1	Comparing Machine-Learning models of different
2	levels of complexity for crop protection : A look
3	into the complexity-accuracy tradeoff
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# 12 1 Abstract

Crop diseases and pests constitute significant causes of yield losses for crops.
To limit the harm incurred by those events, farmers resort to plant protection products. Such products are known to have adverse effects both on the

environment and on human health. Agronomists make continuous efforts 16 to limit the usage of plant protection products to situations where those 17 products are strictly necessary. To determine such situations, agronomists 18 and policy-makers often rely on decision support tools to model and predict 19 the dynamics of plant diseases. Decision support tools are based either on 20 mechanistic models or on statistical approaches learned from large datasets of 21 biotic (e.g., disease incidence, plant phenological stage) and abiotic (meteo-22 rological, soil characteristics) observations in cultures. The surge of powerful 23 machine learning (ML) methods in the last decade makes such approaches a 24 natural pathway to model the dynamics of plant diseases. 25

Machine learning models can reveal the factors that contribute the most to disease and pests outbreaks, provided that those models are simple enough for human inspection. Simplicity, however, may come at the price of lower prediction performances when compared to more complex models.

In this paper, we offer a deep look at the performance of ML models of different complexity when used on two use cases of crop disease prediction: downy
mildew in the grapevine, and Cercospora leaf spot in the sugar beet.

We compare model accuracy and complexity using a year-based cross-validation approach. Our results suggest that interannual meteorological variations are a very important factor in plant disease prediction. Moreover, in line with the observations of the research community in interpretable ML, model complexity stands in clear trade-off with accuracy. This makes models of intermediate
complexity appealing for predicting the dynamics of crop diseases as they
can provide explicit insights about the rationale of their predictions.

# $_{40}$ 2 Introduction

Crop protection against plant diseases is crucial to secure crop yields. To 41 this end, farmers and agronomists make use of plant protection products, 42 i.e., pesticides, to combat plant diseases and pests in cultures. It is well-43 known, however, that the usage of such products has multiple downsides. 44 Besides their impact on farmers' health, and their polluting effect on the en-45 vironment, such products incur an economic cost on both farmers and con-46 summers, not to mention their role in the development of pesticide-resistant 47 breeds [Heap, 2014] and the indirect contamination in other stages of the 48 food supply chain [Parsons et al., 2021]. It follows that minimizing the us-49 age of pesticides in cultures incurs countless benefits. One way to reduce our 50 dependence on such products is to adapt their usage to local factors [Chen, 51 2019] such as the climate/weather, the soil type, or the farming practices. 52 This can be achieved through the deployment of models that can predict dis-53 ease incidence or risk of outbreak. Such tools help farmers and agronomists 54 avoid the usage of pesticides when they are not necessary. 55

<sup>56</sup> There have been multiple efforts to model and predict the risk of outbreak

and the incidence of plant diseases in cultures [Edwards-Jones, 1993]. Exist-57 ing methods can be categorized into two families. On the one hand, mecha-58 nistic models are constructed based on prior observations and knowledge of 59 the diseases or pests' life cycles. These models require extensive agronomical 60 studies and experts intervention, and were the preferred approach to model 61 plant diseases for long time. An inflexion point arose with the emergence 62 of large amounts of data including past observations of diseases in cultures 63 - as human annotations or as images -, but also information about abiotic 64 factors such as the characteristics of the soil and meteorological data. This 65 data abundance has made statistical models, in particular machine learning 66 models, more appealing in the last decade, and has nurtured their steady 67 increase in accuracy and sophistication. 68

ML models used in crop protection are usually trained for a single type of 69 crop and disease. This is due to the fact that different crops develop in 70 different ways, and so do diseases and pests. It is also known that models 71 are typically trained for a given region, and are less accurate when used on 72 data from other regions [Velasquez-Camacho et al., 2023]. Some approaches 73 rely on image classification with deep learning [van Klompenburg et al., 74 2020, Ip et al., 2018, Liakos et al., 2018, van Evert et al., 2017] for disease 75 diagnosis. Other models are designed to predict or forecast the incidence 76 of a disease at a particular period of the year, e.g., before harvest, based 77 on human annotations. This forecast can take the form of an incidence 78

prediction (regression) or a risk of outbreak (classification) [Chen, 2019]. In
those cases the models' outcomes help agronomists decide whether to apply
or not plant protection products in their cultures.

But besides forecasting the incidence of crop diseases, ML models can also help agronomists understand which factors contribute to the development of those diseases. This is possible, however, if the model is simple and interpretable enough to be understood by humans. Examples of interpretable ML models are linear functions and shallow decision trees.

A simple, yet effective proxy to model interpretability is model complexity [Galárraga et al., 2021]. Complexity is usually measured as the number of relevant parameters that play a role in the model's answers, and it is known to be correlated with interpretability. To see why, it suffices to compare the effort of interpreting a linear model with 5 variables versus a linear model with 300 variables.

While complex models such as neural networks or gradient boosting tend to be less interpretable than transparent simple methods such as linear regression or shallow trees, in some cases this complexity pays off in terms of prediction performance [Mori and Uchihira, 2019, Johansson et al., 2011, Galárraga et al., 2021]<sup>1</sup>. This trade-off between complexity and prediction accuracy can happen because more parameters or weaker assumptions en-

<sup>&</sup>lt;sup>1</sup>As shown by Rudin [2019], Bell et al. [2022], the accuracy-interpretability trade-off is not necessarily observed in every application domain and depends on multiple factors such as the quality of the data.

dow models with more expressiveness and flexibility to capture subtle inter-99 actions. Simpler models make assumptions that may not encapsulate the 100 complexity of real data. For example linear models assume there exists a 101 linear relationship between the input features and the target variable i.e., 102 the variable we want to model or predict. This, for instance, excludes any 103 potential interactions between the input features as predictors for the target 104 variable. Between complex approaches and simple models lie pattern-based 105 models [Galárraga et al., 2021, Dong and Taslimitehrani, 2015] that strike an 106 interesting trade-off because they remain relatively simple white boxes that 107 exhibit higher predictive power than linear regression or decision trees. 108

