Daily standardization of milk mid-infrared spectra in a comprehensive regression model framework considering animal related data

A. Mensching¹, J. Braunleder¹, E. Bohlsen², S. Schierenbeck¹, and R. Reents¹

¹ Vereinigte Informationssysteme Tierhaltung w.V. (vit)
² Landeskontrollverband Niedersachsen
MIR spectrometry and its challenges

Y

e.g. fat, protein
... also CH₄ or blood BHB

Y = Xb + e

Same instrument, promptly analyses after calibration...

Same instrument, same samples, but much later in time

Other instrument (same or other model type, other brand...)

\[ \text{Fat [%]} \text{(MIR)} \]

\[ \text{Fat [%]} \text{(Reference)} \]

\[ Y = Xb + e \]
MIR spectrometry and its challenges

**General instrument effects**
- Constructional differences
  - Wavenumber range and number
  - Cuvette material (CaF₂ or diamond)
  - Marginal deviations during production
  - ...

**Temporal instability or deviations**
- Environmental effects like Temperature and humidity
- Technical wear and component changes
- Mechanical or electronic effects (sensor drift)
- ...

Wang et al. (1991): Multivariate Instrument Standardization
Nieuwoudt et al. (2021): Monitoring of Instrument Stability

**Compensation approaches so far**

Post measurement correction of predictions:
- Slope/intercept correction using check samples ('standard milk') with known reference values

<table>
<thead>
<tr>
<th>Spectral standardization:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Manufacturer's own standardization, e.g.: FOSS standardization</td>
</tr>
<tr>
<td>Standardization service of European Milk Recording (EMR) according to Grelet et al. (2015)</td>
</tr>
<tr>
<td>Retroactive standardization according to Bonfatti et al. (2017)</td>
</tr>
</tbody>
</table>

→ Only applicable for known reference values!

→ Enables the use of various models!

But so far only monthly or in even larger time intervals!
The concept of the vit-standardization

What can the observed variance of raw spectra be attributed to?

Aim: Quantify and eliminate variance related to general and temporal instrument effects

How?: Using a framework of regression models on DHI samples considering
• Slope/intercept-corrected laboratory values
• Data on sample origin like DIM and parity of the cow
• Information on the instrument and time of analysis

→ Instrument-wise daily standardization coefficients

Milk main components (fat, protein, lactose)

General and temporal instrument effects

Further associations to other available information (e.g. DIM of the cow)

Absorbance [Log(1/T)]

DIM [d]
Material and methods

All data were provided by the LKV Niedersachsen

- Period: 01/2022 to 06/2022
- Primary breed: Holstein (92%)
- 5 FOSS instruments (2 x MilcoScan™ 7 RM, 3 x MilcoScan™ FT+)

Routine DHI samples
(n = 2.3 M, 5 instruments)

Triple analysed DHI samples
(n = 5.3 k of 7 farms x 3 instruments)

Check samples
(n = 61.0 k, 5 instruments)

Estimation of standardization coefficients

Analysis

I. MIR raw vs. MIR standardized
II. Estimability of fat during calibration

Fat (lab) = Xb + e (→ MIR raw)
Fat (lab) = Xb + e (→ MIR standardized)

Milk fat as an example trait for demonstration purposes

III. Estimability of fat over time
Results I: MIR raw vs. MIR standardized

Principal Component Analysis

• \( n = 4,471 \) per instrument
• 212 of 1,060 wavenumbers

→ Untreated absorbance values
→ 1\textsuperscript{st} gap derivative
Results II: Estimability of fat

Background information

• Splitting of the data
  – 80% calibration, 20% validation

• Separate fat models for raw and standardized spectra

• PLS-regression model properties
  – 1\textsuperscript{st} gap derivative
  – 512/1,060 WN
  – n = 6 latent variables
Results III: Estimability of fat over time

Background information

• n = 53.5 k (balanced over 5 instruments)
• Weekly changed ‘North German Standard Milk’
  – Correspond to bulk milk samples
  – Small range with 3.86 to 4.27% fat

Remark

Check samples were neither used for standardization nor for fat model calibration!
Summary and conclusion

• MIR spectrometric measurements are often impacted by
  – general instrument effects and
  – within instruments over time

• Daily vit-standardization demonstrates
  – A harmonization of MIR spectra across machines and over time
  – An improved ability for the estimation of fat compared to the use of raw spectra
  – Almost similar accuracy as of slope/intercept corrected laboratory fat values

• Further advantages
  – Frequent standardization possible, e.g. daily
  – No need for common milk samples
  – No additional workload for the laboratories

• High potential for the provision of best possible MIR-based predictions as input for
  – genomic evaluations
  – herd management tools
Outlook

• In the meantime …
  – Adaptation of the vit-standardization so that it can handle daily incoming data
  – A first MIR-based tool for monitoring of ketosis on routine DHI-data is active for > 3000 farms
• Comparison with other standardization strategies within the ICAR ExtraMIR project
• Provision of MIR-based predictions as phenotypes for breeding purposes
• Use of vit-standardization coefficients for the qualitative monitoring of spectra?
• Applying the method on
  – bulk milk samples
  – data from other regions and other breeds
  – spectra from instruments of other manufactures
Thank you for your attention!