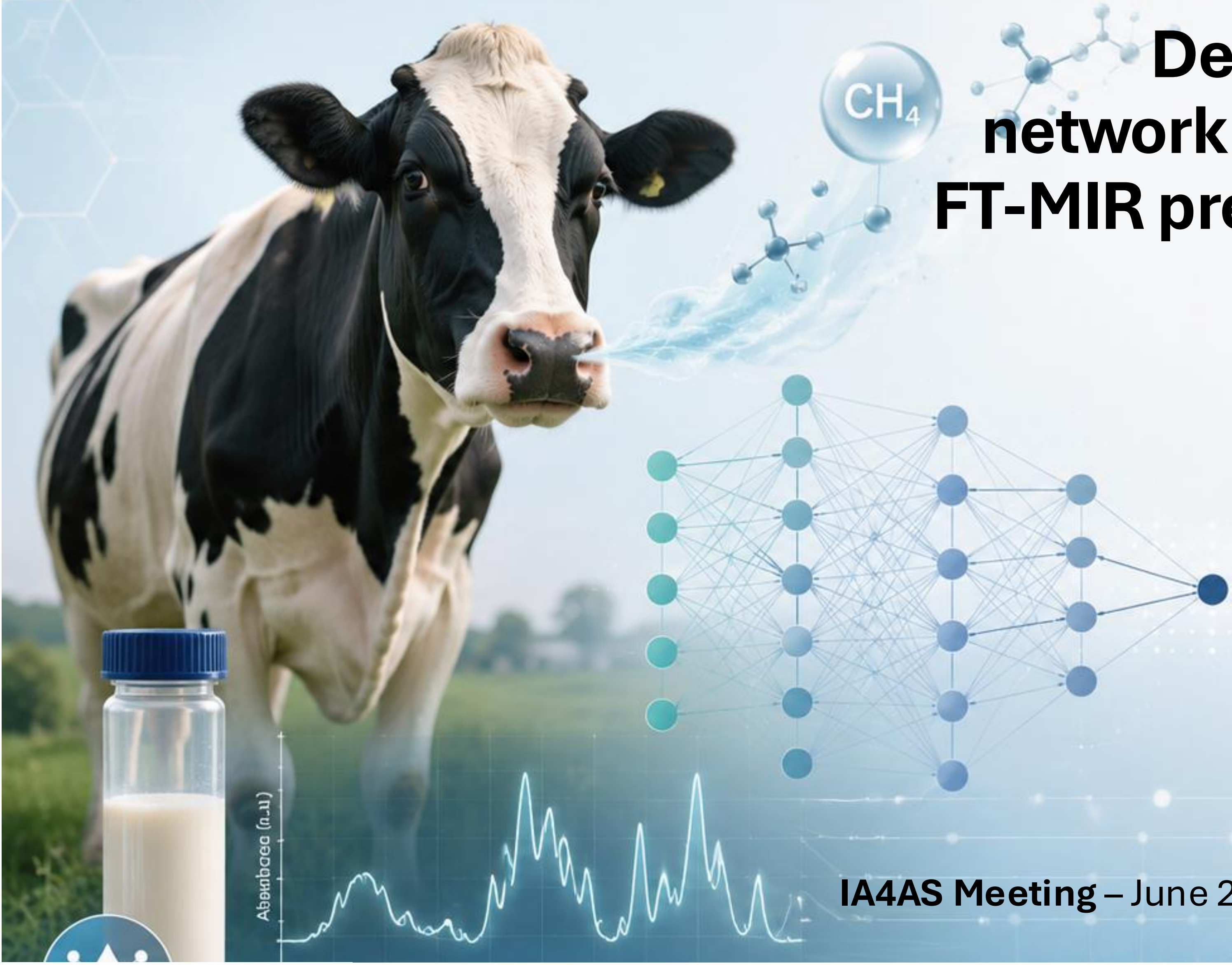
Development of robust neural network architectures for federated FT-MIR prediction of enteric methane emissions in dairy cows

