Understanding Spatiotemporal Patterns of Chemical Attributes in 'Vitis vinifera' L. cv. Cabernet Sauvignon Vineyards in Central California as a Basis for Predicting Fruit Composition

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Abstract

Spatial variability of vine productivity in winegrapes is important to characterise as both yield and quality are relevant for the production of different wine styles and products. Few studies have analysed spatial variability of individual fruit compositional attributes, and even fewer in *Vitis vinifera* L. cv. Cabernet Sauvignon in California, USA. Previous studies have focused on basic chemistry (pH, TA, TSS), groups of attributes (total phenolics), or fruit colour, and few have reported maps of spatial variability of individual aroma precursors or specific phenolic compounds related to mouthfeel in the resulting wines. The overall objectives of the research presented in this thesis were to understand how patterns of variability of Cabernet Sauvignon fruit composition changed over time and space, how these patterns could be characterised with proximal and remote measurements, and how spatial patterns of the variation in specific fruit compositional attributes can aid in improving management decisions.

Prior to the 2017 vintage, 125 data vines were distributed across each of four vineyards in the Lodi American Viticultural Area (AVA) of central California. Each data vine was sampled at commercial harvest in 2017, 2018, and 2019. Yield components and fruit composition were measured at harvest for each data vine, and maps of yield and fruit composition were produced for eight 'objective measures of fruit quality': total anthocyanins, polymeric tannins, quercetin glycosides, malic acid, yeast assimilable nitrogen, β-damascenone, C6 alcohols and aldehydes, and 3-isobutyl-2-methoxypyrazine.

Maps were produced for each compound in each vineyard to assess the temporal stability of their patterns of spatial variability, and to identify which compounds were most useful in describing overall fruit compositional variability. Of all the compounds analysed, patterns of variation in anthocyanins and phenolic compounds were found to be most stable over time. Given this relative stability, management decisions focussed on fruit quality could be based on zonal

descriptions of anthocyanins or phenolics to increase profitability in some vineyards. In addition to the yield and fruit composition measurements in each season, dormant season pruning weights and soil cores were collected at each location. In each vineyard, elevation and soil apparent electrical conductivity surveys were completed, and remotely sensed imagery was captured by fixed wing aircraft and two satellite platforms at major phenological stages. The data collected were used to develop relationships among biophysical data, soil, imagery, and fruit composition. Remote sensing measures provided similar patterns of variability to those obtained by ground measures.

Characterisation of patterns of spatial variability is difficult because of the cost associated with large sampling numbers and densities required to produce geostatistically rigorous maps. The standardised and aggregated samples from four vineyards over three seasons were included in the estimation of 'common variograms' to assess how this technique could aid growers in producing geostatistically rigorous maps of fruit composition variability without cumbersome, single season sampling efforts. Overall, the characterisation of spatial variability of multiple fruit composition parameters is important for the development of prescriptive farming practices aimed at the enhancement of wine quality.

Declaration

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Acknowledgements

List of Publications

Journal articles

Sams, B., Bramley, R.G.V., Sanchez, L., Dokoozlian, N., Ford, C., and Pagay, V. (2022) Characterising spatio-temporal variation in fruit composition for improved winegrowing management in California Cabernet Sauvignon. Australian Journal of Grape and Wine Research, DOI: 10.1111/ajgw.12542.

Sams, B., Bramley, R.G.V., Sanchez, L., Dokoozlian, N., Ford, C., and Pagay, V. (2022) Remote sensing, yield, physical characteristics, and fruit composition variability in Cabernet Sauvignon vineyards. American Journal of Viticulture and Enology 73, 93-105.

Sams, B., Bramley, R.G.V., Aboutalebi, M., Sanchez, L., Dokoozlian, N., Ford, C., and Pagay, V. Facilitating mapping and understanding of within-vineyard variation in fruit composition using data pooled from multiple vineyards. Australian Journal of Grape and Wine Research, DOI 10.1111/ajgw.12556.

Conference Proceedings

Sams, B., Bramley, R.G.V., Pagay, V., Sanchez, L., Ford, C. and Dokoozlian, N. (2019) Can mapping of within-vineyard variability be facilitated using data from multiple vineyards? Stafford, J.V. ed. Proceedings of the twelfth European Conference on Precision Agriculture; 8-11 July 2019; Montpelier, France (Wageningen Academic Publishers) pp. 743-749.

Sams, B., Bramley, R.G.V., Sanchez, L., Bioni, C., Dokoozlian, N., and Pagay, V. (2020) Canopy microclimate vineyard variability in vineyards of the Lodi region of California, USA. Poster presentation. 13th International Terroir Congress; 17-18 November 2020; Virtual Congress; Adelaide, Australia.

Thesis context

Vineyards throughout the old world are grouped into 'appellations' based on regional geographic indicators derived from soil, climate, culture, and historical perceptions of fruit and wine quality. Research conducted over the past two decades suggests that this may be an oversimplification, as several aspects of fruit composition have been shown to vary significantly within a single vineyard. Fruit compositional variability in cultivated winegrapes can be explained by examining environmental and cultural factors. Climate (at the long term and regional scale) and weather (in the seasonal and within-vineyard scale) are major factors in describing the potential of an area or vineyard to produce a certain set of fruit compositional attributes. Thus, cool climates delay or extend the fruit ripening period and hot climates often negatively alter some aspects of fruit composition. The physical environment, like topography and soil, causes variability in fruit composition due to the heterogenous nature of these attributes. In many cases, the heterogeneity of the underlying conditions creates differences in vine size and potential capacity, creating different conditions for fruit maturation, such that vines in soils with different access to water or nutrients grow at different rates and produce fruit with different concentrations of chemical compounds related to quality. Biotic factors, such as viral and fungal pathogens, vertebrate and invertebrate pests, and competition from nearby vegetation, also play a role by affecting the vine's ability to thrive but are difficult to quantify precisely. Cultural practices play a large role in describing variability as practitioners actively manage against the backdrop of the above-mentioned factors. All of the above come together to cause differences in fruit compositional variability, though different chemical attributes related to fruit quality are driven by different environmental factors or cultural practices. This study will attempt to use an understanding of the patterns and drivers of spatial variability in fruit composition at both the regional and single vineyard block scale as a means of developing measures and metrics to predict fruit composition.

Chapter 1: Literature Review

Introduction

The implementation of precision farming was an important advancement for food production, beginning in the late twentieth century. Soil management drove much of the early adoption (Nielsen et al. 1973), but increased capabilities of geographic information systems (GIS) and global position systems (GPS) in the 1980s and 1990s opened the door to more advanced applications (Mulla and Khosla 2016, and references therein). Crop monitoring using remote sensing began in the 1970s (Rouse et al. 1973; Pinter et al. 1979; Idso et al. 1980; Tucker et al. 1980), as well as the first research into automated yield monitoring (Schueller and Bae 1987), but most of these techniques were constrained to large cereal crop farming systems and did not proliferate into winegrapes until the late 1990s-early 2000s (Bramley and Proffitt 1999, Wample et al. 1999, Johnson et al. 2001; Tisseyre et al. 2001). Precision viticulture and the impact of vineyard site variability on vine performance has been the topic of much interest in recent years (Bonilla et al. 2015; Bramley et al. 2017; Bramley et al. 2019; Ferrer et al. 2020) and Bramley (2021) stands as a very useful, and very recent, review. Bramley (2021) described the cyclical process of precision agriculture (Figure 1), and while much work has been conducted in this field, practitioners rarely repeat the cycle, in particular the re-evaluation of the effects of variable rate application on uniformity. This cycle is designed to offer a strategy of effectively measuring site-specific variability of a crop and its environment, developing models and support systems capable of understanding many relationships simultaneously, and to adjust management practices to optimise the desired output. The strategy has been successful in broadacre crop production (Zhang et al. 2002), but the relatively high cost of development and implementation of precision tools for vineyard management has slowed the participation and adoption by grape growers in Australia and is likely similar in other regions of the world (Bramley 2013; Bramley 2021).
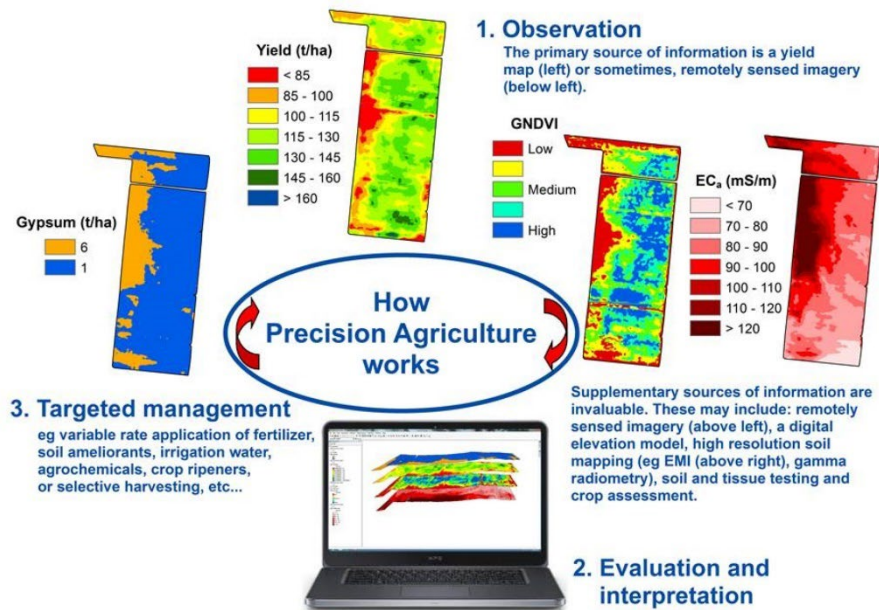
Figure 1. **The cyclic process of precision agriculture circle as described by Bramley (2021). Copyright (2021), with permission from Elsevier.**

Previous research in precision viticulture and vineyard variability has centred around generating useful information from remote and proximal sensors with a variety of mapping capabilities, all based on high accuracy GPS. These capabilities include yield mapping (Bramley and Proffitt 1999), soil apparent electric conductivity and resistivity mapping (McNeill 1980; Corwin and Plant 2005; Ramon Rodriguez-Perez 2011), and canopy characteristics (Lamb 1999; Johnson et al. 2001; Dobrowski et al. 2002; Hall et al. 2002; Bellvert et al. 2013; Zarco-Tejada et al. 2013b; Sun et al. 2017). While remote and proximal sensors can provide high spatial resolution and/or high data density, turning these data into relevant, reliable, and cost-effective management strategies has been challenging due to the need for extensive ground validation.

Progress has occurred in the analysis of these types of data in several forms. Much of this work has occurred in annual broadacre cropping systems, but research into perennial crops has also advanced. Examples include decision support systems for adopting precision management strategies (Andrews et al. 2002; Taylor et al. 2010; Gil et al. 2011; Terribile et al. 2017), clustering multiple layers of geospatial variability for the creation of zones (Oliver and Webster

1989; Fraisse et al. 2001; Bramley and Hamilton 2004; Arno 2011; Herrera Nuñez et al. 2011; Priori et al. 2013; González-Fernández et al. 2017; Oldoni et al. 2021), and computer modelling aimed at predicting canopy characteristics, fruit composition, and climate (Meyers and Vanden Heuvel 2008; Acevedo-Opazo et al. 2010; Barbeau et al. 2014; Le Roux et al. 2015). As the characterisation of vineyard yield and growth variability matured, attention was then focused on the geospatial variability of grape composition and final wine quality (Lamb et al. 2004; Reynolds et al. 2007; Bramley 2010; Bramley et al. 2011a; Scarlett et al. 2014; Bramley et al. 2017; Bramley et al. 2019). While there have been several studies in this area, few have had sufficient sample sizes required to create robust maps (Bramley and Janik 2005). At the time of this review, and to the best of this author's knowledge, research regarding the spatial variability of grape chemistry in California has not been performed with adequate rigour. This gap is at least partially due to several key factors, including but not limited to the time and high costs involved for statistically robust sampling in the field and for subsequent fruit composition quantification in the lab; and the lack of well-established grape composition metrics defining grape and wine quality (Bramley 2021; Niimi et al. 2021).

Vineyard variability

Vineyard variability is extremely complex and involves both abiotic and biotic factors as these influence vines throughout the lifetime of the vineyard (Keller 2015). Environmental conditions related to climate, light, temperature, soil physical and chemical characteristics, pathogenesis, and vineyard management practices constantly impact vine performance (Kliewer and Torres 1972; Jackson and Lombard 1993; Bramley 2001; Downey et al. 2006; Matese et al. 2014). Many studies have focused on these impacts as they relate to the concept of *terroir*, a French term referring to a wine's 'sense of place' (Seguin 1986; Laville 1990; Haynes 1999; Wilson 2001; Goode 2005; Van Leeuwen and Seguin 2006; Bramley and Hamilton 2007; White 2007; Reynolds et al. 2010; Herderich et al. 2015; Bramley 2017; Bramley and Gardiner 2021; Bramley

and Ouzman 2021). The concept of terroir assumes that vines in a region will show commonalities in finished wines based on assumed commonalities in soil, climate, and winemaking practices. While this assumption holds that vineyards in different geographic regions are unique based on different environmental factors, it mostly ignores the variability inherent within the vineyards of each region, as well as the impact of vineyard management (Bramley and Hamilton 2007).

Conventional vineyard management is premised on the default assumption – in the absence of ready access to technologies which facilitate an alternative approach - that vineyards are uniform and that their parcels or sub-blocks are similar in terms of grape quality and value. These vineyards are, therefore, managed uniformly, an approach which often ignores a plethora of factors that can cause variability such as irrigation system inefficiencies, differences in structure and chemistry in heterogenous soils, and in the physical characteristics of the landscape. With access to the tools of precision viticulture, several different strategies can be used to accomplish similar production goals, whether to increase uniformity of the vineyard or to harvest differentially based on zonal differences within a single vineyard.

Vineyard managers have always understood that vineyards are not homogenous, though the tools available to address this variability have not been readily available, and the extent to which this variability is addressed with conventional management is not clear. First, vineyard variability can have several definitions. The main type of variability discussed in the literature is referred to as geospatial or spatial variability. Spatial variability is the level of variation across the vineyard area of some measured variable – perhaps the canopy size or crop level, in any given vineyard in any given season. Climate, soil, and cultural practices are the primary drivers of spatial variability (Bramley 2021). While this type of variability is important, it is imperative to understand whether and how this variation changes between seasons, referred to as temporal variability. Temporal variability is driven primarily by changes in seasonal patterns of weather (Bramley 2021). The

variability that couples the geospatial patterns of variability, and the way in which those patterns vary over time is referred to as 'spatiotemporal variability'. Spatiotemporal variation can then be quantified in terms of how consistent patterns of spatial variability remain between and within seasons.

Several studies have characterised vineyard variability and have identified that some aspects of fruit composition are spatially and temporally stable (Bramley 2001; Ortega et al. 2003; Bramley and Hamilton 2004; Bramley 2005; Taylor et al. 2005; Davenport and Bramley 2007; Tisseyre 2008; Bramley et al. 2011a; Hall et al. 2011; Arno et al. 2012; King et al. 2014; Scarlett et al. 2014; Bramley et al. 2017). One objective of the present study is to understand spatial variability of grape composition at the local (within-vineyard) scale and to further develop our understanding of regional variability in grape composition with implications for wine quality. Within-vineyard variability will be characterised, both spatially and temporally, to understand the level of variability in several vineyards of a region, in this case Lodi, California, with a view to predicting fruit composition. This understanding could underpin management decisions, especially those that might be targeted to discrete areas within a vineyard. This within-vineyard characterisation includes understanding patterns of soil, climate, and other environmental variables, as well as patterns of canopy vigour, yield, and grape composition under uniform management practices. A key objective of this study is to better understand variability of grape composition and chemistry in several vineyards of the Lodi region that can be characterised by patterns of climate and topography. At present, few compounds related to grape composition have been characterised spatially, either within-vineyard or regionally between vineyards.

Remote sensing

Remote sensing is perhaps the most documented form of measuring vineyard variability, utilising aerial images from satellites, airplanes, or unmanned aerial vehicles (UAVs), and remains a key proxy data source for several aspects of vineyard uniformity and performance. Much of this work

has been dedicated to assisting viticulturists with destructive sampling of tissue for yield estimation, vine nutrition, and irrigation scheduling (Baluja et al. 2012b; Zarco-Tejada et al. 2013a; Carrillo et al. 2016; Caruso et al. 2017; Meyers et al. 2020). Due to the relatively coarse resolution of publicly available data, satellite imagery has been used less frequently in California for vineyard management, especially in irrigated winegrape production. The pixel size of most publicly available satellite images is greater than the inter-row distance in most vineyards, making it difficult to separate the vine canopy or growth from the vegetation present in the vineyard inter-row spacing, or indeed in adjacent rows. Large scale patterns have been used for estimation of vineyard parameters like nitrogen content and leaf area (Johnson 2003; Da Silva 2009; Cunha et al. 2010; Arango et al. 2017; Sun et al. 2017; Wang et al. 2017). However, large scale patterns of variability are visible with these relatively coarse resolution images. Higher resolution (<1m ground pixel) imagery available from aerial providers has become increasingly affordable to most growers and can be used for characterising spatial variability. The normalised difference vegetation index (Rouse Jr et al. 1973), or NDVI, and other similar indices are used by many growers and researchers to assess variability in vine vigour using near infrared and visible wavelengths (400–1100 nm). Currently, there is much interest in wavelengths correlated to thermal signatures of plants (8–15 µm). Implications for use in viticulture are mainly in understanding variability in vine water status (Möller et al. 2007; Bellvert et al. 2013; Kustas et al. 2018). Grape canopy characteristics are highly influential in determining final grape composition due to differences in sunlight reaching the canopy interior and fruit zone (Smart 1985; Smart and Robinson 1991; Bergqvist et al. 2001). Therefore, it may be possible to use this type of imagery for characterising differences in light exposure or temperature as related to fruit quality parameters such as colour and phenolics.

Proximal sensing

Proximal sensing of vegetation, in this case typically used to measure some aspect of vine growth or vine status, generally refers to non-destructive measurements recorded using a handheld or vehicle-mounted sensor at less than two metres from the plant. When compared to remote sensing, proximal sensing has several drawbacks, but several important benefits. Proximal sensing is implicitly local, with fewer complications from atmospheric effects and sensor calibrations. On the other hand, proximal sensors must collect data over the course of several hours or days and may need some type of transformation to account for changes in temperature or incoming radiation. Remote sensing provides large amounts of data in a single snapshot. Several studies have used proximal vegetation sensors to further measure vineyard variability and to develop management zones (Bramley et al. 2011b; Rey-Caramés et al. 2016). Others have used hyperspectral radiometers to develop new indices related to plant status (Rodríguez-Pérez et al. 2007; Smart et al. 2007). Several studies have mapped specific attributes of grape composition, chiefly anthocyanins (Stamatiadis et al. 2006; Baluja et al. 2012a), and Bramley et al. (2011c) found correlations between patterns of anthocyanin content measured with the Multiplex® (FORCE-A, Orsay, France) and yield measured by a yield monitor. The use of such a sensor has significant potential as a method to measure an important aspect of grape quality before the fruit reaches the processing facility.

At present, the most widely used measurement obtained via proximal sensor for soil in agriculture is apparent electric conductivity. Soil electric conductivity has been correlated to various aspects of soil texture and chemical composition with application to vineyard management (Bramley 2003; Ramon Rodriguez-Perez 2011; Priori et al. 2013; Ortega-Blu and Molina-Roco 2016). These measurements have been used to characterise soil variability in vineyard studies, specifically for the development of management zones (Bansod and Pandey 2013; Tagarakis et al. 2013), while Bramley et al. (2011b) showed the measurement to be useful

in describing soil depth and vine trunk diameter in a New Zealand vineyard. This measurement is done using one of two sensor types: contact sensors and non-contact sensors (Corwin and Plant 2005; Proffitt et al. 2006; Grisso et al. 2009). The most broadly used commercial sensors include the Dualem (Dualem Inc, Milton, ON, Canada), the EM-38 (Geonics Ltd, Mississauga, ON, Canada), and the Veris (Veris Technologies, Salina, KS, USA).

Yield mapping

Yield monitors attached to mechanical grape harvesters have been deployed in vineyards for two decades (Bramley and Hamilton 2004). The only commercially available vineyard yield monitors operate by weighing fruit as it passes along a set of load cells underneath a discharge belt before being emptied into a collection bin. The loads cells are connected to a GPS unit and assign coordinates to each weight as the harvester moves through the vineyard. The mapping techniques developed and in use today can be found in Bramley and Williams (2001). The data produced from the yield monitors contain weight and location information for the harvester and are interpolated to create digital images of the spatial variability of the crop. The maps produced show the performance of a vineyard in a way not possible with any other data layer. Yield maps show the direct result of all the factors related to seasonal weather and climate variation, physical characteristics of the environment, and cultural practices that led to the crop produced. Several studies have used these maps in understanding vineyard variability (Bramley 2001; Bramley and Hamilton 2004; Bramley et al. 2005; Taylor et al. 2005; Bramley et al. 2011a), but to date, no study of similar depth has been conducted in California.

Characterising the nature of variability

Vineyard variability can have a profound impact on final wine quality (Bramley 2005; Bramley et al. 2011a, 2017). It is well understood that changes in vine canopy characteristics will affect wine quality (Winkler 1958; Smart 1985; Jackson and Lombard 1993; Downey et al. 2006). Previous studies have examined differences in the variability of yield and quality over space and

time (Bramley 2001; Bramley and Hamilton 2004; Bramley 2005; Reynolds et al. 2007; Tisseyre 2008; Trought and Bramley 2011; Smart et al. 2014; Bramley et al. 2017), and have characterised spatial or temporal patterns in specific grape aroma or mouthfeel attributes (Trought and Bramley 2011; Scarlett et al. 2014; Geffroy et al. 2015; Bramley et al. 2017) and methoxypyrazines (Mendez-Costabel et al. 2013). Davenport and Bramley (2007) found spatiotemporal stability in the nutrient content of soil, petioles, and berries in two Australian vineyards. Researchers in Spain found that soil type influences wine composition and quality, specifically that fertile soils can resemble less fertile soils during periods of drought (de Andrés-de Prado et al. 2007). Others have shown that soil texture and depth may have more impact on grape composition and quality than other soil physical characteristics (Reynolds et al. 2007; Bramley et al. 2011b). This relationship can likely be attributed to the impact of soil depth on water available to the plant. Seguin (1986) refers to examples on this point in that quality wine grapes are grown in many different soil types, but that deep, well drained soils can compensate for extreme climatic events like drought or heavy rainfall.

Vineyard variability from air movement at within-vineyard scale is mostly driven by the interaction between canopy and climate. The microscale movement of air in agricultural canopies has been studied to great extent as it relates to vapour pressure deficit (VPD) and evapotranspiration (ET) (Allen et al. 1998; Zhang et al. 2010; Galleguillos et al. 2011; Mahour et al. 2015; Campos et al. 2016). Studies on vine water use have been a focus in using these techniques for understanding variability in vine water status (Acevedo-Opazo et al. 2008; Baluja et al. 2012b; Bellvert et al. 2014; Kustas et al. 2018). Yield prediction and vine productivity studies have advanced as well (Dunn and Martin 2004; Cunha et al. 2010; Bonilla et al. 2015; Carrillo et al. 2016). Results of these and other studies provide the guide for differential management of vineyards for potential final wine quality (Bramley and Hamilton 2004; Tisseyre 2008; Trought and Bramley 2011; Bramley et al. 2019).

The quality of wine can be defined in many ways, and depends, in some ways, on consumer preference. Jackson and Lombard (1993) noted this, and described the myriad problems associated with determining the quality of grapes and wine. Wine quality is also heavily dependent on cultural practices (Downey et al. 2006). Advances in technology have enabled growers to further understand the differences between not only regions, but individual vineyards. There are objective measures of grape chemical compounds that contribute to aroma, mouthfeel, and colour, some of the major drivers of differences in wine sensory perception (Cleary et al. 2015; Harrison 2018; Niimi et al. 2020). Many chemical analytes found in grapes of *Vitis vinifera* L. cv. Cabernet Sauvignon have been identified as important to wine quality including anthocyanins, 2-isobutyl-3-methoxypyrazine (IBMP), β-damascenone, polymeric tannins, quercetin glycosides, carbon 6 alcohols and aldehydes (C6), yeast assimilable nitrogen (YAN), and malic acid (Cleary et al. 2015, Niimi et al. 2020).

Several studies related to vineyard variability have attempted to characterise spatial characteristics of certain aspects of fruit quality (Cortell 2005; Brillante et al. 2017), though with too few samples for sufficient geostatistical rigour according to Webster and Oliver (2007). Webster and Oliver (1992) found a sample size of less than 50 soil samples to be "of little value." According to Webster and Oliver (1992; 2007), at least 100 samples should be used for interpolation using kriging. Kriging is used in geostatistics to "estimate the value of a random variable" (Webster and Oliver 2007) by assigning a weight to a set of subsamples based on their modelled spatial autocorrelation. These larger sampling numbers are required to adequately estimate a variogram, the function from which the weights used in kriging are derived and which characterises the spatial autocorrelation in the data. That is, the variogram, is used to define distances within which samples are similar due to the spatial autocorrelation or beyond which they can be regarded as independent. A tutorial on these techniques can be found in Oliver and Webster (2014). Cortell et al. (2005) used a grid of ~25 soil cores and fruit samples per hectare in

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two vineyards of 1.28 ha (32 cores/ha) and 0.21 ha (six cores/ha). Brillante et al. (2017) used 35

samples to map spatial variability of anthocyanins and several measurements of vine water stress.

Thus, given the low sample numbers, their results need to be treated with caution as they cannot

be regarded as geostatistically rigorous. One might also question the practically of subsequently

implementing some form of differential management (Figure 1) within such small areas.

Reynolds et al. (2007) and Marciniak et al. (2017) applied sufficient sample sizes for vineyard

variability but used inverse distance weighting (IDW) for interpolation. IDW is inferior to kriging

because of the assumption of the distance weighting due to autocorrelation being invariant with

distance (Bramley and Hamilton 2004). The application of a variogram in kriging allows for this

weighting to be quantified based on the relationship between sample variation and their

separation distance; kriging also provides an estimate of the predictive error of interpolation

(Webster and Oliver 2007).

Among the few studies examining spatial variability of a specific wine quality attribute with

adequate geostatistical rigour applied, Scarlett et al. (2014) and Bramley et al. (2017) found

correlations between rotundone, a compound responsible for black pepper aromas in some

Australian cool climate Shiraz, and the physical environment. Using 177 vines in a 6.1 ha

vineyard, the authors characterised rotundone as spatially variable, but with marked spatial

structure, and related to variation in topography. The sample design used in this work, which

derived from earlier work of Bramley (2005), allowed for adequate variogram estimation and

subsequent maps of grape composition, and can be used as a guide for future work in this area.

The aggregation of samples collected from multiple seasons into a 'common variogram' was also

first used by Bramley et al. (2017) to assess spatial variability of rotundone over multiple seasons.

One objective of the research presented in this thesis will be to evaluate the performance of the

common variogram technique across different vineyards over several seasons, and to determine

its usefulness to a group of collaborating vineyard operations.

Cabernet Sauvignon fruit composition

Flavonoids are responsible for several major functions in wine grapes, including ultraviolet (UV) light protection and aiding reproduction (Koes et al. 1994; Downey et al. 2006). These compounds are synthesised through the phenylpropanoid pathway, along with other flavonoids including flavanols and flavonols (Boss et al. 1996; Downey et al. 2006). There are many different types of flavonoids, and anthocyanins are a major subclass. Downey et al. (2006) and references therein, point to the anthocyanin development that occurs in the grape skin as being imperative to winemaking and the main contributor to colour in wine. Anthocyanins in grape skins accumulate rapidly during the ripening phase of development (Mullins et al. 1992) and include the glucosides and acylated forms of anthocyanidins petunidin, peonidin, delphinidin, cyanidin, and malvidin (Boss et al. 1996). While flavonoids develop in seeds, pulp, and other tissues of the grape, most are contained within the skin and development has been shown to coincide with sun exposure (Smart and Robinson 1991; Bergqvist et al. 2001). Additionally, environmental factors greatly affect anthocyanin production and accumulation, specifically related to temperature and nutrition (Boss et al. 1996; Downey et al. 2006; Ristic et al. 2007). Keller and Hrazdina (1998) found that increased nitrogen availability at bloom caused a delay in the accumulation of total phenolics. Other phenolics, like tannins and quercetin, are also affected by light exposure (Koes et al. 1994; Cortell and Kennedy 2006; Ristic et al. 2007). Due to the nature of these compounds and their relationship with light, temperature, and canopy growth, it should be possible to spatially characterise the variation of phenolics in vineyards.

Major aroma compounds in Cabernet Sauvignon

Aroma precursors in wine grapes are important to characterise, especially as they relate to final wine quality. Many compounds associated with flavour and aroma have been identified in Cabernet Sauvignon including IBMP and C6 compounds (green or grassy) (Heymann and Noble 1987; Noble et al. 1995; Ferreira et al. 2000; Reynolds 2010) and β-damascenone (floral or honey)

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(Kotseridis et al. 1999; Sefton et al. 2011; Black et al. 2015). IBMP has been shown to decrease from veraison to harvest with cluster exposure to the sun and because of reduced water application (Noble et al. 1995; Hashizume and Samuta 1999; Brillante et al. 2018), while β-damascenone has been shown to increase from veraison to harvest with increased exposure and water stress (Bindon et al. 2007; Qian et al. 2009; Brillante et al. 2018). Mendez-Costabel et al. (2013) assessed regional variation in IBMP from vineyards in the Central Valley of California at harvest and found the variation between seasons to be more influential than between regions. They also found that green aromas were influenced by spring rainfall and the early onset of irrigation resulting in shading of fruit. While these compounds have been measured in Cabernet Sauvignon, little work has attempted to understand the spatial variability of these compounds either in a single vineyard, set of vineyards, or a grape growing region.

Climate and fruit composition

Models for understanding the relationship between climate and phenology have existed for several decades (Box 1981; Prentice et al. 1992). Many of these models consider some variation in the use of minimum temperatures or temperatures above or below a baseline, such as Huglin (1978). Other studies have linked temperature and climate with a region's ability to produce certain varieties, especially as this relates to climate change (Jones and Davis 2000; Tonietto and Carbonneau 2004; Webb et al. 2008; Jones et al. 2010; Cunha and Richter 2016; Nesbitt et al. 2016; Sturman et al. 2017). While many have attempted to predict yield, climate, or the relationship between these and other factors, little work has investigated how specific compounds related to wine quality vary over a set of vineyards in a region. Jones et al. (2010) mapped differences in climate within American Viticultural Areas (AVAs) of the western United States using the parameter-elevation relationships on independent slopes model (PRISM). A study in New Zealand used several well-known temperature-based models to measure the suitability of grape varieties in the Marlborough region but did not attempt to predict different zones of fruit

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composition or chemistry (Sturman et al. 2017). Acevedo-Opazo et al. (2010) used reference sites of leaf water potential to develop a spatial model for predicting vine water status, but this approach requires excessive field monitoring for use in regional modelling. Bramley and Gardiner (2021) and Bramley and Ouzman (2021) assessed regional differences in growing conditions as they relate to terroir zoning but did not collect fruit samples for analysis. Lamb et al. (2004) found correlations between remotely sensed imagery and characteristics of fruit composition using NDVI taken at different points within a season from manned aircraft. This type of approach could be further explored using more advanced technologies such as thermal imagery and increased spatial resolution from both manned and unmanned aircraft. Several research groups have also incorporated United States Department of Agriculture (USDA) soil data into regional databases of viticultural suitability (Takow et al. 2013; Yau et al. 2014).

Objectives and Significance

The main objectives of this thesis are to: 1) characterise spatial variability of several attributes of Cabernet Sauvignon fruit composition across multiple vineyards and determine which compounds are most important to characterise in order to make optimal management decisions or wine program assignments; 2) link spatial variability of fruit composition to remote sensing and indirect field measurements, so that fewer destructive samples are required for vineyard monitoring; and 3) develop methods for efficiently characterising fruit composition across multiple vineyards in a region. Chapter 2 will assess how remote sensing, yield components, and vine physical characteristics may be useful in understanding variability in Cabernet Sauvignon fruit chemistry. Chapter 3 will examine spatiotemporal variation of fruit composition in Cabernet Sauvignon vineyards and how that variation can be described by thermal and multispectral remote sensing data. Chapters 4 and 5 present a method for collaborating participants to increase the robustivity of maps derived from targeted fruit composition samples by exploring how common variograms may be used to understand spatial variability of fruit composition in

multiple vineyards. We conclude with a general discussion (Chapter 6) of these topics and future research directions.

This research project has the potential to provide new insights into how variability of grape chemistry can be harnessed for optimum winemaking practices. Knowledge about spatial variability of vineyards and grape composition will be furthered by this work, specifically in the realm of spatial structure of chemical compounds. For instance, Bramley et al (2017) found spatially structured patterns of rotundone in Australian Shiraz, but no work of this type has been applied to Cabernet Sauvignon, and no significant research in this area has been published anywhere else in the world. There also exists a significant knowledge gap in the ways variability at the within-vineyard context could aid in understanding variability in other regional vineyards.

While this research will be conducted in California, methods used to understand spatial variability of grape composition could potentially be applied to other regions of the world. Spatial models of grape quality could help wineries and grape growers streamline both the farming of wine grapes, and the winemaking process. Vineyard managers could use within-vineyard information to either manage towards homogeneity, or to optimise the variability in the field by differential harvesting to different wine styles or tiers (Bramley 2011). The benefit to wineries would be derived from a new understanding of fruit streaming for different products. Wineries with estate vineyards would also be able to use this information in a real estate context, with an eye towards buying land in areas with potentially higher levels of desirable fruit characteristics. Overall, this work will improve our understanding of vineyard variability and provide insight on how farm practices may affect the final wine quality.

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Chapter 2: Remote sensing, yield, physical characteristics, and fruit composition variability in Cabernet Sauvignon vineyards

Sams, B., Bramley, R.G.V., Sanchez, L., Dokoozlian, N.K., Ford, C.M., and Pagay, V. (2022) Remote sensing, yield, physical characteristics, and fruit composition variability in Cabernet Sauvignon vineyards. American Journal of Enology and Viticulture 73, 93-105.

Contextual Statement

Though connections have been made between biophysical measurements collected in vineyards (pruning weights, berry weights, etc) and fruit composition, as well as between fruit composition and remotely sensed imagery, few studies have attempted to connect measurements collected at the vine level to those measured in an analytical chemistry lab and to those measured by satellites or airplanes. Further, no study has attempted to compare the capabilities of different remote sensors for describing fruit composition variability. This concept will be further explored in Chapter 3, with the addition of thermal wavelengths. The aims of this study were to: 1) understand which objective measures of fruit quality were correlated with which biophysical measurements; and 2) compare different satellite sensors with different resolutions to a higher resolution manned aircraft. This study uses principal components analysis to describe the relationships between and among other fruit compositional attributes with data from remote sensing and biophysical measurements collected from each vineyard.

