2021

A brief introduction to machine learning and deep learning

David Makowski

INRAE

https://www6.inrae.fr/mia-paris/Equipes/Membres/David-Makowski

Outline

- Definition & main principles
- Several extensions of linear regression
- Trees and forests
- Deep learning

Outline

- Definition & main principles
- Several extensions of linear regression
- Trees and forests
- Deep learning

Artificial intelligence

Machine learning

Artificial intelligence

Machine learning

Supervised learning

Objective: « Learning a function that maps an input to an output based on examples of input-output pairs »

Statistical Modeling: The Two Cultures (Breiman, 2001)

$$y = f(x) + e$$

Modelling approach 1: Try to find the true $f(x)$

Modelling approach 2: Predict y from x as accurately as possible

Statistical Modeling: The Two Cultures (Breiman, 2001)

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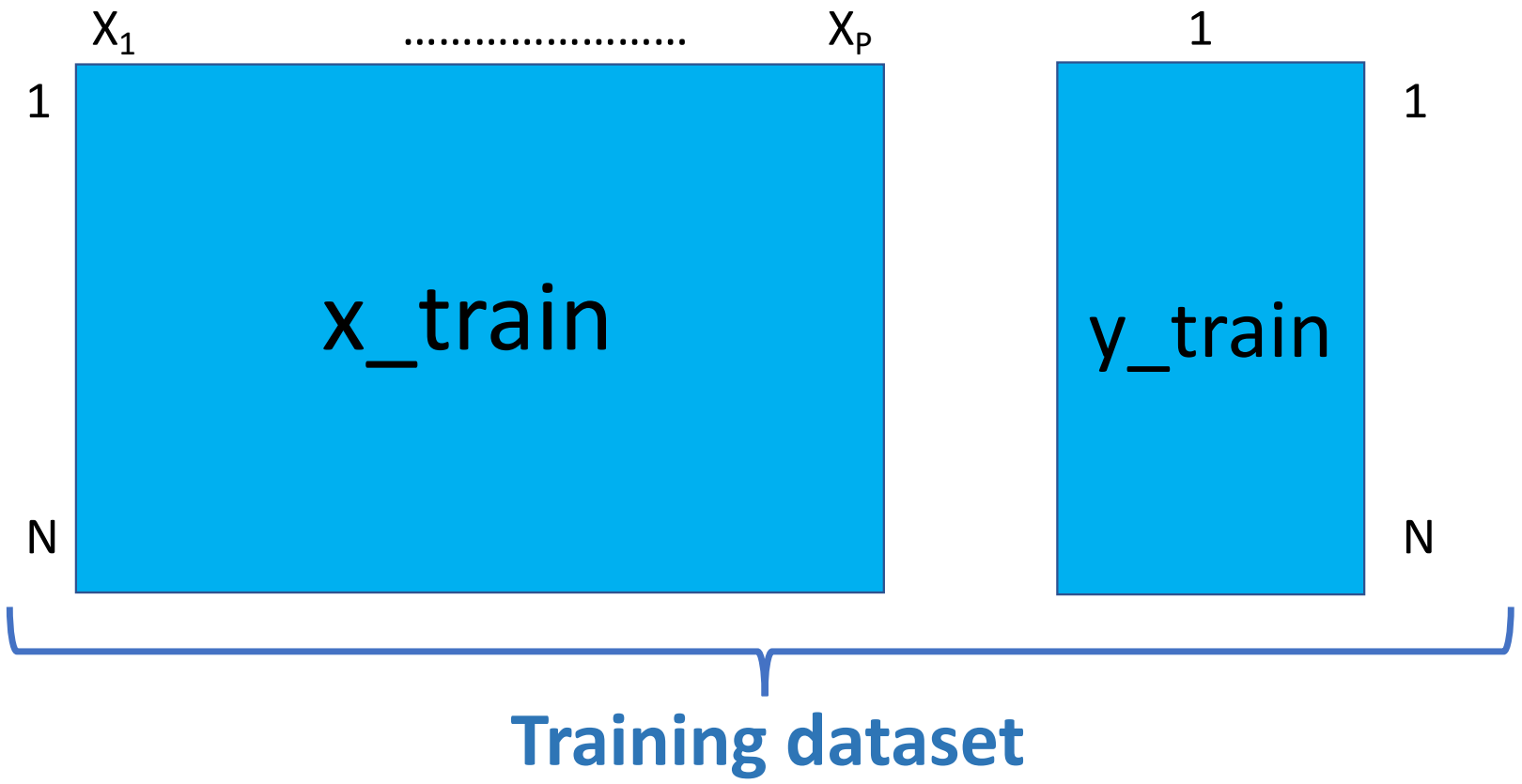
Modelling approach 2: Predict *y* from *x* as accurately as possible

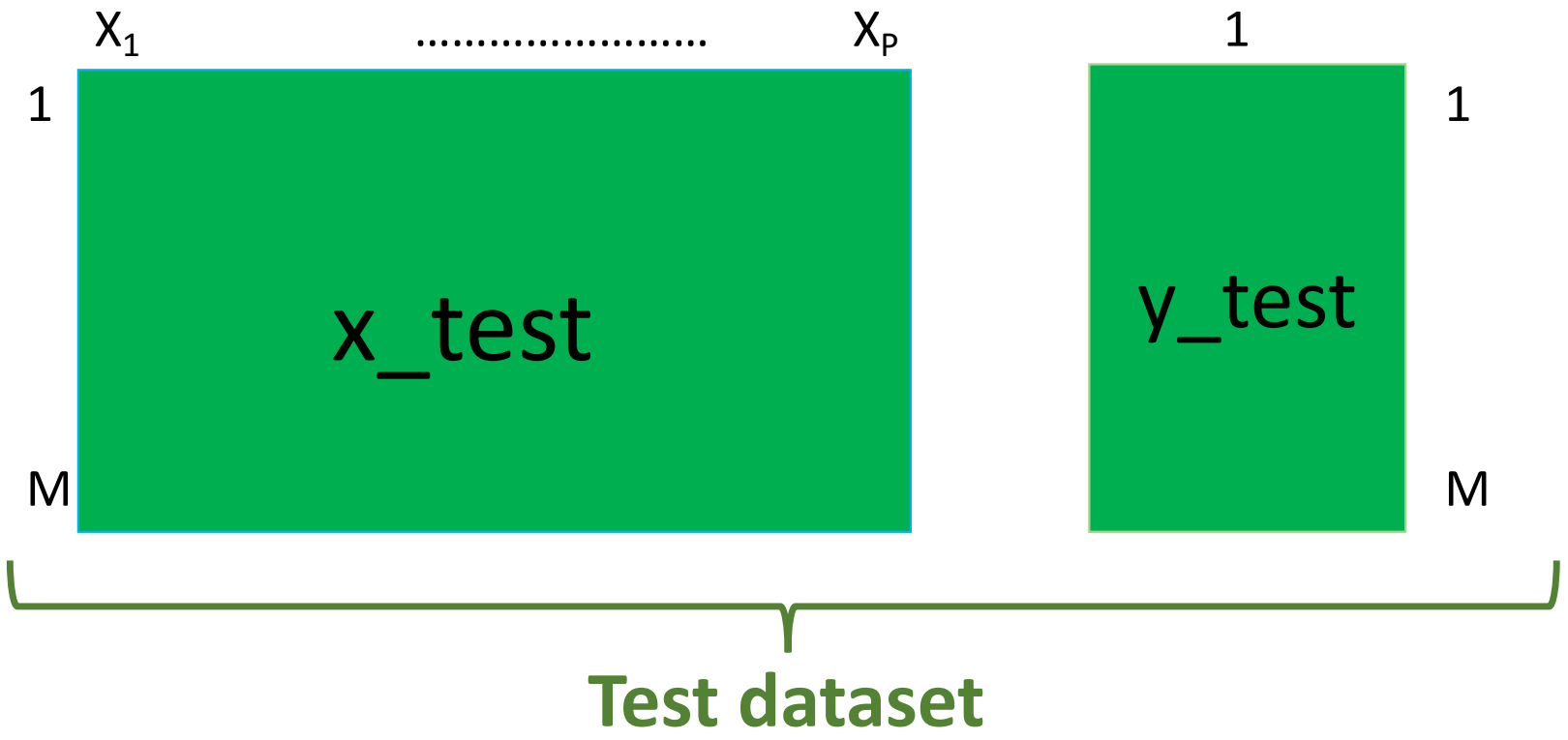
Two main steps

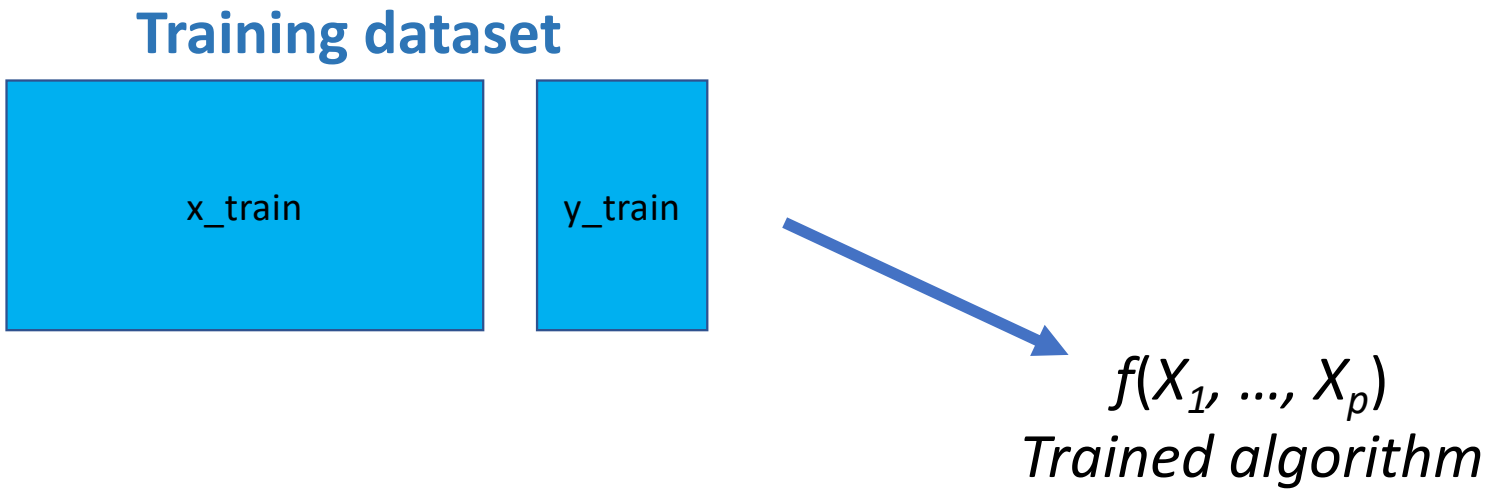
- Step 1: Training
- Step 2: Test

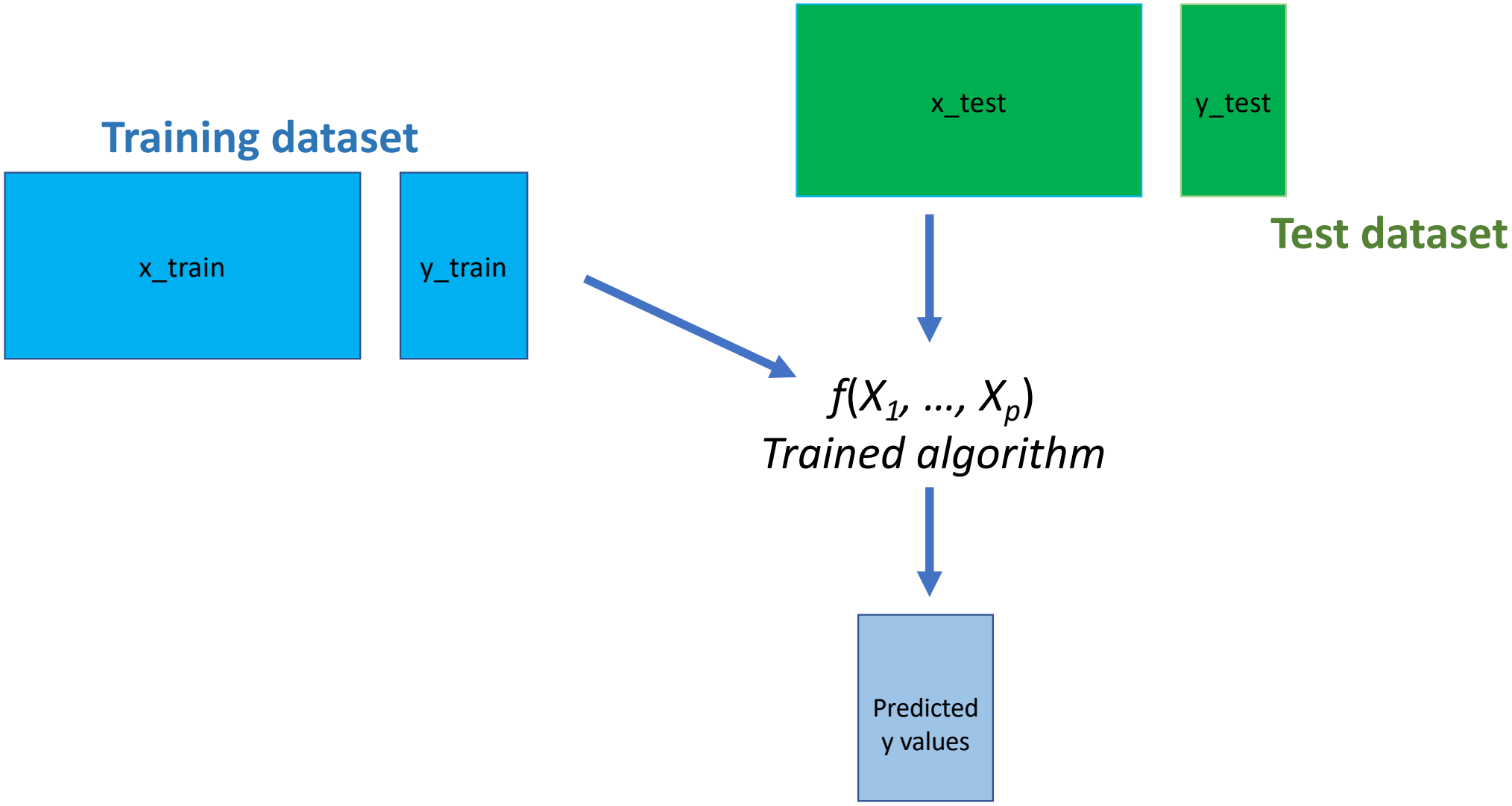
Step 1: Train an algorithm predicting Y as a function of X_1, …, X_P using a **training dataset**