Existing works that use ML methods for crop protection have paid little 109 attention to the potential needs for interpretability and the complexity-110 interpretability trade-off [Fenu and Malloci, 2021, Ip et al., 2018, van Evert 111 et al., 2017]. We therefore contribute to the state of the art by studying 112 this trade-off in the context of crop protection. We train different popular 113 machine learning models of varied complexity for two typical crop protec-114 tion tasks: (i) disease incidence prediction, and prediction of the symptoms 115 appearance date. We predict these target variables for the downy mildew 116 in grapevine cultures, and for the Cercospora leaf spot in sugar beet crops, 117 both in France. In both cases we resort to biotic (e.g., past disease inci-118 dences) and abiotic (e.g., metereological data) predictors. Our tasks are 119 classical regression problems, therefore the studied models include (i) black-120

box ensemble methods such as random forests and gradient boosting trees; 121 (ii) white boxes such as linear regression; and (iii) HiPaR [Galárraga et al., 122 2021], a pattern-based regression method of intermediate complexity. Our 123 experiments confirm a clear complexity-accuracy trade-off in our use cases, 124 and also show different techniques to distill agronomical insights from both 125 white- and black-box ML models. Our results suggest that despite the dif-126 ference in prediction accuracy and model architecture, the models agree on 127 some common insights. Moreover, interannual effects play a very impor-128 tant role, which makes very difficult to have a single model that can predict 129 disease incidence for any arbitrary year. 130

Section 3 describes the datasets used for our study, the methods trained on those datasets as well as their performance. This is followed by a discussion of the different agronomical findings we extracted from the trained ML models in Section 4. Section 5 concludes the paper with avenues for future research in the prediction of disease incidence in cultures.

# <sup>136</sup> 3 Material and Methods

<sup>137</sup> We now describe the agronomical datasets used in our study as well as the<sup>138</sup> machine learning models trained on those datasets.

#### 139 3.1 Data

Our study case builds upon four datasets covering two major plant diseases
observed in French cultures: Grape downy mildew and Sugar beet Cercosporia.

#### <sup>143</sup> 3.1.1 Sugar beet Cercosporia epidemiologic data

Sugar beet Cercosporia (SBC) incidences were observed in several vineyards
located in France by different extension services, including the ITB (Institut Technique de la Betterave). The experimental observations have been
collected from 2009 to 2020 in different regions in France.

For each monitored site, a specific part of the area, further referred to as the 148 "plot", was observed throughout a specific year. Weekly visual inspections 149 were performed on leaves covering one hundred plants in order to assess dis-150 ease incidence. The incidence was calculated as the proportion of sugar beet 151 leaves displaying symptoms of Cercosporia leaf spot (Cercospora beticola). 152 Weekly inspections were conducted in each plot from leaf emergence (which 153 happens in mid-May) until harvest (after mid-September). The collected 154 dataset adds up to 1235 individual plots. We highlight that no plot was 155 observed every year, and that conversely, not all plots can be monitored in 156 a single year. 157

<sup>158</sup> For each plot, we define the date of SBC onset (yearly symptoms apparitions

date) as the first day in which the proportion of infected leaf exceeded 10%.
The end of season incidence for SBC was defined as the maximum incidence
for the period going from the 25th of August to the 15th of September.

#### <sup>162</sup> 3.1.2 Grape downy mildew epidemiologic data

Grape downy mildew (GDM) incidence were observed in several vineyards located in France by different wine extension services including the IFV (Institut Français de la Vigne et du Vin). The data have been collected from 2010 to 2017.

For each considered plot, an untreated row of vines was observed. Each 167 untreated row was surrounded by two other untreated rows to ensure that 168 they were not unintentionally sprayed with fungicides. In the monitored 169 central row, weekly visual inspections were performed on leaves in order to 170 measure disease incidence. The incidence was calculated as the proportion 171 of vine leaves displaying downy mildew symptoms caused by *Plasmopara* 172 viticola. Weekly inspections were conducted in each vineyard from budburst 173 (early March) until at least bunch closing (mid-late July) or stopped when 174 the incidence was close to 100%. The observations consist of around 9407 175 weekly datapoints corresponding to 713 plots. 176

For each plot, date of GDM onset (yearly symptoms apparitions date) was defined as the first week in which the proportion of infected vines leaf exceeded 179 1%. The end of season incidence for GDM was defined as the maximum <sup>180</sup> incidence for each plot.

#### 181 3.1.3 Meteorological data

Meteorological variables were provided by the SAFRAN weather database constructed and maintained by the French national meteorological service (Météo-France). SAFRAN organizes the French territory into a grid of size 8×8 Km and stores meteorological data for each cell in the grid [Quintana-Seguí et al., 2008]. Daily observations on humidity, mean temperature, wind, amount of rainfall, and solar radiation were used to compute different meteorological variables for both diseases.

For SBC, each meteorological variable covers a period of half a month (15 189 days) from January to June. Features in the dataset follow a given conven-190 tion. The first part describes the temporal characteristics of the feature with 191 the first three letters of the corresponding month, followed by an 'A' for the 192 first half of a month or a 'B' for the second half. The second part describes 193 the climatic nature of the feature and how this information was calculated. 194 The feature suffixes are described in Table 1. For example, the variable 195 named JanA-ndRHm60 corresponds to the number of days (nd) such that 196 the relative humidity was higher than 60 percent (**RHm60**) during the first 197 half  $(\mathbf{A})$  of January  $(\mathbf{Jan})$ . 198

Name	Name Feature		
RHm <u>X</u>	Mean Relative Humidity lower than X $(X = \{60, 65, 80, 90\})$		
H87	Humidity index equals to 87		
H87 <u>Y</u>	Humidity index equals to 87 for at least $(Y = \{6, 10\})$ hours		
TmX	Mean Temperature higher than $(X = \{15, 20\})$		
TmVTinfV7	Mean Temperature higher than $(X = \{15\})$ but lower than $(Y = \{10\})$		
$1 \text{ III} \underline{\Lambda} 1 \text{ IIII} \underline{1 \underline{\Lambda}}$	for at least $(Z = \{3\})$ hours		
ThleY	Number of days where temperatures were defined as <i>inhibiting</i>		
TDIOA	to SBC growth for more than $(X = \{3,6\})$ hours.		