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Certification:	This paper reports on original research I conducted during the period of my Higher Degree by Research candidature and is not subject to any obligations or contractual agreements with a third party that would constrain its inclusion in this thesis. I am the primary author of this paper.		
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Remote Sensing, Yield, Physical Characteristics, and Fruit Composition Variability in Cabernet Sauvignon Vineyards

Brent Sams,[1,2]* Robert G.V. Bramley,[3] Luis Sanchez,[2] Nick Dokoozlian,[2] Christopher Ford,[1] and Vinay Pagay[1]

Abstract: Soil texture, topographical data, fruit zone light measurements, yield components, and fruit composition data were taken from 125 locations in each of four *Vitis vinifera* L. cv. Cabernet Sauvignon vineyards in the Lodi region of California during the 2017, 2018, and 2019 seasons. Data were compared against three sources of normalized difference vegetation index (NDVI) with different spatial resolutions: Landsat 8 ($LS8_{NDVI}$; 30 m), Sentinel-2 ($S2_{NDVI}$; 10 m), and manned aircraft (at high resolution, HR) with the interrow removed (HR_{NDVI}; 20 cm). The manned aircraft also captured canopy temperature (CT) derived from infrared (thermal) wavelengths (HR_{CT}; 40 cm) for additional comparisons. HR_{NDVI} was inversely related to HR_{CT}, as well as to several chemical components of fruit composition including tannins and anthocyanins. While some constituents of fruit composition such as anthocyanins may be related to NDVI, canopy temperature, and/or indirect measurements collected in the field, results presented here suggest that yield and fruit composition have a strong seasonal response and therefore environmental conditions should be considered if more accurate predictions are desired. Furthermore, freely available public satellite data sources with mixed canopy and interrow pixels, such as Sentinel-2 and Landsat 8, provided similar information related to predicting specific fruit composition parameters compared to higher resolution imagery from contracted manned aircraft, from which the interrow signal was removed. Growers and wineries interested in predicting fruit composition that accounts for spatial variability may be able to conserve resources by using publicly available imagery sources and small numbers of targeted samples to achieve this goal.

Key words: objective measures of fruit quality, precision viticulture, principal components analysis, remote sensing of vegetation, vineyard variability, *Vitis vinifera* cv. Cabernet Sauvignon

The prediction of winegrape composition in a vineyard, and the resulting wine quality, is difficult for numerous reasons. Manual sampling of fruit quality in vineyards can be complicated and time consuming (Wolpert and Vilas 1992, Meyers et al. 2011), especially for operations comprising many vineyards or many differentiated products. Additionally, comprehensive measures of fruit composition are expensive, requiring either costly commercial lab submissions, or in-house laboratory equipment and personnel. Furthermore, spatial variability exacerbates both of these issues because patterns of variability have shown to be temporally consistent but the magnitude of variability of fruit composition from a vineyard is unlikely to be consistent (Bramley 2005, Arnó et al. 2012, Sams et al. 2022).

Individual destructive vine measurements have long been the industry standard for determining fruit composition and potential wine quality. Commonly used vine measurements to evaluate vineyard performance are berry sizes or mass (Gladstones 1992), total yield estimates (Keller et al. 2005), dormant season pruning weights (Smart and Robinson 1991), and chemical analysis of berries or whole clusters (Niimi et al. 2020). More recently, to describe within-vineyard zones of potentially similar vine performance with a few targeted samples, indirect measurements like apparent electrical conductivity (EC_a) mapping have been shown to be useful in describing soil variability and its relationship with vine performance (Acevedo-Opazo et al. 2008, Bramley et al. 2011). Each of these measurements has an economic cost to vineyard managers and/or wineries, and few commercial operations collect sufficient samples to adequately characterize the full range of variability in a vineyard or have dedicated staff for time consuming surveys that are susceptible to changes in the environment or management practices over time (Ferreira et al. 2020).

Remote sensing can capture information on vineyard variability rapidly and repeatedly, but must be "ground-truthed,"

or validated by measurements collected at the field level, for crop metrics to be useful (Sun et al. 2017), although targeting indirect measurements or samples to vineyard zones based on spatial variability can reduce sample requirements (Meyers et al. 2011). Because all available sources of remote sensing information must be validated by ground measurements, and high-resolution imagery captured by many commercial manned aircraft platforms requires additional spectral and geometric calibrations for quantitative assessment, it would be useful to understand the capabilities of different sensors in predicting fruit composition at harvest to reduce these costs. As imagery from highly calibrated public satellite platforms like the European Space Agency's (ESA) Sentinel and the National Aeronautics and Space Administration's (NASA) Landsat becomes available at increasing spatial and temporal resolution, and at no cost, imagery obtained from manned and unmanned commercial aircraft flying at relatively low altitudes may not be necessary for many applications, such as discriminating zones for differential harvests or zonal vineyard management.

Remote sensing analysis of vineyards began in earnest two decades ago as Dobrowski et al. (2002) used imagery acquired using manned aircraft, and Johnson (2003) used imagery from satellites as tools for understanding grapevine canopies. Lamb et al. (2004), Bramley et al. (2011), Hall et al. (2011), Trought and Bramley (2011), and Song et al. (2014) found relationships between canopy vigor and fruit composition using normalized difference vegetation index (NDVI) and plant cell density derived from imagery acquired from manned aircraft, while Sun et al. (2017) used Landsat-derived products (NDVI and leaf area index) to predict winegrape yield. Sozzi et al. (2020) showed significant relationships in vineyard canopy variability (NDVI) captured by Sentinel-2 versus high-resolution imagery from an unmanned aerial vehicle (UAV), with comparisons of interrow removed and included, but they did not relate these to measurements of yield or fruit composition. Given these findings, and the fact that several compounds found in Cabernet Sauvignon grapes known to influence wine chemistry are related to environmental conditions (Bergqvist et al. 2001, Kliewer and Dokoozlian 2005, Lee et al. 2007, Li et al. 2013, Martínez-Lüscher et al. 2019), we hypothesize that it should be possible to characterize the relationships among vine productivity, seasonal growing conditions, and remote sensing. Principal component analysis (PCA), a method commonly used to reduce dimensionality of large data sets, has been used by others to infer relationships between some aspects of yield and fruit composition with soil variables in Chardonnay in Ontario, Canada (Reynolds et al. 2013), and imagery, water status, soil characteristics, basic grape chemistry, and yield of different varieties in France (Acevedo-Opazo et al. 2008).

We present results of PCA and Pearson correlations combining data from four commercial vineyards in the Lodi region of California with different management strategies, terrains, soil types, and magnitudes of variability. Our objectives were to compare variables from different remote sensing sources with a large volume of spatially distributed and ground-truthed environmental and fruit composition measurements, as well as to determine the most useful and efficient ground-truthing descriptors of vineyard characteristics correlating to fruit composition and quality. To our knowledge, no study exists incorporating yield components, fruit chemistry, soil texture, fruit zone light, and remote sensing with high density ground validation. Additionally, the inclusion of Cabernet Sauvignon grape mouthfeel and aroma precursors differentiates the present analysis from previous studies relying mainly on measures of basic chemistry.

Materials and Methods

Four Cabernet Sauvignon vineyards were selected based on their range of geographic locations and assessments of spatial variability found in aerial imagery and were sampled for yield components and fruit composition at harvest for three consecutive seasons, 2017 to 2019 (Sams et al. 2022). The vineyards were in the American Viticultural Area (AVA) of Lodi, California and were within 40 km of one another and spatially distributed across the AVA. Climate of the region is classified as dry summer subtropical with an average of 190 mm of precipitation annually. Summertime highs regularly exceed 40°C and winter lows rarely dip below 0°C. Climate data were summarized from a centrally located weather station in the Lodi region for the three years in which data were collected (Table 1). Table 2 details the physical characteristics of each vineyard. Briefly, all four vineyards—Vineyards A through D—were drip irrigated and had sprawling, spur-pruned canopies. Vineyard C was planted in 1998, while Vineyards A, B, and D were planted from 2010 to 2013.

Yield and fruit composition. On the commercial harvest dates for each of the four vineyards set by the receiving winery in each season, a three-step process for documenting yield components was completed at each of the spatially distributed 125 georeferenced data vines in each vineyard. Sample distribution maps can be found in Sams et al. (2022). A combined 100-berry sample was collected by randomly selecting 10 clusters and removing 10 total berries from the top, middle, and bottom of each cluster and weighed. Twenty randomly chosen grape clusters were then removed from each data vine, weighed, and transported to the laboratory. Data vines were hand-harvested and total yield per vine and cluster number were recorded. Weights from all three steps were combined for total vine yield. Upon arrival at the laboratory, all berries from the 20 randomly chosen grape clusters were homogenized before extraction with acidified 50% ethanolic solution. Total anthocyanins were measured using a UV-vis based method described by Iland et al. (2000). Polymeric tannins and a combined total of quercetin 3-O-glucoside and 3-O-glucuronide, referred to hereafter as "quercetin glycosides," were measured using reversed-phase high-performance liquid chromatography (HPLC; Peng et al. 2001). Analysis of free-form volatile compounds (C6 and 3-isobutyl-2-methoxypyrazine [IBMP]) was completed using headspace solid-phase microextraction coupled to a gas chromatograph

and a mass spectrometer (HS-SPME-GC-MS) adapted from Kotseridis et al. (2008) and Canuti et al. (2009). Bound form β-damascenone was extracted using solid phase extraction adapted from Whiton and Zoecklein (2002), followed by fast acid hydrolysis and SPME-GC-MS as described by Kotseridis et al. (1999), Ibarz et al. (2006), and Canuti et al. (2009). Total soluble solids (Brix), pH, titratable acidity (TA), yeast assimilable nitrogen (YAN), and malic acid were measured using standard methods of Fourier-transform infrared spectroscopy and calibrated using E. & J. Gallo's reference chemistry standards.

Vineyard physical characteristics. Soil cores were collected between seasons (Vineyards B and C in December 2018; Vineyards A and D in December 2019) from the center of the interrow space ~1 m from each data vine using a 5.7 cm diam soil auger (AMS, Inc.). Each core constituted a single composite sample of soil depths from 0 to 100 cm taken at 20 cm increments, mixed into a 30.5 × 25.4 cm plastic bag, and submitted to a commercial soil analysis laboratory (A & L Western Laboratories) for particle size (texture) analysis. An apparent EC_a survey was conducted in each vineyard prior to the initiation of vine growth in 2018 using a Dualem-1S (Dualem Inc.) and a Trimble Geo7x Global Positioning System (GPS, Trimble Inc.). EC_a data were interpolated in VESPER using local block kriging (version 1.62; Australian Centre for Precision Agriculture, The University of Sydney, New South Wales, Australia). A digital elevation model developed from a range of sources and with a final resolution of ~10 m ground spacing (1/3 arc-second) and a vertical root mean square error of 1.55 m (Gesch et al. 2014) was downloaded from the United States Geological Survey (USGS) and used for topographic analysis (USGS 2019, 3D Elevation Program Digital Elevation Model, accessed 21 March 2020 at https://elevation.nationalmap.gov/arcgis/rest/services/3DEPElevation/ImageServer).

Measurements of photosynthetically active radiation (PAR) in the fruit zone of each data vine were collected in the first week of June in 2018 and 2019 at bloom (modified Eichhorn-Lorenz [E-L] stage 23; Pearce and Coombe 2004), mid-June or fruit set (modified E-L stage 27), and mid-July or veraison (modified E-L stage 35), with measurements occurring only on days with relatively cloudless sky conditions. PAR measurements were taken within two hours of solar noon using an ACCUPAR LP-80 ceptometer (Meter Group, Inc.). In the two bilateral cordon trained vineyards (Vineyards A and D), the ceptometer was placed parallel to the vine cordons in the fruiting zones of the canopies and facing up and on both the north and south sides of the vines, with one above canopy (or ambient) measurement taken before and one after the fruit zone measurements. In the two horizontally divided quadrilateral-cordon trained vineyards (Vineyards B and C), one measurement was taken on the south side of each southern cordon and one measurement on the north side of each northern cordon, with ambient measurements taken before and after fruit zone measurements. The sensor console was aligned horizontally with the vine trunk in all vineyards, ensuring that the main arm from the trunk to the center of the vine was accounted for in each measurement. Measurements from each vine were averaged and fruit zone PAR (PAR_{FZ}) was calculated by dividing the average fruit zone PAR measurements by the average of the ambient PAR measurements. Additional ambient incident PAR measurements were taken in open areas with no overhead sensor obstruction every 15 min throughout each measurement period to ensure above canopy measurements reflected ambient conditions and were not obstructed by neighboring vine rows. Dormant season pruning weights were collected in the first two weeks of December in 2018 and 2019 from each data vine and the Ravaz index was calculated as the ratio of yield:pruning weight (Smart and Robinson 1991).

Table 1 Regional growing degree days, precipitation, radiation, and reference evapotranspiration (ET_o) by annual quarters from 2017 to 2019 in the Lodi region of California.

	Phenology	E-L[a]	Date ranges	Growing degree days (Base$_{10}$)	Precipitation (mm)	Radiation (W m^2)	ET$_o$ (mm)
2017	Leaf fall-budbreak	[43-04]	Nov 2016-March	561	614	3095	282
	Budbreak-fruit set	[05-26]	April-May	476	47	2717	323
	Fruit set-veraison	[27-35]	June-July	690	2	3323	372
	Veraison-harvest	[36-42]	Aug-Oct	959	4	3827	392
	2017 Totals			**2686**	**667**	**12,962**	**1369**
2018	Leaf fall-budbreak	[43-04]	Nov 2017-March	548	298	3395	253
	Budbreak-fruit set	[05-26]	April-May	438	65	3000	279
	Fruit set-veraison	[27-35]	June-July	668	0	3412	372
	Veraison-harvest	[36-42]	Aug-Oct	881	1	3864	382
	2018 Totals			**2535**	**364**	**13,671**	**1286**
2019	Leaf fall-budbreak	[43-04]	Nov 2018-March	500	488	3112	238
	Budbreak-fruit set	[05-26]	April-May	439	67	2812	260
	Fruit set-veraison	[27-35]	June-July	682	0	3419	367
	Veraison-harvest	[36-42]	Aug-Oct	849	7	3628	372
	2019 Totals			**2470**	**562**	**12,971**	**1237**

[a]Modified Eichhorn-Lorenz (E-L) stages, Pearce and Coombe 2004. Source: Lodi Winegrape Commission Weather station network (https://lodi.westernweathergroup.com); Station ID: Valley Oak.

Remote sensing—manned aircraft. High-resolution imagery from manned aircraft (visible/near-infrared = 0.2 m ground resolution, wavelengths = 800, 670, 550 µm, bandwidth =10 nm; thermal infrared/canopy temperature = 0.4 m ground resolution, wavelengths = 7.5 to 13 µm; absolute error ±1°C) was sourced from a commercial provider for each vineyard at phenological stages corresponding to the PAR measurements in 2018 and 2019 (modified E-L stages 23, 27, 35). NDVI was calculated from the near-infrared (800 nm) and red (670 nm) bandwidths (Rouse et al. 1973). Using the histogram for each HR_{NDVI} and HR_{CT}, a bimodal separation of pixels was used to delineate canopy pixels from pixels in the interrow and nonvine signals (Salgadoe et al. 2019). All noncanopy pixels, or those below the histogram separation values in the case of NDVI and above the histogram separation values in the case of thermal infrared, were removed, and the average pixel value of each data vine was derived from the remaining pixels. Image processing was completed using ArcGIS (v10.4, Environmental Systems Research Institute).

Remote sensing—satellites. Sentinel-2 (10-m pixel) and Landsat 8 (30-m pixel) satellite images were processed and downloaded using the Google Earth Engine (Gorelick et al. 2017). Level-1 precision- and terrain-corrected Landsat 8 images were atmospherically corrected to surface reflectance prior to retrieval (Vermote et al. 2016). Because of a lack of available surface reflectance imagery for the study area in 2018, top of atmosphere images from Sentinel-2 were used to maintain a consistent source. Images from satellite overpasses corresponded to acquisition dates closest to PAR measurements and relatively cloudless dates to compare results of each source with phenological stages. NDVI ($S2_{NDVI}$ and $LS8_{NDVI}$) was calculated for each image using each sensor's respective near-infrared (NIR; LS8 = 851 to 879 nm, S2 = 785 to 899 nm) and red (LS8 = 636 to 679 nm, S2 = 650 to 680 nm) bands. Data points corresponding to pixels with more than 20% of each pixel's area outside of each vineyard, i.e., edge pixels, were not included in subsequent analyses.

PCA. PCA was conducted in R statistical software (R Core Team 2020, R Foundation for Statistical Computing, https://www.R-project.org/) using the FactoMineR package (Lê et al. 2008). Because berry weights, cluster counts, and pruning weights were not recorded in 2017, the 2017 data were not included in the further analyses, which used complete data sets for 2018 and 2019. All fruit compositional data, yield components, images, and environmental measurements were standardized by vineyard and season (mean = 0, standard deviation = 1) to eliminate site specific, vintage, and management effects (Carrillo et al. 2016). A modified t-test that accounted for spatial autocorrelation (Dutilleul 1993) was calculated using the SpatialPack package in R (Vallejos et al. 2020) to assess the strength of the relationships among the characteristics of the fruit, yield components, soil, topography, and imagery.

Results

Results from PCA when data were not standardized show that relationships between variables (descriptive statistics can be found in Table 3) were driven by site and seasonal effects (Figure 1A and 1B). However, combined standardized data in PCA from all four vineyards exhibited a typical global response as points from each vineyard and season overlapped and were distributed approximately evenly around the origin (Figure 1C and 1D). Figure 2 revealed similar relationships from the three sources of NDVI imagery (HR_{NDVI}, $S2_{NDVI}$, and $LS8_{NDVI}$), and inverse relationships with HR_{CT}. Imagery from three phenological stages were within ~3% of one another in terms of variance explained by PCA, although no single combination of component one (PC1) and component two (PC2) explained more than 40% of the multivariate variability (Figure 2). NDVI from all three sources of imagery was related to pruning weights, and the relationship strengthened as the seasons progressed. HR_{CT} separated with PAR_{FZ} at bloom and veraison (Figure 2). $LS8_{NDVI}$ showed the weakest relationships with fruit composition and vine performance

Table 2 Physical details, cultural practices, vine characteristics, and irrigation rates applied in 2017 to 2019 in four vineyards in the Lodi region of California.

	Vineyard A	Vineyard B	Vineyard C	Vineyard D
Training method	Single bilateral	Quadrilateral	Quadrilateral	High wire
Trellis system	Sprawl	Sprawl	Sprawl	Sprawl
Vine spacing (m)	2.1	1.2	1.8	2.4
Row spacing (m)	3.1	3.4	3.4	3.1
Vineyard area (ha)	7.4	13.8	11.8	11.2
Sample density (per ha)	17.0	9.0	11.0	11.0
Year planted	2010	2013	1998	2012
Rootstock/ scion clone	039-16/ FPS08	SO4/7	1103P/7	039-16/15
Rootstock parentage	*Vitis vinifera* × *Vitis rotundifolia*	*Vitis berlandieri* × *Vitis riparia*	*V. berlandieri* × *Vitis rupestris*	*V. vinifera* × *V. rotundifolia*
Pruning method	Hand	Hand	Hand	Machine
Floor management	Tilled bare soil	Perennial cover crop	Perennial cover crop	Perennial cover crop
Elevation (min to max; m asl)	6.3 to 7.1	38.9 to 60.4	20.1 to 21.6	39.6 to 47.0
Applied irrigation (mm)				
2017	No data	401	219	No data
2018	No data	415	145	289
2019	No data	423	197	281

Table 3 Fruit composition, crop characteristics, and soil texture measured in 2017 to 2019 in four vineyards in the Lodi region of California.[a]

	Vineyard A			Vineyard B			Vineyard C			Vineyard D		
	2017	2018	2019	2017	2018	2019	2017	2018	2019	2017	2018	2019
Fruit composition												
Total soluble solids (Brix)	24.4 ± 0.5	24.4 ± 0.7	24.4 ± 0.8	24.8 ± 1.0	26.5 ± 0.8	25.4 ± 1.3	24.6 ± 0.9	25.4 ± 0.8	25.0 ± 1.2	24.3 ± 1.2	24.7 ± 1.4	25.3 ± 1.6
pH	3.78 ± 0.06	3.85 ± 0.06	3.87 ± 0.08	3.83 ± 0.07	3.79 ± 0.06	3.63 ± 0.07	3.88 ± 0.12	3.80 ± 0.10	3.73 ± 0.11	3.67 ± 0.14	3.60 ± 0.08	3.63 ± 0.10
Titratable acidity (g/L)	3.7 ± 0.3	3.8 ± 0.5	3.7 ± 0.3	3.2 ± 0.3	3.1 ± 0.3	3.1 ± 0.5	3.8 ± 0.5	3.4 ± 0.5	3.5 ± 0.6	3.8 ± 0.5	3w.8 ± 0.6	3.6 ± 0.5
Anthocyanins (mg/g)	0.79 ± 0.10	1.21 ± 0.19	0.72 ± 0.12	1.15 ± 0.19	2.19 ± 0.21	1.10 ± 0.11	1.34 ± 0.22	2.45 ± .38	1.30 ± 0.20	0.89 ± 0.16	1.89 ± 0.31	0.90 ± 0.14
β-damascenone (μg/g)	46 ± 5	60 ± 7	59 ± 6	59 ± 7	83 ± 12	60 ± 6	57 ± 6	79 ± 10	67 ± 8	48 ± 7	54 ± 7	49 ± 7
C6 (μg/g)	5.3 ± 0.5	5.0 ± 0.8	5.2 ± 0.8	4.2 ± 0.9	3.2 ± 0.6	4.1 ± 0.9	3.1 ± 0.7	3.2 ± 0.8	1.5 ± 0.7	5.2 ± 1.1	4.7 ± 1.1	1.6 ± 0.6
IBMP (pg/g)[b]	5.5 ± 3.3	3.8 ± 3.8	2.1 ± 3.0	0.2 ± 0.9	2.1 ± 2.8	ND[c]	0.1 ± 0.5	0.1 ± 0.7	ND	2.0 ± 2.0	ND	0.1 ± 0.5
Malic acid (g/L)	1.9 ± 0.3	2.2 ± 0.4	1.9 ± 0.3	1.3 ± 0.2	1.6 ± 0.3	0.9 ± 0.3	1.5 ± 0.4	1.7 ± 0.3	1.0 ± 0.5	1.6 ± 0.3	1.7 ± 0.3	1.1 ± 0.4
Polymeric tannins (mg/g)	2.0 ± 0.3	1.4 ± 0.2	1.8 ± 0.2	3.6 ± 0.8	2.2 ± 0.3	2.4 ± 0.3	3.2 ± 0.6	2.7 ± 0.4	3.6 ± 0.6	2.3 ± 0.5	2.2 ± 0.2	2.4 ± 0.5
Quercetin glycosides (μg/g)	35 ± 9	24 ± 7	29 ± 8	102 ± 31	25 ± 9	82 ± 19	59 ± 22	47 ± 18	79 ± 21	50 ± 16	46 ± 7	73 ± 25
YAN (g/L)[b]	0.15 ± 0.03	0.26 ± 0.03	0.17 ± 0.03	0.03 ± 0.01	0.09 ± 0.02	0.02 ± 0.02	0.05 ± 0.02	0.06 ± 0.02	0.04 ± 0.02	0.10 ± 0.03	0.07 ± 0.03	0.04 ± 0.02
Yield components												
Yield (kg/m²)	2.6 ± 0.5	3.0 ± 0.5	3.1 ± 0.6	1.3 ± 0.4	2.1 ± 0.4	2.3 ± 0.6	1.7 ± 0.5	1.9 ± 0.6	1.6 ± 0.5	2.5 ± 0.6	2.8 ± 0.5	2.3 ± 0.6
Cluster weight (g)	NS[c]	173 ± 21	155 ± 16	NS	121 ± 17	101 ± 20	NS	92 ± 16	78 ± 16	NS	131 ± 20	105 ± 25
Clusters (count/m²)	NS	18 ± 3	20 ± 5	NS	18 ± 3	23 ± 4	NS	20 ± 5	20 ± 5	NS	21 ± 3	22 ± 4
Berry weight (g)	NS	1.09 ± 0.08	1.18 ± 0.09	NS	1.13 ± 0.10	1.09 ± 0.10	NS	0.87 ± 0.12	0.95 ± 0.13	NS	1.16 ± 0.09	1.25 ± 0.12
Canopy measurements												
Pruning weight (kg/m²)	NS	0.47 ± 0.08	0.28 ± 0.05	NS	0.19 ± 0.05	0.35 ± 0.07	NS	0.29 ± 0.09	0.24 ± 0.06	NS	0.26 ± 0.05	0.29 ± 0.07
Ravaz index (kg/m²)	NS	6.5 ± 1.1	11.0 ± 2.4	NS	11.8 ± 2.9	6.9 ± 2.2	NS	6.7 ± 1.4	6.7 ± 1.9	NS	10.9 ± 2.2	8.0 ± 2.3
PAR_{FZ}[d] – E-L 23 (% ambient)	NS	0.6 ± 0.9	2.1 ± 2.1	NS	3.4 ± 2.3	4.5 ± 3.7	NS	9.6 ± 10.4	4.0 ± 2.7	NS	1.2 ± 1.1	1.1 ± 0.6
PAR_{FZ} – E-L 27 (% ambient)	NS	0.7 ± 0.6	1.2 ± 1.1	NS	1.8 ± 1.3	6.6 ± 3.9	NS	4.2 ± 6.3	3.9 ± 3.1	NS	1.2 ± 0.7	1.5 ± 1.4
PAR_{FZ} – E-L 35 (% ambient)	NS	1.6 ± 2.9	2.9 ± 2.9	NS	4.3 ± 2.4	9.5 ± 4.8	NS	10.1 ± 7.2	13.9 ± 8.3	NS	4.4 ± 3.8	7.6 ± 6.0
Soil measurements[e]												
Clay (%)		14 ± 2			26 ± 4			20 ± 6			15 ± 3	
Silt (%)		29 ± 6			28 ± 4			33 ± 9			24 ± 7	
Sand (%)		57 ± 7			45 ± 4			47 ± 12			61 ± 8	
EC_a[b] (mS/m²)		96 ± 11			127 ± 19			88 ± 17			92 ± 13	

[a]Values are mean ± SD, n = 125.
[b]IBMP, 3-isobutyl-2-methoxypyrazine; YAN, yeast assimilable nitrogen; EC_a, apparent electrical conductivity.
[c]ND, not detected; NS, not sampled.
[d]PAR_{FZ} = fruit zone photosynthetically active radiation; modified Eichhorn-Lorenz (E-L) stages (Pearce and Coombe 2004).
[e]Soil data were collected in December 2018 at Vineyards B and C, and in December 2019 at Vineyards A and D.

Figure 1 Principal component analysis (PCA) of fruit components (anthocyanins, β-damascenone, C6, malic acid, polymeric tannins, quercetin glycosides, and yeast assimilable nitrogen [YAN]) measured in four vineyards (A, B, C, and D) in the Lodi region of California in 2018 and 2019: (**A**) relationships among nonstandardized variables (loadings), (**B**) distribution of data points from each vineyard and season (scores), (**C**) relationships among standardized (μ = 0, σ = 1) variables (loadings), and (**D**) distribution of standardized (μ = 0, σ = 1) data points from each vineyard and season (scores). n = 1000 (125/vineyard/year).

variables, as evidenced by its limited distance from the center axis (Figure 2) and the weakest Pearson coefficients (Table 4). Visual comparisons of imagery captured at veraison (modified E-L stage 35) in Vineyard C highlight the similarities in the pattern of vigor captured by Landsat 8, Sentinel-2, and high-resolution NDVI, as well as the high-resolution canopy temperature (Figure 3). This similarity was apparent despite the removal of edge pixels in $S2_{NDVI}$ and $LS8_{NDVI}$ and the removal of interrow pixels in the HR_{CT} and HR_{NDVI}. Additionally, high values of HR_{CT} corresponded to low values of HR_{NDVI}, $S2_{NDVI}$, and $LS8_{NDVI}$ (Figure 3), and this visual relationship was mirrored by PCA (Figure 2) and correlation analysis (Table 4).

Quercetin glycosides, polymeric tannins, anthocyanins, and β-damascenone were grouped together and were posi-

tively related to HR_{CT} and inversely related to NDVI from all three sources (Figure 2 and Table 4). Malic acid, YAN, and C6 were typically related with low PAR_{FZ} and were closely related to pruning weights and yield, as well as NDVI in PC1 (Figure 2). Fruit yield per square meter and berry weight were relatively well spread along PC1 when compared with phenolic compounds, which were tightly grouped (Figure 2). While the results from PCA showed many of these variables to be closely related, results from the modified t-test showed that although many of these were significantly correlated ($p < 0.05$), the correlations for many were weak (Table 4). Correlations of fruit composition variables with yield components and pruning weights were generally strong, whereas correlations among most imagery, PAR_{FZ}, and topographic variables produced coefficients <0.2 (Table 4).
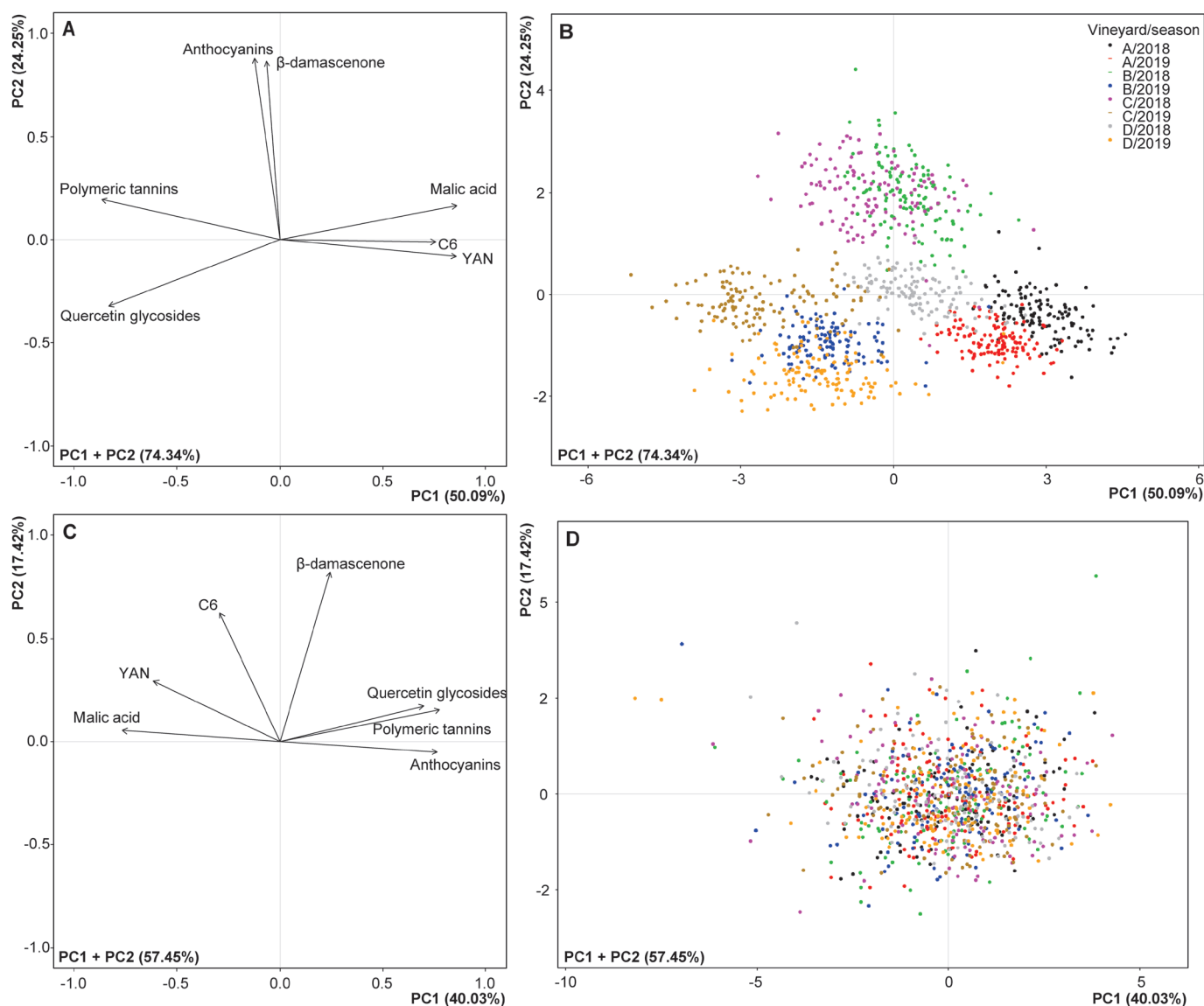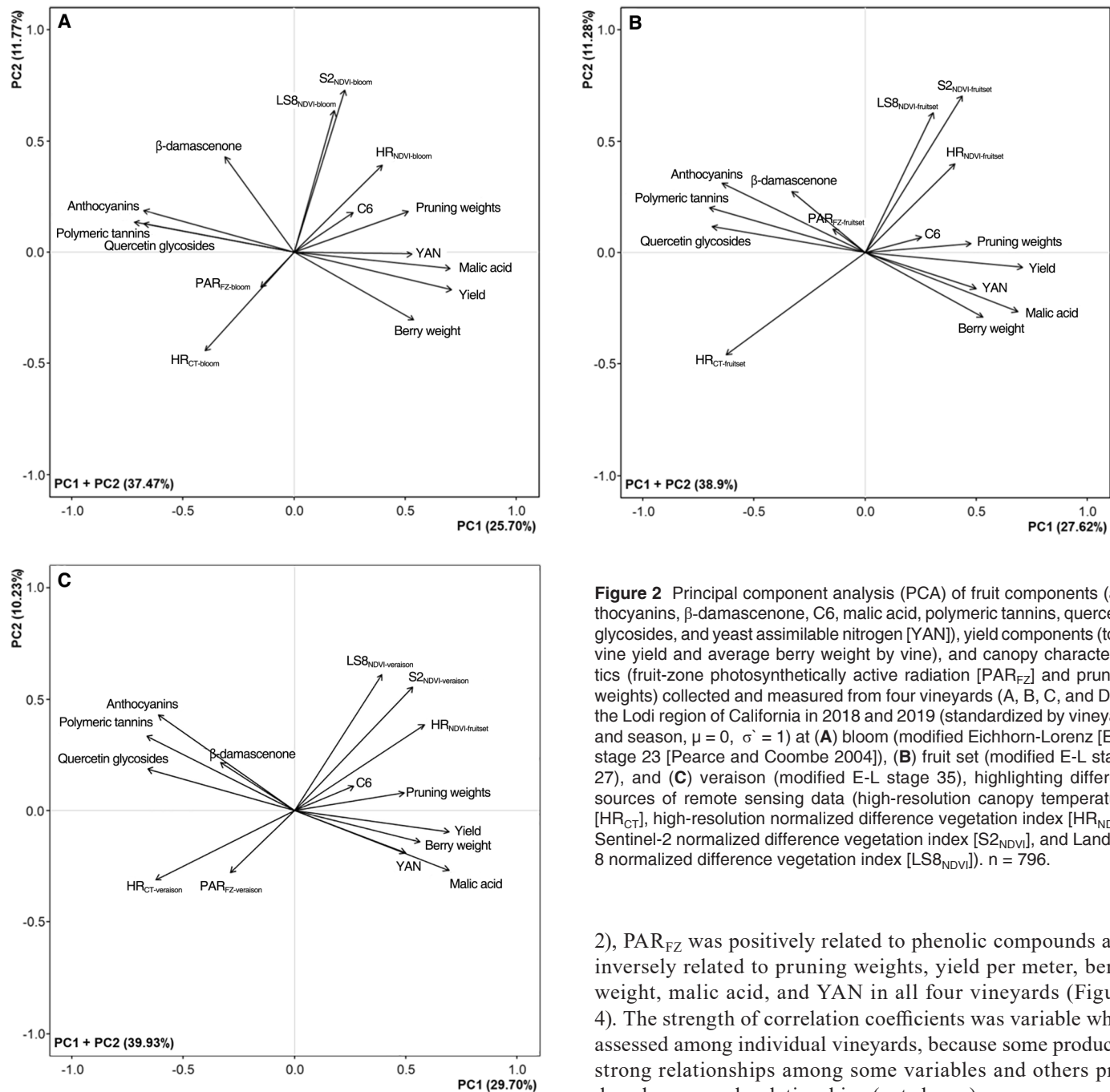
Figure 2 Principal component analysis (PCA) of fruit components (anthocyanins, β-damascenone, C6, malic acid, polymeric tannins, quercetin glycosides, and yeast assimilable nitrogen [YAN]), yield components (total vine yield and average berry weight by vine), and canopy characteristics (fruit-zone photosynthetically active radiation [PAR_{FZ}] and pruning weights) collected and measured from four vineyards (A, B, C, and D) in the Lodi region of California in 2018 and 2019 (standardized by vineyard and season, μ = 0, σ` = 1) at (**A**) bloom (modified Eichhorn-Lorenz [E-L] stage 23 [Pearce and Coombe 2004]), (**B**) fruit set (modified E-L stage 27), and (**C**) veraison (modified E-L stage 35), highlighting different sources of remote sensing data (high-resolution canopy temperature [HR_{CT}], high-resolution normalized difference vegetation index [HR_{NDVI}], Sentinel-2 normalized difference vegetation index [$S2_{NDVI}$], and Landsat 8 normalized difference vegetation index [$LS8_{NDVI}$]). n = 796.