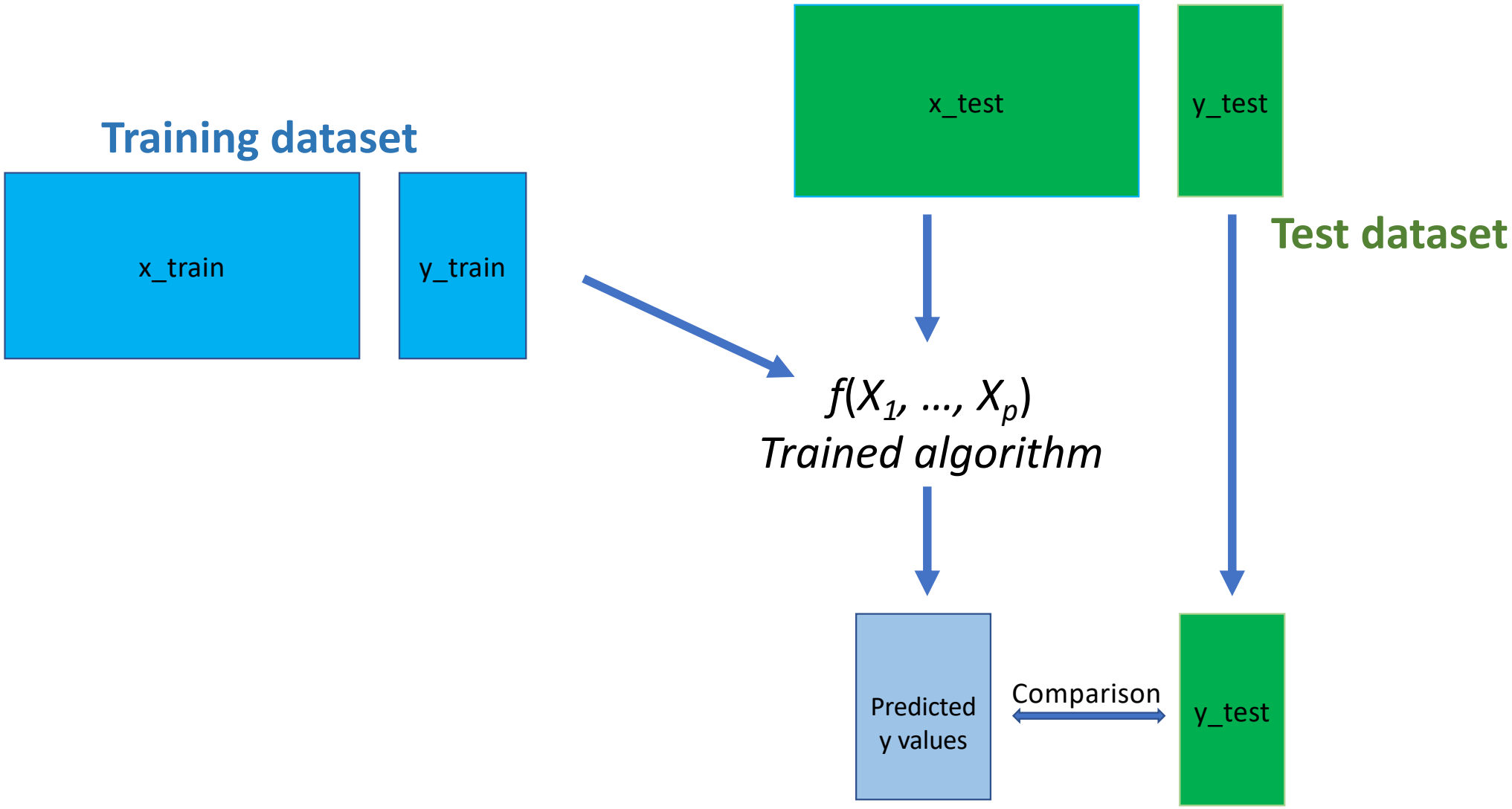


Step 2: Assess the predictive capability of the trained algorithm using a **test dataset**

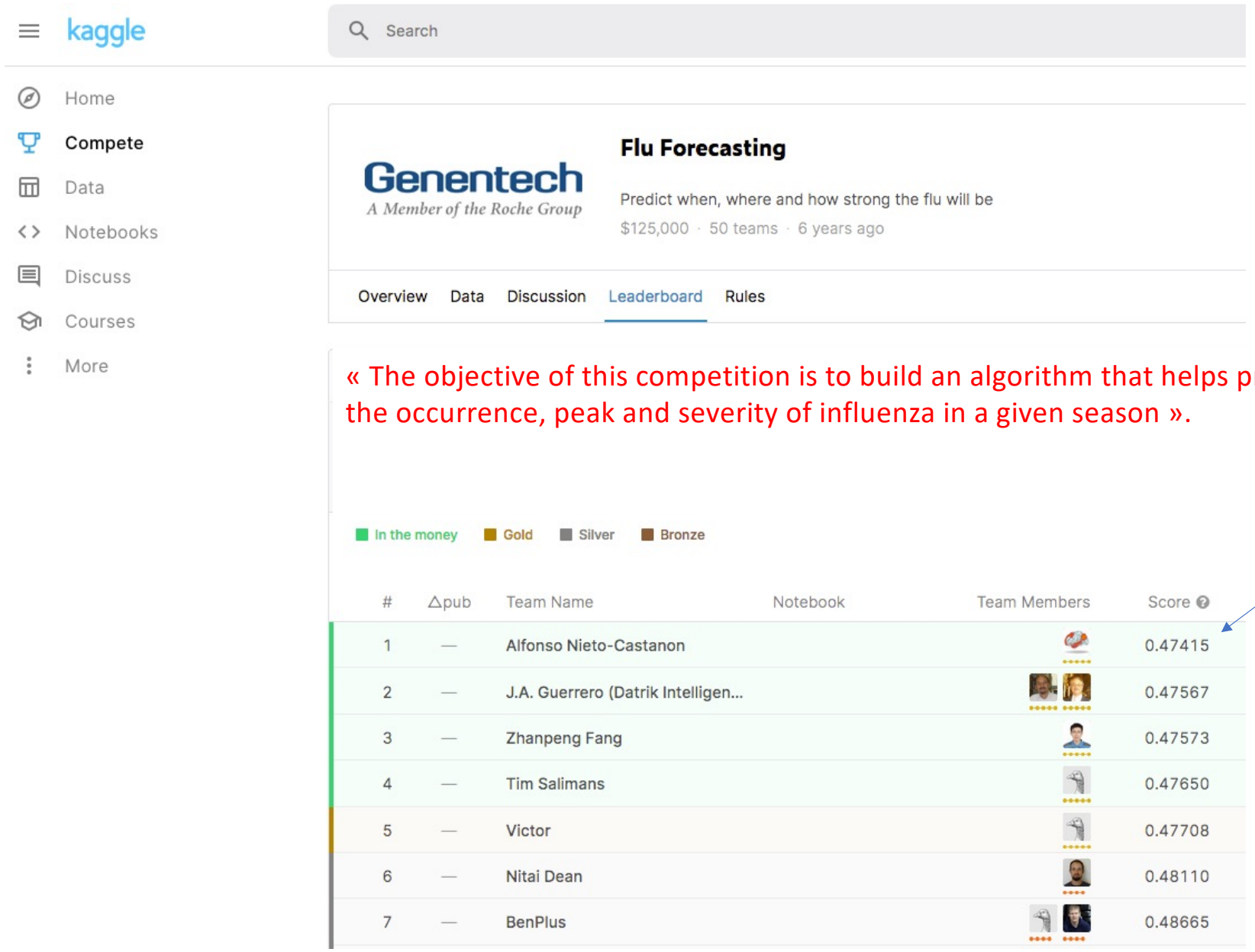



Training dataset
x_train
y_train
$f(X_1, \ldots, X_p)$
Trained algorithm


Training dataset
x_train
y_train
x_test
y_test
Test dataset
$f(X_1, \ldots, X_p)$
Trained algorithm
Predicted
y values


Training dataset
x_train
y_train
x_test
y_test
Test dataset
$f(X_1, \ldots, X_p)$
Trained algorithm
Predicted y values
Comparison
y_test


kaggle
Search
Competitions
Datasets
Notebooks
Competitions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Genentech
A Member of the Roche Group
Flu Forecasting
Predict when, where and how strong the flu will be
$125,000 · 50 teams · 6 years ago
Overview
Data
Discussion
Leaderboard
Rules
« The objective of this competition is to build an algorithm that helps predict the occurrence, peak and severity of influenza in a given season ».
In the money
Gold
Silver
Bronze
RMSE
△pub Team Name Notebook Team Members Score
1 — Alfonso Nieto-Castanon 0.47415
2 — J.A. Guerrero (Datrik Intelligen... 0.47567
3 — Zhanpeng Fang 0.47573
4 — Tim Salimans 0.47650
5 — Victor 0.47708
6 — Nitai Dean 0.48110
7 — BenPlus 0.48665

kaggle

Search

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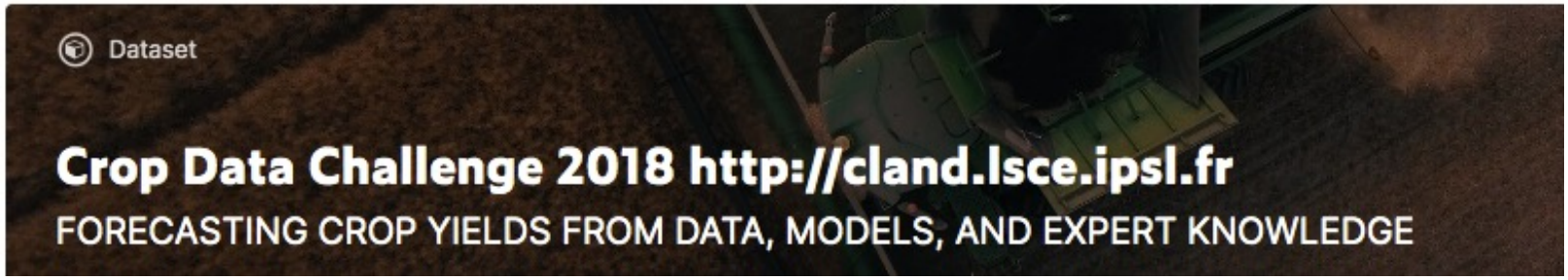
Data