H. Soyeurt, F. Dehareng, N. Gengler, S. McParland, M. Kreuzer, P. Lund, C. Martin, B. Kuhla, A. Vanlierde



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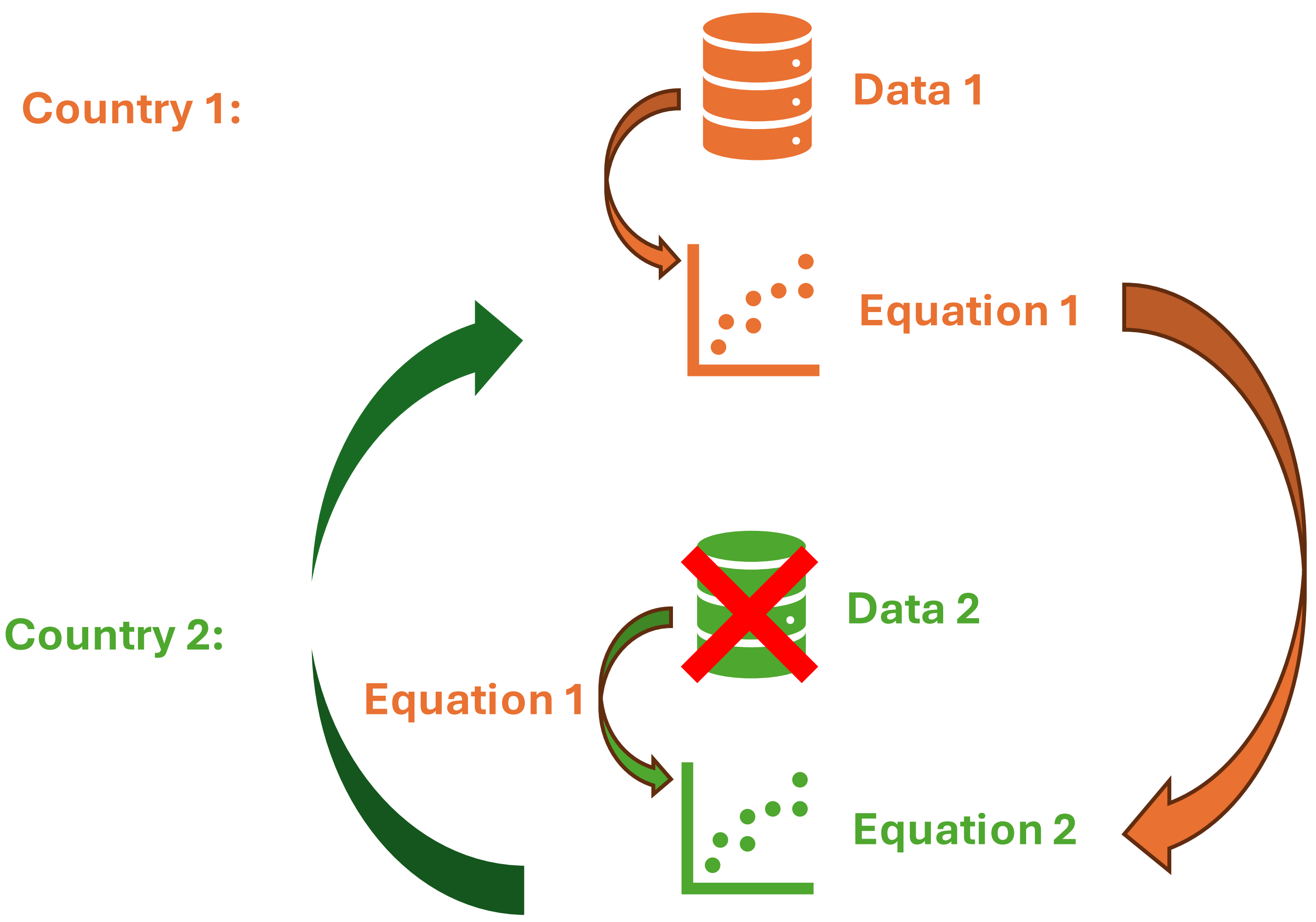
Why neural network ?

- Currently, Partial Least Squares (PLS) Regression
  - High correlation between some spectral points ➔ decrease the dimensionality
  - Known to be robust with low size dataset

- Why neural network ?
  - Considering potential non-linear relationships
  - Transfer learning can facilitate the improvement of models without exchanging data

Transfer learning



This is possible by using neural networks !

Model comparison

- **PLS**
  - **867 features** = 289 spectral points regressed until the second order Legendre polynomials
- Multi-layer neural perceptron (**ANN**)
  - **867 features**
- 1-D Convolutional neural network (**cANN**)
  - 1-D spectral image : **867 pixels**
- 2-D Convolutional neural network (**cANN2**)
  - 2-D spectral image : **289 * 3 pixels**, one row for each Legendre Polynomial

