Data Science In Practice - Model selection

EPF - P2023
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Summary

1. Evaluating a Hypothesis: Metrics
2. Model Selection and Cross Validation
3. Bias vs Variance
4. Regularization
5. Hyperparameter tuning

Evaluating a Hypothesis:

Metrics

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Evaluating a Hypothesis: Metrics

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  - MAE: Mean Absolute Error $\mathrm{MAE} = \frac{1}{N}\sum_{i=1}^{N}|\hat{y}_i - y_i|$
  - R2: Coefficient of Determination $\mathrm{R2} = 1 - \frac{MSE(Model)}{MSE(Baseline)}$

Evaluating a Hypothesis: Classification Metrics

- For **classification**, we use very often the **confusion matrix**

		True condition	
	Total population	Condition positive	Condition negative
Predicted condition	Predicted condition positive	**True positive**	**False positive**, Type I error
	Predicted condition negative	**False negative**, Type II error	**True negative**

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  - **True Positive**: Observation = True && Prediction = True
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- In general, it makes more sense to talk about **ratios**:

$$\mathrm{TPR} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}} \quad , \mathrm{TNR} = \frac{\mathrm{TN}}{\mathrm{TN} + \mathrm{FP}}$$

$$\mathrm{FPR} = \frac{\mathrm{FP}}{\mathrm{FP} + \mathrm{TN}} \quad , \mathrm{FNR} = \frac{\mathrm{FN}}{\mathrm{FN} + \mathrm{TP}}$$

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- We should **carefully choose** our metrics depending on the data

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  - Instead, we should focus on the **Recall** as it evaluates how good is our model at detecting the positives

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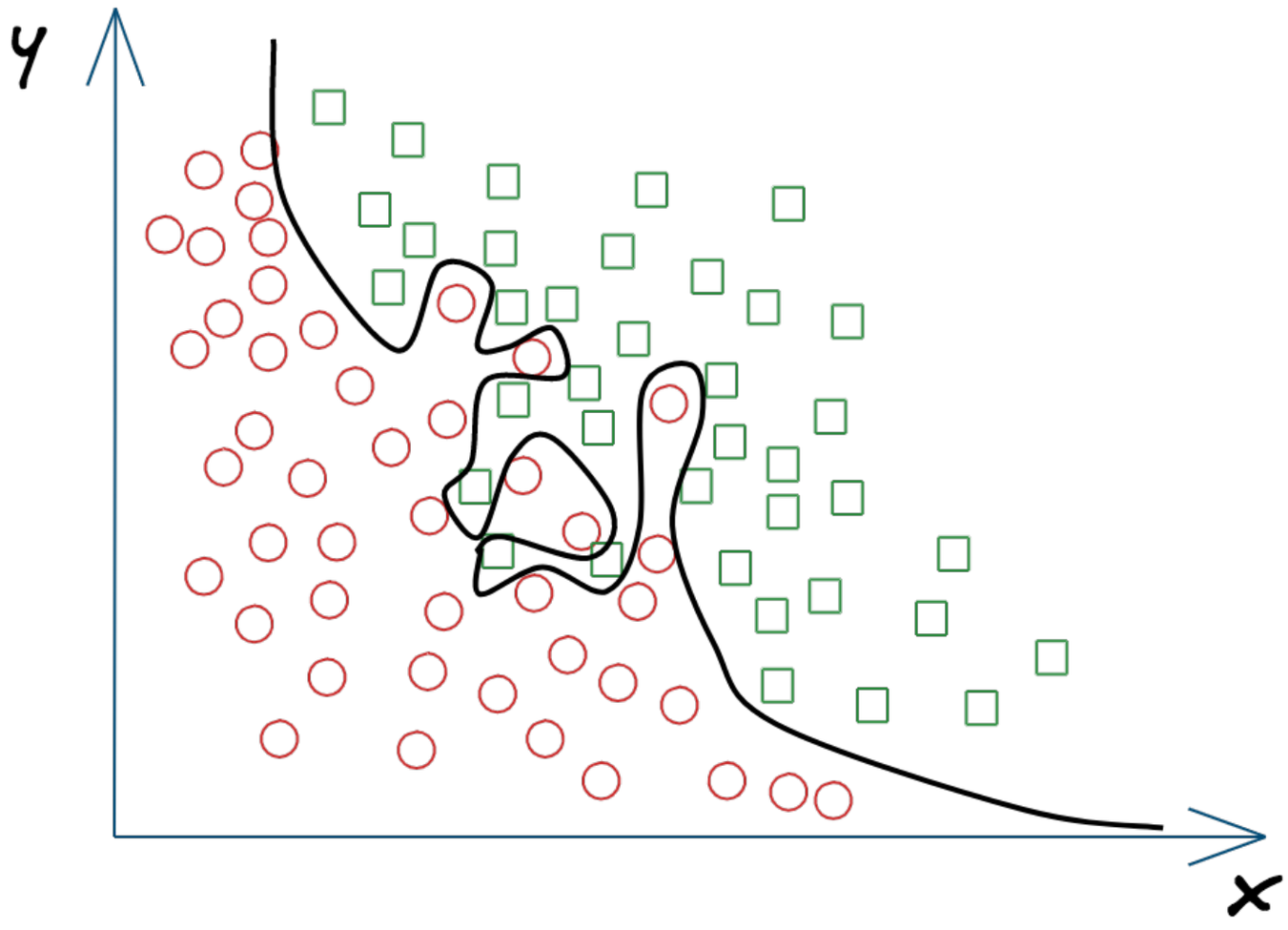
- Let's see an example