Figure 4 shows the relative positions among fruit composition, PAR_{FZ}, and yield components in each of the four vineyards. Vineyards had different mean values and magnitudes of variation in some variables (Table 3). Relationships among fruit compositional variables were similar in all vineyards, specifically along the first principal component (Figure 4). Groups of phenolic compounds (polymeric tannins, quercetin glycosides) segregated on the opposite side of several compounds related to shaded or unripe fruit (C6, malic acid). Larger yields, berry weights, and pruning weights also aligned more closely with characteristics of unripe fruit in all four vineyards (Figure 4). Similar to the relationship when all four vineyards were combined (Table 4 and Figure

2), PAR_{FZ} was positively related to phenolic compounds and inversely related to pruning weights, yield per meter, berry weight, malic acid, and YAN in all four vineyards (Figure 4). The strength of correlation coefficients was variable when assessed among individual vineyards, because some produced strong relationships among some variables and others produced very weak relationships (not shown).

The differences in canopy light environment (PAR_{FZ}) from fruit set (modified E-L stage 23) to veraison (modified E-L stage 35) shows that fruit in Vineyard A received less than 1% of ambient PAR compared with up to nearly 10% during this period in the other vineyards (Table 3). Vineyard D was only slightly more exposed than Vineyard A in the first two measured modified E-L stages (stage 23–bloom, and stage 27–fruit set), but because of canopy management practices, this percentage increased by veraison to levels similar to those observed in Vineyards B and C where fruit color was much higher. PAR_{FZ} was more variable in Vineyards B and C compared with Vineyards A and D, and generally matched the results of anthocyanins and several other variables (Table 3). Soil variables (sand, silt, clay, EC_a) were sometimes statisti-

cally significant and correlated with compositional variables ($p < 0.05$; Table 4), but primarily varied along the less explanatory PC2 (Figure 5). Areas of higher elevation produced fruit with higher concentrations of desirable components, including polymeric tannins and quercetin glycosides (Table 4).

Discussion

Remote sensing. The most significant finding of this study was the relative similarity in the relationships between fruit composition and different remote sensing platforms across multiple seasons and multiple vineyards, although relationships among many variables were not strong. Images captured from satellites, Sentinel-2 and Landsat 8 at 10-m and 30-m ground resolutions, respectively, aligned closely with those from manned aircraft at 20-cm resolution when used

as predictors of fruit composition; that is, there was little, if any, benefit offered by the high-resolution airborne imagery compared to the lower resolution satellite sources. Similar studies in other regions with more diverse soil and climate variability, or in applications where higher resolution imagery is required, may be necessary to broadly extrapolate these findings. Similarly, Sozzi et al. (2020) found that Sentinel-2 images were nearly as useful as UAV imagery captured at <10 cm in describing spatial variability of canopy vigor in vineyards with no grass in the interrow, although no comparisons with fruit chemistry were reported. However, in the PCA with images captured at bloom (Figure 2A) the HR$_{NDVI}$ was somewhat more closely related to pruning weights, unripe and green characteristics (YAN, malic acid, C6), and yield components. The results presented here expand this finding from

Table 4 Pearson correlations accounting for spatial autocorrelation[a] between fruit composition and yield components, canopy characteristics, soil, elevation, and different sources of imagery combining measurements collected in 2018 and 2019 in the Lodi region of California.

	TSS[b] (Brix)	pH	TA[b]	Anth[b]	β-dam[b]	C6	Malic acid	IBMP[b]	Polymeric tannins	Quercetin glycosides	YAN[b]
Yield	-0.27*[c]	-0.41*	0.46*	-0.34*	-0.23*	0.20*	0.03	0.42*	-0.46*	-0.47*	0.30*
Cluster weight	-0.24*	-0.22*	0.26*	-0.26*	-0.23*	0.12*	0.03	0.33*	-0.36*	-0.35*	0.21*
Clusters	-0.16*	-0.27*	0.25*	-0.19*	-0.01	0.17*	-0.09*	0.22*	-0.28*	-0.21*	0.14*
Berry weight	-0.14*	-0.24*	0.30*	-0.40*	-0.48*	0.12*	0.01	0.36*	-0.47*	-0.33*	0.10*
Pruning weight	-0.02	0.08*	0.11*	-0.29*	-0.02	0.03	0.05	0.31*	-0.30*	-0.29*	0.25*
Ravaz index	-0.28*	-0.44*	0.29*	-0.06	-0.14*	0.18*	-0.11*	0.11*	-0.19*	-0.13*	0.02
PAR$_{FZ}$[d] (E-L 23)	-0.00	-0.03	0.02	0.07*	-0.04	-0.05	-0.03	0.00	0.08*	0.10*	0.00
PAR$_{FZ}$ (E-L 27)	-0.07*	0.09*	-0.09*	0.06	0.07*	-0.08*	0.08*	-0.06	0.07*	0.19*	-0.01
PAR$_{FZ}$ (E-L 35)	0.03	0.03	-0.10*	0.12*	0.02	-0.10*	-0.09*	-0.15*	0.11*	0.21*	-0.09*
Clay	0.01	0.05	-0.05*	-0.02	0.11*	-0.00	0.04	-0.03	0.06*	0.01	0.09*
Silt	-0.12*	-0.20*	0.18*	-0.06*	0.00	0.07*	0.04	0.11*	-0.06*	-0.08*	0.16*
Sand	0.10*	0.14*	-0.13*	0.07*	-0.06*	-0.06*	-0.04	-0.07*	0.02	0.05	-0.17*
EC$_a$[e]	-0.00	-0.12*	0.07*	0.08*	-0.12*	-0.00	0.12*	-0.08*	0.05	0.01	-0.01
Elevation	0.12*	0.19*	-0.16*	0.06*	0.18*	-0.17*	-0.05	-0.12*	0.22*	0.19*	0.09*
HR$_{CT}$[e] (E-L 23)	0.10*	0.09*	-0.16*	0.16*	-0.02	-0.11*	-0.07	-0.24*	0.25*	0.20*	-0.19*
HR$_{CT}$ (E-L 27)	0.13*	0.20*	-0.31*	0.21*	0.12*	-0.11*	-0.10*	-0.31*	0.32*	0.36*	-0.19*
HR$_{CT}$ (E-L 35)	0.20*	0.26*	-0.34*	0.27*	0.18*	-0.19*	0.10*	-0.43*	0.35*	0.32*	-0.24*
HR$_{NDVI}$[e] (E-L 23)	-0.02	0.10*	0.07*	-0.16*	-0.08*	0.14*	0.12*	0.19*	-0.21*	-0.26*	0.22*
HR$_{NDVI}$ (E-L 27)	-0.01	-0.01	0.07*	-0.12*	-0.00	0.07*	0.08*	0.15*	-0.14*	-0.25*	0.16*
HR$_{NDVI}$ (E-L 35)	-0.10*	-0.13*	0.24*	-0.18*	-0.10*	0.19*	0.15*	0.38*	-0.26*	-0.40*	0.28*
S2$_{NDVI}$[e] (E-L 23)	0.07*	0.08*	-0.02	-0.05*	0.05	0.09*	0.03	0.03	-0.11*	-0.10*	0.07*
S2$_{NDVI}$ (E-L 27)	0.01	-0.02	0.10*	-0.12*	-0.02	0.12*	0.06*	0.10*	-0.18*	-0.20*	0.10*
S2$_{NDVI}$ (E-L 35)	0.04	-0.05*	0.16*	-0.17*	-0.11*	0.12*	0.11*	0.19*	-0.20*	-0.26*	0.20*
LS8$_{NDVI}$[e] (E-L 23)	0.01	0.04	0.01	-0.01	-0.04	0.10*	0.07*	0.06*	-0.10*	-0.06*	0.03
LS8$_{NDVI}$ (E-L 27)	-0.01	-0.02	0.07*	-0.04	-0.08*	0.09*	0.08*	0.09*	-0.14*	-0.11*	0.04
LS8$_{NDVI}$ (E-L 35)	-0.06*	-0.07*	0.13*	-0.07*	-0.11*	0.13*	0.10*	0.15*	-0.15*	-0.17*	0.09*

[a]Modified t-test (Dutilleul 1993), n = 796.
[b]TSS, total soluble solids; TA, titratable acidity; Anth, anthocyanins; β-dam, β-damascenone; IBMP, 3-isobutyl-2-methoxypyrazine; YAN, yeast assimilable nitrogen.
[c]Asterisks indicate significance ($p < 0.05$).
[d]PAR$_{FZ}$, fruit-zone photosynthetically active radiation; modified Eichhorn-Lorenz (E-L) stages (Pearce and Coombe 2004).
[e]EC$_a$, apparent electrical conductivity; HR$_{CT}$, high-resolution canopy temperature; HR$_{NDVI}$, high-resolution normalized difference vegetation index; S2$_{NDVI}$, Sentinel-2 normalized difference vegetation index; LS8$_{NDVI}$, Landsat 8 normalized difference vegetation index.
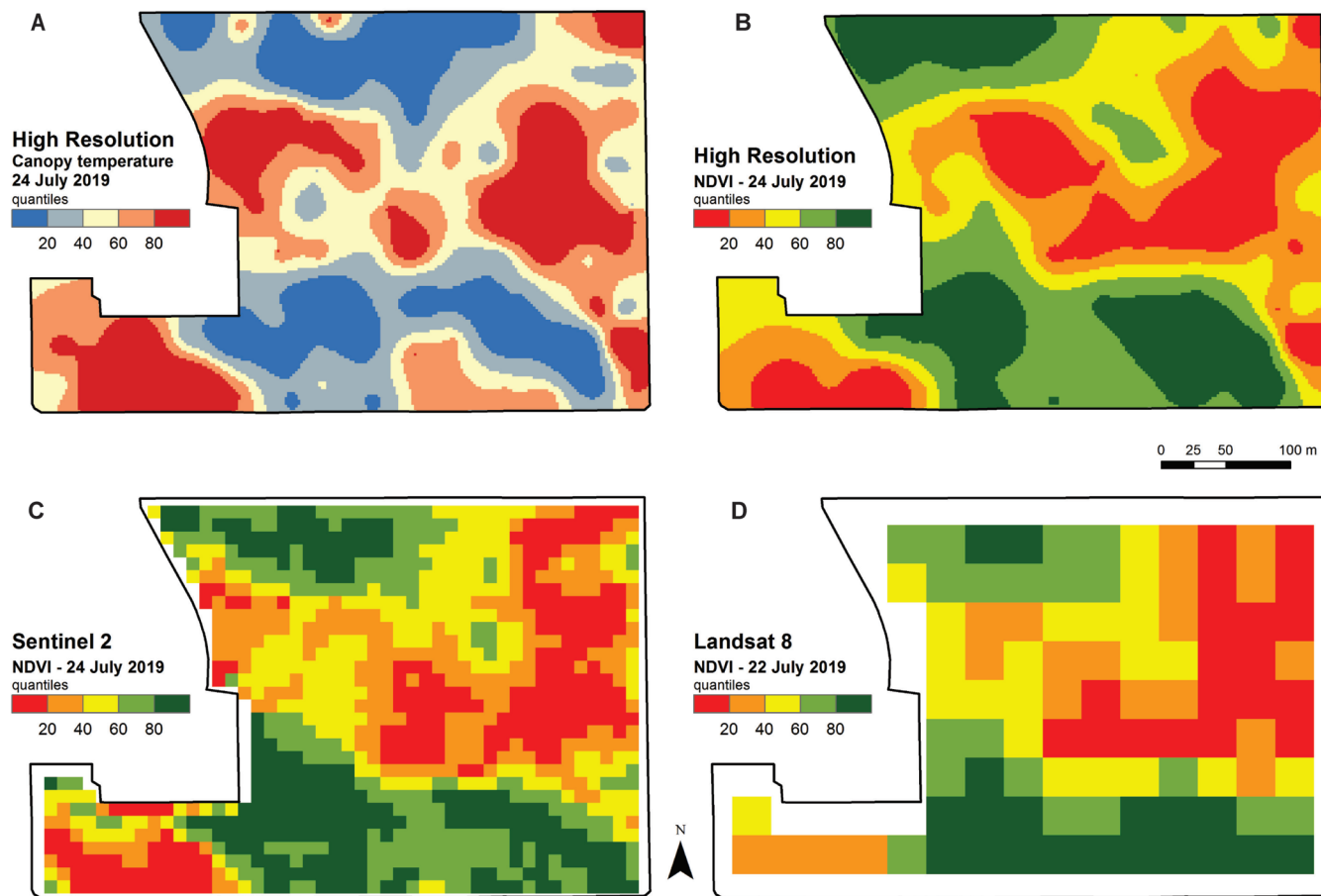
Figure 3 Spatial variation of the normalized difference vegetation index (NDVI) derived from four sources of imagery in a vineyard (Vineyard C) in the Lodi region of California at veraison (modified Eichhorn-Lorenz [E-L] stage 35 [Pearce and Coombe 2004]) in 2019 showing (**A**) high-resolution canopy temperature (HR$_{CT}$), (**B**) high-resolution NDVI (HR$_{NDVI}$), (**C**) Sentinel-2 NDVI (S2$_{NDVI}$), and (**D**) Landsat 8 NDVI (LS8$_{NDVI}$). Note that the map data have been classified as quantiles (20th percentiles).

the spatial variability noted in several fruit compositional parameters (Sams et al. 2022). There may be applications or time sensitive phenological stages where canopy separation from the interrow is imperative for determining vine water status, where an absolute value is necessary to calibrate with ground data, or in vineyards with native, nontilled vegetation occurring in irregular patches, but our results show that this separation may be unnecessary to describe spatial variability of vineyard canopies. Possible explanations for this scenario are that areas comprised of low vigor vines will also cause low vigor of the interrow cover crop, or that by the time of image acquisition at these phenological stages, the interrow cover crop is dead or dormant and provides a mostly bare background. It could be possible that a combination of these two explanations may actually enhance visual patterns of variability because low vigor zones contain more interrow space with soil or dead vegetation as a percentage of ground cover. The separation of nonvine signal from vine canopy is not trivial because image processing represents significant economic cost to imagery providers who then pass this on to customers. Furthermore, a major benefit of the satellite data examined here is the high-level calibration made by those providing the imagery (NASA and ESA), although given the

weak correlations between imagery values and fruit composition, viticulturists may be more interested in spatial patterns found in imagery because absolute values from vegetation indices may vary over multiple images. When compared with maps of fruit composition in these same vineyards shown by Sams et al. (2022), this finding of pattern importance may be even more relevant. With this in mind, growers interested in assessing variability of vineyards may still be better suited to use lower-resolution, publicly available imagery at no cost, rather than purchase higher resolution from vendors because the relationships between imagery and fruit composition described here were not sufficiently strong to give absolute predictive value. For more precise prediction of fruit composition from remote sensing, it is likely that alternatives such as hyperspectral imagery at high resolution may be needed, although neither the precision nor cost-effectiveness of such an approach is known at present.

Similar to our results, Carrillo et al. (2016) found that berry weight, cluster number, and NDVI were similarly aligned along the first principal component in a similar use of PCA. Ballesteros et al. (2020) used NDVI (with other indices) from an unmanned aerial sensor and machine learning techniques to model grapevine yield in *Vitis vinifera* cv. Bobal, but found

contrasting results to those presented here. The authors stated that the soil background was the primary cause for a negative relationship between yield and NDVI when interrow and shadow pixels were included in the analysis, but when those pixels were removed, the relationship was positive immediately prior to harvest. These authors made a similar recommendation to ours, in that seasonal calibration is likely necessary for the most accurate results.

Environmental conditions and fruit composition. Differences in growing degree days, incoming solar radiation, precipitation, and reference evapotranspiration were likely partly responsible for differences in fruit composition among the three years of study (Table 1). In 2018, dormant season precipitation (leaf fall to budbreak) was much lower than in the other dormant seasons. This difference, coupled with the slower accumulation of growing degree days in 2018 and

Figure 4 Principal component analysis (PCA) of fruit components (anthocyanins, β-damascenone, C6, malic acid, polymeric tannins, quercetin glycosides, and yeast assimilable nitrogen [YAN]), yield components (total vine yield and average berry weight by vine), and canopy characteristics (fruit-zone photosynthetically active radiation [PAR$_{FZ}$] and pruning weights) measured in 2018 and 2019 in four vineyards in the Lodi region of California and standardized by season (μ = 0, σ = 1), (**A**) Vineyard A, (**B**) Vineyard B, (**C**) Vineyard C, and (**D**) Vineyard D. n = 250.

higher incoming radiation (Table 1), may explain the large increase in anthocyanin concentration in all four vineyards from 2017 to 2018 (Van Leeuwen et al. 2009; Table 3). However, quercetin glycosides and polymeric tannins were lowest in 2018 in all four vineyards, marking a separation in development between anthocyanins and these phenolic compounds during these seasons, despite the consistent grouping apparent in Figures 2, 4, and 5. Despite the relatively cooler season, a lack of precipitation in the early season (Table 1), and only small differences in irrigation volume (Table 2), yield was also highest in 2018 in all four vineyards (Table 3).

While a case can be made that lower yield equates to an increase in some positive aspects of fruit composition, the reasons for this relationship are somewhat misunderstood (Smart and Robinson 1991). In many cases, low-yielding vines often have small canopies and leaf areas but higher PAR_{FZ}, allowing more light into the canopy interior than a vine with identical yield, larger canopies, and lower PAR_{FZ}. Previous studies have linked light interception with fruit composition in California (e.g., Bergquist et al. 2001, Kliewer and Dokoozlian 2005), and their results complement those presented in this study. Low PAR_{FZ} was likely at least partly responsible for the relatively low values of anthocyanins, polymeric tannins, and anthocyanins in Vineyard A. Extremely high (or low) vigor may affect measurements of light interception through excessive sensor occlusion (or through direct sensor exposure in the case of low vigor). The values of IBMP and C6 are likely elevated in this vineyard due to excessive shading in the fruit zone. Given the low percentage of ambient PAR reaching the fruit zone, large clusters, and relatively high crop load on a single bilateral cordon (Tables 2 and 3), cluster occlusion may also be responsible for these results in Vineyard A (Dunn and Martin 2004). Leaf area can vary greatly between different canopy architectures, and many cultural manipulations are difficult to detect from remote sensing. Trellis design, pruning, leaf removal, irrigation, and crop load management are all parts of this complex system and contribute greatly to the decision-making process as well as to the cost of vineyard management (Jackson and Lombard 1993 and references within).

The relatively weak results from analyses of soil and topographic variables may be related to the way in which they were sampled but also may stem from the adjustment of management practices such as canopy management and irrigation, based on the highly variable soils, which can directly or indirectly influence canopy light interception (Table 4). It may also be possible that the magnitude of variability in soil and topography were insufficient to cause large differences in these vineyards and may differ in other regions or conditions. Shallow soil profiles on slopes and hillsides can produce differences in water holding capacity and lead to smaller vines compared with those on foothills or flat surfaces (Van Leeuwen et al. 2004, Jasse et al. 2021). It also may be responsible for the relationships between elevation, yield, and fruit composition (Figure 5), although soil horizon depths were not measured in this study. Additionally, inherent spatial variability of soil can cause drastic differences in yield and
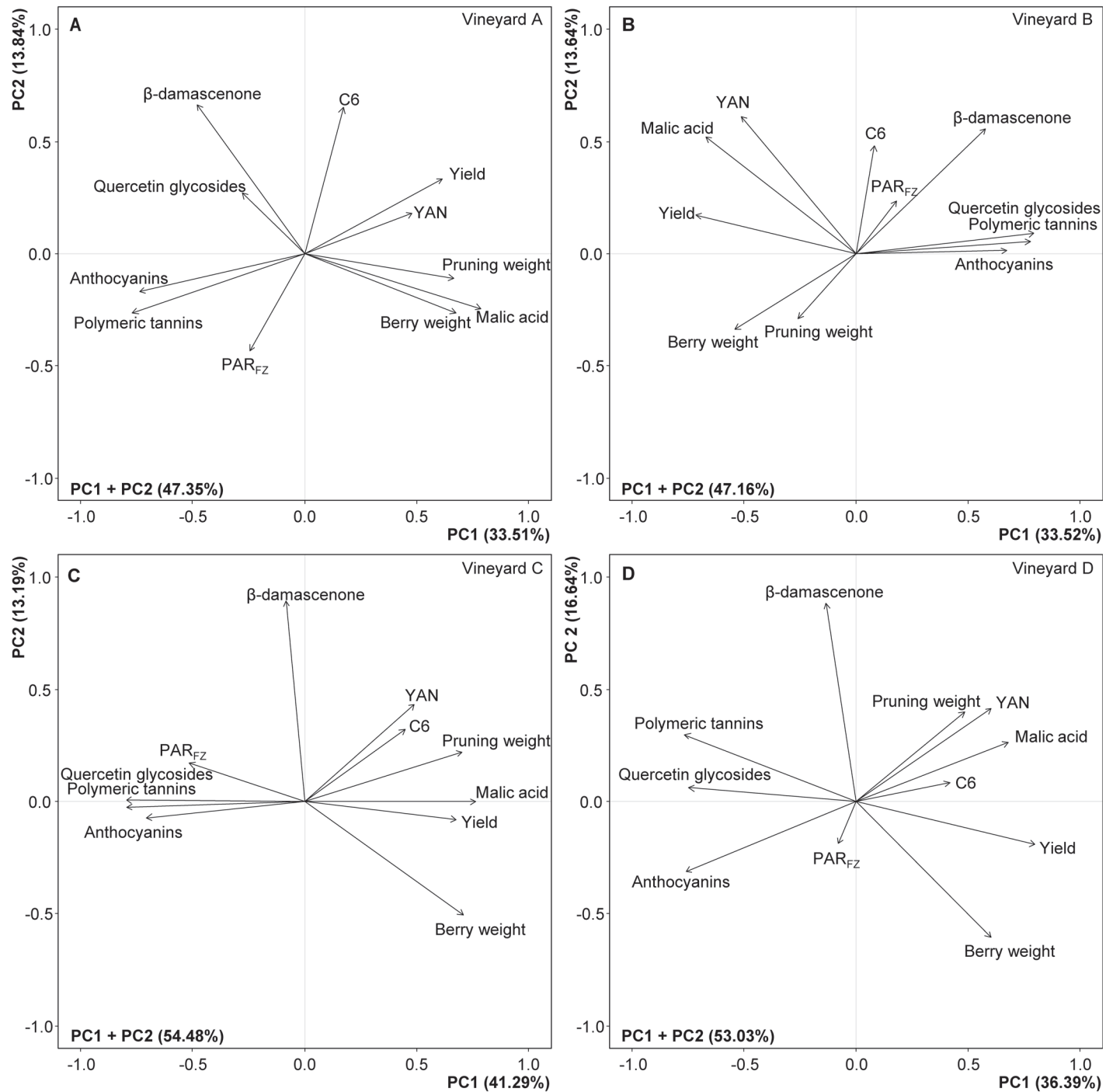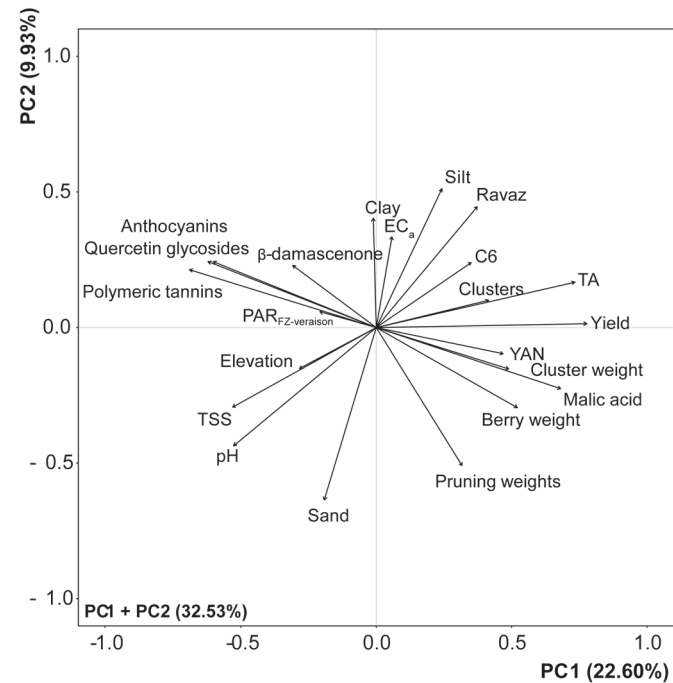

Figure 5 Principal component analysis (PCA) of fruit components (anthocyanins, β-damascenone, C6, malic acid, pH, polymeric tannins, quercetin glycosides, titratable acidity [TA], total soluble solids [TSS], and yeast assimilable nitrogen [YAN]), yield components (total vine yield, average cluster weight by vine, cluster number per vine, and average berry weight by vine), canopy characteristics (fruit-zone photosynthetically active radiation [PAR_{FZ}], pruning weights, and Ravaz index), soil texture (clay, sand, and silt), apparent electrical conductivity (EC_a), and elevation data measured in 2018 and 2019 from four vineyards (A, B, C, and D) in the Lodi region of California, aggregated and standardized ($\mu = 0$, $\sigma = 1$) by vineyard and season. n = 1000

fruit quality, even over short distances, or small changes in topography (Bramley and Hamilton 2004, Bramley 2005); results presented in this study also suggest that elevation and soil texture have a significant effect on many aspects of fruit composition (Table 4). Accordingly, a more detailed investigation using measurements made down the soil profile and using a survey-grade GPS for elevation may lead to more precise understanding of soil and terrain effects.

The combination of high-density fruit composition samples and related vineyard measurements from several large commercial vineyards presented in this study can act as a guide to the industry as to which indirect or destructive measurements are truly useful in describing and predicting fruit composition. Targeted PAR measurements, pruning weights, and/or yield estimates collected from spatially distinct "quality" zones like those shown by Sams et al. (2022), compared with a few fruit composition samples taken with these zones in mind, should provide growers and wineries with a guide to the potential quality variability in a vineyard.

Conclusion

This study illustrates that remote sensing data from low resolution satellites paired with spatially targeted seasonal calibrations of yield components, pruning weights, and/or fruit composition can describe relationships between fruit

composition and vegetative vigor at relatively low cost with sufficient precision to support delineation of within-vineyard zones of different vineyard performance, although additional studies may be necessary in different regions or in different conditions. If calibrations are conducted among different growing conditions and specific cultural and management practices (e.g., trellising, canopy management, water status), it should eventually be possible to model these systems with high precision and accuracy with minimal ground validation. As satellite imagery becomes more widely available and spatial and temporal resolution increases, growers will have even more options available to tailor vineyard management to specific production targets. Data products developed from these sensors, such as estimates of crop evapotranspiration or leaf area index, will also become more useful for more applications such as yield prediction, irrigation management, and environmental damage assessment. The current study may be useful to growers for reducing the costs of acquiring information about how variability affects the magnitude of fruit quality differences in vineyards. Until handheld, proximal sensors capable of detecting fruit composition are readily available at costs suitable for commercial growers and wineries, remote sensing products provide the best platform for capturing this information.

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Chapter 3: Characterising spatio-temporal variation in fruit composition for improved winegrowing management in California Cabernet Sauvignon

Sams, B., Bramley, R., Sanchez, L., Dokoozlian, N., Ford, C. and Pagay, V. (2022) Characterising spatio-temporal variation in fruit composition for improved winegrowing management in California Cabernet Sauvignon. Australian Journal of Grape and Wine Research. https://doi.org/10.1111/ajgw.12542

Contextual Statement

The research presented in the preceding chapter showed how imagery from manned aircraft was correlated with fruit composition in several vineyards. The experiments described in the following chapter expand on these relationships to describe how patterns of spatial variability of several fruit compositional attributes align with patterns of spatial variability found in visible/near infrared and thermal high-resolution aerial imagery. Additionally, maps of fruit composition found in this chapter represent the first known characterisations of the spatial variability of several compounds known to influence Cabernet Sauvignon wines: β-damascenone, C6s, IBMP, polymeric tannins, quercetin glycosides, and YAN. The objectives of this study were to: 1) produce maps of spatial variability of several attributes of fruit composition from several seasons; 2) link them to remote sensing information; and 3) to examine which attributes are most important in driving the overall spatial variability of fruit composition. This study used geostatistical analysis to assess the relationships between fruit composition and imagery.

Statement of Authorship

Title of Paper	Characterising spatio-temporal variation in fruit composition for improved winegrowing management in California Cabernet Sauvignon
Publication Status	☐ Published ☒ Accepted for Publication ☐ Submitted for Publication ☐ Unpublished and Unsubmitted work written in manuscript style
Publication Details	Sams, B., Bramley, R.G.V., Sanchez, L., Dokoozlian, N., Ford, C., and Pagay, V. (2022) Characterising spatio-temporal variation in fruit composition for improved winegrowing management in California Cabernet Sauvignon. Australian Journal of Grape and Wine Research, in press.

Principal Author

Name of Principal Author (Candidate)	Brent Sams		
Contribution to the Paper	Collected samples, performed analysis on grape samples and imagery, interpreted data, wrote manuscript, and served as corresponding author		
Overall percentage (%)	80%		
Certification:	This paper reports on original research I conducted during the period of my Higher Degree by Research candidature and is not subject to any obligations or contractual agreements with a third party that would constrain its inclusion in this thesis. I am the primary author of this paper.		
Signature		Date	29 September 2021

Co-Author Contributions

By signing the Statement of Authorship, each author certifies that:

    i.   the candidate's stated contribution to the publication is accurate (as detailed above);

    ii.   permission is granted for the candidate in include the publication in the thesis; and

    iii.   the sum of all co-author contributions is equal to 100% less the candidate's stated contribution.

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Signature		Date	13 January 2022

Name of Co-Author	Luis Sanchez		
Contribution to the Paper	Supervised project in California, helped to evaluate and edit the manuscript		
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Name of Co-Author	Nick Dokoozlian
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Name of Co-Author	Christopher Ford
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Please cut and paste additional co-author panels here as required.

Name of Co-Author	Vinay Pagay
Contribution to the Paper	Supervised project development, assisted with analyses, helped to evaluate and edit the manuscript
Signature		Date	12/01/2022

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Characterising spatio-temporal variation in fruit composition for improved winegrowing management in California Cabernet Sauvignon

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Abstract

Background and Aims: Spatial variability in yield and fruit composition in winegrape vineyards has been demonstrated, but few chemical compounds responsible for impacting wine composition have been analysed at a sample density high enough to compare with variability in remotely sensed imagery. The aims of this project were to evaluate spatial variability in grape composition at harvest in three seasons and to compare this with remotely sensed canopy vegetation data to assess its utility in underpinning targeted management.

Methods and Results: The composition of fruit samples were analysed to compare their spatial variability with aerial imagery products, the normalised difference vegetation index (NDVI) and the difference between canopy temperature from imagery (T_c) and ambient temperature from ground weather stations (T_a), ($T_c - T_a$). Zonal discrimination of fruit composition using k-means clusters generated from seasonal aerial imagery showed a difference as high as 2.7 kg/m in vine yield, up to 0.3 mg/g anthocyanins and 1.2 pg/g carbon-6 alcohols and aldehydes (C6) with these 'quality zones' reflected by the imagery in some vineyards and/or seasons.

Conclusions: The NDVI and ($T_c - T_a$) data collected at multiple time points were correlated with several attributes of fruit composition evaluated at harvest, but most correlations peaked at veraison. They were also strongest in vineyards in which the spatial variation showed stronger spatial structure.

Significance of the Study: Spatial variations in berry chemistry followed similar patterns to those seen in aerial imagery of vineyards with structured vigour zones. Furthermore, as most of the spatial structure in the variation of fruit composition is dominated by flavanols, opportunities for reduced analytical costs in winery laboratories also arise.

Keywords: *grape composition, precision viticulture, remote sensing of vegetation, vineyard variability,* Vitis vinifera *(cv. Cabernet Sauvignon)*

Introduction

The goal of precision agriculture is to understand variability in crop performance at high spatial resolution so that its management can be optimised (Whelan and McBratney 2000, Bramley 2009). Nonetheless, the challenge remains for practitioners to understand the magnitude of the variability and to decide whether to mitigate it with management or take advantage of it through diversifying the product offering. In winegrapes, this challenge is confounded by the complexity of the highly manipulated cropping system, the lack of broad acceptance of metrics for describing final wine quality and spatial variability in both yield and fruit composition (Bramley 2021). Exploiting patterns of spatial variability through selective harvesting has been shown to be profitable in differentiated wine production systems (Bramley 2005, Bramley et al. 2011b), but has tended to be based on simplistic interactions between yield (and/or vine vigour) and berry chemistry, in spite of this relationship not being well understood (Matthews and Nuzzo 2007). In fact, understanding the spatial variability of key berry compositional and chemical compounds, often referred to as 'objective measures of fruit quality' (OMFQ)

[e.g. Gishen et al. (2002)], is necessary to fully understand how this relationship may vary in both space and time. Due to the high cost and complexity of manual sampling and fruit chemical composition analysis, many studies have attempted to link fruit composition with data obtained from proximal canopy sensors (Stamatiadis et al. 2006, Trought and Bramley 2011), soil sensors (Priori et al. 2013, Yu et al. 2020), or non-destructive fruit sensors (Agati et al. 2007, Gutiérrez et al. 2019, Tuccio et al. 2020). Others have used canopy indices derived from aerial remote sensing to link with some aspects of fruit composition (Lamb et al. 2004, Hall et al. 2011, Fiorillo et al. 2012, Ferrer et al. 2020) and some have linked thermal imagery related to plant water status to resultant fruit composition (Möller et al. 2007, Bellvert et al. 2016). Few studies have addressed spatial variation in OMFQ at a resolution comparable with spatial variation in imagery (Bramley 2005, Trought and Bramley 2011, Baluja et al. 2013, Scarlett et al. 2014, Bramley et al. 2017). Others have attempted this with relatively small sample sizes which may compromise the spatial analysis (Brillante et al. 2017, Martínez-Lüscher et al. 2019, Yu et al. 2020), and even fewer have worked at the commercial

vineyard scale. Only Scarlett et al. (2014) and Bramley et al. (2017) produced geostatistically rigorous maps of a specific compound related to an aroma or aroma precursor, while others focused on basic measures of fruit chemistry (TSS, pH, TA), berry colour (anthocyanins) and/or broad groups of phenolic compounds (flavanols or total phenolics) (Bramley 2005, Trought and Bramley 2011, Baluja et al. 2013). As a result, and despite efforts aimed at development of non-destructive sensors capable of measuring fruit chemistry attributes (Agati et al. 2007, Bramley et al. 2011c, Gutiérrez et al. 2019, Tuccio et al. 2020), growers have little information regarding potential variability of fruit composition in their vineyards, as well as little opportunity to characterise it prior to harvest. Furthermore, given the lack of information on spatial variability in many compounds specifically related to grape and wine quality (i.e. 'objective measures'), growers and wineries may be unsure which compounds to measure. If spatial analysis of an array of compounds shows their spatial structure to be similar, the array of necessary chemical analyses could be reduced leading to a reduction in winery analytical costs. Further, given a lack of commercially available fruit sensors and limited availability of high-quality image collection and analysis services, if patterns of OMFQ are not related to other readily available spatial data far enough in advance of commercial harvest for it to enable decision-making, little can be done to easily remedy or exploit vineyard variability in real time. For this reason, it is important to understand temporal, in addition to spatial variation. Thus, if known patterns from previous seasons are apparent in early- to mid-season imagery obtained in the current season, they could be used to direct sampling to areas of known difference or to direct variable rate management.