Notebooks

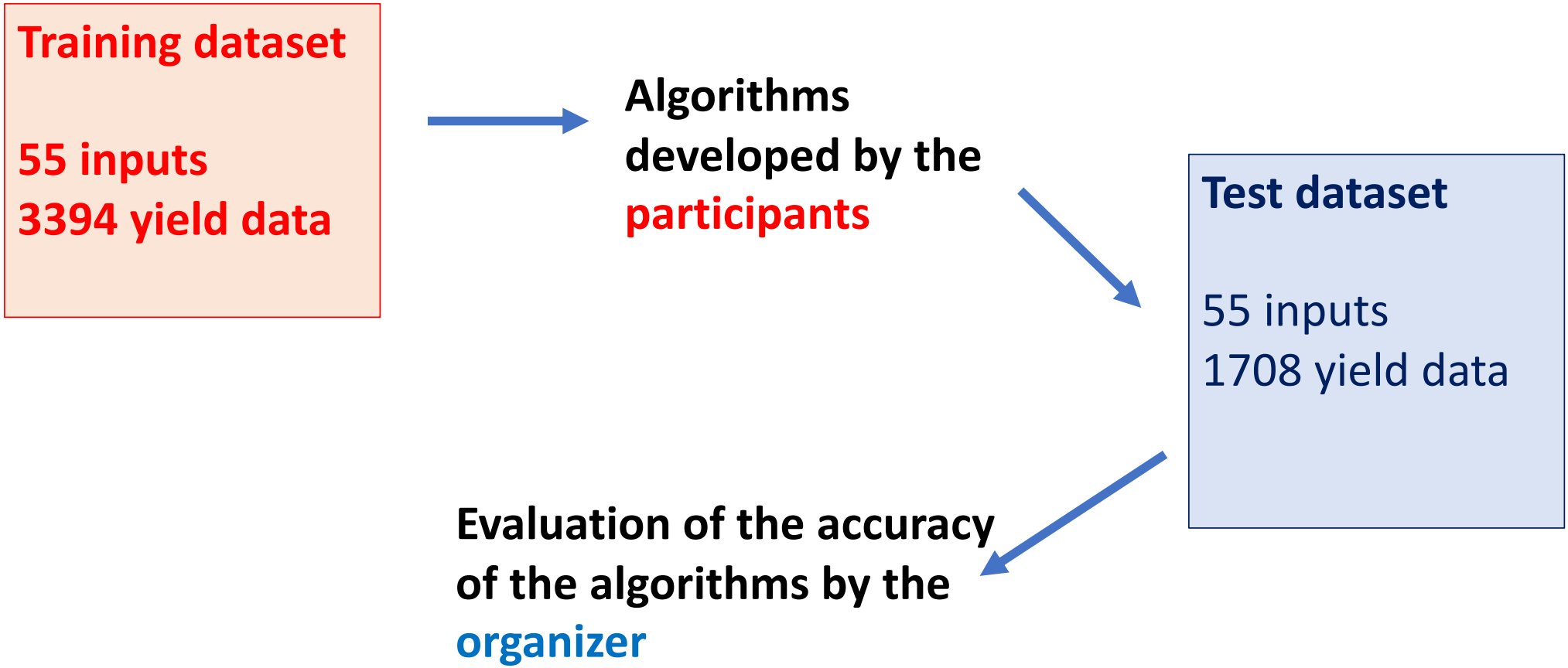


Data (5 MB)

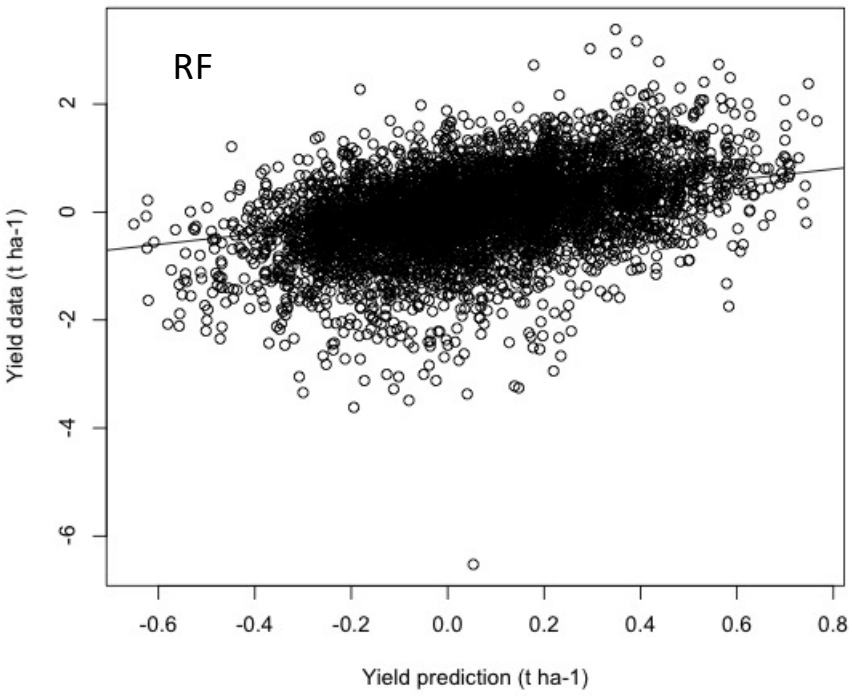
Data Sources

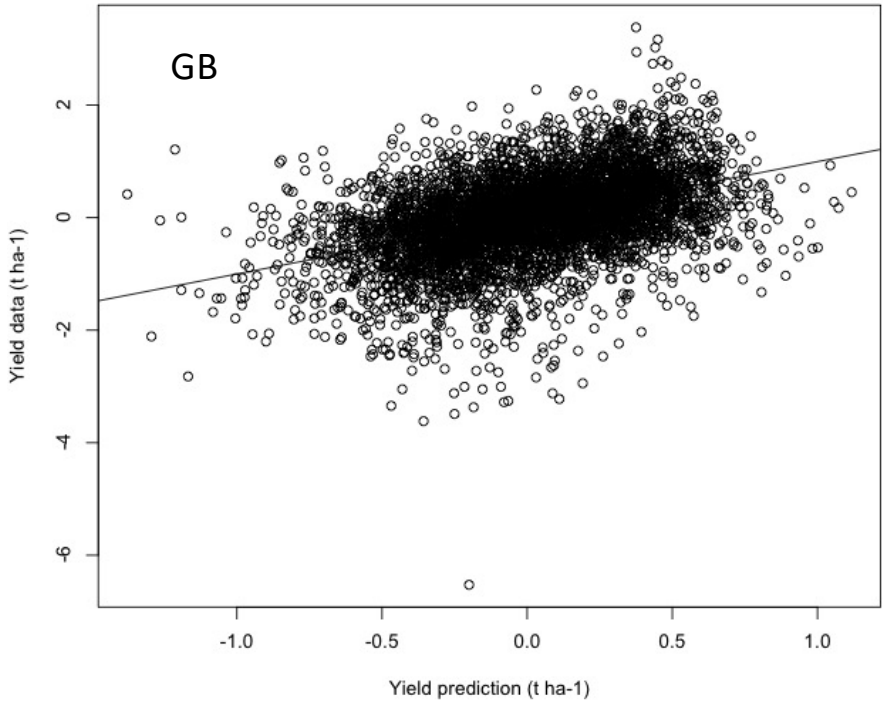
TestDataSet_Ma...	57 columns
TestDataSet_W...	92 columns
TrainingDataSet...	58 columns
TrainingDataSet...	93 columns

French maize yield prediction (départements)



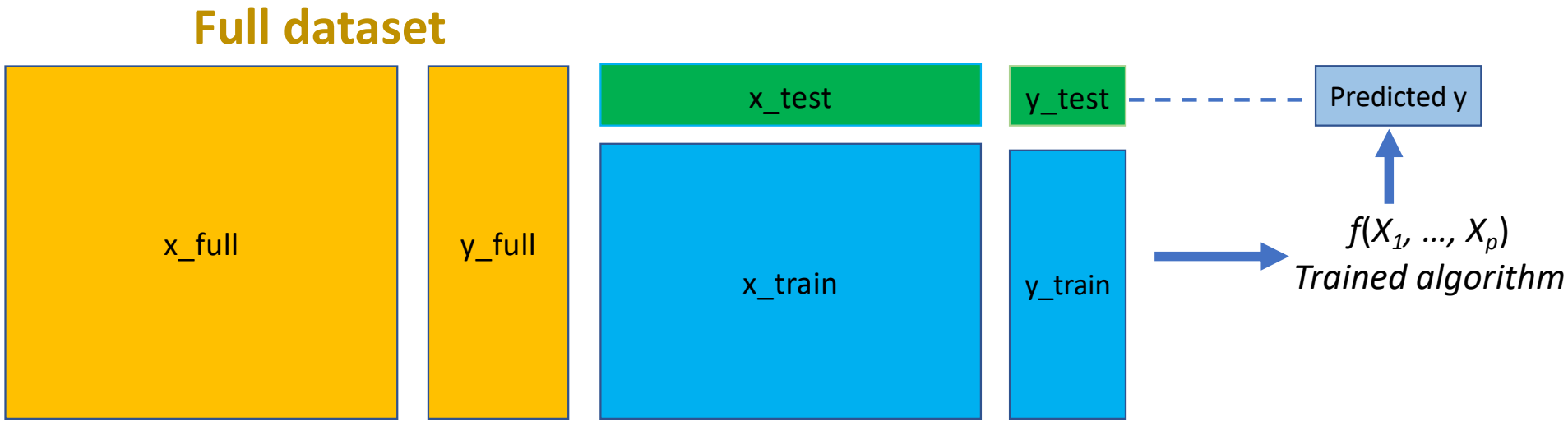
Method	RMSEP (maize yield)
Random Forest (RF)	0.71 t/ha
Gradient boosting (GB)	0.70 t/ha

