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Caio Bustani Andrade

Optimal nutrient levels in soil and plant tissue through boundary line approach using Bayesian segmented quantile regression: a case study on grapevines grown in southern Brazil.

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Caio Bustani Andrade

Optimal nutrient levels in soil and plant tissue through boundary line approach using Bayesian segmented quantile regression: a case study on grapevines grown in southern Brazil.

O presente trabalho em nível de mestrado foi avaliado e aprovado por banca examinadora composta pelos seguintes membros:

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Certificamos que esta é a **versão original e final** do trabalho de conclusão que foi julgado adequado para obtenção do título de Mestre em Agroecossistemas.

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A lógica do vento,
o caos do pensamento,
a paz na solidão.

A órbita do tempo,
a pausa do retrato,
a voz da intuição.

A curva do universo,
a fórmula do acaso,
o alcance da promessa.

O salto do desejo,
o agora e o infinito,
só o que me interessa.

(LENINE, 2008)

RESUMO

O uso ineficiente de fertilizantes na agricultura é um importante problema na produção global de alimentos, pois não apenas dificulta a viabilidade econômica das fazendas, mas também oferece grande risco de poluição ambiental. As recomendações de adubação são guiadas por avaliações nutricionais das plantas, que são comparadas com valores de referência chamados de níveis críticos ou faixas de suficiência, a fim de se decidir sobre quais os nutrientes e em que quantidades devem ser fornecidos. Tradicionalmente, esses valores de referência são definidos por ensaios de campo que são particularmente longos e caros para culturas perenes como a videira. A utilização de dados de vinhedos comerciais combinados a modernos recursos estatísticos e computacionais têm potencial para contornar a necessidade de experimentos no estabelecimento de valores de referência. Esta pesquisa avaliou a aplicação da abordagem Linha de Fronteira (LF) utilizando Regressão Quantílica Segmentada Bayesiana (RQSB) para determinar Níveis Críticos (NC) e Faixas de Suficiência (FS) de nutrientes em solos de vinhedos e folhas de videira (*Vitis vinifera*) a partir de dados obtidos em fazendas comerciais. A abordagem BL usando o modelo BSQR foi minuciosamente definida e posteriormente aplicada a um conjunto de dados provenientes da região da Campanha Gaúcha, Rio Grande do Sul, Brasil. Valores de referência para teores de fósforo (P), potássio (K), cálcio (Ca), magnésio (Mg), enxofre (S), cobre (Cu), zinco (Zn), boro (B) e manganês (Mn) no solo, bem como nitrogênio (N), P, K, Ca, Mg, S, Cu, Zn, B, Mn e ferro (Fe) nas folhas foram determinados com sucesso para o conjunto de dados completo e para uvas brancas e tintas separadamente. O NC para Cu do solo, assim como para Zn e Mn foliar, apresentaram resultados bem acima dos valores de referência regionais, enquanto as estimativas para Ca e Mg no solo foram significativamente menores do que o esperado. Nossos resultados sugerem espaço para aumento de rendimento através da fertilização com S. As uvas tintas apresentaram maiores valores de CL para P do solo, Mn do solo e K foliar, em comparação com as brancas, enquanto os resultados para Zn do solo e Mn foliar foram menores. As avaliações do modelo indicaram que a RQSB foi altamente sensível à seleção dos quantis, mas pouco afetada por mudanças da distribuição *a priori*. Os dados simulados usando modelos ajustados foram consistentemente superdispersos, sugerindo que o particionamento da variabilidade dos dados por meio da reparametrização do modelo, permitindo inclinações e interceptações variáveis, pode levar a um melhor ajuste, maior precisão dos parâmetros e maior acurácia das estimativas. Apesar das limitações atuais, o modelo RQSB fornece uma estrutura flexível para análise de LF, permitindo o uso de conjuntos de dados comerciais no estabelecimento de valores de referência que subsidiem recomendações específicas para grupos e locais, uma valiosa contribuição para o aumento da eficiência e sustentabilidade da fertilização de videiras.

Palavras-chave: nutrição vegetal; adubação de frutíferas; videiras; nível crítico; faixa de suficiência.

ABSTRACT

Inefficient use of fertilizers in agriculture is a major issue in global food production, as it not only hampers economic viability of farms but offers great risk of environmental pollution. Fertilization recommendations are guided by plant nutritional assessments which are compared to reference values, often called critical levels (CL) or sufficiency ranges (SR), so that decisions can be made regarding which nutrient and how much is to be supplied. Traditionally, these reference values are defined by field trials which are particularly long and expensive for perennial crops such as grapevines. The use of data from commercial vineyards, along with modern statistical and computational resources, has the potential to bypass the need for experiments in establishing reference values. This research evaluated the use of Boundary Line (BL) approach using Bayesian Segmented Quantile Regression (BSQR) to determine CL and SR for nutrients in vineyard soils and grapevine (*Vitis vinifera*) leaves from commercial data. The BL approach and BSQR model were thoroughly defined and subsequently applied to a data set obtained from a winery in the Campanha Gaúcha region, Rio Grande do Sul, Brazil. Reference levels of phosphorus (P), potassium (K), calcium (Ca), magnesium (Mg), sulfur (S), copper (Cu), zinc (Zn), boron (B) and manganese (Mn) in soil and nitrogen (N), P, K, Ca, Mg, S, Cu, Zn, B, Mn and iron (Fe) in leaves were successfully determined for the complete dataset as well as for white and red grapes separately. CL for soil Cu, as well as leaf Zn and Mn, showed results well above the regional reference values, while estimates for Ca and Mg in the soil were significantly lower than expected. Our results suggests room for yield increase through S fertilization. The red grapes showed higher CL values for soil P, soil Mn and leaf K, compared to the white ones, while the results for soil Zn and leaf Mn were lower. Model assessments indicated that BSQR was highly sensitive to quantile selection but poorly affected by changes in the *prior*. Data simulated using fitted models were consistently over-dispersed, suggesting that partitioning data variability through model reparametrization, allowing variable slopes and intercepts, may lead to better fit, higher parameter precision and greater accuracy of estimates. Despite current limitations, the BSQR model provides a flexible framework for BL analysis, enabling the use of commercial datasets in establishing reference values to support group- and site specific recommendations, a valuable contribution to increase efficiency and sustainability of grapevine fertilization.

Keywords: plant nutrition; fruit tree fertilization; grapevines; critical level; sufficiency range.

RESUMO EXPANDIDO

Introdução

A videira é uma cultura de suma importância cultural e agronômica, ocupando mundialmente cerca de 7,3 Mha de terra no ano de 2021. Mais da metade (57%) da produção mundial de uvas se destina à fabricação de vinhos, estimada em 26 GL, enquanto as uvas de mesa e uvas passa representaram 36% e 7% respetivamente. Para sustentar os altos rendimentos das videiras é necessário um fornecimento regular e equilibrado de nutrientes. Uma adubação inadequada compromete o tamanho da colheita e a qualidade dos frutos, seja pela pela escassez de nutrientes, toxicidades ou deficiências induzidas, levando a perdas econômicas além de representar grave risco de poluição ambiental. O manejo da adubação é feito com o auxílio de diagnósticos nutricionais, realizadas por meio de análise de solo ou de tecidos, que são comparadas com valores de referência chamados Níveis Críticos (NC) ou Faixas de Suficiência (FS). Estes valores representam as quantidades de nutrientes a partir das quais o fornecimento adicional não se reverte em aumento de produtividade. Apesar de amplamente utilizada, essa abordagem é frequentemente criticada por avaliar deficiência ou excesso para nutrientes isolados, apenas para um determinado estágio fenológico e sem levar em consideração as relações entre os nutrientes e seus possíveis desequilíbrios. Diferentes técnicas buscaram superar essas limitações por meio de métodos bivariados e multivariados, como o Sistema Integrado de Diagnóstico e Recomendação (Diagnosis and Recommendation Integrated System - DRIS) e o Diagnóstico Composicional de Nutrientes (Compositional Nutrient Diagnosis - CND). Esses são, no entanto, aplicáveis a dados composicionais, sendo adequados para análise de tecidos, mas de uso limitado para dados de solo. Para atingir alta eficiência é desejável o estabelecimento de valores de referência específicos do local, idealmente ajustados até o nível de cultivar, uma tarefa difícil devido à natureza perene das videiras, exigindo longos e caros experimentos de calibração. A necessidade de calibração é, portanto, considerada uma grande limitação para a aplicabilidade da abordagem de NC/FS. Fazendas comerciais realizam diagnósticos de fertilidade a fim de orientar o manejo da adubação e aumentar a sua rentabilidade. A disponibilidade deste tipo de informação vem crescendo exponencialmente, tornando oportuno o desenvolvimento de técnicas capazes de aproveitá-las para o estabelecimento de valores de referência. A análise de Linha de Fronteira (LF) é uma abordagem adequada para lidar com dados que possuem a grande variabilidade, permitindo o estabelecimento de NC e FS a partir de condições não controladas, demandando apenas a definição de uma função matemática que relacione os teores de nutrientes com as produtividades e a posterior estimativa dos parâmetros a partir de um conjunto de medidas de obtidas em campo. Regressões Segmentadas (RS) permitem atribuir diferentes comportamentos para diferentes segmentos de uma curva, o que confere grande flexibilidade na definição de uma função dose-resposta. Regressões Quantílicas (RQ), por sua vez, possibilitam a exploração de diferentes extratos da variável resposta e facilitam a obtenção de parâmetros condicionado a altas produtividades. A união destes dois recursos pode alavancar as informações já disponíveis, permitindo a estimativa de valores de referência a partir de dados gerados por fazendas comerciais.

Objetivos

O trabalho teve por objetivo principal o desenvolvimento de uma metologia capaz de gerar valores de referência ajustados para condições locais e que dispense a necessidade de se estabelecer experimentos, de modo a contribuir para o aumento da eficiência e sustentabilidade da fertilização das videiras. Deste modo buscou-se, especificamente: estimar níveis críticos e faixas de suficiência de nutrientes em solos de vinhedo e folhas de videira (*Vitis vinifera*) a partir de dados gerados em fazendas comerciais; investigar se estes valores

de referências diferem entre uvas brancas e tintas; avaliar a adequação e as limitações do método proposto.

Metodologia

A abordagem de Linha de Fronteira (LF) utilizando Regressão Quantílica Segmentada Bayesiana (RQSB) foi empregada na determinação dos NC e FS para nutrientes em solos de vinhedos e folhas de videira (*Vitis vinifera*) a partir de dados comerciais. A abordagem LF usando o modelo RQSB foi descrita com detalhes e posteriormente aplicada a um conjunto de dados advindos de uma vinícola da região da Campanha Gaúcha, Rio Grande do Sul, Brasil. O conjunto de dados contém informações sobre 27 cultivares de uva, todas enxertadas sobre SO4 (Selection Oppenheim), com idade média de 19,5 anos, agrupadas em brancas (11 cultivares) e tintas (16 cultivares). As videiras foram cultivadas em solos arenosos e os teores fósforo (P), potássio (K), cálcio (Ca), magnésio (Mg), enxofre (S), cobre (Cu), zinco (Zn), boro (B) e manganês (Mn) disponíveis no solo (0 – 20cm) para 14 safras (n = 539) foram associados às respectivas produtividades. Os mesmos nutrientes, adicionados nitrogênio (N) e ferro (Fe), disponíveis nas folhas (limbo + pecíolo) foram analisados em relação às produtividades de 3 safras (n = 143). As relações entre os rendimentos das videiras e as concentrações de nutrientes no solo ou nas folhas foram descritas pela função linear-platô. Os NC foram definidos como os valores a partir dos quais o incremento de nutriente não se traduziu em aumento de produtividade. Os parâmetros da função foram estimados pela RQSB utilizando métodos de Monte Carlo via Cadeias de Markov e algoritmo de amostragem de Gibbs. As medianas das probabilidades *a posteriori* foram assumidas como valores de NC e FS foram estimadas calculando-se o intervalo contendo 95% de densidade de probabilidade ao redor do NC. A etapa de amostragem utilizou quatro cadeias com 150.000 iterações cada, onde os primeiros 50% foram descartados (*burn-in*) e apenas uma de cada 30 amostras foi retida para estimativa dos parâmetros. Todas as regressões foram condicionadas ao 98º quantil. NC e FS foram estimados para o número total de observações e para observações divididas em uvas tintas e brancas. A convergência da cadeia foi avaliada por meio de gráficos de traços e estatística de Gelman-Rubin. Distribuições uniformes foram usadas para as distribuições *a priori* de todos os NC, definindo igual probabilidade para toda a faixa entre o menor valor e o 95º quantil das variáveis explicativas. A adequação do método foi avaliada por meio de análises de sensibilidade, onde diferentes quantis e diferentes distribuições a priori foram testadas. A ajuste dos modelos foi aferido utilizando valores-p Bayesianos obtidos pela comparação entre o sumário estatístico dos valores observados versus valores simulados pelos modelos ajustados.

Resultados e Discussão

A Regressão Quantílica Segmentada Bayesiana (RQSB) foi eficaz em estabelecer Linhas de Fronteira e estimar níveis críticos (NC) e faixas de suficiência (FS) para nutrientes em solos – P, K, Ca, Mg, S, Cu, Zn, B, Mn – e folhas de videira – N, P, K, Ca, Mg, S, Cu, Zn, B, Mn, Fe – utilizando dados de vinhedos comerciais da Campanha Gaúcha, Rio Grande do Sul. Níveis críticos de Cu no solo, bem como Zn e Mn foliares apresentaram resultados bem acima dos valores de referência regionais, possivelmente devido a contaminações por fungicidas. Estimativas de NC para Ca e Mg no solo, por sua vez, foram significativamente inferiores ao esperado, indicando um possível efeito de camadas inferiores do solo no suprimento destes nutrientes. Os resultados sugerem espaço para aumento de rendimento através da adubação com S. As uvas tintas apresentaram maiores valores de NC para P e Mn no solo e K foliar, em comparação com as brancas, enquanto os resultados de Zn do solo e Mn foliar foram inferiores. As avaliações do modelo indicaram que a RQSB foi altamente sensível à seleção dos quantis, mas pouco afetado por mudanças na distribuição *a priori*. Dados simulados a

partir dos modelos ajustados apresentaram grande dispersão, resultando em aumentando da incerteza sobre as estimativas dos parâmetros, ampliando a FS e dificultando a diferenciação entre os grupos. Os modelos para dados foliares apresentaram valores-p Bayesianos mais adequados, o que pode ser explicado pela menor variabilidade contida neste subconjunto.

Considerações Finais

Neste estudo, os níveis críticos e as faixas de suficiência de nutrientes em solos de vinhedos e folhas de videira foram estimados com sucesso a partir de dados comerciais. Os resultados foram comparáveis a outros estudos sobre nutrição da videira, indicando a relevância da abordagem LF e a adequação da RQSB na obtenção de valores de referência. O método foi capaz de detectar diferenças entre uvas brancas e tintas em relação aos níveis críticos e faixas de suficiência. Melhorias contínuas do método podem levar a uma maior precisão nas estimativas de NC e FS na detecção de diferenças entre os perfis nutricionais de subgrupos. Neste sentido recomenda-se dar prioridade ao desenvolvimento de uma abordagem sistemática para seleção de quantis, devido ao seu grande efeito nos resultados e conclusões, bem como a reparametrização RQSB para permitir inclinações e interceptos variáveis, de modo a particionar a variabilidade dos dados para obter melhores ajustes, bem como a obtenção de parâmetros referentes a subgrupos específicos. Estudos adicionais podem ainda incluir o desenvolvimento de NC e FS para componentes de qualidade relevantes como acidez titulável, pH, sólidos solúveis totais e concentração de flavonoides, bem como considerar os possíveis efeitos da idade das plantas e o papel das camadas mais profundas do solo na disponibilidade de nutrientes para culturas perenes com sistemas radiculares bem desenvolvidos.

Palavras-chave: nutrição vegetal; adubação de frutíferas; videiras; nível crítico; faixa de suficiência.

LIST OF FIGURES

Figure 1 – Number of soil (a) and leaf (b) samples by harvest and grape skin color.....54
Figure 2 – Boundary lines obtained by BSQR using LP functions to describe the relationships between macronutrients in vineyard soils (0 – 20 cm) and relative yields. Vertical red dashed lines represent nutrient CL and vertical shaded rectangles represent nutrient SR (95% HDI). Data points beyond current x-axis scales were omitted to improve visualization.....59
Figure 3 – Boundary lines obtained by BSQR using LP functions to describe the relationships between micronutrients in vineyard soils (0 – 20 cm) and relative yields. Vertical red dashed lines represent nutrient CL and vertical shaded rectangles represent nutrient SR (95% HDI). Data points beyond current x-axis scales were omitted to improve visualization.....60
Figure 4 – Boundary lines obtained by BSQR using LP functions to describe the relationships between macronutrients in grapevine leaves (blade + petiole) and relative yields. Vertical red dashed lines represent nutrient CL and vertical shaded rectangles represent nutrient SR (95% HDI). Data points beyond current x-axis scales were omitted to improve visualization.....61
Figure 5 – Boundary lines obtained by BSQR using LP functions to describe the relationships between micronutrients in grapevine leaves (blade + petiole) and relative yields. Vertical red dashed lines represent nutrient CL and vertical shaded rectangles represent nutrient SR (95% HDI). Data points beyond current x-axis scales were omitted to improve visualization.....62
Figure 6 – Distribution of the relative differences between red and white grapes CL samples for nutrients in soil (a) and leaves (b) generated by BSQR model. Thick and thin lines represent 68% and 95% probability density respectively.....63
Figure 7 – CL estimates (continuous lines) and 95% credibility intervals (dashed lines) at different quantiles for soil macronutrients (0-20cm). Red diamond highlight the chosen 98th quantile.....67
Figure 8 – CL estimates (continuous lines) and 95% credibility intervals (dashed lines) at different quantiles for soil micronutrients (0-20cm). Red diamond highlight the chosen 98th quantile.....68
Figure 9 – Point interval plots of CL estimates for soil macronutrients at different quantiles by grape skin color. Thick and thin lines represent 68% and 95% probability density respectively. 69
Figure 10 – Point interval plots of CL estimates for soil micronutrients at different quantiles by grape skin color. Thick and thin lines represent 68% and 95% probability density respectively.....70

Figure 11 – CL estimates (continuous lines) and 95% credibility intervals (dashed lines) at different quantiles for leaf (blabe + petiole) macronutrients. Red diamond highlight the chosen 98th quantile.....71
Figure 12 – CL estimates (continuous lines) and 95% credibility intervals (dashed lines) at different quantiles for leaf (blade + petiole) macronutrients. Red diamond highlight the chosen 98th quantile.....72
Figure 13 – Point interval plots of CL estimates for leaf (blade + petiole) macronutrients at different quantiles by grape skin color. Thick and thin lines represent 68% and 95% probability density respectively.....73
Figure 14 – Point interval plots of CL estimates for leaf (blade + petiole) micronutrients at different quantiles by grape skin color. Thick and thin lines represent 68% and 95% probability density respectively.....74
Figure 15 – Effects of *prior* choice in CL estimates and number of effective samples evaluated for soil P an K contents regressed on different quantile values. Thick and thin lines represent 68% and 95% probability density respectively. Red dot highlight the 98^{th} quantile.....75

LIST OF TABLES

Table 1 – Descriptive statistics of yield, nutrient concentrations and properties for soil samples (0-20 cm) collected in commercial vineyards from Campanha Gaúcha, Rio Grande do Sul, Brazil.....56
Table 2 – Descriptive statistics of yield and nutrient concentrations for leaf samples (blade + petiole) collected from commercial vines (*Vitis vinfera*) grown in Campanha Gaúcha, Rio Grande do Sul, Brazil.....57
Table 3 – Descriptive statistics for soil sample data subset divided by grape skin color.....57
Table 4 – Descriptive statistics for leaf sample data subset divided by grape skin color.....58
Table 5 – CL and SR of soil macro and micronutrients (0-20cm) for red and white grapes estimated by BSQR model.....64
Table 6 – CL and SR values of leaf (blade + petiole) macro and micronutrients for red and white grapes estimated by BSQR model.....64
Table 7 – Average vineyard soil nutrient contents by harvest. Blue (bold), black (plain) and red (italic) colors indicate nutrient surplus, sufficiency and deficiency, respectively, when compared to estimated CL and SR.....65
Table 8 – Average grapevine leaf (blade + petiole) nutrient contents by harvest. Blue (bold), black (plain) and red (italic) colors indicate nutrient surplus, sufficiency and deficiency, respectively, when compared to estimated CL and SR.....65
Table 9: Gelman-Rubin statistics () and Effective Sample Size (ESS) for slope ($\beta 1$), change point (*cp*) and plateau ($\beta 0$) parameters estimates obtained by BSQR model.....66
Table 10 – Bayesian p-values for multiple test quantities in posterior predictive checks of BSQR model fit applied to soil and leaf nutrients reference values estimates.....76
Table 11 – CL and SR estimated by BSQR for macronutrients in vineyard soils of Campanha Gaúcha, Rio Grande do Sul, Brazil, compared to national and international reports and guidelines.....77
Table 12 –CL and SR estimated by BSQR for micronutrients in vineyard soils of Campanha Gaúcha, Rio Grande do Sul, Brazil, compared to national and international reports and guidelines.....77
Table 13 – CL and SR estimated by BSQR for macronutrients in grapevine leaves (blade + petiole) grown in Campanha Gaúcha, , Rio Grande do Sul, Brazil, compared to national and international reports and guidelines.....78

Table 14 – CL and SR estimated by BSQR for micronutrients in grapevine leaves (blade + petiole) grown in Campanha Gaúcha, Rio Grande do Sul, Brazil, Brazil, compared to national and international reports and guidelines.....78

LIST OF ABBREVIATIONS

AAS	Atomic Absorption Spectrophotometry
ACF	Autocorrelation Function
ALD	Asymmetric Laplace Distribution
B	Boron
BCP	Bayesian Change Point
BL	Boundary Line
BQR	Bayesian Quantile Regression
BSQR	Bayesian Segmented Quantile Regression
Ca	Calcium
CEC	Cation Exchange Capacity
CI	Credible Interval
CL	Critical Level
CND	Compositional Nutrient Diagnosis
cp	Change Point
Cu	Copper
DRIS	Diagnosis and Recommendation Integrated System
ESS	Effective Sample Size
Fe	Iron
HDI	Highest Density Interval
ICP-OES	Induced Plasma Optical Emission Spectrometry
IQR	Interquartile Range
K	Potassium
LP	Linear-plateau
MCMC	Markov Chain Monte Carlo
Mg	Magnesium
MH	Metropolis-Hastings
Mn	Manganese
N	Nitrogen
Na	Sodium
P	Phosphorus
PPC	Posterior Predictive Check
QDPSR	Quadrant Diagram of the Plant-Soil Relationship

QR	Quantile Regression
Q1	First Quartile
Q3	Third Quartile
RS	Rio Grande do Sul
S	Sulfur
SOM	Soil Organic Matter
SR	Sufficiency Range
Zn	Zinc

SUMMARY

1 INTRODUCTION....20

2 THEORETICAL FRAMEWORK....23

2.1 GRAPEVINE NUTRITION....23

2.2 FERTILIZING PRINCIPLES AND NUTRITIONAL DIAGNOSIS....29

2.3 BOUNDARY LINE ANALYSIS....36

2.4 BAYESIAN INFERENCE AND MCMC METHODS....39

2.5 BAYESIAN SEGMENTED QUANTILE REGRESSION....45

2.6 BAYESIAN MODEL ASSESSMENTS....48

2.6.1 MCMC convergence....48

2.6.2 MCMC accuracy....49

2.6.3 Sensitivity analysis....50

2.6.4 Goodness-of-fit....51

3 OBJECTIVES....52

3.1 GENERAL....52

3.2 SPECIFIC....52

3.3 HYPOTHESIS....52

4 MATERIAL AND METHODS....53

4.1 SITE DESCRIPTION....53

4.2 DATASETS....53

4.2.1 Soil samples....53

4.2.2 Leaf Samples....54

4.3 DATA PROCESSING AND MODELING....55

5 RESULTS....56

5.1 EXPLORATORY DATA ANALYSIS....56

5.2 CRITICAL LEVELS AND SUFFICIENCY RANGES....58

5.2.1 Red vs. white grapes....63

5.3 VINEYARD NUTRITIONAL STATUS....65

5.4 MODEL ASSESSMENTS....66
5.4.1 Chain convergence and efficiency....66
5.4.2 Sensitivity analysis....67
5.4.2.1 Quantile selection....67
5.4.2.2 Prior choice....75
5.4.3 Model fit....76
6 DISCUSSION....77
6.1 NUTRIENT REFERENCE VALUES....77
6.1.1 Soil nutrients....77
6.1.2 Leaf nutrients....78
6.2 GRAPEVINE MINERAL NUTRITION....79
6.3 MODEL SUITABILITY....84
7 FINAL REMARKS....86
7.1 CONCLUSION....86
7.2 FUTURE RESEARCH....86

1 INTRODUCTION

Home to the temperate climate zones of the northern hemisphere, members of the genus *Vitis* are thought to comprise about 60 species, spread mostly throughout Asia and North America (ALLEWELDT; POSSINGHAM, 1988; WAN et al., 2008). DNA analyses suggest that approximately 5,000 grapevine varieties are grown commercially worldwide (THIS; LACOMBE; THOMAS, 2006). Despite that, the Eurasian species *Vitis vinifera* L. gave rise to the great majority of modern grape cultivars that are grown for production of table grapes, raisins, juices, wines and brandies, being eventually crossed with American or Asian species for improvements in rootstocks and disease resistance (KELLER, 2010). Analysis of chloroplast DNA indicates that they may originate from at least two geographically distinct populations of *Vitis sylvestris*: one in the Near and Middle East, and the other in a region comprising the Iberian Peninsula, Central Europe, and Northern Africa (ARROYO-GARCÍA et al., 2006).

In 2021, 7.3 million hectares of land were occupied by vineyards world wide. Total production reached 77.8 Mt with over 57% destined to wine grapes, while table and raisins accounted for 36% and 7%, respectively. World wine production in 2021 was estimated in 26 GL, excluding juices and musts (OIV, 2019, 2022). Viticulture has an enormous socioeconomic importance in Brazil, where vineyard harvested area reached over 83 thousand hectares by the year of 2010. In the past decade this area has shrunk roughly 9.7% and yet national grape production have shown consistent increase since 1990, reaching 1.7 Mt in 2021 (IBGE, 2022), indicating that area reduction was compensated by higher grapevine productivity. Brazilian wine production in 2021 was estimated in 0.36 GL, a significant 60% increase compared to 2020 and the largest volume recorded since 2008. Wine consumption reached 0.41 GL, the highest since 2000, making Brazil the second largest market in South America after Argentina (OIV, 2022). However, if only fine wines are considered – a higher value-added market – 86 of every 100 bottles consumed by brazilians in 2019 were imported (MELLO; MACHADO, 2020), revealing the enormous growth potential for national wineries.