1	2	3	…	867

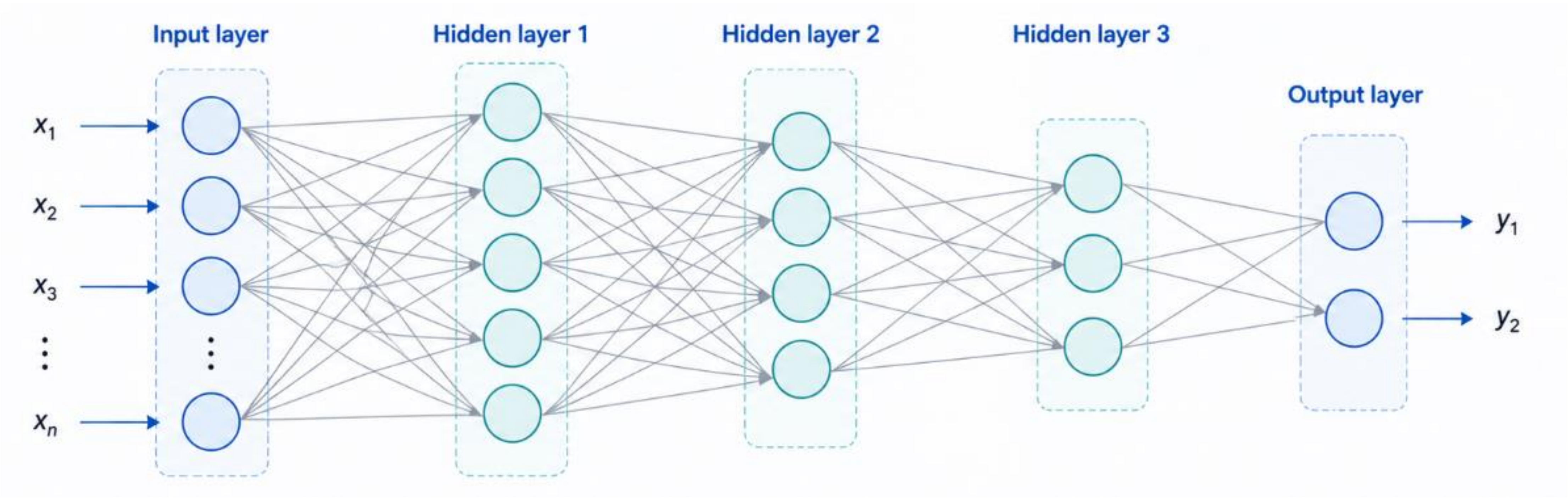
1	2	3	…	289	Raw spectrum
1	2	3	…	289	1st Legendre regressed spectrum
1	2	3	…	289	2nd Legendre regressed spectrum

Define the best structure for PLS

HYPERPARAMETER –
NUMBER OF PLS FACTORS

COW-INDEPENDENT **5-FOLDS** CROSS-VALIDATION

Multi-layer perceptron (ANN) - Theory



For us, only **one output** as it is a regression

Minimum hyperparameters:

- **Number of hidden layers**
- Number of **nodes** in each hidden layers

Define the best structure for ANN

- **Max. 10 hyperparameters** :
  - **Batch size** : 32 , 64 samples
  - **Learning rate**: 1e-4, 1e-2
  - **Weight decay** : 1e-8, 1e-2
  - **Number of hidden layers** : 1 to 5
  - **Number of nodes in each hidden layer** : 16 to 128 (step = 16)
  - **Drop-out importance** : 0 to 0.5 (step = 0.1)

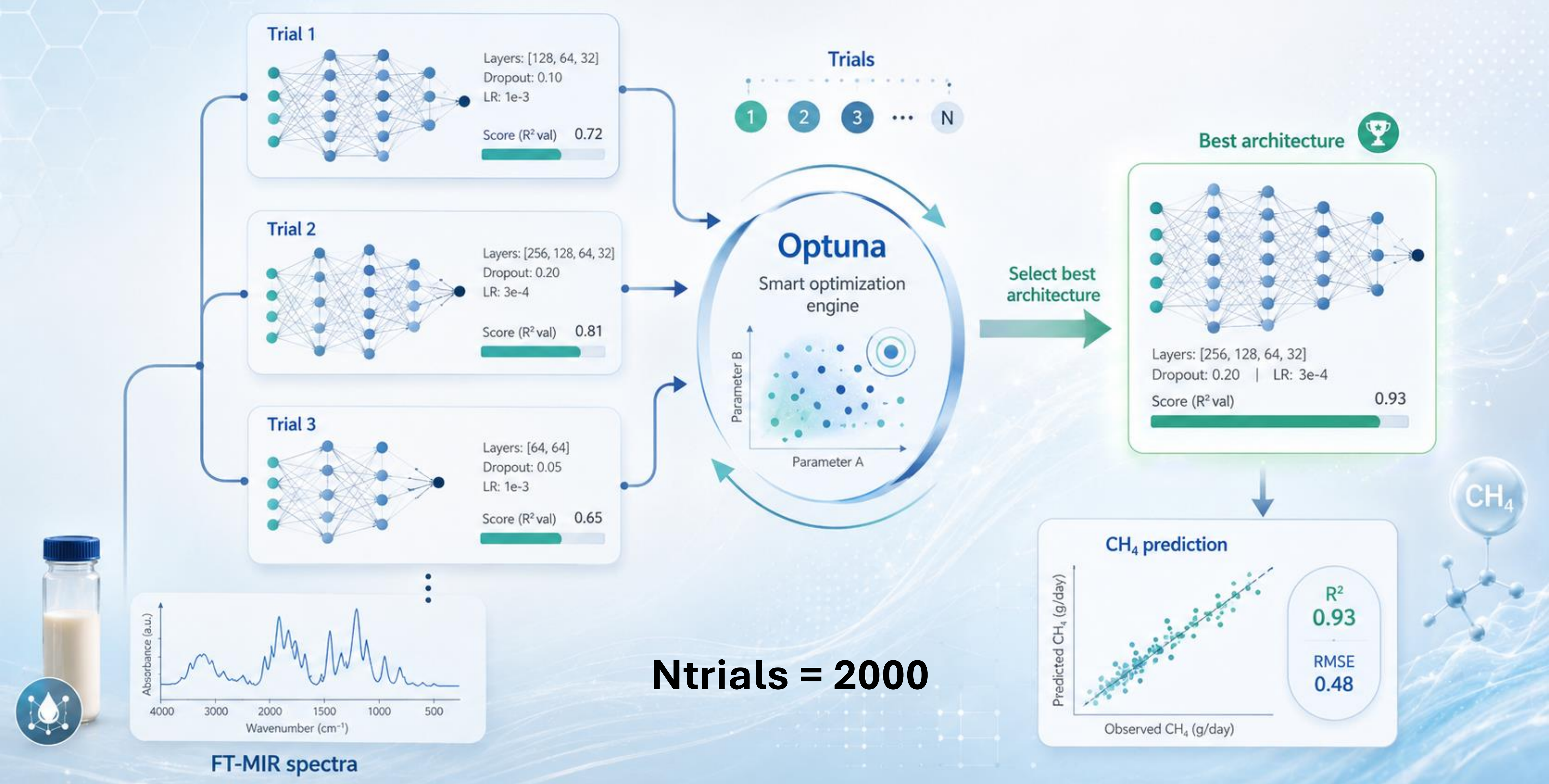
- A lot of possibilities to try :