Table 1: Description of the meterological variables used to model the dynamics of the Sugar beet Cercosporia (SBC). Temperatures are considered as *inhibiting* below  $10^{\circ}$ C or above  $38^{\circ}$ C

For GDM, features either describe meteorological conditions at the date of recording or its sum for the four previous weeks before recording. For example, the predictive variable ETP gives us the evapotranspiration at the time of recording. ETP-4w is the sum of evapotranspiration for the four previous weeks. Two exceptions are the number of rainy and dry days, which are counted from the beginning of January. This length of four weeks was chosen based on expert insights about the growth speed of downy mildew.

#### 206 3.1.4 Four prediction targets

From both diseases data and associated climatic variables, we finally obtained 4 data sets corresponding to our 4 prediction targets.

• Sugar beet Cercosporia (SBC) end of season incidence (% of leaves with diseases) with 1235 plots and 367 variables including one categorical variable and 366 numeric ones. The categorical feature is the

212	risk-exposure, an indicator defined by agronomists based on their own
213	knowledge of each plot's sensitivity to SBC. The numerical variables
214	correspond to the one described in Subsection 3.1.3.
215 •	Sugar beet Cercosporia (SBC) symptoms appearance date (day number
216	of year) with 1235 plots and 367 variables.
217 •	Grape downy mildew (GDM) end of season incidence (% of sick leaves)
218	with 359 plots and 22 variables including two categorical and 20 nu-
219	meric.
220	Grape downy mildew (GDM) symptoms appearance date (week num-
221	ber of year) with the same 359 plots and 22 variables.

Thus, the target variables are numerical. We are thus confronted to a regression problem in all cases.

### 224 3.2 Regression Methods

We assume that the goal is to predict the values of a real variable, that we call the *target variable*, using observations from another set of variables that we call the *predictive variables*. Examples of target variables are given in Subsection 3.1.4. Conversely, the predictive variables constitute the set of meteorological indicators (see Table 1). This scenario constitutes a classical regression problem. We first introduce some notation and then survey the most popular regression methods used in crop protection on tabular data. We extend the discussion with the description of a pattern-aided regression method that deals with the complexity-accuracy trade-off introduced in previous sections.

#### 235 3.2.1 Problem Formulation and Notation

Let us assume that we count on a set of n target observations represented as 236 a column vector  $\boldsymbol{y} \in \mathbb{R}^n$ . Those target observations are associated to a set 237 of observations on the predictive variables, organized in a matrix  $X \in \mathbb{R}^{n \times d}$ . 238 Each row  $\boldsymbol{x}_i^{\top} \in \mathbb{R}^d$  in the matrix stores the observed values of the *d* predictive 239 variables associated to a target observation  $y_i$ . From now on, we denote 240 vectors and matrices with names in **bold** to distinguish them from scalars 241 and functions. Moreover, matrices are denoted with capital letters. If a 242 predictive variable is categorical, e.g., plant variety, we assume its values 243 have been encoded as real numbers, for instance, by resorting to strategies 244 such as one-hot encoding or dimensionality reduction. 245

The goal of regression analysis is to learn a function f such that  $y = f(X) + \epsilon$ and  $\epsilon$  is minimal. The function f is a model of the data designed to predict the target variable for unseen instances  $x^{\top} \in \mathbb{R}^d$  of the predictive variables. The term  $\epsilon$  is the error of the regression model and accounts for potentially unobserved predictors of y. The model f is learned on a set of training and validation observations.

#### 252 3.2.2 Classical Regression Methods

Linear Regression. This method assumes that the relation between the target variable y and the predictive variables X is linear, that is,

$$\boldsymbol{y} = \boldsymbol{\beta} \boldsymbol{X'} + \boldsymbol{\epsilon} \text{ with } \boldsymbol{\beta} = \operatorname{argmin}_{\hat{\boldsymbol{\beta}}} || \boldsymbol{y} - \boldsymbol{X'} \hat{\boldsymbol{\beta}} ||_2^2$$
 (1)

$$\boldsymbol{\beta} = (\boldsymbol{X}^{\top} \boldsymbol{X})^{-1} \boldsymbol{X}^{\top} \boldsymbol{y}, \qquad (2)$$

where  $X' = \mathbb{1} \oplus X$ , i.e.,  $X' \in \mathbb{R}^{n \times (d+1)}$  and  $\beta \in \mathbb{R}^{d+1}$  are the parameters 255 of the model (the operator  $\oplus$  denotes column concatenation), namely the 256 linear coefficients associated to the each of the d predictive variables plus 257 the intercept coefficient  $\beta_0$ . The parameters of the model can be computed 258 by minimizing the loss function  $\mathcal{L}_l(\hat{m{eta}}) = ||m{y} - m{X}' \hat{m{eta}}||_2^2$  with the method of 259 ordinary least squares (OLS) as illustrated in Equation 2. Linear models 260 are among the most popular regression methods due to their simplicity and 261 interpretability. This is because the magnitude of the coefficients tells us ex-262 plicitly how much a predictive variable contributes to the model's prediction. 263 On the downside, the linearity assumption may come at the expense of low 264 prediction accuracy, which is why linear models are often used as baseline 265 methods. 266

Lasso. To reduce the risk of over-fitting in linear regression, Lasso [Tibshirani, 1994] proposes an L1-regularization of the loss function, which favors models with few non-zero coefficients. This is achieved by minimizing the following objective:

$$\boldsymbol{\beta} = \operatorname{argmin}_{\boldsymbol{\hat{\beta}}} \mathcal{L}_l(\boldsymbol{\hat{\beta}}) + \theta ||\boldsymbol{\hat{\beta}}||_1.$$
(3)

By minimizing the L1-norm of  $\beta$  we can obtain sparse models that can not only prevent or mitigate over-fitting, but that are less complex and therefore easier to inspect by humans. The penalization term  $\theta$  is a hyper-parameter that controls the importance of the sparsity constraint in the optimization process. The Lasso method selects the set of parameters  $\hat{\beta}$  that achieves the highest performance in cross-validation.