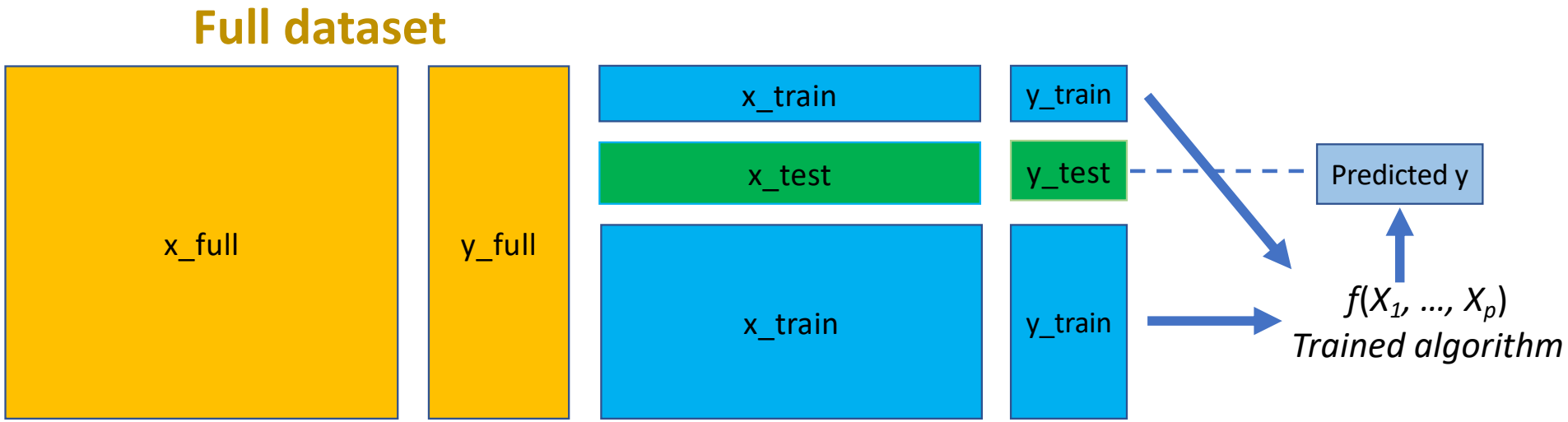




Model testing should be taken seriously to avoid risk of overfitting

Cross-validation is used when no independent test dataset is available


Full dataset
x_full
y_full
x_test
y_test
Predicted y
x_train
y_train
$f(X_1, \ldots, X_p)$
Trained algorithm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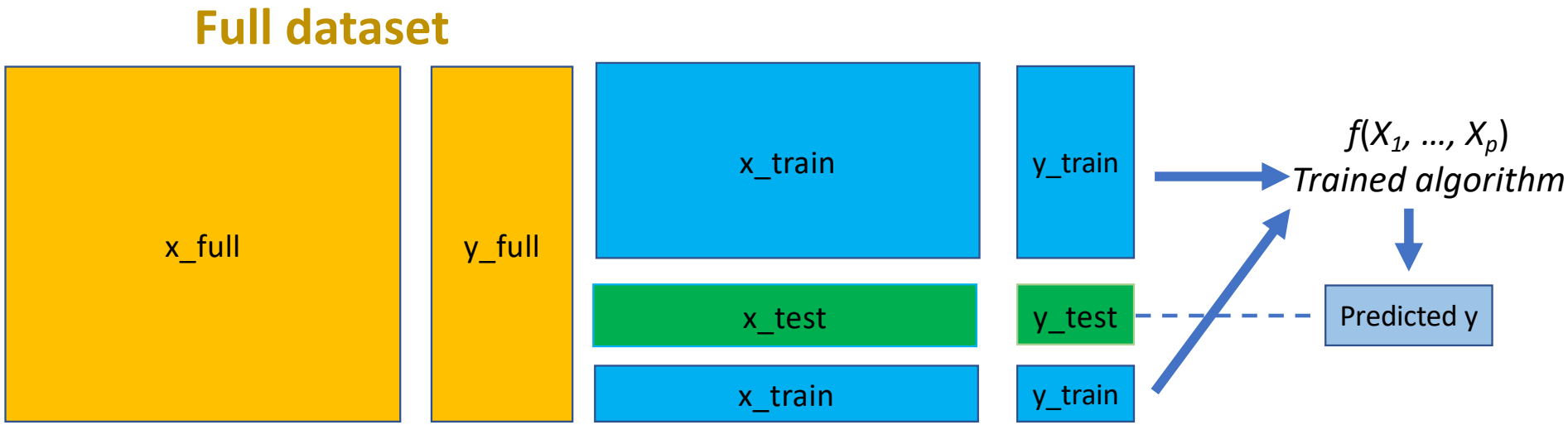
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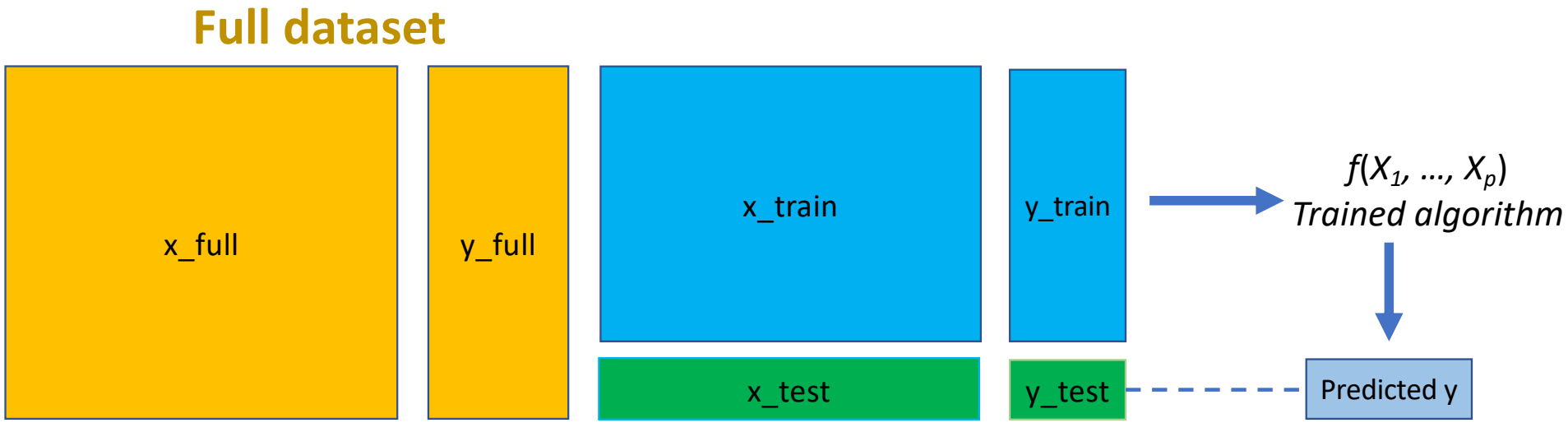
Predicted y


Full dataset
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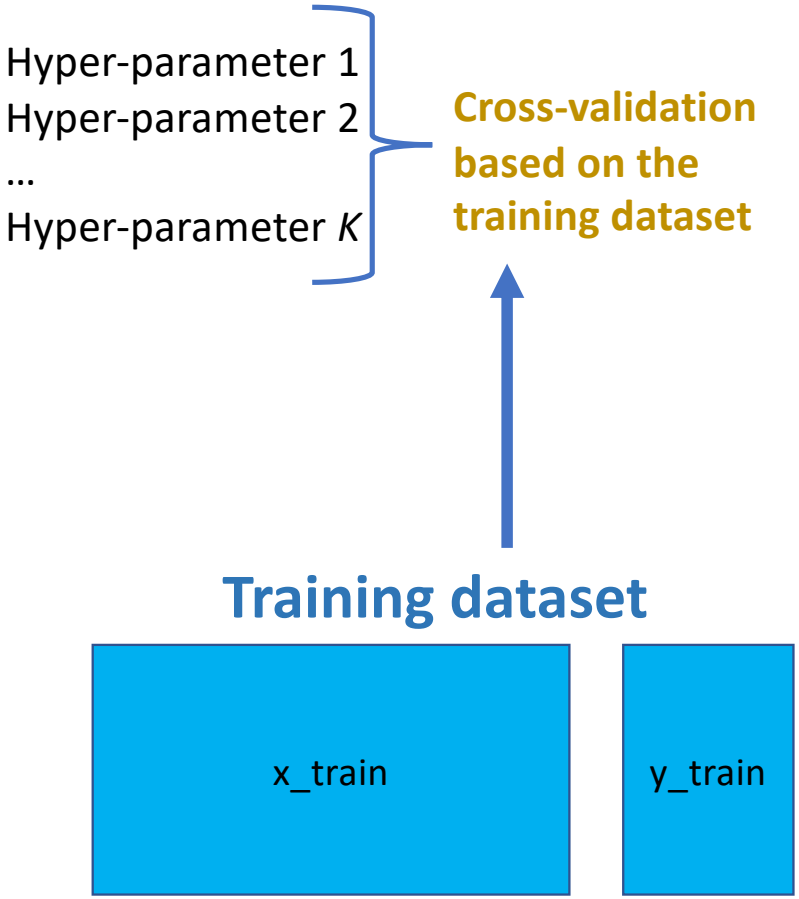
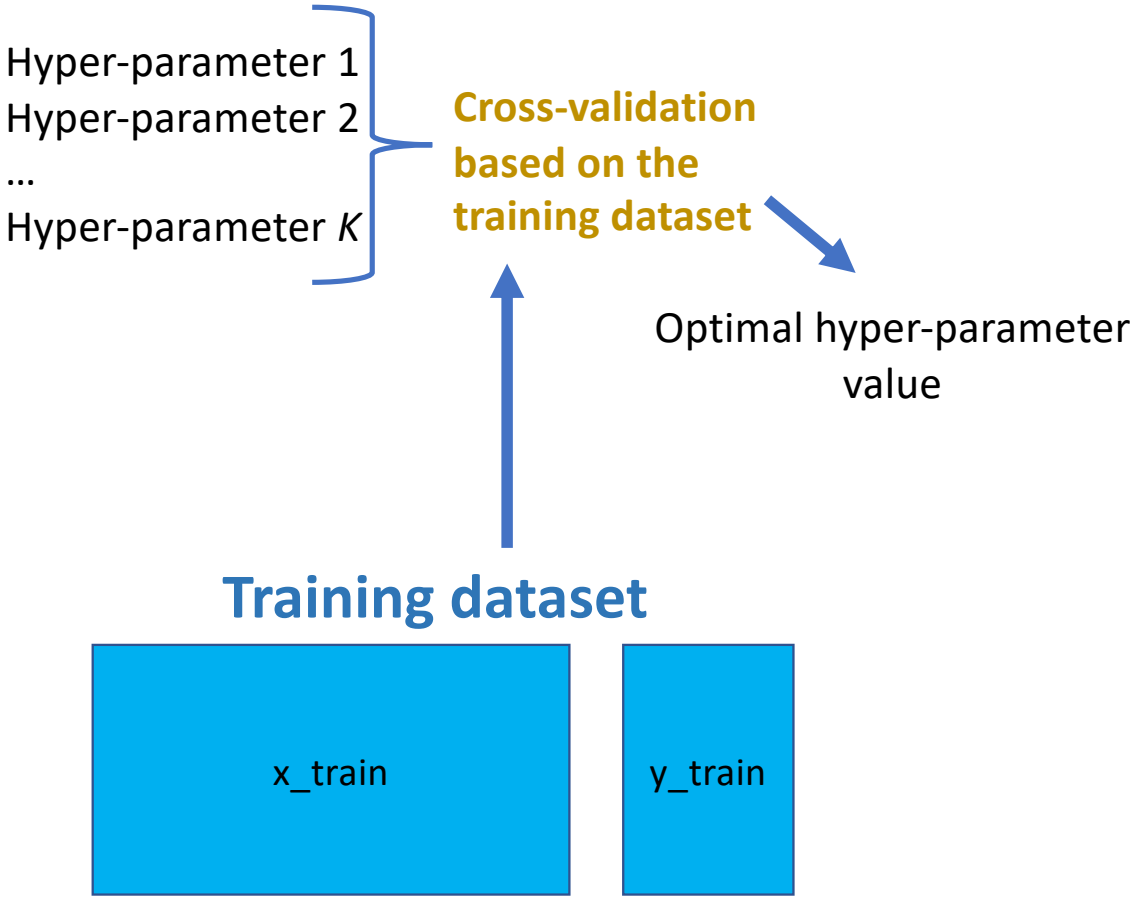
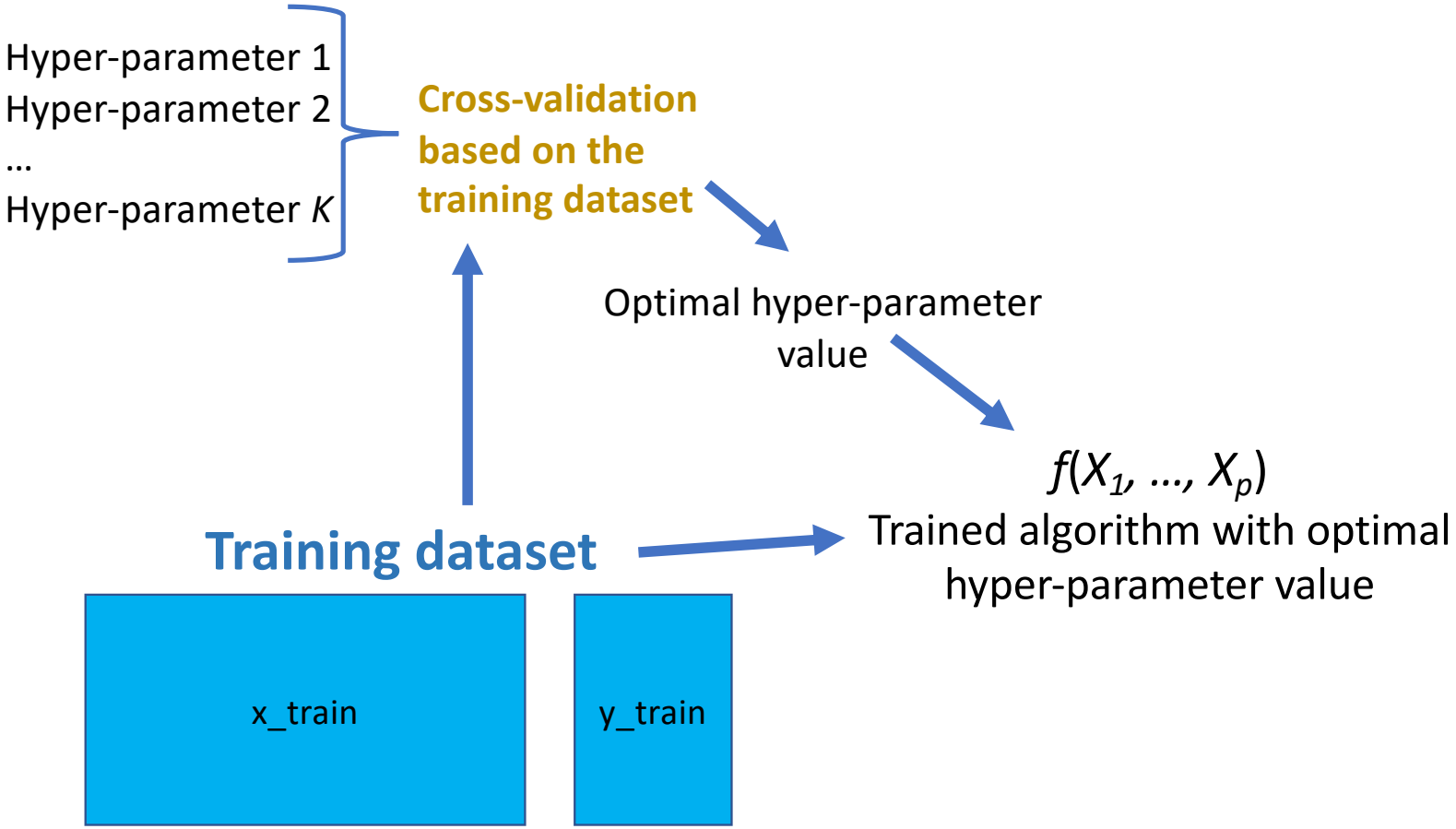
Cross-validation and test dataset can be combined together


Hyper-parameter 1
Hyper-parameter 2
…
Hyper-parameter K
Cross-validation based on the training dataset
Training dataset
x_train
y_train