Model Selection and Cross Validation

- Example: At first sight, the model seems to fit perfectly the training data



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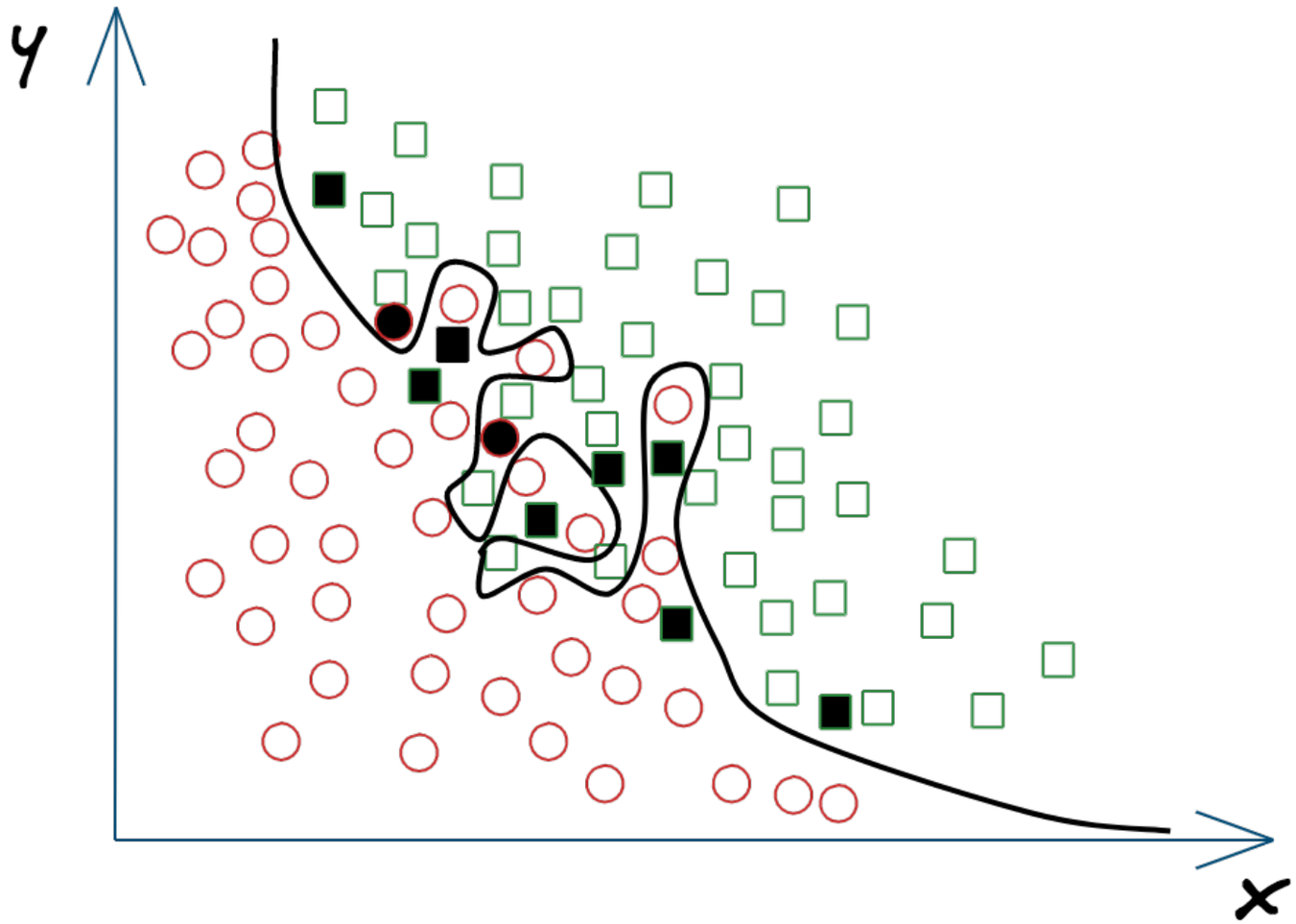
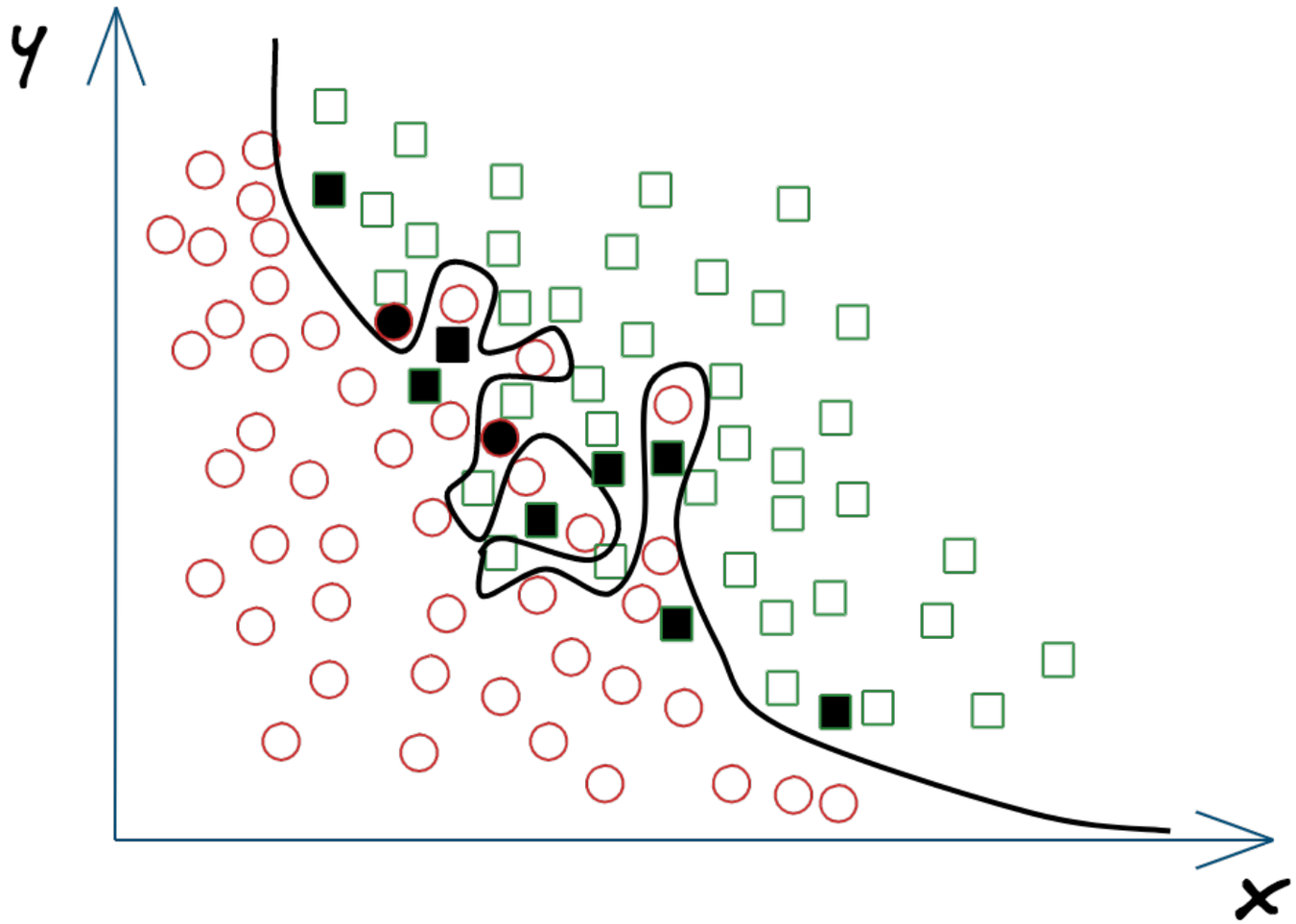


