Objective measures of grape quality
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The need for objective quality measures
A relationship with perceived quality?

In Australia, grape quality assessment is mainly subjective. Chemical measures of grape quality would ensure that both transparency and maximum value are achieved.

Can objective measures be identified?

The research question and procedure
Can existing commercial grading allocations be predicted using previously identified and new chemical measurements?

- Samples sourced from various growing regions across Australia
- 56 Cabernet Sauvignon (CAS), 62 Shiraz (SHZ) and 64 Chardonnay (CHA) grape samples from up to 9 commercially-defined quality grades
- Chemical analyses selected based on a literature review and a survey of the way local and international producers measure quality

- Basic chemical measures:
  - berry weight
  - titratable acidity (TA)/pH/malic acid
  - °Brix
  - nitrogen (alpha amino nitrogen, AAN; ammonia, NH\textsubscript{3}; total = YAN)
- Potential negative quality markers: laccase, chloride, methoxypyrazine
- Targeted compositional measures (dependent on variety):
  - ‘grassy, green’ C6 compounds (C6)
  - volatile thiol precursors (thiol-PRE)
  - β-damascenone (β-dam)
  - the broad flavour measure phenol-free glycosyl-glucose (GG)
  - amino acid profile (aa)
  - phenolics (colour/520nm, UV-visible spectrum, tannin)
- Non-targeted spectral fingerprinting in mid- and near-infrared (MIR/NIR)
- Data analysis with multivariate statistical methods PLS (Partial Least Squares Regression) and Discriminant Analysis (quadratic, QDA)

Results

- PLS models developed for grade had $R^2$ values of validation ($R^2_{val}$) 0.55–0.84, showing that this was not always the best modelling approach
- Due to the fact that grade is not numerically defined, QDA (which predicts categories not values) gave better grade accuracy
- RMSE\textsubscript{val} = root mean sq. error of PLS validation (0.5 would be a perfect fit)
- QDA and PLS results are shown below
- Positive (+ve) variables = subset only

Targeted chemical analysis

MIR and NIR spectra (*only MIR results shown*)

UV-visible spectrum

SHZ

PLS

$R^2_{val} = 0.65$

$RMSE_{val} = 1.39$

+ve variables: °Brix, AAN, YAN, aa, tannin, 280 nm, 520 nm, C6, chloride

QDA prediction = 85%

CAS

PLS

$R^2_{val} = 0.83$

$RMSE_{val} = 0.97$

QDA prediction = 92%

CHA

PLS

$R^2_{val} = 0.78$

$RMSE_{val} = 1.32$

+ve variables: TA, NH\textsubscript{3}, malic acid, thiol-PRE, C6, GG, chloride, β-dam

QDA prediction = 79%

QDA prediction = 95%

QDA prediction = 96%

Only UV-Vis subset determined

Conclusions and future directions

- MIR and UV-Vis scans best predicted CAS and SHZ grade, while targeted chemical analyses best predicted CHA grade using QDA.
- There is potential for objective chemical measures to be defined either by targeted or non-targeted methods.
- A relatively simple analytical grading tool should be available following refinements by grape variety, and calibration across multiple vintages.