Hyper-parameter 1
Hyper-parameter 2
…
Hyper-parameter K
Cross-validation based on the training dataset
Optimal hyper-parameter value
Training dataset
x_train
y_train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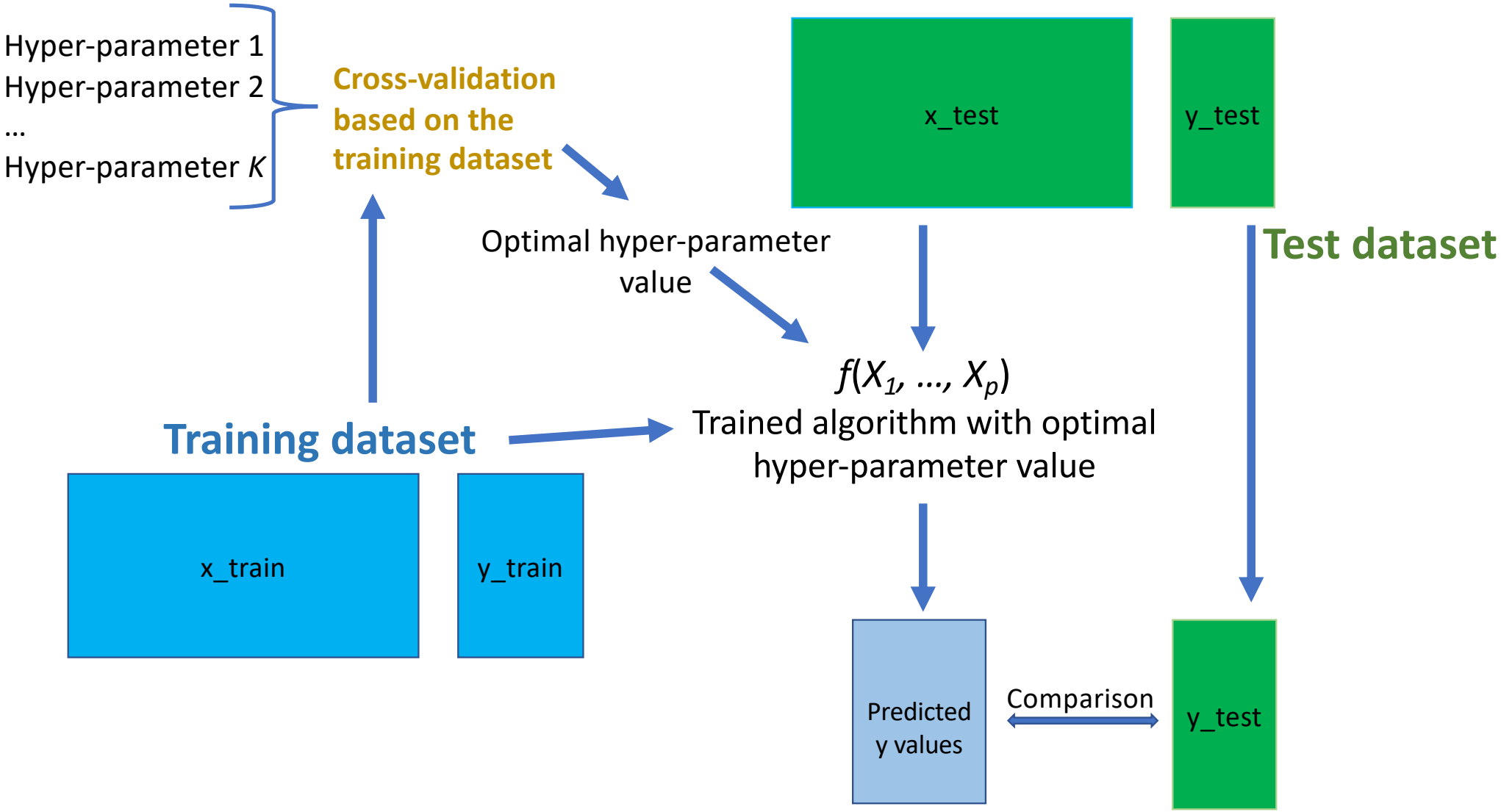
Hyper-parameter 2
…
Hyper-parameter K
Cross-validation based on the training dataset
Optimal hyper-parameter value
f(X1, …, Xp)
Trained algorithm with optimal hyper-parameter value
Training dataset
x_train
y_train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y_test

Why machine learning is powerful?

Very flexible methods

+

Computational power

+

Large datasets

Increased chance to obtain accurate predictions

Why machine learning is powerful?

Prediction error = *g*(Bias, Variance)

Why machine learning is powerful?

Prediction error = g(Bias, Variance)

ML is able to fing a good balance between bias and variance

Several « ML tricks »	Principle	Effect
Regularization	Add information to prevent overfitting and simplify the model	Reduce variance at the cost of a small increase of bias
Bagging	Bootstrap aggregation: average together multiple models fitted to resampled dataset	Reduce variance
Boosting	Fit a sequence of weak models to weighted versions of the data (more weight given to poorly predicted data at earlier rounds).	Reduce bias

Numerous methods available

- Regressions (standard, PLS, LASSO, Elastic net…)
- SVM
- Tree and random forest
- Gradient boosting
- Neural network
- Deep neural network
- Deep learning
- Bayesian classification

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Relatively easy to run these methods with specialized packages (with R or Python)

Are machine learning models « black boxes »?

This is less true than before.

Vizualisation tools:

- Importance ranking
- Partial dependence plots (PDP)
- Accumulated Local Effects (ALE) Plot

Example 1

RESEARCH ARTICLE

Forecasting severe grape downy mildew attacks using machine learning

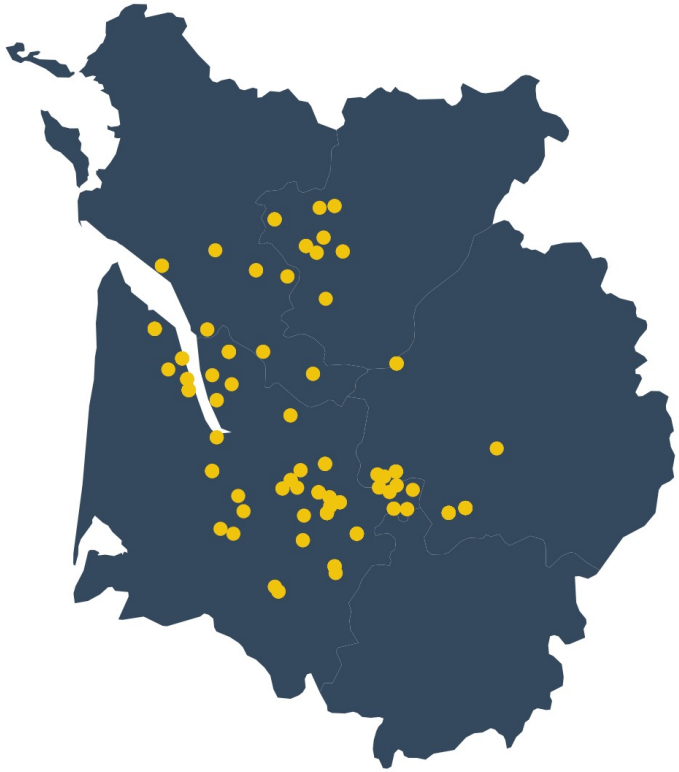
Mathilde Chen[1]*, François Brun[2], Marc Raynal[3], David Makowski[4,5]

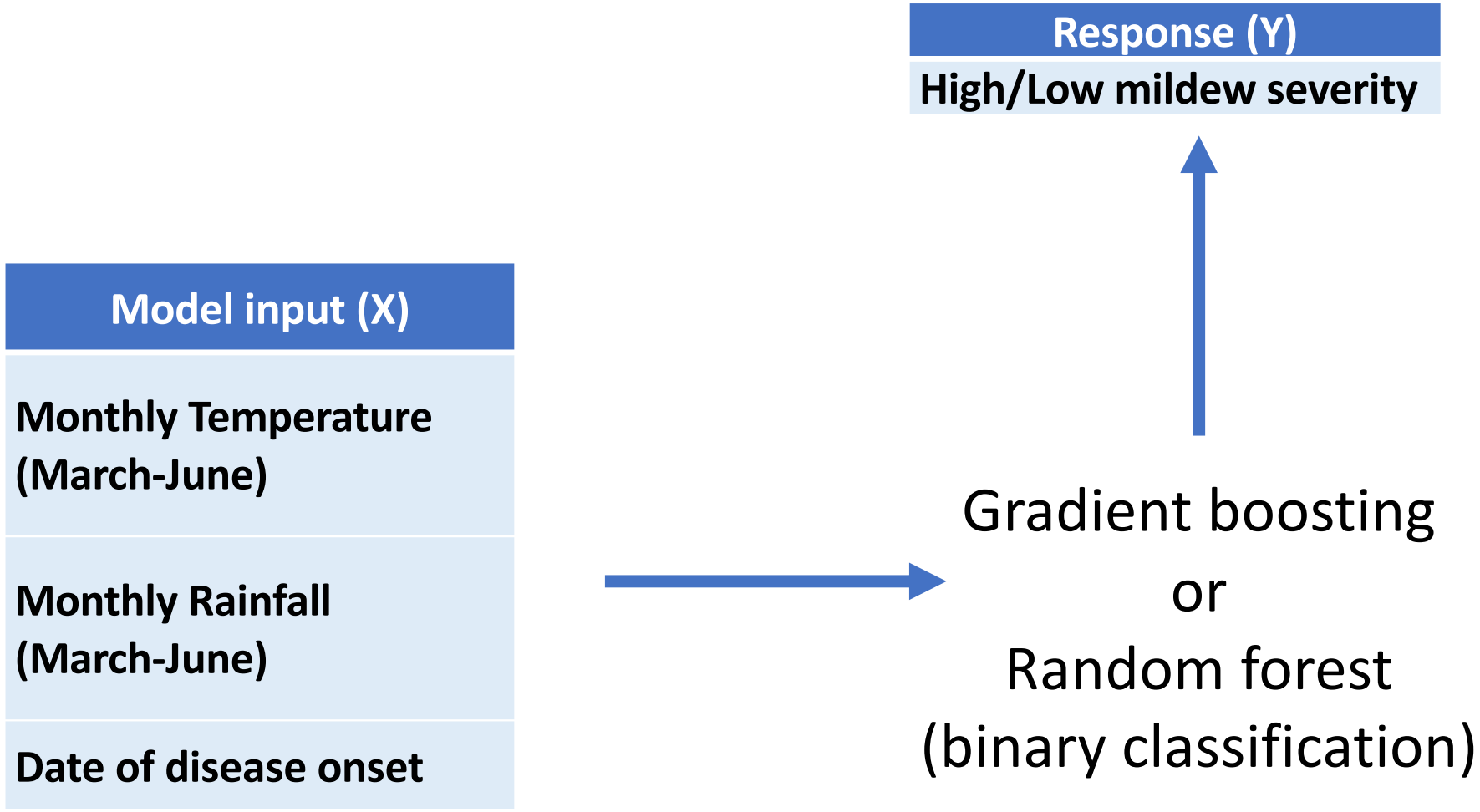
https://doi.org/10.1371/journal.pone.0230254