Model Selection and Cross Validation

- Example: How well will it perform on previously unseen data? Not so good! Why is that?



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- This is one of the reasons we need to evaluate our models on **unseen data** (i.e test data)

Model Selection and Cross Validation

- Let's say we want to choose between these hypothesis functions

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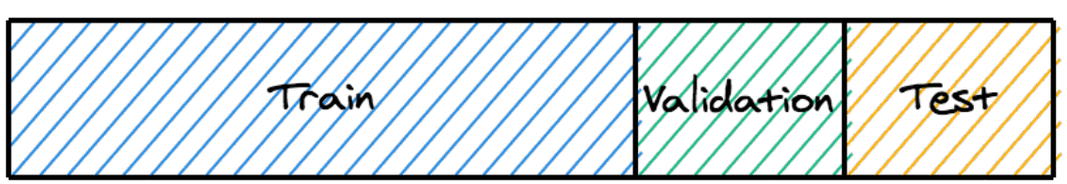
- We need to split our data to 3 parts:
  - Train, Validation, Test (usually: 60%, 20%, 20%)



Model Selection and Cross Validation

- For each of the six hypothesis functions:
  - We train the models on the **training set** to find the best set of **parameters**
  - We then evaluate the models on the **validation** set to choose the best one
  - Finally, we evaluate the **generalization** error on the **test** set

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  - **Model Assessment:** Once the model chosen, assess its generalization error on new data
- The **generalization** error needs to be evaluated on data that **hasn't been seen** by the model and that didn't serve for parameters tuning

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- The data set is divided into k subsets. Each time one of the k subsets is used as a **validation** set and the k-1 remaining are put together to form the **training** set

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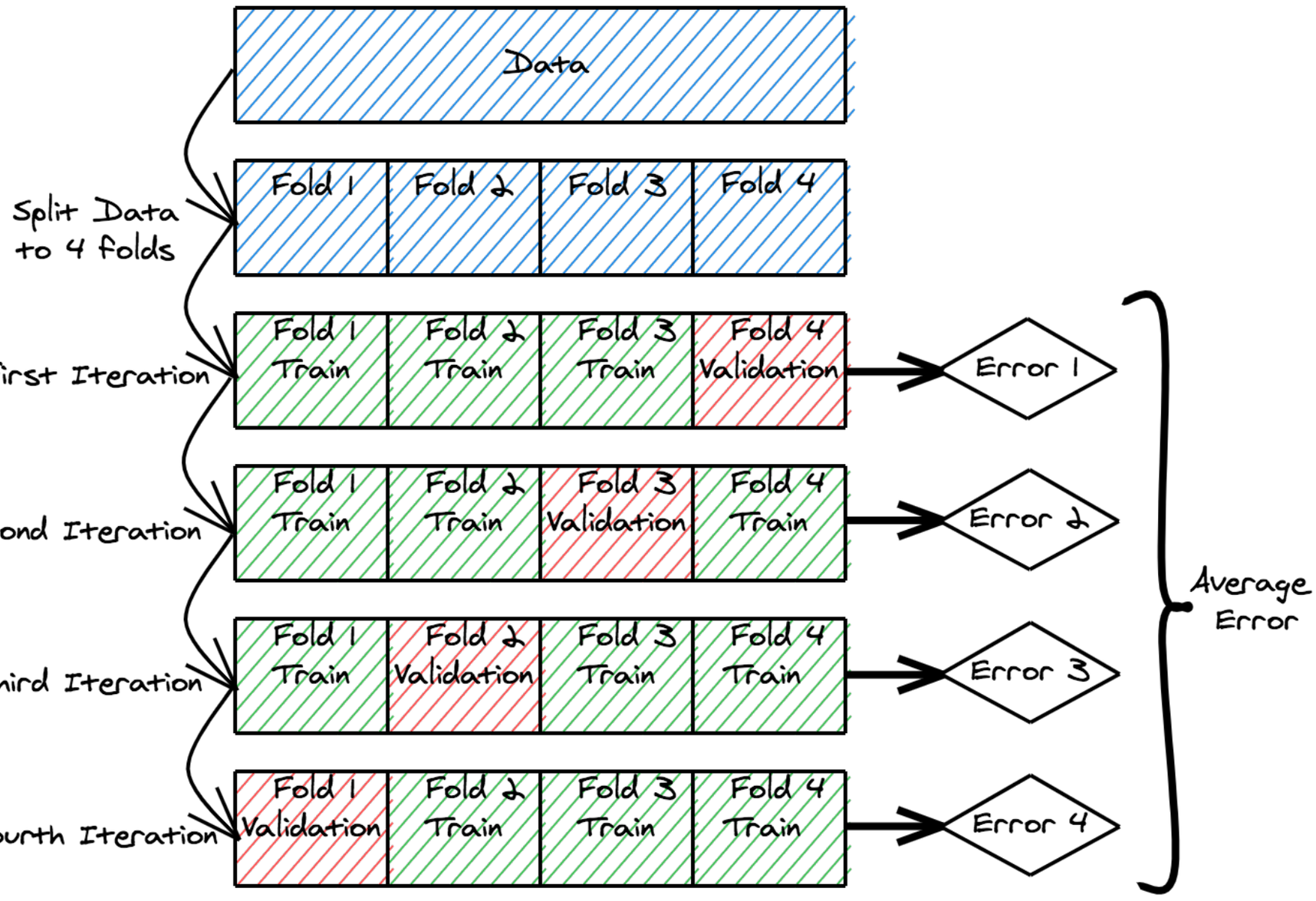
- The method is **repeated** k times, in the end we compute the **average** error across the k trials