**Decision/Regression Trees.** A decision tree is a binary tree where each 277 internal node evaluates a Boolean condition on a predictive variable. The 278 children of a node are decision trees associated to an evaluation outcome, 279 i.e., true or false. Leaves (also called final nodes) are linked to a prediction of 280 the model for the target variable. When the target variable is numerical, we 281 talk about regression trees [Kramer, 1996]. Regression trees are white-box 282 models because the model's prediction on a particular instance  $\boldsymbol{x}^{ op} \in \mathbb{R}^d$  can 283 be explained by following the path from the root to the leaf node that pre-284 dicts the outcome for  $\boldsymbol{x}^{\top}$ . This makes regression trees interpretable models, 285

provided that the tree is not too deep for human inspection. Despite their interpretability, decision trees are prone to over-fitting if not properly parameterized, and are usually outclassed in terms of predictive performance by ensemble methods such as random forests and gradient boosting trees.

Random Forests. Random Forests are ensembles of weak decision tree 290 estimators [Breiman, 2001]. Predictions are computed by averaging the pre-291 dictions of each tree in the ensemble. The weak estimators are learned by 292 applying bagging and random feature selection. In bagging, each tree is 293 learned by sampling from X and y uniformly and with replacement. More-294 over, the trees are trained on different subsets of the features, which gives 295 each tree a "partial" but "unique" view of the data. These techniques make 296 random forests very robust to over-fitting, and a very popular choice for crop 297 protection [Elavarasan et al., 2018]. On the downside, random forests are 298 not interpretable because the aggregation step makes it very difficult to trace 299 the outcome of the model back to the input features – without resorting to 300 post-hoc inspection approaches as we will show later. 301

Gradient Boosting. Another popular ensemble method is gradient boosting [Mason et al., 1999]. Like random forests, the basic principle is to compute a robust prediction from the predictions of a set of weak learners. Different from random forests, learning is based on an additive model where each learner  $h_m$  is fit on the error of the previous learner  $h_{m-1}$  – technically on the negative gradient of the minimized loss function. Put dif-ferently, each new learner is trained to correct the errors of the previous one:

$$\gamma_i = \mathcal{L}(\boldsymbol{y}, f_m(\boldsymbol{X})) \quad (5)$$

$$f_m(\boldsymbol{X}) = f_{m-1}(\boldsymbol{X}) + \gamma_m h_m(\boldsymbol{X}) \quad (4)$$

The individual learners can be of any type, however decision trees are a common choice [Mason et al., 1999]. Gradient boosting models are very robust to over-fitting, and like random forests, behave pretty much like black boxes.

#### 315 3.2.3 Hierarchical Pattern-aided Regression (HiPaR)

Pattern-aided Regression. Pattern-based regression models consist of a 316 set of local models trained on regions of the data. Those regions are charac-317 terized by interpretable patterns, namely logical conditions on the predictive 318 variables, e.g., wind-speed > 50. The local models are usually interpretable 319 functions, e.g., linear functions, that capture local relationships between the 320 target and the predictive variables that cannot be observed at the "global 321 level". As shown in the literature [Galárraga et al., 2021, Dong and Taslim-322 itehrani, 2015], these methods exhibit higher predictive performance than lin-323 ear regression at the price of a manageable increase in complexity. Examples 324 of pattern-aided regression methods include piecewise regression [McGee 325 and Carleton, 1970], regression trees [Breiman, 2001], model trees [Wang 326

and Witten, 1997]<sup>2</sup>, Contrast pattern-aided regression (CPXR) [Dong and
Taslimitehrani, 2015], and HiPaR [Galárraga et al., 2021]. We elaborate on
the latter method in the following.

HiPaR. Hierarchical Pattern-aided Regression Galárraga et al. [2021] estimates the values of the target variable via a compact set of local hybrid
rules on the predictive variables. These rules have the form:

$$p = C_1 \wedge \dots C_m \Rightarrow \boldsymbol{y} = f_p(\boldsymbol{X}_p).$$
 (6)

In this expression, the pattern p is a conjunction of conditions on the pre-333 dictive variables such as wind-speed >  $50 \wedge humidity > 30$ . Those conditions 334 define subsets or regions of the data  $X_p \subset X$ . A hybrid rule is associated 335 to a local linear model  $f_p$  that has been trained on  $X_p$ , and that refines the 336 predictions of a global linear model f trained on X. The model f, called 337 the *default* model, is used to make predictions whenever none of the local 338 hybrid rules applies. After having learned the default model, HiPaR mines 339 a compact set of hybrid rules by means of two phases: 340

1. During the enumeration phase, the learning algorithm explores the space of patterns p in a depth-first hierarchical fashion. When a pattern p is visited, HiPaR learns a hybrid rule of the form  $p \Rightarrow y = f_p(X_p)$ 

<sup>&</sup>lt;sup>2</sup>These are regression trees such that some nodes, usually the leaves, are linear models on the target variable

344		on $X_p$ – the set of observations that satisfy $p$ –, and then explores
345		the sub-regions of $X_p$ . Since the search space is exponential in the
346		number of features, a set of pruning strategies reduces it by avoiding
347		the exploration of unpromising sub-regions; for example a minimum
348		support threshold is enforced to avoid sub-regions with very few points.
349	2.	Despite the pruning strategies carried out during the enumeration
350		stage, the set of resulting hybrid rules can still be very large. For
351		this reason, HiPaR carries out a selection phase that retains a small
352		set of hybrid rules with good performance and minimal overlap. This
353		phase is governed by two hyper-parameters: the support and the over-
354		lap bias. They determine, respectively, to which extent very specific
355		rules are preferred over general rules, and how much overlap between
356		the selected rules is allowed.

Contrary to tree-based models, HiPaR's hybrid rules are extracted from a 357 hierarchy with potentially overlapping regions as depicted in Figure 1. When 358 a new observation  $\boldsymbol{x}^{\top}$  satisfies more than one hybrid rule, the final prediction 359 is the weighted average of the predictions of the individual rules. The weight 360 is inversely proportional to the rule's error on a validation subset. This 361 makes HiPaR models more robust than linear functions and regression trees, 362 but significantly more complex. That said, HiPaR hybrid rules remain white-363 box models that allow for simple inspection of the most important predictive 364 variables in the prediction for an observation  $x^{\top} \in \mathbb{R}^d$ . 365



Figure 1: A depiction of the regions explored by HiPaR for two steps of the enumeration phase. Each rectangle defines a region described by a pattern, on which HiPaR learns a local regression model. Regions can overlap; an example are the regions stage = "b. veraison" and variety = "Grenache". Once a region is explored, e.g., stage = "b. veraison", HiPaR will look at its sub-regions in a depth-first-search manner (figure on the right).

