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Introduction to milk mid-infrared spectroscopy, equations development, and applications

Maria Frizzarin

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Content of the presentation

1. What is the mid-infrared spectroscopy
2. Equation development
3. Some examples
    1. Body condition score change
    2. Nitrogen use efficiency
    3. Methane emissions
4. Applications
    1. Implementation
    2. Share equations across countries
5. Conclusions

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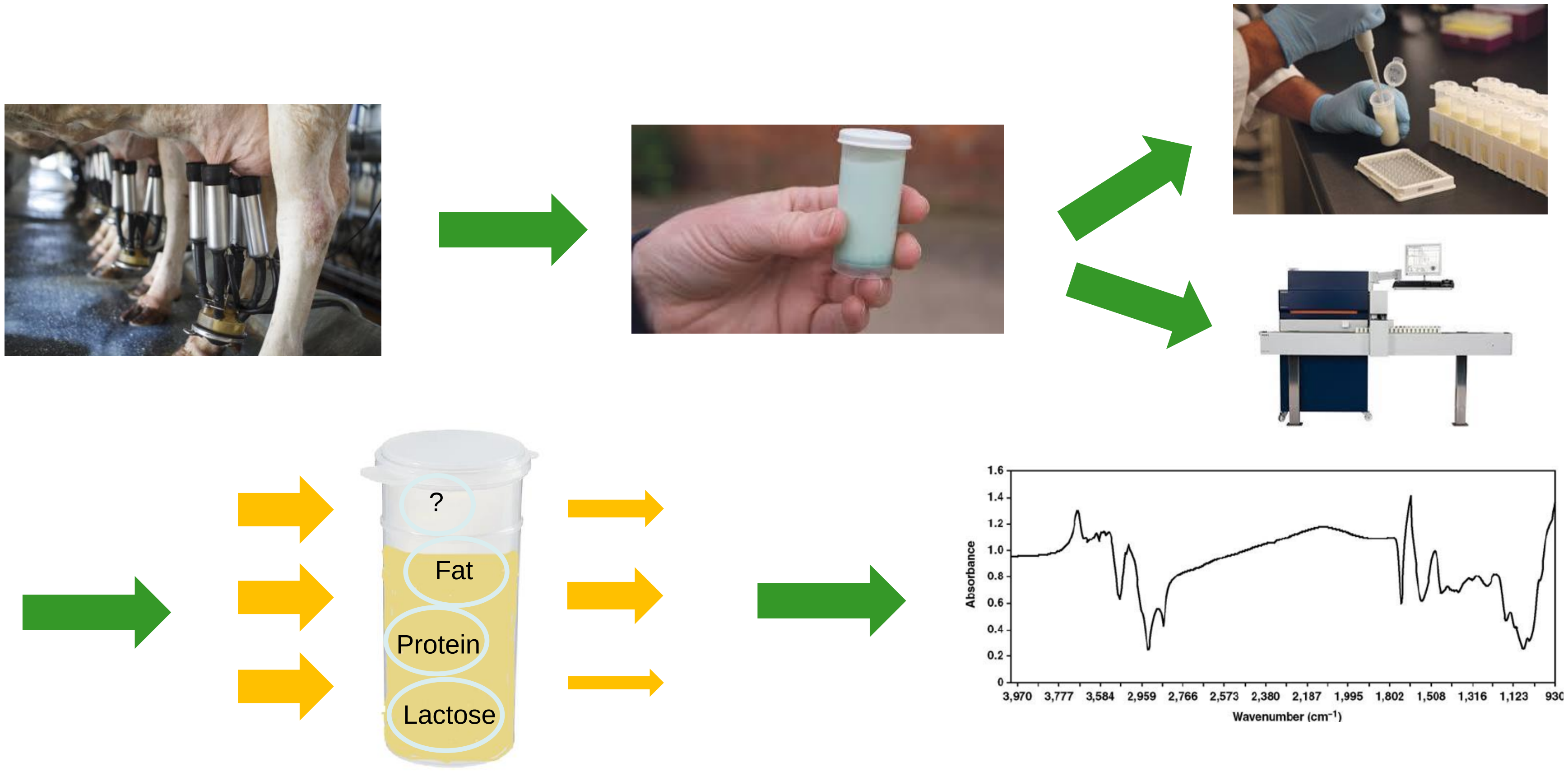
What is MIRS?



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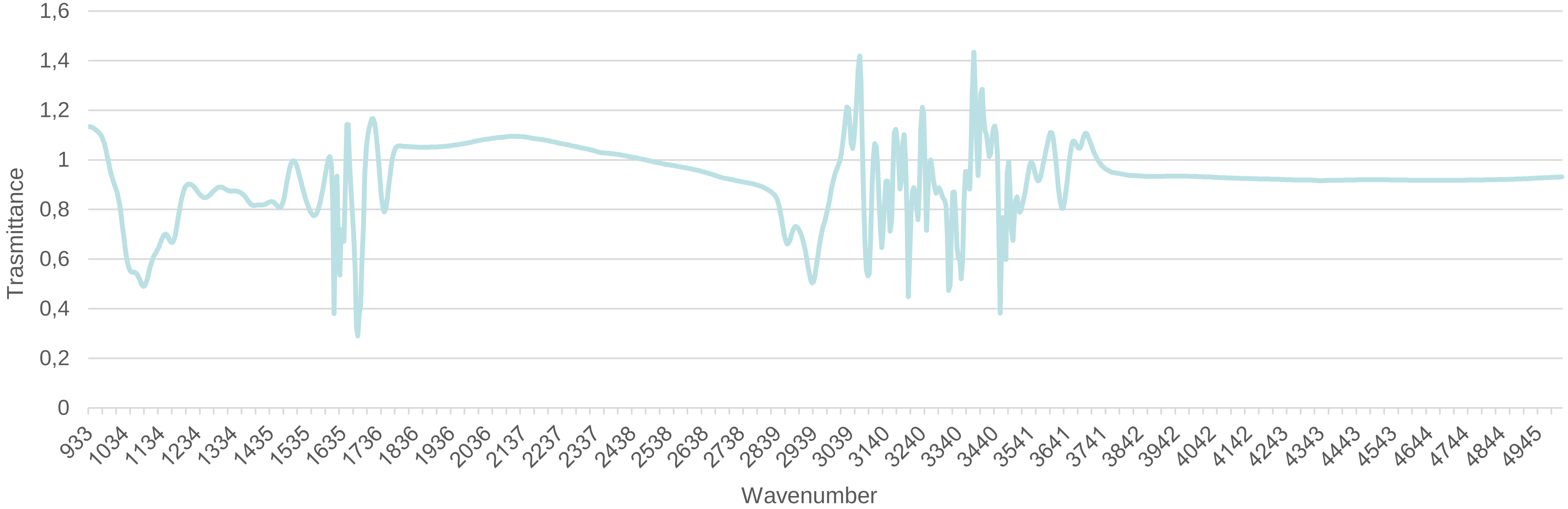
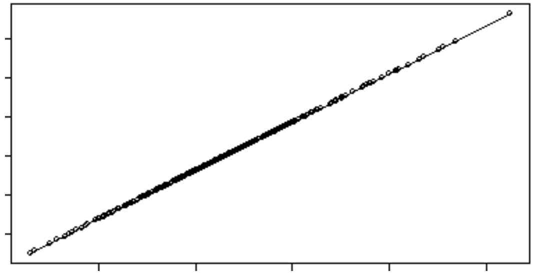
The data



Animal_No_	Sample_ID	Protein	Lactose	Fat	933 cm-1	937 cm-1	941 cm-1	944 cm-1	949 cm-1	953 cm-1	957 cm-1
3519	_2351916920081	3.14	4.49	3.13	1.134182	1.133682	1.132127	1.129342	1.125566	1.121129	1.116232
3784	_2378415020081	3.35	4.37	4.01	1.178803	1.170875	1.162666	1.154521	1.146977	1.140336	1.134607
3837	_2383712720081	3.48	4.54	3.8	1.167817	1.158173	1.147213	1.136616	1.127905	1.121724	1.117787

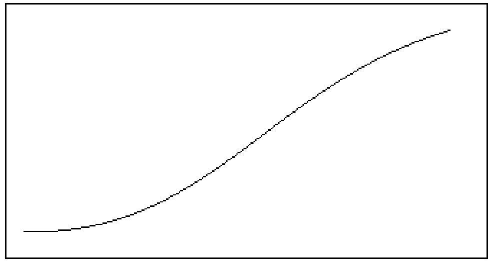
Prediction methods

Linear association



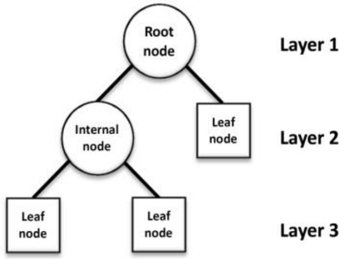
- Partial Least Squares Regression (PLSR)
- Ridge regression
- Lasso
- Elastic Net
- Principal Component Regression (PCR)
- Spike and Slab

Non-linear association



- Neural Network (NN)
- Projection Pursuit Regression (PPR)

Decision trees



- Random Forest
- Boosting Decision Tree

Ensamble models

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Why MIRS?

- Routinely used during milk recording
- Cheap and fast
- A single spectra useful to predict multiple traits
- Application in
  - Milk related traits
  - Animal related traits

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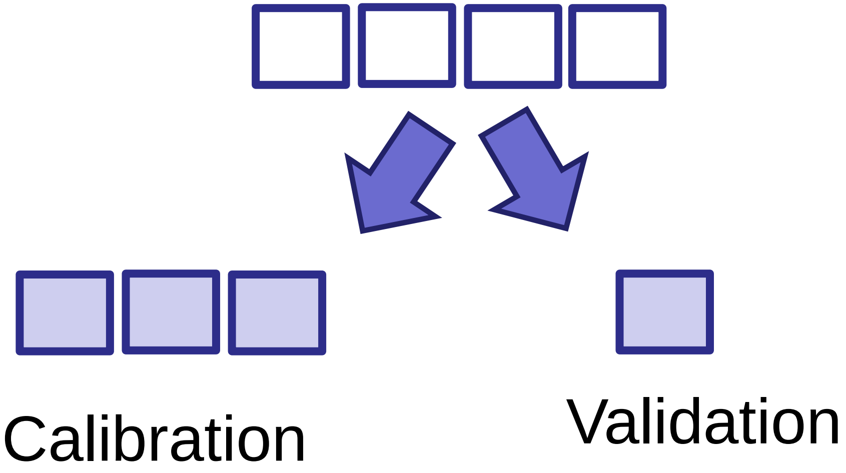
Validation



- Cow independent CV
- Experiment indepenent CV
- Herd independent CV

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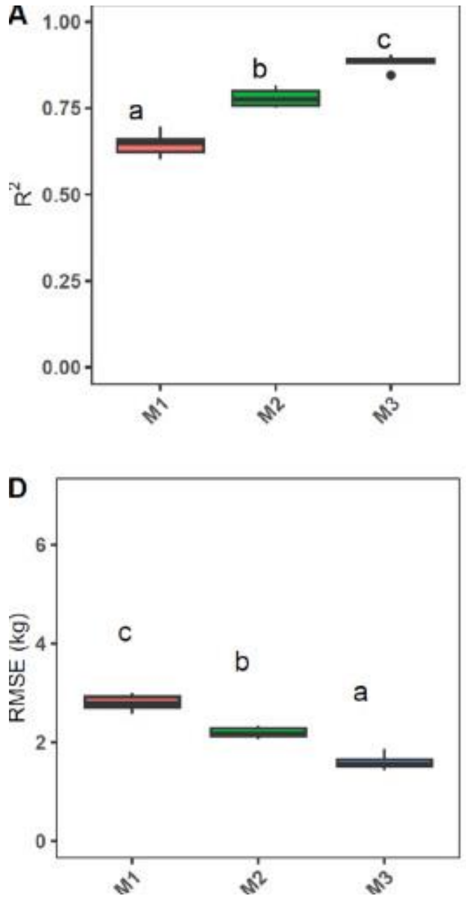
Validation