Model Selection and Cross Validation

- Example: 4-fold cross-validation



Bias Vs Variance

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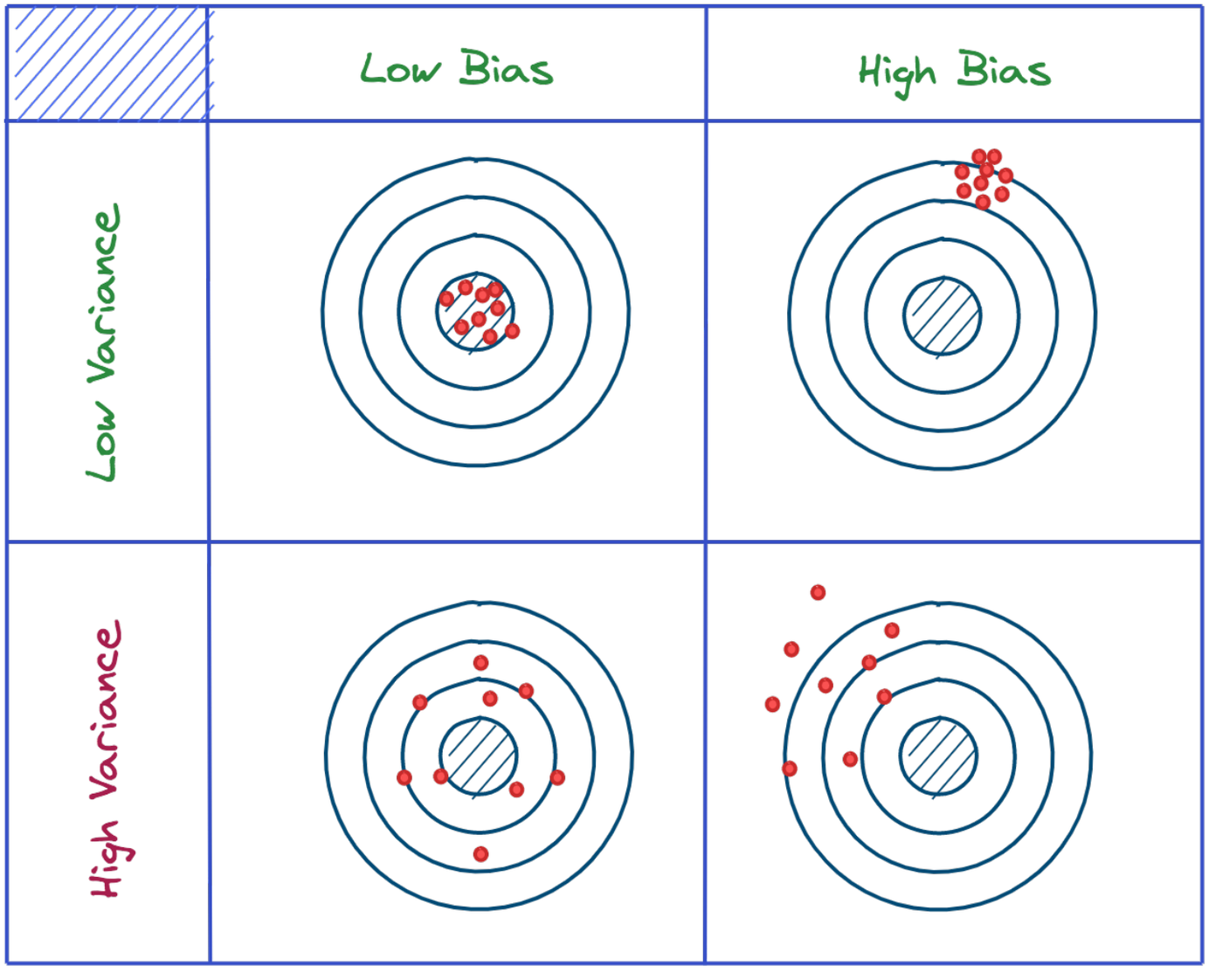
- Typically: The **more complex** the model is, the **lower the Bias**, but **the higher the Variance**. Which one should we choose?