Brazil is the only country in the world where three wine-growing regions with different climatic and pedological conditions can be observed (PEREIRA et al., 2020): traditional, in the South and Southeast regions of Brazil; tropical, in the Northeast (São Francisco valley); and winter wines, from high altitudes (> 700 m) in the Southeast, Midwest and Northeast regions (TONIETTO et al., 2020). National wine market size in 2019 was estimated in R$ 20.3 billion (~US$ 4 billion), employing around 200 thousand people (MELLO; MACHADO, 2020). Regions that produce wines and juices have the opportunity to

develop quickly, as they're able to attract investments in complementary sectors, such as wine tourism and gastronomy, generating additional employment and income that are of especial importance where small family farms are predominant. An example is the municipality of Bento Gonçalves, in Serra Gaúcha region, Rio Grande do Sul state (RS), which has appropriate infrastructure for business, fairs, congresses and wine tourism and guested around 1.67 million visitors in 2019 (PEREIRA et al., 2020). Despite the potential of other Brazilian regions for growth of wine sector, the south is traditionally home to most of country's vineyards (~62.5%), wherein RS accounts for 90% of country's total wine and juice production, as well as 85% of sparklings (MELLO; MACHADO, 2020; PEREIRA et al., 2020)

The production of vines is governed by a series of factors which can be of uncontrollable (*e.g.* climate), partially controllable (*e.g.* irrigation) or controllable (*e.g.* management) nature. High yields require a regular and balanced supply of nutrients, thus efficient fertilization is one of the most effective tools to increase profitability of fruit trees (BRUNETTO et al., 2015). However, without the right information to properly manage fertilization and fearing insufficient yields, farmers may use inputs beyond actual needs. This represents not only an unnecessary expense but may also lead to reduced fruit quality (BRUNETTO et al., 2015; CIOTTA et al., 2016; KODUR, 2011; PICCIN et al., 2017; STEFANELLO et al., 2021a), toxicities or deficiencies of other elements (MARSCHNER, 2012; MILOŠEVIĆ; MILOŠEVIĆ, 2020). Proper fertilizer rates and application practices minimize the adverse effects of nutrient movement out of the fields, reducing environmental pollution risks (GATIBONI et al., 2015a; LASSALETTA et al., 2014; SCHMITT et al., 2014), as well as overall production costs, increasing the profitability and sustainability of the sector and ensuring competitiveness (MEDICI; CANAVARI; TOSELLI, 2020).

Fertilizing management is guided by nutritional assessments, assisted by either soil or plant tissue analysis (BRUNETTO et al., 2020; BRUNETTO; MELO; KAMINSKI, 2011). Recommendations can be made by comparing diagnostic sampling results with reference values called critical levels (CL) or sufficiency ranges (SR) (ULRICH; HILLS, 1967) that represent the quantities from which additional inputs yields very low to no increase in desired response (MUNSON; NELSON, 1990). These reference values are historically established by running experimental trials that correlate nutrient levels with response variables such as yield (ROZANE; PARENT; NATALE, 2015). To attain high efficiency in fertilizing management CL and SR should be developed for site (BETEMPS et al., 2020; DE PAULA et al., 2020; ROZANE et al., 2020) and cultivar (HERNÁNDEZ-VIDAL et al., 2021; PARENT et al.,

2013; STEFANELLO et al., 2021a) specific conditions, a difficult task to accomplish due to the perennial nature of grapevines, requiring long and expensive calibration trials (ROZANE; PARENT; NATALE, 2015).

Data generated in commercial vineyards contains valuable information that, combined with appropriate statistical techniques, can be leveraged to establish or update nutrient reference values (LARK et al., 2019). The limiting effect of an independent variable (*e.g.* nutrient concentrations) on some response variable (*e.g.* yield) under uncontrolled growing conditions can be described by a Boundary Line (BL) (WEBB, 1972),, which considers that the best performance in a population is described by a line at the edge of any data body (WALWORTH; LETZSCH; SUMNER, 1986). The development of a BL comprises the definition of a mathematical function f(X; θ) expressing Y as a function of X and of a set of parameters θ, which can be estimated from a set of field measurements (MAKOWSKI; DORÉ; MONOD, 2007; WEBB, 1972). As nutrient availability increases, yield is expected to increase up to a point where additional inputs does not translate into higher response, defining thus the CL. Linear-plateau function (LP) is a type of regression with two segments separated by a change point (MUGGEO, 2003) that can be used to model such behavior (MAKOWSKI; WALLACH; MEYNARD, 2001). Quantile regressions (QR) (KOENKER, 2005) allow estimation of change rates in all parts of the distribution of the response variable (CADE; NOON, 2003), a feature of great convenience for estimating BL parameters (θ) conditional on high yield expectations (MAKOWSKI; DORÉ; MONOD, 2007). Recently developed Bayesian Segmented Quantile Regression (BSQR) (LIANG et al., 2021) combines the flexibility of QR with the ability to detect change points, enabling the use of LP function under the Bayesian framework. In the Bayesian approach, the unknown parameters of a model are treated as random variables that have a probability distribution (SPADE, 2020). As such, Bayesian data analysis provide an explicit distribution of the credibility across these parameter values, so that inference can be drawn (KRUSCHKE; LIDDELL, 2018).

This study aims were thus to (1) establish CL and SR for nutrients in soils and grapevine leaves based on boundary lines built using data from commercial vineyards and BSQR; (2) investigate whether these reference values differ between white and red grapes and; (3) assess the suitability and limitations of proposed approach.

2 THEORETICAL FRAMEWORK

2.1 GRAPEVINE NUTRITION

Grapevines can be productive for several decades before replacement is needed, but for yields to be proper in size and quality, adequate amounts of water, nutrients, solar radiation and carbon dioxide (CO_2) are required. Some of these factors are out of farmer's control while others, such as soil chemical properties and levels of macro- and micronutrients, can be managed and have decisive impact on vineyards production (KRZYSZCZAK et al., 2018; TYLER; OLSSON, 2001; ZIA et al., 2006). Mineral nutrition is one of the most important factors in fruit production, especially in high-density orchards (EBERT, 2009), as minerals are responsible for several functions in plants, such as tissue constitution, enzymatic activation and osmotic regulation of membranes, playing also important role in energetic processes (FAUST, 1989; MARSCHNER, 2012). The ultimate goal is to achieve balanced nutrition, as both lack and excess of nutrients can compromise yields and quality of grapes, affecting its appearance, color, flavor, size, aroma, post-harvest storage capacity and tolerance to pests and diseases (BRUNETTO et al., 2015; ROZANE; PARENT; NATALE, 2015), which is later reflected in the characteristics of the resulting must and wines (BRUNETTO et al., 2007; CONSIDINE; FOYER, 2015; MPELASOKA et al., 2003; SKINNER et al., 2019).

Among the macronutrients, nitrogen (N) is the element that plants require in largest amount, being the most abundant soil-derived nutrient in grapevine (BELL; HENSCHKE, 2005). It is a component of the plant cell as part of amino acids molecules, proteins, nucleic acids, and other organic compounds (SOUZA; FERNANDES, 2006). Yet, N supply to vines should be carried out with caution, due to its effects on vegetative growth, yield and chemical composition of grapes, must and wine (BELL; HENSCHKE, 2005; BRUNETTO et al., 2007). High rates of N can stimulate vegetative growth, reducing penetration of solar radiation into plant canopy, favoring the incidence of fungal diseases on leaves and fruits (THOMIDIS et al., 2016), reducing the number of pollinated flowers and berries per bunch (BRUNETTO et al., 2015). In addition, yield increase provided by N can correlate negatively with fruit quality, resulting from a dilution effect on berry compounds (SANTESTEBAN; MIRANDA; ROYO, 2011; SOFO et al., 2012; STEFANELLO et al., 2021a), potentially impairing wine quality parameters such as aroma (VILANOVA et al., 2019). Overfertilization of N can delay leaf senescence, plant dormancy and ripening of clusters, reduce the activity of enzymes that regulate the synthesis of some important compounds such as anthocyanins (that colors must and wine), total polyphenols and soluble solids in grape must, as well as increase total titratable acidity (BRUNETTO et al., 2007, 2009; DUCHÊNE; SCHNEIDER;

GAUDILLÈRE, 2001; KELLER; POOL; HENICK-KLING, 1999). On the other hand, N-deficient plants show decreased growth (dwarfism), reduced leaf size, chlorosis, shortening of internodes, poor development of root system and low fertilization of clusters, which may lead to small fruits with early maturation (BRUNETTO et al., 2020).

Phosphorus (P) is a nutrient of great physiological importance, being the second most limiting nutrient to plants, with impacts on cell membrane formation, carbohydrate metabolism, protein synthesis, photosynthesis, respiratory sugar metabolism and energy storage and transfer (ARAÚJO; MACHADO, 2006; MARSCHNER, 2012). Deficiency of P is marked by delayed growth of plants and roots, delayed flowering, early leaf fall, inhibition of sprouting of lateral buds, and decrease in number of fruits (BOTELHO; MÜLLER, 2020; BRUNETTO et al., 2015). Grapevines deficient in P exhibit red-violet coloring in marginal and interveinal leaf areas (especially in old leaves) and red coloring in the petioles and in the primary and secondary veins of the old leaves. Excessive P, in turn, delays ripening of clusters and can reduce Fe, Cu and Zn availability (BALDI et al., 2018a, 2018b; BRUNETTO et al., 2020; HE et al., 2021; LONERAGAN; WEBB, 1993).

Potassium (K) is the most abundant cation in the cytoplasm of plant cells and plays a role in the activation of enzymes, protein synthesis, stomatal movement, photosynthesis and cell extension. It is also the main cation involved in cellular turgor and the maintenance of cellular electric neutrality (MARSCHNER, 2012; SARDANS; PEÑUELAS, 2015; TAIZ; ZEIGER, 2017). It corresponds to roughly 80% of cations present in grape berry (MPELASOKA et al., 2003; ROGIERS et al., 2017), being the most exported macronutrient and, thus, highly demanded by grapevines. Nevertheless, excessive availability of K in the soil can result in equally high levels of it in berries and, consequently, in the must, causing a reduction of sugars, impairing its fermentation (ROGIERS et al., 2017), raising the pH (WALKER; BLACKMORE, 2012) and decreasing the titratable acidity (CIOTTA et al., 2016; KODUR, 2011), which increases susceptibility to must and wine oxidation (MPELASOKA et al., 2003). Furthermore, high levels of exchangeable K in the soil can causes stem desiccation, due to lower Ca and Mg uptake by the grapevine (DALBÓ et al., 2015; MPELASOKA et al., 2003), leading to Mg deficiency in vine leaves and physiological disturbances resulting in rachis desiccation and decreased productivity (HALL; BONDADA; KELLER, 2011). Grapevines K deficiency can eventually occur, especially in alkaline soils where Ca and Mg can be absorbed at higher levels (HANNAN, 2011).

Calcium (Ca) has an important function in the structure and permeability of cell membranes in cell division. Ca regulates the uptake of other cations, due to its ionic charge

(TAIZ; ZEIGER, 2017) and it can cross-link cell wall pectins and fruit cell wall (which is pectin rich), determining the physical and structural properties of the fruit. Thus, Ca is of paramount importance to ensure slow ripening and longer shelf life (KANGUEEHI, 2008). Fruit cell wall layers also play a role in pathogen susceptibility and spraying fruits with Ca can improve their integrity and enhance disease resistance (HOCKING et al., 2016). Grapevines cultivation is often preceded by liming practices to ensure proper soil pH and base saturation and the application of limestone acts as a source of Ca that usually guarantees its supply. Yet, low pH and high availability of K and Mg can induce lack of Ca in plants. Ca deficiency causes new leaf margins to cup and interveinal and marginal chlorosis, followed by necrosis of blade margins. The availability of B, however, helps the translocation of Ca in the plant and for the fruits (BOTELHO; MÜLLER, 2020).

Magnesium (Mg) is the main constituent of the chlorophyll molecule that plays an important role in the enzymatic activation of ribulose diphosphate carboxylase/oxygenase (rubisco) (MALAVOLTA, 2006; TAIZ; ZEIGER, 2017). It is required by fruit plants in quantities lower than Ca, and its uptake is reduced by competition with cations such as K, Ca, and Mn (MARSCHNER, 2012). Leaves of Mg-deficient grapevines have yellowish margins, which are directed toward their center, while the veins remain green. Mg deficiency may cause reduced sugar content in the must and stem desiccation, due to the imbalance of the K/Mg ratio (BRUNETTO et al., 2020).

Sulfur (S) is incorporated into amino acids, proteins and coenzymes, and is also necessary for the synthesis of other compounds, including coenzyme A and vitamin B (TAIZ; ZEIGER, 2017). Deficiency of S causes delayed growth and chlorosis in plants which, although similar to N deficiency, occurs first in the youngest leaves of plants (MARSCHNER, 2012; TISDALE et al., 1993) whereas N is translocated from old to new leaves. Deficiency of S affects both yield and fruit quality (SCHNUG, 1993; ZHAO; HAWKESFORD; MCGRATH, 1999), but the application of S fertilizers is effective in remediating these problems. Sulfur uptake by the roots of the plants occurs almost exclusively in the form of sulfate ion (SO_4^{-2}) which, in well-drained soils, is predominantly adsorbed to clay and oxides or bound to the soil organic matter (SOM). In highly industrialized areas the S requirement of plants is often met fully or to a substantial degree by atmospheric sulfur dioxide (SO_2) pollution and deposition. This element can be toxic at high concentrations though (TISDALE et al., 1993).

Copper (Cu) is a key micronutrient involved in photosynthesis, respiration, hormone signaling, and antioxidant activity (MARSCHNER, 2012; YRUELA et al., 2000). Large

amounts of Cu-based compounds are used to control fungal diseases in vineyards (BRUNETTO et al., 2017; CASALI et al., 2008; MIOTTO et al., 2014), which leads to Cu accumulation in plant leaves and soils (TIECHER et al., 2016, 2017). Excessive soil Cu can damage cell membranes in the roots (DE VOS et al., 1989) impairing its growth, leading to reduced exploration of the soil with significant decrease in the uptake of nutrients and water, reflected in indirect symptoms, such as the reduction of branch growth and the chlorosis (MARTINS et al., 2014), eventually resulting in plant death (KOPSELL; KOPSELL, 2006; MARSCHNER, 2012), especially in young grapevines (MIOTTO et al., 2014). Grape cells exposed to excess of Cu rely on plasma membrane and vacuolar transport for detoxification (MIOTTO et al., 2014) and adult grapevines during the productive season do not exhibit visual symptoms of toxicity caused by Cu, as they can uptake and store it in perennial and annual organs (LAI; JUANG; CHEN, 2010) mostly in roots (BALDI et al., 2018b).

Zinc (Zn) deficiency affects plant development and its symptoms include stunted growth, shortened internodes and petioles and small malformed leaves (ROBSON, 1993). In grapevines it is associated with reduction of berry clusters (BRUNETTO et al., 2020), being the most widespread micronutrient deficiency of raisin vineyards (CHRISTENSEN; PEACOCK, 2000). It should be noted, however, that Zn is generally supplied to grapevines due to application of Zn-based fungicides, which can lead accumulations in soil and plant stress (BRUNETTO et al., 2014; TIECHER et al., 2017). In soils with low pH, Zn solubility and uptake is in increased and so is the potential for Zn phytotoxicity, with consequences on chlorophyll biosynthesis and other biochemical reactions (ROBSON, 1993). Excess Zn in the root system can also inhibit root lengthening, and the roots may have dark coloring, followed by necrosis (TIECHER et al., 2018).

Iron (Fe) is directly involved in grapevine plant growth and carbon assimilation processes and its deficiency can significantly decrease leaf CO_2 exchange rate, chlorophyll photosynthetic efficiency, leaf area, dry matter accumulation and suppress other physiological processes, resulting in increased fruit abscission (BERTAMINI; NEDUNCHEZHIAN, 2005). Iron deficiency–induced leaf chlorosis is a common nutritional disorder in grapevines, especially when cultivated in soils with alkaline pH or high in lime, which reduces plant growth and productivity (TAGLIAVINI; ROMBOLÀ, 2001; TECCHIO; TERRA; MAIA, 2012). In acidic soils, severe Fe-deficiency chlorosis can be caused by excessive Zn (ROBSON, 1993). Mild deficiency of Fe, however, can positively change wine quality due to improvement in traits such as soluble solids, pH, anthocyanins and resveratrol (BRUNETTO

et al., 2020). Symptoms of Fe toxicity include bronzing of the leaves and browning of the roots (SIQUEIRA-SILVA et al., 2012).

Boron (B) is considered to be essential for actively growing regions of plants, such as root tips, new leaf and bud development, playing important role in structural and functional integrity of plasma membranes (AHMAD et al., 2009) and in bonding cell wall components (MATOH, 1997). Deficiency of B is associated with shortening of internodes, death of bud tips, interveinal chlorosis of older leaves and reproductive development impairment, having negative effect on flowering, growth of pollen tube, fruit set and seed set (CHRISTENSEN; PEACOCK, 2000; MOUSAVI; MOTESHAREZADEH, 2020). Symptoms of B toxicity include the formation of a “shell” on new shoots, followed by brown necrotic spots on the leaf margin and yellow stripes between the veins (BRUNETTO et al., 2020). Boron is considered highly immobile in most plants and accumulates in leaves due to transpiration flow (NABLE; BAÑUELOS; PAULL, 1997), especially in leaf edges where necrotic specks may also develop along the leaf margins. Although essential, B can become toxic in excessive amounts and grapevines are classified as sensitive to boron excess (CHRISTENSEN; KASIMATIS; JENSEN, 1978), as plants can only tolerate a narrow range of concentrations within their tissues.

Manganese (Mn) acts as an activator for about 35 enzymes in plants, notably those involved in phenylpropanoid metabolism pathways, leading to the synthesis of various secondary metabolites (*e.g.* flavonoids, lignin) and auxin (BURNELL, 1988). Mn can induce some defense responses (YAO et al., 2012b) and improve flavonoid content in grape berry skins (CHEN et al., 2020). In fact, Mn content in soil is reported to have close relationship with catechin flavonoid content in wine grapes (ACUÑA-AVILA et al., 2016). Furthermore, recent studies suggests that Mn plays a role in enhancing plant’s resistance to water stress (GHORBANI et al., 2019). Many biochemical reactions that involve Mn cannot function properly in Mn-deficient plants. Deficiency often occurs in alkaline soils and interveinal chlorosis on young leaves is the most obvious symptom of severe Mn shortage. However, in recent years, hidden Mn deficiency (with no visible symptoms) has become widespread, and this has affected the yields and quality of many crops, which may lead to substantial economic losses. Grapevines are considered particularly susceptible to Mn deficiency (ALLOWAY, 2008).

One of the main objectives plant mineral nutrition studies is to increase productivity with quality through the efficient management of fertilization. Fertilizer additions contribute to the nutrient stocks held by the soil, from which plants obtain most of their needs, rather

than directly from the added fertilizer (COOKE, 1982; STOCKDALE et al., 2013). However, the evident positive response of plants to fertilization has triggered widespread use of fertilizers with little attention to actual plant needs (BRUNETTO et al., 2015). N fertilization along the grapevine cycle, for instance, increases the mineral N content in soils (especially nitrate) (ROGERI et al., 2015), even in vineyards, which are highly demanding. Part of nitrate may be absorbed by the grapevines, but because it forms outer sphere complexes with functional groups of soil particles, it can be very mobile in the soil profile. N may be lost through leaching and surface runoff (NAPOLI et al., 2017), ammonia volatilisation or nitrous oxide emissions (CAMERON; DI; MOIR, 2013; NAPOLI et al., 2017), causing decreased soil fertility, atmospheric pollution and eutrophication of the water bodies.

In addition, excessive application of N can lead to higher susceptibility to fungal disease, which may result in successive fungicide applications and the consequent increase in Cu and Zn bioavailability in vineyard soils, contributing to environmental contamination (BRUNETTO et al., 2014, 2017; FERNÁNDEZ-CALVIÑO et al., 2008; MIRLEAN; ROISENBERG; CHIES, 2007). High Cu and Zn concentrations can affect soil biological activities (DUMESTRE et al., 1999) and be toxic to grapevines and other existing plants within the vineyards (BRUN; LE CORFF; MAILLET, 2003; CHAIGNON; HINSINGER, 2003), damaging the entire production system. This toxicity is maximized in sandy, acidic soil with low soil organic matter, conditions found in various sites where grapevines are grown (TIECHER et al., 2017, 2018).

Phosphorus applied via fertilizers in vineyard soils tends to be adsorbed to the reactive particles of the colloidal fraction, especially Fe and Al oxides (BARROW, 1999; SPARKS, 2003). However, continuous P fertilization, without technical criteria and above the exportation rates may result in soil P accumulation (PAVINATO et al., 2020), increasing the likelihood of P loss to water (GATIBONI et al., 2015b; SCHMITT et al., 2014), where it can cause the proliferation of algae. P losses, either of inorganic or organic forms, can occur in vineyard soils both by surface runoff (NAPOLI et al., 2017; RAMOS; BENITO; MARTÍNEZ-CASASNOVAS, 2015) and leaching (ESTELLER et al., 2009).

Thus, there is a great demand for methodologies to help winegrowers with soil amendments and fertilizer management in order to achieve a production of grapes, must and wine in satisfactory quantities and qualities (PICCIN et al., 2017), increasing profitability, reducing negative impacts on the environment and providing quality products to the consumer, meeting the principles of sustainable fruit production (MEDICI; CANAVARI; TOSELLI, 2020).

2.2 FERTILIZING PRINCIPLES AND NUTRITIONAL DIAGNOSIS

By the year of 2018, acquisition of fertilizers and lime corresponded, on average, to 38% of the expenses with inputs and about 16% of total maintenance costs of productive vines (4 years and older) (AGRIANUAL, 2019). Brazil imports nearly 81% of total fertilizer used in agriculture (ANDA, 2021) being thus highly vulnerable to international price fluctuations. Indeed, the Russian invasion of Ukraine in 2022 triggered a supply shock that led to an astonishing increase of 288% in fertilizer prices in the country between 2020 and 2022 (CNA, 2022), highlighting the urge to increase resource use efficiency.

The aim of fertilizing recommendations is to attain adequate soil nutrient levels, capable of properly nourishing plants while rationalizing the use of inputs, leading to profitable yields with least negative environmental impacts. An early proposal of a fertilization recommendation system developed for southern Brazil consisted in dividing the landscape in physiographic regions and establishing reference values (critical levels) for soil analysis in each of them (MOHR, 1950). The use of soil sampling for recommendation purposes became widespread in the 1960s. In the 1970s the system was sensibly improved and recommendations were then based on crop type, with fertilization further divided in corrective and maintenance applications, where the underlying philosophy was to “fertilize the soil”. During the 1980s there were restrictions on agricultural credit, making it difficult to correct soil fertility in a single application, so a mixed system, based on correction and replacement (or restitution) was established. Gradual increment of soil P and K was recommended, aiming to achieve reference levels over three crops or years, shifting the philosophy to “fertilizing the crop”.

In the beginning of 2000s techniques such as irrigation, no-till, protected cultivation, hydroponics, organic farming and crop-livestock integration where already consolidated and applied for a diverse set o crops, including fruits, flowers, ornamental, medicinal and aromatic species, which lead to a new update in the recommendation system. The new version supported correction, maintenance and replacement fertilization adjusted as a function of expected yield and included various new crop types, providing recommendation for double cropping, hydroponics and protected cultivation for different production systems. In mid 2010s the most recent version of the “Manual de Calagem e Adubação para os Estados do Rio Grande do Sul e Santa Catarina” was released to catch up with the continuous intensification of the fields and the availability of new technology that allows high resolution soil maps and application of inputs at a variable rate, making precision agriculture a reality in many farms (CQFS-RS/SC, 2016).

Fertilization for grapevines is currently divided into correction, growth and maintenance applications. Correction fertilization aims to increase nutrient availability to sufficiency levels prior to the planting of seedlings, typically P, K and, due to the high demand and the characteristics of Brazilian the soils, B (MELO, 2003). After vineyard establishment, growth fertilization takes place, being N the most important nutrient of this phase. Maintenance fertilization replenishes the nutrients that left the vineyard through harvest exportation or losses. Macro and micro nutrients are then applied to soil or leaves depending on specific conditions or management system, generally guided by plant nutrition assessments (BRUNETTO et al., 2020; BRUNETTO; MELO; KAMINSKI, 2011) reliant on both soil and tissues analysis (CQFS-RS/SC, 2016).

The traditional soil analysis approach is based on the assumptions that the chemical extractants simulate the root system acquisition of soil nutrients and that soil sampling represents the soil portion explored. For perennial crops such as grapevine, however, this may not always hold true, as root systems can grow beyond usual sampling layer and reach over a meter deep (BASSOI, 1998), although small and shallow root systems can occur in high plant density (EBERT, 2009) and in drip irrigated vineyards (BASSOI, 1998). Moreover, traditional methods require sample preparation with subsequent analysis in laboratory (*i.e., ex-situ*). In such arrangements the nutrient contents of samples can be accurately determined but may not reflect the actual availability under field conditions, since nutrient availability is greatly affected by soil properties such as pH, cation exchange capacity (CEC) and organic matter (SOM) (SPARKS, 2003), root colonization by mycorrhizae (BALZERGUE et al., 2011), interactions between nutrients (GRANSEE; FÜHRS, 2013; HE et al., 2021), among others.

Most of these conditions are independent and can individually affect the availability of nutrients, whilst their combined effects result in the actual soil nutritional capacity (MILOŠEVIĆ; MILOŠEVIĆ, 2020). As a result, the dynamics of nutrient uptake, plant growth and its response to climate and management are not fully captured by a soil sample (MALAVOLTA, 2006; MOURÃO FILHO, 2004; ROZANE; PARENT; NATALE, 2015). Hence, despite being globally used to estimate nutrient availability, these limitations, along with the nutritional stability acquired by adult grapevines (MARSCHNER, 2012) may hinder the relationship between soil nutrient concentrations with culture growth and yield parameters. Sensor systems for mapping soil fertility is currently an active field of research that have the potential to circumvent the limitations of traditional sampling methods, delivering a more realistic determination of soil nutrition capacity under field conditions in

the near future (MOLIN; TAVARES, 2019). Nevertheless, the considerable amount of data obtained by traditional methods can and must be leveraged to improve fertilizer recommendations through innovative data analyses techniques (KYVERYGA et al., 2013; MAKOWSKI; DORÉ; MONOD, 2007; PADARIAN; MINASNY; MCBRATNEY, 2020; THEOBALD; TALBOT, 2002).

Analysis of plant tissues have proven to be a useful guide to nutrient management and typically aims to detect nutritional problems that are not expressed visually, to identify the cause of the visual symptoms observed in the field, to verify if a given nutrient was absorbed by the plant, to identify interactions between nutrients, to characterize the specific cause of a nutritional problem, and, along with soil analysis, to guide a rational soil fertilization and correction programmes (CARMO et al., 2000). It is considered a more direct method of plant nutritional status evaluation and is often more closely related to crop performance than soil analysis (VAN MAARSCHALKERWEERD; HUSTED, 2015). Any shortage in soil nutrient supply will be reflected in different parts of the plant, but the freshly mature leaves (petioles, blades or complete leaves) are considered to be the center of physiological activities that better reflects crop nutritional status, constituting the main plant sampling material (ROZANE; PARENT; NATALE, 2015). In grapevines, leaf collection is suggested at full flowering or at berry veraison (CQFS-RS/SC, 2016). The results of leaf analysis can be interpreted by several methods, especially univariate ones such as critical level or sufficiency range (CL/SR), bivariate methods such as the Diagnosis and Recommendation Integrated System (DRIS), and multivariate methods such as the Compositional Nutrient Diagnosis (CND) (ROZANE; PARENT; NATALE, 2015).

