Predicting ketosis from milk mid-infrared (MIR) spectra using multivariate mixed models

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Third DairyCare Conference 2015 Zadar, Croatia
October 5th and 6th 2015

Introduction

- Ketosis:

  ➢ metabolic disease in early-lactation dairy cows.

  ➢ impact on production, reproduction and overall health status of cows:
    - ✓ Reduced milk production(Duffield et al., 2009)

    - ✓ Reduced reproduction performances (Walsh et al., 2007) and

    - ✓ Increased risk for displaced abomasum (LeBlanc et al., 2005).

Introduction (2)

- Ketosis:

    ➢ caused by mobilization of body fat to compensate for negative energy balance.

        ❖ increased blood concentration of ketone bodies (β-hydroxybutyrate (BHB), acetone…).

- BHB is the most common ketone body that used as indictor for ketosis.
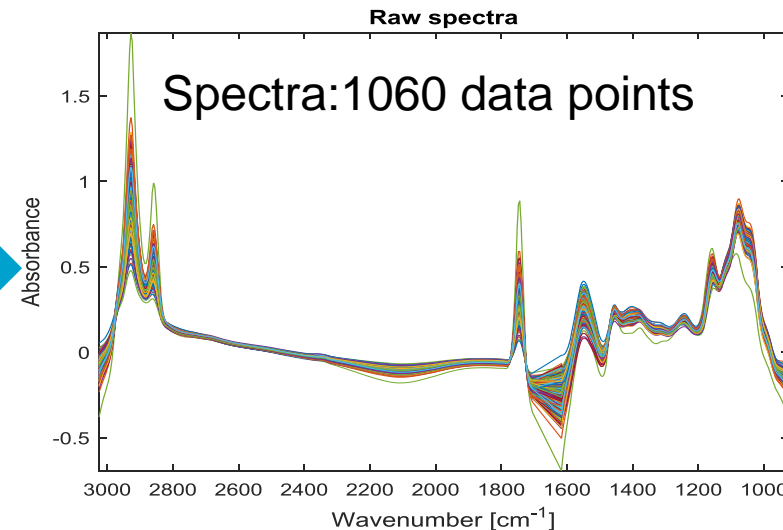
Introduction(3)

- Blood BHB concentrations (μM/L) of cows are not routinely available.

- Milk concentrations of BHB could routinely available by **FTIR** spectroscopy.

- Infrared reading of the milk sample is very multivariate.

Milk sample

FTIR spectroscopy

Raw spectra

Spectra:1060 data points

Absorbance

Introduction(4)

- Multivariate mixed modelling may benefit from the multivariateness of the spectra.

- E.g. 2-5% better accuracy in predicting breeding values for fat%, protein% and lactose% than univariate modeling (Dagnachew et al, 2013).

- However, independent reference values for the fat%, protein% and lactose% were not available in that study.

Objective

To verify whether multivariate modeling of milk spectra (Direct Prediction – DP) gives better prediction of BHB than the common univariate (Indirect Prediction – IP) approach.

Materials and Methods

Table 1. Structure of datasets: number of herds, cows and records

Datasets	#herds	#cows	#records
Dataset1 (with blood BHB): September 2013 and June 2014			
Calibration	31	496	496
Evaluation	24	330	330
Total	**55**	**826**	**826**
Dataset2 (without blood BHB): September to December 2014			
Dimension reduction	12,059	147,946	218,174
Bivariate	8,916	103,017	146,587
Multivariate	5,726	41,896	83,406

Datasets are from *Polish Federation of Cattle Breeders and Dairy Farmers* in Poland.

Data analysis

- A link between blood BHB and milk spectra developed by PLS regression using part of dataset1 (calibration set).

- Cross-validated with 10-fold random segments.

- Root mean square error prediction ($RMSEP_{cv}$) and R^2_{cv} computed.