- Table 2 summarizes the strengths and weakness of the methods discussed in
- 367 this section.

Models	Characteristics	${f Advantages}$	Disadvantages
Lasso	Sparse linear regression	Simple/interpretable	Baseline method
HiPaR	Pattern-based	Medium-complexity	High computation time
Random Forests	Ensemble-, tree-based	High accuracy, Built-in feature importance values	Black-box model
Gradient Boosting	Ensemble-based	High accuracy	Black-box model

Table 2: Overview of the machine learning methods used in this study.

#### 368 3.3 Training and testing procedures

#### 369 3.3.1 Optimization and performance evaluation

- 370 One of the challenges of evaluating different machine learning models is to
- <sup>371</sup> select the best configuration so that comparisons are fair and meaningful. In

an agronomical scenario the important interannual differences make standard cross-validation unadapted. Therefore, we use cross-validation by year, that is, each year is used as a fold in the process. The data from a given year is separated from the rest of the dataset for testing, whereas the observations from remaining years are used to train the algorithm. That way we are able to estimate the actual capacity of the algorithms to predict for unseen scenarios, e.g., for a new year.

Inside each fold, we select the best model by optimizing the hyper-parameters of each method. HiPaR's enumeration phase can take long for very low support thresholds. Therefore we run the enumeration phase with a support threshold of 30% the size of the dataset once – i.e., regions covering fewer points are not explored –, and we then optimize the hyper-parameters of the selection phase to pick the most performing set of rules.

We use the coefficient of determination  $(\mathbf{R}^2)$  as prediction performance met-385 ric. The R<sup>2</sup> score is defined as the proportion of the variance in the predicted 386 target variable explained by the independent variables. Contrary to the root 387 mean square error (RMSE), R<sup>2</sup> values can be compared among different pre-388 diction tasks (e.g., disease incidence and symptoms appearance). Indeed, the 389 closer to 1 the  $\mathbb{R}^2$  is, the better the model fits the data. Values close to zero 390 denote a performance comparable to predicting the mean of the target vari-391 able, whereas negative scores mean the model is worse than a mean-based 392 simple predictor. 393

#### 394 3.3.2 Complexity measure

To measure the complexity of the studied machine learning models, we resort 395 to the complexity measure for pattern-based models proposed by Galárraga 396 et al. [2021] that counts the number of elements in the model. An element 397 is either a non-zero coefficient or a condition on a predicting variable. We 398 remark that this measure is also applicable to tree-based methods such as 399 random forests or gradient boosting trees because each node of each tree of 400 the ensemble defines either a condition on one attribute or a linear model 401 - for simple regression trees this linear model is a single constant. The 402 number of elements can be very large when the ensemble consists of many 403 trees, which points out the complexity of such models. 404

<sup>405</sup> Under this principle, a Lasso model is generally less complex than a HiPaR<sup>406</sup> model with several rules. This is the case because for Lasso we only need to<sup>407</sup> count the non-zero coefficients in the linear function, whereas for HiPaR we<sup>408</sup> must consider both the number of conditions and the coefficients of each of<sup>409</sup> the local models.

<sup>410</sup> If we consider the following regression tree T:



<sup>412</sup> Then its complexity c(T) is 5. Likewise, if we consider the rule R:

$$C_1 \wedge C_2 \wedge C_3 \wedge C_4 \Rightarrow y = 3x_1 + 4x_2 - 4x_3 + 8.$$
 (7)

then its complexity c(R) is 8 because the rule consists of 4 conditions and 4 linear coefficients.

#### 415 3.4 Results

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### 416 3.4.1 Performance-Complexity Trade-off

Figure 2 depicts the trade-off between the complexity and accuracy of the studied machine learning methods. On the x-axis we show the complexity of the models (in log scale). The y-axis corresponds to the median R<sup>2</sup> coefficient of each model in cross-validation. Models located in the top-left part of the space strike a better accuracy-complexity trade-off as they predict the data more accurately with fewer elements. As suggested by Galárraga et al. [2021], more complex models such as random forests or gradient boosting trees achieve the best performance at the price of high complexity. Lasso regression, our baseline, is often the least accurate model. HiPaR positions itself in between linear regression and ensemble methods striking a very interesting trade-off for 3 of the 4 prediction tasks.

We highlight that accuracy varies drastically across tasks: All models strug-428 gle when it comes to predicting the date of apparition of downy mildew in 429 vine cultures, as the median R<sup>2</sup> for all methods is negative (bottom-right fig-430 ure). We observe  $\mathbb{R}^2$  scores between 0.12 and 0.26 for the final downy-mildew 431 incidence (on the bottom-left) with gradient boosting as the winner. HiPaR 432 lies close to Lasso, which means that it did not find many regression rules 433 improving performances marginally over the baseline. The performance dif-434 ferent between the two target variables in the downy-mildew dataset could 435 be explained by the relatively low number of observations for the date of 436 symptoms apparition – 359 versus 700 observations for the end-of-season 437 incidence. 438

The reach of the aggregated variables is relatively limited too. By this we mean most of these variables over a range of 4 weeks before data collection. While this confirms the trade-off, the low R<sup>2</sup> makes this dataset less interesting to study further.

The results for the sugar beet Cercospora are more encouraging. The R<sup>2</sup> median scores for the apparition date vary between 0.13 and 0.18 with gradient boosting leading the rank and followed by HiPaR (top-right figure).
For the prediction of the end-of-season incidence performance ranges from
0.05 to 0.35. In this use case HiPaR outperforms all methods and finds a
large number of rules that improve performance significantly when compared
to a single linear model, and without incurring as much complexity as the
ensemble methods.