Forecasting severe grape downy mildew attacks using machine learning

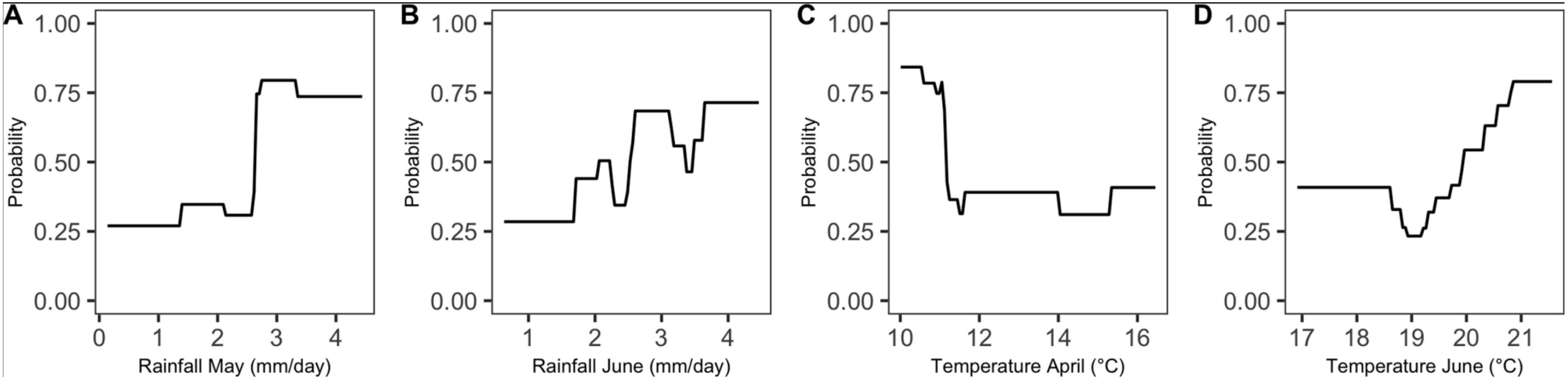
Incidence data collected on

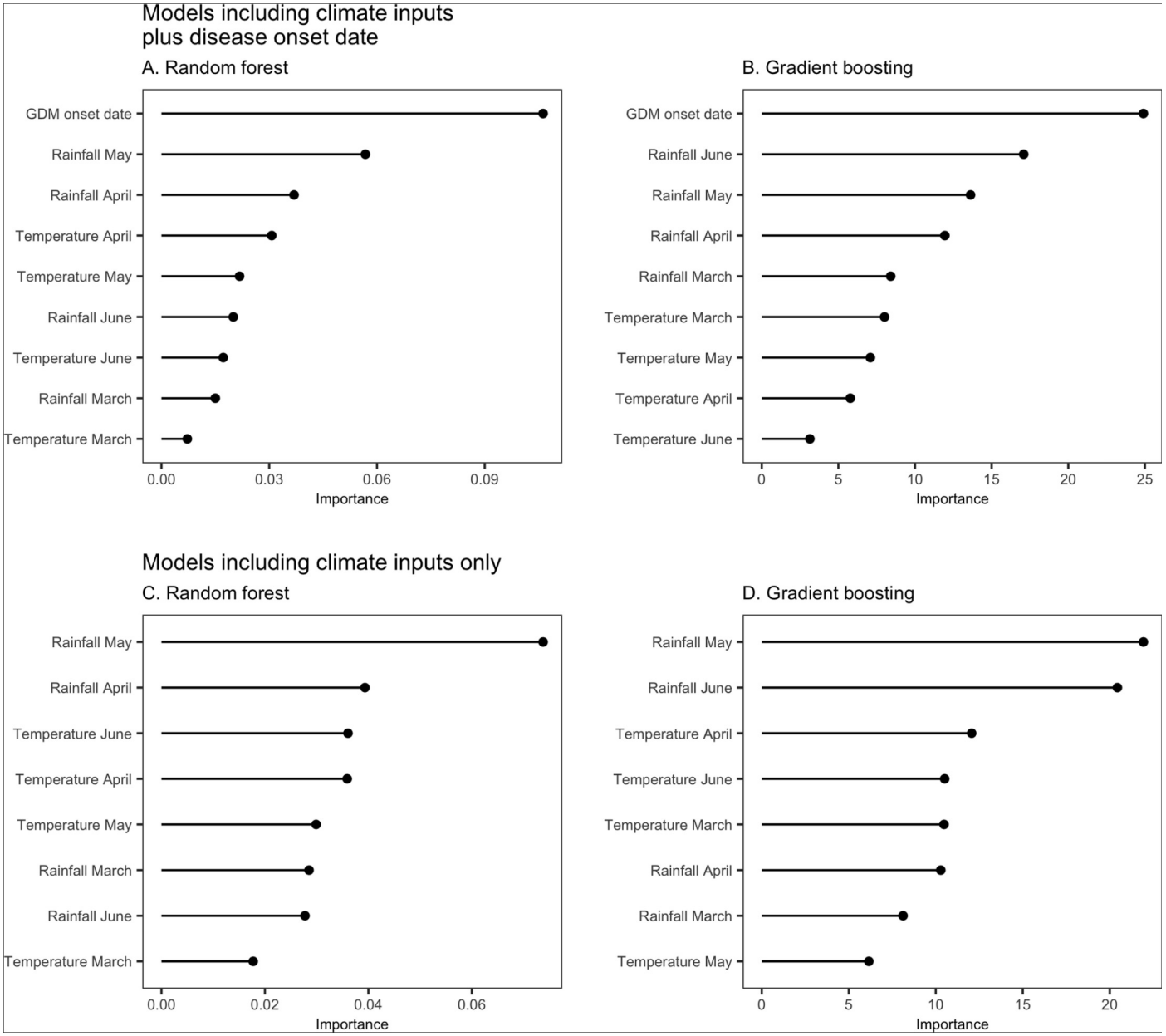
266 untreated plots between 2010 and 2017




Response (Y)
High/Low mildew severity
Model input (X)
Monthly Temperature (March-June)
Monthly Rainfall (March-June)
Date of disease onset
Gradient boosting
or
Random forest
(binary classification)

Probability of high severity on leaves as a function of climate inputs




Models including climate inputs plus disease onset date
A. Random forest
GDM onset date
Rainfall May
Rainfall April
Temperature April
Temperature May
Rainfall June
Temperature June
Rainfall March
Temperature March
0.00
0.03
0.06
0.09
Importance
B. Gradient boosting
GDM onset date
Rainfall June
Rainfall May
Rainfall April
Rainfall March
Temperature March
Temperature May
Temperature April
Temperature June
0
5
10
15
20
25
Importance
Models including climate inputs only
C. Random forest
Rainfall May
Rainfall April
Temperature June
Temperature April
Temperature May
Rainfall March
Rainfall June
Temperature March
0.00
0.02
0.04
0.06
Importance
D. Gradient boosting
Rainfall May
Rainfall June
Temperature April
Temperature June
Temperature March
Rainfall April
Rainfall March
Temperature May
0
5
10
15
20
Importance

« Results show that the use of this forecasting tool would reduce the number of treatments against grape downy mildew in the Bordeaux vineyards compared to current practices **by at least 50**%. »

Example 2: Prediction of root biomass

https://doi.org/10.5194/essd-2021-25
Preprint. Discussion started: 29 March 2021

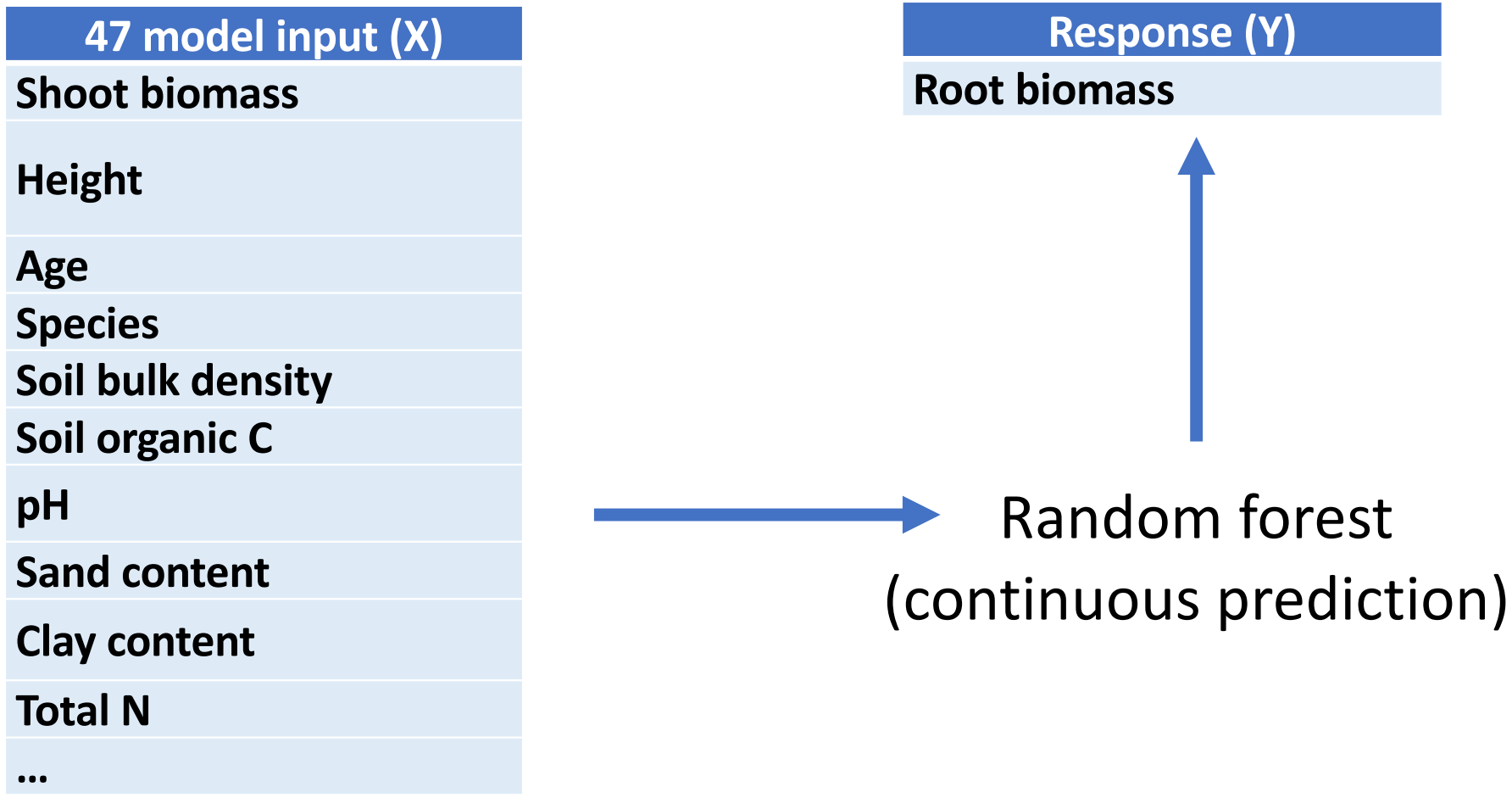
Open Access Earth System Science Data Discussions

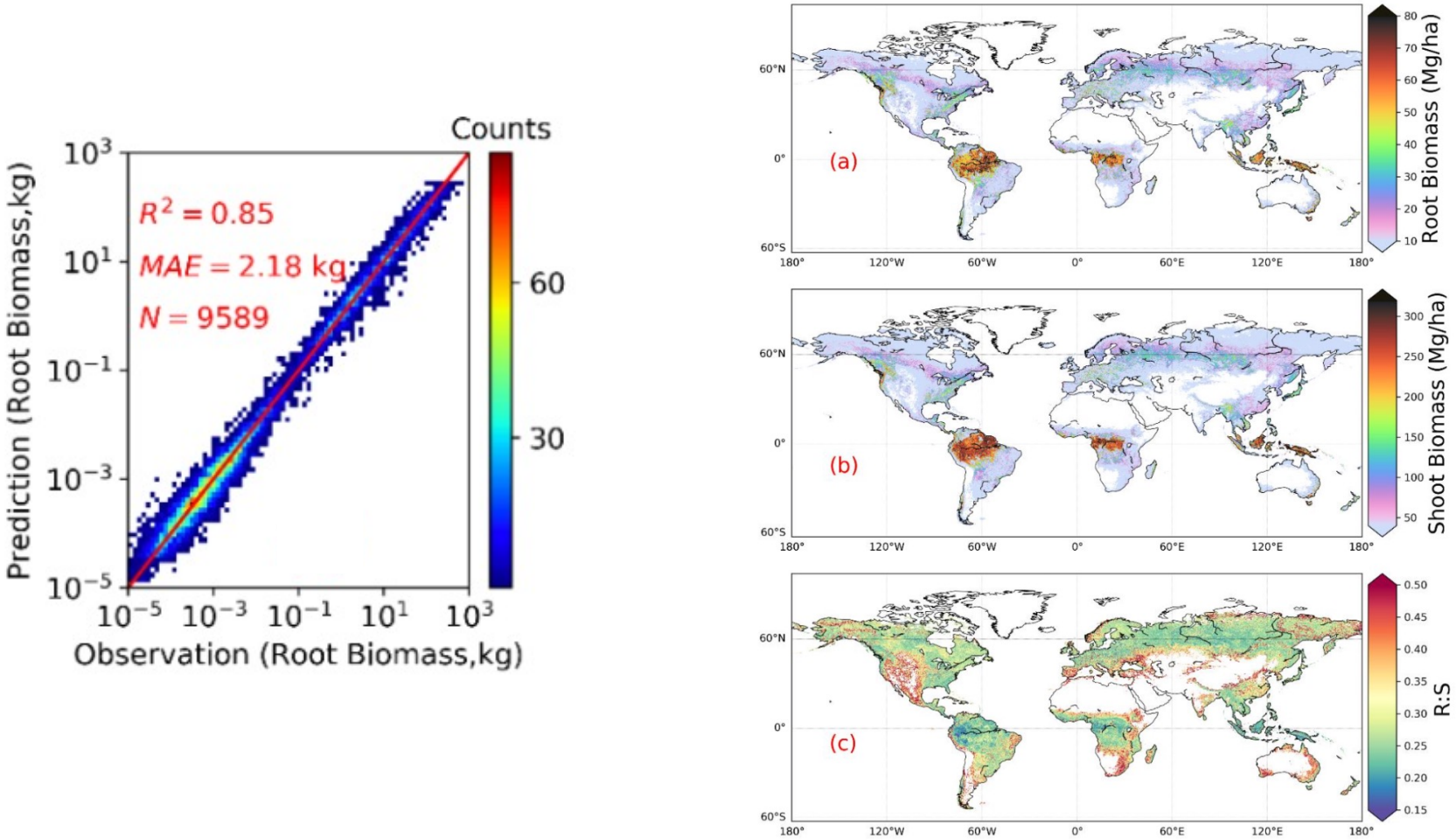
A global map of root biomass across the world's forests

Yuanyuan Huang[1,2], Phillipe Ciais[1], Maurizio Santoro[3], David Makowski[4,5], Jerome Chave[6], Dmitry Schepaschenko[7,8,9], Rose Z. Abramoff[1], Daniel S. Goll[1], Hui Yang[1], Ye Chen[10], Wei Wei[11], Shilong Piao[12,13,14]

Dataset:

10,307 in-situ measurements of the biomass of roots and shoots for individual woody plants, covering 465 species across 10 biomes.


47 model input (X)
Shoot biomass
Height
Age
Species
Soil bulk density
Soil organic C
pH
Sand content
Clay content
Total N
…
Response (Y)
Root biomass
Random forest
(continuous prediction)



Global maps of **forest root biomass** generated through a machine learning model (a), shoot biomass from GlobBiomass-AGB(Santoro, 2018b) (b) and Root:Shoot ratio (c).