Remote sensing may provide vineyard managers with a solution to these problems as many chemical attributes related to fruit quality are related to vine canopy size and shape (Johnson 2003, Hall et al. 2011, Caruso et al. 2017, Romboli et al. 2017). Efforts have been made at directing optimal fruit sampling by use of aerial imagery (Meyers et al. 2020), but without high-resolution ground validation of grape composition, such imagery is unlikely to be sufficiently accurate to provide actionable information for precision management. Data clustering techniques, such as *k*-means, have been used to identify zones of relative consistency in yield and fruit composition (Bramley 2005, Arno et al. 2011, Bramley et al. 2017, González-Fernández et al. 2017) and could provide a link between fruit composition and an easily acquired spatial data source necessary to fully characterise yield and quality variability.

A common approach to fruit quality assessment, both in California and elsewhere, is to focus on a range of grape analytes. In the context of understanding vineyard variability and the idea that some areas of vineyards have inherently different fruit composition than others, there is value in understanding whether different aspects of composition follow similar patterns of spatial variation, thus potentially enabling a reduced analytical load in the winery laboratory, and in knowing whether their variation can be described by remotely sensed imagery. In order to test the relationship between imagery and fruit composition, for the present study, several of these compounds known to be related to canopy size and structure (Bergqvist et al. 2001, Kliewer and Dokoozlian 2005, Yu et al. 2016, Martínez-Lüscher et al. 2019) were selected for spatial analysis and comparisons with imagery-derived vegetation indices and canopy temperature.

Our objectives were to produce geostatistically rigorous maps showing spatial variability of fruit composition in vineyards in the Lodi region of California and to relate the spatial patterns of these compounds to patterns of canopy variability as measured with remote sensing. Thus, the goal was to determine whether key compositional parameters influencing winegrape quality showed consistent structural patterns across multiple commercially farmed vineyards, and to relate those patterns to a data source with the operational potential to guide targeted vineyard management. We were also interested to explore options for reducing the analytical load on laboratories in characterising 'fruit quality', both for more targeted vineyard management and/or fruit streaming at receiving wineries.

Materials and methods

Vineyards
Four Cabernet Sauvignon vineyards were selected for the study (Figure 1), which was conducted over 3 consecutive years culminating in the 2017–2019 vintages. The vineyards were located in district 11 of the American Viticultural Area of Lodi, California (38°7′44″N, 121°16′51″W) and within 40 km of one another. General vineyard characteristics are listed in Table 1. All management practices, such as fertilisation, weed control and other amendments, were spatially uniform in application. Vineyard A was the only vineyard without a perennial cover crop in the inter-row, though the cover crops in Vineyards B, C and D were mostly dormant by berry set (modified E-L stage 27) (Pearce and Coombe 2004) in each season.

Sampling design
A detailed scheme for fruit sampling was developed for each vineyard (Figure 1). Each vineyard scheme contained sufficient data for variogram estimation ($n = 125$) based on the criteria of Webster and Oliver (2007). First, a regularly spaced grid, based on the number of rows and vines in each vineyard, was produced to best distribute the predetermined 125 sample number. Points were then given a random offset of up to half the distance between the next row of points in both x and y directions to randomise 'data vine' selection and to create a sampling grid with a wide range of distances between sampling points for variogram estimation. Finally, approximately 20 randomly selected points from each vineyard's sampling grid were removed and reassigned to a randomly chosen position adjacent to another data vine (i.e. either one row space or one vine space from the adjacent data vine). This method (Bramley 2005) allows for the estimation of an experimental variogram for each fruit quality attribute in each vineyard over distances ranging from the vine separation to the farthest distance between any two sampling points in a vineyard. It also provides adequate numbers of point pairs at short distances for characterising short-range spatial variation.

Vineyard sampling and laboratory analysis
Each vineyard was sampled based on the commercial harvest date set by the receiving winery. Each data vine was hand-harvested and total vine yield and the number of bunches were recorded. Twenty randomly chosen bunches from each data vine were then transferred to the laboratory for subsequent chemical analysis of selected fruit compositional attributes which, henceforth, we refer to as OMFQ; that is, through these analytes, fruit quality can be
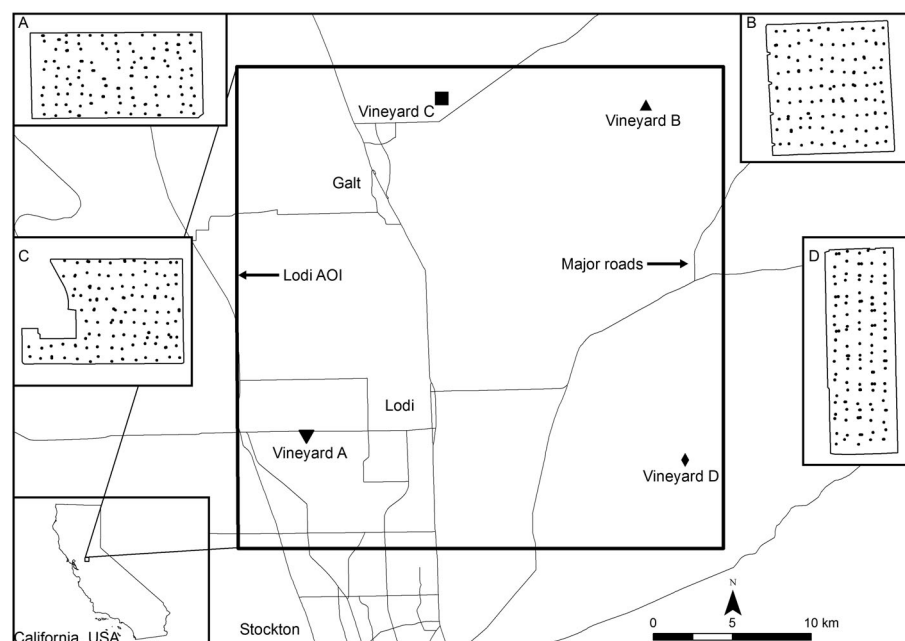
Figure 1. Location and data vine (●) distribution of the four Cabernet Sauvignon vineyards in the Lodi appellation of California (□) used in the study: Vineyard A (▼), Vineyard B (▲), Vineyard C (■) and Vineyard D (◆). Major roads (──).

quantitatively assessed as opposed, for example, to assessing wine quality through informal sensory evaluation (Gishen et al. 2002). The OMFQ used here were those commonly used in Californian wine production and comprised total anthocyanins, polymeric tannins, quercetin glycosides, six carbon alcohols and aldehydes (C6), 3-isobutyl-2-methoxypyrazine (IBMP), β-damascenone, malic acid and yeast assimilable nitrogen (YAN). Once the fruit arrived at the laboratory, whole bunches were mechanically destemmed and homogenised before extraction with acidified 50% ethanolic solution. Total anthocyanins were measured using a UV–Vis based method described by Iland et al. (2000). Polymeric tannins and quercetin glycosides (combined total of quercetin 3-O-glucoside and 3-O-glucuronide) were measured using reverse-phase HPLC (Peng et al. 2001, Chong et al. 2019). The free-form volatile compounds (C6 and IBMP) were analysed using headspace solid-phase microextraction (HS-SPME) coupled to a GC/MS as described by Kotseridis et al. (2008) and Canuti et al. (2009). The bound form of

β-damascenone was extracted using solid-phase extraction adapted from Whiton and Zoecklein (2002), followed by fast acid hydrolysis and SPME-GC/MS as described by Kotseridis et al. (1999), Ibarz et al. (2006) and Canuti et al. (2009). A WineScan FT-120 Fourier Transform Infrared Spectroscopy (FOSS North America, Eden Prairie, MN, USA) was used for the analysis of TSS, pH, TA, YAN and malic acid. The calibration for each attribute was created by WinISI II software (FOSS, Hillerød, Denmark) using E&J Gallo's internal grapes and reference chemistry quality standards.

Descriptive and spatial analysis
Descriptive statistics, coefficients of variation (CV%) and spread [range as per cent of the median (Bramley 2005)], were calculated to describe the relative statistical variation between vineyards. Experimental variograms (Webster and Oliver 2007) were then estimated for each fruit quality compound in each vineyard using VESPER (Minasny et al. 2005). Preliminary exploratory variogram fitting led to the

Table 1. Physical characteristics of the vineyards used in the study.

	Vineyard A	Vineyard B	Vineyard C	Vineyard D
Training method and trellis system	Single bilateral sprawl	Quadrilateral sprawl	Quadrilateral sprawl	High wire sprawl
Vine spacing (m)	2.1	1.2	1.8	2.4
Row spacing (m)	3.1	3.4	3.4	3.1
Vineyard area (ha)	7.4	13.8	11.8	11.2
Year planted	2010	2013	1998	2012
Rootstock/scion clone	039-16/FPS08	SO4/7	1103P/7	039-16/15
Rootstock parentage	*V. vinifera* × *V. rotundifolia*	*V. berlandieri* × *V. riparia*	*V. berlandieri* × *V. rupestris*	*V. vinifera* × *V. rotundifolia*
Pruning method	Hand	Hand	Hand	Machine
Floor management	Tilled bare soil	Perennial cover crop	Perennial cover crop	Perennial cover crop
Soil texture (% clay/silt/sand)	14/29/57	26/28/45	20/33/47	15/24/61
Elevation [min–max (masl)]	6.3–7.1	38.9–60.4	20.1–21.6	39.6–47.0
Applied water (L/m)				
2017	No data for all 3 years	1485	535	No data
2018		1387	608	881
2019		1418	658	856

spherical model being chosen as appropriate for characterising spatial structure in fruit quality; that is, the spherical model either gave the best fit to the experimental variogram or one that was not significantly inferior to an alternative such as the exponential model. Model choice was standardised in an attempt to minimise any effects of the artefacts of variogram fitting from subsequent comparison of maps across sites and seasons. Maps were then interpolated for each vineyard in VESPER, based on these variograms and the 125 sample points, using global point kriging. A maximum distance setting was applied to each variogram model based on vineyard size in order to maximise the number of pairs in each lag class. This resulted in a 250 m maximum in vineyards A, C and D, while a 350 m maximum distance was applied to vineyard B.

Nugget [measurement and sampling error (c_0)], partial sill [spatially dependent variance (c_1)] and effective range [distance at which samples are no longer considered spatially dependent (a_1) (Webster and Oliver 2007)] were derived during the variogram fitting process in VESPER, and the Cambardella index (CAM) was calculated using the formula

$$\left(\frac{c_0}{c_0 + c_1} \right) \times 100$$

to describe the degree to which variability is spatially structured (Cambardella and Karlen 1999, Santos et al. 2012, Santesteban et al. 2013, Sams et al. 2019). In general, lower values of CAM represent stronger spatial structure (Han et al. 1994, Taylor et al. 2007).

Remote sensing

High-resolution imagery (VIS/NIR, 0.2 m ground resolution; wavelengths = 800, 670, 550 nm; bandwidth = 10 nm; thermal/canopy temperature, 0.4 m ground resolution, bandwidth = 7.5–13 μm; absolute accuracy ±1°C) was sourced from a commercial provider for each vineyard at major phenological stages in 2018 and 2019, and one image in 2017 collected at a modified E-L stage 27 [Table 2 (Pearce and Coombe 2004)]. Images were collected as close to solar noon as possible on each date and only on cloudless days. Given the distance between vineyards and the time necessary to fly each using a single aircraft on a single day, as well as other customer vineyards, acquisition times ranged from approximately 1 h before solar noon to approximately 1 h past solar noon. The normalised difference vegetation index (NDVI), a ubiquitous vegetation index used across many disciplines of plant science, was used as a proxy for canopy size and vigour (Johnson 2003). Following histogram analysis of

each image, the estimated non-vine signal was classified and masked using a thresholding process to enable assessment of the correlation between vine canopy values and OMFQ. Images were classified into 'vine' and 'non-vine' signals based on the bimodal distribution in each image. The centre of the trough between the two peaks in the histogram was used as the cut-off value in each image. While it was not possible to definitively remove all mixed pixels, the histogram thresholding process eliminated all pixels dominated by non-vine signals. The masking layer created in the non-vine signal removal was then used to remove the same areas from imagery layers of surface temperature. The difference between canopy and air temperature ($T_c - T_a$) for each image was calculated by subtracting the ambient temperature at the time of image acquisition (T_a) from canopy temperature of the sensor (T_c) according to Idso et al. (1977), where T_c was derived using a nearly identical histogram separation method (the difference being proximal vs aerial imagery) to that proposed in Salgadoe et al. (2019), and T_a was from a central weather station near Lodi, California (Lodi Winegrape Commission Weather station network at www.lodi.westernweathergroup. com, Station ID: Valley Oak). As would be the case with nearly all commercial image providers and growers in this region, no ground reflectance targets were in the image scenes, and subsequent analyses are dependent on the calibrations and atmospheric corrections provided by the source (Bramley et al. 2019).

Following the image correction described above, NDVI and ($T_c - T_a$) values were extracted from a neighbourhood of pixels in the imagery corresponding to each 'data vine' using the Spatial Analyst toolbox available in the ArcGIS software suite (v10.4, Environmental Systems Research Institute, Redlands, CA, USA). In Vineyard A, for example, based on the row and vine spacing (Table 1), each vine occupies 6.5 m^2 which equates to thirty-three 0.2 m^2 pixels in the NDVI images and seventeen 0.4 m^2 pixels in the ($T_c - T_a$) maps, although roughly half of these pixels were removed as inter-row. These data were used to calculate two-tailed Pearson's correlations using a modified *t*-test to account for spatial autocorrelation with fruit composition and yield values for those vines (Dutilleul et al. 1993, Sozzi et al. 2020).

Clustering

Each set of annual image data (2018–2019; only one image was collected in 2017) was clustered into two- and three-zone solutions using *k*-means cluster analysis for two separate analyses in R (R Core Team 2020). The first analysis clustered data from only the 125 data vines in each vineyard (see above). In the second analysis, each image layer (with

Table 2. Dates of remote imagery overpasses and associated phenological stages based on the modified E-L phenological scale 2017–2019.

Season	>50% Budburst	Imagery overpass	Days post-budburst†	Modified E-L stage‡	Stage description
2017	27 March–3 April	15 June	73–79	27	Berry set
2018	28 March–4 April	14 May	40–46	19	Initial flowering
		3 June	60–66	23	>50% Flowering
		13 June	70–76	27	Berry set
		24 July	111–117	35	Veraison
		29 August	147–153	36	Ripening
2019	30 March–8 April	14 May	38–47	19	Initial flowering
		2 June	57–66	23	>50% Flowering
		13 June	68–77	27	Berry set
		24 July	109–118	35	Veraison

†The range of dates post-budburst represents differences in phenological advancement among vineyards; ‡Pearce and Coombe (2004).

Table 3. Spatial statistics for fruit composition at all data vine locations in each of the four vineyards over the 3 years of the study.

		Vineyard A					Vineyard B				
		Nugget (c_0)	Sill (c_1)	ER (a_1)	CAM	RMSE	Nugget (c_0)	Sill (c_1)	ER (a_1)	CAM	RMSE
Yield	2017	1.8	0.4	150	83	0.23	1.2	0.6	178	68	0.26
	2018	2.1	0.3	102	89	0.16	1.4	0.8	240	64	0.14
	2019	2.9	0.7	51	81	0.27	1.6	1.9	61	47	0.29
AN	2017	0.01	0.00	41	54	0.00	0.02	0.02	97	44	0.00
	2018	0.01	0.03	131	19	0.01	0.03	0.02	56	65	0.00
	2019	0.00	0.01	52	14	0.00	0.01	0.01	43	59	0.00
PT	2017	6.6	4.1	108	62	0.80	0.2	0.5	231	27	0.09
	2018	1.6	1.5	205	51	0.31	0.0	0.2	606	18	0.02
	2019	0.6	3.4	24	15	0.23	0.1	0.0	410	67	0.00
QG	2017	71	7	178	91	7.56	773	188	185	80	134.00
	2018	15	46	164	25	5.82	51	23	116	69	22.80
	2019	63	9	20	88	4.42	195	120	112	62	74.10
MA	2017	5.7	5.3	82	52	1.00	0.0	0.0	216	40	0.01
	2018	1.8	12.0	73	13	1.36	0.0	0.1	361	18	0.03
	2019	3.7	5.1	80	42	0.55	0.1	0.1	42	49	0.03
BD	2017	19	7	80	73	1.79	18	27	78	40	3.68
	2018	6	43	21	12	3.85	78	149	673	34	16.50
	2019	19	23	215	44	5.15	26	15	102	64	3.86
C6	2017	21.7	9.5	118	70	2.26	0.3	0.5	65	35	0.06
	2018	54.8	47.5	350	54	8.78	0.3	0.1	573	73	0.09
	2019	50.4	8.1	224	86	2.83	0.6	0.3	300	67	0.07
IBMP	2017	8.7	2.2	72	80	0.73	0.3	0.4	37	43	0.15
	2018	8.7	6.1	129	59	1.32	1.7	6.6	133	21	1.34
	2019	8.7	2.2	72	80	0.73			n.d.		
YAN	2017	4	5	68	47	0.95	22	216	494	9	42.70
	2018	97	685	48	12	95.20	213	272	197	44	33.50
	2019	153	649	36	19	59.10	364	210	107	63	239.00

		Vineyard C					Vineyard D				
		Nugget (c_0)	Sill (c_1)	ER (a_1)	CAM	RMSE	Nugget (c_0)	Sill (c_1)	ER (a_1)	CAM	RMSE
Yield	2017	0.9	1.7	148	34	0.21	1.5	1.8	111	46	0.37
	2018	1.4	2.2	122	40	0.35	0.7	1.6	42	30	0.28
	2019	1.4	1.1	122	56	0.19	0.4	3.0	65	12	0.26
AN	2017	0.02	0.03	128	44	0.00	0.02	0.01	88	76	0.00
	2018	0.07	0.08	107	48	0.02	0.01	0.07	57	15	0.01
	2019	0.01	0.03	124	19	0.00	0.00	0.02	38	16	0.00
PT	2017	0.0	0.30	56	13	0.05	0.1	0.1	86	49	0.02
	2018	0.1	0.09	108	49	0.02	0.0	0.0	59	23	0.01
	2019	0.1	0.18	125	40	0.02	0.1	0.2	109	29	0.04
QG	2017	165	310	84	35	34.80	125	230	481	35	22.50
	2018	171	140	165	55	23.60	43	10	155	82	5.46
	2019	114	322	58	26	30.10	196	416	85	32	52.50
MA	2017	0.0	0.2	154	15	0.02	0.0	0.1	45	36	0.02
	2018	0.0	0.1	174	24	0.01	0.0	0.1	62	12	0.01
	2019	0.0	0.2	117	5	0.02	0.0	0.1	41	7	0.02
BD	2017	22	17	68	56	4.05	28	13	178	68	4.91
	2018	12	84	124	12	15.90	24	20	291	55	3.46
	2019	33	28	261	54	4.39	11	25	202	30	2.84
C6	2017	0.3	0.2	252	55	0.03	0.5	1.6	457	24	0.11
	2018	0.1	0.5	100	15	0.06	0.3	0.9	113	28	0.11
	2019	0.1	0.3	81	17	0.12	0.1	0.2	115	27	0.03
IBMP	2017			n.d.			1.5	2.5	73	38	0.30
	2018	0.3	0.2	140	54	0.08			n.d.		
	2019			n.d.			0.0	0.8	52	32	0.15
YAN	2017	213	731	185	23	63.60	257	778	39	25	73.20
	2018	47	307	87	13	27.00	202	452	96	31	102.00
	2019	83	315	125	21	24.20	29	230	68	11	59.70

$n = 125$; n.d., not detected or too few samples with detectable compound. AN, anthocyanins; BD, β-damascenone; C6, six carbon alcohols and aldehydes; CAM, Cambardella index; ER, effective range (m); IBMP, 3-isobutyl-2-methoxypyrazine; MA, malic acid; PT, polymeric tannins: QG, quercetin glycosides; RMSE, root-mean-square error; YAN, yeast assimilable nitrogen.

the non-vine signal removed) was resampled to the same 2 m grid used to interpolate the fruit chemistry and clustered using the same k-means clustering process in R. This process allowed for a full vineyard comparison between imagery and fruit composition both in terms of entire map layers, and in respect of the specific 125 sample locations.

All three seasons of all fruit composition variables (OMFQ) in each vineyard (2017–2019) were clustered to provide an overall assessment of fruit quality variability with which to compare clusters generated from all imagery (2017–2019). Clustered maps were generated in ArcGIS v10.4 using the 2 m gridded map data.
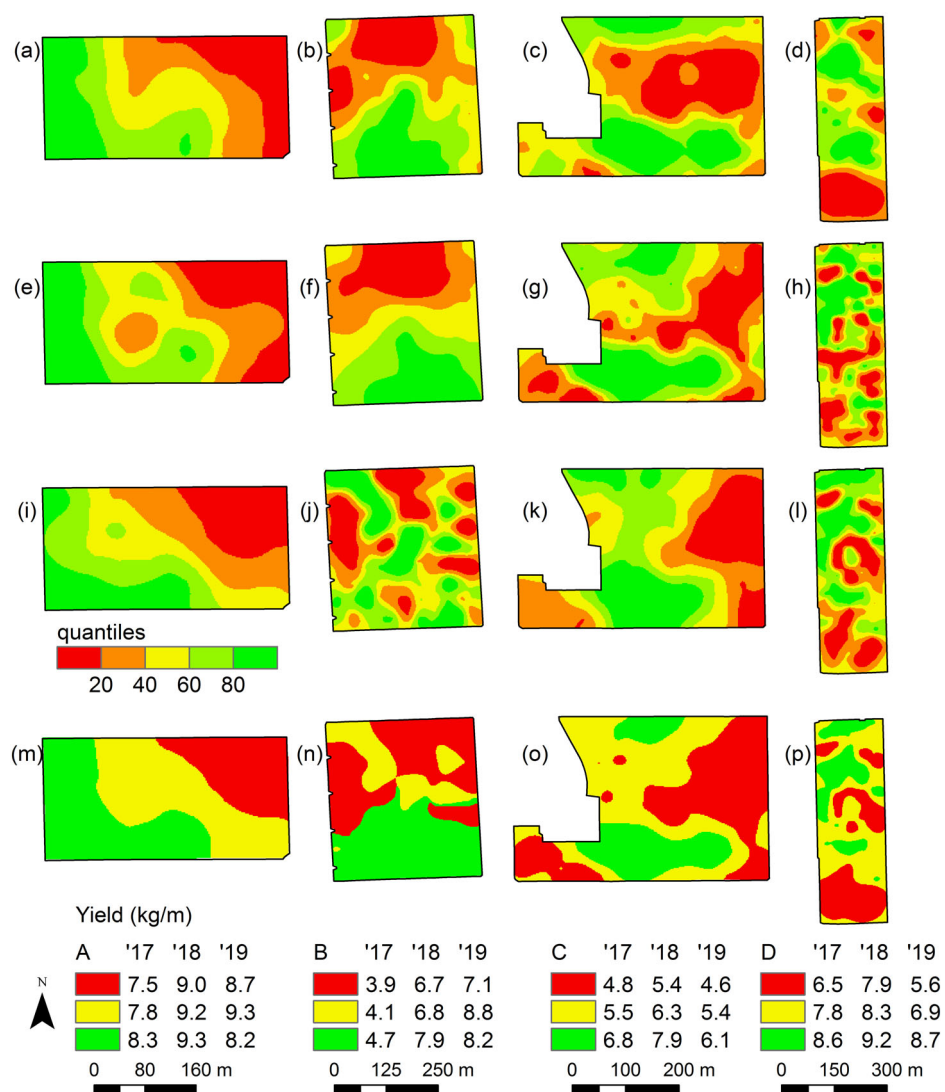
Figure 2. Patterns of yield variability in Vineyard A [(a) 2017, (e) 2018, (i) 2019], Vineyard B [(b) 2017, (f) 2018, (j) 2019], Vineyard C [(c) 2017, (g) 2018, (k) 2019] and Vineyard D [(d) 2017, (h) 2018, (l) 2019] ($n = 125$), and k-means clusters, with cluster means (kg/m), from all three seasons using the 2 m gridded data [(m)–(p)]. Note that the map data [(a)–(l)] have been classified as quantiles (20th percentiles).

Results

Spatial variability

The patterns of spatial variation were most temporally stable in Vineyard C as compared with the other three vineyards with relatively consistent CAM values that were also representative of strong to moderate spatial structure [CAM < 50 (Table 3)]. The effective range was more consistent in Vineyard C than in other vineyards across most compositional variables (Table 3). Additionally, Vineyard C showed strong patterns of spatial variability in yield (Figure 2c,g,k) and in most fruit chemistry variables (Figure 3). Short-range variation, however, and low concentration of β-damascenone and C6 in three seasons resulted in clusters unlike those of most other compounds (Figure 3). Measures of TSS and pH showed low CV and spread in all vineyards (Table 4). Though the patterns in seasonal yield (Figure 2a,e,i,m) were visually similar to those of IBMP (Figure 4a,e,i,m), spatial statistics showed that Vineyard A was not strongly spatially structured based on inconsistent effective ranges and high CAM values for fruit compositional attributes (Table 3). Relatively low spread and CV (Table 4) resulted in clusters of NDVI that were unable to partition fruit composition in this

vineyard (Figure 5b). In Vineyard B, some compounds, such as anthocyanins, were reasonably consistent in terms of the CAM, though the values were not typically indicative of strong spatial structure (Table 3). Vineyard D showed a relatively stable spatial structure of β-damascenone (Figure 4) when compared with other aroma compounds in this and the other vineyards, though the mean values in the three clusters identified using k-means were similar (Figure 4). Variogram root-mean-square error was generally less than one-third of the nugget variance, though the average root-mean-square error for YAN was 70% (Table 3).

Temporal variation

Though significant correlations were found for each variable between seasons ($P < 0.05$), yield, TSS, pH and malic acid were the strongest interseasonally correlated variables across all four vineyards (average Pearson correlation >0.5), while C6 and IBMP were the only variables with average correlations across seasons below 0.2 (Table 5); that is, the concentration of C6 and IBMP in 1 year was generally a poor indicator of their concentration in other years. β-Damascenone was the only variable related to an aroma or

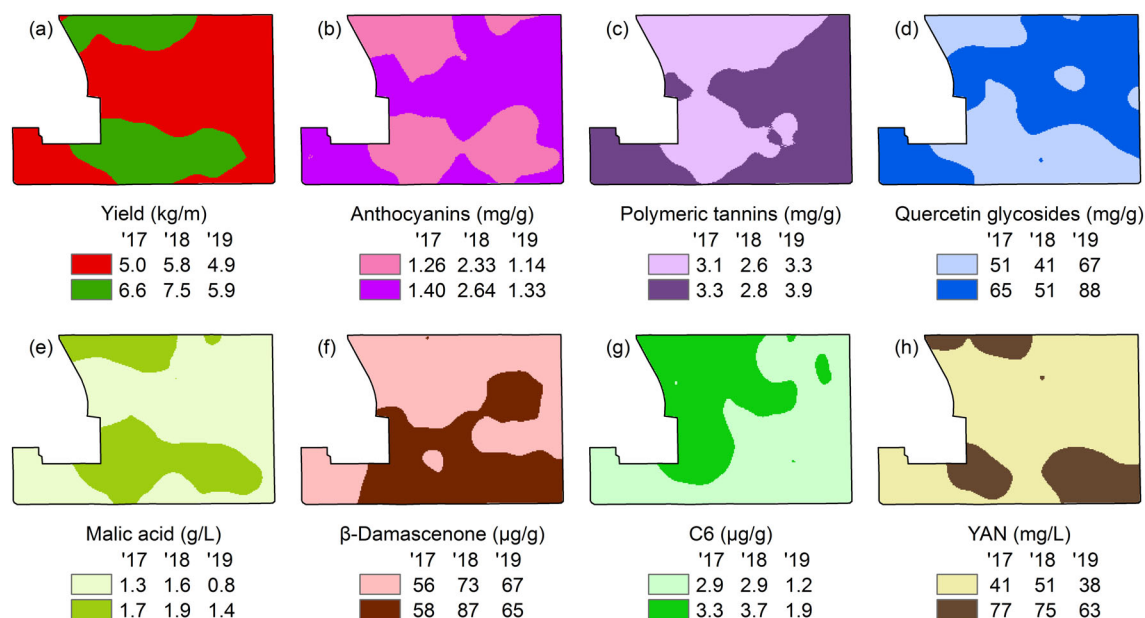**Figure 3.** Results of *k*-means clustering using two-cluster solutions in all three seasons (2017–2019) using the 2 m gridded data from seven individual fruit compositional attributes and yield in Vineyard C. Numbers in figure legends are cluster means. Numbers in figure legends are cluster means (a) yield, (b) anthocyanins, (c) polymeric tannins, (d) quercetin glucosides, (e) malic acid, (f) β-damascenone, (g) C6 (six carbon alcohols and aldehydes), and (f) yeast assimilable nitrogen (YAN).

aroma precursor with an average correlation coefficient between seasons above 0.3 (Table 5).

In terms of gross variability, Vineyard A exhibited the lowest average CV (21%) and spread (Table 4). Vineyard A also produced the highest yield each season, and the highest concentration of IBMP, C6 compounds and YAN, as well as malic acid. A lower concentration of anthocyanins (colour), β-damascenone and polymeric tannins was found in Vineyard A compared to the other three vineyards (Table 4). In Vineyard A, only malic acid and YAN showed a Pearson correlation between seasons above 0.5 and most other variables did not have a significant correlation between seasons ($P < 0.05$; Table 5). Vineyard B showed high seasonal variability with the highest average CV (Table 4), and interseasonal yield was most highly correlated in this vineyard despite a large increase from 2017 to 2018 (Table 5, Figure 2). Vineyard C showed remarkable temporal stability compared with the others and some of the highest concentration of positive fruit quality attributes, including quercetin glycosides, polymeric tannins and anthocyanins, as well as the lowest yield, in most seasons (Table 4). Correlations between seasons were also generally stronger and more consistent in Vineyard C than in the other vineyards (Table 5). On average, Vineyard D was slightly more consistently correlated (average absolute Pearson correlation = 0.54) between seasons than the other vineyards (average absolute Pearson correlations of A = 0.31, B = 0.32, C = 0.51) (Table 5), but spatial statistics did not reflect this consistency over the three seasons (Table 3).

Relationship between fruit composition and remotely sensed imagery

Spatial statistics for NDVI and $(T_c - T_a)$ extracted from imagery at the 'data vine' locations, showed general agreement by vineyard with those of fruit composition and yield, though with more erratic effective ranges and CAM values (Table 6). The CAM often decreased with phenological development during the 2018 and 2019 seasons, but the pattern was not always consistent and was even reversed in several cases by modified stage 35 or 36 in 2018 (Table 6).

Values of the CAM again proved to be most consistent, as well as indicating strong spatial structure, in Vineyard C relative to other vineyards (Table 6). Extremely low nugget variance in the $(T_c - T_a)$ imagery in Vineyard C caused the CAM value to be low in 2017 and 2018 but $(T_c - T_a)$ showed high spatial structure in all 2019 images (Table 6). Imagery from vineyards A and B were most inconsistent across seasons and phenological stages, while imagery from Vineyard D exhibited the lowest average effective ranges and relatively small CAM values (Table 6).

Modified *t*-tests between both NDVI and $(T_c - T_a)$ imagery at different stages and fruit composition at harvest showed that correlations peaked (generally between ±0.3 and ±0.6) at modified E-L stage 35 (veraison) in 2018 and 2019 and were significant ($P < 0.05$) for yield, anthocyanins, polymeric tannins, quercetin glycosides and malic acid in most vineyards. The compounds C6, β-damascenone and IBMP were rarely significantly correlated ($P < 0.05$) with imagery from any phenological stage, and correlation coefficients were mostly below ±0.2 (data not shown). In nearly every case, correlation coefficients between the two types of imagery and fruit composition were the inverse of one another, that is fruit composition variables that were positively correlated with NDVI were nearly always negatively correlated with $(T_c - T_a)$, and vice versa.

Mapping fruit 'quality'

Mean cluster values for indices of fruit composition in two-cluster solutions generated from the 125 data points (Table 7) were similar to those generated from the 2 m interpolated data and resampled imagery (Table 8). Importantly though, the 2 m interpolated data provided a full visual representation of the clustered zones that would be necessary for developing prescriptive maps for variable rate management (Figure 4). There were some small differences in the partitioning of fruit composition based either on NDVI or $(T_c - T_a)$, but cluster means were generally similar (Tables 7,8, Figure 5). The separation of TSS, pH and TA by NDVI or $(T_c - T_a)$ from 125 data points or 2 m interpolated

Table 4. Descriptive statistics for yield and fruit composition parameters in the vineyards used in the study (2017–2019).