$$N_{models} = n_1 * n_2 * \ldots * n_k$$

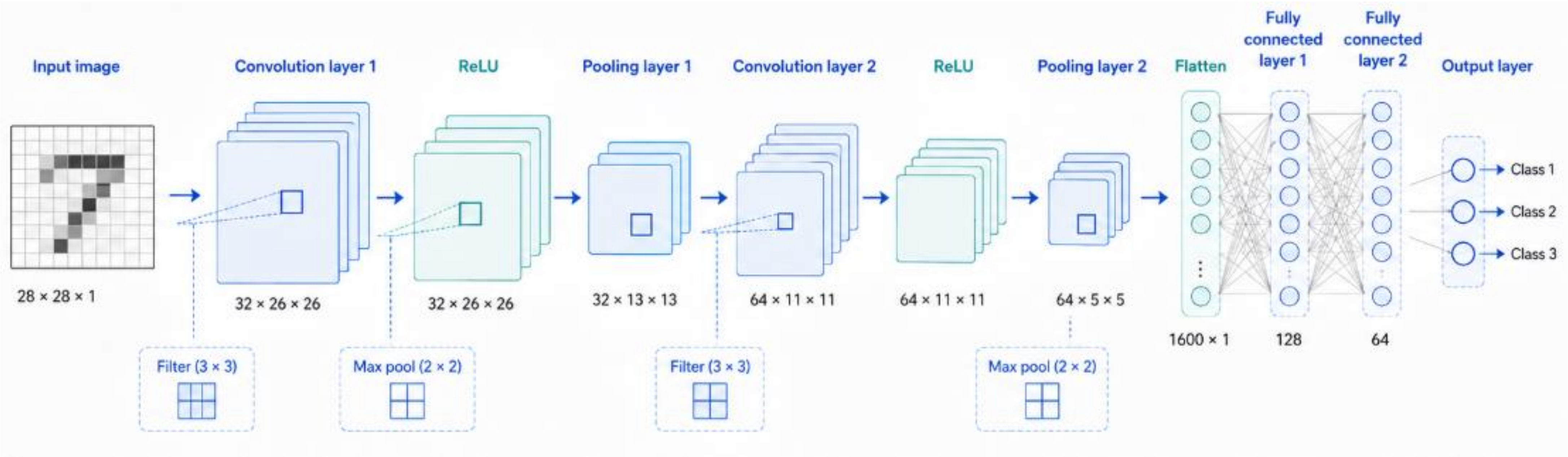
$n_1 = number\ of\ possibilities\ for\ hyperparameter\ 1$
$n_2 = number\ of\ possibilities\ for\ hyperparameter\ 1$
$n_k = number\ of\ possibilities\ for\ hyperparameter\ k$