Figure 2:  $\mathbb{R}^2$  of different machine learning models compared against their complexity. The x-axis correspond to the number of elements that compose each model (log scale). The y-axis are the median  $\mathbb{R}^2$  values in cross-validation. GBR stands for gradient boosting regression, and RFR for random forests regression.



Figure 3: Mildew symptoms apparition date



Figure 4: Mildew end of season incidence





(b)  $\mathbf{R^2}$  year-to-year cross-validation distribution

Figure 5: Cercosporia symptoms date of apparition



Figure 6: Cercosporia end of season incidence

When we look at the performance of the methods per year (Figures fig. 2), we notice that performance can vary drastically from one year to another, and that both end-of-season incidence and date of apparition are very hard to model for some years. This is true for all methods. As a general trend, we can observe that Cercospora end of season incidence predictions seem to follow a downward trend in performance. The performance variability across folds (Figures fig. 2) for the different methods is comparable and does notseem to follow a noticeable pattern.

Now that we have illustrated the accuracy-complexity trade-off present in our 459 use cases, we delve into the knowledge captured by the different methods. 460 To do so we analyze the models trained to predict year 2009 for the end-461 of-season incidence of the sugar beet Cercospora, as these models exhibit 462 the highest explained variance across all years ( $\mathbb{R}^2$  scores of 0.67 and 0.66 463 for gradient boosting trees and random forests, 0.3 for Lasso, and 0.47 for 464 HiPaR). For white-box models such as Lasso and HiPaR, we conduct direct 465 inspection of the models' elements. For the complex black-box approaches, 466 we resort to classical model inspection techniques and assess whether our 467 models agree on the relationships between the predictive variables and the 468 target variables. 469

#### 470 3.4.2 Use case: Incidence of the Sugar Beet Cercospora

In this section we carry out an inspection phase aimed to distill agronomical insights from the experimental machine learning models trained to predict the incidence of sugar beet Cercospora. These models were trained on all years except 2009 and correspond to the most performing cross-validation round of our experiments. We resort to classical interpretation techniques including feature importance rankings, partial dependence plots, and simple rule inspection. The first technique tells us which are the most important

variables that play a role in the prediction. PDPs and rule inspection allow 478 us to identify threshold effects on the predicting variables, that is, cases 479 when the behavior of the target variable varies in a piece-wise manner, i.e., 480 according to thresholds on the predicting variables. Pattern-based regression 481 methods such as HiPaR are good at detecting such kind of effects. Moreover, 482 such methods allow us to study more fine-grained interactions among the 483 predicting variables present in the rules. Our observations set the ground 484 for the discussion in Section 4. 485

Feature importance. A simple way to interpret the knowledge captured 486 by a machine learning model is to construct a feature-importance ranking 487 that tell us how much the model's input variables affect the model's out-488 put. This ranking can be based on the actual contributions of a variable 489 to the answers of a model, e.g., the coefficients of a linear regression, or 490 on model-aware scores computed a posteriori for black-box models. In this 491 spirit we contrast the feature-importance rankings of Lasso, RFR and GBR 492 and depicted them in Figure 7. Lasso's linear coefficients encode the ac-493 tual contributions of the input features to the answers of the model. They 494 are therefore signed. To turn the linear coefficients into importance scores, 495 we take their absolute value. Conversely, RFR and GBR are based on tree 496 ensembles for which different importance scores have been developed. We 497 choose the permutation feature importance method as implemented in the 498

scikit-learn library. This approach estimates the importance of a feature by shuffling its values across rows in X. The resulting decrease in accuracy is then used to determine how much the model relies on a feature to make predictions – the higher the decrease, the informative the feature is for predicting the target variable.



Figure 7: Parallel coordinates chart comparing feature-importance rankings for Lasso, random forests, and gradient boosting trees when predicting endof-season incidence for the sugar beet Cercospora. For each model we chose the top-4 most important features. For each model, features below the 4 can be further down the importance order than what is displayed

As we can see, RFR and GBR yield very similar rankings – their top-4 504 variables are the same even though the order is not identical. The variable 505 threshold-1 is the most important feature for all three models. This variable 506 represents the day in which the first symptoms of Cercospora were detected 507 in the culture. Conversely RFR and GBR's accuracy rely on the risk-zone 508 expert-based indicator, which is less important for linear regression. While 509 importance scores tells us which information the model is looking at, it 510 does not tell whether those features tend to increase or decrease the model's 511 incidence prediction. We can, however, obtain this information by looking 512

513 at the linear coefficients learned by Lasso.

<sup>514</sup> Table 3 shows the top-5 most important linear coefficients:

Variable	Coefficient
Threshold-1	-41
AprA-STm10	27.64
JunA-ndW2	-23.39
JunB-STm10	22.24
AprB-ndRHm60	14.73

Table 3: Top-5 important linear coefficients learned by Lasso

515 We remind the reader the meaning of these variables:

516 Threshold-1 : The symptoms apparition date

AprA-STm10 : The sum of the daily average temperatures of the days
above 10°C during the first half of April.

JunB-ndW2 : The number of days in the first half of June such that the average wind speed was higher than 2 m/s.

JulB-STm10 : The sum of the daily average temperatures above 10°C
during the second half of June.

AprB-ndRHm60 : The number of days in the second half of April such
that the relative humidity is higher than 60%.

Table 3 tells us that the later symptoms appear, the lower the final incidence tends to be. The predicted incidence tends to increase when temperature and humidity in June and April increase, whereas faster winds seem to hinder the development of Cercospora. This results must be taken with a grain of salt given the fact that our baseline Lasso model can explain only 30% of the target variable's variance. That said, these variables are used by more accurate models such as RFR and GBR, which means that we are not uncorrelated with the target variable.