		Vineyard A			Vineyard B			Vineyard C			Vineyard D		
		Median	CV%	Spread	Median	CV%	Spread	Median	CV%	Spread	Median	CV%	Spread
Yield (kg/m)	2017	7.8	19	95	4.1	31	206	5.4	28	129	7.4	25	137
	2018	9.2	16	102	7.2	20	106	6.1	30	128	8.3	18	107
	2019	9.0	20	100	7.6	24	116	5.2	30	162	6.9	27	120
TSS (°Brix)	2017	24.4	1	10	24.8	4	24	24.6	3	31	24.3	5	35
	2018	24.4	3	16	26.5	3	16	25.4	3	19	24.7	6	34
	2019	24.4	4	16	25.4	5	40	25.0	5	26	25.3	6	40
pH	2017	3.77	2	9	3.83	2	10	3.88	3	18	3.67	4	19
	2018	3.85	2	7	3.79	2	9	3.80	3	13	3.60	2	16
	2019	3.87	2	9	3.63	2	12	3.73	3	16	3.63	3	12
TA (g/100 mL)	2017	0.37	7	38	0.32	8	44	0.38	12	81	0.38	13	78
	2018	0.38	13	66	0.31	8	53	0.34	15	85	0.38	16	111
	2019	0.37	9	41	0.31	17	165	0.35	16	89	0.36	13	75
Anthocyanins (mg/g)	2017	0.79	13	79	1.15	16	94	1.34	16	94	0.89	18	79
	2018	1.21	16	78	2.19	10	52	2.45	16	109	1.89	16	94
	2019	0.72	17	81	1.08	10	54	1.25	16	74	0.89	16	113
Polymeric tannins (mg/g)	2017	2.0	16	78	3.6	22	103	3.2	17	100	2.3	21	112
	2018	1.4	12	66	2.2	15	104	2.7	15	89	2.2	10	52
	2019	1.8	11	53	2.4	11	54	3.7	16	72	2.4	21	113
Quercetin glycosides (mg/g)	2017	34	25	135	97	30	143	57	37	184	48	32	156
	2018	26	30	136	23	37	208	45	38	225	46	16	84
	2019	29	29	149	81	23	124	80	27	153	69	34	216
Malic acid (g/L)	2017	1.9	17	99	1.3	17	109	1.4	29	169	1.6	20	113
	2018	2.1	17	98	1.5	19	89	1.7	17	91	1.7	17	85
	2019	1.9	16	85	0.9	32	315	0.9	50	231	1.1	33	252
β-Damascenone (μg/g)	2017	46	11	58	59	11	67	57	11	64	47	13	76
	2018	60	12	77	84	14	86	79	13	72	53	12	69
	2019	59	10	53	60	11	63	66	11	55	48	13	67
C6 (μg/g)	2017	5.3	10	54	4.1	22	122	3.0	22	101	5.2	25	115
	2018	4.8	18	97	3.2	19	127	3.2	24	130	4.6	24	104
	2019	5.1	15	69	4.0	22	112	1.5	45	170	1.5	35	181
IBMP (pg/g)	2017	5.4	60	263	0.0	452	n.a.	0.0	673	n.a.	1.8	100	442
	2018	3.7	100	384	1.3	132	1060	0.0	512	n.a.	n.d.	n.a.	n.a.
	2019	0.0	145	n.a.	n.d.	n.a.	n.a.	n.d.	n.a.	n.a.	0.0	887	n.a.
YAN (mg/L)	2017	144	19	110	25	47	504	40	60	383	92	32	173
	2018	252	11	63	86	24	156	53	34	193	64	41	296
	2019	171	15	78	21	95	1210	37	45	251	36	49	421
Mean		n.a.	21	84	n.a.	35	169	n.a.	54	115	n.a.	46	123

$n = 125$; n.a., not applicable; n.d., not detected. C6, six carbon alcohols and aldehydes; CV, coefficients of variation; IBMP, 3-isobutyl-2-methoxypyrazine; YAN, yeast assimilable nitrogen.
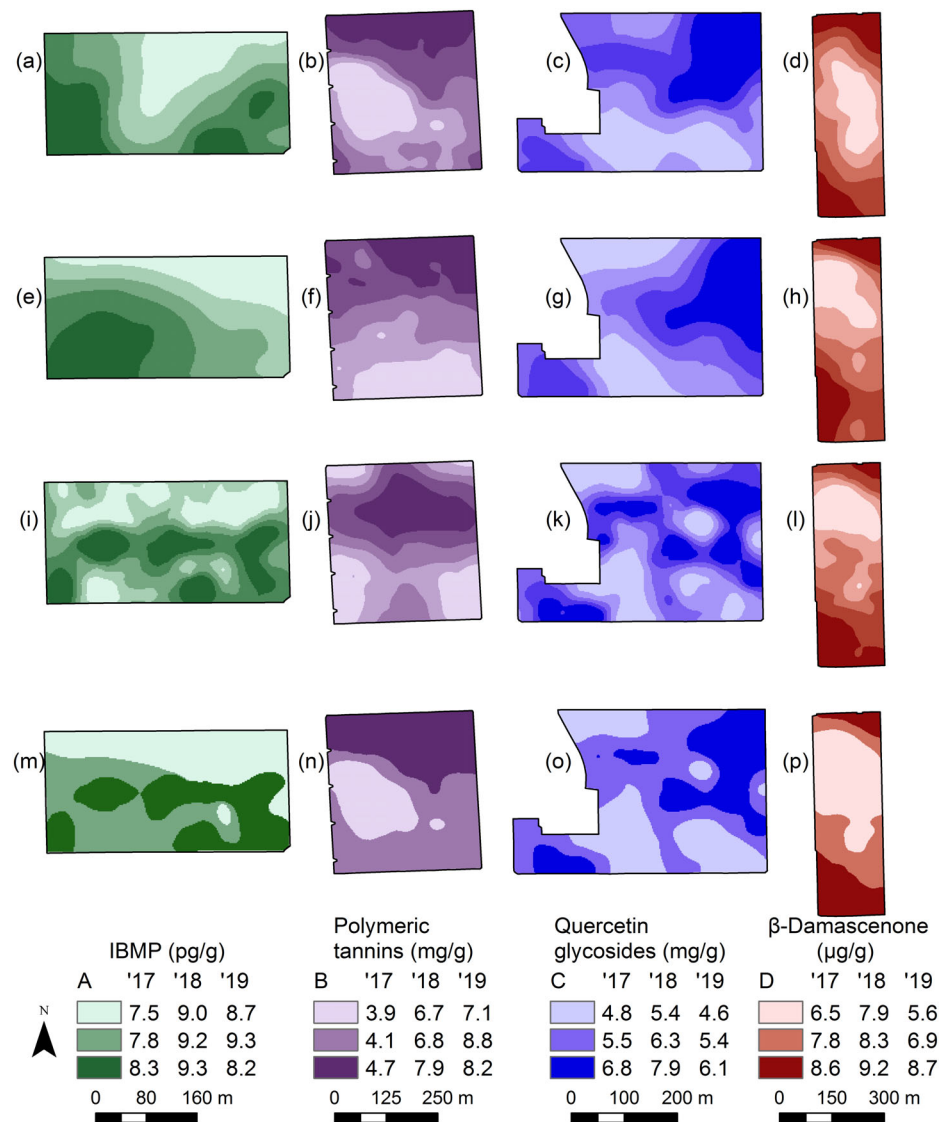
Figure 4. Illustrations of spatial variability noted in this study: 3-isobutyl-2-methoxypyrazine (IBMP) in Vineyard A [(a) 2017, (e) 2018, (i) 2019]; polymeric tannins in Vineyard B [(b) 2017, (f) 2018, (j) 2019]; quercetin glycosides in Vineyard C [(c) 2017, (g) 2018, (k) 2019]; and β-damascenone in Vineyard D [(d) 2017, (h) 2018, (l) 2019] (*n* = 125); and results of *k*-means clustering (3 cluster solutions), for all three seasons (2017–2019) using the 2 m gridded data [(m)–(p)]. Note that the map data [(a)–(l)] have been classified as quantiles (20th percentiles). The numbers in the legends to maps (m)–(p) are the cluster means.

data were generally weak compared with other variables (data not shown). Fruit composition and imagery in Vineyards B and D were generally spatially and statistically erratic. Vineyard A was relatively homogenous whilst, in contrast, Vineyard C showed strong zonal differences (Tables 7,8). Accordingly, Vineyards A and C provide a useful comparison of the utility of remote sensing to describe zonal differences in fruit composition (Figure 5). As is clear from the small zonal differences of vine productivity in Vineyard A, along with the lack of visual similarity between imagery clusters and fruit compositional clusters, imagery was not successful in delineating zones in this vineyard. In contrast, and consistent with most analyses presented here, classifications generated from imagery showed greater separation in most compositional attributes in Vineyard C (Tables 7,8, Figure 5).

Discussion

Vineyard variability is an important and complex issue for several reasons. First, vineyard managers must ask whether a

vineyard is variable enough in compounds that impact fruit quality to warrant further investigation and, if consistent, possible differential management. Ranges of statistical variability in additional compounds can be useful because they provide the initial clues into how variable a vineyard might be. For instance, Vineyard A is relatively uniform compared to the other vineyards as evidenced by the relatively low CV and spread (Table 4), high CAM values, inconsistent effective ranges in most fruit quality attributes (Tables 3,6), and small differences between zones (Tables 7,8, Figure 5). Although Vineyard A was consistently lower than the other vineyards in the study in terms of phenolic compounds, it would not be a candidate for variable rate management under its present production system due to a small range in both yield and the various measures of fruit composition. Second, practitioners must be confident that any patterns of variability persist over time. Vineyard C was spatially consistent and variable enough (Tables 3–6) to be a suitable candidate for increasing its economic productivity by means of variable rate management and/or selective harvesting, as shown by the spatial patterns
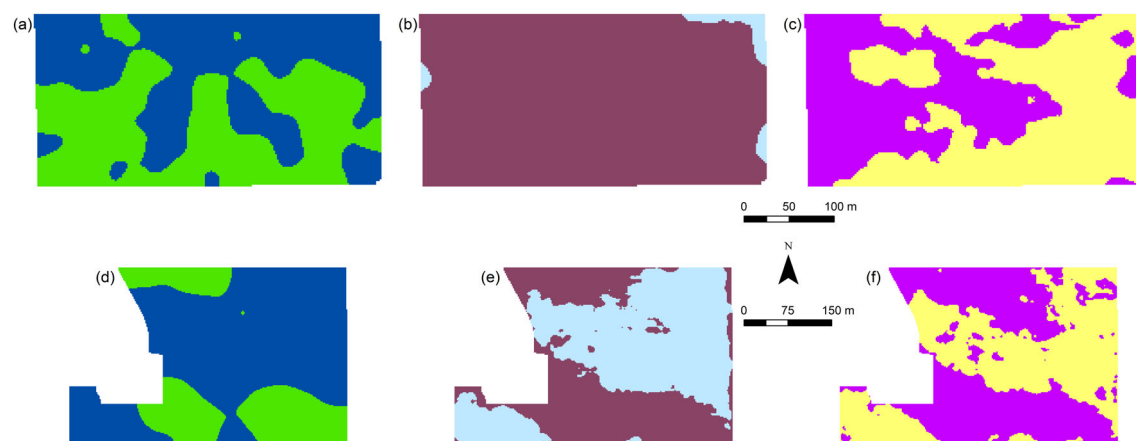
Figure 5. Results of *k*-means clustering in Vineyard A using: (a) all objective measures of fruit quality 2017–2019, (b) all NDVI imagery 2017–2019 and (c) all ($T_c - T_a$) images 2017–2019; and in Vineyard C using (d) all objective measures of fruit quality 2017–2019, (e) all NDVI imagery 2017–2019 and (f) all ($T_c - T_a$) images 2017–2019. Note that the cluster means are reported in Table 8. All objective measures of fruit quality: 1 (■), 2 (■); all NDVI: 1 (□), 2 (■); all $T_c - T_a$: 1 (□), 2 (■). NDVI, normalised difference vegetation index; $T_c - T_a$, canopy temperature − air temperature.

in yield (Figure 2c,g,k) and most fruit chemistry variables (Figure 3). This finding, combined with an average CV of 54% (Table 4), is useful because for a vineyard to be a strong candidate for variable rate management there must be enough variation in fruit composition to warrant that decision as well as some consistency (i.e. predictability) of spatial patterns of these variables between seasons. The CV in measures of basic fruit chemistry (TSS, pH, TA) were low in these four vineyards (Table 4). This is arguably the expected result as the fruit was considered appropriately ripe for commercial harvest. It also makes clear that the other OMFQ are necessary to characterise vineyard variability if differential management strategies targeting fruit composition are to be employed. Since the season to season correlation of these variables was high in most cases (Table 5), but the patterns of variability did not align with yield or imagery as well as variation in other variables such as anthocyanins or malic acid (data not shown), those interested in vineyard performance should perhaps put less weight on measures of basic chemistry for management decisions.

Several attributes of fruit composition measured at harvest, including quercetin glycosides and malic acid, show promise for understanding potential wine quality from a spatial perspective and across seasons. Additionally, some compounds may be more important for decision-making with respect to grape processing and final wine quality and/or style. The spatial variability of phenolic compounds was fairly consistent and potentially predictable using NDVI and ($T_c - T_a$) generated from remote sensing techniques. These compounds are major drivers of positive mouthfeel characteristics in wine (Chong et al. 2019), making them potential targets for precision management. We hypothesise that some parameters, such as IBMP, may not be useful for this purpose unless measured earlier in fruit development. When these compounds are found in samples from a vineyard, they present a warning for wineries or growers looking to collect a single fruit sample to accurately reflect the composition of the entire vineyard. An excessive concentration of IBMP is considered a negative attribute in California Cabernet Sauvignon, and vineyard managers generally avoid this issue by harvesting fruit at higher than

Table 5. Pearson correlations between fruit composition measured in different seasons in each of the four vineyards (2017–2019).

| | Pearson coefficient (*r*) | | | | | | | | | | | |
| | Vineyard A | | | Vineyard B | | | Vineyard C | | | Vineyard D | | |
	17/18	17/19	18/19	17/18	17/19	18/19	17/18	17/19	18/19	17/18	17/19	18/19
Yield	0.41*	0.41*	0.49*	0.68*	0.56*	0.66*	0.64*	0.46*	0.71*	0.52*	0.58*	0.68*
TSS	0.20*	0.43*	0.15	0.48*	0.33*	0.44*	0.61*	0.73*	0.73*	0.81*	0.78*	0.89*
pH	0.25*	0.44*	0.38*	0.34*	0.45*	0.44*	0.76*	0.66*	0.72*	0.84*	0.85*	0.80*
TA	0.11	0.21*	0.08	0.50*	0.36*	0.17	0.65*	0.74*	0.56*	0.61*	0.76*	0.70*
AN	0.27*	0.16	0.10	0.18	−0.04	0.28*	0.29*	0.29*	0.21	0.65*	0.57*	0.59*
PT	0.41*	0.16	0.20	0.45*	0.17	0.45*	0.29*	0.41*	0.43*	0.35*	0.28*	0.47*
QG	0.19	0.28*	−0.12	0.56*	0.31*	0.18	0.62*	0.59*	0.59*	0.42*	0.20*	0.39*
MA	0.63*	0.64*	0.65*	0.71*	0.37*	0.34*	0.49*	0.72*	0.58*	0.46*	0.57*	0.65*
BD	0.14	0.28*	0.15	0.38*	0.07	0.49*	0.49*	0.44*	0.19	0.47*	0.45*	0.59*
C6	0.19	−0.08	−0.19*	0.07	0.01	0.11	0.19	0.28	0.31	0.55*	0.01	0.35*
IBMP	0.11	0.35*	0.31*	0.13	n.d.	n.d.	−0.03	n.d.	n.d.	n.d.	−0.09	n.d.
YAN	0.62*	0.63*	0.59*	0.18	0.08	0.03	0.56*	0.72*	0.65*	0.43*	0.37*	0.62*

*$P < 0.05$; n.d., not detected. $n = 125$; subheadings below the vineyard letter (A, B, C, D) designations refer to comparisons between seasons (2017/18, 2017/19, 2018/19). Note that a modified *t*-test corrected for spatial autocorrelation (Dutilleul et al. 1993) was used for this analysis. AN, anthocyanins; BD, β-damascenone; C6, six carbon alcohols and aldehydes; IBMP, 3-isobutyl-2-methoxypyrazine; MA, malic acid; PT, polymeric tannins: QG, quercetin glycosides; YAN, yeast assimilable nitrogen.

Table 6. Spatial statistics from points extracted from imagery at all data vine locations in each of the four vineyards.

		Vineyard A					Vineyard B				
	E-L stage	Nugget (c_0)	Sill (c_1)	ER (a_1)	CAM	RMSE	Nugget (c_0)	Sill (c_1)	ER (a_1)	CAM	RMSE
NDVI											
2017	27	0.00001	0.00008	188	10	0.00001	0.00014	0.00011	30	57	0.00001
2018	19	0.00003	0.00002	191	52	0.00001	0.00036	0.00015	262	70	0.00006
	23	0.00002	0.00004	388	35	0.00000	0.00005	0.00004	80	55	0.00001
	27	0.00003	0.00001	8	73	0.00000	0.00000	0.00001	0	6	0.00000
	35	0.00004	0.00001	20	79	0.00000	0.00005	0.00003	218	63	0.00001
	36	0.00003	0.00026	252	11	0.00003	0.00005	0.00004	151	52	0.00001
2019	19	0.00003	0.00002	141	59	0.00000	0.00041	0.00072	92	36	0.00008
	23	0.00002	0.00002	231	1	0.00000	0.00001	0.00006	0	15	0.00005
	27	0.00002	0.00002	226	48	0.00000	0.00001	0.00003	14	15	0.00001
	35	0.00004	0.00012	131	22	0.00001	0.00017	0.00002	511	90	0.00002
$T_c - T_a$											
2017	27	0.12	0.94	41	11	0.13	0.83	1.68	138	33	0.25
2018	19	0.16	0.27	201	37	0.03	0.70	1.69	316	29	0.12
	23	0.14	0.72	47	16	0.12	0.69	2.23	263	23	0.13
	27	0.59	1.63	51	27	0.61	0.40	2.93	192	12	0.18
	35	0.00	1.50	21	0	0.23	0.23	1.39	144	14	0.21
	36	0.22	0.37	71	37	0.15	0.24	0.54	549	31	0.07
2019	19	0.11	0.27	184	28	0.03	0.66	1.00	258	40	0.29
	23	0.27	0.64	71	29	0.21	0.51	0.57	245	47	0.12
	27	0.36	0.40	56	47	0.10	0.57	3.85	449	13	0.29
	35	0.00	2.07	22	0	0.22	0.55	1.84	185	23	0.20

		Vineyard C					Vineyard D				
	E-L stage	Nugget (c_0)	Sill (c_1)	ER (a_1)	CAM	RMSE	Nugget (c_0)	Sill (c_1)	ER (a_1)	CAM	RMSE
NDVI											
2017	27	0.00004	0.00013	190	21	0.00002	0.00002	0.00007	48	23	0.00001
2018	19	0.00021	0.00025	187	46	0.00003	0.00020	0.00015	55	57	0.00003
	23	0.00007	0.00008	244	46	0.00001	0.00003	0.00005	41	41	0.00001
	27	0.00001	0.00001	62	49	0.00000	0.00001	0.00001	56	45	0.00000
	35	0.00013	0.00037	272	26	0.00007	0.00004	0.00009	232	32	0.00001
	36	0.00013	0.00079	612	14	0.00005	0.00006	0.00007	162	45	0.00001
2019	19	0.00017	0.00028	150	39	0.00005	0.00005	0.00004	117	57	0.00001
	23	0.00005	0.00007	219	44	0.00001	0.00004	0.00010	189	31	0.00002
	27	0.00002	0.00005	313	31	0.00001	0.00002	0.00005	129	30	0.00001
	35	0.00014	0.00064	117	18	0.00008	0.00004	0.00021	36	16	0.00002
$T_c - T_a$											
2017	27	0.00	5.09	105	0	0.60	0.64	1.95	243	25	0.27
2018	19	0.00	2.20	215	0	0.26	0.00	1.97	64	0	0.19
	23	0.00	5.38	490	0	0.45	0.00	0.82	46	0	0.08
	27	0.00	3.22	188	0	0.46	0.12	0.97	35	11	0.12
	35	0.00	0.88	155	0	0.07	0.06	1.25	35	4	0.15
	36	0.00	0.46	178	0	0.06	0.08	0.41	37	16	0.03
2019	19	0.59	0.98	176	38	0.15	0.04	0.74	87	5	0.10
	23	0.13	1.20	96	10	0.12	0.01	1.61	61	0	0.24
	27	0.31	2.81	106	10	0.21	0.00	2.32	42	0	0.23
	35	0.42	3.19	108	12	0.38	0.05	2.16	34	2	0.26

$n = 125$. CAM, Cambardella index; ER, effective range (m); NDVI, normalised difference vegetation index; RMSE, root-mean-square error.

normal maturity level to allow the compound to degrade prior to processing (Bindon et al. 2013). This is likely the reason that few vineyards in this study contained a measurable concentration of IBMP at harvest, since average TSS values indicated the vineyards were fully ripe as all were above 24°Brix (Table 4). In contrast, C6 compounds, also responsible for green aroma characteristics in grapes, were present at a detectable concentration allowing spatial maps to be reliably constructed. Both C6 compounds and IBMP are related to fruit exposure and maturation (Bindon et al. 2013), so it is possible the two may exhibit similar patterns of spatial variability. Malic acid, YAN and β-damascenone were individually correlated with NDVI and $(T_c - T_a)$ in some vineyards, but not in others, an indication that other layers or indices are needed to guide management decisions for these compounds. While some have found good relationships between canopy vigour, yield and fruit chemistry (e.g. Trought and Bramley 2011, Gatti et al. 2017, Sun et al. 2017), the results presented here more closely align with those of Acevedo-Opazo et al. (2008) and Bonilla et al. (2015) in suggesting that imagery alone is likely insufficient to fully characterise spatial variability in individual compounds related to fruit quality, except in cases with strong spatio-temporal patterns of variability (as in Vineyard C). This finding supports the need to develop alternative sensors capable of detecting compounds of interest. Of course, if deployment of these is dependent on large ground-truthing campaigns such as reported here,

Table 7. Cluster means of yield and fruit compositional attributes in each of the four vineyards for two- and three-cluster solutions generated from seasonal normalised difference vegetation index and canopy temperature − air temperature in 2018 and 2019.

| | | Vineyard A | | | | | | | | Vineyard B | | | | | | | |
| | | NDVI | | $T_c - T_a$ | | | | | | NDVI | | $T_c - T_a$ | | | | | |

Two-cluster

		NDVI 1	NDVI 2	T_c-T_a 1	T_c-T_a 2	NDVI 1	NDVI 2	T_c-T_a 1	T_c-T_a 2
Yield (kg/mL)	2018	9.0	9.3	8.9	9.5	7.0	7.3	6.7	7.4
	2019	8.7	9.7	9.5	9.1	8.2	7.5	8.1	7.0
AN (mg/g)	2018	1.26	1.16	1.23	1.17	2.18	2.20	2.21	2.18
	2019	0.74	0.71	0.71	0.73	1.07	1.09	1.08	1.08
PT (mg/g)	2018	1.5	1.4	1.4	1.4	2.2	2.2	2.4	2.1
	2019	1.9	1.8	1.8	1.8	2.4	2.4	2.4	2.4
QG (mg/g)	2018	24	25	23	26	26	23	28	23
	2019	30	28	27	30	82	82	85	75
MA (g/L)	2018	2.1	2.2	2.1	2.2	1.5	1.6	1.4	1.6
	2019	1.8	2.0	1.8	1.8	1.6	1.4	1.0	0.8
BD (µg/g)	2018	60	60	61	59	85	82	87	81
	2019	59	59	58	60	59	60	59	60
C6 (µg/g)	2018	4.8	5.1	5.1	4.8	3.3	3.2	3.2	3.2
	2019	5.2	5.2	5.1	5.3	4.1	4.0	4.1	4.0
IBMP (pg/g)	2018	4.2	3.6	3.0	5.0	ND	ND	ND	ND
	2019	1.3	2.6	2.0	2.1	ND	ND	ND	ND
YAN (mg/L)	2018	255	255	253	260	89	86	86	88
	2019	162	180	173	171	21	26	24	24

Three-cluster

		NDVI 1	NDVI 2	NDVI 3	T_c-T_a 1	T_c-T_a 2	T_c-T_a 3	NDVI 1	NDVI 2	NDVI 3	T_c-T_a 1	T_c-T_a 2	T_c-T_a 3
Yield (kg/mL)	2018	9.3	8.1	9.3	9.1	8.8	9.6	7.3	7.4	6.9	7.1	6.7	7.7
	2019	9.1	9.8	8.6	9.4	8.5	10.0	8.5	7.8	7.2	7.0	8.7	7.0
AN (mg/g)	2018	1.29	1.09	1.13	1.27	1.21	1.16	2.16	2.20	2.21	2.17	2.20	2.22
	2019	0.74	0.71	0.70	0.68	0.74	0.73	1.06	1.10	1.07	1.08	1.09	1.07
PT (mg/g)	2018	1.5	1.3	1.4	1.5	1.4	1.4	2.2	2.2	2.2	2.2	2.4	2.1
	2019	1.9	1.8	1.8	1.8	1.9	1.7	2.4	2.4	2.4	2.5	2.4	2.4
QG (mg/g)	2018	23	25	26	19	26	26	25	24	25	25	28	22
	2019	30	26	32	27	30	31	81	86	74	87	82	73
MA (g/L)	2018	2.2	2.1	2.2	2.3	2.1	2.2	1.5	1.6	1.6	1.6	1.4	1.7
	2019	1.8	2.0	1.7	1.9	1.7	2.0	1.0	1.0	0.8	0.8	1.0	0.8
BD (µg/g)	2018	60	58	60	59	61	60	85	83	83	85	88	8
	2019	61	57	59	57	59	65	60	59	61	60	59	61
C6 (µg/g)	2018	4.8	6.1	5.1	5.1	5.1	4.8	3.3	3.3	3.1	3.2	3.3	3.2
	2019	5.2	5.2	5.2	5.0	5.3	5.4	4.1	4.1	4.0	4.1	4.2	3.8
IBMP (pg/g)	2018	5.1	0.0	3.1	2.9	2.5	5.5	ND	ND	ND	ND	ND	ND
	2019	1.4	3.0	1.2	2.1	1.7	2.5	ND	ND	ND	ND	ND	ND
YAN (mg/L)	2018	262	237	252	265	243	260	97	88	80	89	87	86
	2019	167	185	153	170	167	183	21	25	23	7	9	7

| | | Vineyard C | | | | | | | | Vineyard D | | | | | | | |
| | | NDVI | | $T_c - T_a$ | | | | | | NDVI | | $T_c - T_a$ | | | | | |

Two-cluster

		NDVI 1	NDVI 2	T_c-T_a 1	T_c-T_a 2	NDVI 1	NDVI 2	T_c-T_a 1	T_c-T_a 2
Yield (kg/mL)	2018	5.2	6.8	7.3	5.5	8.6	8.0	8.5	8.3
	2019	4.6	6.1	6.0	4.5	6.4	7.2	6.8	7.2
AN (mg/g)	2018	2.49	2.4	2.40	2.49	1.96	1.75	1.89	1.89
	2019	1.34	1.1	1.16	1.35	0.94	0.87	0.89	0.90
PT (mg/g)	2018	2.9	2.6	2.6	2.8	2.2	2.2	2.2	2.1
	2019	3.9	3.4	3.4	3.9	2.5	2.4	2.5	2.4
QG (mg/g)	2018	59	41	37	54	45	48	47	45
	2019	90	66	67	92	81	69	74	72
MA (g/L)	2018	1.5	1.8	1.8	1.6	1.7	1.7	1.7	1.7
	2019	0.7	1.3	1.3	0.7	1.0	1.2	1.2	1.1
BD (µg/g)	2018	78	79	82	75	52	58	54	54
	2019	67	67	66	67	47	50	52	46
C6 (µg/g)	2018	2.7	3.5	3.7	2.9	5.0	4.0	4.7	4.7
	2019	1.5	1.5	1.5	1.4	1.4	1.6	1.6	1.6
IBMP (pg/g)	2018	ND	ND	ND	ND	ND	ND	ND	ND
	2019	ND	ND	ND	ND	ND	ND	ND	ND
YAN (mg/L)	2018	49	60	66	49	66	70	74	63
	2019	37	52	51	36	31	42	42	36

		Three-cluster											
		1	2	3	1	2	3	1	2	3	1	2	3
Yield (kg/mL)	2018	5.3	5.9	7.5	7.6	6.1	5.2	7.8	8.7	8.0	8.7	7.7	8.5
	2019	5.0	6.2	4.6	4.3	6.2	5.1	5.6	7.3	7.2	8.3	6.7	5.6
AN (mg/g)	2018	2.54	2.48	2.34	2.17	2.62	2.42	1.82	1.96	1.77	1.90	1.87	1.89
	2019	1.27	1.11	1.36	1.38	1.11	1.28	1.00	0.89	0.87	0.86	0.90	0.94
PT (mg/g)	2018	2.9	2.8	2.5	2.5	2.9	2.8	2.1	2.1	2.2	2.2	2.2	2.1
	2019	3.7	3.3	3.9	4.0	3.3	3.7	2.6	2.4	2.4	2.2	2.5	2.6
QG (mg/g)	2018	59	49	34	34	49	56	45	45	48	48	46	45
	2019	79	63	94	97	62	80	86	73	69	65	74	82
MA (g/L)	2018	1.4	1.7	1.9	1.9	1.7	1.6	1.6	1.7	1.7	1.7	1.8	1.7
	2019	0.9	1.4	0.7	0.7	1.4	0.9	0.9	1.1	1.3	1.3	1.2	0.9
BD (µg/g)	2018	77	77	2	82	79	75	58	52	57	53	56	54
	2019	67	67	66	68	65	67	46	47	51	45	52	47
C6 (µg/g)	2018	2.6	3.2	3.7	3.9	3.0	2.8	4.0	5.0	4.1	4.4	5.0	4.7
	2019	1.5	1.4	1.5	1.5	1.5	1.5	1.2	1.5	1.7	1.8	1.5	1.4
IBMP (pg/g)	2018	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	2019	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
YAN (mg/L)	2018	47	2	68	72	49	48	56	66	73	73	68	63
	2019	38	59	35	37	59	36	27	34	45	42	39	33

$n = 125$; ND, not detected or too few samples with detected compound. AN, anthocyanins; BD, β-damascenone; C6, six carbon alcohols and aldehydes; IBMP, 3-isobutyl-2-methoxypyrazine; MA, malic acid; NDVI, normalised difference vegetation index; PT, polymeric tannins; QG, quercetin glycosides; $T_c - T_a$, canopy temperature − air temperature; YAN, yeast assimilable nitrogen.

they may not present as favourable due to time, complexity and cost. In vineyards with patterns of fruit composition variability that remains consistent, the potential for differential management exists, including selective harvesting in cases where differences in cluster means is sufficiently large to warrant separation. Many wineries already tailor vineyard management practices to wine style, but the results presented here suggest that this could be further developed into targeting specific fruit compositional attributes on a location-specific basis and cognisant of within-vineyard variation.

An important distinction between the present work and other previous studies assessing vineyard variability is that many were confined to single vineyards of less than 10 ha (Baluja et al. 2013, Brillante et al. 2017, Yu et al. 2020). The present results present a view from 'broad scale' viticulture and therefore represent a view of vineyards that has not been commonly described. This broad scale is also the reason why remote sensing approaches to fruit compositional characterisation were sought, given the potentially large sampling requirement if composition were to be manually monitored in such large vineyards. The present results are consistent with the idea that NDVI is a useful tool in describing canopy variability in vineyards throughout the growing season, but they also suggest that NDVI is a somewhat 'blunt instrument' if the aim is to identify oenologically meaningful differences in some attributes of fruit composition. In making this statement, we nonetheless recognise that our sampling intensity was, for reasons of logistics, somewhat lower than the 26 samples/ha used by Bramley and Hamilton (2004) and Bramley (2005). Canopy temperature converted to some measure of plant water status, as in the $(T_c - T_a)$ imagery used in the present study, has been shown to be useful in irrigation scheduling (Bellvert et al. 2016) and can also be useful in describing variability (Tables 6,7). As a tool for separating zones of differing fruit composition, however, the present results point to similar limitations as for NDVI. If imagery is inconsistently variable, it is unlikely that confident precision management decisions can be made from imagery alone. When patterns in imagery, or other spatial data layers, are consistently spatially similar, variable rate management is possible and perhaps even suggested when patterns persist over several seasons. In this situation, persistent zones are likely to produce different fruit compositional characteristics. Vineyard C shows this to be the case but was the only one to do so in the four vineyards in this study. In these specific cases with strong patterns of variability, the specific type of imagery (i.e. NDVI, canopy temperature, other indices) may not even matter as patterns may be visible with publicly available software or maps, like Google Maps (Alphabet, Mountain View, CA, USA). Where the patterns of vegetative vigour are predictable, fruit chemistry will almost certainly differ. Conversely, if patterns are not predictable, fruit chemistry is likely to be difficult to manage.

Since several aspects of fruit composition measured in the present study were spatially stable while others were not, growers and winemakers could potentially reduce the number of fruit composition attributes measured in the laboratory and/or used for spatial analysis because many of these variables will provide little additional information beyond that provided by others. For instance, since anthocyanins and polymeric tannins exhibit similar spatial patterns (Figure 3), testing only for colour could be more cost-effective and deliver similar actionable information. While the main objective in Bramley et al. (2011a) was to evaluate an 'on-the-go' sensor for anthocyanin detection, this work also referred to the hand-held version which could accomplish a similar goal provided sampling could be appropriately targeted, perhaps using a targeted scheme such as that proposed by Meyers et al. (2020). Using this and other similarly engineered sensors, and assuming the availability of imagery or other covariates of utility in predicting indices of fruit quality, high-density maps for potential fruit quality could be derived from a few key attributes, which could be collected at appropriate scale efficiently and economically, and result in differential management as proposed in Trought and Bramley (2011). Due to the short range of spatial variation and relatively low concentration of some compounds in the fruit, as in the aroma precursors shown here, it may be necessary to develop a more precise sampling strategy in order to adequately characterise the true variability of these analytes.

Table 8. Cluster means of yield and fruit composition in vineyards A and C for two-cluster solutions generated from all fruit composition in 2017–2019 using the 2 m gridded data.

		Vineyard A						Vineyard C					
		OMFQ		NDVI		$T_c - T_a$		OMFQ		NDVI		$T_c - T_a$	
		1	2	1	2	1	2	1	2	1	2	1	2
Yield (kg/m)	2017	7.8	8.0	7.4	7.9	7.8	8.1	5.1	6.5	4.9	6.2	5.0	6.0
	2018	9.2	9.2	9.0	9.2	9.1	9.2	5.9	7.3	5.7	7.0	5.7	6.9
	2019	9.2	9.4	8.8	9.3	9.2	9.4	5.1	5.7	4.9	5.7	4.9	5.6
Anthocyanins (mg/g)	2017	0.79	0.78	0.81	0.79	0.80	0.78	1.39	1.23	1.39	1.28	1.40	1.29
	2018	1.17	1.24	1.15	1.21	1.22	1.18	2.49	2.35	2.49	2.40	2.48	2.42
	2019	0.73	0.71	0.69	0.72	0.72	0.73	1.30	1.14	1.32	1.17	1.35	1.17
Polymeric tannins (mg/g)	2017	2.0	2.1	2.0	2.0	2.1	2.0	3.2	3.2	3.3	3.3	3.3	3.2
	2018	1.4	1.5	1.4	1.4	1.4	1.4	2.8	2.6	2.8	2.6	2.8	2.6
	2019	1.8	1.8	1.9	1.8	1.8	1.8	3.7	3.5	3.8	3.5	3.8	3.5
Quercetin glycosides (mg/g)	2017	35	35	37	35	36	34	64	49	65	52	64	54
	2018	25	23	25	24	26	26	49	40	51	41	51	42
	2019	58	60	58	59	60	58	84	67	87	71	87	72
Malic acid (g/L)	2017	1.9	2.0	1.8	1.9	1.9	2.0	1.3	1.8	1.3	1.7	1.3	1.6
	2018	2.2	2.2	2.0	2.2	2.1	2.2	1.7	1.8	1.6	1.8	1.6	1.8
	2019	1.9	1.9	1.7	1.9	1.9	1.9	0.9	1.3	0.8	1.2	0.8	1.2
β-Damascenone (μg/g)	2017	46	45	46	46	46	46	57	58	57	57	57	57
	2018	60	60	60	60	60	60	76	85	76	83	77	81
	2019	58	60	58	59	60	58	66	67	66	67	66	67
C6 (μg/g)	2017	5.4	5.2	5.3	5.3	5.3	5.3	3.0	3.0	3.0	3.0	3.0	3.0
	2018	5.1	4.8	5.1	5.0	4.9	5.0	3.0	3.7	2.9	3.6	2.9	3.5
	2019	5.1	5.3	5.2	5.2	5.3	5.1	1.5	1.3	1.5	1.4	1.5	1.5
IBMP (pg/g)	2017	5.3	5.7	5.2	5.5	5.5	5.5	0.0	0.2	0.0	0.2	0.0	0.1
	2018	3.3	4.4	2.1	3.9	3.6	4.2	0.1	0.1	0.1	0.2	0.1	0.2
	2019	1.5	2.7	1.3	2.1	1.8	2.3	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
YAN (mg/L)	2017	137	163	138	150	151	150	40	74	39	63	40	59
	2018	250	263	247	257	255	258	50	73	50	65	48	65
	2019	159	186	154	173	172	174	37	60	37	52	37	51

Note that these data relate to the clusters shown in Figure 5. n.d., not detected or too few samples with detected compound. C6, six carbon alcohols and aldehydes; IBMP, 3-isobutyl-2-methoxypyrazine; NDVI, normalised difference vegetation index; OMFQ, objective measures of fruit quality; $T_c - T_a$, canopy temperature − air temperature; YAN, yeast assimilable nitrogen.