The usual method for analysis interpretation presupposes a comparison between the nutrient concentrations obtained through leaf sampling with reference values, often called Critical Levels (CL) or Sufficiency Ranges (SR) (ULRICH; HILLS, 1967) which describes the levels above which the probability of economic return of additional nutrient supply is small or none (MUNSON; NELSON, 1990). These methods are often criticized as they evaluate nutrient concentration in isolation and only for a certain phenological stage (CARVAJAL; ÁLVAREZ; GUTIÉRREZ, 2021). In fact, the validity of nutrient assessments using CL/SR seems to be affected, to a large extent, by nutrient interactions and plant age (BATES, 1971; PARENT; DAFIR, 1992), therefore, to monitor plant nutritional status would require reference values for several different stages and, although simple in theory, this procedure is of difficult application. For instance, the precise definition of plant phenological stage under field conditions is not always straightforward and the influence of scion-cultivars

combinations in the nutrient concentration in a given stage is still largely unknown (MOURÃO FILHO, 2004).

DRIS is another method used to assess crops nutrient status. By taking into account dual interactions expressed as nutrient ratios (*e.g.* P/K), DRIS (BEAUFILS, 1973) is considered an improvement in diagnosis compared to CL/SR approach, generally showing greater diagnostic efficiency (WALWORTH; SUMNER, 1987). It conveys results of plant nutritional diagnosis through indices in a continuous numeric scale, which represent the effect of each nutrient in the nutritional balance of the plant, where positive or negative values indicate excess or deficiency, respectively. The closer to zero are the indices for all the nutrients, the closer the plant will be to the adequate nutritional balance (MOURÃO FILHO, 2004). The use of DRIS in grapevine nutrition is not new (SCHALLER; LÖHNERTZ, 1985) and the method has been widely used in Brazil, aiding fertilization of many fruit crops such as atemoya (SANTOS; ROZANE, 2017), banana (PEREIRA et al., 2015; RODRIGUES et al., 2021), cactus pear (TEIXEIRA et al., 2019), cocoa (OLIVEIRA et al., 2019), conilon coffee (PARTELLI et al., 2018), guava (SOUZA et al., 2015), orange (CAMACHO et al., 2012; DIAS et al., 2013; RAGOZO; LEONEL; TECCHIO, 2014), pitaya (ALMEIDA et al., 2016), and, unsurprisingly, grapes (MELO; ROZANE; BRUNETTO, 2018; TEIXEIRA et al., 2015; TERRA et al., 2007).

In general, DRIS has some advantages such as easy interpretation, ability to rank nutrients from the most deficient up to the most excessive and to detect cases of yield limitation due to nutrient unbalance, rather than nutrient insufficiency (MOURÃO FILHO, 2004). An additional advantage of DRIS, acknowledged by some authors but rebutted by others, is that it is generally not very sensitive to tissue aging (WALWORTH; SUMNER, 1987). It has, however, some limitations, such as the inability to exclude outliers using mathematical procedures, the arbitrariness in selecting reference subpopulations, the incompatibility with multivariate analysis methods and the dependence between ratios that may lead to inadequate diagnoses (PARENT, 2011). Indeed, the definition of reference subpopulation in DRIS is vague, since no specific criteria to partition high and low productivity groups was originally proposed (WALWORTH; SUMNER, 1987). As a result, the reference population definition is still largely subjective (ROZANE; PARENT; NATALE, 2015) and suggestions include using 10% of high-yielding specimens in the database (LETZSCH; SUMNER, 1984), 80% of maximum productivity (MALAVOLTA, 2006), population mean ± 0.5 standard deviation (SILVA et al., 2005) or simply the population mean (SERRA et al., 2010).

DRIS provides a single correction factor for any nutrient given information about another nutrient and indices are computed as the mean value of these dual ratio functions, which are derived independently (PARENT; DAFIR, 1992). Nutrient contents in tissue, however, constitute compositional data, that is, vectors whose components are the proportion or percentages of some whole. Their peculiarity is that their sum is constrained to the be some constant, equal to 1 for proportions, or 100 for percentages (AITCHISON, 1982). DRIS fails to recognize this dependence structure and, therefore, may convey spurious correlations that obscure results in biology (ROZANE; PARENT; NATALE, 2015).

CND expands the DRIS concept from a bidimensional to a multidimensional space using tools of compositional data analysis (AITCHISON, 1982), eventually increasing diagnostic consistency by involving larger number of elements (HOLLAND, 1966). The CND (PARENT; DAFIR, 1992) is able to recognize high-order interactions between nutrients, which CL/SR fails to account for and it is only partially addressed by DRIS. Since it diagnoses one “nutrient imbalance” rather than one crude component at the time, the interpretation is as simple as, but theoretically more robust than CL/SR and with greater potential for improving tissue diagnosis (PARENT; DAFIR, 1992). In Brazil, CND was applied in studies on nutrition of guava (ROZANE et al., 2012), mango (PARENT et al., 2013), banana (DE LIMA NETO et al., 2022) and grapevines (ROZANE et al., 2020).

Despite highly valuable, leaf analysis is still limited as a tool to diagnose nutritional status, since relationship between leaf nutrient content and yield may be weak. For instance, fertilization of grapevines with increasing N doses leads to increased N content in leaves which do not necessarily translate into higher grape yields, probably as a result of partial N compartmentalization in cell organelles (BRUNETTO et al., 2007, 2008). Similar behavior can occur with P, K (BRUNETTO et al., 2020) and Mn (YAO et al., 2012a) whenever absorption surpasses physiological demand. Another drawback to leaf analysis is that results can seldom be used to the benefit of the plant-population from which the sample was taken, because greatest part of the growing season has already passed (SCHALLER; LÖHNERTZ, 1985). Moreover, different diagnostic methods based on leaf samples fail to provide direct information on the amount of nutrients to be supplied to plants (WADT, 2011), acting as an indirect assessment of nutrient supply.

It would be more appropriate to interpret the results of plant tissue analysis in combination with those determined by soil analysis, however, systematic studies on the relationships between leaf chemical analysis, soil nutrient availability and yield are lacking (SOUSA et al., 2018). The Quadrant Diagram of the Plant-Soil Relationship (QDPSR)

(SOUSA, 2016) was developed as an attempt to address the issue. In this method the data is plotted in a Cartesian system divided into four quadrants. Two of theses quadrants are considered to convey two types of errors: false positive, when nutrient accumulates in plant tissues due to low yields; and false negative, when very high yields lead to nutrient dilution effects. Accordingly, these two quadrants are ignored and only data points in the remaining quadrants are used to model plant-soil relationship, improving reliability of system diagnosis by eliminating possible biases (SOUSA, 2016).

The QDPSR has been recently applied to obtain optimal leaf nutrient concentrations for coffee (SOUSA et al., 2018), banana (DEUS et al., 2018) and eucalyptus (NETO et al., 2020) based on estimated soil CL. Application of the method in the reverse way, that is, to obtain soil CL from leaf data hasn't been reported thus far. Concurrent sampling of soil and leaves is required for establishing the soil-plant relationship, which is a limitation of the method, given that it is not common practice out of experimental or research setups. Also, the assumption of direct relationship between current soil nutrient availability and pending production does not always hold for perennial crops, as nutrient translocation occurs within plants (SCHREINER, 2016; SCHREINER; SCAGEL; BAHAM, 2006).

Reasonably, one can realize that, although, some soil properties can be considered compositional, such as texture (sand + silt + clay) and subcompositions like base saturation (Ca + Mg + K + Na), most of essential nutrients in soil are considered unconstrained, making unsuitable the application of CND and DRIS to obtain reference values. On the other hand, the need for calibration is regarded as a major limitation for the applicability of the CL/SR approach, a disadvantage compared to CND and DRIS, which are considered less dependent on it (WADT, 2011). In order to calibrate nutrient applications and secure maximum economic return on the long run, nutrition studies in fruit crops must be conducted in long-term experiments where genetic and environmental characteristics and their interactions with nutrients are controlled, often restricting the use of such diagnostics beyond the experimental conditions (ROZANE; PARENT; NATALE, 2015) Yield, for instance, is affected by approximately 52 production factors and the nutritional aspect is only one of them (TISDALE et al., 1993). Given the sheer effect of non nutritional factors on productivity, it is reasonable to also assume that reference values will hardly be universally applicable (BATAGLIA; SANTOS, 2001; OLIVEIRA et al., 2019; RODRIGUES et al., 2021; SILVA et al., 2005) and must be updated regularly because new genetic material and management or cultivation techniques are being constantly introduced (ROZANE; PARENT; NATALE, 2015).

Grapevine cultivars are known to exhibit wide differences in biochemical composition. Anthocyanins, for instance, tend to be the main polyphenolics in purple grapes, whereas flavanols (*i.e.* catechins) are the more abundant class of polyphenols in white varieties (CANTOS; ESPÍN; TOMÁS-BARBERÁN, 2002). This change in metabolic profile points to genotype effect on nutrient signatures, suggesting that, ideally, nutrient standards should be elaborated at cultivar level (MELO et al., 2018; PARENT et al., 2013; ROZANE et al., 2015; STEFANELLO et al., 2021b). Likewise, the use of rootstocks can also have a major influence on the mineral nutrient status of scion cultivar (IBACACHE; VERDUGO-VÁSQUEZ; ZURITA-SILVA, 2020), affecting vegetative growth, precocity, productivity, fruit quality, resistance to negative biotic and abiotic factors, physiological and phonological traits, nutrient uptake, as well as leaf and shoot nutrient composition (MILOŠEVIĆ; MILOŠEVIĆ, 2020). As such, establishing reference values for specific combinations of environment, genetic and management is a daunting task, unfeasible by means of traditional experimentation.

Commercial data bases can be used to relate production and quality to specific site characteristics and management practices (COCK et al., 2011; COOK et al., 2013; JIMÉNEZ et al., 2016). Large amounts of data about soil (from sampling and analysis), plant tissue and yield are acquired by farm businesses to improve management (INGRAM; MAYE, 2020). This data can be used to establish optimum fertilization practices for particular crops and conditions (LARK et al., 2019). Such arrangement avoids the need for large number of costly experiments that would be required in traditional research methods (COCK et al., 2011). Therefore, there is growing interest in the potential of such data sources to improve the efficiency of farm enterprises (WOLFERT et al., 2017) and it is expected to take primary sector to move to the next level of farm productivity and profitability (HIMESH et al., 2018). However, whereas a field fertilizer trial is carefully designed to reduce the yield variation induced by limiting factors other than the controlled treatment, avoiding biases on fertilizer effect, this is not necessarily the case in data generated by commercial farms (LARK et al., 2019). It is thus mandatory to devise innovative data analytics tools able to characterize the relationship between productive factors and crop responses from commercial data sets (CHERGUI; KECHADI; MCDONNELL, 2020; PADARIAN; MINASNY; MCBRATNEY, 2020).

2.3 BOUNDARY LINE ANALYSIS

Boundary Line (BL) analysis (WALWORTH; LETZSCH; SUMNER, 1986; WEBB, 1972) is a modeling approach which considers that the best performance in a population is described by a line at the edge of any body of data – that is, the boundary – and occurs whenever there is a cause-effect relationship between the two variables under study. This line represents the limiting effect of an independent variable (*e.g.* nutrient concentrations), on some response variable (*e.g.* yield) under uncontrolled conditions. The BL is thus a function interpreted as the possible response of a single variable when the other factors are not limiting (*e.g.* strong winds during flowering phase).

BL has been applied to assess yield gaps (CAO et al., 2019; CASANOVA et al., 1999; HAJJARPOOR et al., 2018; YOUSEFIAN et al., 2021; ZHANG; WANG; LI, 2019) as well as to obtain sufficiency ranges for both leaf (ALI, 2018; ALMEIDA et al., 2016; BLANCO-MACÍAS et al., 2010; DE SOUZA et al., 2020; HERNÁNDEZ-VIDAL et al., 2021; MAIA; DE MORAIS, 2016; MANORAMA; BEHERA; SURESH, 2021; NIELSEN; FRIIS-NIELSEN, 1976) and soil nutrients (DEUS et al., 2018; EVANYLO; SUMNER, 1987; LARK et al., 2019; MANORAMA; BEHERA; SURESH, 2021; NETO et al., 2020; RODRIGUES FILHO et al., 2021).

Regarding grapevines, the BL approach has been used to study the effects of water supply (LI; HAO; KANG, 2017; OLIVO; GIRONA; MARSAL, 2009) and soil salinity related variables (MYBURGH; HOWELL, 2014; URDANOZ; ARAGÜÉS, 2009). More recently the effects of N application modes on yield, concentration of anthocyanins and soluble solids in grapes was assessed using leaf samples (STEFANELLO et al., 2021a) and reference values for leaf N, P and K concentrations were obtained (STEFANELLO et al., 2021b, 2022). Despite the simplicity and univariate nature, reference values estimated by BL were considered comparable to those estimated by CND for sugar maple (VIZCAYNO-SOTO; CÔTÉ, 2004), coniferous trees (QUESNEL et al., 2006), opuntia fig (BLANCO-MACÍAS et al., 2009, 2010) and mango (ALI, 2018).

The BL is a function where $Y_{MAX} = f(X; \theta)$ such that, when Y is measured without error, all the measurements of Y obtained for a given value of X are lower than or equal to $f(X; \theta)$, and the difference between Y and $f(X; \theta)$ is due to limiting factors such as low water, pest attack, frost incidence, heat stress or weed competition. When Y is measured with error, some measurements may be higher than $f(X; \theta)$ but only due to measurement errors. Thus, when the measurement errors are small, a value of Y lower than $f(X; \theta)$ indicates that the crop was probably affected by one or several limiting factors (BRANCOURT-HULMEL;

LECOMTE; MEYNARD, 1999). For grapevines, measurement errors in Y (yield) may arise during collection and weighing of the grapes as well as a consequence of the yield sampling scheme adopted, as they generally do not consider the variability at field level (ARAYA-ALMAN et al., 2019).

The development of a BL then comprises two steps: the definition of a mathematical function f(X; θ) that expresses Y as a function of X and of a set of unknown parameters θ; and the estimation of the value of θ from a set of N measurements of Y and X obtained in field (MAKOWSKI; DORÉ; MONOD, 2007; WEBB, 1972). The f(X; θ) function must be flexible enough to give a good representation of the dependence between variables, in this case between crop yield and nutrient levels. Strictly increasing functions, such as exponential and inverse linear functions, tend to give a poor fit to the data (BOYD; YUEN; NEEDHAM, 1976), while quadratic functions, commonly used for fertilizer optimization (ALI, 2018; DEUS et al., 2018; NETO et al., 2020) consistently overestimate the fertilizer level for maximum yield (CERRATO; BLACKMER, 1990; THEOBALD; TALBOT, 2002). Moreover, quadratic functions fail to describe accurately the yield response to fertilizer addition, as a much more gradual change in is expected after the critical level than below it.

Makowski, Wallach and Meynard (2001, 1999) used linear-plateau, quadratic and quadratic-plateau functions to evaluate the response of wheat to fertilization with N and did not identify significant differences between models performance. Similarly, Theobald and Talbot (2002) found comparable results when using linear-plateau, inverse quadratic (BOYD; YUEN; NEEDHAM, 1976; NELDER, 1966; SPARROW, 1979) and inverse linear functions with descending linear function (GREENWOOD et al., 1971; SPARROW, 1979).

A linear-plateau (LP) function is a type of segmented regression – also known as segmented, piecewise, broken-line or multi-phase regression – with two segments separated by a change point (MUGGEO, 2003). The LP function can be generally defined as in (1). In this study, f(X; θ) is the (relative) yield obtained when the independent variable nutrient concentration is equal to X. θ is a set of parameters $(\theta_1,\theta_2,\theta_3)^T$, where θ_1 is the maximum (relative) yield (the "plateau"), θ_2 is the slope of the linear part of the function, and θ_3 is the change point (*i.e.* the critical level).

$$f(X;\theta) = \begin{cases} \theta_1 + \theta_2(X-\theta_3), & X \leq \theta_3 \\ \theta_1, & X > \theta_3 \end{cases} \quad (1)$$

For a given model, calibration describes the process of finding a set of parameters that provide the best description of the relationship between variables, which can be achieved by using field data. Early methods for BL calibration include estimation of parameters “by eye” or using only the most extreme measured values of Y (WEBB, 1972). While the first is highly subjective, the latter may not account for measurement errors and is likely to overestimate the true parameter values. In such scenario, deficiency will always be diagnosed but maximum estimated yield is never to be attained, leading to inefficient resource use.

Another method consists of selecting a subset of data and fitting a model with it. The principle is to divide the domain of variation of X into Q intervals and, for each X interval, calculate the value of Y corresponding to a high quantile value, say, the 90^{th} quantile. The resulting data subset is then used to estimate the BL parameters by least squares (ALI, 2018; BHAT; SUJATHA; JOSE, 2012; BLANCO-MACÍAS et al., 2010; DE SOUZA et al., 2020). The drawbacks of this method are, firstly, that the parameters are not estimated from the original dataset and, secondly, the method is based on an arbitrary number of Q intervals and an arbitrary quantile value (MAKOWSKI; DORÉ; MONOD, 2007).

Makowski, Doré and Monod (2007) proposed the use of Quantile regression (QR) models to avoid having to subset the data, given QR explores the effect of one or more predictors on any quantile of the response variable distribution (BENOIT; VAN DEN POEL, 2017; DAS; KRZYWINSKI; ALTMAN, 2019; KOENKER; BASSETT, 1978). Compared with mean regression methods, QR can provide a more complete view of possible causal relationships (KOENKER, 2005; TOMAL; CIBOROWSKI, 2020) and can reveal useful predictive relationships at some parts of the response variable distribution, even when there is a weak or no predictive relationship between the predictor(s) and the mean of the response variable distribution (CADE; NOON, 2003). In addition, QR appears more robust to outliers of the response variable (DAS; KRZYWINSKI; ALTMAN, 2019; YU; MOYEED, 2001).

The principle of QR is to define $f(X; \theta)$ satisfying $P[Y < f(X; \theta)] = \tau$ for all values of X. With this definition, $f(X; \theta)$ represents the τth quantile of the response variable Y, so that a proportion τ of the measurements of Y are below and a proportion $1 - \tau$ of the measurements are above the boundary line. Parameters θ can then be estimated by using quantile regression techniques (DAS; KRZYWINSKI; ALTMAN, 2019; KOENKER, 2005) which make use of the whole dataset, weighting observations according to the chosen quantile value (MAKOWSKI; DORÉ; MONOD, 2007), in such way that the upper bound of the data dispersion can be examined. However, in order to parameterize a LP function while benefiting from the advantages of QR, a method with the ability to detect a change point is

required, but it has rarely been explored (TOMAL; CIBOROWSKI, 2020; ZHOU; WANG; TANG, 2015).

2.4 BAYESIAN INFERENCE AND MCMC METHODS

Proper estimation of model parameters is necessary to ensure accurate predictions and adequate reliability for modeling-based decisions. An objective summary of the model parameters with confidence intervals and other statistical information is desired, so they can be weighted in terms of probabilities. In the Bayesian approach, the unknown parameters of a model are treated as random variables that have a probability distribution, as opposed to considering them as fixed quantities that need to be estimated in classical frequentist statistics (SPADE, 2020). The goal of Bayesian data analysis is then to provide an explicit distribution of the credibility across possible model parameter values, so that inference can be drawn (KRUSCHKE; LIDDELL, 2018).

Consider there is some data to be explained and one must deliberate over multiple possible explanations, encoded as parameter values of a model. Before any data is observed, each of these candidates have some initial credibility of being the best explanation, commonly referred as *prior*. This prior belief can be built from previous information available to the researcher, general understanding of the phenomenon, prior experience and expert opinion. When no information is available, the *priors* can assume very wide distributions and are often called “vague” or “weakly informative”. After considering the data, credibility reasonably shifts towards the candidate explanations that better account for it and this distribution, derived after new data are taken into account, is called *posterior*. The *posterior* distribution can then be directly interpreted and examined to see which parameter values are most credible and which values delimit high credibility ranges.

A mathematical description for this process of credibility reallocation is given by Bayes’ theorem (2), named in honor of the 18th century minister Thomas Bayes (1701–1761) who first wrote it:

$$\pi(\theta \mid X) = \frac{\pi(X \mid \theta)\pi(\theta)}{\pi(X)} \tag{2}$$

Where $\pi(\theta)$ is the *prior*, that is, the probability of values for parameter θ without the data X. The *likelihood* – $\pi(X|\theta)$ – describes the joint probability of the observed data X as a function of the parameters θ of the chosen model, therefore it assigns a probabilistic prediction to the observed data X for each specific parameter value θ in the parameter space.

The *posterior* – $\pi(\theta|X)$ – is the probability of θ values given that we have the data X (GELMAN et al., 2013; GILKS; RICHARDSON; SPIEGELHALTER, 1995; KRUSCHKE, 2014).

In other words, the *posterior* is obtained by an averaged combination of the *prior* and the observed data. If we observe data that corroborate with our *prior*, confidence grows and the *posterior* becomes "narrower". Accordingly, if data contradict our *prior*, since we believe in it, but we also believe in the data, the logical conclusion is that the truth lies somewhere in between, and that is exactly what the math does. New data can thus be systematically incorporated to update the *posterior* which, in turn, affect our beliefs, becoming our *prior* for the next iteration.

The denominator – $\pi(X)$ – is the overall probability of the data according to the model, also called *marginal likelihood* of the data. For continuous variables it can be obtained by integrating the *likelihood* $\pi(X|\theta)$ weighted by the prior probability of θ over all values of θ (CONGDON, 2003; GELMAN et al., 2013; KRUSCHKE, 2014), so (2) can be rewritten as (3).

$$\pi(\theta \mid X) = \frac{\pi(X \mid \theta)\pi(\theta)}{\int_{\theta} \pi(X \mid \theta)\pi(\theta)\, d\theta} \tag{3}$$

Hence, the determination of a proper *posterior* distribution directly from Bayes' rule involves computing the *marginal likelihood*, a task than can rarely be done analytically in the usual case of continuous parameters due to intractable integrals (ELLIS et al., 2020; GELFAND, 2000; GILKS; RICHARDSON; SPIEGELHALTER, 1995). The difficulty of the integration was historically addressed by restricting models to relatively simple *likelihood* functions with corresponding formulas for *prior* distributions called *conjugate priors*, which were mathematically sound, with reasonable theoretical properties and proper behavior, resulting in tractable integrals, but not necessarily reflecting the phenomena under study (KRUSCHKE, 2014; SPADE, 2020).

In such situations, *posterior* distributions can be alternatively obtained by Monte Carlo integration, including Markov chain Monte Carlo (MCMC) methods. Monte Carlo is a technique for randomly sampling from a probability distribution to approximate a desired quantity. The appellation Monte Carlo is attributed to the mathematicians Stanislaw Ulam (1909–1984) and John von Neumann (1903–1957) (KRUSCHKE, 2014), referencing the famous Casino in Monaco. Monte Carlo methods typically assume that we can efficiently

draw samples from a target distribution and, when the samples are independent, the law of large numbers ensure that the approximation of a desired quantity is accurate, as long as large Monte Carlo sample size is provided (GILKS; RICHARDSON; SPIEGELHALTER, 1995). Eventually, drawing samples independently from the *posterior* may not feasible, as the density may be overly complicated or unavailable analytically. Fortunately, an integral can be approximated by a possibly dependent sample that properly reflects the proportions associated with the *posterior* (GILKS; RICHARDSON; SPIEGELHALTER, 1995; SPALL, 2003). This less stringent requirement opens up the possibility of efficient Markov chain-based schemes that avoid the need to directly sample from the *posterior*.

A Markov chain, named after the mathematician Andrey Markov (1856–1922), is a stochastic model describing a sequence of possible events (the state space) in which the probability of each event depends only on the state attained in the immediately preceding iteration, that is, in a sequence of random variables $\{X_0, X_1, X_2,...\}$, X_{i+1} is generated from the (conditional) distribution $P(X_{i+1} \mid X_i)$, called the transition kernel of the chain, and X_0 represents some initial state. If the transition kernel is invariant over the length of i, than the Markov chain it is said to have stationary transition probabilities (GEYER, 2011; GILKS; RICHARDSON; SPIEGELHALTER, 1995; SPALL, 2003).

Under standard conditions, the dependence of X_i on any fixed number of earlier states disappear as $i \rightarrow \infty$. Hence, the density (distribution) of X_i will approach a stationary form. For the distribution of X_i to converge to a stationary form, the chain needs to satisfy three important properties. First, it has to be irreducible, meaning that every state can be reached from every other state in n steps with probability greater than zero. Second, the chain needs to be aperiodic, thus independent from i. This prevents the Markov chain from oscillating between different sets of states in a regular periodic movement. Finally, and most importantly, the chain must be positive recurrent, that is, the expected time to return to a state (recurrence time) is finite (ROBERTS, 1995). If the Markov chain has one recurrent class and is aperiodic, it is called ergodic and it will converge to the stationary distribution regardless of the initial state X_0. Thus, after n iterations, a sufficiently long chain yields points $\{X_i; i = m + 1,..., n\}$ that look increasingly like dependent samples from the target stationary distribution. The first m iterations in the chains (called the *burn-in* period) can be discarded to avoid retaining samples that were taken before convergence. We can now use the output from the Markov chain to form an ergodic average (4), which converge to their expectations and are representative of the entire population (GEYER, 2011; SPALL, 2003).

$$\bar{\theta} = \frac{1}{n-m} \sum_{i=m+1}^{n} \theta_i \quad (4)$$

The choice of *m* and *n* numbers is not straightforward and previous works have suggested *m* around 1 or 2% of *n* (GEYER, 1992), at least 20% of *n* (RAFTERY; LEWIS, 1995), up to *m* = *n*/2 (MAKOWSKI; WALLACH; TREMBLAY, 2002) in order to avoid retaining parameter values that are far from the *posterior* distribution. One method to determine *n* is to run several strings with different initial values and different lengths and then compare the results obtained with these different strings, for instance, the average value of the generated parameters (GELMAN, 1995). If the results do not agree properly, the number of iterations *n* must be increased.

MCMC is essentially Monte Carlo integration using Markov chains that have the *posterior* as its stationary distribution (GILKS; RICHARDSON; SPIEGELHALTER, 1995). An important benefit from MCMC method is that the *posterior* density need only to be known to within a scale factor (KRUSCHKE, 2014). Effectively, since the *marginal likelihood* in (3) consider all possible θ values and the data is constant, π(X) is also constant, acting as a scaling factor so that the results are normalized and have a proper probability distribution, that is, the sum of the probabilities across all events in the entire sample space is ensured to be 1 (KOLMOGOROV, 1956). So, alternatively, the proportional sign (∝) can be used instead of equal sign (=) and (3) can be written as (5), meaning that the *posterior* probability is proportional to the product of *likelihood* and *prior* probability.

$$\pi(\theta \mid X) \propto \pi(X \mid \theta)\pi(\theta) \quad (5)$$

The exemption from computing the *marginal likelihood* makes MCMC very relevant to Bayesian applications and allow Bayesian statistical methods to gain practical use. MCMC assumes that the *prior* – π(θ) – is specified by a function that is easily evaluated and that the value of the *likelihood* – π(X|θ) – can be computed for any specified values of X and θ. Conditions met, the method produces an approximation of the *posterior* distribution – π(θ|X) – in the form of a large number of θ values sampled from that distribution. Representative θ values can then be used to estimate any features of the *posterior*, such as central tendency, highest density interval (HDI), etc (KRUSCHKE, 2014).