373,160 models

Too many possibilities


Trial 1
Layers: [128, 64, 32]
Dropout: 0.10
LR: 1e-3
Score (R² val) 0.72
Trial 2
Layers: [256, 128, 64, 32]
Dropout: 0.20
LR: 3e-4
Score (R² val) 0.81
Trial 3
Layers: [64, 64]
Dropout: 0.05
LR: 1e-3
Score (R² val) 0.65
Trials
1 2 3 ... N
Optuna
Smart optimization engine
Parameter B
Parameter A
Select best architecture
Best architecture
Layers: [256, 128, 64, 32]
Dropout: 0.20 | LR: 3e-4
Score (R² val) 0.93
CH₄ prediction
Predicted CH₄ (g/day)
Observed CH₄ (g/day)
R² 0.93
RMSE 0.48
CH₄
Absorbance (a.u.)
4000 3000 2000 1500 1000 500
Wavenumber (cm⁻¹)
FT-MIR spectra
Ntrials = 2000

Convolutional neural network



Minimum Hyperparameters:

- **Number of filters**
- Number of **nodes** in the hidden layer

For us, only **one output** as it is a regression. We tried only **one fully connected hidden** layer.

Define the structure for **cANN**

Hyperparameters :

- **Batch size** : 8, 16, 32, 64 samples
- **Learning rate**: 1e-4, 1e-2
- **Number of filters in the conv layer**: 16, 32, 64
- **Drop-out rate (ndrop)**: 0.3, 0.5, 0.75
- **Number of neurons in the hidden later (nout)** : 10, 50, 100, 150, 200, 250, 300, 350, 400, 450, 500, 550

- Number of possibilities : 864 models
- Optuna selection – Ntrials : 200 models

Hyperparameters :

- **Batch size** : 8, 16, 32, 64 samples
- **Learning rate**: 1e-4, 1e-2
- **Number of filters in the conv layer**: 16, 32, 64
- **Drop-out rate (ndrop):** 0.3, 0.5, 0.75
- **Number of neurons in the hidden later (nout)** : 10, 50, 100, 150, 200, 250, 300, 350, 400, 450, 500, 550
- **Weight decay** : 1e-8,1e-2

Define the structure for **cANN2**

- Number of possibilities : 1,728 models
- Optuna selection – Ntrials : 200 models

Dataset used in a previous study

- N=**1,089 records**
- Respiration chambers and SF_6
- 7 countries
- Different breeds
- Different diets

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Research Article

Improving robustness and accuracy of predicted daily methane emissions of dairy cows using milk mid-infrared spectra

Amélie Vanlierde, Frédéric Dehareng, Nicolas Gengler, Eric Froidmont, Sinead McParland, Michael Kreuzer, Matthew Bell, Peter Lund, Cécile Martin, Björn Kuhla, Hélène Soyeurt

First published: 22 November 2020 | https://doi.org/10.1002/jsfa.10969 | VIEW METRICS