Clustering multiple images in a growing season may have some benefit to assess the spatial variation in fruit chemistry, though the inconsistent results shown here warrant further investigation into why this technique works in some vineyards and not in others, as well as the degree to which patterns in imagery change over the course of a growing season. The use of two clusters was most often deemed a better reflection of differences between zones as a third cluster was generally either insufficiently distinct from another in terms of differences between cluster means, or represented areas of vineyards that would likely be deemed too small to warrant consideration for differential management. The use of three or more k-clusters will likely be dependent on the drivers of variation in vineyard performance, the style targets desired by growers or winemakers and, in the case of selective harvesting, the market opportunity for different wines. More than a small number of clusters will almost certainly increase the complexity of a typical farming operation, as well as logistics at the receiving winery. Such complexity will likely present as a disincentive for adoption.

Overall, winemakers and vineyard managers have two major strategies when given information regarding grape yield and quality variability in vineyards. The first is to characterise fruit quality variability in order to separate higher quality grapes from lower-quality grapes or to separate based on suitability to different wine styles. This allows the fruit to be harvested and delivered to the winery in separate lots of different but more consistent fruit quality. Patterns of spatial variability of objective measures of fruit composition presented in this study can act as an initial guide for this purpose. Vineyards with relatively high or low values in certain compounds could be also be used to drive different wine styles and products. Vineyard areas with a high level of negative attributes could be downgraded or managed separately if a reduction in attribute concentration was possible—perhaps through blending at the winery. The second strategy is to practice variable rate management of inputs in order to reduce vineyard variability and increase the uniformity of yield and fruit composition across the entire vineyard. Variable rate irrigation (Sanchez et al. 2017) is one such example. The first strategy requires the characterisation of vineyard variability and the ability to separate fruit at harvest based on spatial information. Where harvest is performed manually, it is relatively easy to separate the fruit from different areas of the vineyard. Large or highly mechanised vineyards require the same level of information, but also require some coordination of harvest logistics to perform this separation successfully (Bramley 2005, Bramley et al. 2011b). The second strategy of attempting to reduce variability to deliver more consistent fruit quality requires differential management. Vineyard managers also need a more advanced understanding of variability for this approach to work. As White (2020) has noted, for example, few quantitative relationships between soil properties and grape or wine composition have been identified, which suggests that considerable further work may be needed for targeted management to be robustly implemented in the vineyard, perhaps rendering selective harvesting a more favourable option. None of these strategies are possible without the characterisation and quantification of the variability of yield and/or fruit composition.

Conclusions

The results presented here support the findings of previous studies that, assuming patterns of variation in fruit composition in vineyards are temporally stable, they are potentially manageable. The results also suggest that most berry chemical compounds associated with canopy characteristics, or which can be characterised using canopy related variables such as NDVI or $(T_c - T_a)$, are also temporally stable and potentially manageable, even in large vineyards. The latter also suggests that some OMFQ may be accurately predicted using airborne remote sensing data and characterised by clustering into relatively uniform parcels but may require additional information in order to make meaningful separations of fruit quality. Conversely, measures of basic chemistry (TSS, pH, TA) are unlikely to provide much insight related to differences in fruit composition, nor is imagery likely to be useful at separating variables with such low spatial and statistical variability at harvest. The description of fruit composition could be used by vineyard managers to increase the value of their crop by targeting areas of low productivity for increased yield without sacrificing quality, while simultaneously managing high vigour areas to improve potential fruit quality without sacrificing yield. Wineries could also gain value by streaming deliveries of grapes to the winery into separate categories of potential quality for product differentiation (Bramley 2021).

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Chapter 4: Can mapping of within-vineyard variability be facilitated using data from multiple vineyards?

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Stafford, J.V. ed. Proceedings of the twefth European Conference on Precision Agriculture; 8-11

July 2019; Montpelier, France (Wageningen Academic Publishers) pp. 743-749.

Contextual Statement

The previous two chapters presented the results of research that examined how indirect measurements of canopy and vine perfmorance could be useful in predicting and describing relationships among fruit compositional attribues and to describe how patterns of spatial variability are related to these measurements. The research described in the following chapter describes how multiple vineyards within a region could work together to produce these maps of spatial variability by aggregating samples into the same model of spatial dependence, referred to here as a 'common variogram'. This was considered important given the potential impediment to a commercial vineyard adopting pursuit of understanding of variability due to the high sampling demand. This research used spatial and geostatistical analysis to understand how patterns of variability of anthocyanin concentration in grapes would differ using a within-vineyard only variogram versus a common variogram comprised of all samples collected in 2017 from all four vineyards in the study.

Statement of Authorship

Title of Paper	Can mapping of within-vineyard variability be facilitated using data from multiple vineyards?
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Principal Author

Name of Principal Author (Candidate)	
Contribution to the Paper	Sample collection, data processing, statistical analysis, wrote manuscript
Overall percentage (%)	75
Certification:	This paper reports on original research I conducted during the period of my Higher Degree by Research candidature and is not subject to any obligations or contractual agreements with a third party that would constrain its inclusion in this thesis. I am the primary author of this paper.
Signature	Date 8 December 2021

Co-Author Contributions

By signing the Statement of Authorship, each author certifies that:

i. the candidate's stated contribution to the publication is accurate (as detailed above);

ii. permission is granted for the candidate in include the publication in the thesis; and

iii. the sum of all co-author contributions is equal to 100% less the candidate's stated contribution.

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Can mapping of within-vineyard variability be facilitated using data from multiple vineyards?

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Abstract

Variogram estimation requires extensive sampling that may limit its practical uses in agriculture. During the 2017 harvest, 125 grape samples were collected for the analysis of chemical composition from each of four vineyards in the Lodi area of the Central Valley of California. Maps of grape colour (anthocyanins) of each block were produced using variograms derived from data from each individual vineyard (n=125), as well as from the aggregated dataset containing all samples from all four vineyards (n=500). The resulting grape colour maps show differences in spatial patterns, although the impact of these on vineyard decision making would be minimal. Aggregation of data from multiple vineyards in a region may therefore offer a means of cost-effectively examining within-vineyard variation in individual vineyards.

Keywords: vineyard variability, kriging, precision viticulture

Introduction

The cost-effectiveness of collecting and analysing sufficient samples for characterization and mapping of within-vineyard variation in crop attributes is a major constraint to understanding variability in commercial vineyards. However, several studies have mapped specific attributes of grape composition, chiefly anthocyanins (Bramley, 2005; Stamatiadis *et al.*, 2006; Bramley *et al.*, 2011; Baluja, *et al.*, 2012) or of other attributes of fruit quality (Cortell, *et al.*, 2005; Reynolds *et al.*, 2007; Brillante *et al.*, 2017). However, according to Cressie (1993) and Webster and Oliver (2007), too few samples have been collected in a majority of these studies for sufficient rigour in variogram estimation and thus, map interpolation using kriging. Cressie (1993) suggested 30-50 pairs of samples for each distance class, whilst Webster and Oliver (2007) recommended that 100 samples should be regarded as the minimum for adequate variogram estimation. Most of the aforementioned studies fail to meet these criteria. Exceptions were those of Bramley *et al.* (2011) using a prototype on-the-go sensor and Bramley (2005), whose vine sampling design allowed for adequate variogram estimation and subsequent kriging of maps of grape composition; this can be used as a guide for future work in this area. However, anecdotal evidence suggests that such a sampling design presents an impediment to commercial operations, especially when, in addition to collection of samples, some sort of laboratory analysis is also required. There would therefore be much value if an understanding of variability in an attribute of interest in one vineyard could inform similar understanding in another, especially if this understanding could assist in reducing the sampling and analytical demand. McBratney and Pringle (1999) attempted to address this problem in the case of soil mapping by using the magnitude of different soil properties to estimate proportional and average variograms for other properties. Similarly, Walter *et al.* (2007) explored using combined data from different years and regions to better estimate variograms to predict oyster abundance. However, to the authors' knowledge, no study of this type has been applied to agriculture. The objective of this study was to compare the predictions between two variogram estimation methods and their impact on characterisation and

mapping of spatial variability in four vineyards in the Lodi region of California. In particular, the main interest was to see whether samples collected in one vineyard could assist in the mapping of variability in another from the same region.

Materials and methods

In the 2017 harvest season, four Cabernet Sauvignon vineyard blocks were selected for high density sampling of grape anthocyanins as shown in Figure 1. All four vineyards are in the American Viticultural Appellation (AVA) of Lodi, California (38° 7' 44' N, 121° 16' 51' W) and occur within <25 km of each other.

A detailed scheme for fruit sampling was developed for each vineyard as shown in Figure 2. This sampling scheme assumed no prior knowledge of vineyard variability and contained enough points, or 'data vines', for adequate variogram estimation (n=125) based on the criteria of Webster and Oliver (2007). To develop this scheme, the points were first spread out in a common square grid across each vineyard. Next, each point was given a random offset in both *x* and *y* directions – both to randomise aspects of data vine selection, and to create a sampling grid with different distances between points for more robust variogram estimation, especially at shorter distances. Finally, approximately 20 sample points from each sampling grid were then randomly removed and randomly reassigned to a position adjacent to another data vine (i.e. either one row space or one vine space from the adjacent data vine). This method allowed for the estimation of an experimental variogram for grape anthocyanin content in each vineyard over lags ranging from a single vine spacing to as far as the farthest two points from each other. Importantly, it provided adequate numbers of pairs of points at short distances for characterising short-range spatial variation. Total anthocyanins were measured by collecting 20 clusters from each data vine and subsequent analysis according to Iland *et al.* (1996). Experimental variograms were then estimated for the anthocyanin data of each
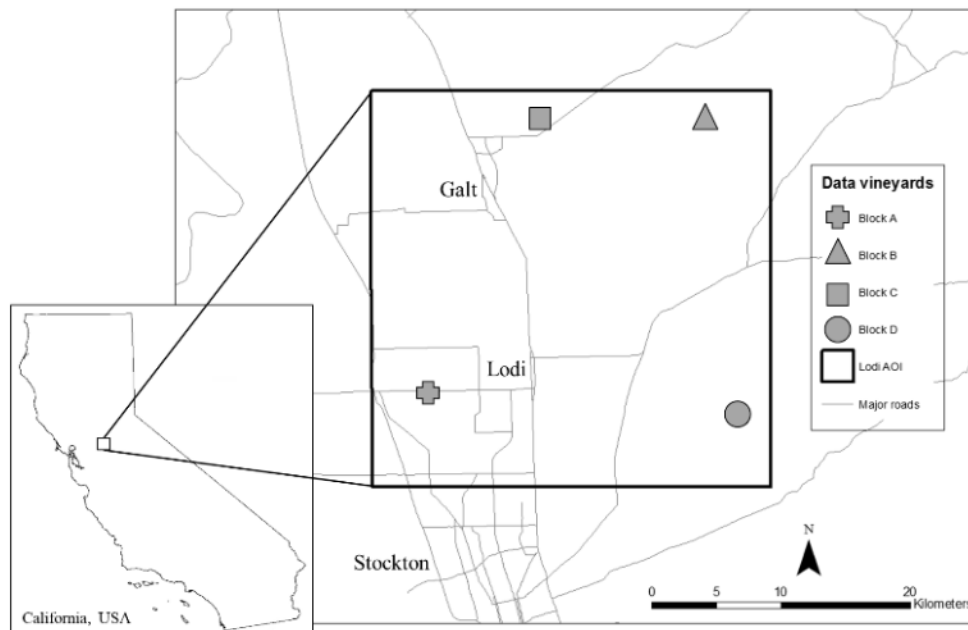
Figure 1. Each of the four selected vineyards in the Lodi area of interest.

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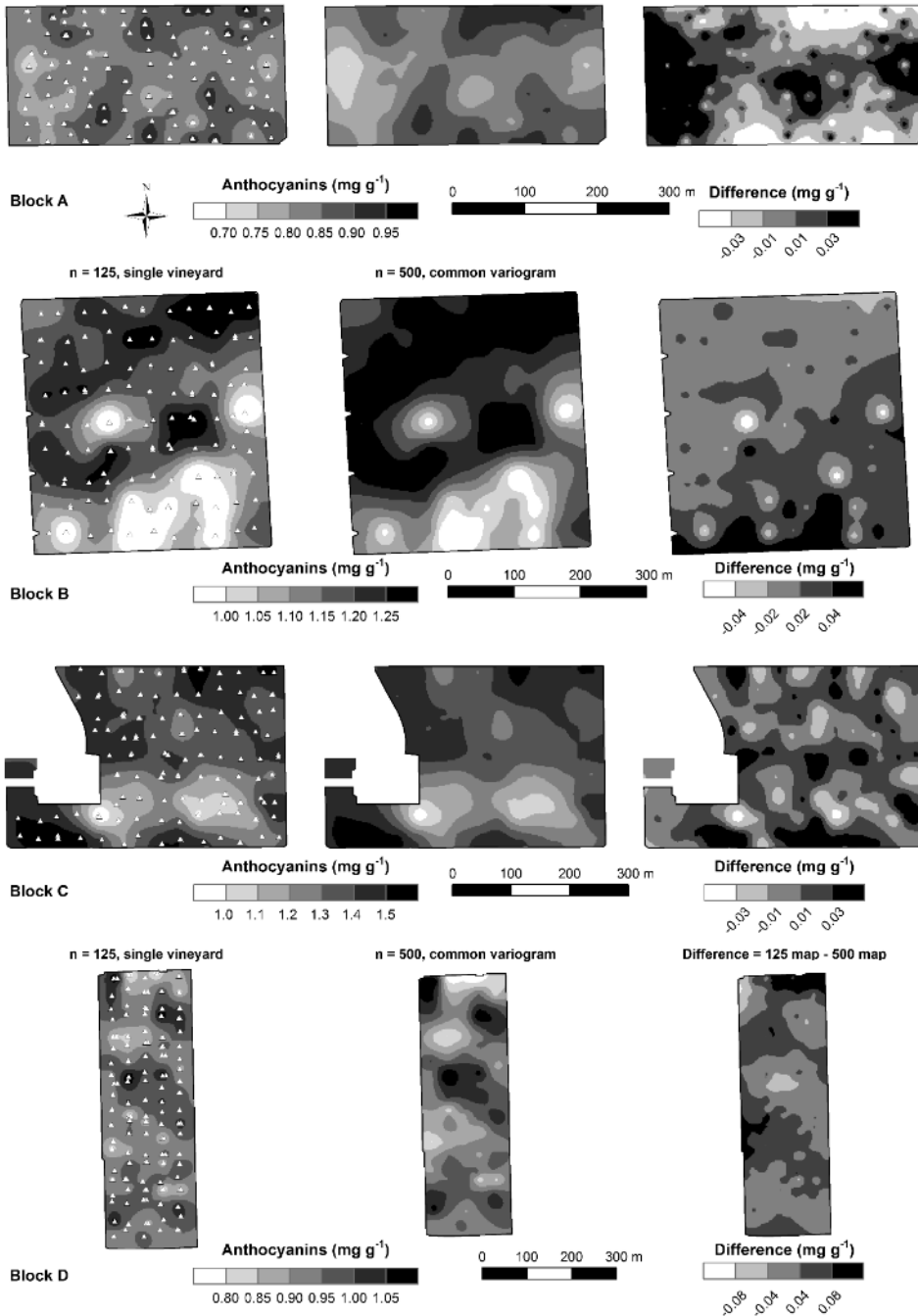
Figure 2. Anthocyanin maps using variograms derived either from only sample points within the vineyard (n=125) or from all four vineyards (n=500) and the difference between these maps.

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vineyard using VESPER (Minasny, *et al.,* 2006). Preliminary exploratory variogram fitting led to the assumption of the exponential model being appropriate for characterising spatial structure in anthocyanin variation. Maps were then interpolated for each vineyard in VESPER using global point kriging, based on the 125 samples within.

Aside from the assumption of an exponential variogram, several constraints were applied to the variogram estimation. The number of lag classes (20) and the lag tolerance (10%) were set for each model, as was a maximum distance for variogram estimation (250 m); that is, the largest lag class was set at 250 m. The choice in variogram settings was based on initial exploratory analysis and to provide a consistent set of parameters for method comparison. A further variogram was then produced by combining all 500 points from all four vineyards into a 'common variogram' which was nevertheless estimated using the same settings in VESPER as for the vineyard-specific variograms, viz. number of lag classes, lag tolerance and maximum distance. From the variogram parameters fitted in VESPER, (nugget, sill and effective range), the nugget/sill ratio, sometimes referred to as the 'Cambardella Index', was calculated to give a measure of spatial structure, where a value less than 25 was deemed to represent 'strong' spatial structure, and a value greater than 75 representing 'low' spatial structure (Cambardella, *et al.,* 1994).

Results

Differences between the maps generated using either the vineyard-specific or common variograms were small (Figure 2 and 3). Absolute differences in mapped anthocyanin concentration were generally of the order of analytical error or smaller, and the difference ranges in all four vineyards were similarly spaced from 0 (Figure 2). However, in terms of providing a platform for winery decision making, when the maps were classified on a 'low', 'medium' and 'high' anthocyanin basis (derived from 33rd percentiles), the misclassification of 'anthocyanin zones' when using the common variogram was minimal (Figure 3). Block C represents the smallest level of misclassification, over the entire area of 11.9 ha, where only 0.7 ha (i.e. 5.9%) were assigned to a different zone when using the map derived from the common variogram (n=500). In Blocks A, B, and D, the misclassifications represented 1.3 ha 10.0%), 0.9 ha (12.4%), and 1.6 ha (18.4%) respectively. Figure 3 also shows that the misclassifications generally occurred on zone boundaries, as might be expected.

Table 1 shows the difference between parameters of both variograms and the effect on spatial structure. Effective range was between 12.5 m and 49.5 m when using the individual within-vineyard variograms, while the effective range in the common variogram was higher (66.6 m) than all four within-vineyard variograms. The change in Cambardella index in Block D was the highest (10.3), with the lowest in Block B (1.18). All four values of the Cambardella index were in the medium to low range indicating moderate to strong spatial structure. These small changes would have no impact on the interpretation of each map.

Discussion

The difference maps in Figure 2 and 3 show the largest difference in anthocyanins to be less than 0.1 mg/g, which would be considered insignificant to winemakers and vineyard managers. The key finding of this work is that, in practice, vineyard managers would do nothing differently based on the changes between maps produced by the two models, yet the maps derived from the common variogram reduce the need for expensive and time-consuming sampling in an individual vineyard. While the overall variance amongst the 500 data points used to construct the common variogram was greater than in the individual blocks (n=125), the effect on spatial structure in the resulting map and on the characterisation of spatial structure (i.e. Cambardella index) was minimal. The difference in predicted anthocyanins was also very low, further making the case for use of the common variogram. The increase in the number of points in the shortest distance classes in the
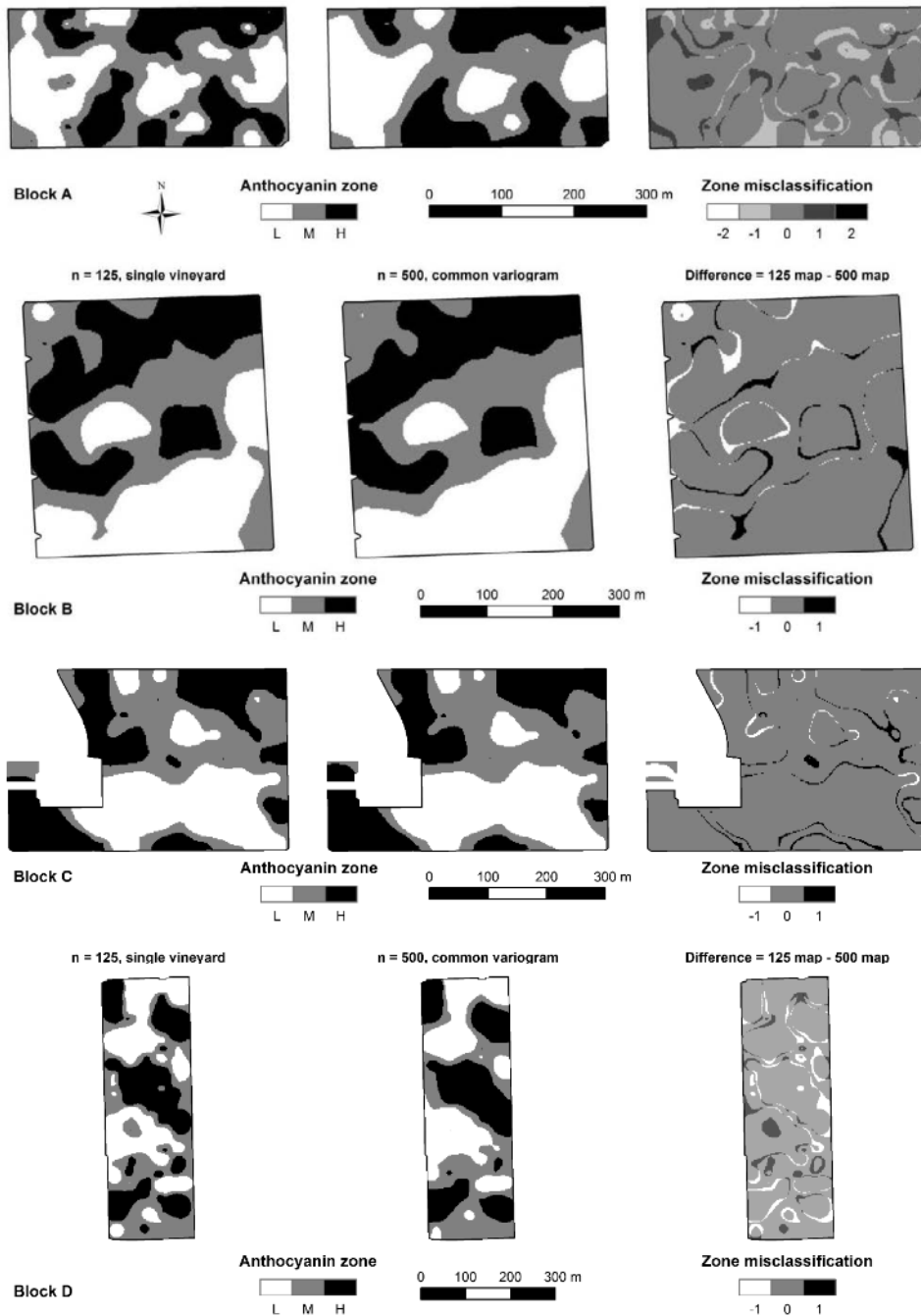
Figure 3. Maps of 'high', 'medium', and 'low' zones of anthocyanins derived either from only sample points within the vineyard (n=125) or from all four vineyards (n=500) and the misclassification of zones due to use of the common variogram.

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Table 1. Comparison of descriptive and spatial statistics from each of the four vineyard blocks.

		Vineyard block			
		A	B	C	D
Variogram 125	Mean (μ)	0.7907	1.1460	1.3433	0.8913
	Variance (σ^2)	0.0106	0.0350	0.0477	0.0244
	c_0 (nugget)	0.00423	0.01303	0.01676	0.01162
	$c_0 + c_1$ (sill)	0.00978	0.03414	0.04790	0.02334
	Effective range (m)	12.50	35.05	49.46	16.23
	Cambardella index	43.25	38.17	34.99	49.79
Variogram 500	Mean (μ)	1.0428			
	Variance (σ^2)	0.0762			
	c_0 (nugget)	0.01204			
	$c_0 + c_1$ (sill)	0.03060			
	Effective range (m)	66.57			
	Cambardella index	39.35			
		A	B	C	D
Difference	Mean (μ)	0.2521	0.1030	0.3010	0.1515
	Variance (σ^2)	0.0656	0.0412	0.0285	0.0518
	c_0 (nugget)	0.00781	0.00100	0.00470	0.00042
	$c_0 + c_1$ (sill)	0.02082	0.00350	0.01730	0.00730
	Effective range (m)	54.07	31.52	17.11	50.34
	Cambardella index	3.90	1.18	4.36	10.44

common variograms improved the robustness of the prediction due to the importance of properly characterising variation at lags less than the range of spatial dependence. Thus, this approach could be used as a default for anthocyanin prediction in Lodi vineyards. Samples could be continuously added to the common variogram for an increasingly robust predictive capability. The Cambardella index in all four blocks indicated moderate to high spatial structure, and the difference between the two variograms showed a very small change in each block. Differences in the effective range could have the greatest effect on vineyard decision making or sample design, since this distance could potentially be used in optimizing any measurements or tissues to sample.

The common variogram approach offers several promising improvements to sample based design and future sampling schemes. As more and more data are collected with geospatial analysis in mind, they could be combined in multiple ways. This type of data combination, along with normalisation, could also be used in temporal analysis by combining data from multiple seasons for a different type of common variogram. The inclusion of additional data over time could greatly increase the effectiveness of smaller sampling campaigns, as the relationships over multiple distances could be integrated into the same variogram. In cases where samples are taken prior to harvest, these values could be normalised and included into the regional variogram for an estimate of where to expect the relative colour ranges in that region and then streamed into appropriate wine programs. These additions could also be used to build spatial databases of key vineyard attributes to include, among many others, fruit quality, soil characteristics or plant nutrition.

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Conclusions

The finding that a common variogram may be applied to mapping grape anthocyanins in single vineyards may enhance the robustness of further anthocyanin mapping, especially in previously unsampled Cabernet Sauvignon vineyards in Lodi. Using 500 data values from four vineyards enabled more robust variogram construction than when the data from individual blocks were used separately, with very small differences seen between maps kriged using either individual or common variograms; these differences were inconsequential for decision making.

Acknowledgements

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Chapter 5: Facilitating mapping and understanding of within-vineyard variation in fruit composition using data pooled from multiple vineyards

Sams, B., Bramley, R., Aboutalebi, M., Sanchez, L., Dokoozlian, N.K., Ford, C.M. and Pagay, V. (2022) Facilitating mapping and understanding of within-vineyard variation in fruit composition using data pooled from multiple vineyards. Australian Journal of Grape and Wine Research. https://doi.org/10.1111/ajgw.12556

Contextual Statement

While the research presented in the previous chapter dealt with the use of a common variogram to produce maps of anthocyanin variability in four vineyards, the following chapter describes experiments that expand on this concept by: 1) increasing the data pool from a single year of data collection (n = 500) to three years (n = 1500); 2) canvassing the merits of the approach using two additional compounds, β-damascenone and malic acid, in addition to anthocyanins; and 3) simulating a scenario where multiple vineyards could cooperate in order to optimise sampling strategies and reduce single season sampling volumes but still produce geostatisically rigorous maps. Spatial and geostatistical analysis, as well as Monte Carlo simulations, were used to assess the accuracies of maps produced using within vineyard variograms to compare with those produced using common variograms.

Statement of Authorship

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Overall percentage (%)	80%
Certification:	This paper reports on original research I conducted during the period of my Higher Degree by Research candidature and is not subject to any obligations or contractual agreements with a third party that would constrain its inclusion in this thesis. I am the primary author of this paper.
Signature	Date 8 December 2021

Co-Author Contributions

By signing the Statement of Authorship, each author certifies that:

i.   the candidate's stated contribution to the publication is accurate (as detailed above);

ii.   permission is granted for the candidate in include the publication in the thesis; and

iii.   the sum of all co-author contributions is equal to 100% less the candidate's stated contribution.

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Facilitating mapping and understanding of within-vineyard variation in fruit composition using data pooled from multiple vineyards

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Abstract

Background and Aims: A large number of fruit samples is required for adequate variogram estimation, making the development of prescriptive maps for vineyard management cost prohibitive for most growers. The project assessed the efficacy of aggregating samples from multiple vineyards, over multiple years, to estimate a 'common' variogram that could be generated and applied more efficiently.

Methods and Results: Fifteen hundred berry samples were collected over 3 years (2017–2019) in four vineyards in California for analysis of fruit composition and spatial variability. Maps were produced for anthocyanins, malic acid and β-damascenone in each vineyard using four separate aggregations of samples and showed only subtle changes in patterns of spatial variability in any of the three analytes assessed. A common variogram generated without points from the vineyard to be mapped indicated lower kriging variances over 100 simulations and was able to correctly classify up to 70% of sample values.

Conclusions: The use of a common variogram in describing spatial variability in vineyards adds important statistical support to the generation of robust maps that could be used for targeted vineyard management. Grower collaboration across multiple regional vineyards could therefore improve mapping support for all involved. Though high-density sampling may still be required in some cases, once stable zones of fruit quality have been characterised, the sample size could potentially be reduced in subsequent years.

Significance of the Study: Maps produced from combined datasets collected from multiple vineyards and years could provide growers and wineries more confidence in zonal management by showing the temporal stability of the spatial variability of several aspects of fruit quality.

Keywords: *common variogram, kriging, map interpolation, precision viticulture, vineyard variability, Vitis vinifera* Cabernet Sauvignon

Introduction

Understanding spatial variability in perennial crops, such as winegrapes, is important for farmers and those downstream of the crop, but in the absence of appropriate sensors, the cost of sample collection necessary to create maps of productivity constrains most operations (Bramley 2021). Vegetation indices, derived from remote or proximal sensors, are tools that can alleviate some of this burden by allowing practitioners of precision agriculture to collect strategic samples based on the assignment of management zones to areas considered to contain similarly productive plants (Acevedo-Opazo et al. 2008, Tagarakis et al. 2013, Bonilla et al. 2015, Meyers et al. 2020, Oldoni et al. 2021, Sams et al. 2022b). Nevertheless, direct measurements may be necessary to characterise variability in regions where image collection is difficult due to atmospheric conditions, or where the variable of interest is not closely related to the spectral response of canopies (Sams et al. 2022a,b). In these cases, mapping support must meet some minimum criteria in order to be trustworthy. Kriging (e.g. Webster and Oliver 2007) is regarded as the optimal method for map interpolation in agriculture (Whelan et al. 1996), and relies on the function known as the 'experimental variogram' which describes the relationship between the variance among sample measurements as a function of the distance between the locations at which the samples were collected. This function is used in the kriging interpolation process to give appropriate weighting to neighbouring sampled locations in estimating the values of the variable of interest at unsampled locations. Robust estimation of the experimental variogram requires a minimum of 100 samples (Webster and Oliver 2007), though more statistically complex techniques such as the residual maximum likelihood (REML) variogram estimation have shown promise in reducing sample size requirements in soil science (Pardo-Igúzquiza and Dowd 1998, Kerry and Oliver 2007). Additionally, at least 30 pairs of points per distance class, or lag, may be necessary to fully characterise this variability (Cressie 1993). Some published studies have included maps with a resolution far lower than the smallest distance between any two sample points (Cortell et al. 2005, 2007, Martínez-Lüscher et al. 2019, Brillante et al. 2020, Yu et al. 2020), and/or with far fewer than 100 samples used

for mapping, making both the maps and subsequent analysis potentially unreliable. A method for aggregating samples from many vineyards would therefore be useful to the grapegrowing community, as it could allow for a more robust estimation of the spatial structure of fruit composition and other indices of vineyard performance with low sampling requirements for individuals.

Taylor et al. (2005) found similarities in several geostatistical metrics (effective range, Cambardella index, and opportunity index) related to yield variability between vineyards in Europe and Australia. Accordingly, they suggested that it would be useful to also develop an understanding as to how fruit composition varies across regions, cultivars and production. While McBratney and Pringle (1999) provided a basis for the estimation of 'average' and 'proportional' variograms, Bramley et al. (2017) pioneered the use of a 'common' or 'across-years' variogram in vineyards to assess the spatial patterns of berry rotundone concentration over several years and to reduce the potential for artefacts of subjective variogram fitting to data from any single year on analysis of the temporal stability of patterns of spatial variability. Sams et al. (2019) used this common variogram approach in order to assess the effect of aggregating samples on the spatial patterns of anthocyanins in four vineyards in central California and found the method to add robustness to the variogram estimation as suggested by Cressie (1993) without compromising the characterisation of spatial patterns of variability when mapping each vineyard individually.

The first objective of the current study was to expand the results presented by Sams et al. (2019) to include multiple years to determine the effect of the common variogram estimation on spatial patterns of variability over time. The second objective was to determine the effectiveness of this method to generate more robust and useful maps of fruit compositional attributes that Sams et al. (2022a) found to be somewhat spatially and temporally erratic—possibly due to artefacts of the variogram fitting process rather than due to annual variation in the pattern of spatial variation. Simulation studies were also conducted to assess and to demonstrate the ability of the common variogram method to produce maps suitable for characterising spatial variability in an unknown or unsampled vineyard.

Materials and methods

Vineyards and sample collection

Immediately prior to commercial harvest, 125 samples per year were collected in 2017, 2018 and 2019 from each of four *Vitis vinifera* L. cv. Cabernet Sauvignon vineyards in the Lodi American Viticultural Area in central California (38° 7′ 44″ N, 121° 16′ 51″ W). The vineyards and samples were the same as those presented in Sams et al. (2022a,b). Briefly, all four vineyards were drip-irrigated, spur-pruned, and machine harvested. Vineyard A, planted in 2010 on the rootstock 039-16 and to clone FPS 08, was pruned to a single bilateral sprawling training system and had no inter-row cover crop. Vineyard B, planted in 2013 on SO4 rootstock and to clone 7, and Vineyard C, planted 1998 on 1103P and to clone 7, were trained to quadrilateral sprawling systems with a perennial inter-row grass cover crop. Vineyard D, planted in 2012 on rootstock 039-16 and to clone 15, was a mechanised high-wire sprawling canopy with the same inter-row cover crop as Vineyards B and C. Elevation in Vineyards A and C varied by less than 2 m, Vineyard B

sloped about 20 m downward from north to south, and Vineyard D was characterised by rolling hills with an elevation range of about 8 m.