- Spectral dimension(523 wavenumber) reduced into few latent traits (8) by PCA for dataset2.
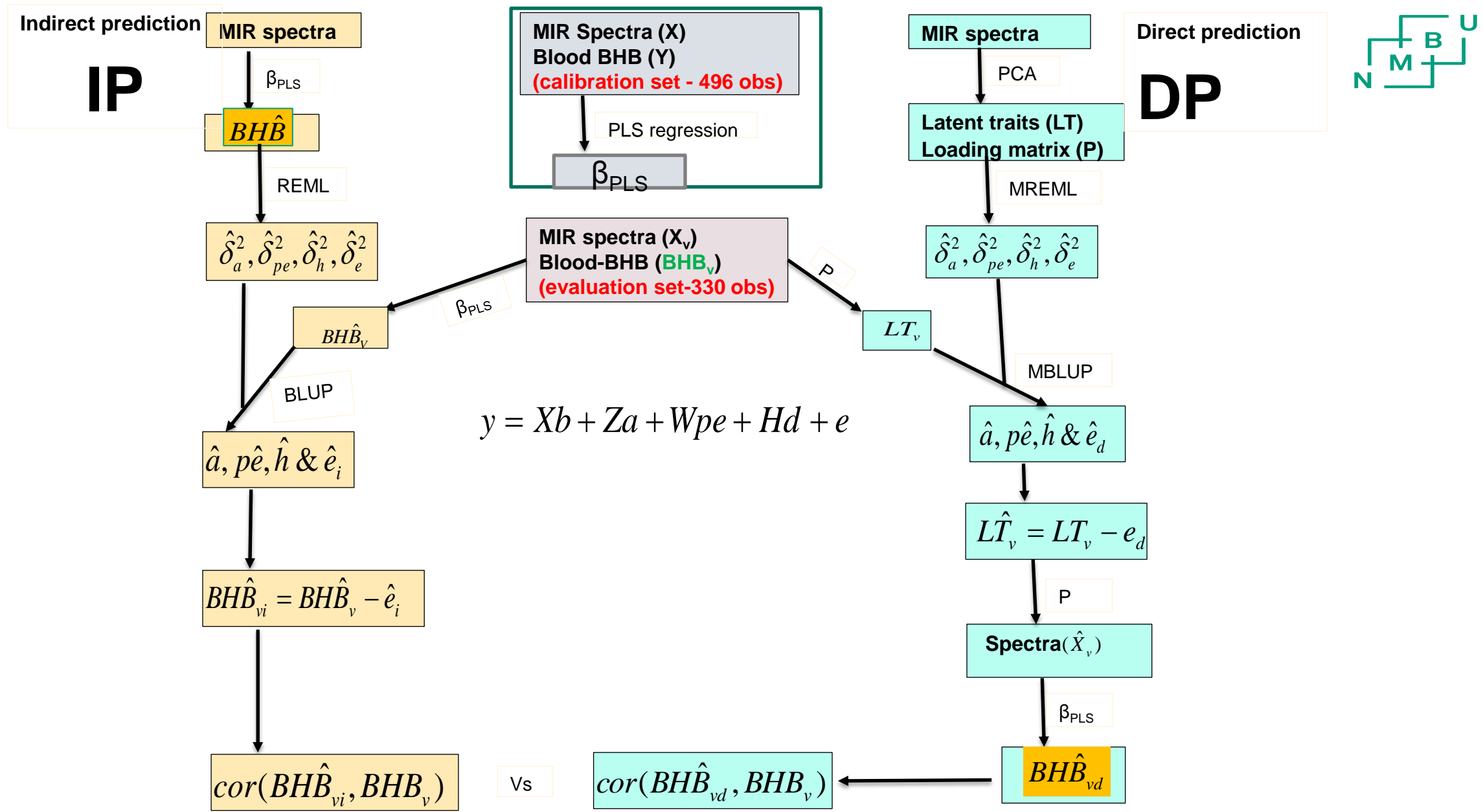
Data analysis…
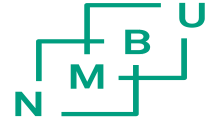
- REML estimate of (co)variance components of latent traits for dataset2 and BLUP of the latent traits for dataset1 (evaluation set) by Wombat (Meyer, 2007).
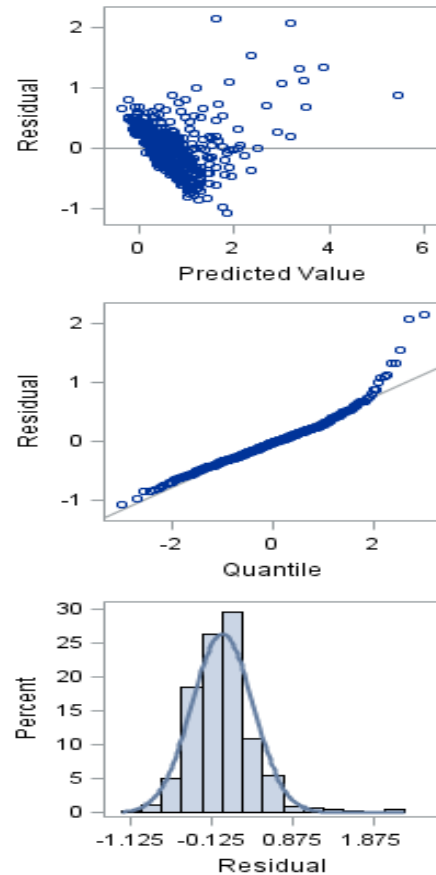
- Test day animal model fitted:

$$y = Xb + Za + Wpe + Hd + e$$

- **Fixed effects**: b : lactation stage, lactation number, season (month) & breed