Cow independent CV



Predicting 28-d DMI

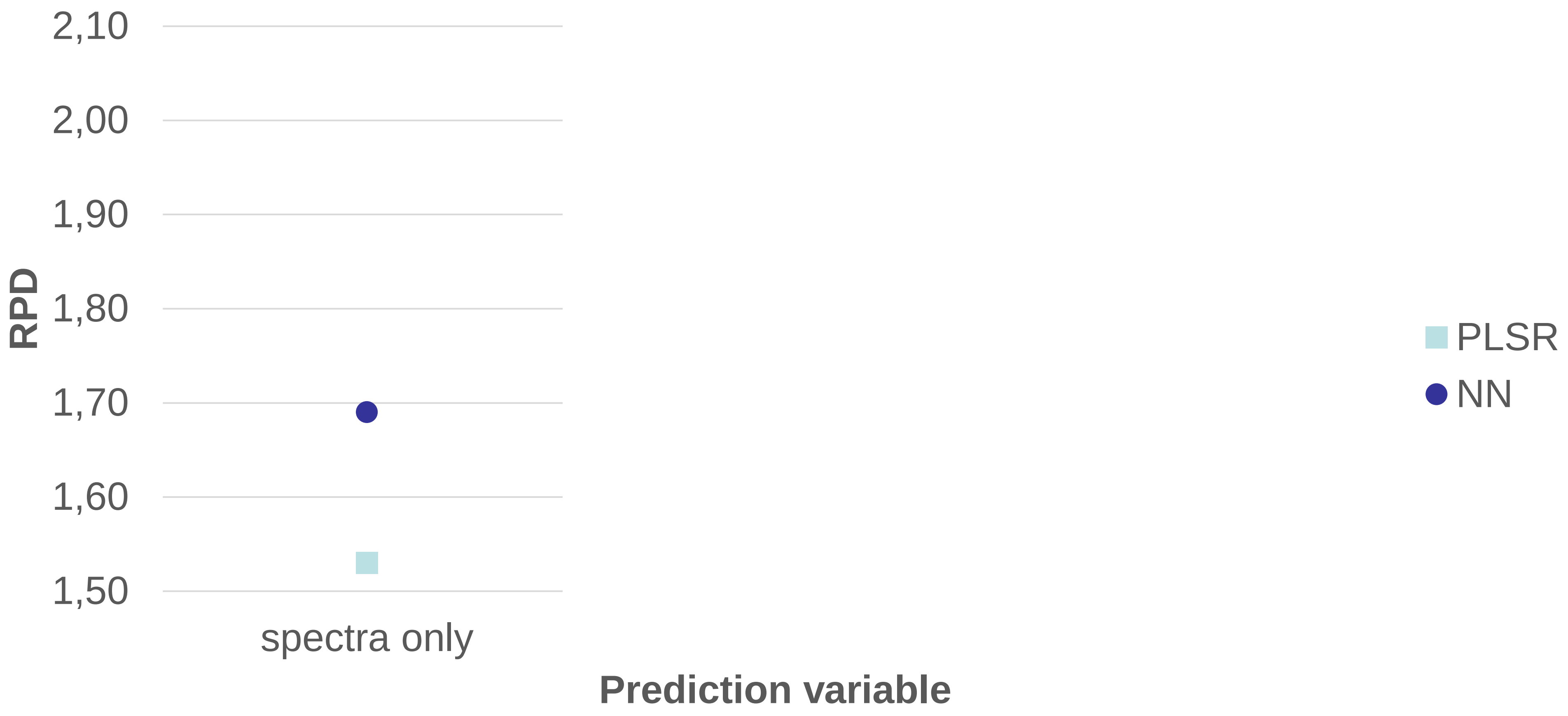
- M1, milk mid-infrared (MIR) spectral data only
- M2, energy sinks
- M3, MIR data and energy sinks

Models M2 and M3 also included parity class and first- and second-order terms on age at calving and DIM.

Adkinson et al., 2024 JDS
Assessing different cross-validation schemes for predicting novel traits using sensor data: An application to dry matter intake and residual feed intake using milk spectral data - ScienceDirect

How useful is actually the MIR?

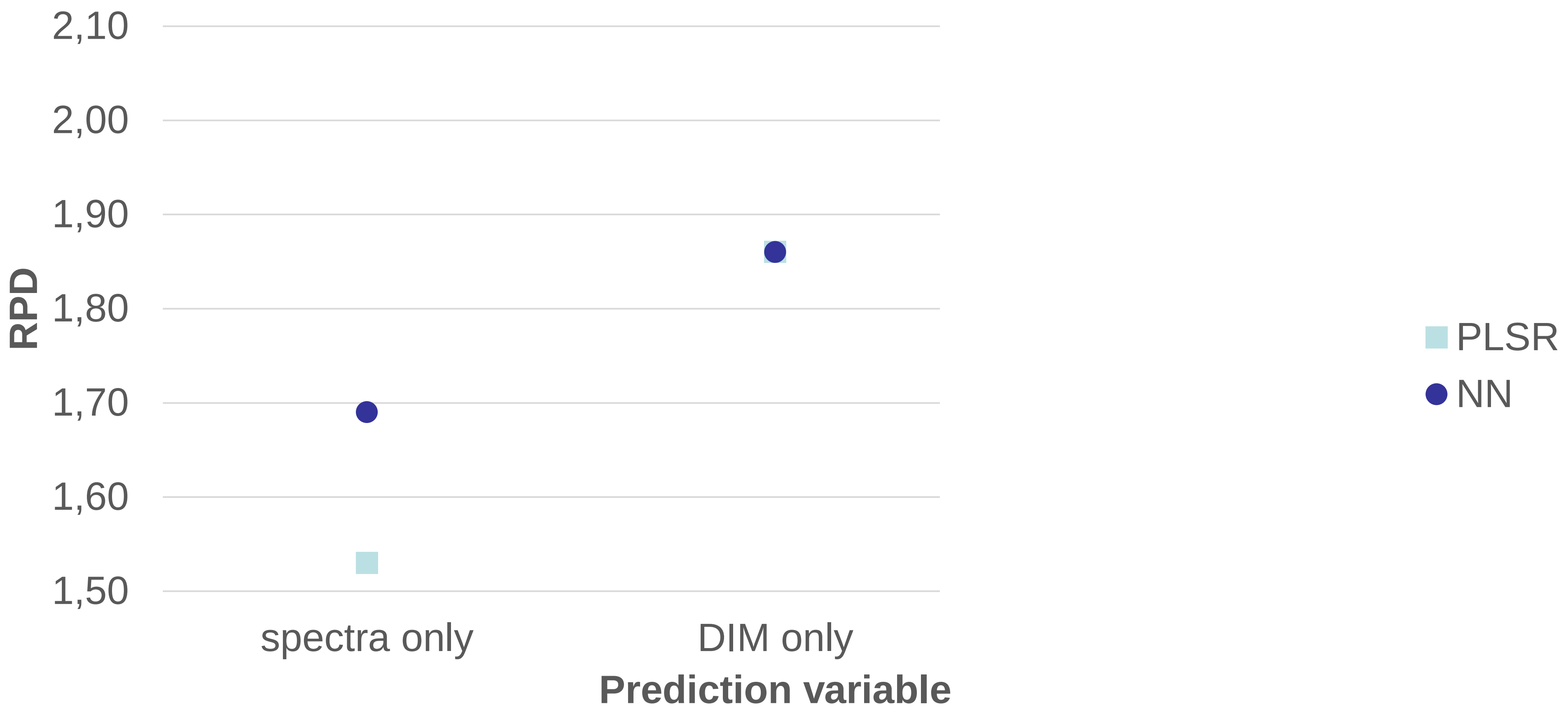
Example with body condition score change prediction



Frizzarin et al., 2023 JDS
[Estimation of body condition score change in dairy cows in a seasonal calving pasture-based system using routinely available milk mid-infrared spectra and machine learning techniques - ScienceDirect]

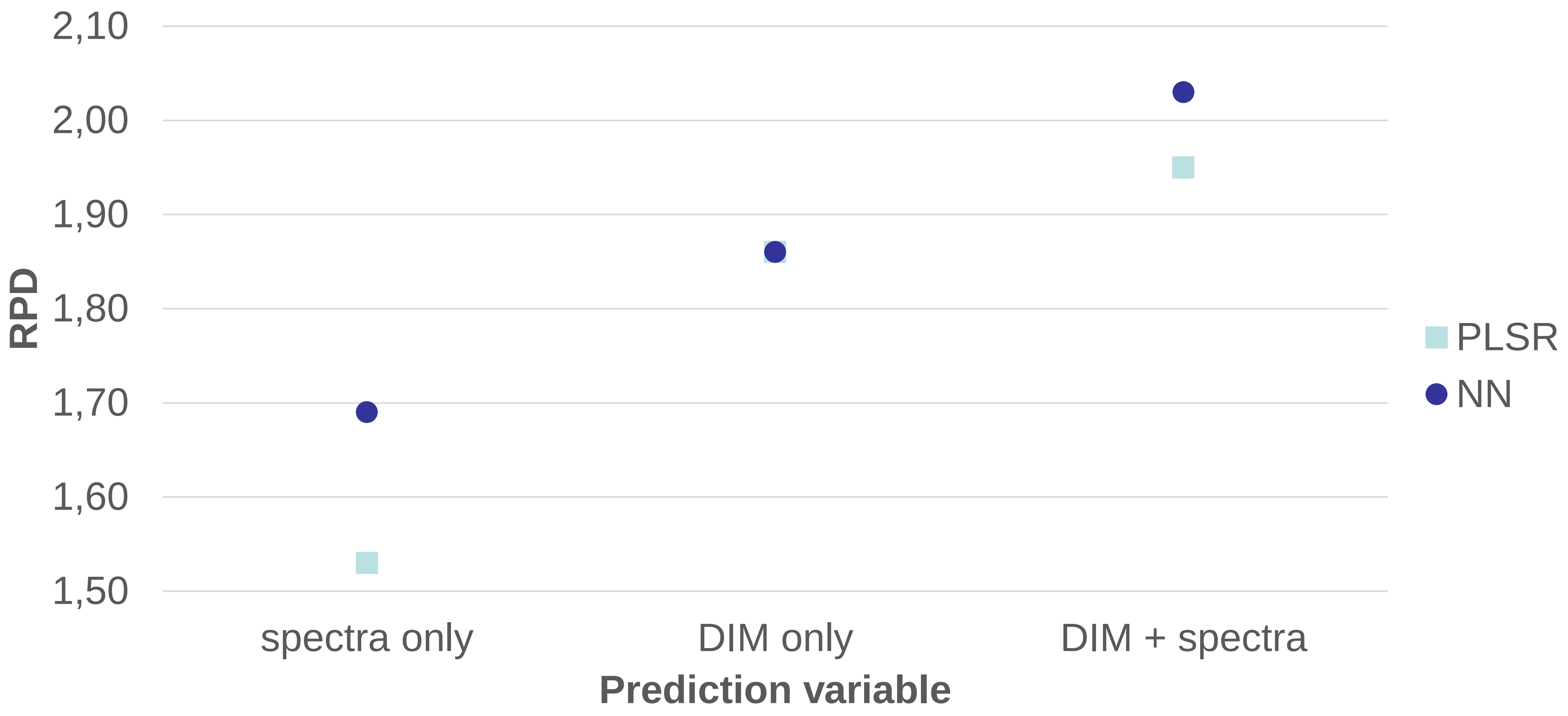
How useful is actually the MIR?

Example with body condition score change prediction



How useful is actually the MIR?