Despite having over 250 years of age, Bayesian methods stayed in the background of statistical practice until recently. The advent of high-speed computers, associated with the

introduction of general-purpose MCMC algorithms in the 1990s, including general purpose software, such as BUGS (LUNN et al., 2013), JAGS (PLUMMER, 2003, 2017), and Stan (STAN DEVELOPMENT TEAM, 2022), allowed Bayesian methods to be used in realistic applications with seamless facility that would have been effectively impossible 30 years ago (KRUSCHKE; LIDDELL, 2018). Two useful techniques for generating MCMC samples are the Metropolis-Hastings algorithm (MH) and the Gibbs sampler.

In the MH algorithm (HASTINGS, 1970; METROPOLIS et al., 1953) sample values from the target distribution are generated by taking random walks through the parameter space. The walk starts at some arbitrary vector value θ_0, specified by the user, and proceeds at each step by generating a vector of candidate parameters θ^* from a proposal distribution $q(\theta^* \mid \theta_{i-1})$, which can take on many different forms but should be designed to efficiently explore regions of the parameter space where highest densities lies.

$$T = \frac{\pi\left(X \mid \theta^*\right)\pi\left(\theta^*\right)q\left(\theta_{i-1} \mid \theta^*\right)}{\pi\left(X \mid \theta_{i-1}\right)\pi\left(\theta_{i-1}\right)q\left(\theta^* \mid \theta_{i-1}\right)} \tag{6}$$

Then T is calculated as in (6), where $\pi(X \mid \theta^*)$ and $\pi(X \mid \theta_{i-1})$ are the *likelihoods* of θ^* and θ_{i-1} respectively, and $\pi(\theta^*)$ and $\pi(\theta_{i-1})$ are the previous densities values of θ^* and θ_{i-1}, respectively. If min $(1, T) > u$, where u is interpreted as an "acceptance threshold" extracted from a uniform distribution on the interval (0, 1), then the proposed move is accepted and $\theta_i = \theta^*$, otherwise, the proposed move is rejected and $\theta_i = \theta_{i-1}$. Thus, a sequence of n vectors of parameter θ_i, i = 1, ..., n, is generated.

Before using the MH algorithm it is then necessary to choose the initial value θ_0 and the proposal distribution $q(\theta^* \mid \theta_{i-1})$. The choice of θ_0 is not very critical, given that the chains will eventually "forget" their starting point (GILKS; RICHARDSON; SPIEGELHALTER, 1995). On the other hand, the choice of the proposed distribution $q(\theta^* \mid \theta_{i-1})$ is an important issue. A common practice is to use a normal (Gaussian) distribution with mean θ_{i-1} and constant covariance matrix Σ, which is equivalent to assuming that $q(\theta^* \mid \theta_{i-1}) \sim N(\theta_{i-1}, \Sigma)$. The choice of Σ should done so that the algorithm acceptance rate is in the range of 20–70% (MAKOWSKI; WALLACH; TREMBLAY, 2002). While MH is very general and broadly applicable, it is mandatory that the proposal distribution is properly tuned to the *posterior* if the algorithm is to work well, otherwise the method can become very inefficient as sample proposals are hardly accepted and the chains get "stuck", which may be difficult when there are multivariate distributions involved (KRUSCHKE, 2014). Alternatively, the Gibbs sampler

can be used, which is a special case of Metropolis-Hastings, applicable when we have all known conditionals.

The Gibbs sampler (GEMAN; GEMAN, 1984), named after the physicist Josiah Willard Gibbs (1839–1903), is a special case of MH algorithm that simplifies a complex, high-dimensional problem by breaking it down into simpler, smaller-dimensional problems. The basic idea of the Gibbs sampler is to partition the set of unknown parameters and then sample them, one at a time, with each estimated parameter conditional on all others (CONGDON, 2003; GELFAND, 2000; GEYER, 2011; SPALL, 2003; TADDY; KOTTAS, 2010), given that it is much easier to propose an update for one parameter at a time (Gibbs) than all parameters simultaneously (MH). Gibbs sampling generally works as follows:

Consider a three-component density $\pi(\theta_1,\theta_2,\theta_3)$. The full conditional distributions associated with this density are $\pi(\theta_1|\theta_2, \theta_3)$, $\pi(\theta_2|\theta_1, \theta_3)$, and $\pi(\theta_3|\theta_1, \theta_2)$. If our current state is $(\theta_1^{(n)}, \theta_2^{(n)}, \theta_3^{(n)})$ at the nth iteration, then we update our parameter values with the following steps:

1. Sample $\theta_1^{(n+1)} \sim \pi(\theta_1|\theta_2^{(n)}, \theta_3^{(n)})$
2. Sample $\theta_2^{(n+1)} \sim \pi(\theta_2|\theta_1^{(n+1)}, \theta_3^{(n)})$
3. Sample $\theta_3^{(n+1)} \sim \pi(\theta_3|\theta_1^{(n+1)}, \theta_2^{(n+1)})$

For the Gibbs sampler to work it is necessary to know each of the conditional probability distributions and to be able to independently sample from them. This makes Gibbs a very versatile algorithm, as it is not necessary for $(\theta_1^{(n)},..., \theta_k^{(n)})$ to be scalars, since θ_1 could be bivariate, trivariate or have arbitrary large dimensions, as long as it is possible to sample from their full conditional distributions.

Gibbs sampling has the potential to sample much more efficiently than MH. It doesn't propose updates only to reject them and doesn't suffer from poor tuning that can make MH explore the parameter space very slowly. Instead, Gibbs works its way around by using the marginal *posteriors*. On the other hand, samples are constructed by changing one parameter at a time – meaning that subsequent samples are very close in the search space – so its progress can be stalled by highly correlated parameters and there is risk of the chain getting "stuck". Single parameter update also makes it hard for the samplers to quickly move along "diagonal ridges" in the *posterior* that would be theoretically feasible using MH. In the infinitely long run, the Gibbs and MH generally converge to the same distribution, what differs is the efficiency of getting to any desired degree of approximation accuracy in a finite run.

2.5 BAYESIAN SEGMENTED QUANTILE REGRESSION

In principle, any parameterized model of data can have its parameters estimated via Bayesian methods. As described earlier, for the definition of a BL using a LP function we could take advantage of quantile regression (QR) models (MAKOWSKI; DORÉ; MONOD, 2007) with the ability to detect a change point. Bayesian inference may be undertaken in the context of QR by putting the Bayesian quantile regression (BQR) problem in the framework of the generalized linear model and using the asymmetric Laplace distribution (ALD) to form the likelihood function, irrespective of the actual distribution of the data (BENOIT; VAN DEN POEL, 2017; YU; MOYEED, 2001).

Although a standard conjugate *prior* is not available for the QR formulation, MCMC methods can be used for parameter posterior approximation. This, in fact, allows the use of virtually any *prior* distribution, so, in the absence of any realistic information, one could use improper uniform *priors* for parameters. This choice is appealing as the resulting joint *posterior* distribution is proportional to the likelihood surface, thus equivalent to a frequentist approach, since no information other than the data is provided (YU; MOYEED, 2001). So one might say that Bayesian approach also covers the frequentist results.

There is an apparent contradiction between ALD assumptions (*i.e.* independent and identically distributed error terms) and the motivation for using QR (*e.g.* in case of error heteroskedasticity) and it is true that there are other Bayesian approaches to QR (BENOIT; VAN DEN POEL, 2017), nevertheless, the ALD approach is a valuable and relatively simple alternative that does not need complex choices of *prior* distributions and *prior* (hyper-)parameters (YU; STANDER, 2007). Additionally, misspecified likelihood in the ALD approach is proved to lead to posterior consistency under fairly general conditions (SRIRAM; RAMAMOORTHI; GHOSH, 2013; YU; MOYEED, 2001).

Recently a Bayesian Segmented Quantile Regression model (BSQR) was proposed (LIANG et al., 2021), enabling the detection of change point in BQR by integrating it with the well-developed Bayesian change point (BCP) model (BARRY; HARTIGAN, 1993; ERDMAN; EMERSON, 2007). The BSQR model inherits advantages of both BQR and BCP models and is able to provide a complete view on the variable-response relationship (LIANG et al., 2021; MULLER; CADE; SCHWARZKOPF, 2018; XU et al., 2015) while making possible the detection of any change point in the regression intercept, slopes, and/or variance of residuals (BECKAGE et al., 2007; LIANG et al., 2019, 2021). Additionally, BSQR is not constrained by the equal variance assumption, *i.e.* homoscedasticity (CADE; NOON, 2003; LIANG et al., 2021).

The main functions of BSQR model to estimate the relationship between an independent variable x_i and a response variable y_i at a specific regression quantile τ ($0 < \tau < 1$) in which there is a change point can be expressed by (7) and (8), where cp^τ represents the change point, $\beta^\tau_{1,1}$ and $\beta^\tau_{1,2}$ are regression slopes before and after the change point, respectively, $\varphi^\tau[i]$ is the step function controlling the index of regression slope, β^τ_0 is the estimated value of the response at the change point and ε_i^τ represents the error.

$$y_i = \beta_0^\tau + \beta^\tau_{1,\phi^\tau[i]}\left(x_i - cp^\tau\right) + \varepsilon_i^\tau \tag{7}$$

$$\phi^\tau[i] = \begin{cases} 1\,, x_i \le cp^\tau \\ 2\,, x_i > cp^\tau \end{cases} \tag{8}$$

Estimation of parameters is based on the minimization of weighted sums of absolute deviations (BENOIT; VAN DEN POEL, 2017; KOENKER; BASSETT, 1978), which can be expressed by (9), where ρ_τ is the loss function expressed by (10) for a given value u, with I ($u < 0$) meaning that the value will be one if $u < 0$, and zero otherwise. The minimization of the loss function in (10) is equivalent to the maximization of a likelihood function formed by combining independently distributed ALD (YU; MOYEED, 2001; YU; ZHANG, 2005).

$$\min_\beta \sum_i \rho_\tau\left(\varepsilon_i^\tau\right) = \min_\beta \sum_i \rho_\tau\left(y_i - \beta_0^\tau + \beta^\tau_{1,\phi^\tau[i]}\left(x_i - cp^\tau\right)\right) \tag{9}$$

$$\rho_\tau(u) = u\left(\tau - I\left(u < 0\right)\right) \tag{10}$$

A random variable u is said to follow the ALD if its probability density is given by (11), where $0 < \tau < 1$ and $\rho_\tau(u)$ is as defined in (10). When $\tau = \frac{1}{2}$, (11) reduces to $\frac{1}{4}\exp\left(\frac{-|u|}{2}\right)$, which is the density function of a standard symmetric Laplace distribution. For all other values of τ, the density in (11) asymmetric and the mean (μ_u) and variance (σ^2_u) are defined as in (12), with μ_u being positive only for $\tau > \frac{1}{2}$, while σ^2_u increases quite rapidly as τ approaches 0 or 1.

$$\pi_\tau(u) = \tau(1-\tau)\exp\{-\rho_\tau(u)\} \tag{11}$$

$$\mu_u = \frac{1-2\tau}{\tau(1-\tau)}\,, \qquad \sigma_u^2 = \frac{1-2\tau+2\tau^2}{\tau^2(1-\tau)} \tag{12}$$

Benefiting from this feature of ALD, the error ε_i^{τ} can be expressed by (13) where $\delta^{\tau}_{\varphi\tau[i]}$ represents the precision parameter of the ALD, W_i is an exponentially distributed random variable with rate of $\delta^{\tau}_{\varphi\tau[i]}$ and Z_i is random variable with a standard normal distribution. It is noteworthy that the two random variables W_i and Z_i are independent and that the marginal distribution of ε_i^{τ} remains ALD, while ε_i^{τ} follows a normal distribution on condition of the latent weight W_i (KOTZ; KOZUBOWSKI; PODGÓRSKI, 2001; LIANG et al., 2021; WANG et al., 2016; YANG; WANG; HE, 2016; ZOU; SHI, 2020).

$$\varepsilon_i^{p} = \frac{1-2\tau}{\tau(1-\tau)} W_i + \sqrt{\frac{2\,W_i}{\delta^{\tau}_{\phi^{\tau}[i]}\tau(1-\tau)}}\,Z_i \tag{13}$$

As such, from equations (7) and (13), the distribution of y_i can be expressed by (14)

$$y_i \sim N\left(\beta_0^{\tau} + \beta^{\tau}_{1,\phi^{\tau}[i]}\left(x_i - cp^{\tau}\right) + \frac{(1-2\tau)W_{\phi^{\tau}[i],i}}{\tau(1-\tau)},\ \frac{2\,W_{\phi^{\tau}[i],i}}{\delta^{\tau}_{\phi^{\tau}[i]}\tau(1-\tau)}\right) \tag{14}$$

Accordingly, *posterior* distributions of all the parameters in the BSQR model can be expressed by (15) and estimated using MCMC methods.

$$\begin{aligned} & \pi\left(\beta_0^{\tau}, \beta_{1,1}^{\tau}, \beta_{1,2}^{\tau}, \delta^{\tau}, cp^{\tau}\right) \\ \propto\ & \prod_{i=1}^{n} N\left(y_i; \beta_0^{\tau} + \beta^{\tau}_{1,\phi^{\tau}[i]}\left(x_i - cp^{\tau}\right) + \frac{(1-2\tau)W_{\phi^{\tau}[i],i}}{\tau(1-\tau)}, \frac{2\,W_{\phi^{\tau}[i],i}}{\delta^{\tau}_{\phi^{\tau}[i]}\tau(1-\tau)}\right) \times \\ & \pi\left(\beta_0^{\tau}\right) \times \pi\left(\beta_{1,1}^{\tau}\right) \times \pi\left(\beta_{1,2}^{\tau}\right) \times \\ & \pi\left(W_{\phi^{\tau}[i],i} \mid \delta^{\tau}_{\phi^{\tau}[i]}\right) \times \pi\left(\delta^{\tau}_{\phi^{\tau}[i]}\right) \times \\ & \pi\left(cp^{\tau}\right) \end{aligned} \tag{15}$$

The Bayesian framework provides the convenience for parameters estimation using MCMC methods (QIAN; STOW; BORSUK, 2003) and allow explicit representation of the uncertainty of all parameters, including the change point (ELLISON, 2004; UNDERWOOD et al., 2017). Measures of uncertainty are based directly on posterior credible intervals (CI) obtained by computing the highest density interval (HDI) of parameters *posterior* distributions (KRUSCHKE; LIDDELL, 2018). All the values inside the HDI have higher probability density than any value outside the HDI, being thus the most credible. Interpretation of CI differs from that of confidence interval from frequentist statistics, which is a measure of the interval, not the parameter of interest (KRUSCHKE, 2014). The 95% HDI

thus contains a total probability of 95%, that is, the 95% most credible values of the parameter. In principle any probability density could be directly extracted from the *posterior*, the 95% is merely due to familiarity by analogy to 95% confidence intervals of frequentist statistics.

These features of Bayesian statistics are of practical use for estimating nutrient CL for soil and leaf nutrients, as they allow not only the calculation of the most probable CL value (the change point parameter) but also the definition of SR as a degree of uncertainty around it, rather than calculated from a fitted equation. In addition, comparison of parameters based on their *posterior* distributions is straightforward (ALAMEDDINE; QIAN; RECKHOW, 2011; LIANG et al., 2021; QIAN et al., 2009), making it possible to differentiate groups regarding their optimal nutrition levels. Finally, the incorporation of all available prior knowledge during model development can be seamlessly done (ELLISON, 1996, 2004) leveraging existing data bases and previous research results.

2.6 BAYESIAN MODEL ASSESSMENTS

2.6.1 MCMC convergence

The goal of MCMC is to draw samples from some probability distribution without having to know its exact value at any point. The method aims to generate samples proportional to the *posterior* density, such that the distribution of the final samples is stationary, meaning that it converges to something while retaining consistency. There is currently no certain way to prove convergence, but it is possible to ascertain when convergence has not been achieved. This is done first by examining if the MCMC chains appear to be well mixed and representative of the *posterior* distribution (KRUSCHKE, 2014).

Convergence (or lack of) can be assessed by either visual or numerical means. The visual inspection of the chain trajectory is aided by trace plots, which are graphs displaying the parameter values as a function of steps in the chain, called iterations. Representative chains overlap and mix well, although the converse is not necessarily true, as the chains might overlap, but all be stuck in the same unrepresentative part of parameter space. One popular numerical convergence check is the Gelman-Rubin statistic (GELMAN; RUBIN, 1992), also called Brooks-Gelman-Rubin statistic (BROOKS; GELMAN, 1998), eventually called potential scale reduction factor and usually denoted as $\hat{R}$. The $\hat{R}$ statistic measures the ratio of the average variance of samples *within* each chain to the variance of the pooled samples *between* chains. If all chains are at equilibrium, these will be very similar and $\hat{R}$ will be very

close to one. If the chains have not converged to a common distribution, the $\hat{R}$ statistic will be greater than one. The condition of $\hat{R}$ being near 1.0 depends on the problems at hand, but usually values below 1.1 can be satisfactory for practical purposes (GELMAN et al., 2013).

2.6.2 MCMC accuracy

After we have some assurance that the chains are genuinely representative samples from the *posterior* distribution, the second main goal is to have a large enough sample size for stable and accurate numerical estimates of the distribution. In MCMC methods, samples will typically be autocorrelated within a chain, increasing the uncertainty of the estimation of posterior quantities of interest such as means, variances, or quantiles (GEYER, 2011). Autocorrelation measures the value of a chain in a current iteration with its values after a certain number of iterations called *lag*. The autocorrelation can be computed for any *lag* of interest using autocorrelation function (ACF). When the chains have high autocorrelation, ACF values remain well above zero for large *lags*, meaning that parameter values at successive steps in the chain are not providing independent information about the *posterior* distribution, because each successive step is partially redundant with the previous one (KRUSCHKE, 2014).

The effective sample size (KASS et al., 1998) (ESS) measures how much independent information there is in autocorrelated chains. It divides the actual sample size by the amount of autocorrelation and indicates the sample size of a completely non-autocorrelated chain which yields the same information. In principle, the larger the ESS the better but exactly how large is enough to result in estimates of good statistical quality is still unclear, since it can vary depending on the problem at hand and even for quantities of interest within the same problem, so it is unwise to rely on a mere “rule of thumb”. Zitzmann and Hecht (2019) argue that 1,000 samples would be optimal, but 400 samples could eventually be sufficient. Raftery and Lewis (1992) suggest that reasonable accuracy can be frequently achieved with 1,000 samples and, more generally, with 5,000, though authors point out that highly correlated posterior parameters may require even larges samples. Accordingly, Kruschke (2014) states that for aspects of the distribution that are strongly influenced by sparse regions, such as the limits of the 95% HDI, an ESS of 10,000 is recommended.

MCMC practitioners very often tackle the autocorrelation issue by thinning the chains, that is, discarding all but every *k*th observation (LINK; EATON, 2012). This approach is historically known to be unnecessary, and always inefficient to reduce autocorrelation

(GEYER, 1992). Essentially, thinning throws away information and might be more detrimental effects on the estimates than unthinned correlated samples (LINK; EATON, 2012), unless there is severe autocorrelation, *e.g.*, high correlation with *lag* = 30, for instance (CHRISTENSEN et al., 2011). However, thinning merely produces correct results less efficiently (on average) than using the full chain from which the thinned chain was extracted (KRUSCHKE, 2014). High autocorrelation might be unavoidable, requiring very long chains to attain appropriate ESS, which can be constrained by limitations in computer memory and storage. In such conditions, thinning can be used not as a strategy for avoiding these long chains, but it as a strategy for dealing with the otherwise overwhelming amount of MCMC output (JACKMAN, 2009). Nevertheless, for extreme autocorrelation, it's best not to rely on long-run averaging out, but instead to use other techniques that actually get rid of the autocorrelation, usually involving model reparameterization (KRUSCHKE, 2014).

2.6.3 Sensitivity analysis

As previously discussed, all the measurements of Y should be lower than or equal to the values estimated by the BL function and the only exceptions occur given the existence of measurement errors in Y. In addition, the application of QR requests that the BL function should satisfy $P[Y < f(X; \theta)] = \tau$ for all values of X. In such arrangement, the choice of quantile (τ) bares relationship with the implicit tolerance to errors, with potential effects on model outcomes. In the absence of a defined methodology for quantile selection, a reasonable approach is to assess the effects of different quantile values on the BL parameters.

In addition, the *prior* distribution of a given parameter component θ_k represents the explicit encoding of previous knowledge about it in the model. If very little is known about θ_k, then one may reasonably choose a prior distribution that has little impact on the *posterior* (SPADE, 2020). *Priors* that are broad relative to the *posterior* are called “vague” or only “mildly informed” by the typical scale of the data. The use of these innocuous broad *priors* for typical data analysis in which the focus is on estimation of continuous parameters is recommended (KRUSCHKE; LIDDELL, 2018). A good *prior* helps, a bad one hurts, but the *prior* matters less as available data increases. Still, because the choice of *prior* may be deemed somewhat subjective, a sensitivity analysis should then be performed to determine to what extent it affects the modeling results (ELLIS et al., 2020).

2.6.4 Goodness-of-fit

If the model has a good fit, replicated data generated under the model is expected to look similar to observed data or, to put it differently, the observed data should look plausible under the posterior predictive distribution (GELMAN et al., 2013). Posterior predictive checks (PPC) are a way of measuring whether a model does a good job of capturing relevant aspects of the data, such as means, standard deviations, and quantiles (GELMAN; MENG; STERN, 1996). The PPC works by simulating new replicated data sets based on the fitted model parameters and then comparing statistics, called test quantities, applied to both data sets. A test quantity T(·) is a scalar summary of parameters and data that is used to compare between observed (y) and replicated data (y^{rep}). Any systematic differences between the simulations and the data indicate potential failings of the model (KRUSCHKE, 2014).

In practice, PPC is usually computed using simulations. Let y be the observed data and θ be the vector of parameters, if we already have simulations from the posterior density of θ, we just draw one y^{rep} from the predictive distribution for each simulated θ to obtain draws from the joint posterior distribution $\pi(y^{rep}, \theta|y)$. The PPC is the comparison between the realized test quantities – $T(y, \theta)$ – and the predictive test quantities – $T(y^{rep}, \theta)$. The proportion of simulations for which the test quantity equals or exceeds its realized value is often called Bayesian p-value (16) (GELMAN et al., 2013).

$$p_B = Pr\left(T\left(y^{rep}, \theta\right) \geq T\left(y, \theta\right)|y\right) \tag{16}$$

It is important to note that the Bayesian p-values are not classically calibrated statistics, and thus its uniform distribution under the true model is only assured in very special cases (GELMAN et al., 2013). For general conditions, the distribution of the Bayesian p-value is more concentrated near the middle the range, that is, the p-value is more likely to be near 0.5 than near 0 or 1 if the model is true. This is an intuitive interpretation: in a good fit, $T(y^{rep}, \theta)$ would have a symmetrical distribution around $T(y, \theta)$, being greater only about half of the time, thus p-values would approach 0.5.

3 OBJECTIVES

3.1 GENERAL

The main objective of the work was to propose and test a new method for generating nutrient reference values adjusted to local conditions and cultivar groups using commercial farm data, aiming to increase grapevine fertilization efficiency and sustainability.

3.2 SPECIFIC

I. Estimate critical levels and sufficiency ranges for nutrients in vineyard soils and grapevine leaves (*Vitis vinifera*) cultivated in the Campanha Gaúcha, Rio Grande do Sul, using data generated by commercial farm.

II. Investigate whether critical level and sufficiency range estimates differ between white and red grapes.

III. Assess suitability and limitations of the proposed method.

3.3 HYPOTHESIS

A) Commercial farm data can be leveraged to update fertilizing recommendation systems and account for specific conditions.

A) Current regional recommendations are too broad. Tailored recommendations will have narrower sufficiency ranges.

B) Due to different biochemical profiles of red and white grapes cultivars, reference values will vary based on grape skin color.

4 MATERIAL AND METHODS

4.1 SITE DESCRIPTION

The data used in this study came from a commercial vineyard (*Vitis vinifera*) cultivated on sandy textured Alisol (*Argissolo*) (IUSS WORKING GROUP WRB, 2015; SANTOS et al., 2018) located in the municipality of Santana do Livramento, in the Campanha Gaúcha region, Rio Grande do Sul (RS), southern Brazil (latitude 30°53'27" S, longitude 55°31'58" W). The Campanha Gaúcha has altitudes ranging from 100 to 300 m and climate described by Köppen-Geiger classification as humid subtropical with hot summers and no dry seasons (Cfa). Average annual temperatures ranges between 16 and 18°C with annual precipitation of 1600 to 1900 mm (ALVARES et al., 2013). Over 86% of RS territory is classified as Cfa climate, with the remainder classified as Cfb (warm summer), therefore, current study area can be considered representative of the Campanha Gaúcha region.

4.2 DATASETS

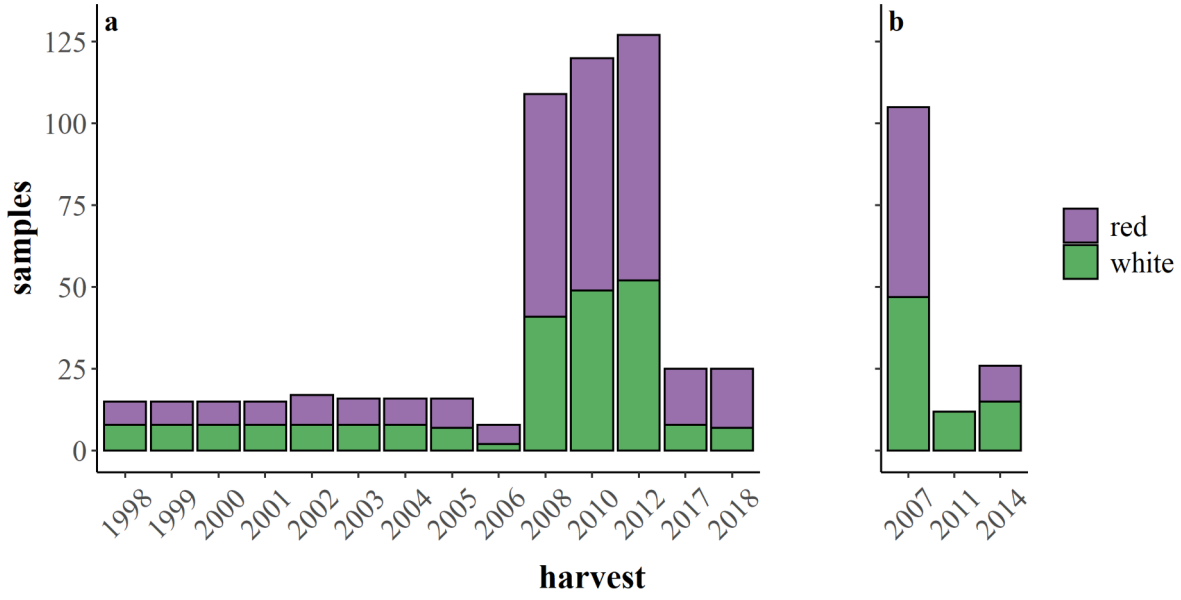
Complete dataset consisted of 682 yield observations regarding 17 harvests between 1998 and 2018, registered for 27 grape cultivars, which were grouped based on their skin color, *i.e.* white, (11) and red (16). Grapevines were all grafted onto Selection Oppenheim 4 rootstocks and conducted in espalier system. Plant age ranged from 2 to 40 years old, with mean of 19.8 years. Relative yields were calculated based on the highest values recorded.