Bias Vs Variance

- A good visualization tool for this is the bulls-eye diagram



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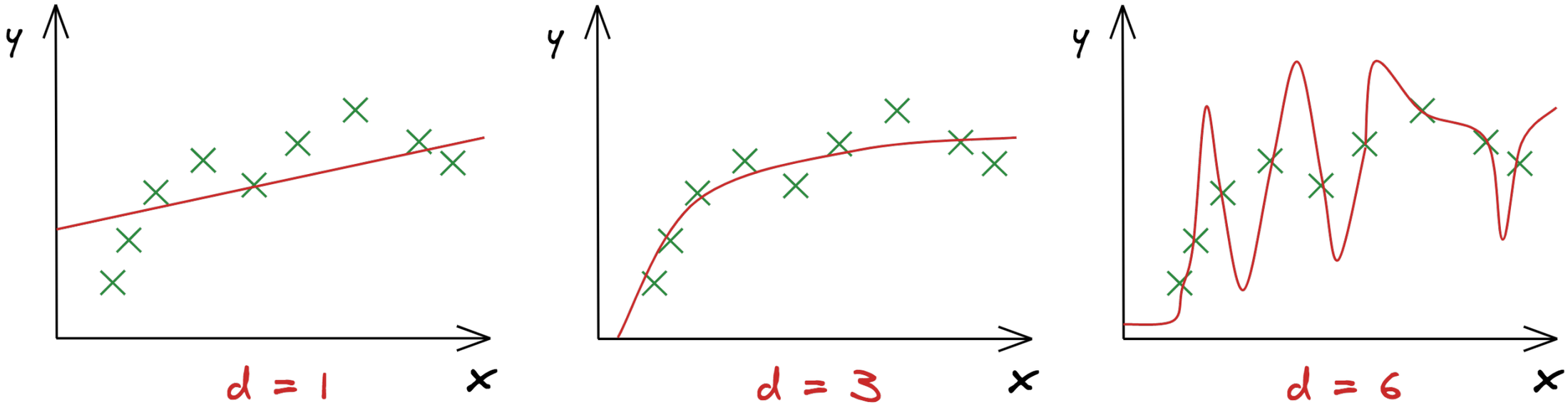
- Here the **complexity** of the model is represented by the **degree** of the polynomial (d). The higher the degree, the higher the complexity

Bias Vs Variance

- We need to carefully choose d



Small d
High Bias (underfit)

Intermediate d
Equilibrium

High d
High Variance (overfit)

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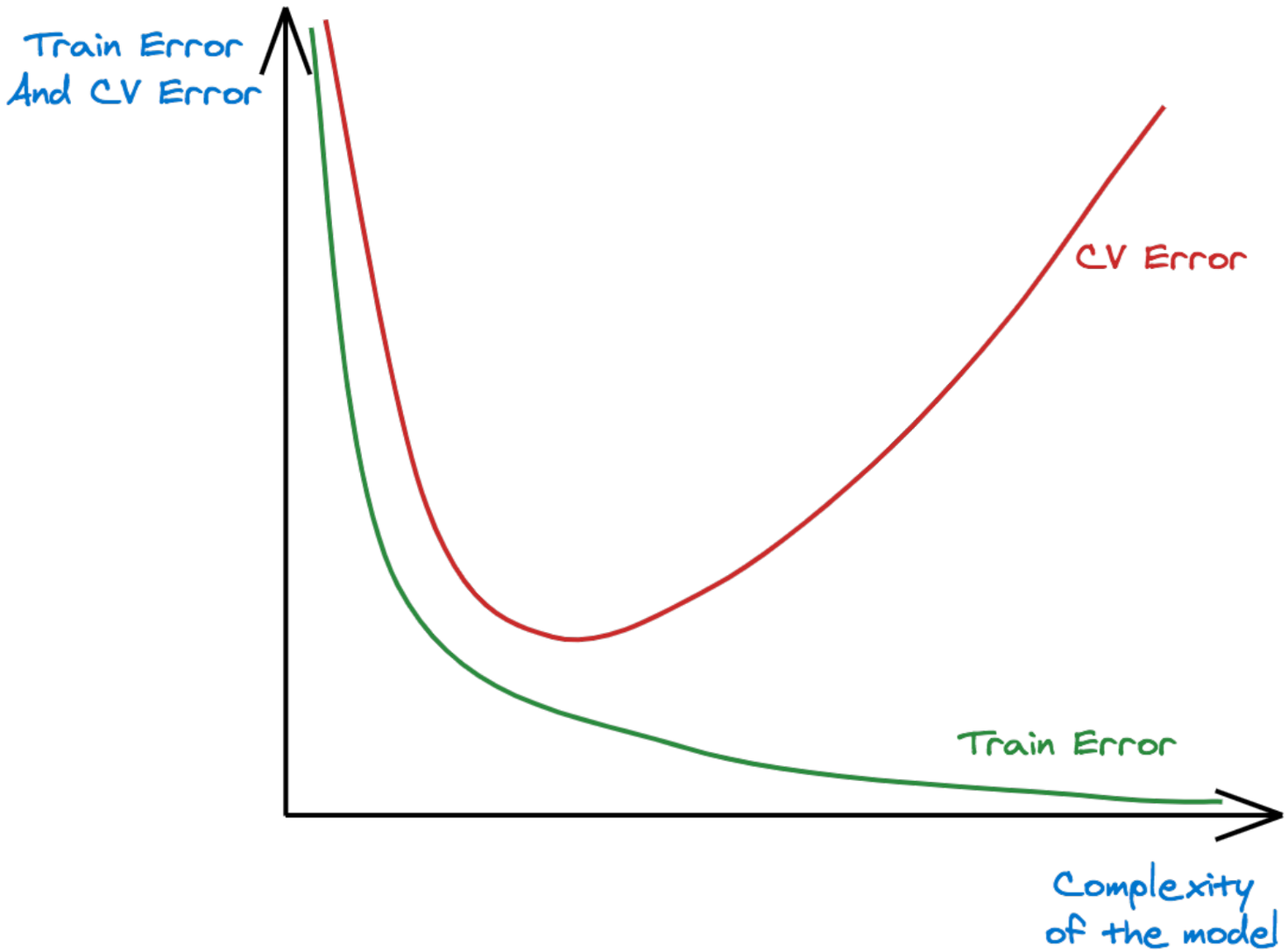