As stated before, pattern-based regression methods Threshold Effects. 533 are constructed to detect predicting variable threshold effects on the target 534 variable. In HiPaR such effects are explicitly stated in the rule conditions. 535 To observe whether our models captured such effects we have a deep look 536 at the hybrid rules learned by HiPaR on our studied use case, and con-537 trast those thresholds to those learned by the more complex models, namely 538 RFR and GBR. Since those models are actually based very large ensembles 539 of threshold-based estimators, we observe those threshold effects by means 540 of partial dependence plots (PDP). This widely-used inspection technique 541 allows us to visualize the behavior of a model's prediction (y-axis) for the 542 different values of a predicting variable (x-axis). 543

In our use case, HiPaR learned 3 hybrid rules whose conditions are listed in Table 4. As displayed before, thresholds (in red) used in HiPaR's rules roughly fits with changes in the PDPs behaviour. While they not the most important features as seen before, it seems to indicate that these thresholds are not insignificant (according to RFR and GBR models). We suppose that these features might act as proxies for other features, or simply have an indi-

<sup>550</sup> rect influence on the final result that is not detectable by using PDPs.

Rule 1	$\mathit{JunA}\mathit{-ndTm15} < 8, \mathit{risk}\mathit{-zone}{=}\mathit{false}$
Rule 2	JulB-STm10<324
Rule 3	$MarB-ndW2 \ge 4, JunB-ndTm15 < 13$

Table 4: Conditions of the hybrid rules learned by HiPaR when predicting the end-of-season incidence of the sugar beet Cercospora.

In other words, HiPaR detected different linear behaviors based on whether a plot lies or not within a region deemed risky by experts (*risk-zone*), or whether the number of hot days in June and July are below certain thresholds (*JunA-ndTm15*, *JulB-STm10*, *JunB-ndTm15*), or whether the second half of March was windy (*MarB-ndW2*). We now construct PDPs for the numerical variables on RFR and GBR, which we depict in Figure 8.





(a) Number of days where average temperatures were higher than 15° during the first half of july

(b) Number of hours where average temperatures were higher than  $10^{\circ}$  during the second half of june





(c) Number of days where average wind speed were higher than 2km/h during the 2nd half of march

(d) Number of days where average temperatures were higher than  $10^{\circ}$  during the 2nd half of june

Figure 8: Partial Dependence Plots for the predicting variables MarB-ndW4, JulB-STm10, JunA-ndTm15 and JunB-STm10 on random forests and gradient boosting trees. The red line — represents a threshold learned by HiPaR.

**Feature Interactions.** Each of the conditions listed in Table 4 is associ-

ated to a local linear model (learned using Lasso). Those models reveal local

interactions between the variables in the conditions and the linear coefficients, and are designed to refine the baseline linear (called also the default) model learned on the entire dataset. Out of 368 features used as input in the models, Lasso selects between 25 and 55. This represents between 6.7% and 15% of the available features. Moreover, local models are systematically less complex than the default model as Table 5 shows.

	Rule 1	Rule 2	Rule 3	Default Model
Rule 1	25	8	3	6
Rule 2		28	6	16
Rule 3			26	12
Default Model				55

Table 5: Number of common non-zero coefficients of the linear models learned by HiPaR for the prediction of the end-of-season sugar beet Cercospora.

We can also observe that coefficients overlap between the different hybrid rules is low. This means that each local model is relying on different signals to make predictions on the end-of-season incidence. Figure 9 depicts the intensity and polarity of 16 of those coefficients for both the default and local models.



Figure 9: A color encoding for the linear coefficients of the three hybrid rules learned by HiPaR. Cells in white  $\Box$  denote features with a linear coefficient strictly equal to 0, which means those features aren't used by the model

<sup>570</sup> Our first observation is that the apparition date (*threshold-1*) is consistently <sup>571</sup> important across all models – and always correlated negatively with the <sup>572</sup> predict incidence. The features *risk-zone* and *JunA-ndW2* (wind speed in <sup>573</sup> the first half of June) are used in all models except the first rule because <sup>574</sup> these variables appear in the conditional part of this rule (Table 4).

This rule can be interpreted as follows: Plots with lower disease exposure (*risk-zone=false*) and lower temperatures in the first half of June (*JunAndTm15* < 8), experience an aggravated development of Cercosporia as humidity in May (*MayA-ndRHm60*), wind speed in March (*MarA-ndW4*), and rainfall in February (*FebA-SR*) increase. Wind during June (*JunB-ndW2*) is associated to a slow down of the disease.

The second rule suggests that lower temperatures in July (JulB-STm10 < 324) make Cercosporia sensitive to wind in January, February, June, and July (JanB-ndW2, FebA-ndW2, JunA-ndW2, JulA-ndW2). Conversely, a wet June (JunA-ndRHm65) or a windy March (MarA-ndW4) appear as aggravating factors. A windy July (JulA-ndW4), a rainy February (FebA-SR) and a hotter April (AprA-STm10) have a mitigated effect on the development of Cercosporia.

The third rule triggers when the month of March is windy (MarB-ndW4589  $\geq 4$ ) June is not very hot (JunB-ndTm15 < 13). In that case, higher tem-590 peratures in May (MayB-ndTm20) and a wet April (AprB-ndRHm60) are correlated with the growth of Cercosporia growth. Conversely, wind in June (*JunA-ndW2*) and July (*JulA-ndW4*) exhibit a negative correlation with growth.

Finally, we observe that the default model combines signals from all the lo-594 cal rules, even though it does not always relies on the same variables. This 595 happens because the learning objective of this model must fit the observa-596 tions from all the sub-regions. This translates into selecting variables (such 597 as JunB-STm10) that explain incidence for all the observations, i.e., at the 598 global level, but that have little to no explanation power when limited to 599 subsets of the data such as the observations on regions not deemed risky by 600 the experts (*risk-zone=false*). 601

## 602 4 Discussions

We structure our discussion along three axes: (a) the complexity-accuracy trade-off discussed in Subsection 3.4.1, (b) the implications of complexity in interpretability, and (c) the agronomical insights offered by the models trained.