As outlined in Sams et al. (2022a), the sampling scheme was designed and intended for spatial analysis of fruit chemistry using modified regular grids based on row and vine distance (i.e. Vineyard A had a spacing of 2.1 m between vines and 3.1 m between rows, so the grid was 2.1 × 3.1 m), but with random offsets assigned to each data vine location. This method allowed for the characterisation of spatial dependence and variability at short, uneven distances for robust variogram generation at low sample separation of 'lags'. Commercial harvest for the four vineyards occurred within 10 days of one another in all 3 years, with the entire 2019 sample collection occurring over just 5 calendar days. In most cases, the vineyards were sampled either the day before or on the day of commercial harvest. Fruit from each data vine was completely removed and yield for each vine recorded. Twenty bunches, sampled at random from each vine, were then set aside for laboratory analysis.

Laboratory analysis

Total anthocyanins were measured using the UV-Vis method of Iland et al. (2000). Malic acid was analysed by Fourier-transform infrared spectroscopy using a WineScan FT-120 (FOSS North America, Eden Prairie, MN, USA) using a calibration created in WinISI II (FOSS, Hillerød, Denmark) using the reference chemistry quality standards of E&J Gallo Winery. Quantification of bound form β-damascenone was completed following a method of solid phase extraction derived from Whiton and Zoecklein (2002), fast acid hydrolysis, and headspace solid-phase microextraction (SPME) coupled to GC/MS (Kotseridis et al. 1999, Ibarz et al. 2006, Canuti et al. 2009).

Variogram analysis

Experimental variograms for individual constituents of fruit composition in each year were estimated as part of Sams et al. (2022a). Building on this work, and that of Bramley et al. (2017) and of Sams et al. (2019), the focus of the current study was to explore the application of the common variogram to multiple sites, seasons, and an expanded number of variables. The choice of the variables used in this study followed Sams et al. (2019) with the addition of 2018 and 2019 anthocyanins, but malic acid (2017 to 2019) and β-damascenone (2017 to 2019) were chosen as they showed high vine to vine variability where higher sample numbers may be necessary to generate zonal maps with high confidence and may be aided by the use of a common variogram. Bramley et al. (2017) used 1000 m offsets, applied sequentially to data from additional seasons to both the *x* and *y* coordinates, to combine data from multiple years from a 6.1 ha vineyard. These offsets enabled the derivation of a common variogram from multiple years by incorporating the semivariance from multiple years into the same spatial model. A larger number of point pairs in each lag class was achieved and any artefacts of variogram fitting in a single season were removed from the overall analysis. The larger set of point pairs is especially important at short distances as these are typically those at which the fewest pairs exist, yet characterising spatial dependence at short distances is critical to robust definition of the variogram and of the range of spatial dependence—the distance beyond which, samples can be regarded as independent. In the present context with multiple vineyards in multiple seasons, a much larger offset

was required to ensure that the data contribution from any single vineyard/season was spatially discrete in relation to the others. Given that the four vineyards lie within approximately 40 km of each other, common variograms were generated by adding a 100 km offset to the eastings and northings of each vineyard to combine data from 2017 to 2019 such that the original coordinates were used for the 2017 data, +100 km to each coordinate in 2018, and +200 km to each coordinate in 2019. Data from each vineyard and year were standardised [mean (μ) = 0, SD (σ) = 1] to eliminate issues related to site or season specificity such as inherent differences in the absolute values of compositional metrics, or differences due to seasonal weather. Common settings of lag size (20), lag tolerance (10%), and maximum distance (250 m) were applied to the variogram estimation of each dataset in VESPER (Minasny et al. 2005) with the maximum distance of 250 m being appropriate both in terms of expected patterns of variation (Sams et al. 2022a) and as a means of ensuring data from the different vineyards remained discrete. As in Sams et al. (2022a), a spherical model was found to be suitable for the spatial characterisation of fruit composition, and spatial statistics were produced for each variable and associated variogram. Each variable from each vineyard was then interpolated using each set of variogram parameters derived from the single and combined datasets [single vineyard–single year (SVSY), $n = 125$; single vineyard–multiple year (SVMY), $n = 375$; multiple vineyard–single year (MVSY), $n = 500$, multiple vineyard–multiple year (MVMY), $n = 1500$] to assess differences in map products. Variogram statistics were calculated for all four classes of variograms listed above. These include the nugget [measurement and sampling error (c_0)], partial sill [spatially dependent variance (c_1)], effective range [distance at which samples are no longer spatially dependent (a_1) (Webster and Oliver 2007)], and root-mean-squared-error (RMSE). Cambardella index was calculated as the nugget divided by the sum of the nugget plus the sill and multiplied by 100 and was used as a descriptor of the spatial structure of variability (Cambardella and Karlen 1999, Sams et al. 2019). Low values of Cambardella index indicate high spatial structure and can be used to assess the potential suitability of a farm for variable rate management (Han et al. 1994).

To further demonstrate the utility and application of the approach, two case study simulations were carried out for an 'unknown' vineyard and analyte. The first was conducted in order to simulate how a common variogram could be used for a practical purpose. For this, the 2019 anthocyanin concentration in the 'unknown' vineyard (Anth2019D in Vineyard D) was predicted based on different numbers of sample points ($n = 10$ to 120 with intervals of 10) and common variograms using Monte Carlo simulations (100 iterations per n). To ensure that selected sample points (n) in each simulation were uniformly spread out in the 'unknown' vineyard, a ten-cell grid of five rows and two columns was used to label all 125 points (Figure 1). The grid labelling system mimicked a sampling strategy where samples were spread across the vineyard but also that each section of the vineyard would be represented in each simulation. In each Monte Carlo simulation, three steps were defined as selection, prediction, and evaluation. In the selection step, $n/10$ points were randomly selected from each grid cell and used as inputs for the kriging model. Next, Anth2019D was predicted using three different models: a common variogram produced from using data from 2017 to
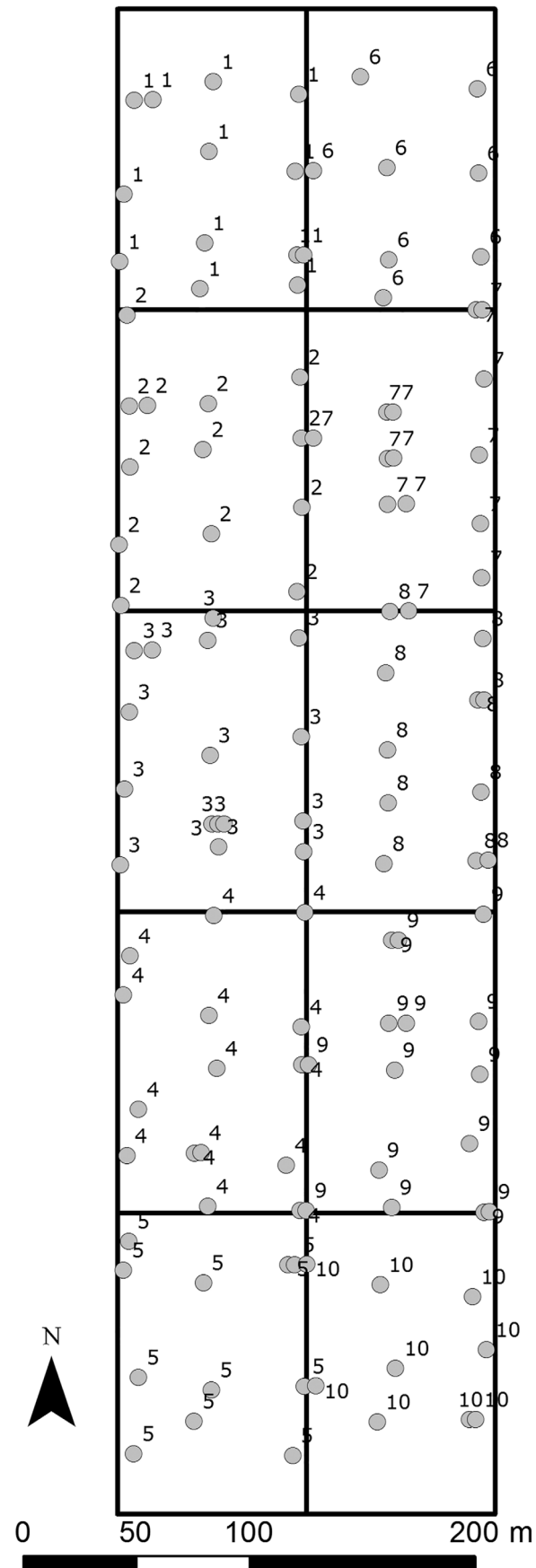

Figure 1. Sample points labelled by grid cell for the Monte Carlo simulation to ensure whole vineyard coverage in the 'unknown' vineyard. Each iteration of single vineyard–single year (SVSY$_n$), from 10 to 120 sample points included, consisted of increasing numbers of sample points coming from each grid cell.

2019 in Vineyards A, B, and C (CV); a common variogram produced using data from 2017 to 2019 in Vineyards A, B and C with the (n) points from the 'unknown' vineyard (CV+); and the SVSY variogram of the 'unknown' vineyard with the (n) points (SVSY$_n$, where n represents the increasing number of included points from 10 to 120). Finally, Anth2019D maps produced from three different variograms were classified by histogram analysis into 33rd percentiles (low, medium and high) and compared to the classified 2019 anthocyanin map in Vineyard D using the SVSY of Vineyard D with all 125 points. Kriging estimates from simulated maps of each model were compared against the SVSY using the 'accuracy' metric from a confusion matrix, where accuracy is equal to the proportion of predictions the model was able to classify correctly (Fawcett 2006). Average kriging variance and average variance of estimated anthocyanins were also calculated from the resulting layers.

The second simulation study was conducted to illustrate how a grower might take advantage of the common variogram and the reduced annual sampling requirement that it enables. Using the same target vineyard (Vineyard D) as in the first simulation, 35 sample points were randomly selected from each of the four vineyards and each year (2017–2019), with no repeated samples, and were standardised ($\mu = 0$, $\sigma = 1$) by vineyard and year. The standardised data from Vineyard D, obtained over 3 years,

were combined into a single dataset and a SVMY variogram was fitted and a combined map of total anthocyanins from 2017 to 2019 was produced. To simulate how a group of growers may cooperate for the derivation of a common variogram, samples from the other three vineyards (Vineyards A, B and C) were added to the combined Vineyard D dataset and a MVMY variogram was fitted and applied to the combined Vineyard D sample points for interpolation.

Results

Spatial variability
Maps produced from different variogram models were similar, with small deviations among the maps derived from the different variograms (Figures 2–4). The spatial variability of anthocyanin concentration did not change dramatically with different variogram settings in Vineyards B and D in 2018 (Figure 2) and the same was true for β-damascenone in Vineyards A and C in 2017 (Figure 3). The variability of malic acid in Vineyard C changed little from 2017 to 2019 using the SVSY compared with the MVMY (Figure 4). In general, patterns of spatial variability could be characterised as 'smoother' as the number of vineyards or years included in each variogram model increased from 125 points in the SVSY variograms to the MVMY variograms with 1500 points used to determine spatial structure (Figures 2–4).
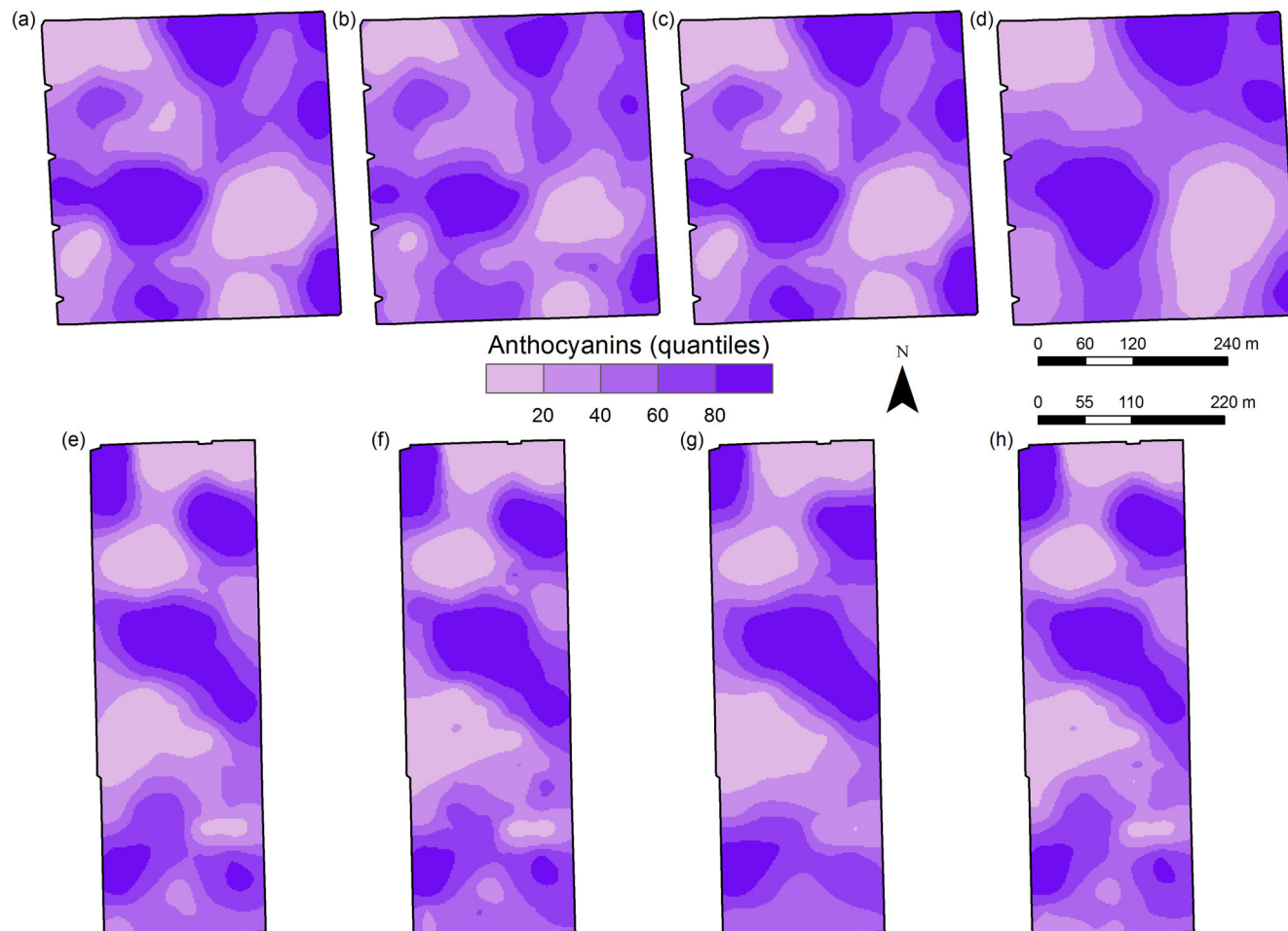

Figure 2. Maps showing spatial variability of standardised ($\mu = 0$, $\sigma = 1$) anthocyanin concentration in 2018 in (a–d) Vineyard B and in (e–h) Vineyard D derived from experimental variograms derived from (a, e) single vineyard–single year (SVSY) $n = 125$; (b, f) single vineyard–multiple year (SVMY) $n = 375$; (c, g) multiple vineyard–single year (MVSY) $n = 500$; (d, h) multiple vineyard–multiple year (MVMY) $n = 1500$.
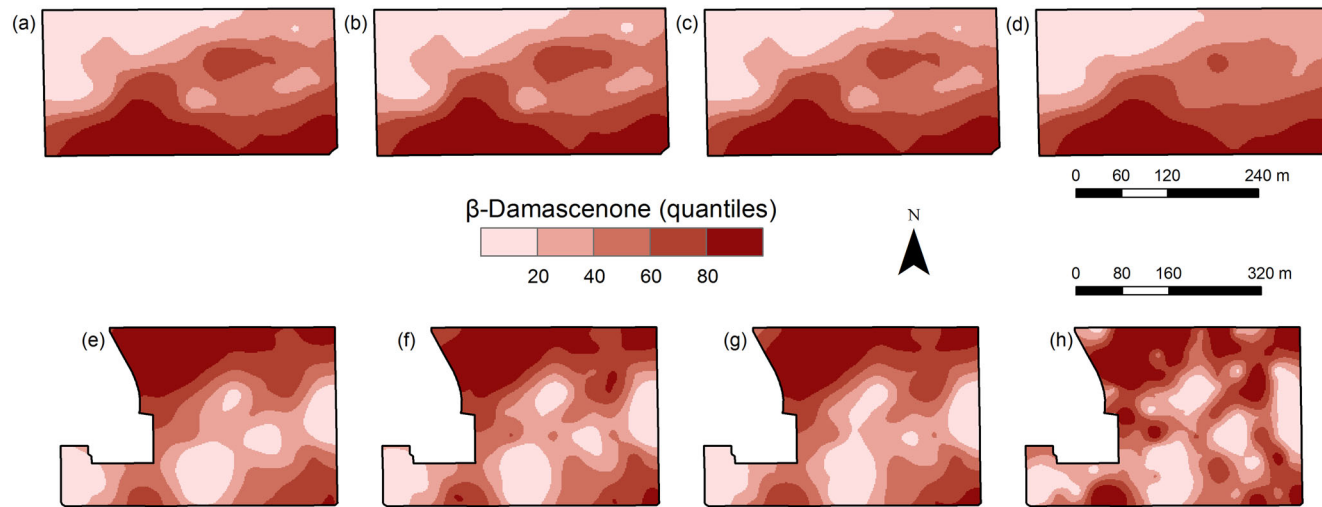
Figure 3. Maps showing spatial variability of standardised ($\mu = 0$, $\sigma = 1$) β-damascenone concentration in 2017 in (a–d) Vineyard A and in (e–h) Vineyard C derived from experimental variograms derived from (a, e) single vineyard–single year (SVSY) $n = 125$; (b, f) single vineyard–multiple year (SVMY) $n = 375$; (c, g) multiple vineyard–single year (MVSY) $n = 500$; (d, h) multiple vineyard–multiple year (MVMY) $n = 1500$.

Variograms

Spatial statistics showed that although there were differences between SVMY variograms and those from SVSY variograms, differences between them in terms of RMSE were small, with those for multiple years (SVMY) typically lower than the highest error of any single year (SVSY) (Table 1). Results from multiple vineyard variograms showed that RMSE was also similar between any MVSY and the MVMY (Table 2). In general, the nugget, sill, and Cambardella index of each SVMY variogram were somewhere between those of the highest and lowest values of the SVSYs, though anthocyanin concentration in Vineyard A was an exception (Table 1). Nugget (c_0) and partial sill (c_1) variance, along with effective range (a_1), were more consistently similar among multiple

vineyard variograms (Table 2) as compared with single vineyard variograms (Table 1). Since 3 years were included in the SVMY, the number of pairs of points in each lag class increased exactly threefold (Table 1), with the largest number of point pairs per distance class (lag) occurring in the MVMY variogram (Table 2)—as would be expected. Variograms derived from total anthocyanins were similar in shape and in ranges of spatial dependence (Figure 5), though the 2017 effective range in Vineyard B separated from the others in Vineyard B (Figure 5b). Variograms derived from β-damascenone data and malic acid (not shown) exhibited some differences between vineyards, and variogram settings were similar to those found for anthocyanins, but these did not result in any major changes in mapped outputs.
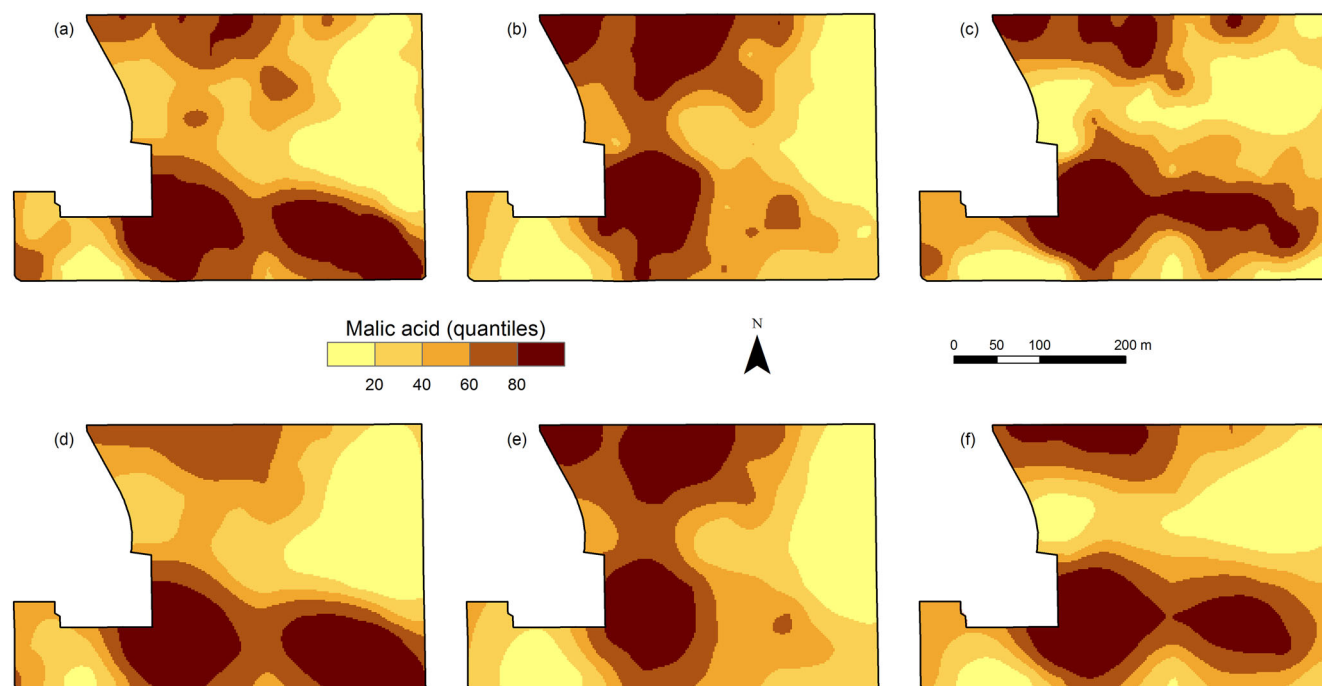

Figure 4. Maps showing spatial variability of standardised ($\mu = 0$, $\sigma = 1$) malic acid concentration in Vineyard C derived from experimental variograms derived from (a) single vineyard–single year (SVSY) in 2017, (b) SVSY in 2018, (c) SVSY in 2019, (d) multiple vineyard–multiple year (MVMY) in 2017, (e) MVMY in 2018, (f) and MVMY in 2019. All SVSY $n = 125$; and all MVMY $n = 150$.

Table 1. Spatial statistics from each single vineyard–single year variogram and from each single vineyard–multiple year variogram incorporating data from 2017 to 2019.

Analyte	Statistic	Vineyard A				Vineyard B				Vineyard C				Vineyard D			
		2017 $n=125$	2018 $n=125$	2019 $n=125$	17/18/19 $n=375$	2017 $n=125$	2018 $n=125$	2019 $n=125$	17/18/19 $n=375$	2017 $n=125$	2018 $n=125$	2019 $n=125$	17/18/19 $n=375$	2017 $n=125$	2018 $n=125$	2019 $n=125$	17/18/19 $n=375$
Anthocyanins	Nugget (c_0)	0.43	0.19	0.13	0.57	0.03	0.59	0.38	0.45	0.43	0.48	0.20	0.37	0.73	0.15	0.04	0.46
	Sill (c_1)	0.55	0.88	0.84	0.47	0.88	0.44	0.65	0.54	0.55	0.52	0.82	0.63	0.23	0.76	0.85	0.46
	Range (a_1) (m)	48	130	51	153	65	106	86	87	128	107	125	120	88	58	38	84
	CAM	44	18	13	55	3	57	37	45	44	48	20	37	76	16	4	50
	RMSE	0.08	0.13	0.10	0.08	0.13	0.06	0.10	0.05	0.08	0.15	0.07	0.07	0.10	0.10	0.11	0.10
β-Damascenone	Nugget (c_0)	0.74	0.02	0.49	0.56	0.46	0.45	0.6	0.56	0.54	0.11	0.57	0.38	0.65	0.54	0.25	0.49
	Sill (c_1)	0.27	0.98	0.62	0.44	0.57	0.55	0.42	0.47	0.44	0.79	0.49	0.57	0.30	0.44	0.59	0.43
	Range (a_1) (m)	80	21	215	76	98	149	103	126	68	124	259	111	178	293	202	216
	CAM	73	2	44	56	45	45	59	54	55	12	54	40	68	55	30	53
	RMSE	0.07	0.07	0.14	0.08	0.07	0.09	0.50	0.19	0.10	0.15	0.08	0.09	0.11	0.08	0.07	0.06
Malic acid	Nugget (c_0)	0.52	0.14	0.41	0.39	0.47	0.32	0.12	0.34	0.15	0.23	0.05	0.22	0.34	0.11	0.06	0.17
	Sill (c_1)	0.48	0.90	0.56	0.62	0.68	0.83	0.90	0.85	0.85	0.76	0.98	0.79	0.59	0.86	0.72	0.74
	Range (a_1) (m)	83	73	80	80	341	388	50	305	154	174	117	147	45	62	41	51
	CAM	52	13	42	39	41	28	12	29	15	23	5	22	37	11	8	19
	RMSE	0.09	0.10	0.06	0.07	0.11	0.14	0.23	0.12	0.10	0.11	0.07	0.06	0.16	0.12	0.14	0.07
Lag minimum		24	24	24	72	10	10	10	30	18	18	18	54	35	35	35	105

Simulation study

Monte Carlo simulations to predict Anth2019D were completed using two common variogram approaches, one derived from the 2017–2019 data in Vineyards A, B and C, that is, without data from Vineyard D (CV) included for variogram modelling, and one with data from Vineyard D included (CV+) (Figure 6). Both CV and CV+ produced maps with a tighter range of accuracy than that of the SVSY from 2019 anthocyanins in Vineyard D alone (Figure 6), regardless of the number of points included. This indicated that the common variogram approach provided a more confident set of maps than single vineyard data alone, and that information from regional vineyards without data from the unknown vineyard produced a similar result. Ranges of accuracies between each method overlapped until the number of points used to derive the local variogram exceeded 100 sample points (Figure 6), equivalent to the number recommended by Webster and Oliver (2007). The predictive capability, however, of the local variogram (SVSY$_n$) with more than 100 samples reached nearly 90% of the accuracy of standard (SVSY) as compared with a top-level prediction of about 70% for the common variograms (Figure 6). The addition of data from Vineyard D into the CV+ variogram method was slightly better than the common variogram without Vineyard D data (CV), though the difference was small (Figure 6).

Figure 7 provides a comparison of the variance in mapped (i.e. estimated) anthocyanin concentration and the average kriging variance (i.e. confidence of prediction) between the three variogram approaches over 100 simulations using 120 sample points. The average variance of kriged anthocyanin values was lower in the common variogram approaches (CV in Figure 7a; and CV+ in Figure 7b) compared with the SVSY (Figure 7c) as few pixels in the common variogram maps showed values above 0.05 mg/g compared with those in the SVSY map. While the two common variograms (CV in Figure 7d; and CV+ in Figure 7e) produced maps with only a few pixels with average kriging variances in the lowest class of prediction confidence (<0.014), they showed no pixels in the highest two classes (>0.022). Conversely, average kriging variances in the SVSY (Figure 7f) showed many pixels to be in the highest class (>0.026) reflecting increased uncertainty when only one vineyard was included in the variogram estimation. In summary, the SVSY approach resulted in higher anthocyanin variance by pixel (Figure 7c) and in a large portion of pixels in the bottom two classes of kriging variance (Figure 7f), indicating that both the confidence in prediction and the variance of predicted anthocyanins was improved with the use of a common variogram. Note here that Figure 7a–c show the variance of the predicted anthocyanin values and Figure 7d–f shows the kriging variance following 100 iterations of kriging, not the variances obtained from single simulations.

In order to provide a use case scenario for practitioners interested in deploying a common variogram without the large sampling ($n > 100$) required for variogram estimation in a single year, two additional maps were created using common variograms to simulate how this may be achieved. Figure 8 shows two maps of anthocyanin concentration derived from a dataset ($n = 105$) comprised of 35 samples randomly selected and normalised by year in each of 2017–2019 from a single vineyard. In Figure 8a, the map was interpolated using a variogram obtained from the 105 samples. The map in Figure 8b was produced using the same

Table 2. Statistics from common variograms that include all four vineyards in each year (multiple vineyard–single year) and an aggregated common variogram (multiple vineyard–multiple year) with all four vineyards across all 3 years (2017–2019).

Analyte	Statistic	2017 $n = 500$	2018 $n = 500$	2019 $n = 500$	17/18/19 $n = 1500$
Anthocyanins	Nugget (c_0)	0.65	0.51	0.38	0.79
	Sill (c_1)	0.34	0.51	0.60	0.21
	Range (a_1) (m)	109	110	94	159
	CAM	66	50	39	79
	RMSE	0.05	0.05	0.07	0.05
β-Damascenone	Nugget (c_0)	0.58	0.45	0.49	0.78
	Sill (c_1)	0.42	0.47	0.51	0.27
	Range (a_1) (m)	82	105	184	269
	CAM	59	49	49	74
	RMSE	0.06	0.09	0.05	0.03
Malic acid	Nugget (c_0)	0.60	0.33	0.44	0.67
	Sill (c_1)	0.44	0.62	0.54	0.33
	Range (a_1) (m)	212	119	95	139
	CAM	58	35	45	67
	RMSE	0.08	0.06	0.10	0.04
	Lag minimum	111	111	111	675

35 normalised random samples per season, but with the inclusion of 35 additional random samples, normalised by year and vineyard, obtained from three other vineyards in the region each year and included for variogram estimation ($n = 420$). A strong resemblance is evident between the map derived from the common variogram fitted with 420 points (Figure 8) and those found in Figure 2e–h, which used a larger statistical support.

Discussion

The practical utility of a common variogram was assessed for a vineyard and analyte (2019 anthocyanins in Vineyard D) to simulate mapping done for a vineyard manager with interest in combining their data with that of others in the region to characterise within-vineyard spatial variability. Results show that the predictive capability of the common variograms could correctly classify nearly 50% of input points with relatively high confidence compared to SVSY, and with as few as 30 samples (Figure 6). Compared against the results from SVSY, which reached only a mean prediction above 70% similar with 90 points, this simulation showed that the common variogram could be a useful tool in describing the spatial variability of anthocyanins even in a vineyard where high density sampling has not occurred, providing sufficient samples are available from nearby vineyards over several years to support creation of the common variogram. In the absence of further study, caution should be taken in determining the appropriate spatial extent
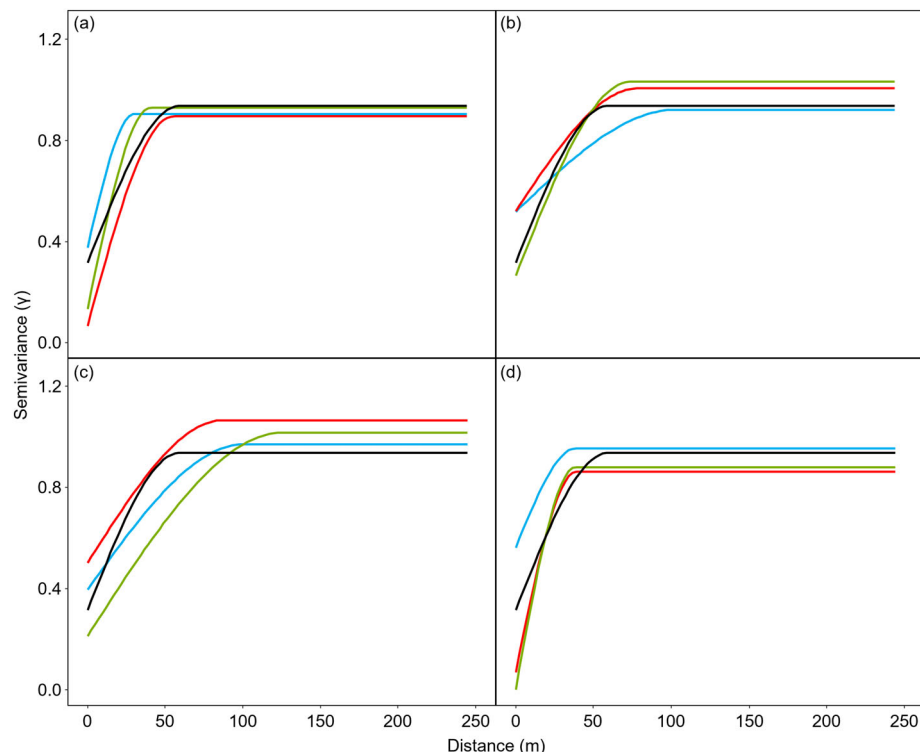

Figure 5. Common ($n = 1500$) (——) and single year ($n = 125$), 2017 (——), 2018 (——) and 2019 (——), variogram models of standardised ($\mu = 0$, $\sigma = 1$) anthocyanin concentration in Vineyards (a) A, (b) B, (c) C and (d) D.
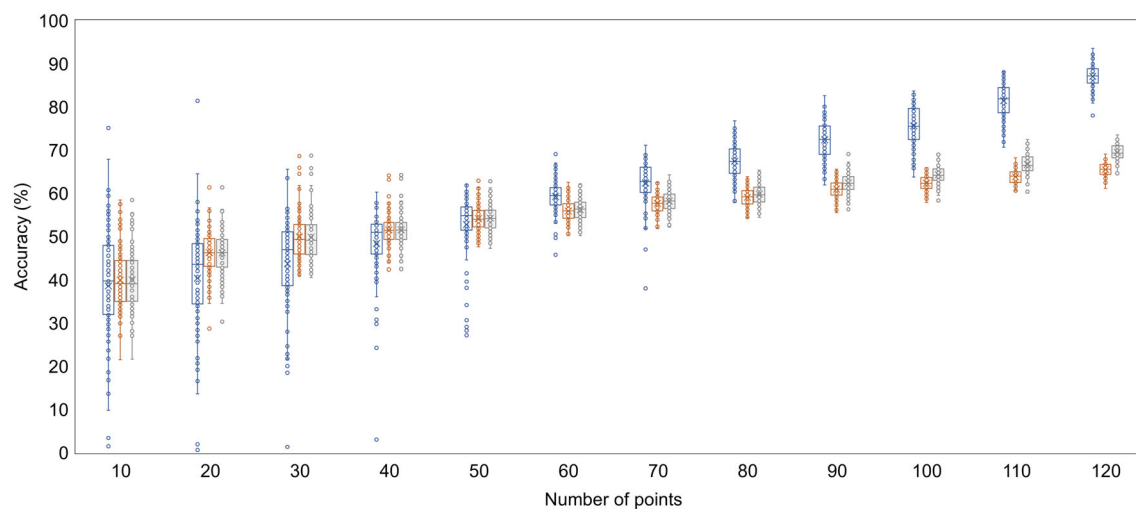
Figure 6. Change in the accuracy of predictions of two common variogram methods (common variogram without Vineyard D, CV; and common variogram with Vineyard D, CV+) and the site specific single vineyard–single year variogram with increasing numbers of points (SVSY$_n$), compared against the anthocyanin maps produced with the site specific variogram from all 125 points in Vineyard D (SVSY). (□) SVSY versus SVSY$_n$, (□) SVSY versus CV, (□) SVSY versus CV+. Note that sample points were selected from the locations shown in Figure 1 using Monte Carlo simulation. $n = 100$ simulations.

within which to group vineyards for data aggregation. For example, samples from vineyards in the Lodi region should probably not be included for common variogram generation with those from vineyards in Napa Valley. Examining this issue presents an interesting opportunity for future study. In situations where a vineyard manager does have more than 100 samples and can estimate a local variogram with some confidence, results presented here indicate they would have higher confidence in maps produced using the common variogram approach (Figures 6–8) if data were available from other nearby vineyards. Additionally, the inclusion of those points into a regional variogram could help others to generate maps with more confidence. To take advantage of this technique, groups of growers, vineyard managers, or wineries could target samples in a subset of vineyards over a few years in such a way as to provide the group with at least a baseline common variogram from which predictions and maps could be generated to the benefit of all participants, as the example in Figure 8 illustrates. Importantly, this may be achieved with a reduced annual sampling requirement, though care should be taken regarding the size of the region within which vineyard data are pooled. Thus, 35 samples per year from each vineyard could be collected over the course of 3 years to collect the minimum 100 samples for variogram estimation (Figure 8a), but the robustness of the maps could be improved by a cooperative effort from other growers/vineyards (Figure 8b). Both maps illustrate how an individual grower might take advantage of the common variogram approach, coupled with a more manageable annual sampling requirement of 35 samples per year compared to more than 100. The fact that Figure 8b delivers a smoother map with strong similarities to Figure 2e–h, indicates how a cooperative sampling strategy could provide robust results, which represent the variability of this vineyard over the course of 3 years, but without the requirement for a large sample number in a single year. Given that the typical capital cycle of a vineyard is of the order of 30 years, we think this approach may be both attractive and useful. This sample number could potentially be reduced even further using techniques like REML variogram estimation (Kerry and Oliver 2007), but the present objective was to provide a practical method for understanding vineyard

variability using simple techniques and software available to growers. This pragmatic approach is important given the results from recent conversations with growers about field experimentation in Australian vineyards (Song et al. 2022). Nonetheless, the use of more advanced techniques is of interest, especially since there are few, if any, studies incorporating these methods into the characterisation of spatial variability of vineyard productivity.