Example with body condition score change prediction



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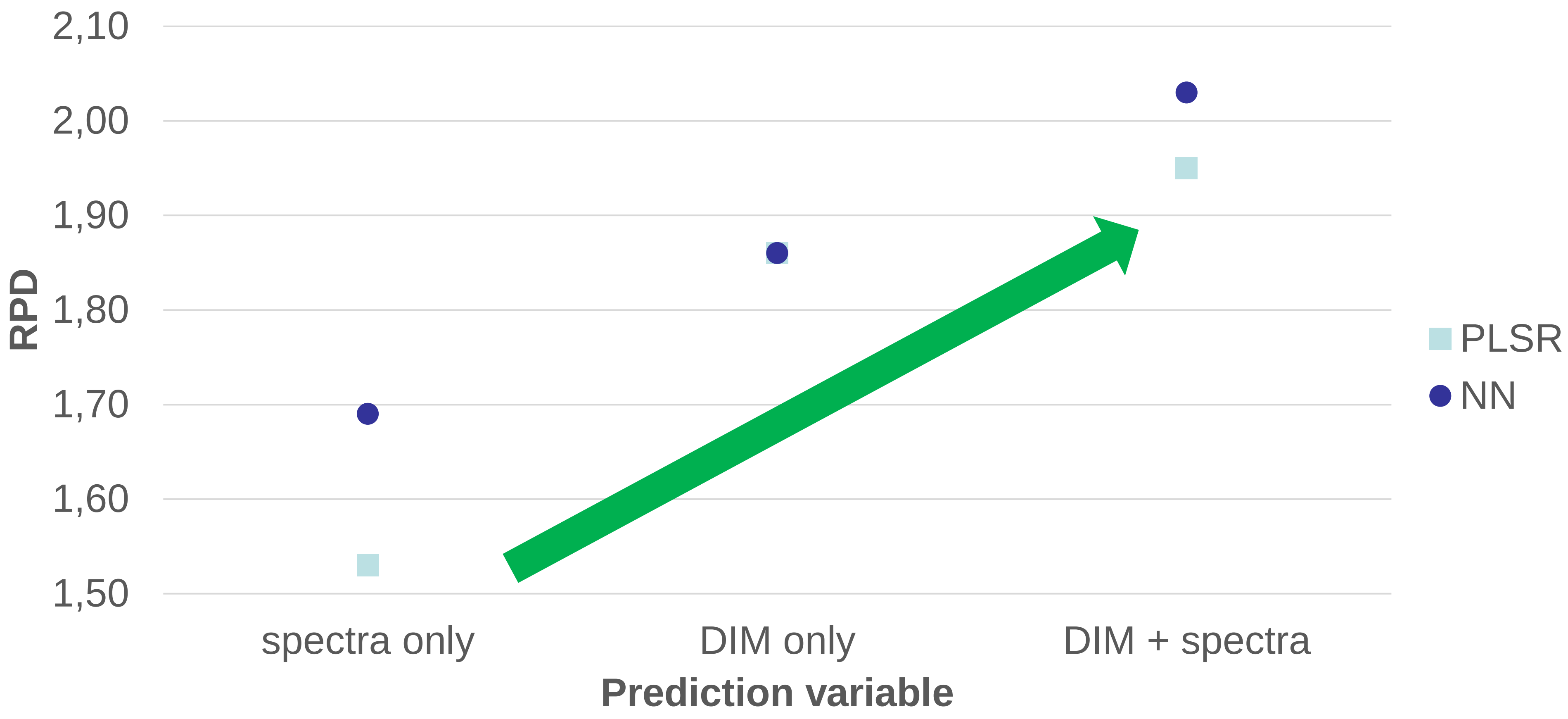
How useful is actually the MIR?

Example with body condition score change prediction



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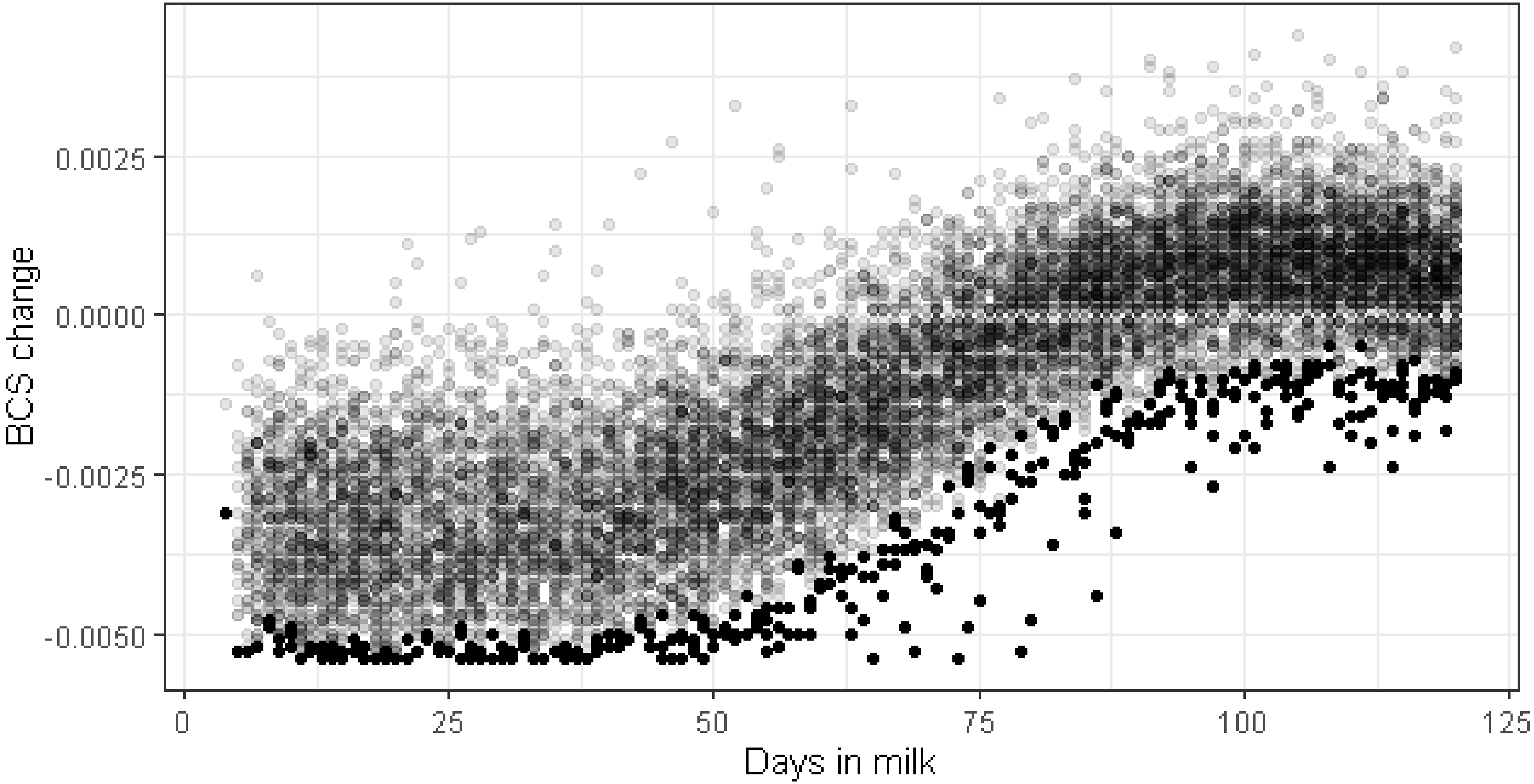
How useful is actually the MIR?

Example with body condition score change prediction



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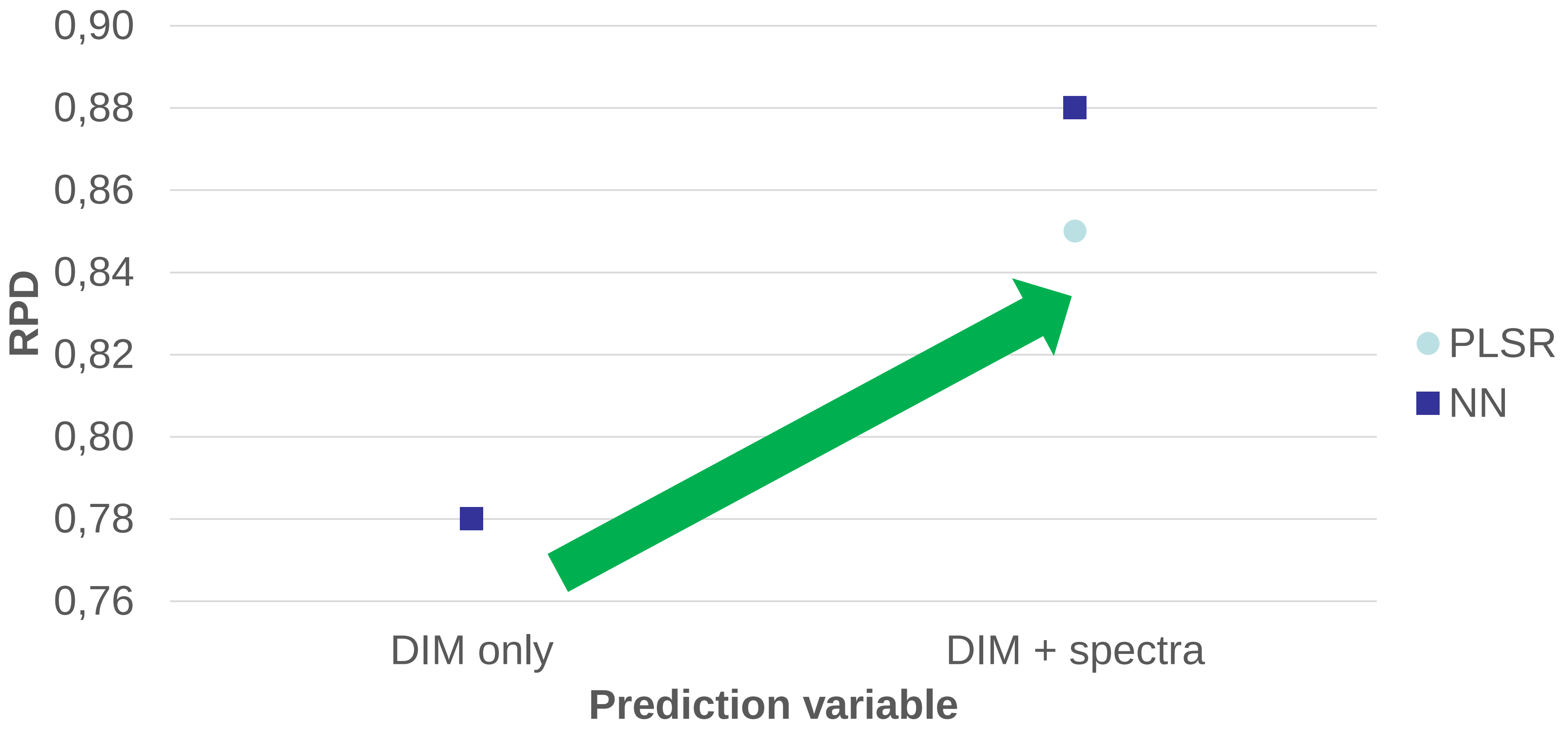
How useful is actually the MIR?

Example with body condition score change prediction



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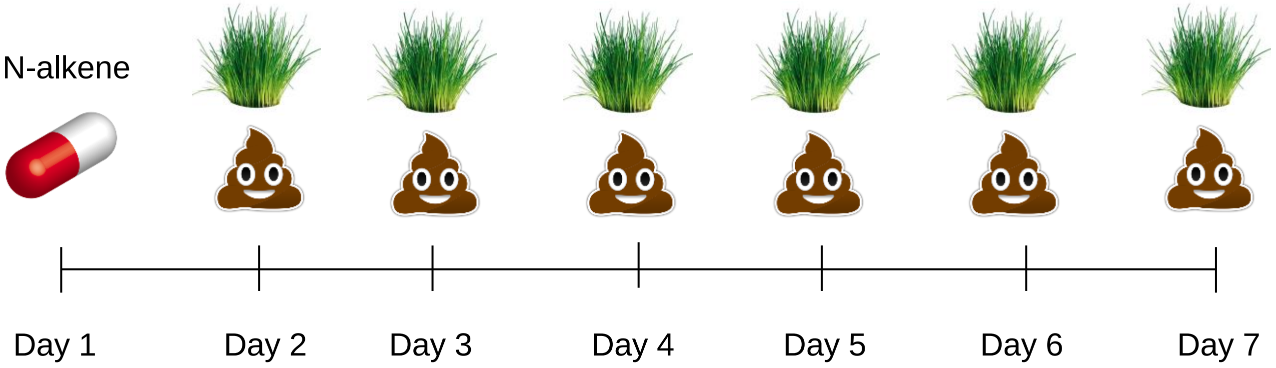
Prediction of nitrogen use efficiency



- NUE = (N in milk + N in the conceptus + N used for the growth + N stored in the reserves) / (N intake + N mobilized from the reserves)

Teagasc
Agriculture and Food Development Authority

Frizzarin et al., 2024 JDS
Using milk mid-infrared spectroscopy to estimate cow-level nitrogen efficiency metrics - ScienceDirect

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Prediction of nitrogen use efficiency

4 fold CV
NN algorithm

Trait	Prediction variable	Spectra type								
		Morning			Evening			Morning and evening		
		RMSEcv[1]	R^2	RPIQ	RMSEcv	R^2	RPIQ	RMSEcv	R^2	RPIQ
NUE	Spectra	3.16[a]	0.58	2.29	3.12[a]	0.58	2.32	3.02[c]	0.61	2.40
	Spectra + MY	2.68[b]	0.59	2.70	2.59[b]	0.71	2.79	2.49[d]	0.74	2.90
	Spectra + DIM	3.12[a]	0.58	2.31	3.10[a]	0.59	2.33	2.98[c]	0.61	2.43
	Spectra + MY + DIM	2.66[b]	0.69	2.72	2.64[b]	0.71	2.74	2.49[d]	0.74	2.90
	Spectra + MY + par	2.59[b]	0.84	2.80	2.58[b]	0.72	2.80	2.50[d]	0.74	2.89
	Spectra + MY + par + DIM	2.62[b]	0.71	2.76	2.67[b]	0.59	2.71	2.48[d]	0.74	2.92