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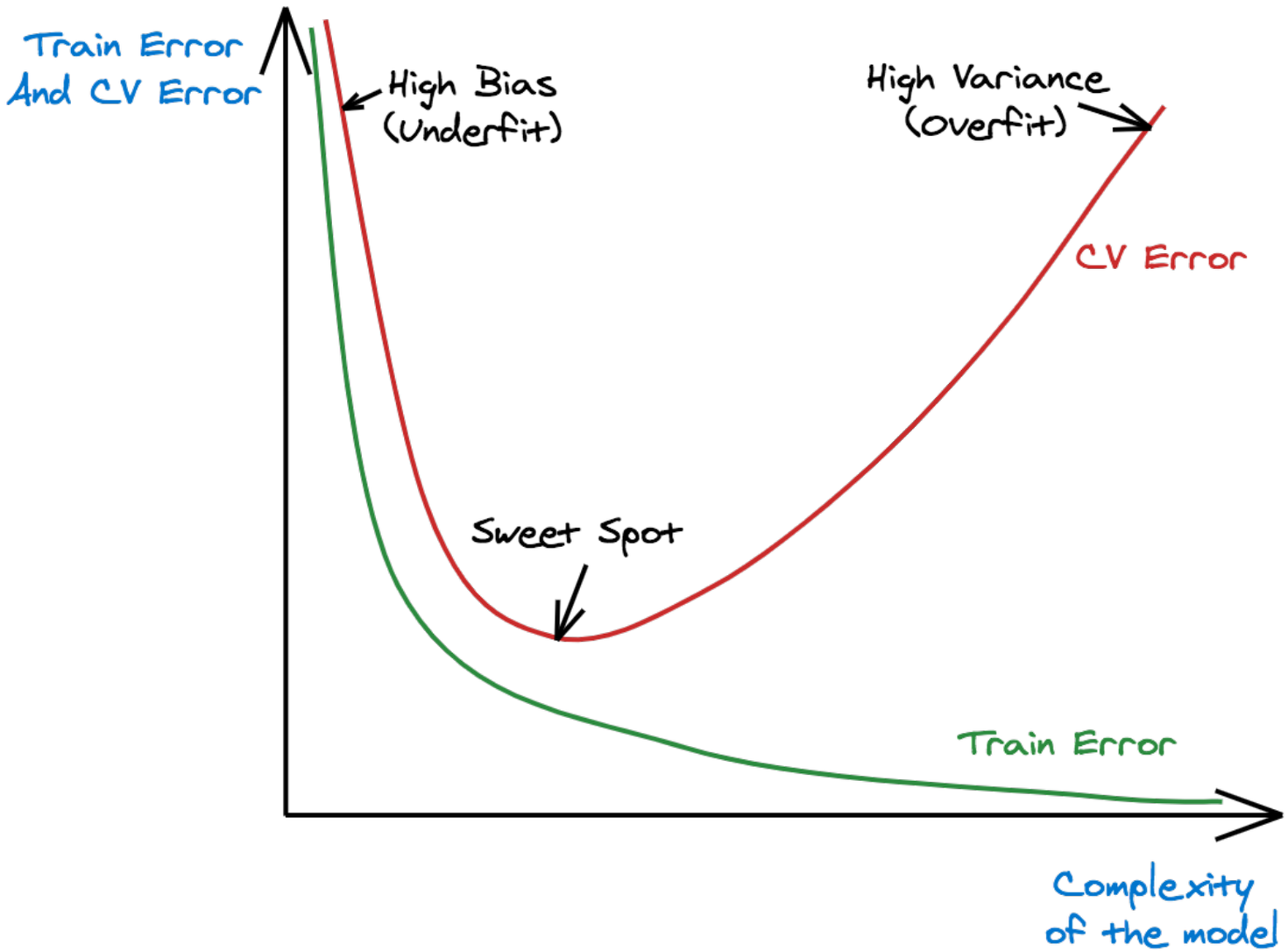