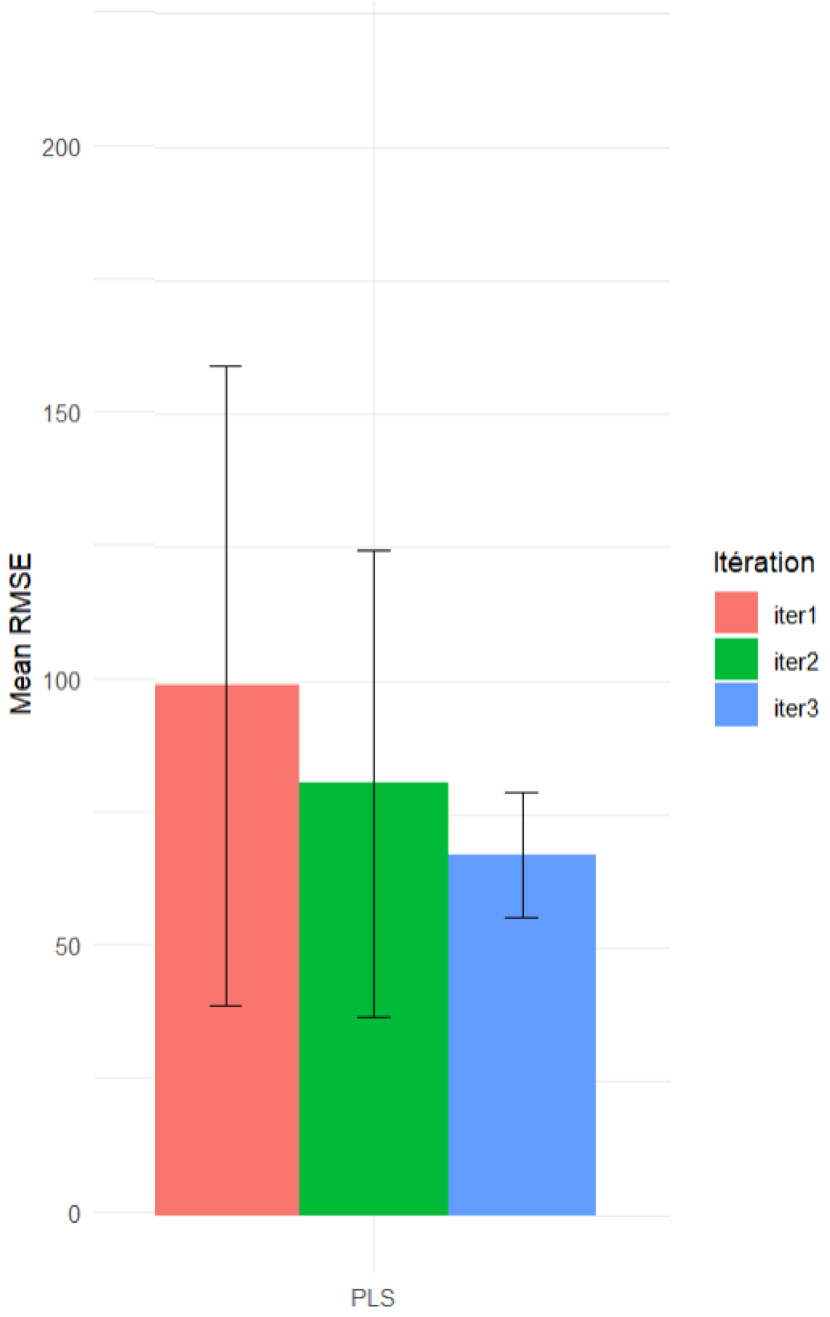
Data splitting

- Separation of dataset per country
  - 7 datasets

- Split between training and test sets for each dataset
  - 20 % for test set
  - 80 % for training set

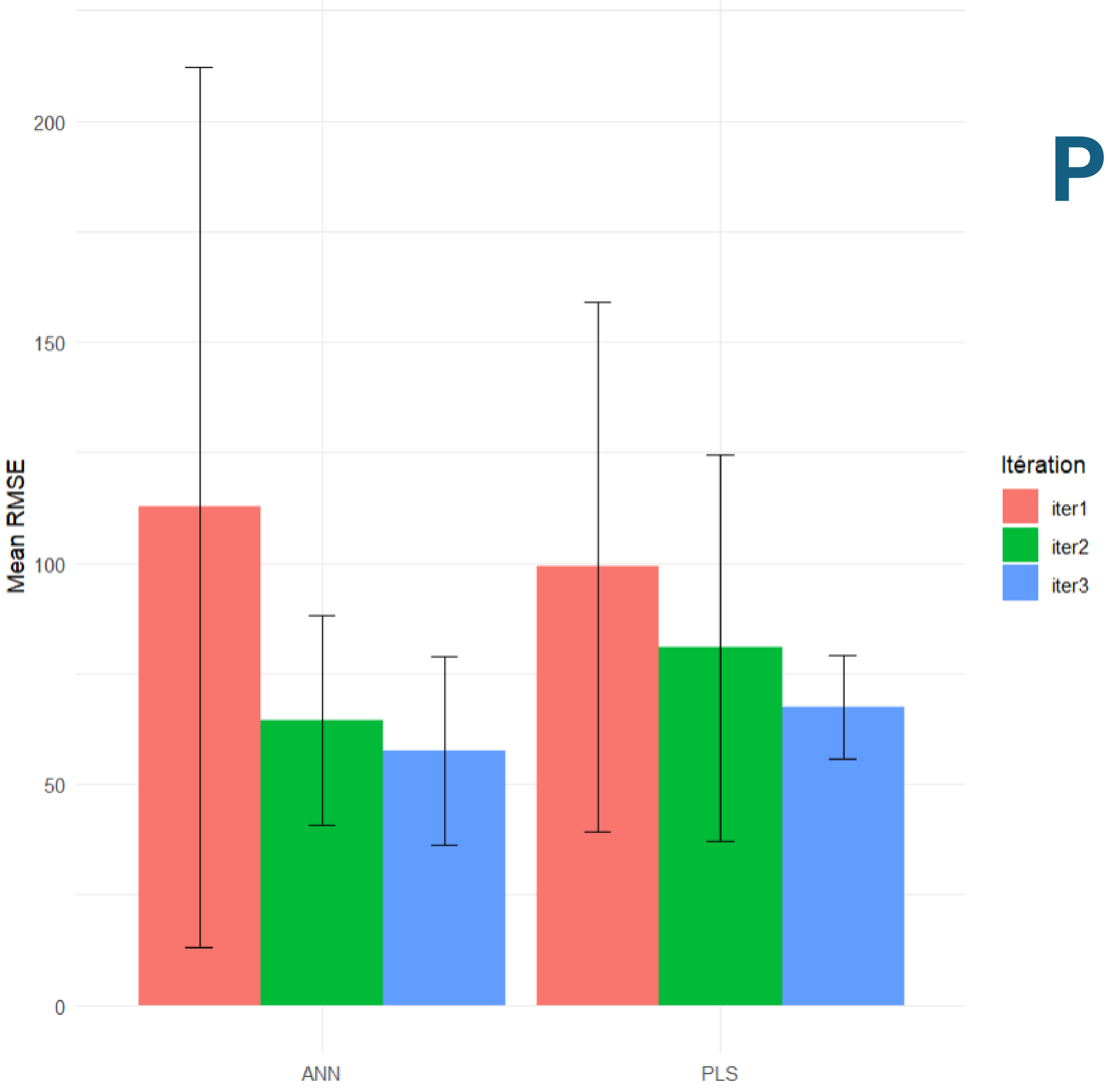
- Hyper-parameters optimization
  - Cow-independent 5-folds cross-validation