Complexity and Accuracy. Our results go in line with what has been observed in other works on model complexity [Dong and Taslimitehrani, 2015,
Galárraga et al., 2021], that is, the tendency of complex models to outperform simple models in terms of prediction accuracy. It is crucial to highlight

though, that such a trend holds under the assumption that the models have 611 been properly parameterized and trained. For instance, a complex model 612 trained on very little data will surely over-fit that data specially if there 613 are as many or more parameters than data points. Conversely if the data 614 adheres to the learning hypothesis of a simple model, e.g., linearity, such 615 model will surely shine in terms of performance regardless of its complexity. 616 Finally, even if a model was trained under a reasonable learning hypothesis, 617 testing it on data that diverges from the training distribution will result in 618 unsatisfactory prediction performance. We can observe such a phenomenon 619 for the models tested on years 2013 and 2015 for the prediction of both 620 the incidence and the date of apparition in both cultures. The observations 621 collected those years are atypical because some of the predicting variables 622 exhibited measures outside the amplitudes observed other years. This trans-623 lated into a clear under-fitting with the lowest  $\mathbb{R}^2$  scores registered in our 624 experiments. 625

Interpretability. It is widely-assumed that interpretability and model complexity are positively correlated. An illustration of such phenomenon can be observed from our use case. Both linear and pattern-based model allowed us to distill insights easily and directly from the structures of the models themselves. For more complex models such as random forests and gradient boosting trees we had to resort to external inspection tools such as

the permutation-based accuracy decrease and the partial dependence plots 632 (PDPs). Albeit effective, those techniques have limitations. Importance 633 scores do not tell us if a variable is positively or negatively correlated with 634 the prediction of the model. PDPs can be applied to up to two variables at 635 the same time, and make independence assumptions that often do not hold 636 on the data. This happens because each point in the curve is the result of 637 averaging the model answers over all possible values of the remaining pre-638 dicting variables. Since some combinations of values may be unlikely, PDPs 639 must be taken with a grain of salt, specially when the predicting variables 640 exhibit some correlation. That said, the PDPs for RFR and GBR in our 641 experiments were in concordance with the threshold effects observed when 642 using HiPaR. It should be noted that while RFR, GBR, and HiPaR resort 643 to thresholds on the predicting variables, the fact they all outperform Lasso 644 significantly suggest that threshold effects are a reasonable hypothesis for 645 the prediction of plant diseases based on meteorological data. 646

Agronomical insights. Based on our use case study on the sugar beet
Cercospora, we observe that aggregating the meteorological indicators according to the seasons, i.e., winter, spring, and summer can effectively explain some of the variation in disease incidences.

<sup>651</sup> Winter defines the initial conditions: This is the period in which the primary <sup>652</sup> inoculum of Cercospora lies in the soil in the form of spores. Spring defines the development period for both crops and the Cercospora. Finally, summer
encompasses the end of the season, and the moment in which the disease's
symptoms, as well as its effects, are obvious.

As a general rule, dry summers seem to hinder the growth of Cercospora. 656 This follows from the importance assigned by the models to the wind and 657 temperature factors during June and July. Dry winters also seem to mitigate 658 the disease's spread. Conversely, a hot and humid spring stands as the 659 main aggravating factor in Cercospora's incidence. Thanks to the hybrid 660 rules provided by HiPaR, we can obtain more nuanced relationships between 661 the incidence and the predicting variables. Rule 2 in Table 4 tells us that 662 a mild month of July should make us focus the attention on the initial 663 conditions (winter), in particular the wind and the sun exposure and the 664 temperature – the two latter factors contributing positively to the presence of 665 the primary inoculum. Moreover, a windy spring with mild temperatures in 666 June should target our attention towards the development phase (spring) in 667 particular towards temperature and humidity, which are positively correlated 668 with incidence. In all cases, the date of apparition is the best predictor of the 669 final incidence, which means that early detection is the best weapon against 670 Cercospora. 671

We could not draw insights from the prediction of the downy-mildew on the vine because the transparent models explain no more than 14% of the observed variance for the incidence – the results for the date of apparition are

worse. We think this performance gap is due to the fact that the dataset 675 relies only on meteorological measures for the four weeks that precede the 676 end of the season. In other words, this dataset lack the richness of the me-677 teorological signals available for the sugar beet Cercospora dataset. This 678 observation confirms the importance of accurate and complete meteorolog-679 ical measurements when modeling the dynamics of plant diseases. We also 680 believe that the studying the impact of the granularity of the meteorological 681 indicators in such tasks remains an interesting research avenue. 682

# 683 5 Conclusions

In this paper, we have shown the interest of exploring the complexity trade-684 off for machine learning models when applied to predicting the incidence 685 of plant diseases. It is accepted that in some applications, complex mod-686 els such as neural networks or gradient boosting generally perform better 687 than simpler ones such as linear regression. This comes, however, at the 688 cost of interpretability, which (a) is vital when we need to draw insights 689 from the prediction model, and (b) fosters transparency, which can in turn 690 favor acceptability by users. Post-hoc explanation methods can help us ex-691 tract insights from accurate black-box models, but they are not the only 692 solution as we have shown in this work: medium-complexity models based 693 on pattern-aided regression can achieve competitive prediction performance 694 while remaining simple and interpretable. Moreover, our experiments with 695

post-hoc explainability techniques such as partial dependence plots suggest 696 that pattern-aided regression can reveal threshold effects that are also ex-697 ploited by the more accurate black-box ensemble methods. Using those mod-698 els, we have also shown that medium-complexity methods are well suited to 699 extract more pertinent information compared to simpler models. Likewise 700 medium-complexity models are easier to interpret compared to more com-701 plex methods. This shows the utility of pattern-aided regression and makes 702 it appealing for crop prediction. Since there is a direct correlation between 703 interpretability and acceptability, evaluating the complexity of a model is 704 not trivial and should be taken into account. This aspect has been already 705 addressed from the angle of learning complexity [Kearns, 1990] or from the 706 perspective of data complexity [Dwivedi et al., 2020], but rarely in terms 707 of the complexity of the resulting model. Finally, our study suggests that 708 the meteorological inter-annual variations make disease incidence prediction 709 very challenging, and that predicting disease incidence for any year requires 710 more research as well as more historical (quality) data. 711

In the future we envision to study whether increasing the temporal and spatial granularity of the meteorological attributes can help us improve the quality of our predictions. An interesting research avenue could be to apply representation learning techniques in order to learn novel and useful meteorological indicators that predict disease incidence more accurately. Given the inter-annual variations of weather patterns, future approaches should be able to categorize prediction models based on the meteorological profile of the
data used to train them. We believe that unsupervised learning techniques
could be adapted in that regard. Such approaches may be even necessary in
the light of a climate that will keep changing in the upcoming years.

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