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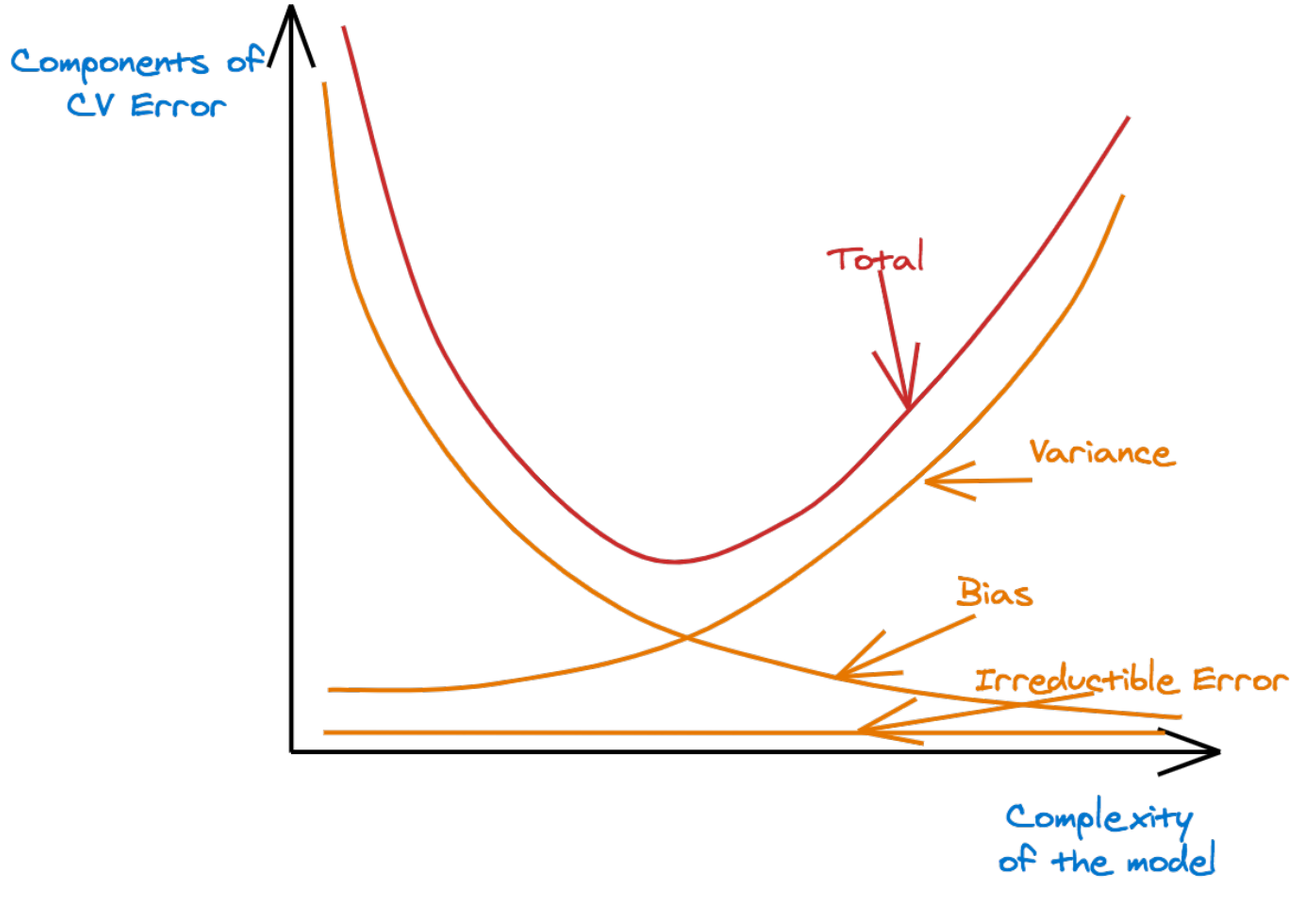

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- The principle of **Regularization** is to accept a slight increase of Bias to get a bigger decrease of Variance => **The overall error is reduced**

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- By only keeping the most important, the model is **less complex** and **more explainable**

Regularization

	Ridge	Lasso
Advantages	- Helps shrink parameters of variables that are less important - Handles well high number of parameters	- Serves as a shrinkage method - Serves as a feature selection method as unimportant features are set to 0
Inconvenients	- It helps shrink the parameters but does not set them to 0 - This leads to poor model interpretability	- It struggles when there are too many predictors - If there are two or more highly collinear variables, it will randomly select one and set the rest to 0

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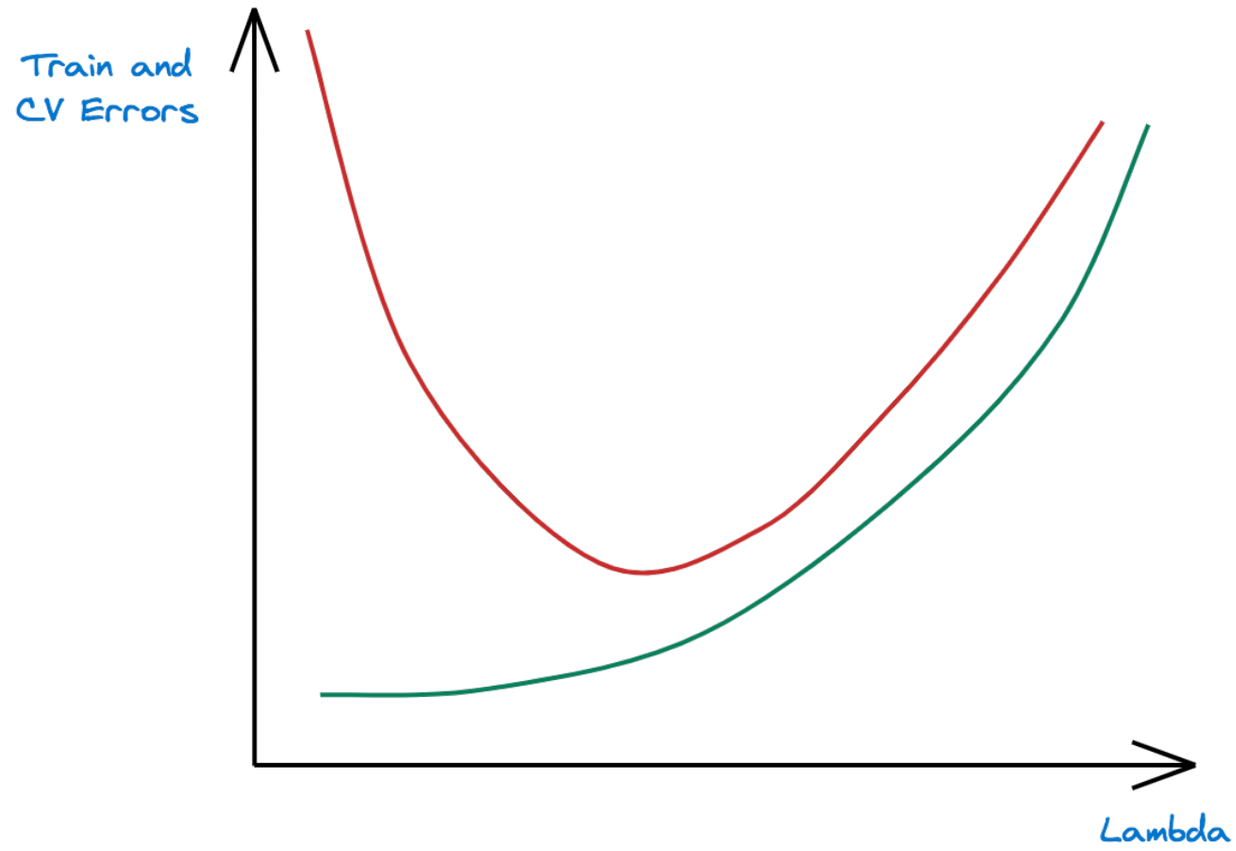
- Let's vary the parameter λ and evaluate our non-regularized loss function on the train and cross-validation sets