- See the impact of increasing the datasets
  - 3 iterations : [countries 1 & 2], [iter1 + countries 3,4 & 5], [iter2 + countries 6 & 7]



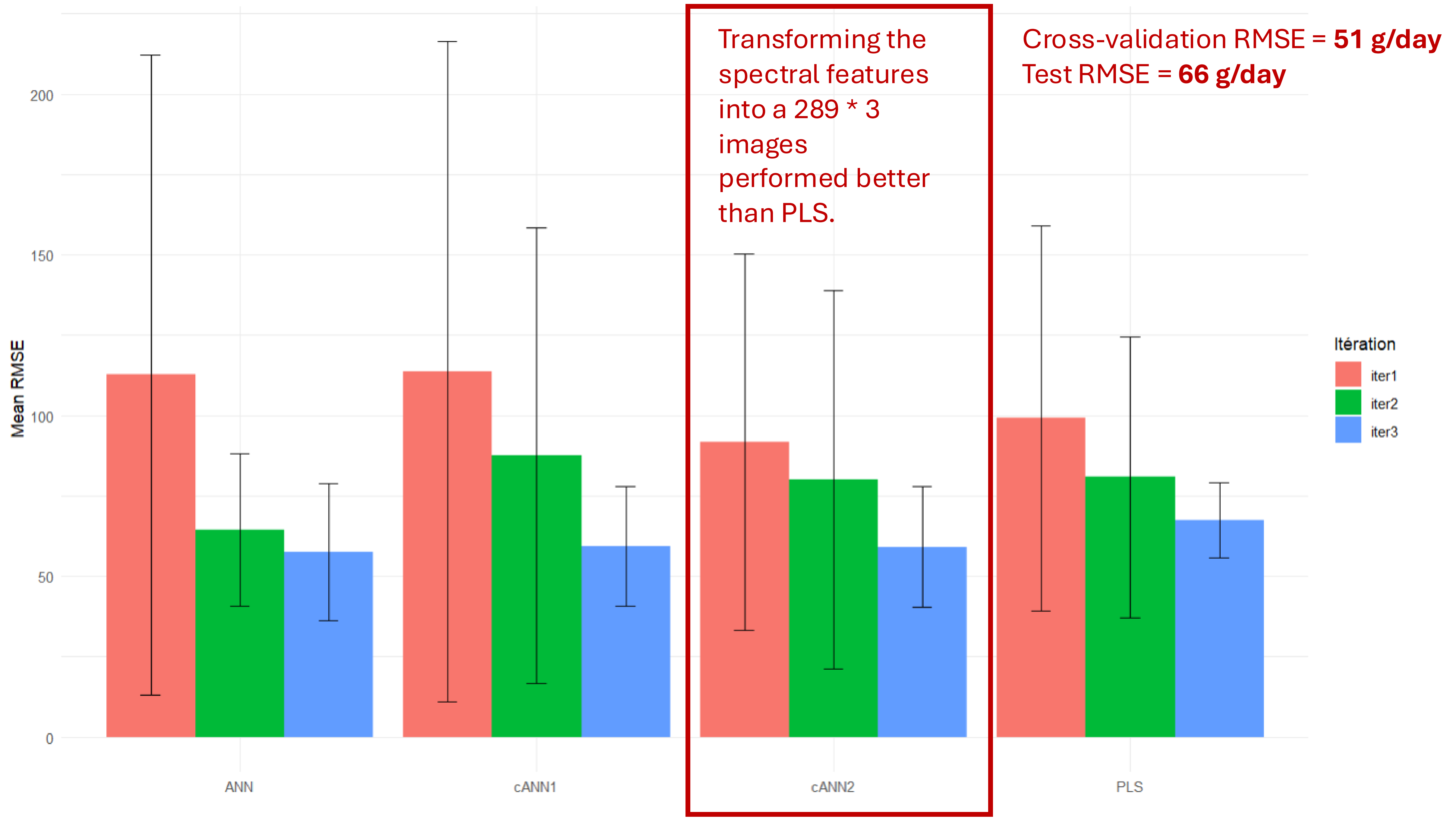
PLS model

- Different training set:
  - Iteration 1 : 410 samples
  - Iteration 2 : 611 samples
  - Iteration 3 : 890 samples
- Same dataset for each iteration (N= 199)
- Test RMSE ↓ when the training dataset increases as well as the SD



PLS vs. ANN model

- Same dataset for each iteration (N= 199)
- Test RMSE ↓ when the training dataset increases as well as the SD
- The performance is better when the training dataset is sufficient.