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Prediction of nitrogen use efficiency

Farm independent CV

Trait and farm ID	n[1]	Mean	SD	PLSR				NN			
				RMSEV	R^2	Slope (SE)	RPIQ	RMSEV	R^2	Slope (SE)	RPIQ
1	893	19.03	3.31	4.90	0.10	0.25 (0.02)	0.88	6.43	0.14	0.26 (0.02)	0.67
2	1,023	23.47	4.60	4.17	0.31	0.67 (0.03)	1.38	4.87	0.18	0.46 (0.03)	1.18
3	1,009	21.33	4.27	5.23	0.07	0.28 (0.03)	1.23	4.85	0.25	0.41 (0.02)	1.33
4	572	26.97	3.52	5.37	0.28	0.79 (0.05)	0.82	5.62	0.24	0.67 (0.05)	0.78

Previously R2 of 0.74

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Prediction of methane - Data

- 93,888 individual methane spot measures (>2 minutes)
  - 384 lactations from 277 dairy cows

n≥20

Methane

n≥10 n≥10

-6 0 +6

AM & PM Milk sample
- Yield & composition
- Spectrum
- Days post calving

AM only
PM only
AM+PM
―――――
AM&PM

Agriculture and Food Development Authority

McParland et al., 2024 JDS
Predicting methane emissions of individual grazing dairy cows from spectral analyses of their milk samples - ScienceDirect

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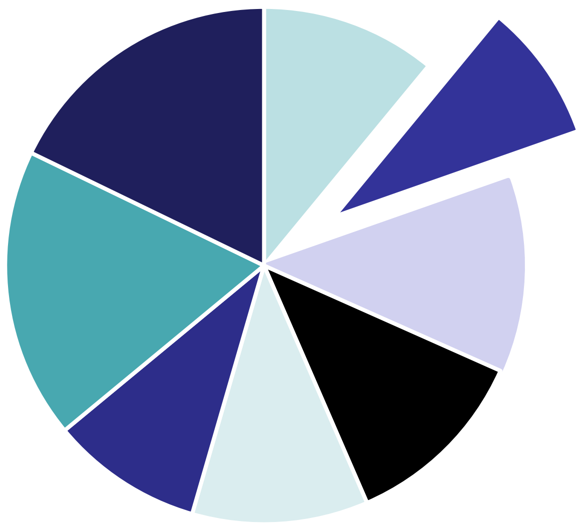
Prediction of methane - Approach

One experiment out



$$\text{Methane} = \int (\text{spectrum, days in milk, yield, fat\%, protein \%})$$

Partial least squares or neural networks

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Prediction of methane - Results

- μ = 323.4 g/d
- σ = 75.2 g/d
- Average of 30 spot measures to ±6 days
  - 111 minutes
- Repeatability = 28%

- Little difference
  - AM v PM, neural networks v partial least squares
- Flanking 6 days > previous 6 days > subsequent 6 days

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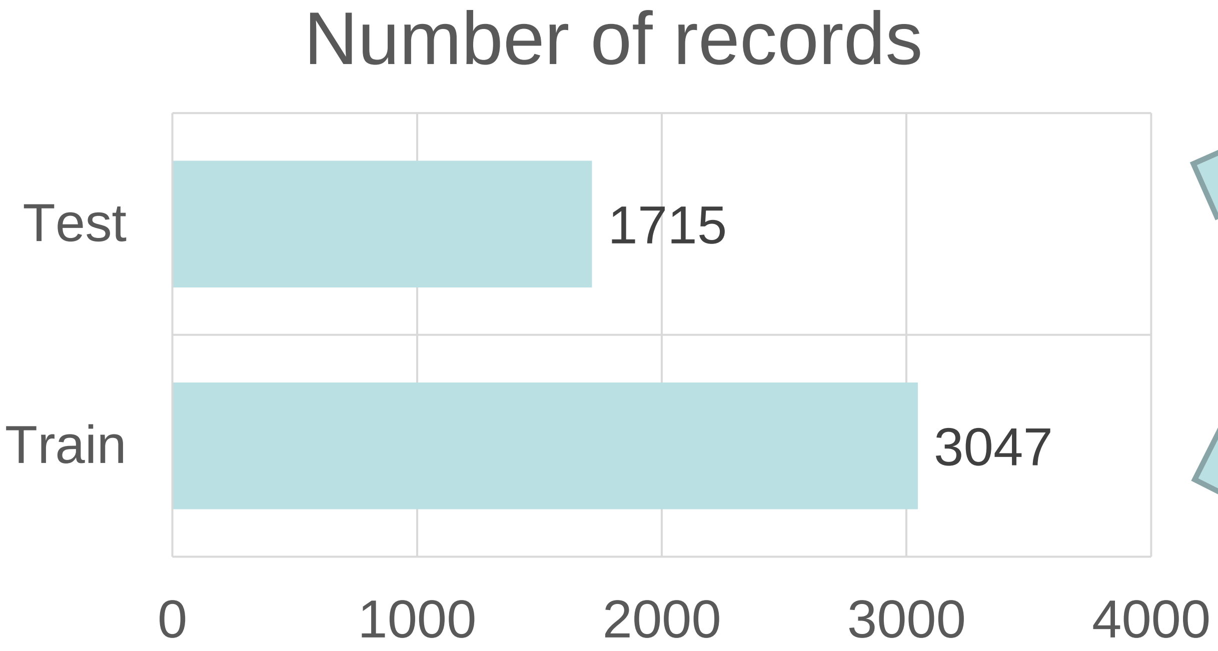
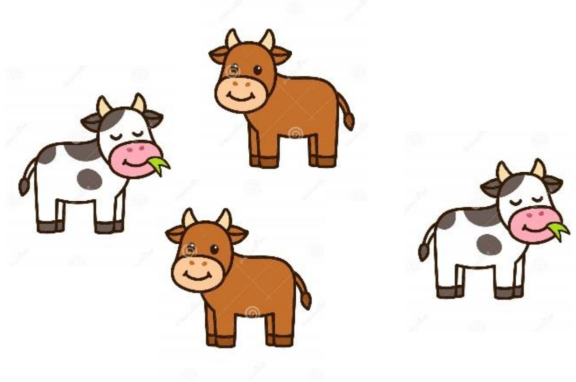
Prediction of methane – results

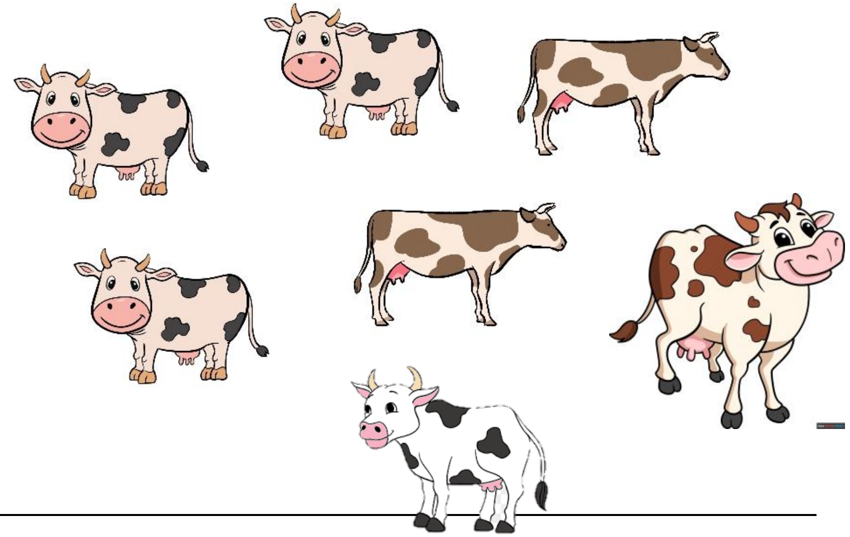
Using NN, average AM and PM spectra, and flanking 6 days

Model	No spectra	With spectra
Spectra		0.55 (0.07)
DIM	0.32 (0.13)	0.55 (0.06)
Yield	0.10 (0.18)	**0.64 (0.05)**
Composition	0.32 (0.13)	0.57 (0.06)
DIM + yield	0.52 (0.10)	0.64 (0.06)
DIM + composition	0.41 (0.10)	0.55 (0.06)
Yield + composition	0.32 (0.07)	0.62 (0.05)
DIM + yield + composition	0.54 (0.09)	0.64 (0.05)

Prediction of methane – new validation

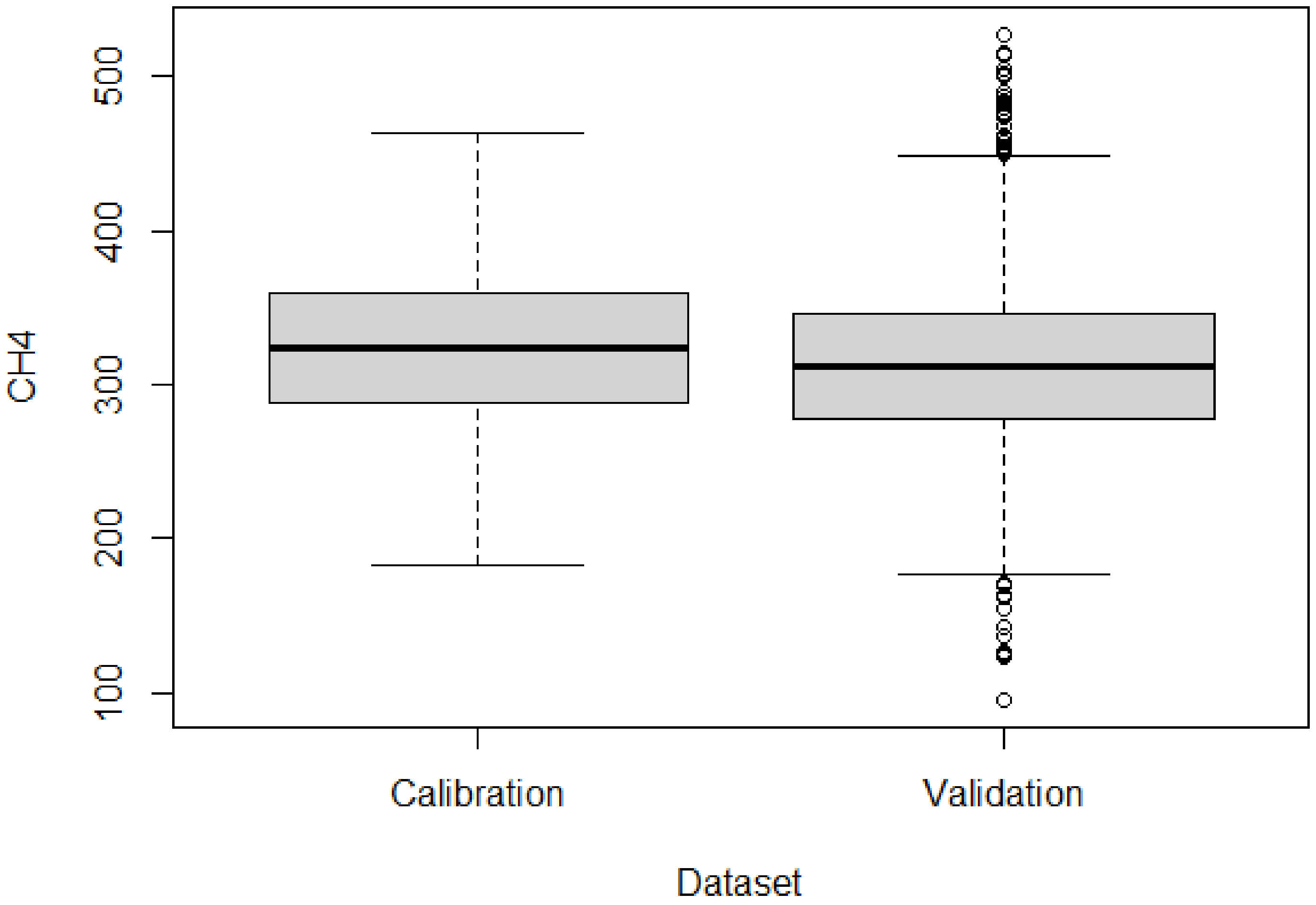






Prediction of methane – new validation

- Calibration
  - N = 3,047
  - From 2020 to 2022
- Validation
  - N = 1,715
  - From 2023