The small differences in mapped patterns of spatial variability between each of the common variogram methods used to interpolate each fruit compositional analyte are important for the characterisation of spatial variability in vineyards. First, the increase in pairs of points per distance class means that the sample density to meet minimum variogram robustness requirements (Cressie 1993) can be met in large commercial vineyards without more excessive sampling campaigns. Those interested in variability maps need collect only the number of samples necessary to provide the accuracy desired. Some may choose to sample less densely and still achieve a zonal classification of at least 50% accuracy (Figure 6). The minimum number of pairs of points per lag class doubled with the addition of a second year and tripled when all 3 years were included, either when all four vineyards were included in the variogram estimation or from an estimation composed from a single vineyard (Tables 1, 2). In a study from the same four vineyards shown in this study, Sams et al. (2019) found that differences between anthocyanin maps derived from a single vineyard variogram and one from a common variogram of all four vineyards in a single year were primarily located on the edges of classified zones and would not have altered zonal prescriptions such as those used to underpin selective harvesting. Second, the common settings applied to each analyte or vineyard assessed in this study helped to reduce the effect of any potential subjective variogram fitting (Bramley et al. 2017, Sams et al. 2019). Since information from multiple vineyards (MVSY and MVMY) and/or years (SVMY and MVMY) was included in the analysis, there was less reliance on the fit of a single variogram (SVSY) for the characterisation of spatial variability of compounds found to have short ranges of spatial dependence (Bramley 2005, Sams et al. 2022a). These results suggest that pooling data
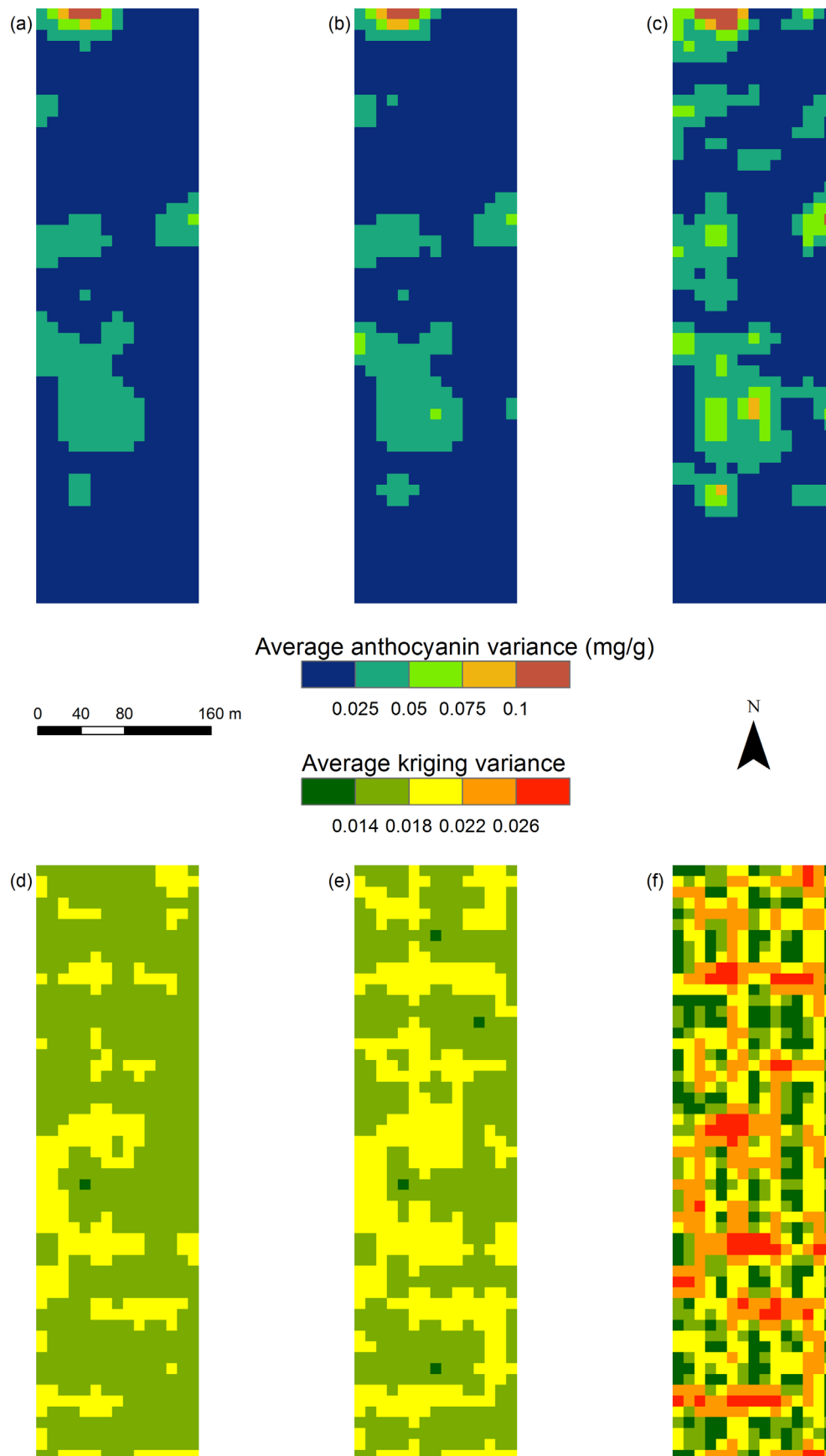
Figure 7. Variance in predicted anthocyanin concentration and the average kriging variance (prediction confidence) from simulations of each variogram class using (a, d) common variogram without Vineyard D (CV), (b, e) common variogram with Vineyard D (CV+), and (c–f) single vineyard–single year from vineyard D in 2019 (SVSY) with 120 points included in the interpolations. $n = 100$ simulations.
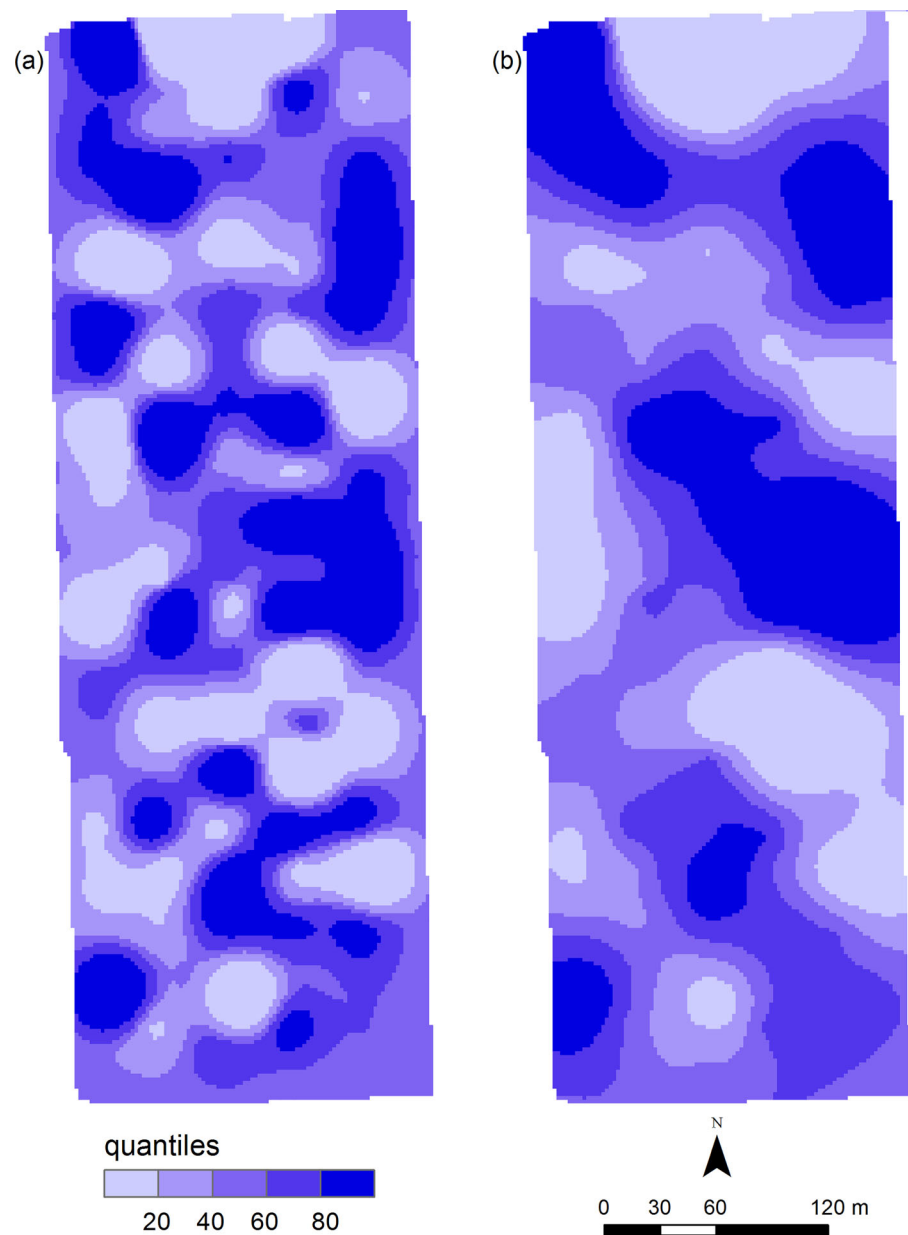
Figure 8. Maps of anthocyanin concentration derived from 35 samples collected each year for 3 years (2017–2019) in a single vineyard and standardised ($\mu = 0$, $\sigma = 1$) on an annual basis. In (a), the map was produced using a single vineyard–multiple year variogram derived from the 105 multi-year combined samples, whilst in (b) the data used to derive the multiple vineyard–multiple year variogram were supplemented by an additional 35 randomly selected samples per year for 3 years (2017–2019) from four different vineyards in the same region ($n = 420$). In the latter case, the data were again standardised ($\mu = 0$, $\sigma = 1$) by vineyard and year.

into common variograms could be beneficial to those interested in characterising spatial variability by adding the geostatistical support necessary for robust variogram estimation. As suggested by Taylor et al. (2005) for yield mapping, the advantages of building a database for variability of regional fruit composition are numerous. Individual vineyard managers would be less reliant on small numbers of samples to characterise variability while at the same time achieving a more robust idea of the variability of local and regional fruit composition. Additionally, regional information about the range of spatial dependence of certain compounds would be beneficial even when only a few samples were collected by acting as a guide to how far apart samples should be in order to be considered independent.

Given the requirements established by Cressie (1993) and Webster and Oliver (2007), of a minimum 100 samples per variogram and at least 30 pairs of points per lag class, maps describing spatial variability of grape composition must be based on sample numbers which are likely to be financially prohibitive to most winegrowing businesses. This is especially true in large commercial vineyards, since the sample number of 125 geolocated samples per vineyard in this study amounted to 9–17 vines/ha, which is somewhat lower than the 26 samples/ha used by Bramley (2005) or 28 samples/ha by Scarlett et al. (2014). Although these studies did not consider this density to be the absolute minimum number of samples required per hectare, they have been viewed as something of a guide for the geospatial analysis of fruit composition in vineyards. While the sample density per hectare used for this and related studies (Sams et al. 2022a, b) was similar to those collected by others in California (Santos et al. 2012, Martínez-Lüscher et al. 2019, Yu et al. 2020),

though nearly double in the case of Vineyard A, this study is, so far, the only one conducted in California which meets the100-sample threshold (Webster and Oliver 2007). Another study in North America used a high sample number but in a small vineyard (Reynolds et al. 2007) not representative of commercial conditions in the California Central Valley. Our study sought a compromise to these sampling issues by pooling data into common variograms in order to satisfy the large sample number requirements necessary for the characterisation of spatial variability, but without the need for even more intensive and expensive ground sampling. The variograms produced from this exercise, or other similar studies in other regions of the world, could be considered the typical variograms for those analytes and regions with which others in these areas could compare against their own degrees of spatial variability. Additionally, if suitable covariates such as soil electrical conductivity surveys, high-density yield maps from a yield monitor, or remotely sensed imagery (Sams et al. 2022b) exist for their sites, they could be used to further increase confidence that patterns of spatial variability are stable.

While Sams et al. (2022a) found that NDVI and canopy temperature measurements made from a fixed wing aircraft were sufficient to describe differences in variability of fruit composition in vineyards with highly structured and temporally stable zones, many samples had to be collected at great expense to demonstrate this. Thus, the development of fruit composition sensors may be increasingly necessary in vineyards with less distinct patterns and/or where imagery is difficult to acquire as a means of reducing the cost of sampling and analysis. Since the labour cost and complexity of sample collection involved in such a strategy may not decrease at the level needed to add value for smaller producers, either an advancement in the capabilities of remote sensing instruments or a high throughput proximal sensor may be necessary to accommodate the needs of characterising variability in fruit composition. The examples shown in Figure 8 could be produced with even less effort from collaborating entities, if they used sensor-based estimates of fruit composition rather than being reliant on sampling and laboratory analysis.

The simulations presented here show that additional vineyards could be added to a regional variogram without large sample numbers and could aid smaller operations in understanding spatial variability with higher confidence than from a single vineyard alone. Compounds with high nugget variance, either from measurement error, high local variation, or low concentration in the fruit, and no defined range of spatial dependence, may require either additional sampling or a separate approach to destructive sampling completely, that is, remote or proximal sensing. One potential remedy is to increase the sampling density to account for this variability, but results shown here point to the application of a common variogram to aid in the statistical support necessary for the description of vineyard spatial variability. As Sams et al. (2022a) pointed out, fruit compositional variability is largely influenced by a small number of key attributes such as anthocyanins, making it potentially unnecessary to map less important compounds unless a specific flavour or aroma is desired for winemaking.

Conclusions

Simulations were used to demonstrate how a common variogram could be applied to the mapping of fruit composition in a vineyard. It was found that such an approach led to an increase in the confidence that could be attached to the resulting maps. While a higher number of point pairs per lag class enabled the most robust variogram fits in this study, the impact on maps of spatial variability was small. Along with comparison between the various forms of common variogram explored here, this indicates that data from multiple vineyards and years can add to the statistical support of map interpolation without changing the patterns of variation in individual vineyards. In turn, this may lead to an enhanced understanding of longer-term patterns of spatial variability as the inclusion of multiple years lends weight to these patterns. Vineyard managers and wineries could have increased confidence in zonal management with the added statistical weight provided by a common variogram where patterns of variability continue to hold over several years. This is an especially important finding given the errors found in maps derived from the data collected from a single year, even with the relatively large sample size shown in this study. There is also potential for a smaller annual sampling effort with data combined over the course of few years with a common variogram for a particular grape analyte obtained from a group of vineyards if data from existing or cooperating vineyards are available.

Acknowledgements

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Chapter 6: General Discussion and Future Directions

General Discussion

The research presented in this thesis examined spatial variability of several components of grape composition related to Cabernet Sauvignon wine quality in central California, though these techniques could be applied to specific attributes found in other cultivars and in other winegrowing regions. Each of the studies presented here attempted to increase our understanding of how mapping spatial variability of fruit composition can be exploited to the benefit of growers by linking fruit composition to indirect measurements from proximal data or remote sensing (Chapters 2 and 3) and showing how sample collection strategies can be leveraged by multiple vineyards or growers to aid those involved in developing knowledge of the spatial variability of fruit composition across a region (Chapters 4 and 5). Though expensive and time-consuming sample collection will be unavoidable for the foreseable future, the information presented in these studies should act as a guide for how to make the most of targeted samples to achieve optimal results.

Characterising the spatial variability of fruit composition

Fruit composition (or quality) mapping is a necessary step towards true precision management of wine grapes. As opposed to many other cropping systems, particulary broadacre crops on annual cycles, the main factor used to evaluate vineyard productivity is how well the fruit perfoms after a secondary process (fermentation); i.e. the quality of the wine. Whereas in many crops, a yield map may be sufficient to characterise the productivity of a farm, in wine grapes this is only part of the story as the fruit from a single vineyard is then mixed (possibly with fruit from other vineyards) and made into wine. Additionally, cultural practices in vineyards complicate the relationship between yield and fruit composition or quality since one side or other of the yield-quality relationship is manipulated by different canopy management practices, irrigation, or nutrient management. All of these influences together make it necessary to produce maps of fruit

composition over a few years, if the full potential of a vineyard is to be realised. This need for spatial characterisation of fruit chemistry brings with it several challenges, many of which have been described in the preceding chapters. As a summary, these include complex and costly chemical analyses, a lack of settled-upon chemical attributes, high sampling volumes and densities, and difficulty scaling these procedures to multiple vineyards or across broad acreages, among others. The first two of these have a partial solution described in Chapters 2 and 3; that is, to measure only those chemical attributes that have significant impacts on the final wines and/or those which dominate the patterns of spatial variation. Further, only those compounds which can be connected to indirect or remote measurements should be characterised since many of the compounds presented in this thesis did not show temporally stable patterns of spatial variation over the course of three seasons. The main driver for this conclusion is that without temporal stability of spatial patterns that resemble those derived from soil or imagery, confidence in the prescriptions for differential management will be low. Chapters 4 and 5 also provide partial solutions to the problem of sampling and assessment of spatiotemporal variation in vineyard productivity, through the development of common variograms. This technique could drastically reduce the sample volume and demand on laborartory time required of individual growers in a single season by combining them with those collected from other growers in the region. Adding to this benefit is that each cooperating grower ends up with more robust maps of fruit composition than a single grower conducting a similar trial on their own. Common variograms, coupled with a targeted approach to selection of which chemical attributes to measure, make sampling much less expensive and therefore more attainable for a larger number of precision viticulture practitioners or potential adopters.

Linking indirect measurements with fruit composition

Perhaps the most economical method of understanding spatial variability of fruit composition is to target fruit composition sampling to areas with known environmental or biophysical similarities that can be measured without excessive lab analysis. Conversely, areas of known fruit composition could be targeted for environmental or biophysical measurements. As shown in Chapter 2, and consistent with some of the earlier work, dormant season pruning weights, average berry weights, and vine yield measurements are correlated with major fruit compositional attributes and could be used with some confidence to derive zones for differential management. Vineyard managers could collect a few samples for fruit compositional analysis in zones with similar vigour, as determined by differences in dormant season pruning weights, and extrapolate to the rest of the vineyard. While this method is not perfect, vineyards with distinct vigour zones are likely to produce differences in fruit chemistry, as shown in Chapter 3. A similar method could be used with average berry weights collected near harvest. Samples collected for yield estimates could also work for this objective, though yield maps derived from a harvester mounted yield monitor provide data for entire vineyards with little additional effort. As with targeted pruning weights or berry weights, the relationship between yield and fruit composition or quality is not well-established or consistent, but is certainly more desirable than the alternative, if full vineyard optimisation of yield and quality is to be achieved.

Building on the relationships derived from proxy measurements like pruning weights and berry weights, Chapters 2 and 3 also dealt with how remote sensing may be employed to assess vineyard spatial variability. The major advantage of remote sensing is that images capture large areas in a single snapshot and require little effort on the part of the vineyard manager. This advantage is particularly useful to large farming operations in places like the Central Valley of California where vineyards are very often larger than 30 ha. Freely and publicly available imagery (i.e., Landsat, Sentinel) adds to this advantage, as emphasised by the information

provided in Chapter 2. The disadvantage, however, is similar to those of pruning weights and berry weights in that the relationship between canopy derived vegetation indices is indirect and must be validated by ground measurements. A combination of these methods, linking imagery to pruning weights and pruning weights to fruit composition may help with these issues, at least on a relative scale in vineyards with two or three distinct zones.

Proximal canopy sensors may also be used to this effect, especially in areas with regular cloud cover. One major advantage of proximal canopy sensing, as opposed to remote sensing, is that sensors can be placed at angles other than directly above the canopy. Since grapevines are a heavily manipulated cropping system, with a particular emphasis on canopy size and structure, this advantage could be even greater in vineyards with a higher degree of canopy manipulation i.e., vineyards geared towards premium fruit production. Other proximal sensors, like apparent electric conductivity soil sensors, can be used in similar fashion to produce zones with similar productive characteristics. A more direct approach to mapping fruit quality was provided by Bramley et al. (2011), but advancements in this area have been slow. No commercially available fruit quality sensor is available at present, leaving the collection of fruit samples and indirect measurements as the only viable options currernly available to vineyard managers.

Characterising fruit composition across multiple vineyards

As shown by the research presented in Chapters 4 and 5, multiple vineyards or wineries in a region, particularly those without sophisticated private laboratories, could collaborate to more effectively utilise any fruit composition samples collected by including their data in a local common variogram. Local and regional grower cooperatives or industry groups could direct sampling and spread costs even more effectively to the benefit of all. These types of interactions will likely produce more interest in managing fruit quality variability as growers and wineries gain a better understanding of how to exploit it, whether by variable rate management of

differential harvest. Those involved could potentially gain more exposure to how fruit composition changes in their own regions and further optimise growing practices. The common variogram approach could potentially be used for other types of samples such as cluster counts or pruning weights and compared against previous vintages or remote sensing data.

Precision management

Regardless of the techniques employed to characterise spatial variability, the aim of all of them is to allow for the implementation of precision management for the eventual aim of optimising productivity to benefit the farming operation. Cost and complexity are the major limitations to this process, but the information provided by this thesis should help to alleviate some of these challenges. The question then becomes: How do I use information about vineyard spatial variability to my advantage? Do I take advantage of strong patterns of variability to differentiate fruit for different wine styles or do I attempt to use differential management strategies to 'homogenise' the vineyard? Depending on the size, scale, complexity, and aims of the operation, either or both of these mangament philosiophies are likely to be advantageous to realise the full potential of vineyard productivity and can be realised guided by the material presented in this thesis.

The main objectives of this thesis were to: 1) characterise spatial variability of several attributes of Cabernet Sauvignon fruit composition across multiple vineyards and determine which compounds are most important to characterise; 2) link spatial variability of fruit composition to remote sensing and indirect field measurements; and 3) to develop methods for characterising fruit composition across multiple vineyards within a region. Chapter 1 reviewed appropriate literature and background to these aims, Chapter 2 provided a set of proxy variables that can be useful at describing differences in fruit composition, Chapter 3 assessed the capabilities of remote sensing at discriminating zonal differences in fruit composition, and Chapters 4 and 5 described a

method for reducing sampling requirements for a collaborating group of vineyards/growers to map spatial variability in other local vineyards. The use of a large sample volume from relatively large commercially managed vineyards sets this study apart from others in this area and should enable growers to more readily incorporate precision viticulture practices into real world application.

Future Directions

As laid out in the general discussion, destructive sampling of fruit for chemical analysis is presently necessary for the advancement of precision management aimed at capitalising on spatial variability in vineyards and will remain so until appropriate fruit compositional sensors are available. This, however, does not mean that options are limited to large sampling campaigns as described in Chapter 4 and 5. The cooperation and collaboration among growers, wineries, and researchers could advance the capabilties of everyone involved. Proximal and remote sensing techniques are advancing in several areas including the use of micro-satellites (Aragon et al. 2021), estimates of satellite derived vine water use over entire vineyards (Kustas et al. 2018), spatial measurements of pruning mass (Demestihas et al. 2018), smart phonse based canopy measurements applications (De Bei et al. 2016), and computer vision techniques (Ballesteros et al. 2020), among others, that should increase our ability to map and subsequently predict fruit compositional variability.

The outcomes of these efforts should then lead into the next logical steps in precision viticulture: variable rate management and prescription farming. To date, most efforts at precision viticulture have been aimed at providing growers with decision support systems or characterising vigour classes, and few trials have attempted to put variable rate technology into practice. Examples of these include Sanchez et al. (2017), who showed how variable rate technology could be used to increase water use efficiency by differentially directing irrigation to small zones, or pixels, and

Sozzi et al. (2020) who used the information from a front mounted proximal canopy sensor to apply fertiliser at variable rates. Balafoutis et al. (2017) used different nutrient and water application rates to reduce the carbon footprint in two small Greek vineyards, but did not asssess the effects on fruit composition. More studies of this nature are likely to appear in the coming years as the effects of climate change and calls for more sustainable food production drive producers to alter long standing cultural practices.

Regional characterisation of fruit composition and quality also looks to be a ripe opportunity for the further understanding of how spatial variability may differ over time and space. Though Jones et al. (2010) assessed differences in climate in the western United States, and Mendez-Costabel et al. (2013) examined regional differences of IBMP concetrations collected from vineyards throughout California, no study similar to those of Bramley et al. (2020), Bramley and Gardiner (2021), or Bramley and Ouzman (2021) have been conducted in California. Brillante et al. (2020) argued for more of these objective, data-driven types of research projects in regions around the world and they should be a logical next step for the California grape industry to truly understand how fruit quality differs from place to place.

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Canopy microclimate and fruit quality variability in vineyards of the Lodi region of California, USA

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Aim: The aim of this project was to evaluate the microclimatic effects on objective measures of fruit quality within different vigour classes of multiple vineyards and to compare the results across the Lodi region of California, USA.

Methods: In May 2019, small temperature sensors recording hourly were installed in the fruit zones of nine vineyards in the Lodi region of California. Sensor locations were selected by classifying early season Sentinel-2 multispectral imagery into high and low vigour zones. To assess differences in canopy temperature between high and low vigour areas (Figure 1), three sensors were installed in each vineyard, two in the fruit zone (high and low vigour) and one above the canopy (ambient control). Photosynthetically active radiation in the fruit zone was measured at veraison and harvest on 15 vines surrounding each sensor and compared with the temperature data. At harvest, two randomly selected clusters were collected from each of the 15 data vines, combined into one composite sample per temperature sensor, and analysed for individual objective measures of grape quality. Additionally, commercial samples were included in the analysis as they were geolocated and based on an algorithm (Meyers and Vanden Heuvel, 2014) to identify optimum sample locations based on normalised difference vegetation index.

Temperature sensor locations

Figure 1. Average canopy temperature Δ (max – min) across all nine vineyards for both high and low vigour classes.
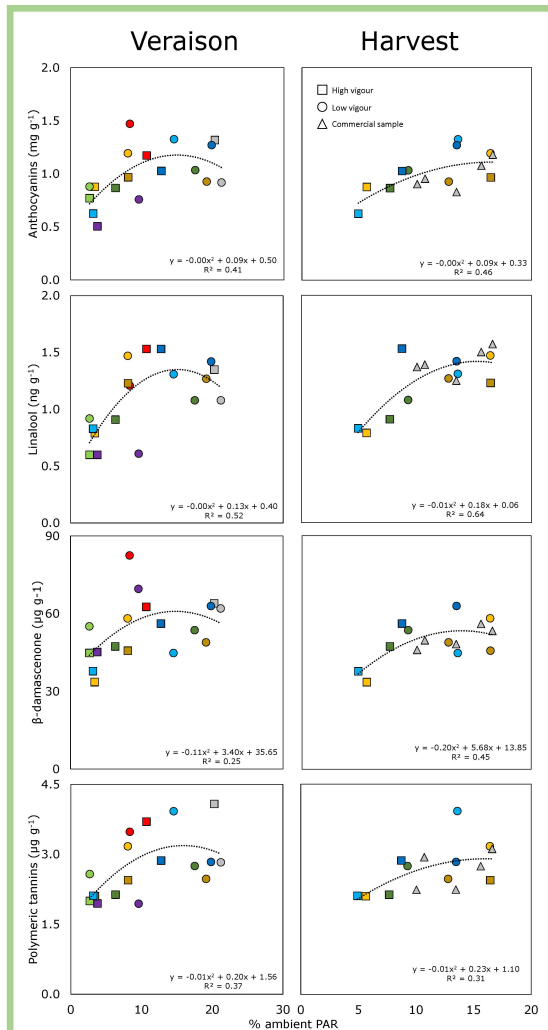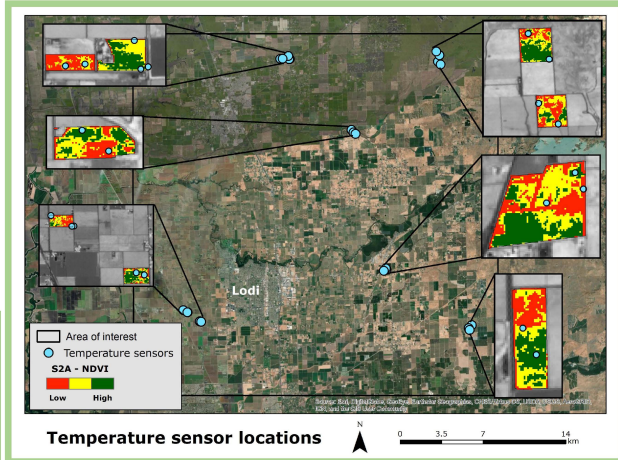
Figure 2. Comparisons between photosynthetically active radiation (PAR) and fruit chemistry. High and low vigour zones within a block are represented with the same colour.
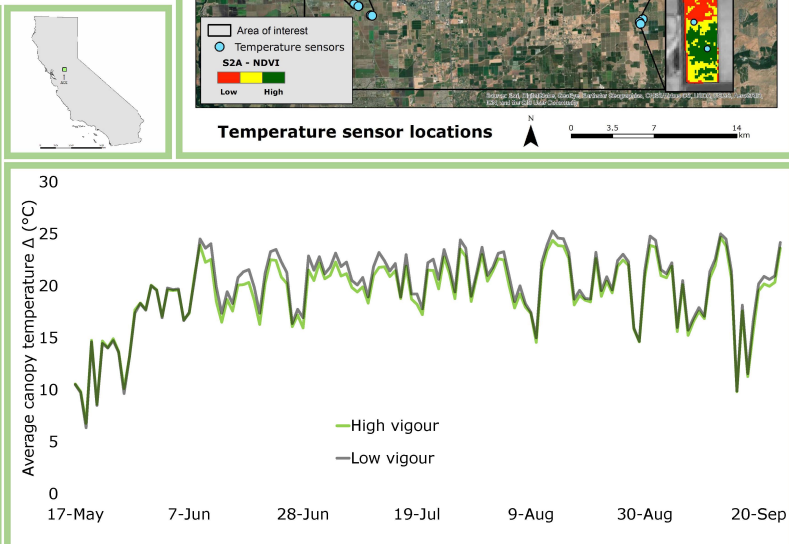
Veraison — **Harvest**

Veraison plots equations:
- $y = -0.00x^2 + 0.09x + 0.50$, $R^2 = 0.41$ (Anthocyanins)
- $y = -0.00x^2 + 0.13x + 0.40$, $R^2 = 0.52$ (Linalool)
- $y = -0.11x^2 + 3.40x + 35.65$, $R^2 = 0.25$ (β-damascenone)
- $y = -0.01x^2 + 0.20x + 1.56$, $R^2 = 0.37$ (Polymeric tannins)

Harvest plots equations:
- $y = -0.00x^2 + 0.09x + 0.33$, $R^2 = 0.46$ (Anthocyanins)
- $y = -0.01x^2 + 0.18x + 0.06$, $R^2 = 0.64$ (Linalool)
- $y = -0.20x^2 + 5.68x + 13.85$, $R^2 = 0.45$ (β-damascenone)
- $y = -0.01x^2 + 0.23x + 1.10$, $R^2 = 0.31$ (Polymeric tannins)

High vigour · Low vigour · Commercial sample

% ambient PAR

Table 1. Pearson correlations between temperature and fruit composition. Bold indicates $P < 0.05$.

Temperature	Anthocyanins	β-damascenone	Polymeric tannins	Linalool
May minimum	0.20	0.38	0.28	0.06
May average	0.01	-0.33	-0.01	0.03
May maximum	0.12	-0.15	0.07	0.14
May delta	**-0.56**	-0.39	**-0.57**	-0.40
June minimum	0.05	0.23	0.11	-0.12
June average	**0.67**	0.33	**0.51**	**0.67**
June maximum	0.44	0.13	0.36	**0.57**
June delta	0.21	0.40	0.07	0.28
July minimum	0.30	0.22	0.32	0.13
July average	0.49	0.37	0.42	0.49
July maximum	**0.54**	0.34	0.44	**0.56**
July delta	0.26	0.43	0.21	0.29
August minimum	0.18	0.16	0.21	-0.01
August average	0.32	0.09	0.28	0.35
August maximum	0.26	0.06	0.25	0.27
August delta	0.12	0.12	0.08	0.18
September minimum	0.14	0.22	0.10	-0.01
September average	0.25	0.00	0.28	0.33
September maximum	0.23	0.03	0.25	0.38
September delta	0.10	0.02	0.10	0.16

Table 2. Anthocyanin prediction using linear regression

Coefficients:	Estimates	Std Error	t value	Pr(>|t|)
(Intercept)	5.8799	1.7861	3.29	0.030 *
May ΔT	-0.1781	0.0401	-4.44	0.011 *
Jun Average T	-0.1664	0.0860	-1.94	0.125
Veraison PAR	0.0208	0.0072	2.89	0.045 *
Harvest PAR	0.0570	0.0148	3.84	0.019

$* P < 0.05$

Residual standard error: 0.0678 on 4 degrees of freedom
Multiple R-squared: 0.935   Adjusted R-squared: 0.869
F-statistic: 14.26 on 4 and 4 DF, p-value: 0.0123

Canopy shading · Sensor placement · Measuring PAR

Conclusions: The results showed differences in fruit quality between vigour zones (Figure 2). The correlation matrix in Table 1 shows significant variability in early to mid season temperatures and the variability in fruit zone light environment affected colour, aroma, and mouthfeel compounds related to Cabernet Sauvignon wine quality (Cleary et al, 2015).

Significance and impact of the study: The combination of early season image classification with measurements of temperature and fruit zone light environment are potentially capable of predicting fruit colour (Table 2). This method could be used as a cost-effective strategy to replace destructive sampling. Understanding how differences in canopy microclimate within vineyards affect fruit composition can aid vineyard managers and winemakers in optimizing streaming processes to wineries.

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