Transforming the spectral features into a 289 * 3 images performed better than PLS.
Cross-validation RMSE = 51 g/day
Test RMSE = 66 g/day
Mean RMSE
200
150
100
50
0
ANN
cANN1
cANN2
PLS
Itération
iter1
iter2
iter3

Conclusions

2D-convolutional neural network (cANN2) can improve the performances of PLS

- Cow-independent 5-folds cross-validation for cANN2 gives a prediction error of **51 g of CH_4/day**.
- The test error for cANN2 was of **66 g of CH_4/day**.
- The test RMSE SD was greater than PLS ➔ check the robustness
- When the structure of cANN2 will be fixed, transfer learning approaches could be tested.

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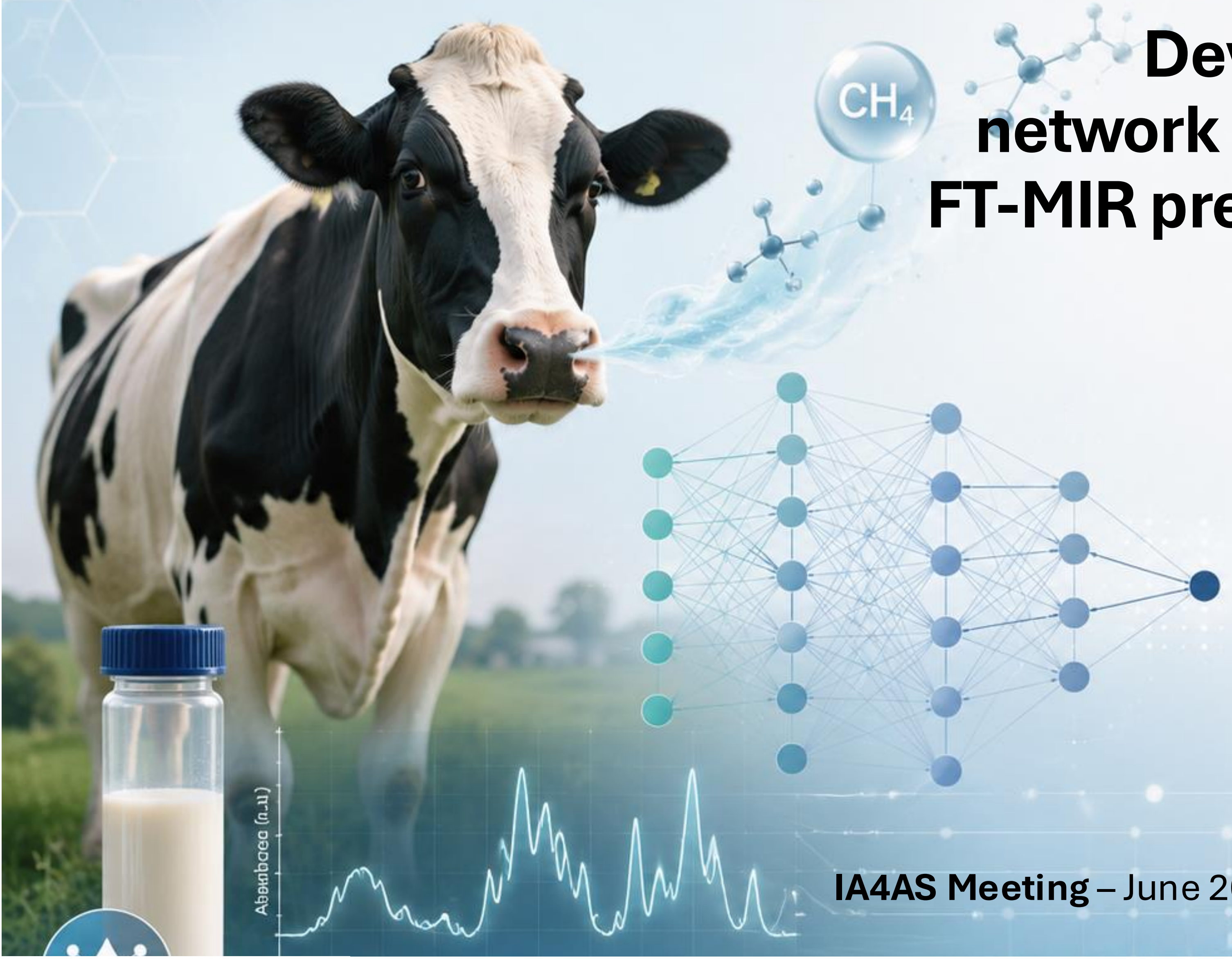

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