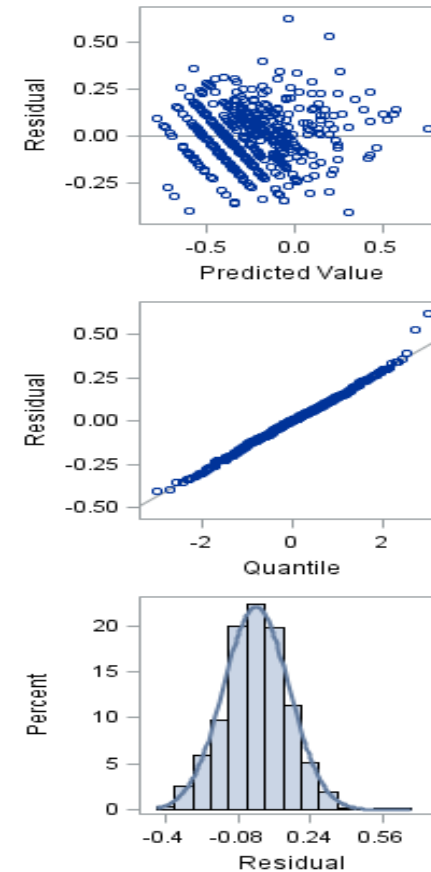- **Random effects**: a, pe, d, e : additive animal, permanent env't, herd*test day and residual.

Results from preliminary analysis:

Diagnostic plot for BHB

Diagnostic plot for logBHB

Calibration results

#PLS factors	N	RMSEP$_{CV}$	R$^2_{cv}$
6	496	0.2422	0.33
10	496	0.2286	0.43
14	496	0.2206	0.49
31	496	0.2051	0.63

Models with *diffrent number of PLS factors found* (3-31 factors)

Spectra explain ≤33% of BHB variation at the optimal number of factors ≤6 ?

Calibration results…

• Why only a proportion of the BHB variation is explained?

- lack of clear information and/or non-linear relationships between milk spectra and blood BHB.

- due to the scale on which blood BHB was measured (kind of discrete variable with few digits: 0.1, 0.2, ..).

- there might be some *baseline variation and/or multiplicative* effects in the spectra.

REML estimates:

Latent traits (LT)	%var explained	Variance components			
		δ_a^2	δ_{pe}^2	δ_h^2	δ_e^2
1	57.08	0.089	0.094	0.194	0.547
2	27.29	0.158	0.136	0.144	0.405
3	8.45	0.110	0.110	0.236	0.436
4	4.05	0.102	0.089	0.163	0.514
5	0.87	0.050	0.036	0.703	0.220
6	0.66	0.201	0.136	0.184	0.456
7	0.39	0.132	0.099	0.131	0.465
8	0.31	0.009	0.002	0.798	0.131
Total variance explained	99.09%				

Estimated variance ratios:

Latent traits (LT)	%var explained	Variance ratios			
		h_a^2	h_{pe}^2	h_h^2	h_e^2
1	57.08	0.096	0.102	0.210	0.592
2	27.29	0.187	0.162	0.170	0.481
3	8.45	0.123	0.124	0.264	0.489
4	4.05	0.118	0.103	0.188	0.591
5	0.87	0.050	0.035	0.697	0.218
6	0.66	0.206	0.139	0.188	0.468
7	0.39	0.158	0.121	0.159	0.563
8	0.31	0.009	0.002	0.850	0.139
Total variance explained	99.09%				

Results…

Correlation coefficients between measured BHB and predicted BHB

#PLS factors	Indirect prediction-IP	Direct prediction-DP	
	Univariate	Multivariate	Bivariate
6	0.5384	0.3889	0.3998
10	0.6536	0.4086	0.4156
14	0.6698	0.4126	0.4203
31	0.5691	0.4186	0.4297

This result contradicts what has been reported in literature and what we expected
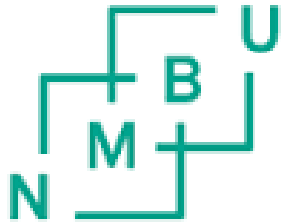
Results…

- The contradiction might be due to difference in :

  – Criteria used for the methods comparison(PEV Vs correlation)

  – What is predicted (breeding value Vs phenotype).

  – Type of data used (only phenotype predicted from spectra Vs both predicted and measured phenotype).

  – The retained 8 latent traits (99.09%) might not contain the required info(BHB) i.e. the remaining 0.91% might contain it.
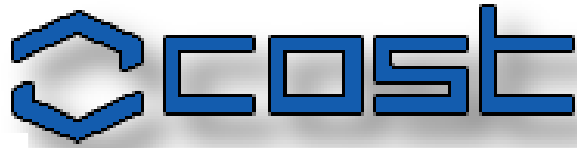
Conclusion

- Calibration model developed was unstable: relationship between milk spectra and blood BHB?

- Better prediction of BHB found when univariate variance structure used than when multivariate covariance structures used.

- However, this is not final conclusion since the work is still in progress.

- Final remark on importance of keeping spectral data multivariate in prediction of phenotype and/or model components (BLUP) such as breeding values, herd*test-day, and residuals will be given.
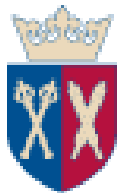
Acknowledgements

Thank you for your attention!