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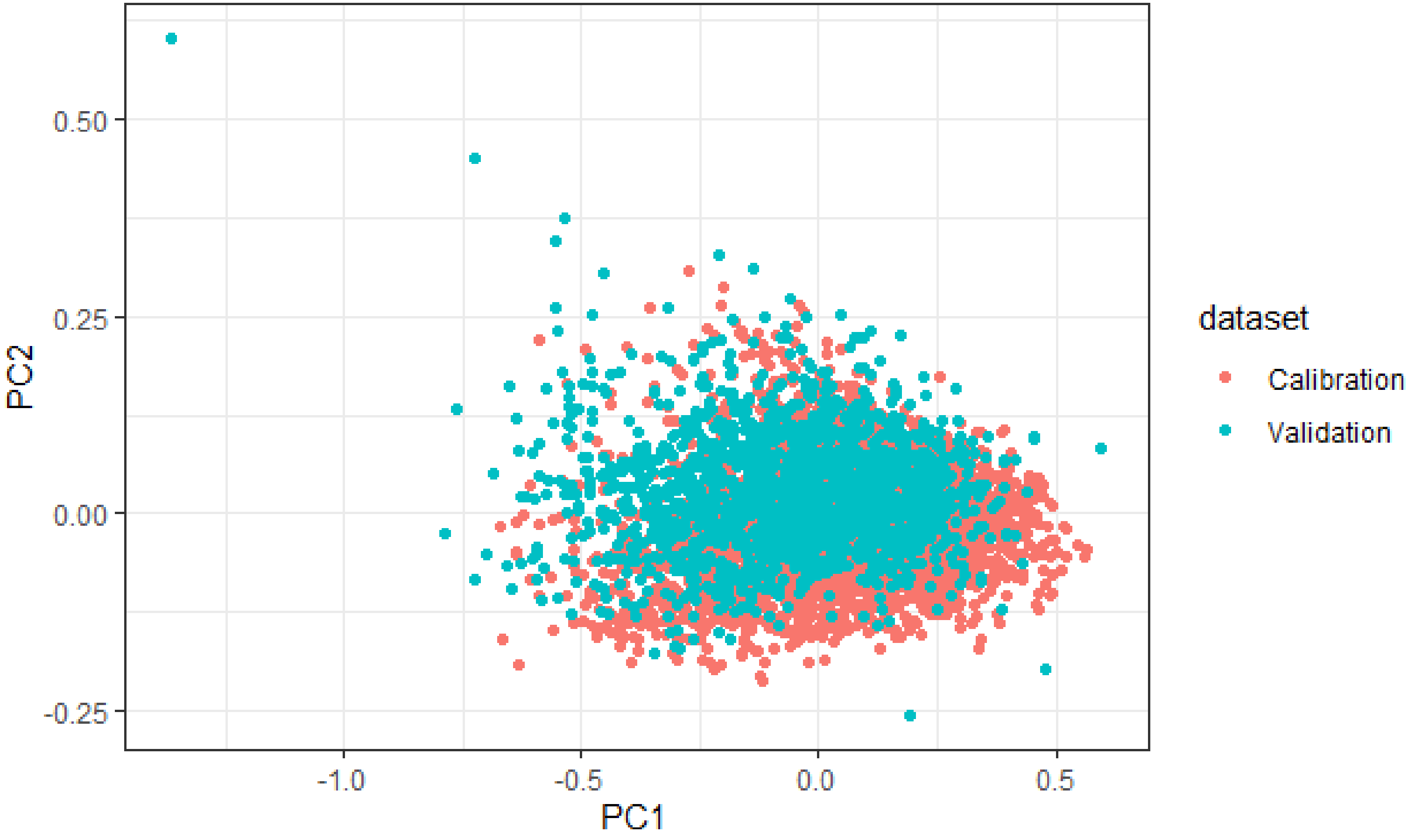
Prediction of methane – new validation



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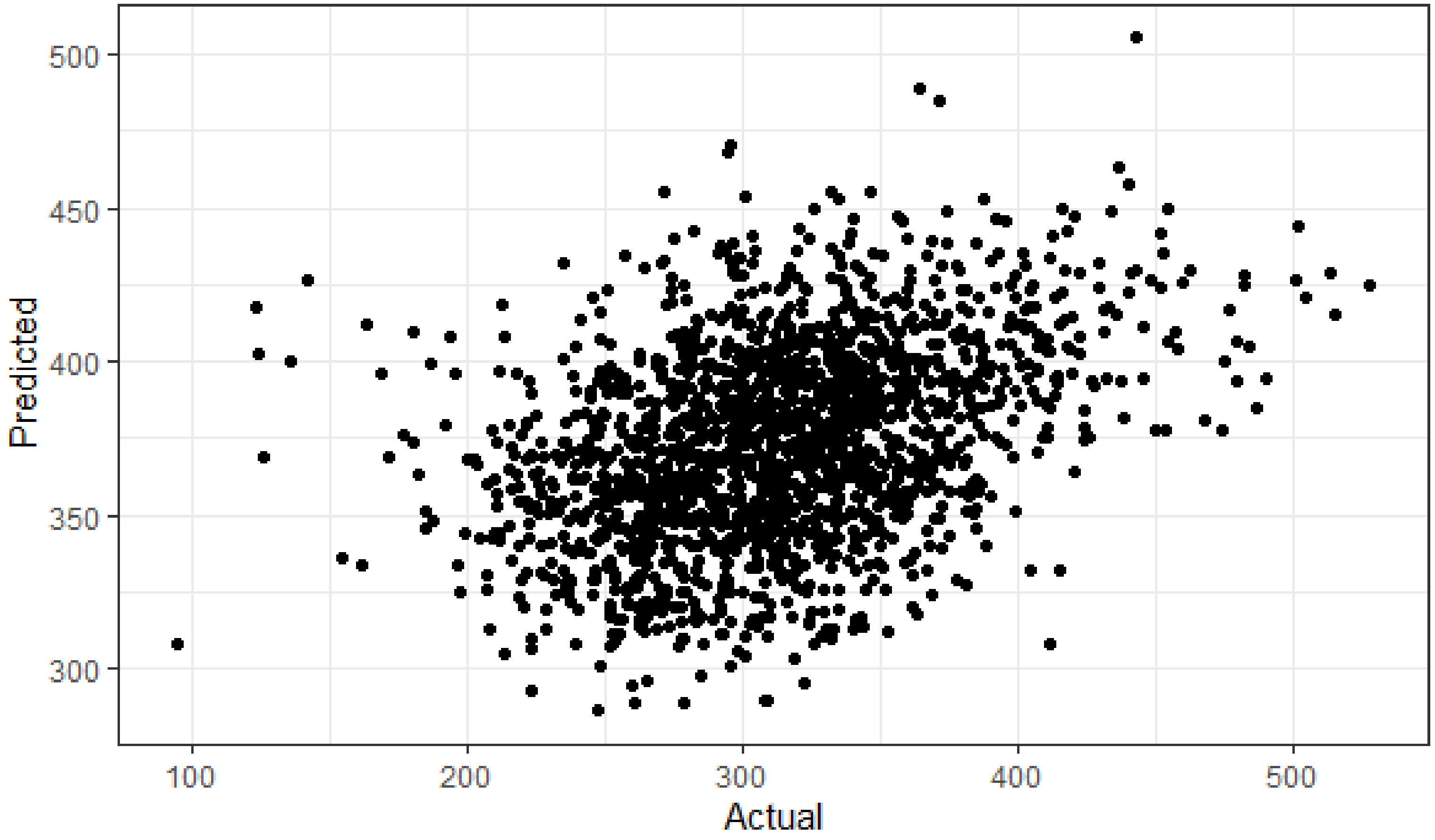
Prediction of methane – new validation

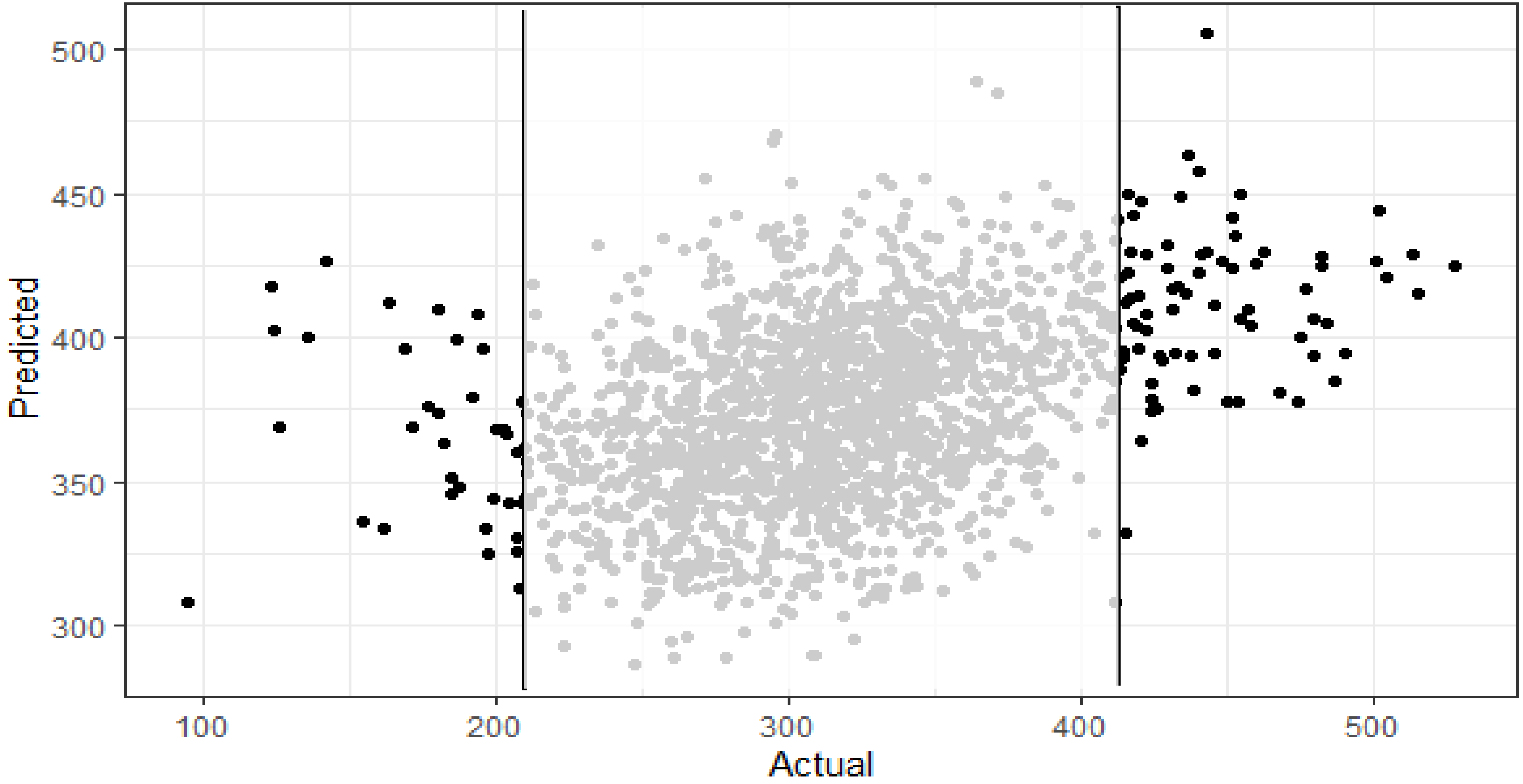


- Correlation between actual and predicted of 0.38 *
- Root mean square error of 78.76 g/d