4.2.1 Soil samples

Soil samples (n = 539) were collected from top layer (0 – 20 cm) after harvest, close to the grapevine or inside the canopy projection. In total 14 harvests had associated soil samples, which were distributed unevenly, with three harvests (2008, 2010 and 2012) comprising 66% of total observations (over 100 each), whereas the remainder contained 25 observations (2017 and 2018) or less. Grapes with white skin had smaller number of soil samples (n = 222) compared to red ones (n = 317) (Figure 1a). Exchangeable concentrations of soil phosphorus (P), potassium (K), calcium (Ca), magnesium (Mg), sulfur (S), copper (Cu), zinc (Zn), boron (B) and manganese (Mn) were determined through laboratory routine analyisis. For P concentrations, samples were submitted to Mehlich-1 extraction and analyzed by colorimetry or UV-visible spectrophotometry, using ammonium molybdate and ascorbic acid as reagents. Available K was determined by either flame photometry, atomic absorption spectrophotometry (AAS) or induced plasma optical emission spectrometry (ICP-OES), after Mehlich-1 extraction. The exchangeable contents of Ca and Mg were determined by

extraction with a concentrated solution of potassium chloride (KCl 1 mol/L) followed by AAS or ICP-OES. S availability was obtained through dissolving samples in calcium phosphate solution (500 mg P/L) followed by digestion and sulfate determination by turbidimetry. Micronutrients Cu and Zn were determined by AAS or ICP-OES after Mehlich-1 extraction while available Mn was determined by AAS after KCl 1 mol/L extraction. Available B was determined by extraction with hot water submitted to colorimetric analysis in the presence of the curcumin dye. Exchangeable Mn was determined by AAS of KCl extract (1 mol/L) acidified with 2% HCl, keeping the extract:acid ratio of 1:1.

Figure 1 – Number of soil (a) and leaf (b) samples by harvest and grape skin color.



4.2.2 Leaf Samples

Leaf samples (n = 143) were collected (blade + petiole) opposite to the first cluster of a fruit branch at veraison, prior to 3 harvests. Samples were unevenly distributed along the years, as a single harvest (2007) accounted for over 73% of total observations, albeit the difference between white (n = 74) and red grapes (n = 69) was less pronounced (Figure 1b). The concentrations of nitrogen (N), P, K, Ca, Mg, S, Cu, Zn, B, Mn and iron (Fe) in leaves were determined by laboratory analysis. Samples were first subjected to sulfuric digestion (for N, P, K, Ca and Mg), nitric-perchloric digestion (for P, K, Ca, Mg, S, Cu, Fe, Mn and Zn) or incineration (for B). Leaf N concentration was determined by semi-micro-Kjeldahl or colorimetry methods. P was determined by colorimetry of extract treated with ammonium molybdate and reducing agent or by ICP-OES. K was determined by either flame photometry of sodium enriched diluted extract, AAS or ICP-OES. Ca and Mg were quantified by AAS,

using lanthanum or strontium solution to avoid interference caused by the presence of phosphates, or by ICP-OES. S was determined by sulfate turbidimetry in the presence of barium chloride or by ICP-OES. Leaf micronutrients Cu, Fe, Mn and Zn were determined by AAS or ICP-OES whereas B was determined by colorimetry after curcumin dye reaction in the presence of oxalic acid.

4.3 DATA PROCESSING AND MODELING

The relationships between crop (relative) yields and soil or leaf nutrient concentrations were described by a segmented function known as linear-plateau (MAKOWSKI; DORÉ; MONOD, 2007), in which nutrient increments lead to increasing response up to a change point, after which the function becomes flat. Function parameters were estimated by Bayesian Segmented Quantile Regression (BSQR) (LIANG et al., 2021) using Markov Chain Monte Carlo (MCMC) methods through Gibbs sampling algorithm (GELMAN; HILL, 2007). Posterior probability medians of the change point parameters were assumed as CL values and SR were estimated by calculating the 95% highest density (continuous) interval around it. The sampling stage used four chains with 150,000 iterations each, where the first 50% were discarded (*burn-in*) and only one of every 30 draws were retained (*thinning*) to estimate model parameters. All models regressed over the 98^{th} quantile. The 98^{th} quantile was arbitrarily chosen as it balances high productivity expectations while accommodating some measurement errors, whereas the 99^{th} quantile was avoided given the instability of model in extreme quantile levels (MAKOWSKI; DORÉ; MONOD, 2007). CL and SR were estimated for the total number of observations and for observations divided by grape skin color. Chain convergence was assessed through trace plots (KRUSCHKE, 2014) and Gelman-Rubin statistics (GELMAN; RUBIN, 1992) while ESS was used to measure chain effectiveness.

Uniform distributions were used for change point *priors*, defining equal probability to the entire range between the lowest and the 95^{th} quantile values of the explanatory variables, *i.e.* the nutrient concentrations, in order to reduce the impact of outliers. In such strategy it is assumed that the advantage of prior knowledge is not being leveraged and the parameter derives almost entirely from the data, thus similar to the frequentist approach. Sensitivity analysis were performed to evaluate the impact of *prior* and quantile changes on results. Goodness-of-fit was measured by comparing statistical summaries – mean, standard deviation (sd), first quartile (Q1), median, third quartile (Q3), interquartile range (IQR), maximum, minimum and the 98th quantile (τ_{98th}) – between observed (y) and simulated data (y^{rep}) generated by the fitted models (KRUSCHKE, 2014).

Modeling was performed using JAGS program (PLUMMER, 2003), implemented through the 'R2*rjags'* package (SU; YAJIMA, 2021), and *posterior* density intervals were obtained using *'HDInterval'* package (MEREDITH; KRUSCHKE, 2020). Data pre-processing and statistical analysis were performed in R (R CORE TEAM, 2021) using RStudio environment (RSTUDIO TEAM, 2020).

5 RESULTS

5.1 EXPLORATORY DATA ANALYSIS

Average yield for the soil sample subset was 9.08 Mg ha^{-1} (n = 539), ranging from 1.98 Mg ha^{-1} (2002, n = 17) to 18.70 Mg ha^{-1} (1999, n = 15). All soil samples had clay content ≤ 20%, cation exchange capacity (CEC) ≤ 7.5 $cmol_c$ dm^{-3} and soil organic matter (SOM) ≤ 2.5g kg^{-1} (Table 1). The average yield of the leaf sample subset was 10.83 Mg ha^{-1}, ranging from 6.09 Mg ha^{-1} (2014, n = 26) to 12.21 Mg ha^{-1} (2007, n = 105) (Table 2).

Table 1 – Descriptive statistics of yield, nutrient concentrations and properties for soil samples (0-20 cm) collected in commercial vineyards from Campanha Gaúcha, Rio Grande do Sul, Brazil.

	n	unit	mean	sd	min	Q1	median	Q3	max	histogram
yield	539	*Mg ha^{-1}*	9.08	4.80	0.14	5.74	8.65	11.92	26.13	
P	539	*mg dm^{-3}*	30.86	13.43	3.70	21.80	29.00	37.00	94.20	
K	539	*mg dm^{-3}*	65.41	18.50	28.00	52.00	64.00	76.00	136.00	
Ca	539	*$cmol_c$ dm^{-3}*	2.05	0.74	0.54	1.52	1.94	2.45	5.10	
Mg	539	*$cmol_c$ dm^{-3}*	0.72	0.30	0.19	0.51	0.68	0.90	2.60	
S	523	*mg dm^{-3}*	6.57	4.02	0.20	3.70	6.00	8.10	28.60	
Cu	523	*mg dm^{-3}*	20.57	14.08	0.20	6.45	21.30	30.74	71.01	
Zn	523	*mg dm^{-3}*	5.07	2.83	0.80	3.00	4.50	6.80	25.00	
B	523	*mg dm^{-3}*	0.36	0.19	0.10	0.30	0.30	0.40	1.40	
Mn	226	*mg dm^{-3}*	18.43	10.66	2.00	11.00	15.00	24.50	53.10	
pH	539	–	5.73	0.47	4.40	5.50	5.80	6.10	6.90	
CEC	539	*$cmol_c$ dm^{-3}*	2.99	0.98	1.00	2.30	2.80	3.50	7.90	
clay	523	*%*	10.28	2.60	6.00	8.00	10.00	12.00	21.00	
SOM	523	*%*	0.83	0.23	0.40	0.70	0.80	1.00	2.10	

For all variables, white and red grapes were compared using Welch's t-test, since it does not assume equal variance nor equal number of observations between groups. In the soil sample subset white grapes recorded significantly higher average yield (10.2 Mg ha^{-1}, n = 222) when compared to red ones (8.27 Mg ha^{-1}, n = 317). White grapes also had higher soil concentrations of Ca, K, Cu and Zn as well as higher CEC compared to red ones, while no difference was found for P, S, Mg, B, Mn, soil pH, clay content and organic matter (Table 3).

Table 2 – Descriptive statistics of yield and nutrient concentrations for leaf samples (blade + petiole) collected from commercial vines (*Vitis vinfera*) grown in Campanha Gaúcha, Rio Grande do Sul, Brazil.

	n	unit	mean	sd	min	Q1	median	Q3	max	histogram
yield	143	$Mg\ ha^{-1}$	10.83	4.37	1.3	7.62	11.36	13.58	20.61	
N	143	$g\ kg^{-1}$	26.22	5.77	16.0	22.00	26.00	29.00	51.00	
P	143	$g\ kg^{-1}$	3.40	1.09	1.4	2.60	3.30	4.10	7.10	
K	143	$g\ kg^{-1}$	13.25	3.83	1.0	11.00	13.00	15.00	29.00	
Ca	143	$g\ kg^{-1}$	14.40	3.49	8.3	12.00	14.00	16.10	25.00	
Mg	143	$g\ kg^{-1}$	2.93	0.69	1.3	2.40	2.90	3.40	4.90	
S	143	$g\ kg^{-1}$	3.43	0.64	2.3	3.00	3.40	4.00	4.90	
Cu	143	$mg\ kg^{-1}$	100.64	227.09	7.0	11.00	13.00	17.00	1,100.00	
Zn	143	$mg\ kg^{-1}$	195.10	88.45	50.0	134.00	170.00	245.00	504.00	
B	142	$mg\ kg^{-1}$	40.20	14.32	15.0	30.00	37.50	49.00	77.00	
Mn	143	$mg\ kg^{-1}$	524.17	166.19	236.0	397.50	514.00	589.50	1,370.00	
Fe	143	$mg\ kg^{-1}$	110.59	33.50	52.0	90.00	105.00	124.50	299.00	

Table 3 – Descriptive statistics for soil sample data subset divided by grape skin color.

	unit	n_{red}	μ_{red}	n_{white}	μ_{white}	| t |	df	p-value	
yield	$Mg\ ha^{-1}$	317	8.27 b	222	10.24 a	4.59	405.98	0.000	****
P	$mg\ dm^{-3}$	317	30.01 a	222	32.06 a	1.79	516.54	0.074	*ns*
K	$mg\ dm^{-3}$	317	64.09 b	222	67.30 a	2.01	493.32	0.045	*
Ca	$cmol_c\ dm^{-3}$	317	1.99 b	222	2.14 a	2.20	414.12	0.028	*
Mg	$cmol_c\ dm^{-3}$	309	0.71 a	214	0.74 a	1.11	441.35	0.268	*ns*
S	$mg\ dm^{-3}$	309	6.34 a	214	6.89 a	1.53	439.84	0.126	*ns*
Cu	$mg\ dm^{-3}$	309	17.22 b	214	25.42 a	6.96	486.52	0.000	****
Zn	$mg\ dm^{-3}$	309	4.63 b	214	5.71 a	4.39	480.16	0.000	****
B	$mg\ dm^{-3}$	309	0.35 a	214	0.38 a	1.90	472.29	0.058	*ns*
Mn	$mg\ dm^{-3}$	128	17.91 a	98	19.12 a	0.83	189.19	0.407	*ns*
pH	-	317	5.73 a	222	5.73 a	0.09	430.08	0.928	*ns*
CEC	$cmol_c\ dm^{-3}$	317	2.91 b	222	3.10 a	2.20	421.05	0.028	*
clay	%	309	10.22 a	214	10.36 a	0.62	474.38	0.538	*ns*
OM	%	309	0.82 a	214	0.86 a	1.81	414.72	0.070	*ns*

In the row, means followed by the same lowercase letter are not statistically different according to Welch's t-test at 95% confidence interval.
Significance levels: ns ($p > 0.05$), * ($p \leq 0.05$), ** ($p \leq 0.01$), *** ($p \leq 0.001$), **** ($p \leq 0.0001$).

Yields did not differ between grape skin colors in the leaf sample subset. Red grapes had slightly higher N leaf concentration than white ones, while the opposite was true for Ca and B. Average leaf Cu was notoriously higher in white grapes (166.85 mg kg^{-1}) compared to red ones (29.64 mg kg^{-1}), which can be largely explained by the fact that all observation from the 2011 harvest were of white grapes and, in that year, an abnormal high average leaf Cu concentration was registered (562 mg kg^{-1}). No differences between white and red grapes were found for concentrations of P, K, Mg, S, Zn, Mn and Fe in leaves (Table 4).

Table 4 – Descriptive statistics for leaf sample data subset divided by grape skin color.

	unit	$\mathbf{n_{red}}$	$\boldsymbol{\mu_{red}}$	$\mathbf{n_{white}}$	$\boldsymbol{\mu_{white}}$	**| t |**	**df**	**p-value**	
yield	*Mg ha^{-1}*	69	11.11 a	74	10.56 a	0.76	136.13	0.451	*ns*
N	*g kg^{-1}*	69	27.20 a	74	25.31 b	1.99	141.00	0.049	*
P	*g kg^{-1}*	69	3.49 a	74	3.31 a	0.99	137.62	0.326	*ns*
K	*g kg^{-1}*	69	12.87 a	74	13.61 a	1.15	140.97	0.252	*ns*
Ca	*g kg^{-1}*	69	13.75 b	74	15.00 a	2.16	139.26	0.033	*
Mg	*g kg^{-1}*	69	2.81 a	74	3.03 a	1.97	137.58	0.051	*ns*
S	*g kg^{-1}*	69	3.51 a	74	3.36 a	1.36	140.53	0.177	*ns*
Cu	*mg kg^{-1}*	69	29.64b	74	166.85 a	3.89	84.15	0.000	***
Zn	*mg kg^{-1}*	69	194.67 a	74	195.50 a	0.06	140.46	0.955	*ns*
B	*mg kg^{-1}*	68	36.84 b	74	43.30 a	2.75	139.12	0.007	**
Mn	*mg kg^{-1}*	69	528.45 a	74	520.18 a	0.30	140.23	0.767	*ns*
Fe	*mg kg^{-1}*	69	113.93 a	74	107.49 a	1.15	137.16	0.254	*ns*

In the row, means followed by the same lowercase letter are not statistically different according to Welch's t-test at 95% confidence interval.
Significance levels: ns ($p > 0.05$), * ($p \leq 0.05$), ** ($p \leq 0.01$), *** ($p \leq 0.001$), **** ($p \leq 0.0001$).

5.2 CRITICAL LEVELS AND SUFFICIENCY RANGES

Boundary lines were successfully generated using BSQR model to estimate LP function parameters from commercial vineyard's data. Nutrient CL and SR for macro (Figure 2) and micronutrients (Figure 3) in vineyard soils (0 – 20 cm), as well as in grapevine leaves (blade + petiole) (Figures 4 and 5) were estimated in relation to grape relative yields conditional on the 98th quantile for all nutrients under study.

Figure 2 – Boundary lines obtained by BSQR using LP functions to describe the relationships between macronutrients in vineyard soils (0 – 20 cm) and relative yields. Vertical red dashed lines represent nutrient CL and vertical shaded rectangles represent nutrient SR (95% HDI). Data points beyond current x-axis scales were omitted to improve visualization.

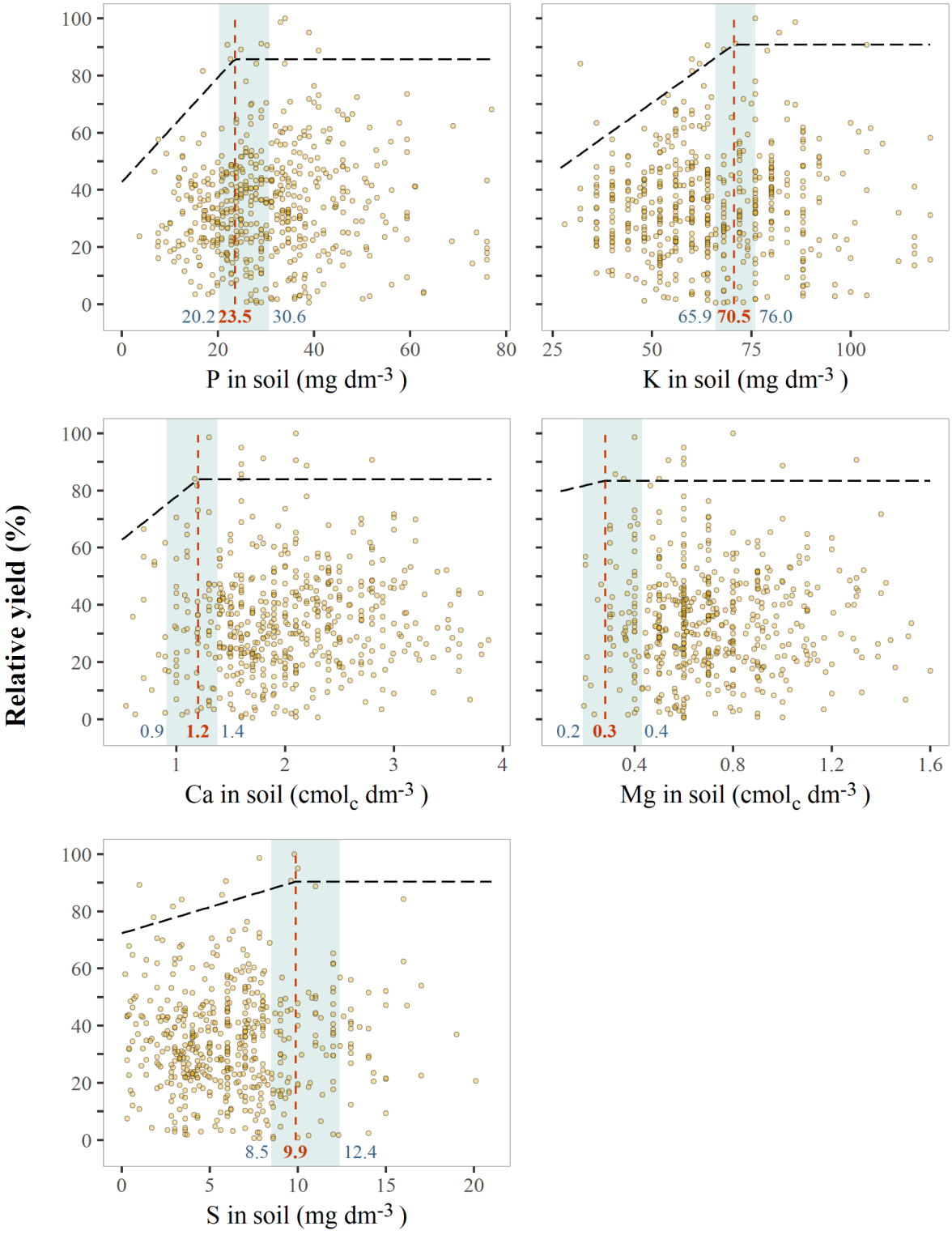


Figure 3 – Boundary lines obtained by BSQR using LP functions to describe the relationships between micronutrients in vineyard soils (0 – 20 cm) and relative yields. Vertical red dashed lines represent nutrient CL and vertical shaded rectangles represent nutrient SR (95% HDI). Data points beyond current x-axis scales were omitted to improve visualization.

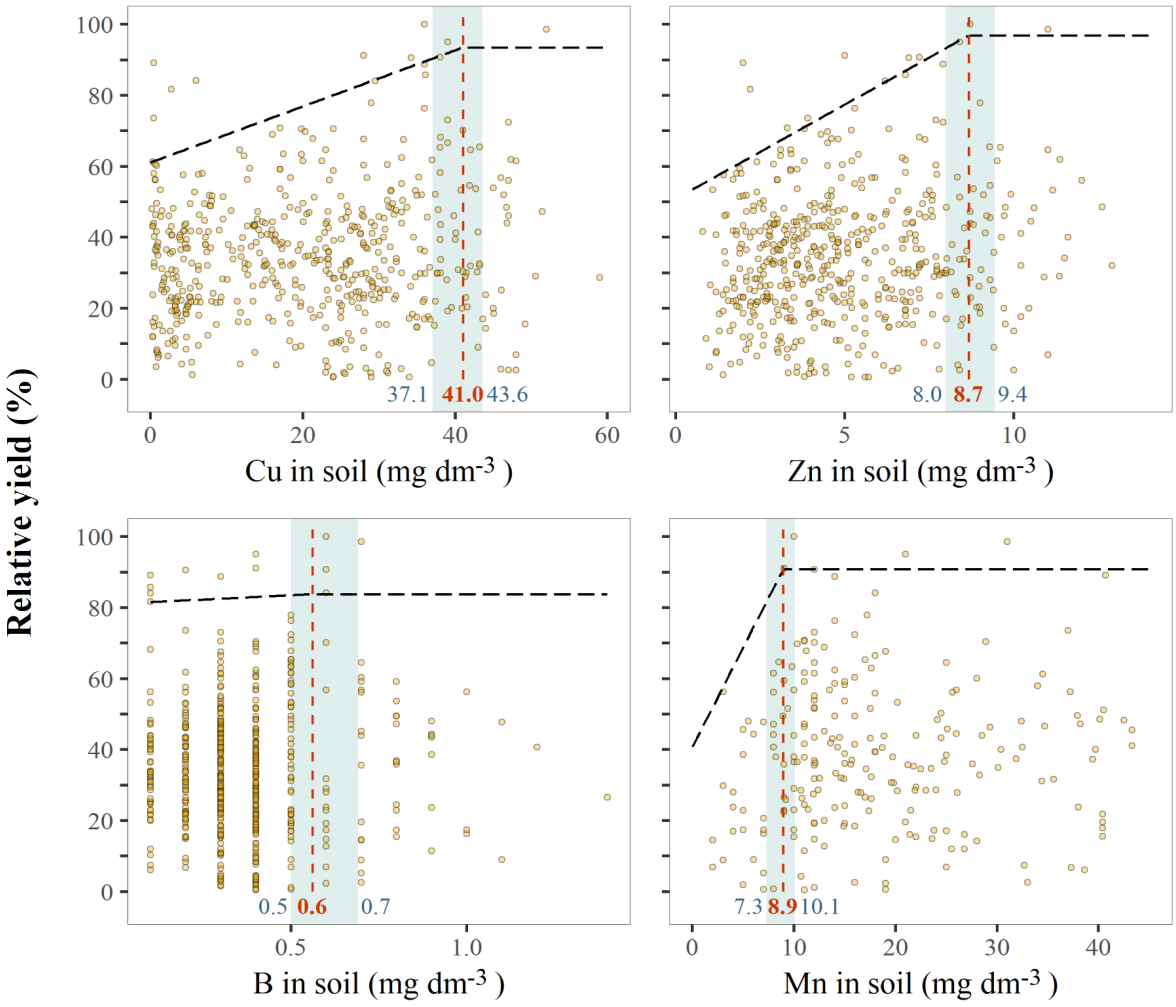


Figure 4 – Boundary lines obtained by BSQR using LP functions to describe the relationships between macronutrients in grapevine leaves (blade + petiole) and relative yields. Vertical red dashed lines represent nutrient CL and vertical shaded rectangles represent nutrient SR (95% HDI). Data points beyond current x-axis scales were omitted to improve visualization.