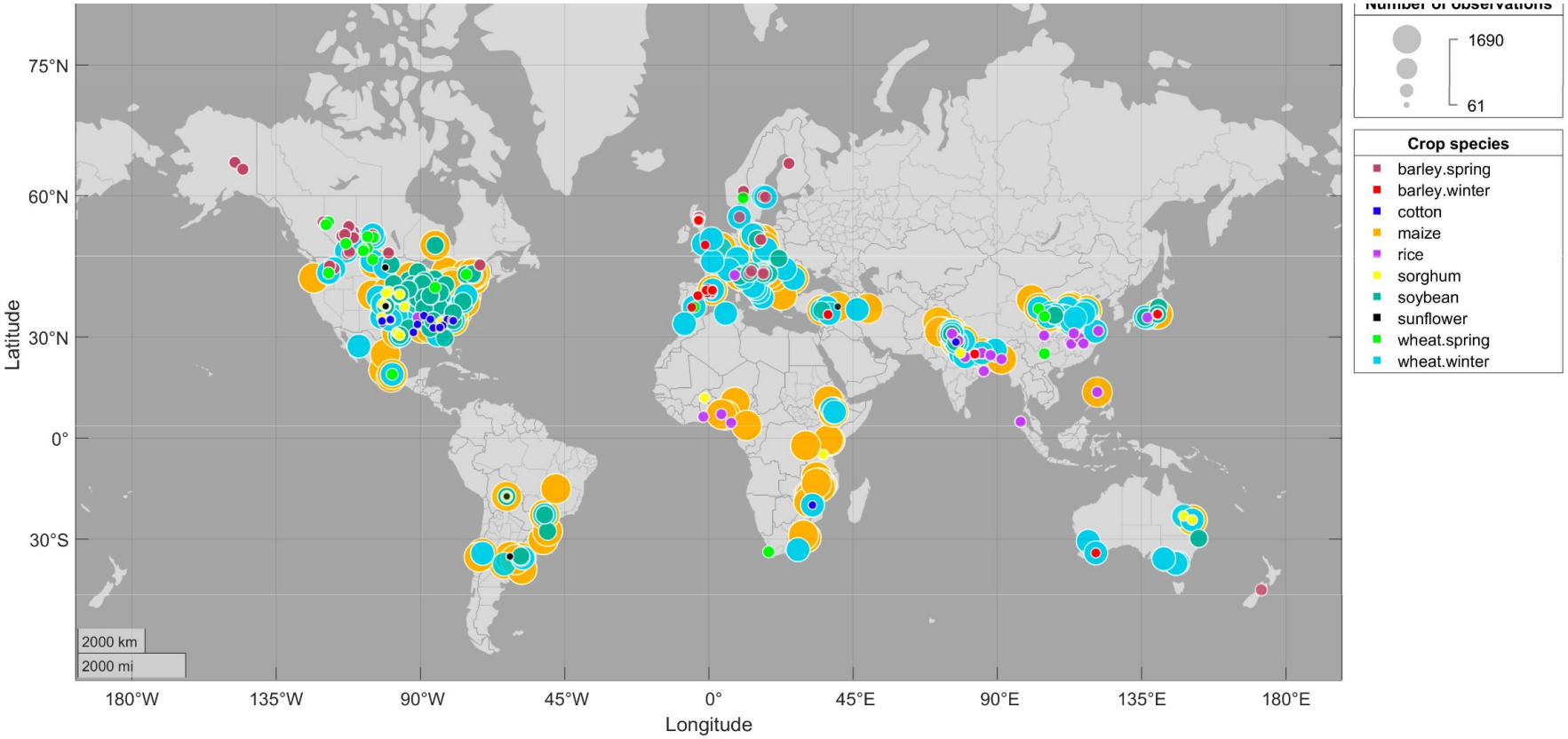
Example 3: Map the probability of yield increase of converting “conventional tillage system” to “conservation agriculture” at the global scale

https://www.nature.com/articles/s41598-021-82375-1.pdf

Locations of the experiments included in the dataset

Each experiment includes yield data for

- a conservation agriculture system
- a conventional tillage system



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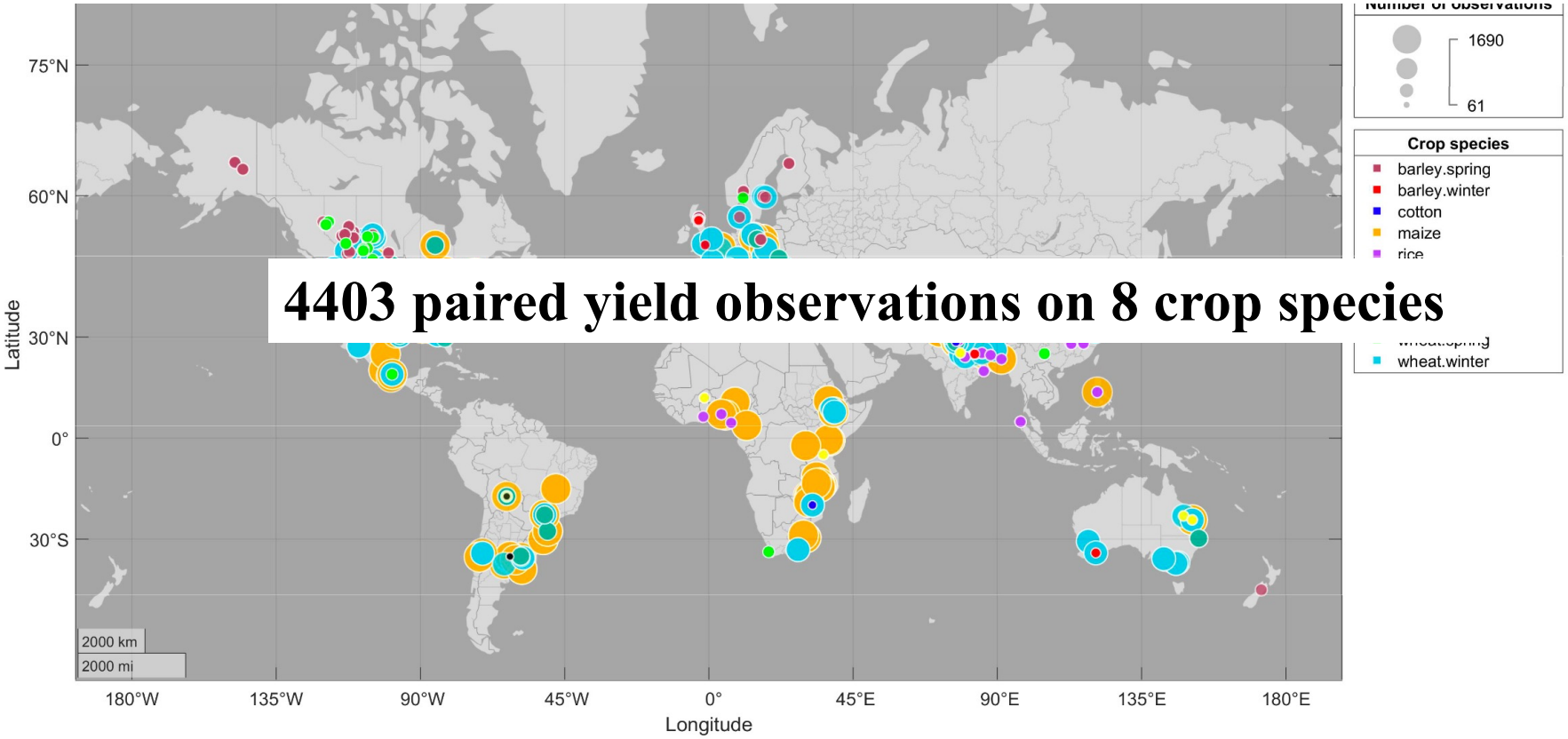

Model input (X)	Response (Y)
Avg. Precipitation	Yield gain vs. yield loss (1/0) induced by no tillage
Avg. Evapotranspiration	
Average temperature	
Avg. Maximum temperature	
Avg. Minimum temperature	
Soil texture	
Crop type (Barley, maize, soybean, wheat, rice, sorghum, cotton, sunflower)	
Fertilizer utilization (Y/N)	
Herbicide and pesticide application (Y/N)	
Crop rotation (Y/N)	
Crop residue management (Y/N)	

Model input (X)
Avg. Precipitation
Avg. Evapotranspiration
Average temperature
Avg. Maximum temperature
Avg. Minimum temperature
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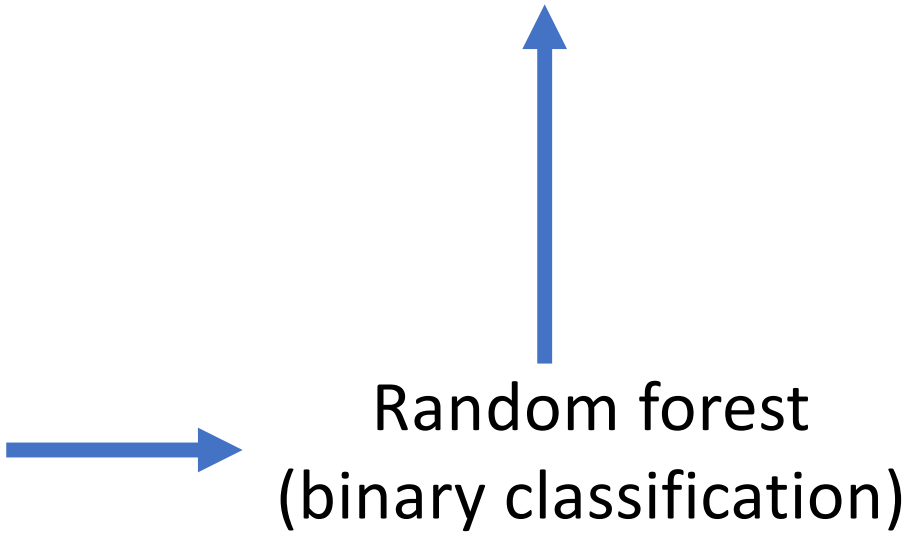
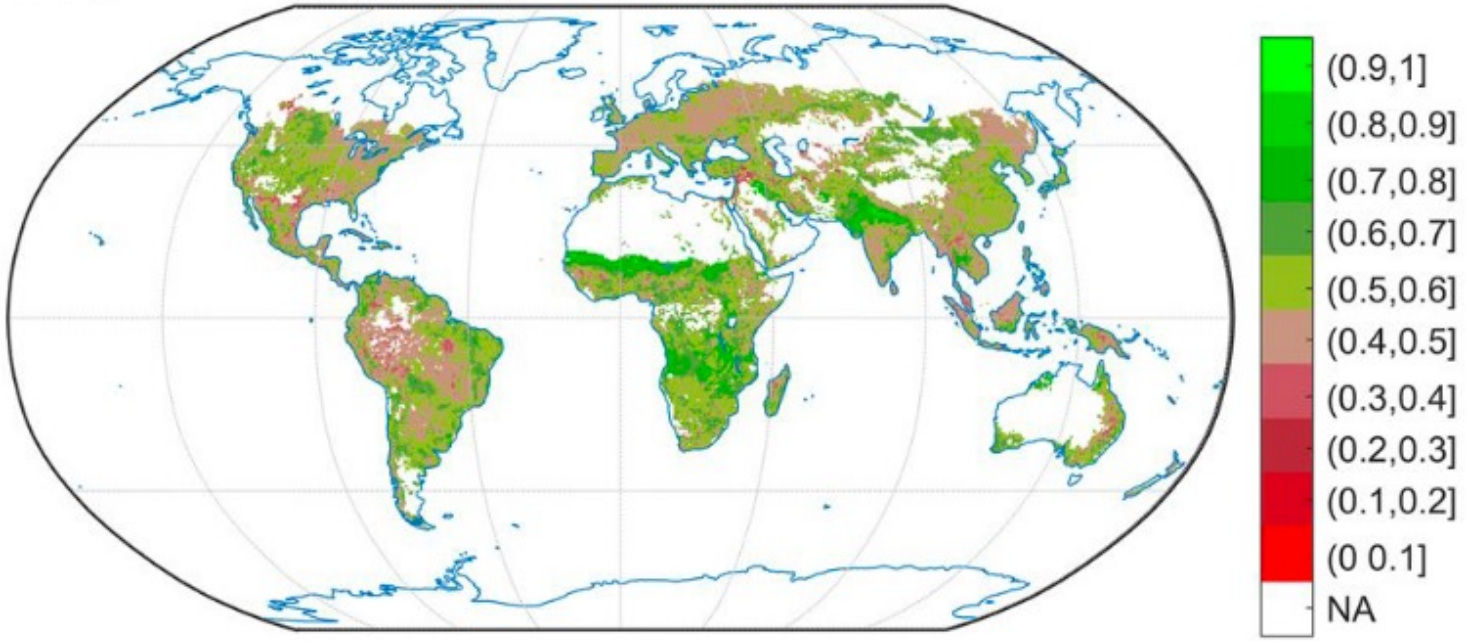
Herbicide and pesticide application (Y/N)
Crop rotation (Y/N)
Crop residue management (Y/N)