* Correlation in the training dataset of 0.64

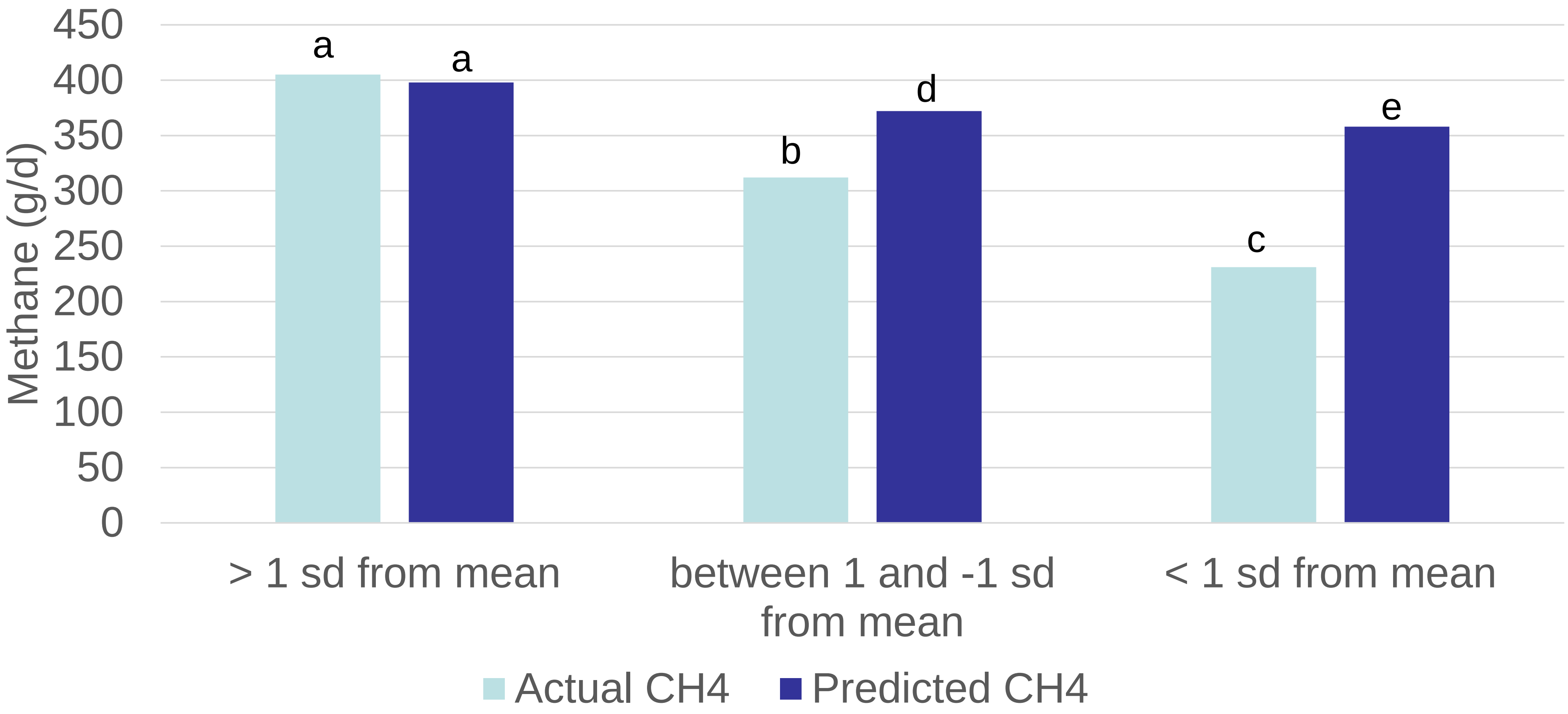
Low 10% emitting cows

High 10% emitting cows



- Mean methane predicted high 10% emitting cows = 402.59 g/d
- Mean methane predicted low 10% emitting cows = 358.29 g/d

Prediction of methane – new validation



Considerations

- Spectra provides additional information to just animal data
- Different spectra available (AM and PM)
- Different ways of combining the spectra and the phenotype
- Validations scenarios essentials to have realistic results
- Often accuracies of prediction are relatively low
- Ability in identify high and low emitting cows
- Ability in identifying groups of cows

Application

How to use it for farm milk recording?

- Different protocolos across farms
  - Collection of both morning and evening milk
  - Collection of just morning milk
  - Collection of just evening milk
  - One time collection of just morning milk, following time collection of evening milk
  - Milking robots

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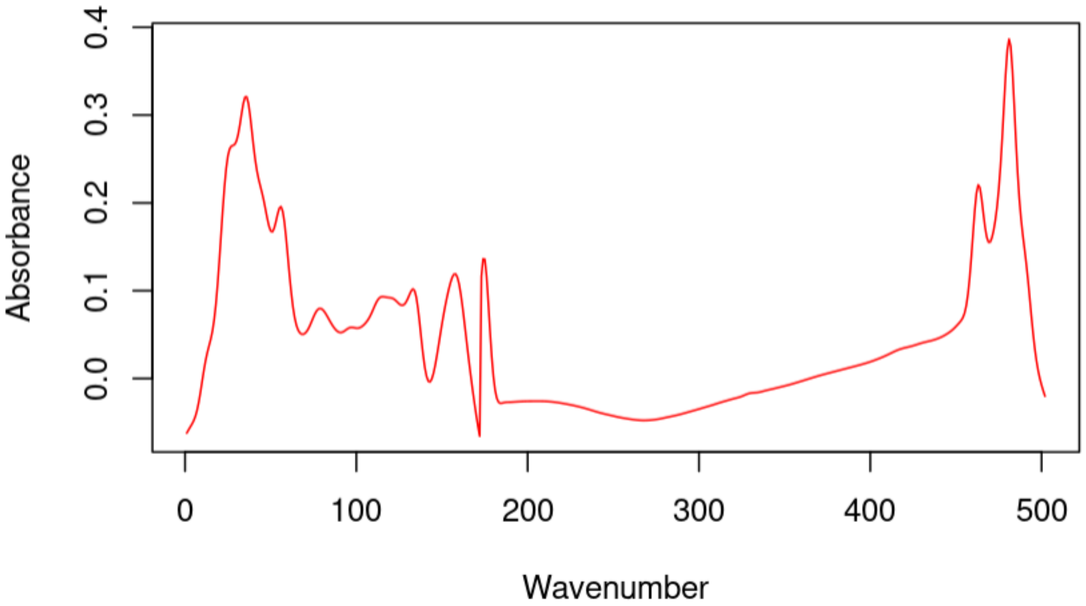
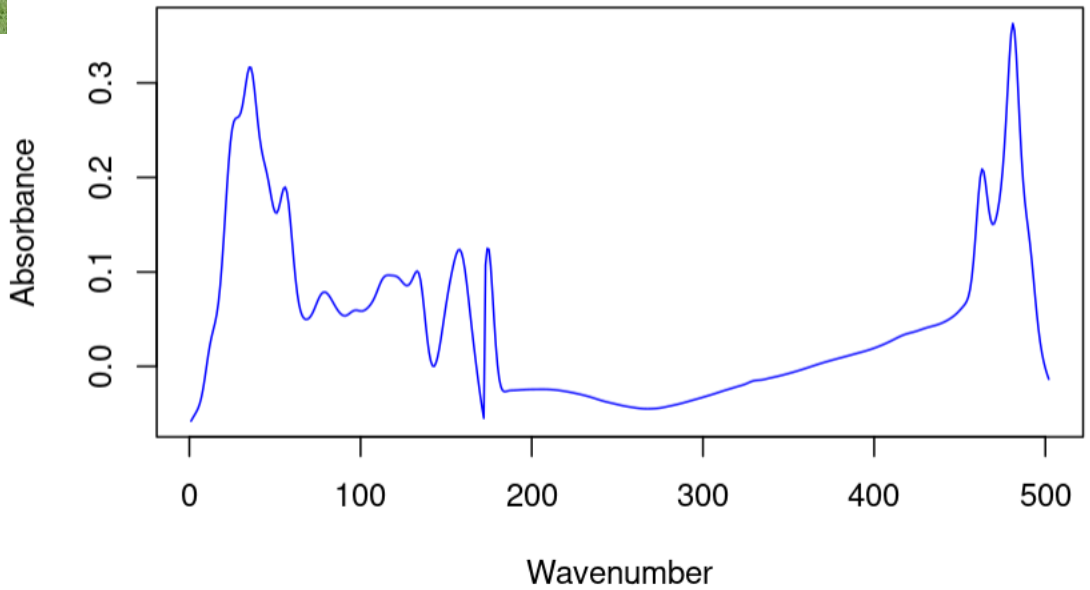


Yield

Fat

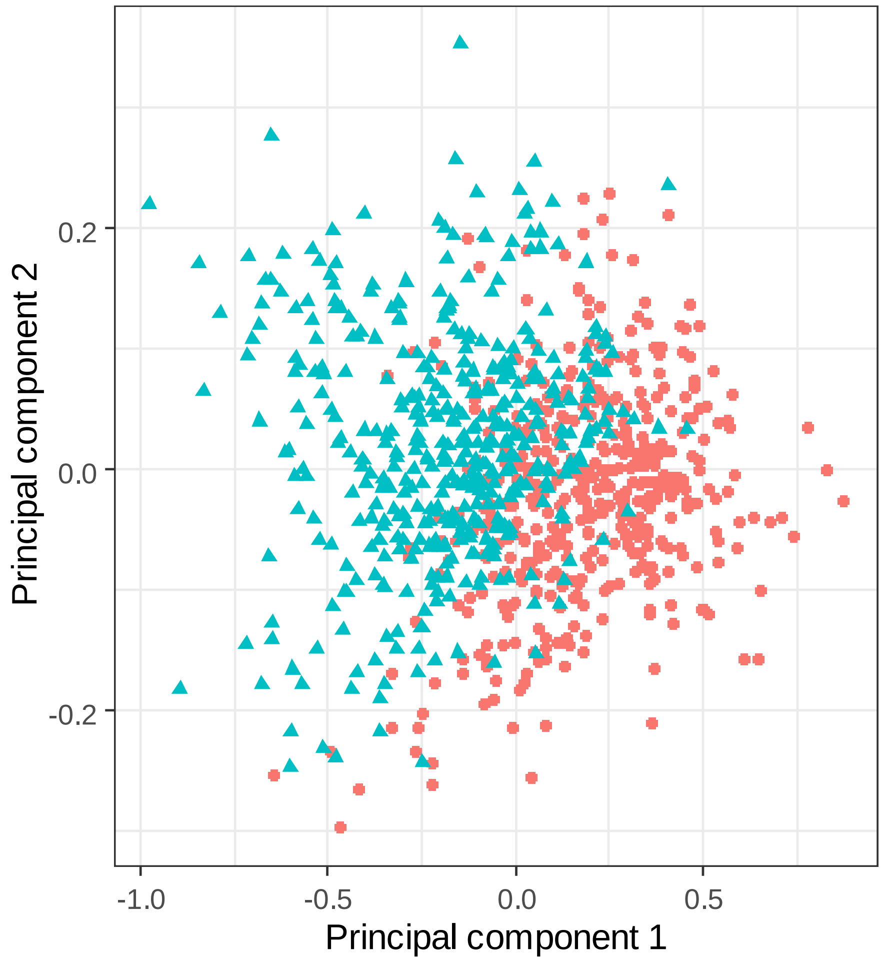
Protein



Frizzarin et al., 2025 JDS
[Comparison of the mid-infrared spectra and prediction equations developed from morning and evening milk samples from twice-a-day milked dairy cows - ScienceDirect]

Data

- 199,288 morning spectrum
- 199,288 evening spectrum
- 2,602 cows
- From 2016 to 2020
- 7 Teagasc research farms



Red = Morning

Blue = Evening

Analyses

- Internal correlation between morning wavelength values vs internal correlation between evening wavelength values
- Difference between morning and respective evening wavelength values
- Pearson correlation between morning and respective evening wavelength values
- Quantified for
  - Entire dataset
  - Within lactation stage, farm, year

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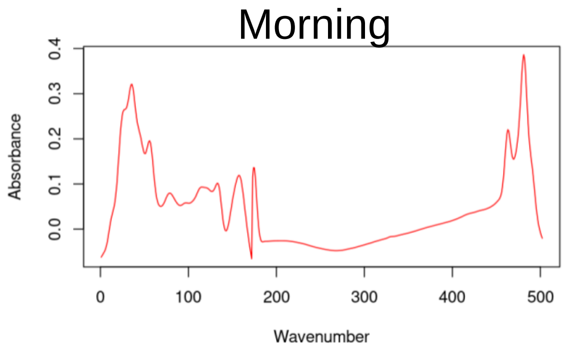
Analyses

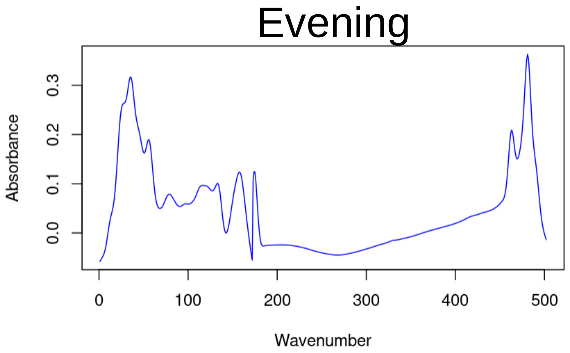
- Prediction equations for nitrogen use efficiency (NUE)
- NUE = (N in milk + N in the conceptus + N used for the growth + N stored in the reserves) / (N intake + N mobilized from the reserves)