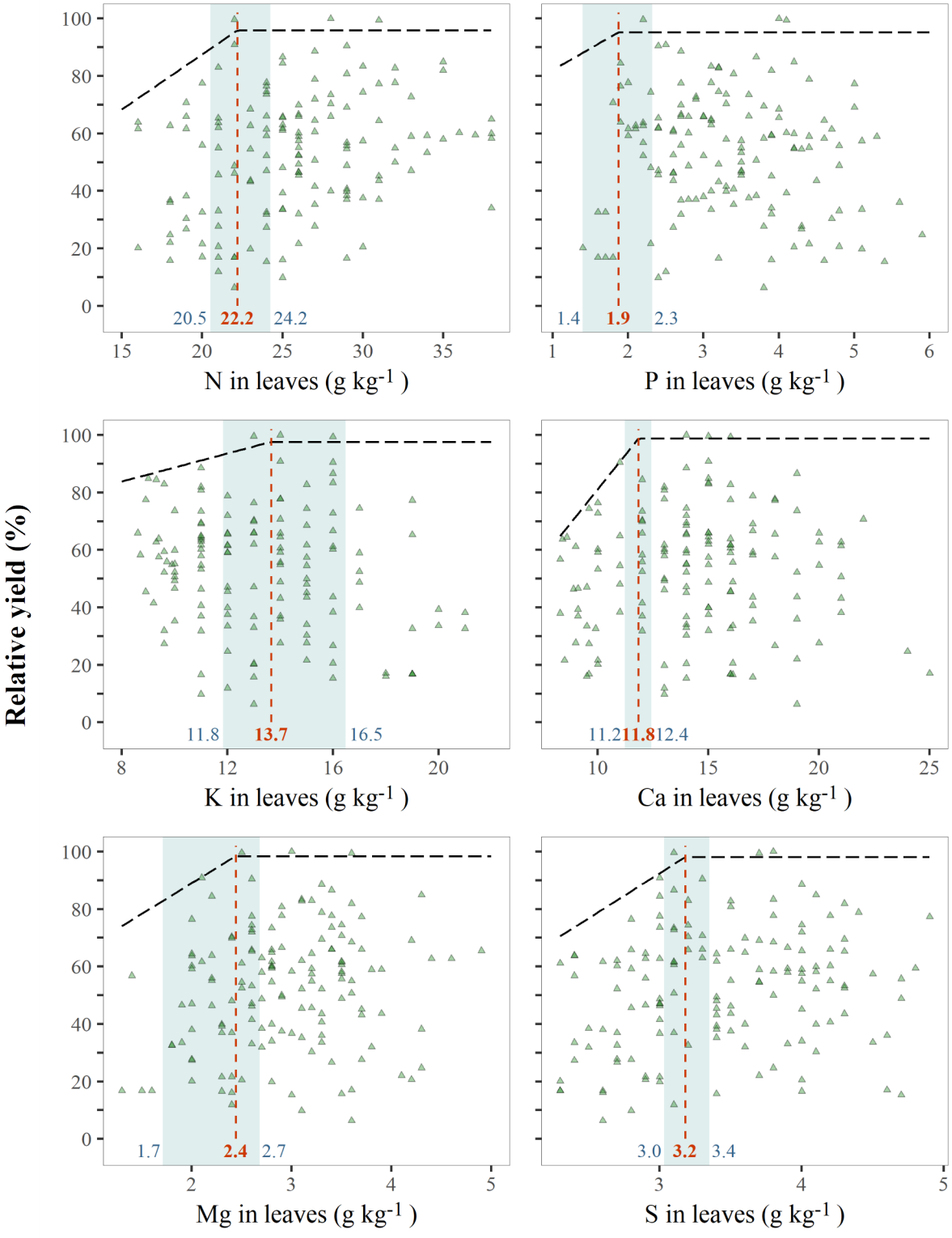
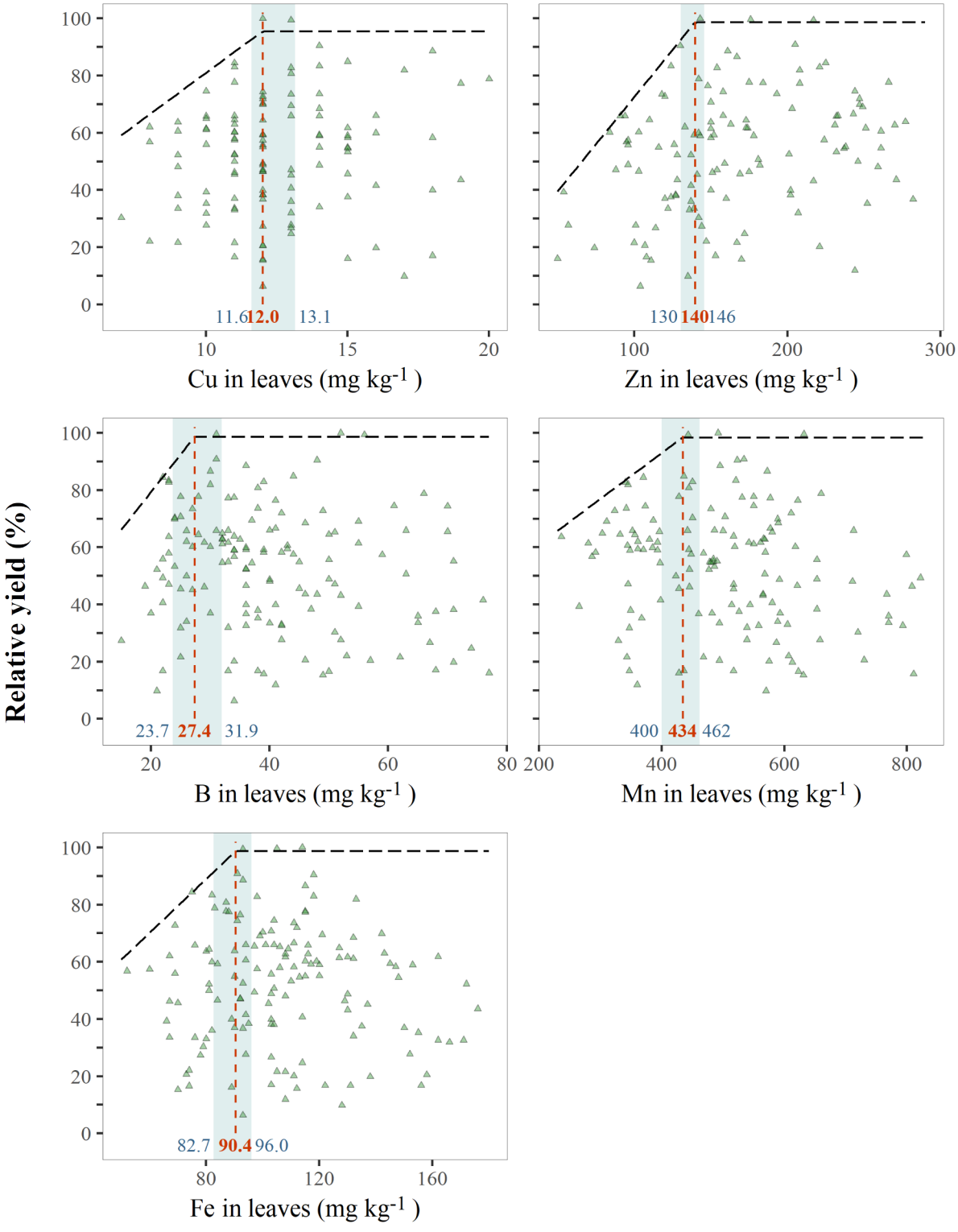


Figure 5 – Boundary lines obtained by BSQR using LP functions to describe the relationships between micronutrients in grapevine leaves (blade + petiole) and relative yields. Vertical red dashed lines represent nutrient CL and vertical shaded rectangles represent nutrient SR (95% HDI). Data points beyond current x-axis scales were omitted to improve visualization.



5.2.1 Red vs. white grapes

Soil and leaf nutrients CL and SR were estimated separately for white and red grapes. For each nutrient, full posterior distributions of the differences between the two groups were calculated from the simulated samples to verify whether densities did include zero. Clear non-zero differences were observed in soil nutrients, where red grapes had higher CL for P and Mn compared to white ones while Zn was lower (Table 5). Regarding leaf nutrients, red grapes had higher K and lower Mn CL values than white grapes (Table 6). All the remainder variables included zero in their 95% HDI, therefore no distinction between grape skin color groups could be assumed (Figure 6).

Figure 6 – Distribution of the relative differences between red and white grapes CL samples for nutrients in soil (a) and leaves (b) generated by BSQR model. Thick and thin lines represent 68% and 95% probability density respectively.

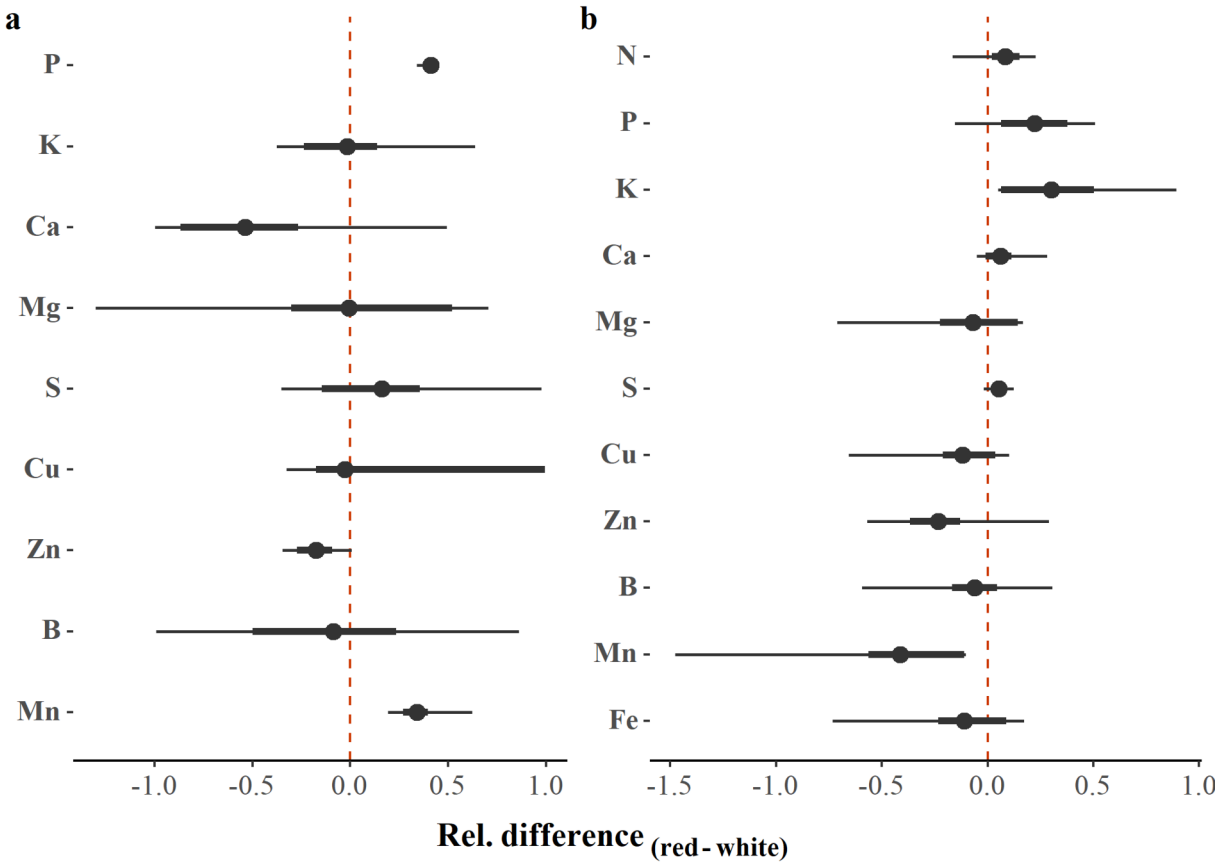


Table 5 – CL and SR of soil macro and micronutrients (0-20cm) for red and white grapes estimated by BSQR model.

	unit	CL_{red}	SR_{red}	CL_{white}	SR_{white}
			Macronutrients		
P	$mg\ dm^{-3}$	38.3	36.7 – 39.0	22.5	20.9 – 25.0
K	$mg\ dm^{-3}$	77.1	59.4 – 82.0	76.2	28.0 – 93.5
Ca	$cmol_c\ dm^{-3}$	0.8	0.7 – 1.9	1.3	0.5 – 1.5
Mg	$cmol_c\ dm^{-3}$	0.3	0.2 – 0.5	0.3	0.2 – 0.6
S	$mg\ dm^{-3}$	9.7	8.6 – 10.0	8	0.2 – 12.6
			Micronutrients		
Cu	$mg\ dm^{-3}$	35.7	32.9 – 39.0	37.3	0.2 – 46.3
Zn	$mg\ dm^{-3}$	7.8	7.1 – 8.4	9.2	8.3 – 10.2
B	$mg\ dm^{-3}$	0.5	0.3 – 0.8	0.6	0.2 – 0.7
Mn	$mg\ dm^{-3}$	14.1	12.6 – 15.3	9.3	5.5 – 10.7

Table 6 – CL and SR values of leaf (blade + petiole) macro and micronutrients for red and white grapes estimated by BSQR model.

	unit	CL_{red}	SR_{red}	CL_{white}	SR_{white}
			Macronutrients		
N	$g\ kg^{-1}$	24.1	19.1 – 27.1	22.2	19.9 – 23.3
P	$g\ kg^{-1}$	2.8	1.9 – 3.3	2.2	1.4 – 2.4
K	$g\ kg^{-1}$	14.7	12.8 – 17.9	10.8	1.7 – 13.0
Ca	$g\ kg^{-1}$	11.8	11.2 – 12.4	11.1	8.4 – 12.2
Mg	$g\ kg^{-1}$	2.4	1.4 – 2.8	2.5	2.4 – 2.8
S	$g\ kg^{-1}$	3.3	3.1 – 3.5	3.1	3.0 – 3.2
			Micronutrients		
Cu	$mg\ kg^{-1}$	11.9	8.1 – 13.2	13.1	11.3 – 15.7
Zn	$mg\ kg^{-1}$	135	110 – 147	168	105 – 180
B	$mg\ kg^{-1}$	27	15.0 – 31.9	28.7	25.3 – 31.0
Mn	$mg\ kg^{-1}$	426	247 – 460	592	480 – 667
Fe	$mg\ kg^{-1}$	87	56.2 – 96.1	93.8	77.9 – 108.1

5.3 VINEYARD NUTRITIONAL STATUS

Estimated CL and SR were compared to average nutrient concentrations in both soil and leaves in each harvest to assess the nutritional status of the vineyards if these new reference values were to be applied. Regarding soil nutrients, concentrations of P, Ca, Mg and Mn would be consistently above needs for optimal yields, where few harvests had average values within SR but mostly beyond SR upper limit. Soil K oscillated between sufficiency, surplus and deficit along the years while S, Zn and B were consistently below recommendations from 2004 and on. Soil Cu was the only nutrient reported deficient for all harvests (Table 7). Nutrient concentrations in leaves were mostly above or within SR in all harvests, with only a few exceptions in 2011 (N and S) and 2014 (Zn) (Table 8).

Table 7 – Average vineyard soil nutrient contents by harvest. Blue (bold), black (plain) and red (italic) colors indicate nutrient surplus, sufficiency and deficiency, respectively, when compared to estimated CL and SR.

	unit	1998	1999	2000	2001	2002	2003	2004	2005	2006	2008	2010	2012	2017	2018
P	$mg\ dm^{-3}$	**32.7**	**33.3**	24.6	25.6	**31.2**	**48.5**	**39.6**	**39.6**	**37.3**	**33.4**	21.8	**32.8**	**36.6**	27.5
K	$mg\ dm^{-3}$	*65.7*	**81.3**	*60.1*	*59.9*	*59.7*	*62.6*	*58.8*	**79.6**	69.0	**81.3**	*51.0*	68.7	*61.1*	*49.3*
Ca	$cmol_c\ dm^{-3}$	**1.6**	**1.9**	**1.9**	**1.6**	**1.7**	**2.6**	1.3	**2.3**	**1.5**	**2.4**	**2.2**	**2.0**	**1.7**	**2.0**
Mg	$cmol_c\ dm^{-3}$	**0.7**	**0.8**	**0.9**	**0.7**	**0.7**	**0.8**	**0.5**	**0.9**	**0.6**	**0.7**	**0.8**	**0.8**	0.4	**0.5**
S	$mg\ dm^{-3}$	9.4	11.3	8.6	*5.6*	9.1	–	8.5	*7.3*	*7.5*	*4.4*	*5.5*	8.5	*4.6*	*4.5*
Cu	$mg\ dm^{-3}$	*17.9*	*35.7*	*16.8*	*29.6*	*25.8*	–	*29.2*	37.2	*25.9*	*11.1*	*18.5*	*24.5*	*25.4*	*14.7*
Zn	$mg\ dm^{-3}$	8.1	8.1	*3.6*	*5.8*	*4.9*	–	*4.7*	*7.4*	*4.5*	*4.6*	*3.4*	*6.3*	*6.3*	*3.6*
B	$mg\ dm^{-3}$	0.6	0.5	**0.9**	0.7	0.6	–	*0.4*	0.5	*0.4*	*0.3*	*0.3*	*0.3*	*0.1*	*0.3*
Mn	$mg\ dm^{-3}$	**13.7**	**15.9**	8.3	7.6	**16.4**	–	**13.1**	**13.1**	**14.0**	**24.5**	–	–	–	–

Table 8 – Average grapevine leaf (blade + petiole) nutrient contents by harvest. Blue (bold), black (plain) and red (italic) colors indicate nutrient surplus, sufficiency and deficiency, respectively, when compared to estimated CL and SR.

	unit	2007	2011	2014
N	$g\ kg^{-1}$	**27.8**	*19.7*	23.1
P	$g\ kg^{-1}$	**3.3**	1.8	**4.7**
K	$g\ kg^{-1}$	12.4	14.2	16.4
Ca	$g\ kg^{-1}$	**14.0**	**15.7**	**15.3**
Mg	$g\ kg^{-1}$	**2.9**	2.5	**3.1**
S	$g\ kg^{-1}$	**3.5**	*2.7*	**3.5**
Cu	$mg\ kg^{-1}$	**69.9**	**562.0**	11.9
Zn	$mg\ kg^{-1}$	**204.0**	**292.0**	*116.0*
B	$mg\ kg^{-1}$	**37.5**	**32.8**	**54.4**
Mn	$mg\ kg^{-1}$	**483.0**	**525.0**	**692.0**
Fe	$mg\ kg^{-1}$	**113.5**	**125.7**	92.1

5.4 MODEL ASSESSMENTS

5.4.1 Chain convergence and efficiency

Gelman-Rubin statistics suggest convergence of nearly all chains for all model parameters, *i.e.* slope (β_1), change point (*cp*) and plateau (β_0). Leaf Mn was the only exception, with $\hat{R}$ values slightly above 1.1 for *cp* and β_1, indicating that part of the chains settled in different values and a longer run should be performed (Table 9). ESS values point to ineffective chains affected by autocorrelation in the *cp* estimates of soil P and leaf Cu and Mn, which reduces parameter precision. It is worth noting that CL of white and red grapes were different for soil P and leaf Mn, which may have interfered in chain behavior when data was analyzed altogether. Moreover, leaf Cu and Mn had samples with few extreme values, resulting in uniform *prior* distributions with wide ranges and parameter estimation may suffer when small datasets are modeled with too vague *priors*.

Table 9: Gelman-Rubin statistics ($\hat{R}$) and Effective Sample Size (ESS) for slope (β_1), change point (*cp*) and plateau (β_0) parameters estimates obtained by BSQR model.

	cp		***β₁***		***β₀***	
	R̂	**ESS**	**R̂**	**ESS**	**R̂**	**ESS**
			soil nutrients			
P	1.004	740	1.002	1,600	1.004	750
K	1.002	2,400	1.002	3,400	1.002	3,200
Ca	1.004	2,300	1.002	8,500	1.001	6,700
Mg	1.003	2,700	1.002	3,900	1.001	5,200
S	1.001	9,700	1.002	2,900	1.001	6,000
Cu	1.003	1,300	1.001	10,000	1.002	1,700
Zn	1.001	5,400	1.002	2,100	1.001	5,300
B	1.004	2,600	1.002	2,900	1.001	5,400
Mn	1.003	10,000	1.001	6,200	1.001	10,000
			leaf nutrients			
N	1.002	3,600	1.001	5,200	1.002	2,800
P	1.001	5,300	1.001	10,000	1.001	6,900
K	1.001	10,000	1.001	10,000	1.001	4,100
Ca	1.001	9,100	1.001	10,000	1.001	7,000
Mg	1.002	2,400	1.001	10,000	1.001	7,100
S	1.001	4,200	1.001	10,000	1.001	7,500
Cu	1.007	390	1.001	5,900	1.007	420
Zn	1.002	3,800	1.002	3,200	1.001	10,000
B	1.001	10,000	1.001	9,400	1.001	10,000
Mn	1.156	170	1.137	230	1.002	2,700
Fe	1.005	10,000	1.001	7,200	1.001	10,000

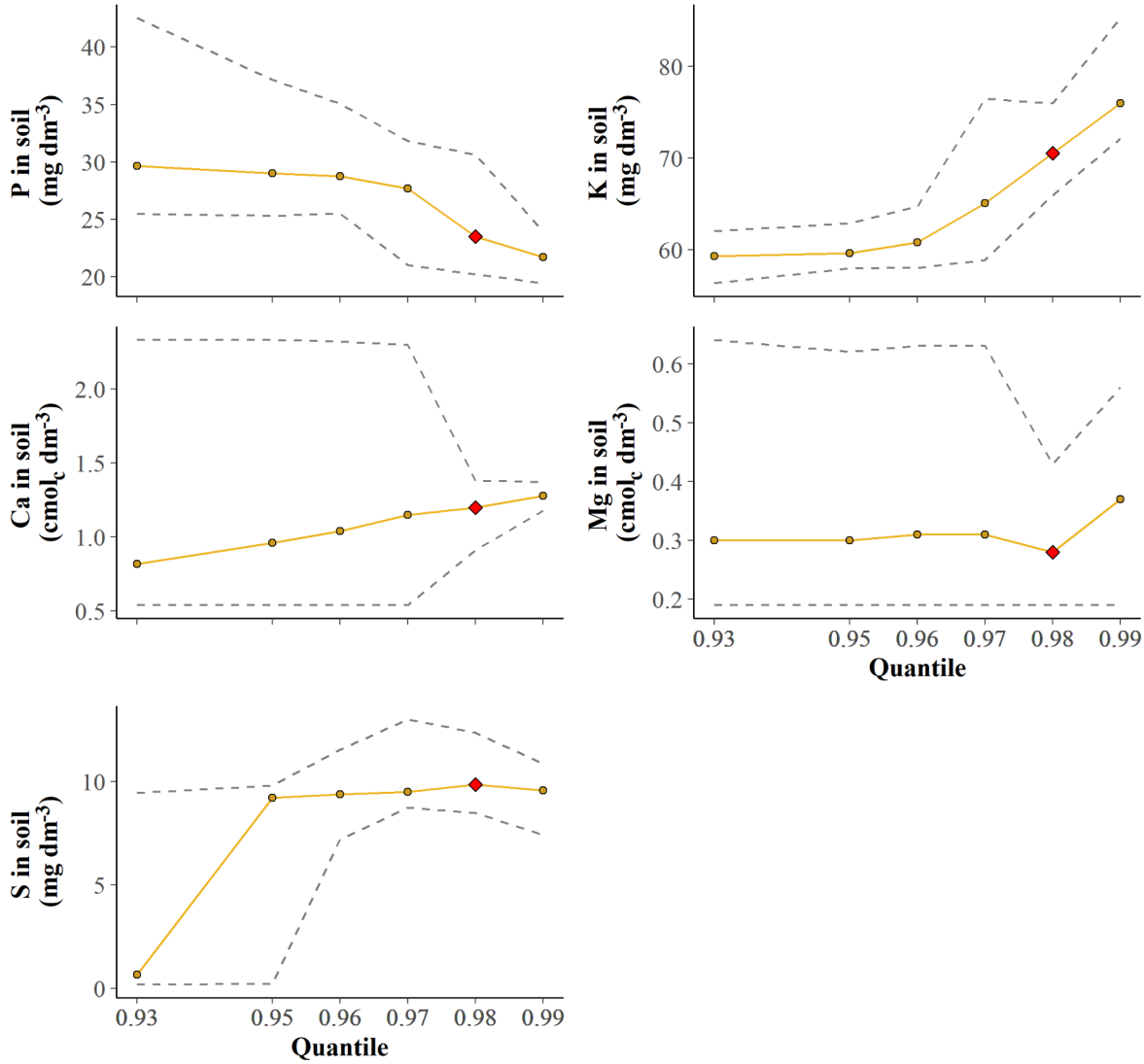
5.4.2 Sensitivity analysis

5.4.2.1 Quantile selection

Soil nutrients

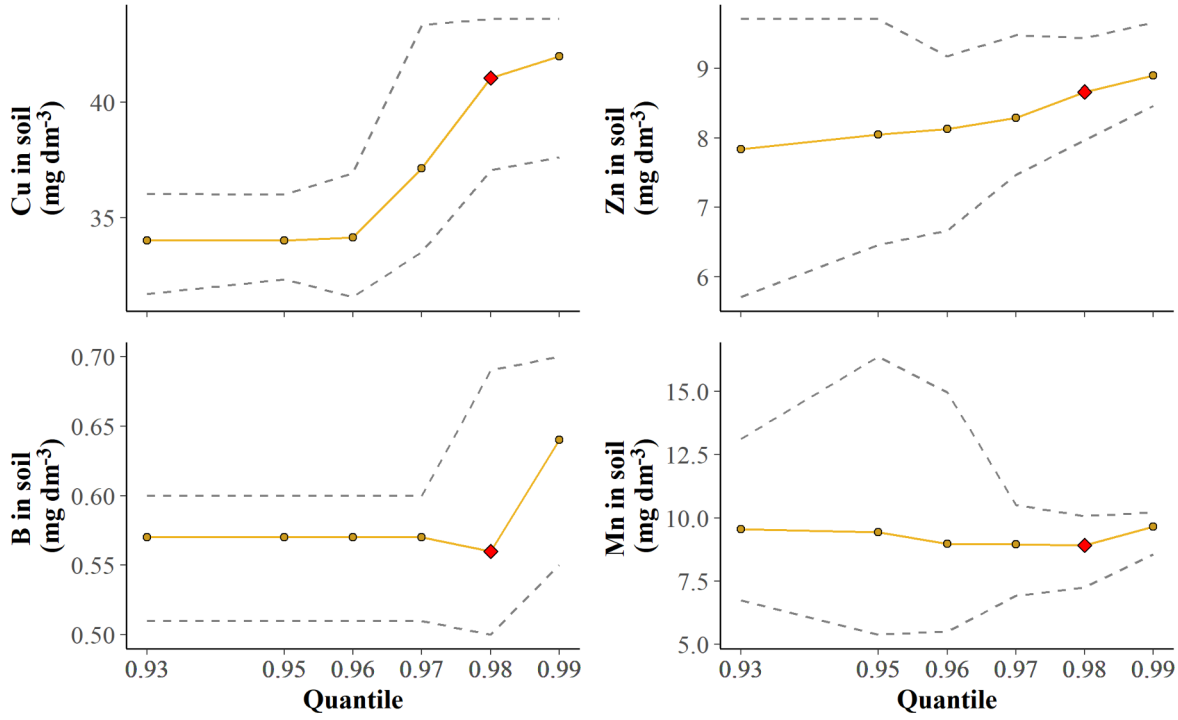
The current model application has shown variable sensitivity to quantile selection regarding soil nutrients (Figures 7 and 8). The expected behavior was that an increase in quantile would lead to an increase in CL estimates, that is, defining the BL on higher yield levels would allow the curve to keep on increasing before reaching plateau. Interestingly, Mg, B and Mn didn't show dramatic changes in CL between 93th and 98th quantiles, although changes in SR were clear, reflecting different levels of parameter credibility across tested values. S was also less sensitive, but there was a steep increase from 93th to 95th quantile. K,

Figure 7 – CL estimates (continuous lines) and 95% credibility intervals (dashed lines) at different quantiles for soil macronutrients (0-20cm). Red diamond highlight the chosen 98th quantile.



Ca, Cu and Zn showed increase in CL with increase of quantile, with most SR narrowing towards the upper values. P had opposite trend, decreasing CL as quantile increases. This behavior can arise from the differences found between red and white grapes, since the predominance of data from one group over another under a particular quantile may vary, leaning the pooled results towards the most influential group at that level. In fact, this behavior disappears when data analysis is performed for each skin color group separately.

Figure 8 – CL estimates (continuous lines) and 95% credibility intervals (dashed lines) at different quantiles for soil micronutrients (0-20cm). Red diamond highlight the chosen 98th quantile.



Clear differences in CL of soil P were exists between white (lower) and red (higher) grapes in all quantile but the 99th (Figure 9). As for Mn, white grapes remained insensitive to quantile selection whereas red grapes show increasing CL, diverging from white grape values from the 97th quantile and on (Figure 10). For Zn, white and red grapes have different CL at lower quantiles but they seem to convergence as quantile rises. A differentiation between red and white grapes is suggested for soil Ca, but the great uncertainty around the parameter values leads to overlaps that do not allow such inference. The remainder soil nutrients didn't show remarkable features that would imply in differentiating red and white grapes.

Figure 9 – Point interval plots of CL estimates for soil macronutrients at different quantiles by grape skin color. Thick and thin lines represent 68% and 95% probability density respectively.