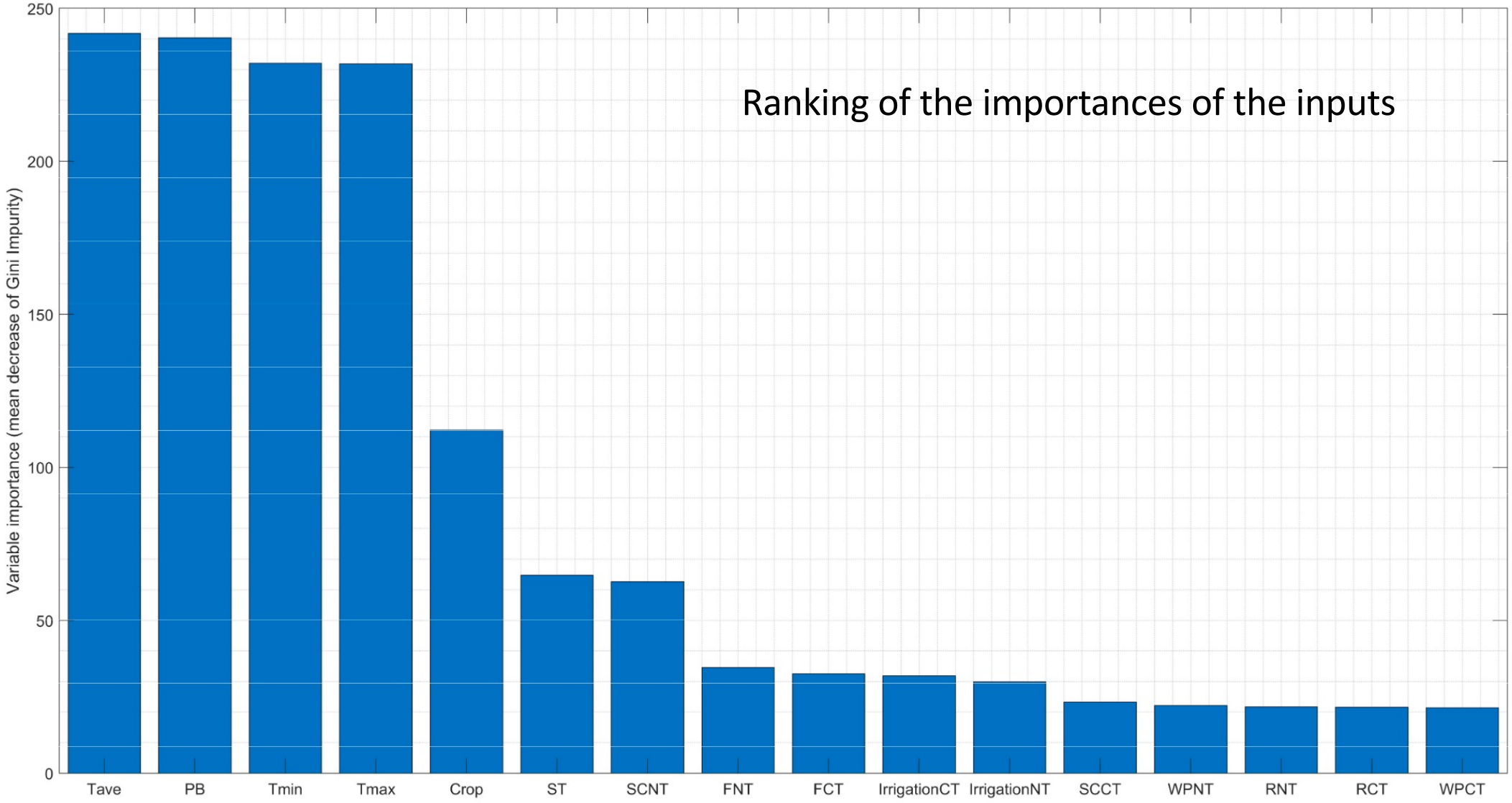
Response (Y)
Yield gain vs. yield loss (1/0) induced by no tillage



probability of yield increase for maize with Conservation agriculture vs. Tillage

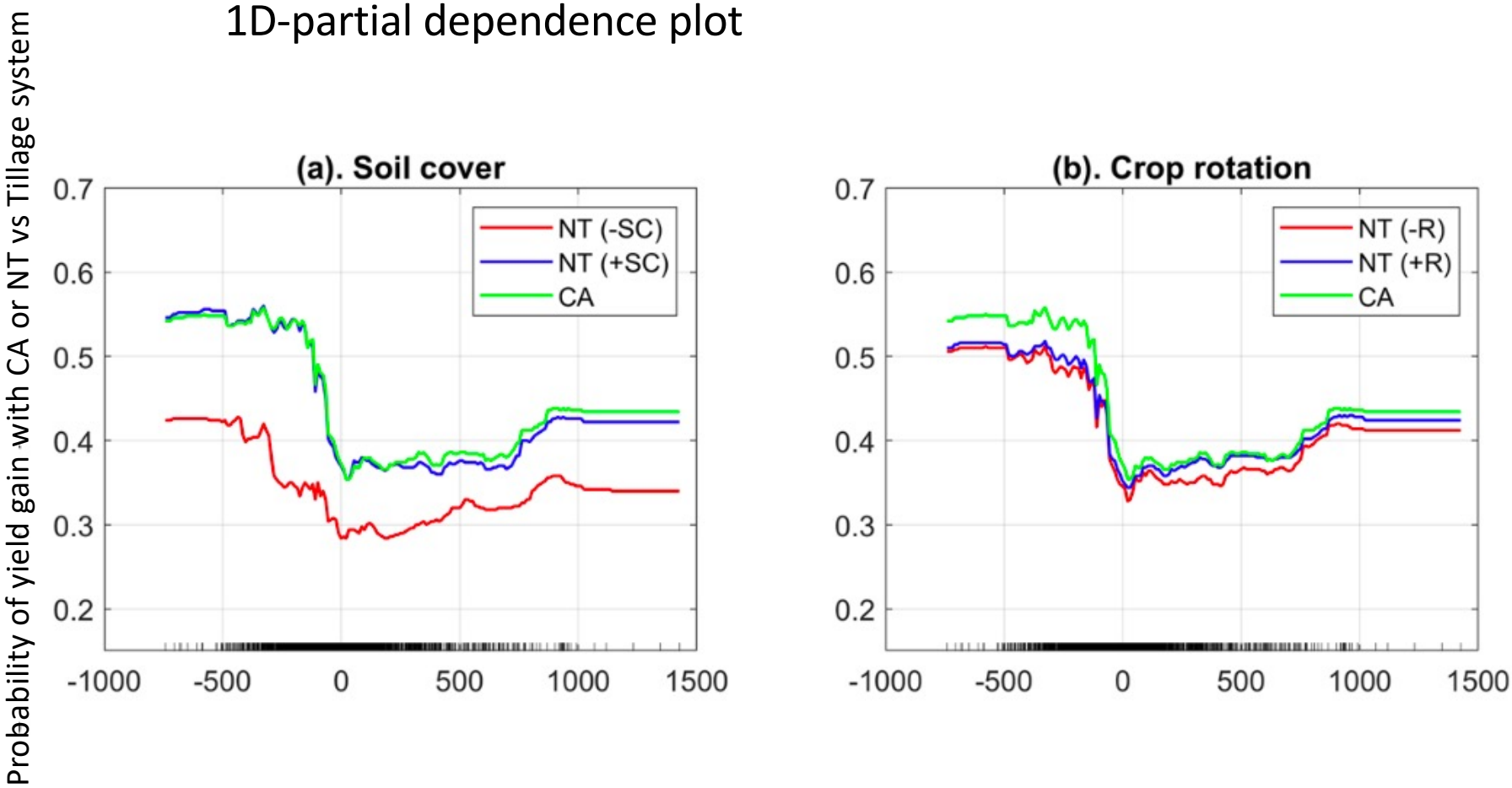


https://www.nature.com/articles/s41598-021-82375-1.pdf



https://www.nature.com/articles/s41598-021-82375-1.pdf

1D-partial dependence plot



NT: No tillage system
R: Rotation
SC: Soil cover
CA: Conservation agriculture (NT+R+SC)

https://www.nature.com/articles/s41598-021-82375-1.pdf

Main challenges in machine learning projects

- Choose a relevant question (Which Y? Which X?)
- Find reliable data
- Calibrate the hyper-parameters
- Assess prediction accuracy without bias
- Optimize computation time
- Vizualisation of output responses

Start simple

Start with two simple methods:

- Penalized linear regression (ex: LASSO)
- Random forest

Some trends

- Visualization tools (to open « the black boxes »)
- Image and text analyses (text mining, deep learning)
- Packages to streamline the development of predictive models (keras, caret, H2O…)
- Including expert knowledge in machine learning

Machine learning to emulate complexe models

Contents lists available at ScienceDirect

Journal of Environmental Management

journal homepage: www.elsevier.com/locate/jenvman

Research article

Meta-modeling methods for estimating ammonia volatilization from nitrogen fertilizer and manure applications

Maharavo Marie Julie Ramanantenasoa[a,b], Sophie Génermont[a,*], Jean-Marc Gilliot[a], Carole Bedos[a], David Makowski[c,d]

ACCEPTED MANUSCRIPT • OPEN ACCESS

Maize yield and nitrate loss prediction with machine learning algorithms

Mohsen Shahhosseini[1], Rafael A Martinez-Feria[2], Guiping Hu[3] and Sotirios Archontoulis[1]

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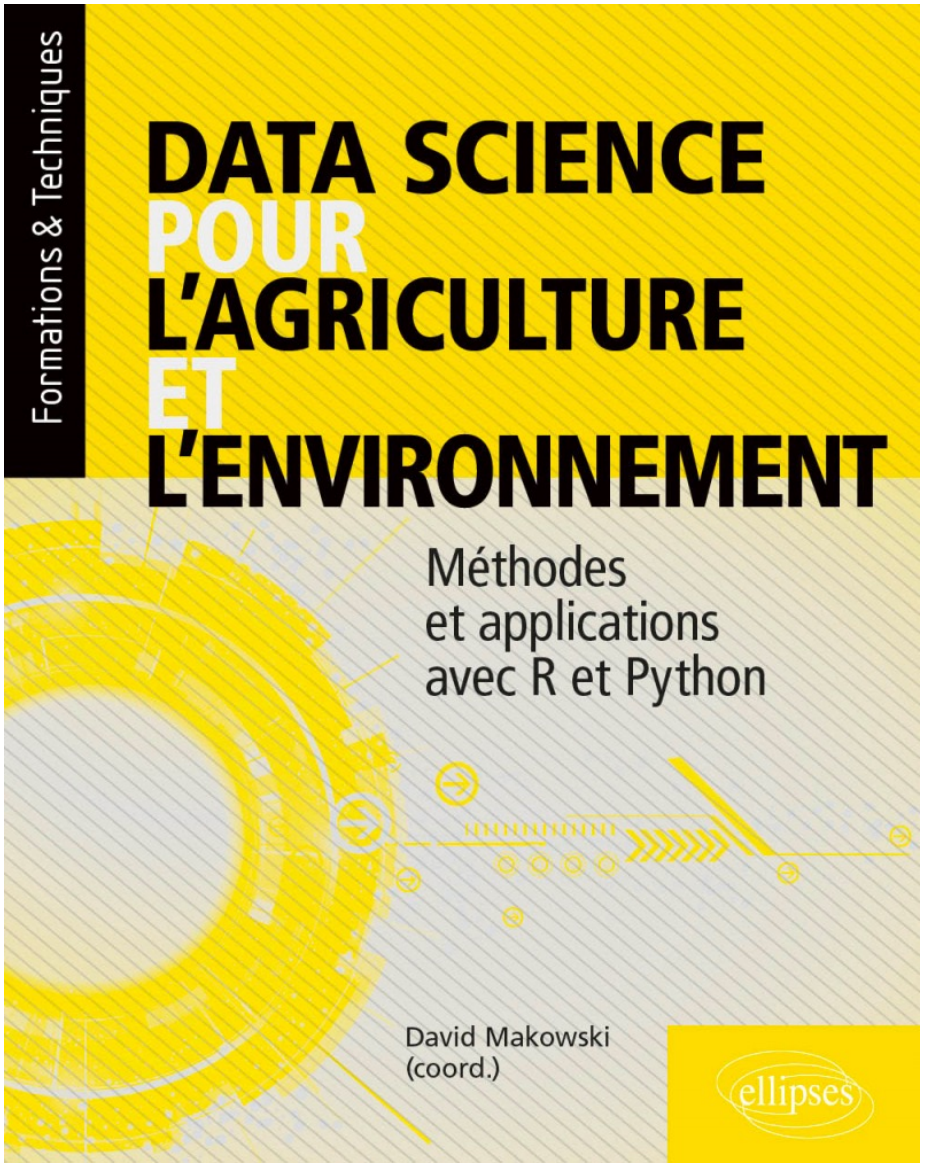
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