Predicted from equations developed on

NUE

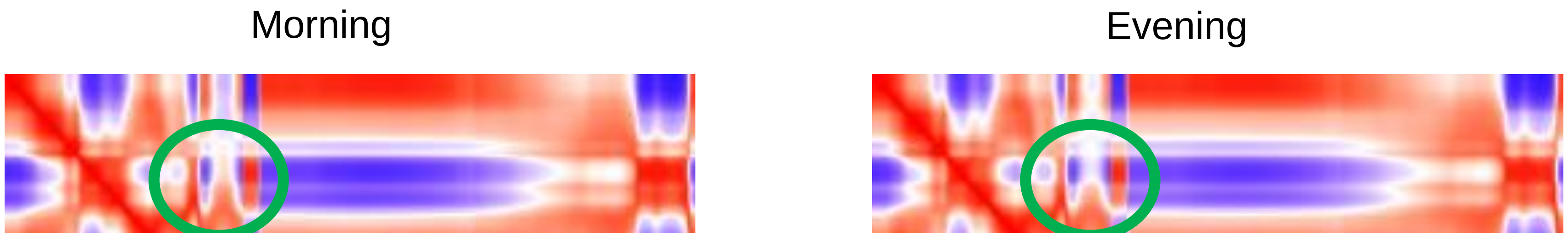


Morning spectra
Evening spectra
Weighted morning and evening

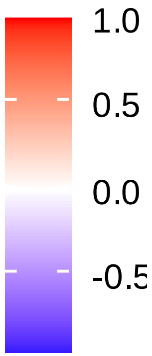


Morning spectra
Evening spectra
Weighted morning and evening

Results



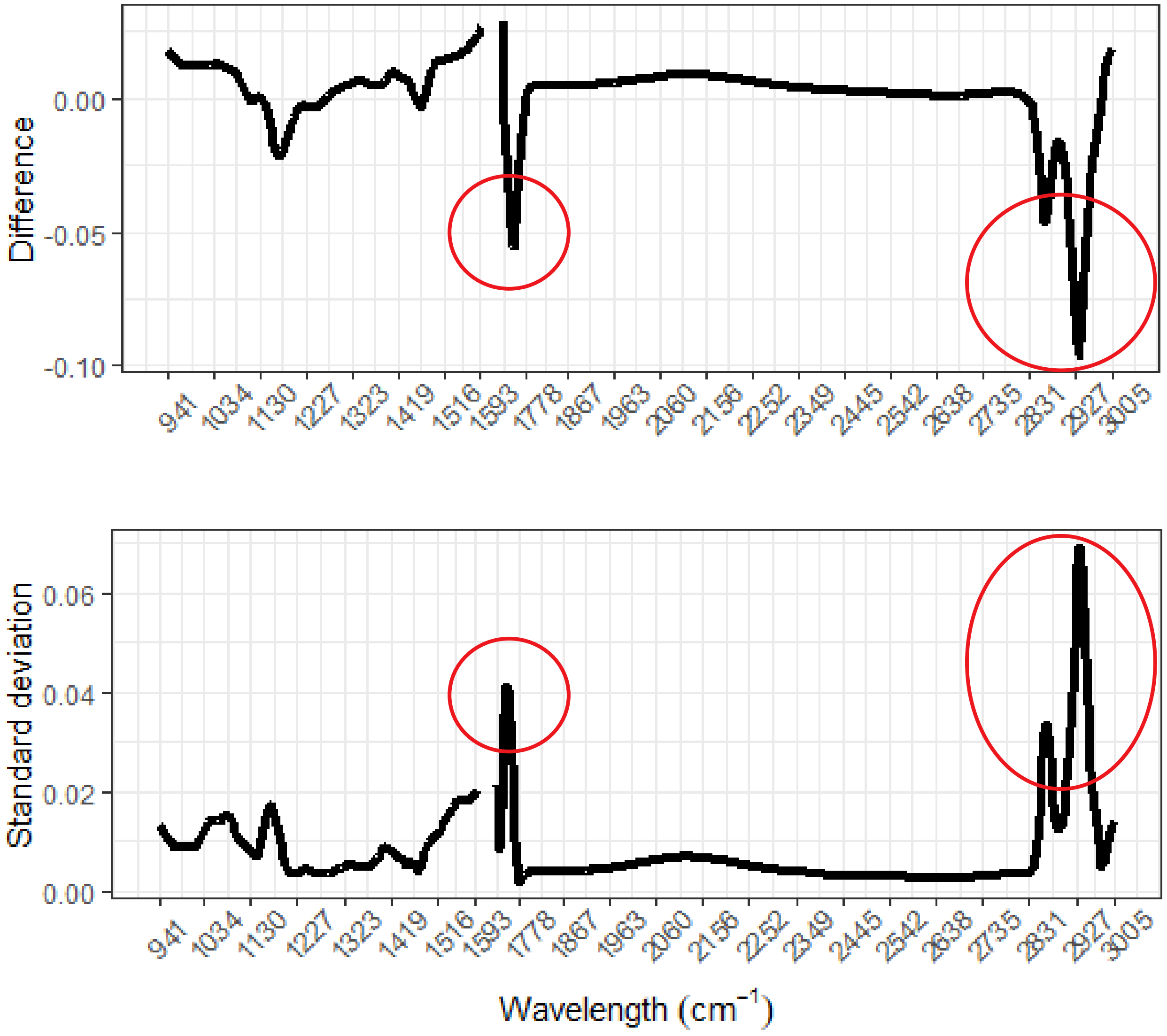
Internal relationships among the absorbance values for the morning spectra differed ($P < 0.05$) from those among the absorbance values for the evening spectra



Results

Morning minus evening wavelenght values

SD morning – evening wavelenght values



Fat

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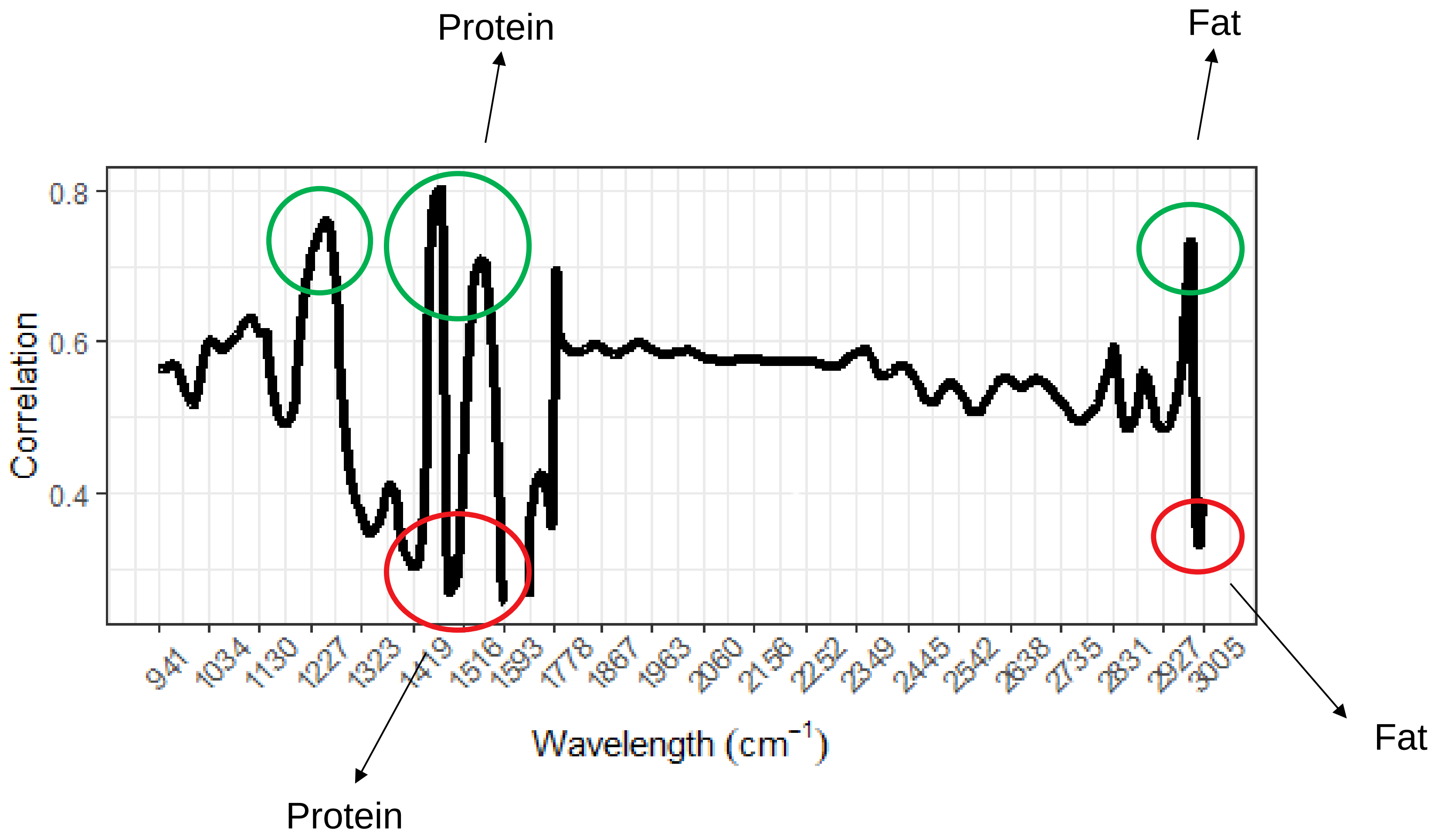
Results



Correlation

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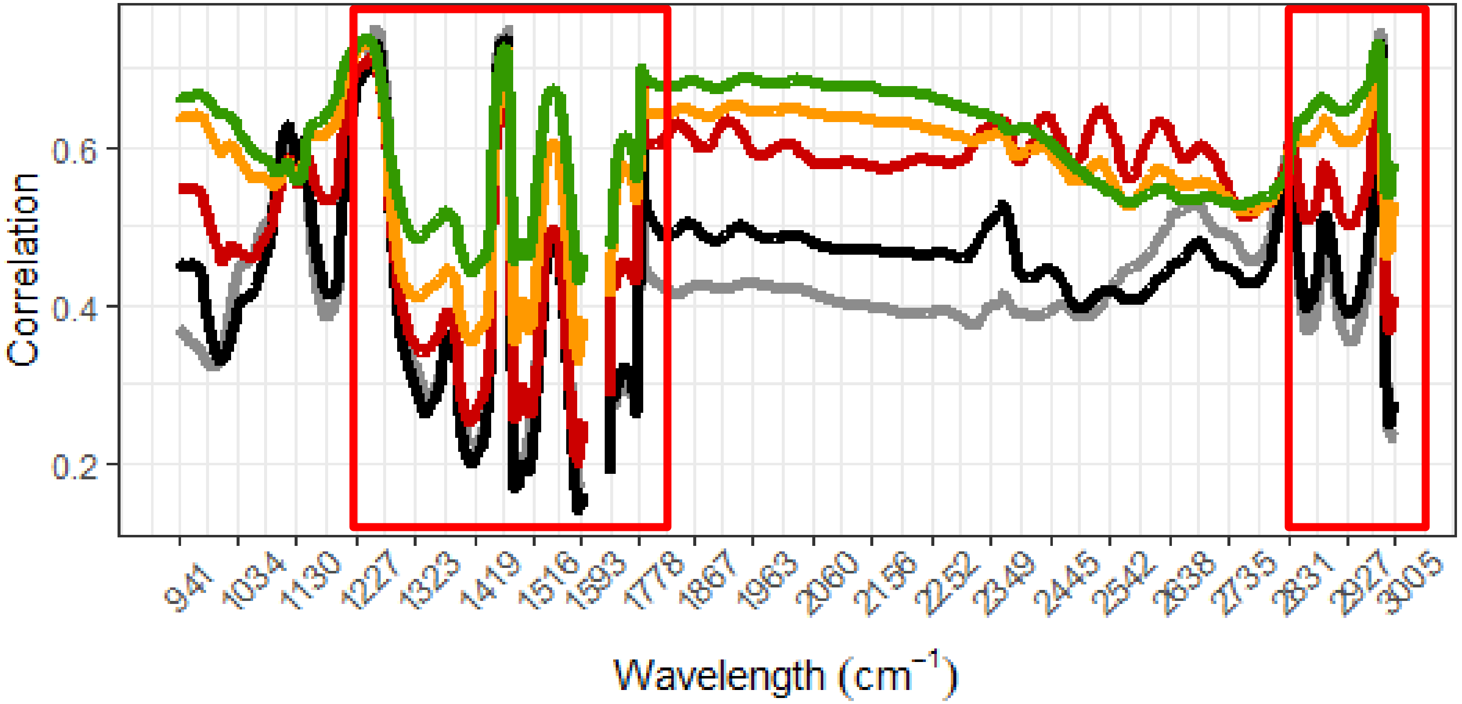
Results