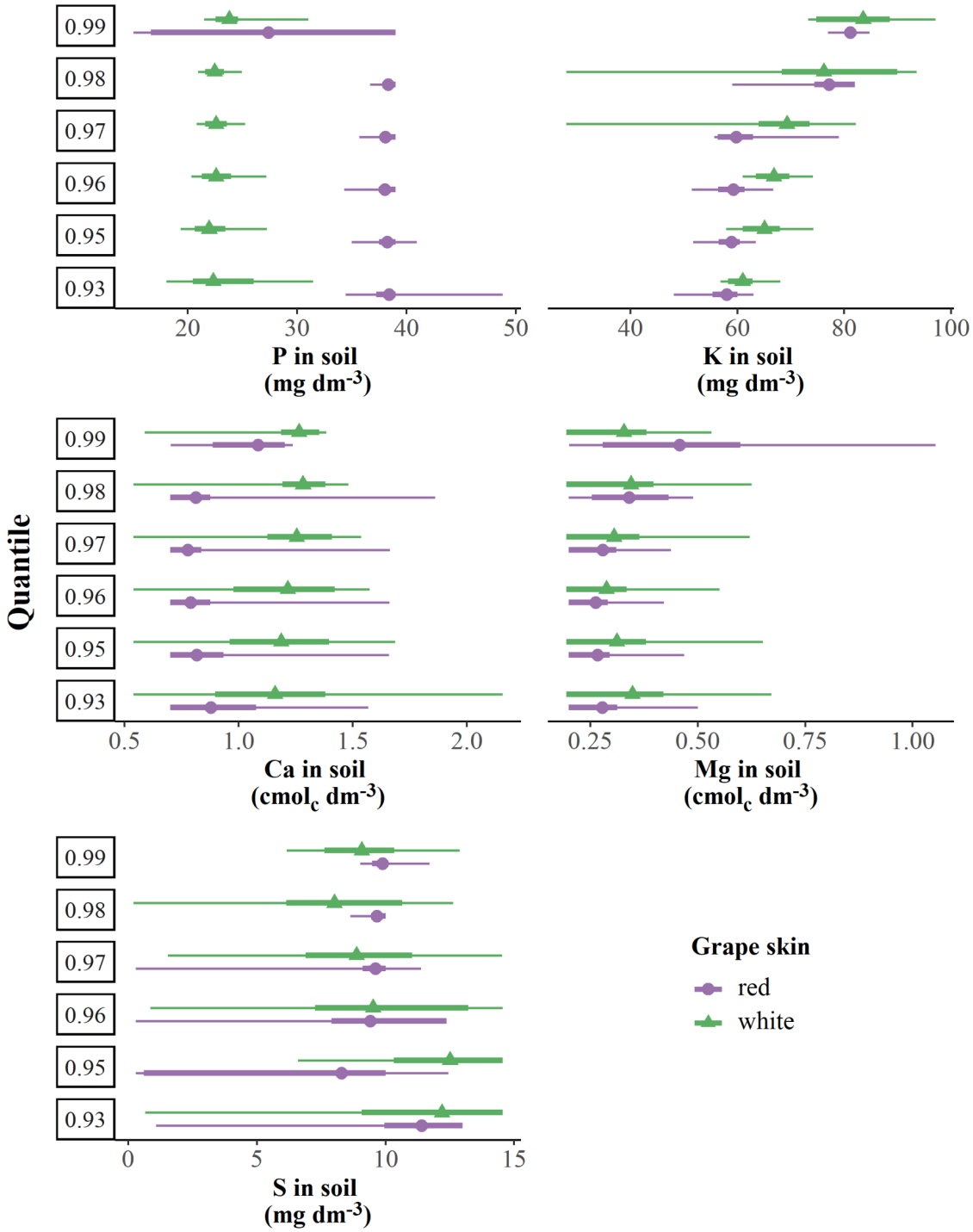
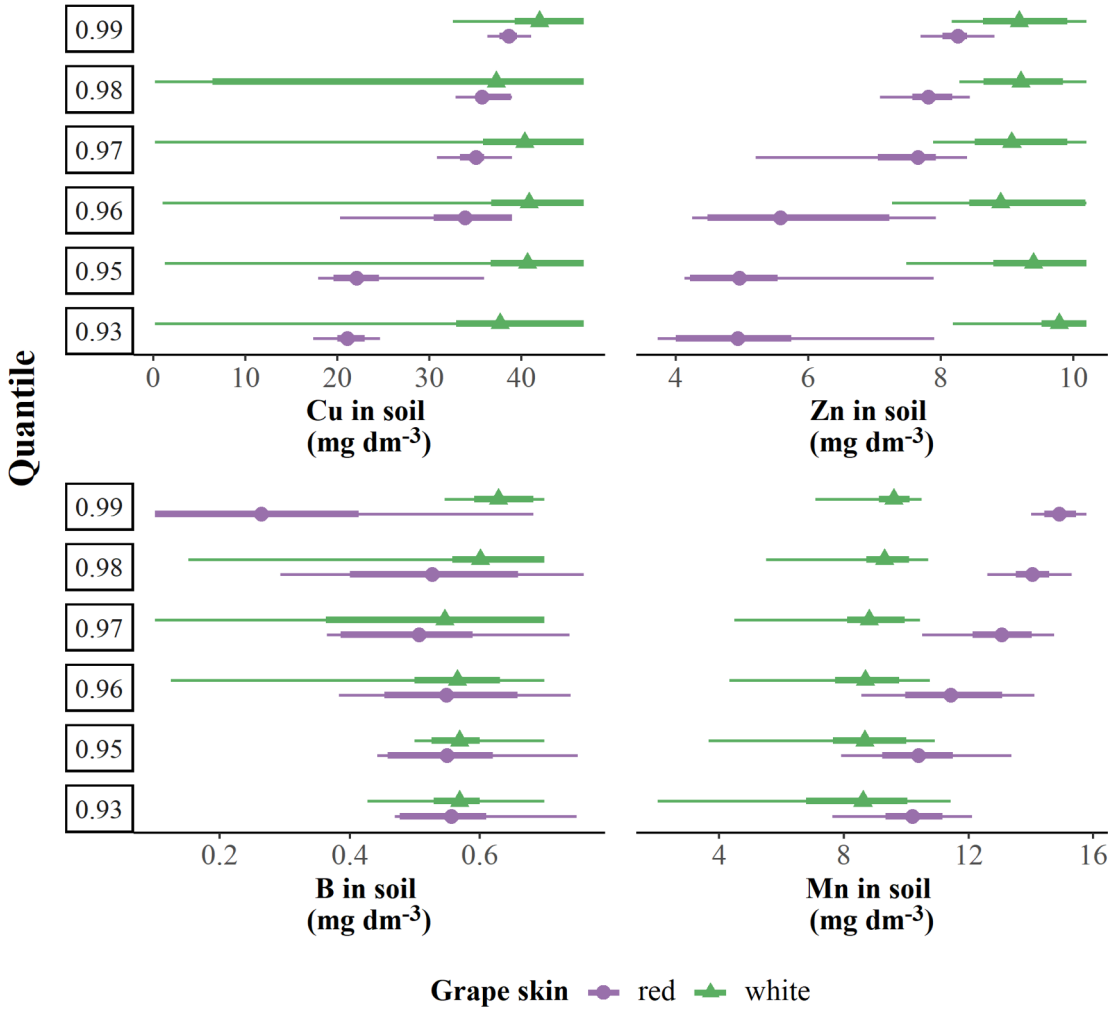


Figure 10 – Point interval plots of CL estimates for soil micronutrients at different quantiles by grape skin color. Thick and thin lines represent 68% and 95% probability density respectively.



Leaf nutrients

Most of estimated CL and SR for leaf nutrient concentrations were also sensitive to quantile selection, being N, P, S and Cu the least affected, with the remainder showing roughly the same increasing pattern as quantile rises (Figures 11 and 12). Leaf Mg is the single exception in which CL drops until the 97th quantile, being followed by a steep increase.

Figure 11 – CL estimates (continuous lines) and 95% credibility intervals (dashed lines) at different quantiles for leaf (blabe + petiole) macronutrients. Red diamond highlight the chosen 98th quantile.

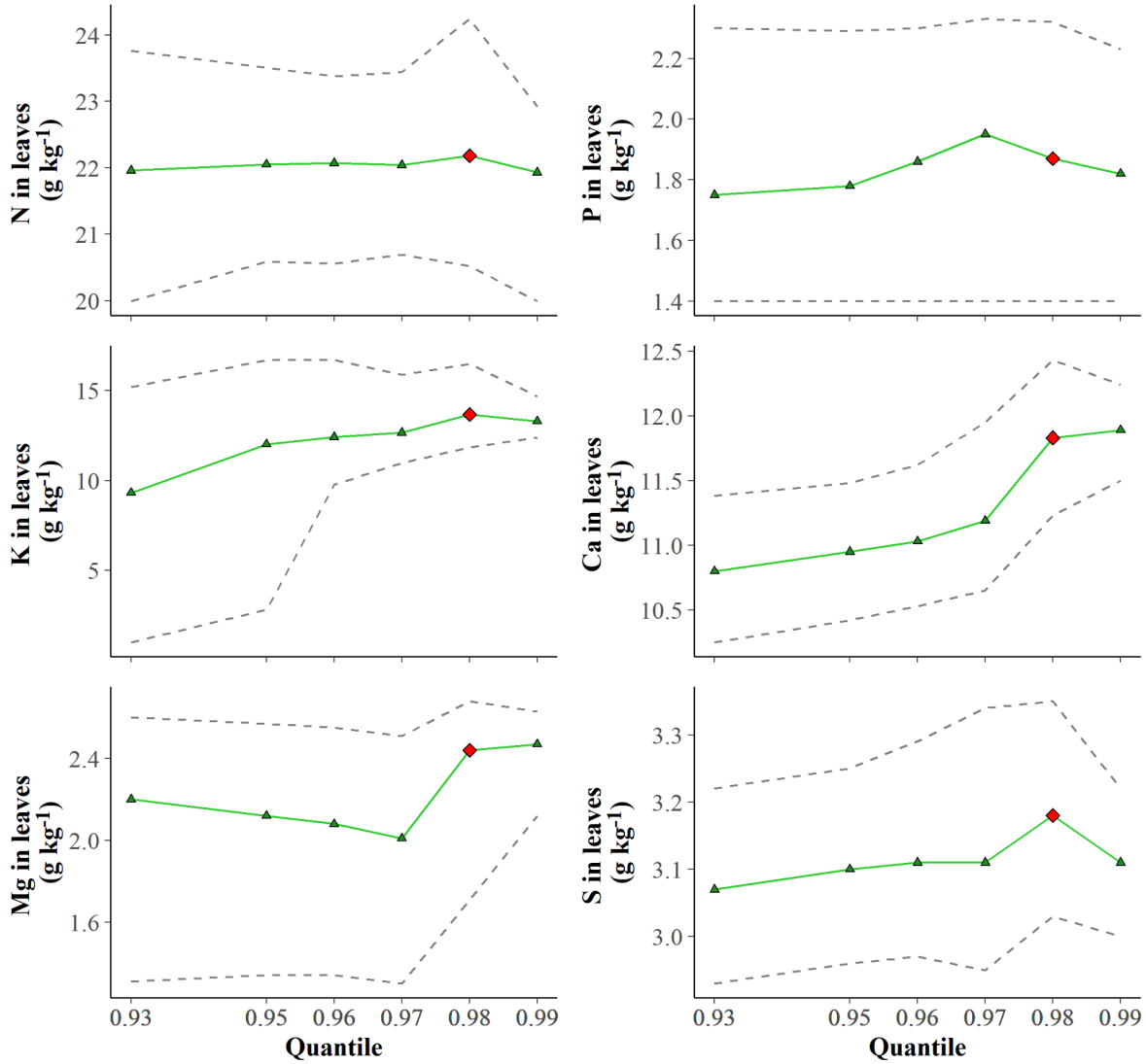
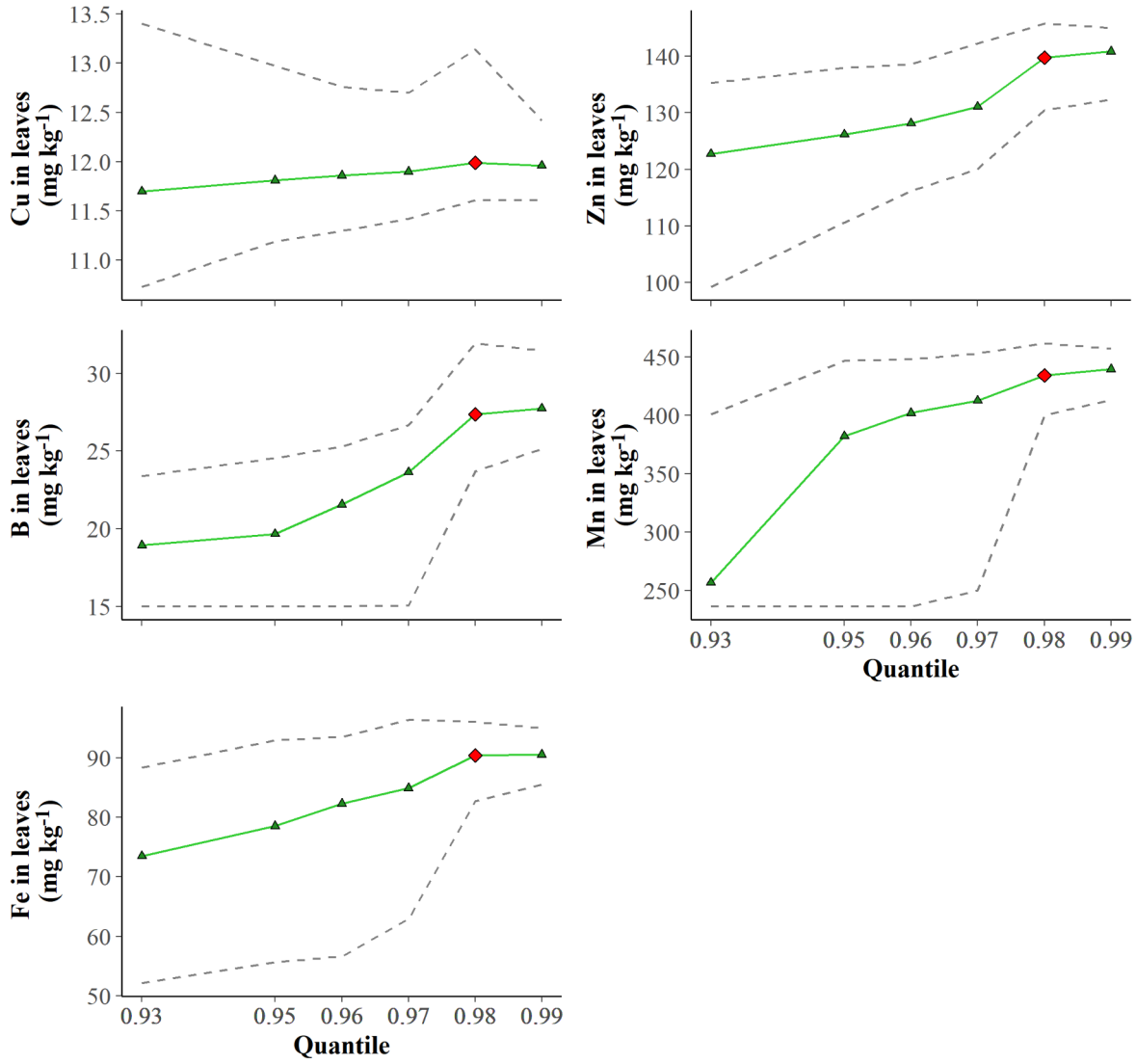


Figure 12 – CL estimates (continuous lines) and 95% credibility intervals (dashed lines) at different quantiles for leaf (blade + petiole) macronutrients. Red diamond highlight the chosen 98th quantile.



When analyzed separately, CL values for leaf K in red grapes remained stable whereas white grapes had an apparent increasing behavior as quantile rises (Figure 13). A diverging pattern is seen in leaf Mn, where white grapes start off with higher values but difference increases together with quantile (Figure 14). CL for Mg in leaves start off showing apparent differentiation between white and red grapes but converges at higher quantiles, whereas Zn, despite not showing clear differences, suggests that CL of white grapes is more dramatically affected by quantile. Nevertheless, parameter uncertainty prevent further differentiation.

Figure 13 – Point interval plots of CL estimates for leaf (blade + petiole) macronutrients at different quantiles by grape skin color. Thick and thin lines represent 68% and 95% probability density respectively.

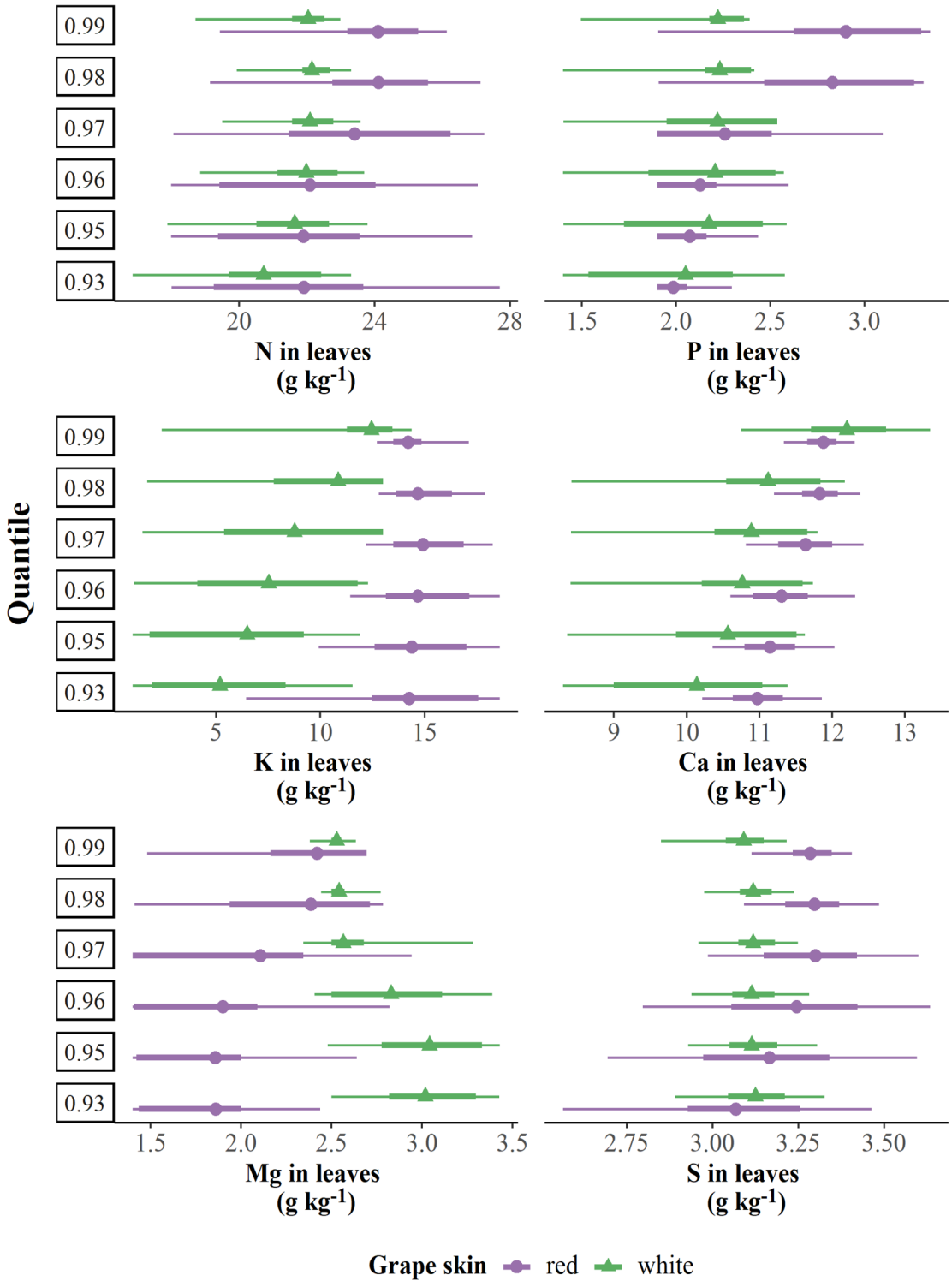
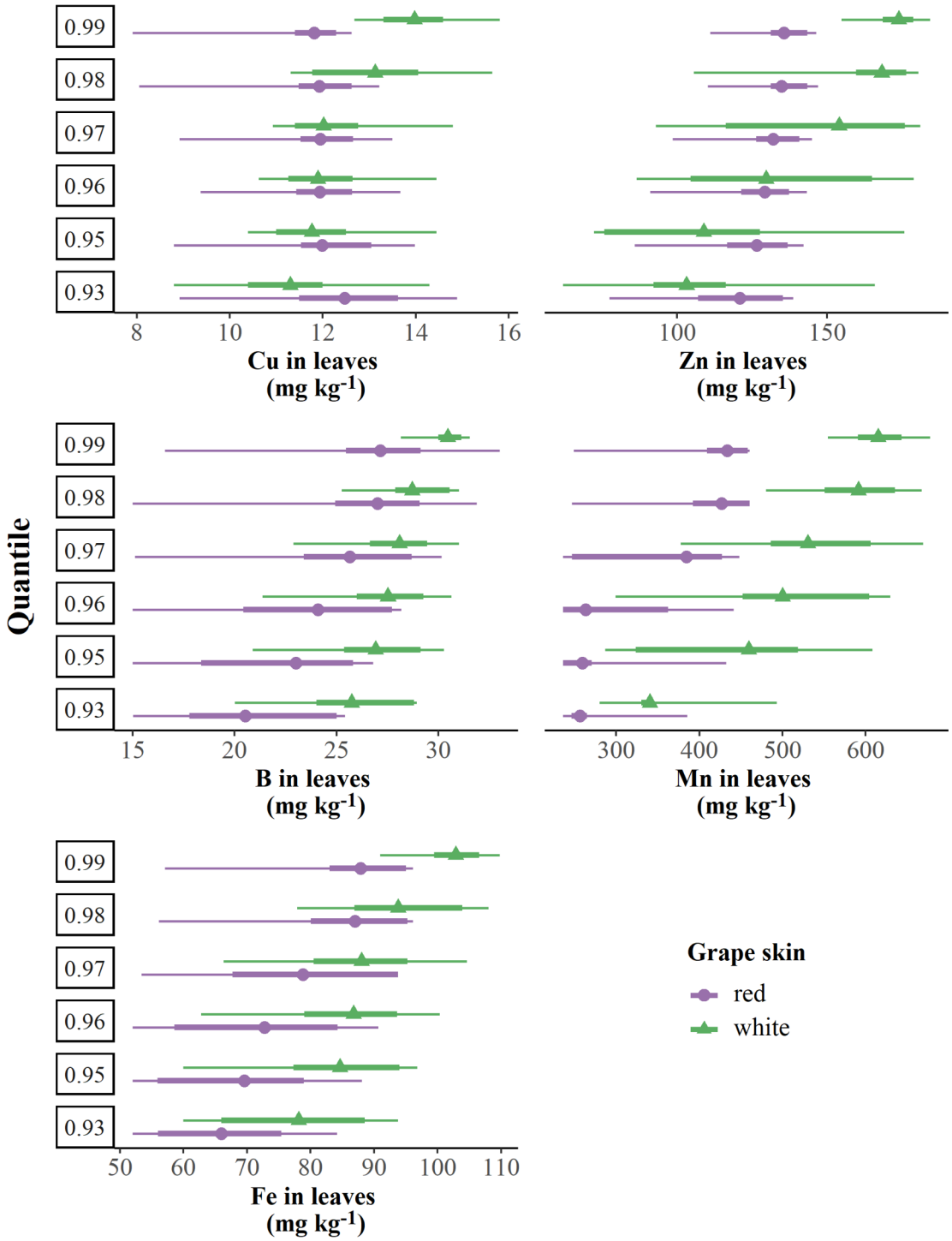


Figure 14 – Point interval plots of CL estimates for leaf (blade + petiole) micronutrients at different quantiles by grape skin color. Thick and thin lines represent 68% and 95% probability density respectively.

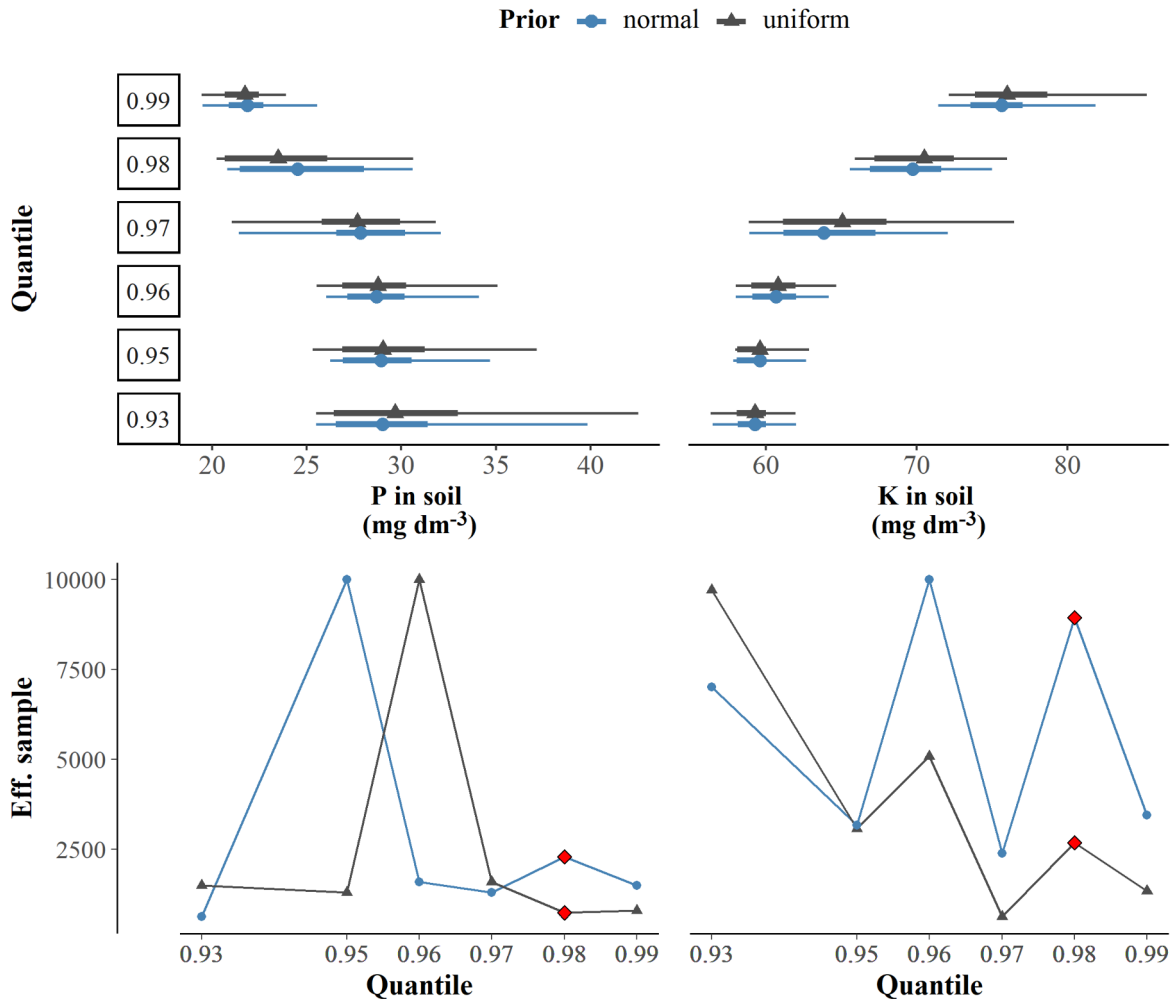


5.4.2.2 Prior choice

In order to evaluate model sensitivity to *prior* choice, the BSQR was used to estimate CL and SR for soil P and K using two different *prior* distributions for the change point (*cp*) parameter, namely normal and uniform. Normal distributions were centered at current CL values proposed in (CQFS-RS/SC, 2016) with reasonably large variance, whereas uniform distribution limits were determined by the minimum and the 95th quantile of the data distribution (17).

$$cp_K \begin{cases} \sim U(28, 97) \\ \sim N(60, 10^2) \end{cases} \qquad cp_P \begin{cases} \sim U(4, 56) \\ \sim N(30, 8^2) \end{cases} \tag{17}$$

Figure 15 – Effects of *prior* choice in CL estimates and number of effective samples evaluated for soil P an K contents regressed on different quantile values. Thick and thin lines represent 68% and 95% probability density respectively. Red dot highlight the 98th quantile.