Correlation within lactation stage



5 to 60 DIM (grey line)
61 to 120 DIM (black line)
121 to 180 DIM (red line)
181 to 240 IM (orange line)
240 to 305 DIM (green line)

Consistent profiles

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Results

Calibration	Validation		r	RMSE
Morning	Morning		0.70	3.49[a]
Evening	Morning		0.62	3.85[b]
Average	Morning		0.67	3.63[c]
Evening	Evening		0.70	3.46[a]
Morning	Evening		0.66	3.85[b]
Average	Evening		0.67	3.79[b]

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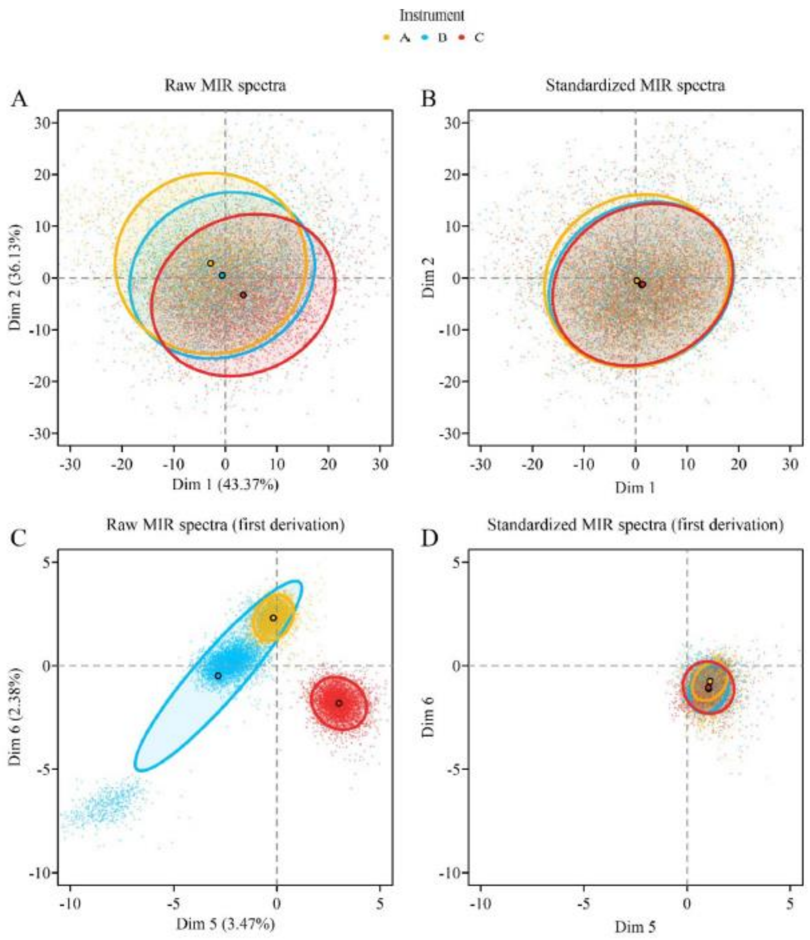
Application

How to use it for farm milk recording?

- Distinct internal relationships among the absorbance values for morning and evening milk spectra
- Certain spectral regions exhibit substantial differences in absorbance values between morning and evening milk samples
- Other spectral regions had weak correlations between the absorbance values of morning and evening spectra
- More pronounced differences in early lactation
- Variability in absorbance values at different wavelengths between morning and evening samples can influence the accuracy of predicting animal-related traits from milk MIR

Share equations across countries

Spectra standardization



Mensching et al., 2025 JDS
[Daily standardization of routinely collected milk mid-infrared spectra from dairy herd improvement testing in a statistical framework - ScienceDirect]

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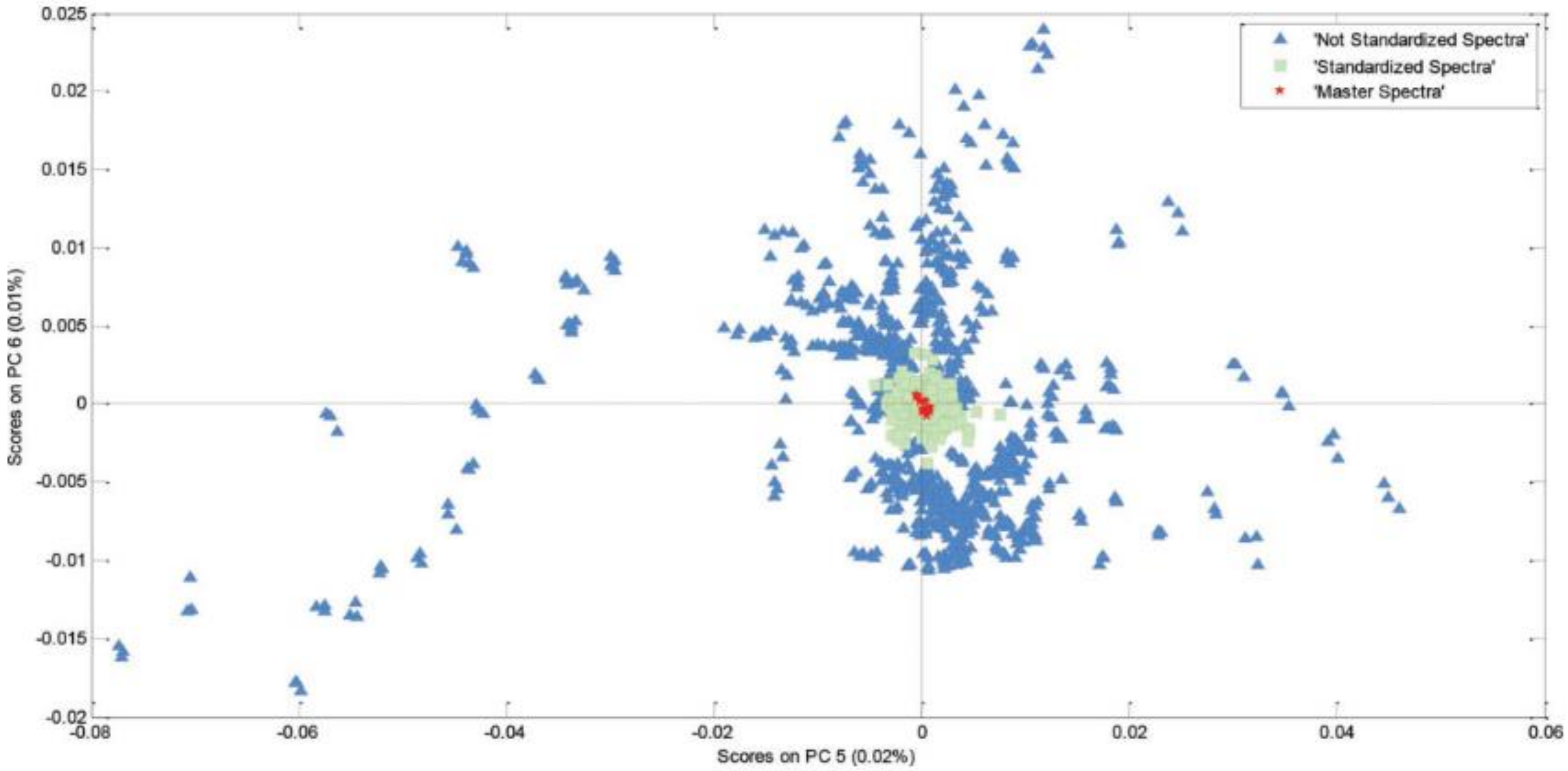
Share equations across countries

Spectra standardization



Grelet et al., 2017 JDS
Standardization of milk mid-infrared spectrometers for the transfer and use of multiple models - ScienceDirect

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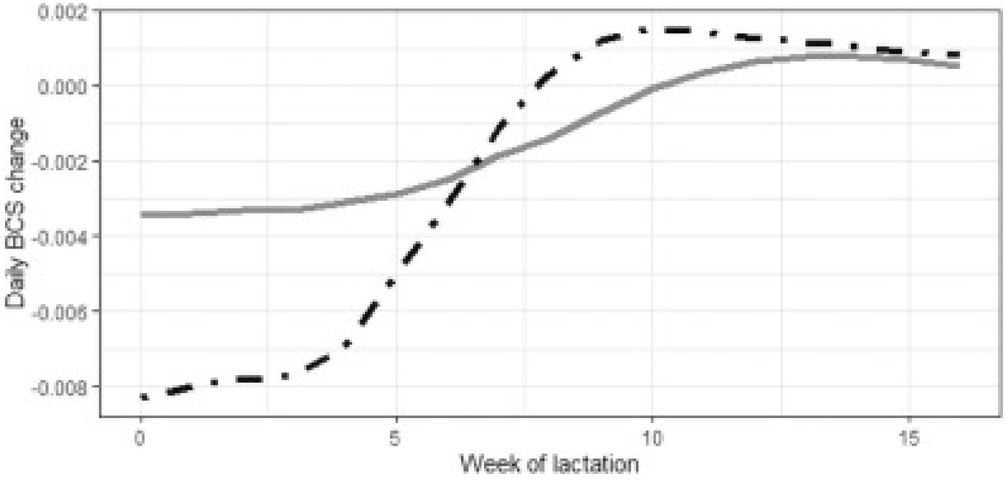
Share equations across countries

Differences in the phenotype



Canadian daily BCS change (black dashed-dotted line)

Irish daily BCS change (gray continuous line)

Mean and SD of daily ΔBCS

Canadian cows -2.30×10^{-3} and 4.26×10^{-3} BCS units

Irish data were -1.19×10^{-3} and 2.00×10^{-3} BCS units

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Frizzarin et al., 2024 JDS
Transferability across countries of equations developed using milk mid-infrared spectroscopy to estimate daily body condition score change in dairy cows - ScienceDirect

Share equations across countries

Differences in the phenotype

Canadian data to predict Canadian data

Calibration	Pretreatment	Method	RMSEV[2, 3] (SD)	Bias[2] (SD)	r (SD)	Slope (SE)	RPIQ (SD)
Canadian only	None	PLSR	1.68[d] (0.026)	0.00 (0.041)	0.92 (0.006)	1.00 (0.008)	2.54 (0.03)
		NN	1.47[e] (0.038)	0.00 (0.027)	0.94 (0.003)	1.00 (0.006)	2.91 (0.07)
	First derivative	PLSR	1.70[d] (0.032)	0.00 (0.048)	0.92 (0.003)	1.00 (0.007)	2.51 (0.05)
		NN	1.47[e] (0.021)	0.00 (0.044)	0.94 (0.002)	1.00 (0.004)	2.90 (0.04)

No bias, slope of 1, r > 0.92

Irish data to predict Canadian data

Pretreatment	Std	Method	RMSEV[2, 3]	Bias[2]	r	Slope (SE)	RPIQ
None	No	PLSR	4.99[a]	3.98	0.80	1.83 (0.012)	0.85
		NN	3.52[b]	1.84	0.78	1.71 (0.012)	1.21
First derivative	No	PLSR	3.41[c]	1.04	0.67	1.31 (0.013)	1.25
		NN	3.57[d]	0.66	0.62	1.67 (0.019)	1.19
None	Yes	PLSR	11.17[e]	10.85	0.80	0.86 (0.006)	0.38
		NN	6.88[f]	6.29	0.78	0.80 (0.006)	0.62
First derivative	Yes	PLSR	5.86[g]	4.59	0.67	0.62 (0.006)	0.73
		NN	5.10[h]	3.78	0.62	0.78 (0.009)	0.84

Large bias, slope largly different from 1, r < 0.81

Frizzarin et al., 2024

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Conclusions

- MIR spectra of milk is already available in many countries
  - Pipeline already existing
  - No extra cost in collecting new data

- Prediction equations not always easy to develop for animal features (e.g., methane emissions, NUE)

- Difficulties in implementation when different protocols exist for milk recording

- Difficult of sharing equations across countries if no spectra standardization and if very different production systems (different phenotypes)

Thank you for your attention

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