Estimated CL and SR weren't different between *priors* in any quantile (Figure 15), confirming that the BSQR model using asymmetric Laplace distribution (ALD) to form the likelihood function yields proper *posteriors* even from improper uniform *priors*. The effect of *prior* in the model performance was also assessed using the number of effective samples in a total of 10,000 draws from 4 different chains. The normal *priors* seems to have a very slight advantage over the uniform, but effective samples varied considerably between different quantiles.

5.4.3 Model fit

Model goodness-of-fit was assessed by retrieving 500 simulated samples of relative yield from each fitted model (*i.e.* one for each nutrient) and comparing its summary statistics to the original data. Bayesian p-values were then calculated as the rate in which simulated data exceeded real data, therefore, values close to 0.5 indicate a good fit.

Table 10 – Bayesian p-values for multiple test quantities in posterior predictive checks of BSQR model fit applied to soil and leaf nutrients reference values estimates.

	Test quantity								
	mean	**sd**	**Q1**	**median**	**Q3**	**IQR**	**min**	**max**	τ_{98th}
				soil nutrients					
P	0.230	1.000	0.022	0.982	1.000	1.000	0.000	0.000	0.006
K	0.206	1.000	0.038	0.982	1.000	1.000	0.000	0.000	0.018
Ca	0.244	1.000	0.020	0.994	1.000	1.000	0.000	0.000	0.000
Mg	0.192	1.000	0.010	0.988	1.000	1.000	0.000	0.000	0.000
S	0.218	1.000	0.026	0.982	1.000	1.000	0.000	0.000	0.000
Cu	0.070	1.000	0.034	0.980	1.000	1.000	0.000	0.002	0.004
Zn	0.194	1.000	0.056	0.984	1.000	1.000	0.000	0.060	0.006
B	0.164	1.000	0.026	0.988	1.000	1.000	0.000	0.000	0.000
Mn	0.384	1.000	0.268	0.902	0.994	0.988	0.000	0.000	0.020
				leaf nutrients					
N	0.376	0.988	0.474	0.462	0.986	0.924	0.000	0.048	0.288
P	0.422	0.984	0.506	0.484	0.990	0.944	0.002	0.062	0.288
K	0.348	0.984	0.562	0.428	0.984	0.876	0.000	0.106	0.282
Ca	0.464	0.994	0.490	0.434	0.986	0.942	0.006	0.234	0.712
Mg	0.486	0.994	0.448	0.468	0.990	0.928	0.000	0.152	0.630
S	0.372	0.988	0.444	0.484	0.978	0.918	0.004	0.138	0.428
Cu	0.354	0.956	0.494	0.466	0.976	0.868	0.002	0.060	0.298
Zn	0.490	0.990	0.500	0.446	0.982	0.888	0.004	0.190	0.660
B	0.450	0.998	0.498	0.408	0.992	0.940	0.002	0.210	0.636
Mn	0.492	0.996	0.534	0.578	0.996	0.896	0.000	0.200	0.614
Fe	0.476	0.994	0.514	0.446	0.996	0.932	0.004	0.208	0.658

6 DISCUSSION

6.1 NUTRIENT REFERENCE VALUES

6.1.1 Soil nutrients

Estimated CL and SR for soil nutrients using BSQR on commercial data from vineyards grown in Campanha Gaúcha were in general, consistent with regional reference values for grapevines indicated in CQFS-RS/SC (2016) (Tables 11 and 12), excepted Ca and Mg, which would be classified as "low availability". Estimated CL for soil P is slightly below recommendations of CQFS-RS/SC (2016) as well as Stefanello et al. (2021), whose estimates refer to the Campanha Gaúcha, while K has compatible values and a narrower SR. S and Mn have only minimal thresholds in CQFS-RS/SC (2016) while current BSQR estimates include SR and suggest higher CL for both nutrients. Zn and especially Cu are considerably higher than reviewed references, whereas B is in accordance with most reports and guidelines, providing a very narrow SR.

Table 11 – CL and SR estimated by BSQR for macronutrients in vineyard soils of Campanha Gaúcha, Rio Grande do Sul, Brazil, compared to national and international reports and guidelines.

	Scope	P	K	Ca	Mg	S
	ISO 3166	*mg dm^{-3}*		*cmol$_c$ dm^{-3}*		*mg dm^{-3}*
CL_{BSQR}	**BR-RS**	**23.5**	**70.5**	**1.2**	**0.3**	**9.9**
SR_{BSQR}	**BR-RS**	**20.2 – 30.6**	**65.9 – 76.0**	**0.9 – 1.4**	**0.2 – 0.4**	**8.5 – 12.4**
CQFS-RS/SC (2016)	BR-RS/SC	30.1 – 60.0	61 – 120	> 4.0	> 1.0	> 5.0
Stefanello et al. (2021)	BR-RS	35 – 45	60 – 80	–	–	–
Raij et al. (1997)	BR-SP	31 – 60	121 – 234	> 0.7	> 0.8	> 10
Ribeiro et al. (1999)	BR-MG	22.6 – 33.8	71 – 120	2.4 – 4.0	0.9 – 1.5	14.5 – 21.6
Kurtural et al. (2004)	US-KY	22 – 28	140 – 168	–	0.9 – 1.2	–
Moyer et al. (2018)	US-WA	6 – 8	100 – 220	3 – 9	1 – 2	5 – 20

Table 12 –CL and SR estimated by BSQR for micronutrients in vineyard soils of Campanha Gaúcha, Rio Grande do Sul, Brazil, compared to national and international reports and guidelines.

	Scope	Cu	Zn	B	Mn
	ISO 3166	*mg dm^{-3}*			
CL_{BSQR}	**BR-RS**	**41**	**8.7**	**0.6**	**8.9**
SR_{BSQR}	**BR-RS**	**37.1 – 43.6**	**8.0 – 9.4**	**0.5 – 0.7**	**7.3 – 10.1**
CQFS-RS/SC (2016)	BR-RS/SC	> 0.4	> 0.5	06 – 1.0	> 5.0
Raij et al. (1997)	BR-SP	> 0.8	> 1.2	> 0.6	> 5.0
Ribeiro et al. (1999)	BR-MG	1.3 – 1.8	1.6 – 2.2	0.6 – 0.9	9 – 12
Kurtural et al. (2004)	US-KY	–	4.5 – 5.6	0.8 – 1.1	–
Moyer et al. (2018)	US-WA	0.50 – 0.75	1 – 2	0.6 – 1.0	15 – 20

6.1.2 Leaf nutrients

Estimated CL for grapevine leaf (blade + petiole) concentrations of N, P, K, Mg and Fe obtained by BSQR were consistent with CQFS-RS/SC (2016), presenting narrower SR, while divergences were observed for the other nutrients (Tables 13 and 14). On the other hand, BSQR results related well with standards specifically developed for the Campanha Gaúcha region (ROZANE et al., 2020; STEFANELLO et al., 2021b).

Table 13 – CL and SR estimated by BSQR for macronutrients in grapevine leaves (blade + petiole) grown in Campanha Gaúcha, , Rio Grande do Sul, Brazil, compared to national and international reports and guidelines.

	Scope	N	P	K	Ca	Mg	S
	ISO 3166			*g kg^{-1}*			
CL_{BSQR}	**BR-RS**	**22.2**	**1.9**	**13.7**	**11.8**	**2.4**	**3.2**
SR_{BSQR}	**BR-RS**	**20.5 – 24.2**	**1.4 – 2.3**	**11.8 – 16.5**	**11.2– 12.4**	**1.7 – 2.7**	**3.0 – 3.4**
CQFS-RS/SC (2016)	BR-RS/SC	16 – 24	1.2 – 4.0	8 – 16	16 – 24	2.0 – 6.0	–
Rozane et al. (2020)	BR-RS	24 – 30	2.9 – 3.8	11 – 14	12 – 16	2.6 – 3.3	3.1 – 3.8
Stefanello et al. (2021)	BR-RS	18.2 – 21.7	1.1 – 1.4	15.3 – 18.2	–	–	–
Pauletti and Motta (2017)	BR-PR	28	2	12	20	4	2
Malavolta et al. (1997)	BR-SP	25 – 27	2.0 – 3.0	15 – 20	30 – 40	3.0 – 4.0	2.0 – 3.0
Raij et al. (1997)	BR-SP	30 – 35	2.4 – 2.9	15 – 20	13 – 18	4.8 – 5.3	3.3 – 3.8
Ribeiro et al. (1999)	BR-MG	25	2	15	4	4	–
Moyer et al. (2018)	US-WA	22.5 – 32.5	1.5 – 3.0	5 – 10	2.5 – 5.0	10 – 30	–
García-Escudero et al. (2013)	ES-LO	9.4 – 11.0	3.0 – 3.4	13.2 – 17.5	14.2 – 15.5	5.6 – 6.6	–

Table 14 – CL and SR estimated by BSQR for micronutrients in grapevine leaves (blade + petiole) grown in Campanha Gaúcha, Rio Grande do Sul, Brazil, Brazil, compared to national and international reports and guidelines.

	Scope	Cu	Zn	B	Mn	Fe
	ISO 3166			*mg kg^{-1}*		
CL_{BSQR}	**BR-RS**	**12**	**140**	**27.4**	**434**	**90.4**
SR_{BSQR}	**BR-RS**	**11.6 – 13.1**	**130 – 146**	**23.7 – 31.9**	**400 – 462**	**82.7 – 96.0**
CQFS-RS/SC (2016)	BR-RS/SC	–	25 – 60	30 – 65	30 – 300	60 – 150
Rozane et al. (2020)	BR-RS	10 – 14	148 – 254	27 – 41	398 – 586	91 – 142
Pauletti and Motta (2017)	BR-PR	14	20	30	30	60
Malavolta et al. (1997)	BR-SP	–	25 – 40	30 – 40	40 – 100	–
Raij et al. (1997)	BR-SP	18 – 22	30 – 35	45 – 53	67 – 73	97 – 105
Ribeiro et al. (1999)	BR-MG	15	25 – 40	100	40 – 100	–
Moyer et al. (2018)	US-WA	6 – 20	15 – 50	30 – 100	30 – 100	> 75
García-Escudero et al. (2013)	ES-LO	8.3 – 10.0	14 – 17	40 – 42	23 – 29	22 – 25

6.2 GRAPEVINE MINERAL NUTRITION

Phosphorus

Current findings suggest that lower P and higher Zn concentrations in soil would lead to increased grape yields. Interestingly, P-Zn interactions in soil-plant systems can influence their bioavailability and, therefore, have been a recurrent study subject (HE et al., 2021; LONERAGAN; WEBB, 1993) and few mechanisms have been proposed, not without controversy. High doses of P can promote Zn sorption and reduce plant uptake (CHEN et al., 2019) but the addition of P fertilizers to soils has been reported to have had variable effects on Zn retention (ROBSON, 1993), probably as result of changes in soil pH and surface charges. Additionally, plant responses to nutrient imbalance, such as exudation of carboxylates, can affect Zn and P availability in soil (DUFFNER; HOFFLAND; TEMMINGHOFF, 2012). The only mechanism that has been shown unequivocally to induce Zn deficiency in plants is the suppression of root infection by vesicular arbuscular mycorrhizae due high levels of soil P (BALZERGUE et al., 2011). As a rule, all factors which impair root colonization by mycorrhizae tend to increase the risk of Zn deficiency in plants grown on soils low in extractable zinc, since mycorrhizae hyphae greatly expands roots surface and is responsible for up to 50% of Zn uptake in crop plants (MARSCHNER, 2012).

In this study, white grapes requirements of P were lower than the mean soil content in the subset, indicating possible excess and thus affecting Zn requirements as compensation for reduced Zn uptake. Soil rich in P lead to its accumulation in roots, being remobilized to supply canopy development in subsequent cycles (SCHREINER, 2016; SCHREINER; SCAGEL; BAHAM, 2006). Red grapes on the other hand may be suffering from moderate P shortage, hampering higher yields. Nonetheless, moderate P deprivation may have positive effect on fruit quality, as it has proven to stimulate anthocyanin synthesis (ZHENG et al., 2020). Red wines are rich in anthocyanins and their oxidation products which are responsible for major characteristics such as hue, color stability, and taste (JEZEK et al., 2018). Sensory differences are detectable between red and white wines made from P-sufficient and P-deficient vines (SKINNER et al., 2019).

Potassium

Plant K uptake occurs in roots tips, either though ion channels or carriers proteins, depending on the soil K status (MARSCHNER, 2012). Berries appear to be the strongest sink for K, especially between veraison and harvest (ROGIERS et al., 2006), with clusters at harvest accounting for 60% or more of the total K content of the above-ground organs

(MPELASOKA et al., 2003). During this period, K content in the clusters increases and levels accumulated are higher than the total amount taken up by the vine, at the same time, content in the trunk, roots, shoots, and leaves decreases, suggesting that a significant amount of K that accumulates in the berries is re-translocated from other organs (CONRADIE, 1981). Our results suggests that current recommendations for soil K concentrations could be slightly increased to attain higher yields, but product quality is also an important factor for market competition. Given the high sink capacity of berries, excessive availability of K in the soil can result in equally high levels of it in the must, causing a reduction of sugars, impairing its fermentation (ROGIERS et al., 2017), raising the pH (WALKER; BLACKMORE, 2012) and decreasing the titratable acidity (CIOTTA et al., 2016; KODUR, 2011), which increases susceptibility to must and wine oxidation, compromising quality parameters such as taste (MPELASOKA et al., 2003)

In grapevines, differences in the K status of vines, berries, juice or must have been reported for different varieties grafted onto the same rootstock (ARROYO et al., 1997; WALKER et al., 1998). In terms of berry K accumulation, the same rootstock may have variable effects on different scion varieties, thus vines of different vigour, and crop production may respond differently to specific levels of soil K availability, which is corroborated by our results. The higher CL for leaf K in red grapes should be considered with caution though, as the high pH of grape juice and wine promoted by K also decreases the colour quality of red wines due to reduced ionization of anthocyanins (SOMERS, 1977). Absorbed K accumulates in berry skin (ROGIERS et al., 2006), thus berry K levels are of special importance to red wines, since during its fermentation the skin is left for some period after crushing for the extraction of anthocyanins, potentially increasing K transport to wine (MPELASOKA et al., 2003).

Calcium and Magnesium

The estimated CL for soil Ca and Mg would be classified as “low availability” according to (CQFS-RS/SC, 2016). In fact, these value is considerably lower than what most recommendations reviewed in this study would deem appropriate. Ca canopy supply derives mainly from soil uptake (SAURE, 2005), driven by high transpiration rates, as contribution of stored reserves is considered negligible due to its low phloem mobility (MARSCHNER, 2012; SCHREINER, 2016). Mg canopy supply also rely heavily on soil uptake (SCHREINER; SCAGEL; BAHAM, 2006) but, different from Ca, it is stored in more mobile forms, as only about 20% of the total Mg is bound to chlorophyll through chelation, being

readily translocated to actively growing plant parts whenever shortage occurs (MARSCHNER, 2012).

Calcium is an essential plant nutrient mainly for cell wall formation, cellular signaling responses and cell membrane stability. Fruit cell walls are pectin rich, and calcium-pectin cross-links are a major factor in determining the physical and structural properties of fruit (HOCKING et al., 2016). Mg, on its turn, is the main constituent of the chlorophyll molecule thus it is expected that healthy and highly productive grapevines require high amounts of these nutrients. Our results contradicts this assumption and suggest that very low soil concentrations in the 0 – 20 cm layer would suffice. However, Ca uptake decreases with increasing distance from the root apex, being much higher in apical than in basal root zones (MARSCHNER, 2012; SAURE, 2005), whereas Mg ionic radius is smaller than that of other cations like Ca, K or Na, but its hydrated radius is substantially larger. This weakens its bounds to soil charges (CEC) and facilitates leaching processes, especially in wet seasons (GRANSEE; FÜHRS, 2013). CL and SR estimated for leaf Ca and Mg indicates that current supplies were above optimal. Acidity correction is the main external source of Ca and Mg in soil, generally applied prior to vineyard establishment and no systematic increase in soil concentrations of those nutrients were observed (Table 7). These facts indicate a possible role of deeper soil layers in the supply of Ca and Mg to grapevine roots.

Sulfur

Sulfate (SO_4^{2-}) is the most abundant inorganic forms of S in soil and it is the preferred form for plant uptake (AMÂNCIO et al., 2009; RIBEIRO et al., 2001). In surface horizons, soluble and adsorbed S forms usually represent < 10% of total S, and the remainder is dominated by organic forms that usually form its major reserve (SCHERER, 2001). Apart from crop removal, leaching represents the main S exportation mechanism from the soil system, highly influence by soil texture and precipitation regime. As such, soils with low in organic matter, coarse-textured and well drained, such as the ones from this study, are prone to exhibit sulfur deficiencies (DICK; KOST; CHEN, 2008).

Plants are able to incorporate the greater part of absorbed S into cysteine, used in protein synthesis (AMÂNCIO et al., 2009), hence, the efficient use of carbon and N in plant growth depends on the absorption and assimilation of appropriate amounts of S (BRUNOLD, 1993). Several S-secondary plant metabolites are also of major importance in defense against pathogens (HELL; KRUSE, 2007), although there may exist distinct patterns of gene expression between genotypes (GOES DA SILVA et al., 2005). According to our results,

there is room for yield increase through S fertilization. In addition, quality parameters may be positively affected as many compounds responsible for typical aromas, flavor and texture of *Vitis vinifera* wines are sulfur containing substances, which play important role in the abundance and stability of components, such as tannins, phenolic acids, anthocyanins, and aldehydes (CONSIDINE; FOYER, 2015).

Copper and Zinc

Copper-based fungicides (*e.g.* Bordeaux mixture) are largely used against crop diseases, such as downy mildew (*Plasmopara viticola*) (BRUNETTO et al., 2017) and Cu inputs from applications can reach up to 30 kg ha^{-1} in a grapevine cycle (CASALI et al., 2008), often leading to increase in the total and available Cu in the soil (PIETRZAK; MCPHAIL, 2004). Alternatively, grape producers may use Zn-based fungicides to avoid Cu toxicity risk (TIECHER et al., 2017). The occurrence of high contents of both Cu and Zn in vineyard soils has been reported, especially in the last decade (BRUNETTO et al., 2014, 2017; TIECHER et al., 2016, 2017, 2018), increasing the environmental risk of surface and groundwater contamination (MIOTTO et al., 2014). Young grapevine plants grown in Cu contaminated soil demonstrate reduced growth of roots and shoots and leaf chlorosis. In early stages, accumulation of Cu in roots can damage cell membranes, impairing nutrient and water uptake, occasionally leading to plant death (MIOTTO et al., 2014). Adult grapevines, in contrast, may avoid toxicity effects by adopting an exclusion strategy, accumulating Cu in perennial and annual organs (LAI; JUANG; CHEN, 2010), mostly in roots (BALDI et al., 2018b).

Current results show no apparent deleterious effects from soil Cu and Zn concentrations up to 41.0 mg dm^{-3} and 8.7 mg dm^{-3}, respectively. These values are considerably lower than preventive threshold concentrations of 60 mg dm^{-3} (Cu) and 300 mg dm^{-3} (Zn) defined by Brazilian government regulatory agencies (CONAMA, 2009). Moreover, no significant translocation of Cu from soil to leaves was observed, as tissue concentrations were close to optimal levels which, in turn, were coherent with CND estimates (ROZANE et al., 2020). Therefore, the correlation between vineyard disease control and higher yields may be affecting CL and SR estimates for soil concentrations, given the model is unable to isolate nutritional from phytosanitary effects in contaminated samples. As for Zn, leaf mean concentrations were beyond estimated CL in 2007 and 2011 harvests (Table 8). These results contrast with the apparent insufficient supply suggested by soil Zn CL/SR estimates (Table 7). Adsorption of Zn occurs predominantly on functional groups of minerals

such as Fe oxides and clay (MELO et al., 2016), thus leaching is higher in sandy soils, carrying Zn to deeper layers, out of sampling depth but still available for plant uptake. Furthermore, Zn absorbed from soil by grapevines tend to accumulate in woody stems rather than leaves, although it is still unknown whether or not the Zn that reaches the trunk and woody canes is immediately sequestered in cell walls or by chelating ligands, or if it is first transported to leaves (primary site for transpiration delivery) and then remobilized back to these woody tissues via the phloem. Regardless, high levels of Zn accumulation in woody stems act as reserve, maintaining the long term viability of the plant and allowing leaves and fruits to be shed without compromising growth from buds in future years (SCHREINER, 2016).

Boron

Due to the high demand and the characteristics of the soils, B is typically added in correction fertilization of Brazilian vineyards (MELO, 2003). Current results suggest shortage of soil B from 2004 on, yet no systematic decrease in yield was identified (Table 7) and leaf B concentrations were above the estimated CL/SR (Table 8), indicating a sufficient supply. In most plants, B is considered highly immobile and its movements are restricted to transpiration flow, subject to accumulation in leaves (NABLE; BAÑUELOS; PAULL, 1997). Moreover, in coarse-textured soils with low organic matter content and soil pH values between 5.5 and 7.5, B is highly soluble, leaching off during irrigation or rainfall (MOUSAVI; MOTESHAREZADEH, 2020), indicating a possible role of deeper soil layers in B supply to roots.

Manganese

Ethylenebisdithiocarbamate of manganese and zinc – $[C_4H_6N_2S_4Mn]_x(Zn)_y$ – also known as Mancozeb, is a fungicide used in agriculture that can contribute to both Zn and Mn leaf and soil contamination (LA PERA et al., 2008). Mn content in soil is closely related to the content of phenolic compounds (catechin, epicatechin, resveratrol, piceid) in wine grapes (ACUÑA-AVILA et al., 2016) while leaf absorption can increase the contents of acetylated, methylated, total anthocyanins, and total flavonols in grape skins (CHEN et al., 2020). Anthocyanins have a crucial role in determining the color of red grapes and wines (CHENG et al., 2014) while flavonols contribute to wine color as copigments and are related to the health-promoting properties of wine (CASTILLO-MUÑOZ et al., 2007).

Berry seeds are the largest sink for the xylem-mobile elements, such as Mn, followed by skin and pulp, with most of its deposition occurring prior to veraison, followed by an additional stream during late ripening (ROGIERS et al., 2006). Xylem tracer studies indicated that xylem flow occurs along the central bundles leading to the seeds in pre-veraison grape berries (ROGIERS et al., 2001), suggesting continuous xylem flow to this component. Xylem anatomical and derived hydraulic parameters, as well as total vascular tissue area vary between cultivars and in receptacle/berry components (XIAO et al., 2021), which may explain the differences found between white and red grapes regarding Mn optimal concentrations in soil and leaves, although further elicitation is needed.

In this study soil Mn supply was considered sufficient or above sufficiency in all reported years, leading to high plant uptake (Tables 7 and 8). The reduced Mn flow to berries during veraison may lead to its accumulation in leaves (SCHREINER, 2016). Grape species are, however, tolerant to Mn excess due to its detoxification mechanisms, which include compartmentalization into cell vacuole, exclusion into cell wall, secretion on leaf surface and deposition in vascular wall. In cellular organ, excess Mn in chloroplast can be detoxified by deposition in starch granule (YAO et al., 2012a). This may result in high Mn levels in leaves without detrimental effects to yield. Still, Mn at high concentrations plays a role in the destabilization of wines and in their oxidative evolution (BENÍTEZ; CASTRO; BARROSO, 2002), especially in red wines where Mn concentration may be higher due to its transfer during the extended contact with grape skin and seed.

6.3 MODEL SUITABILITY

Sensitivity assessments have shown that quantile choice can have direct impact on parameter estimates (MAKOWSKI; DORÉ; MONOD, 2007), therefore in resulting CL and SR values. Since the BL is interpreted as the potential response when there are no limiting factors, the choice of quantile bares relationship with desired yield level as well as with tolerance to errors in Y measurements, however no systematic approach to its selection has been defined. The devise of utility functions which considers application doses, fertilizer costs and product selling prices could allow a more objective quantile selection through modeling (THEOBALD; TALBOT, 2002), although it would arguably require more data to obtain reference values. In the absence of such models, the sensitivity analysis is a valid approach to assess the behavior of parameters estimates and can lead to valuable insights, enabling a richer comprehension of the relationship between variables at different strata of the data (LIANG et al., 2019, 2021).

In terms of sensitivity to *prior* distribution, BSQR model using asymmetric Laplace distribution (ALD) to form the likelihood function indeed yielded proper *posteriors* even from improper uniform *priors* (YU; MOYEED, 2001). This a feature is of great convenience since it avoids the need of defining and justifying a proper *prior*, easing the application of the model in the absence of previous knowledge through a more Frequentist approach while still retaining the ability to incorporate newly generated knowledge in a later research stage.

Bayesian p-values suggest that the models yielded y^{rep} with consistently higher standard deviations, indicating over-dispersion of replicated data (Table 10). The model fit was apparently better for leaf than soil nutrients, very likely an effect of a smaller number of harvests considered in leaf analysis and the fact that a single harvest (2007) accounted for over 73% of total observations, resulting in less variability in the data subset. Such poor performance may be a result of the complete pooling strategy, as data from different cultivars in different harvests were analyzed altogether, ignoring variation between groups, increasing overall data variability with impacts o model parameter estimations. The no-pooling alternative on the other hand would overstate it and the increasing number of models would overfit the data within each group (GELMAN; HILL, 2007). A reasonable approach is to partition the data variability using partial pooling and incorporating layers into the hierarchical structure of the model. The further development of model's hierarchical structure would allow varying slopes and intercepts which may account for group differences regarding cultivars and harvests, potentially improving model fit and estimates accuracy (GELMAN, 2006).

7 FINAL REMARKS

7.1 CONCLUSION

Bayesian Segmented Quantile Regression (BSQR) was effective in establishing Boundary Line functions and estimating critical levels (CL) and sufficiency ranges (SR) for nutrients in soils and grapevine *(Vitis vinifera)* leaves (blade + petiole) using data from commercial vineyards in Campanha Gaúcha, Rio Grande do Sul. CL and SR for soil Ca, Mg, Cu and leaf Zn and Mn were the most divergent results compared to literature. Reference values for red and white grapes were different for soil P, Zn and Mn, as well as leaf K and Mn. The BSQR model was highly sensitive to quantile selection but poorly affected by *prior* choice. High data variability resulted in poor model fit, increasing uncertainty over parameter estimates, enlarging SR and hampering the differentiation between groups. Despite current limitations, the BSQR model provides a flexible framework for BL analysis, enabling the use of commercial datasets in establishing reference values to support group- and site specific recommendations, a valuable contribution to increase efficiency and sustainability of grapevine fertilization

7.2 FUTURE RESEARCH

Continuous improvements of the BSQR model can lead to greater accuracy and precision in critical levels and sufficiency range estimates as well as enhance the detection of differences between nutrition profiles of subgroups. To further development, suggested priorities are:

a) Development of a systematic approach for quantile selection, due to its large effect on results and conclusions.

b) Reparametrization of the Bayesian Segmented Quantile Regression hierarchical structure, in order to allow varying slopes and intercepts, so that model fit can be improved and more accurate inferences can be made at cultivar- and site specific levels.

To further comprehension on plant nutrition and improve the efficiency and efficacy of fertilizing practices, future studies and applications should include:

c) The development of reference values for yield quality components that are relevant to production purpose, such as titratable acidity, pH, total soluble solids and concentration of flavonoids.

d) Establishing nutrient critical levels and sufficiency ranges for other fruit crops.

e) Investigating whether, given nutritional stability of perennial crops, plant age has impact on nutrient critical levels and sufficiency ranges.

f) Investigating the role of deeper soil layers in nutrient supply to perennial crops with well developed root systems.

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