$$J_{train}(\theta) = \frac{1}{2m_{train}}\sum_{i=1}^{m_{train}}(h_\theta(x^{(i)}) - y^{(i)})^2$$

$$J_{cv}(\theta) = \frac{1}{2m_{cv}}\sum_{i=1}^{m_{cv}}(h_\theta(x^{(i)}) - y^{(i)})^2$$

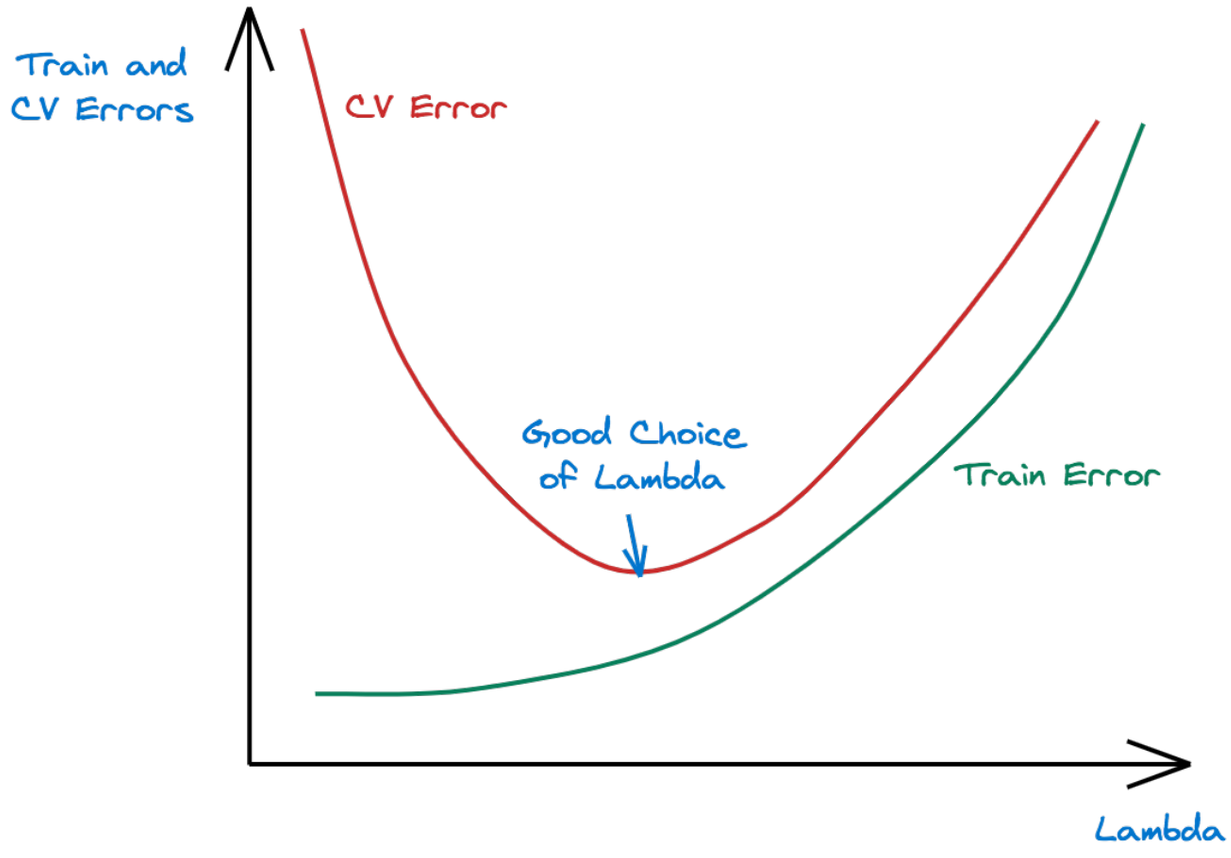
Regularization

- Which one is which? (as λ increases, what happens to train and cv errors ?)



Regularization

- As λ increases, the complexity (variance) of the model decreases, the cross validation error decreases, until a point where it starts increasing again. At some point, the decrease of variance is not enough to compensate for the bias increase



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- All these features help us **control the complexity** of our Decision Trees or Random Forest model. The more **complex** our model is, the more likely it is to be **overfitting**

Hyperparameters Tuning

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- Conceptually, Hyperparameters tuning can be seen as an **optimization loop** on top of ML model learning to find the set of hyper-parameters leading to the **lowest validation error**

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- We cannot rely on a gradient like we did for training the model. Instead, at each iteration the system must try **blindly** a new configuration in the search space, or make an educated guess of where the most interesting configuration might be

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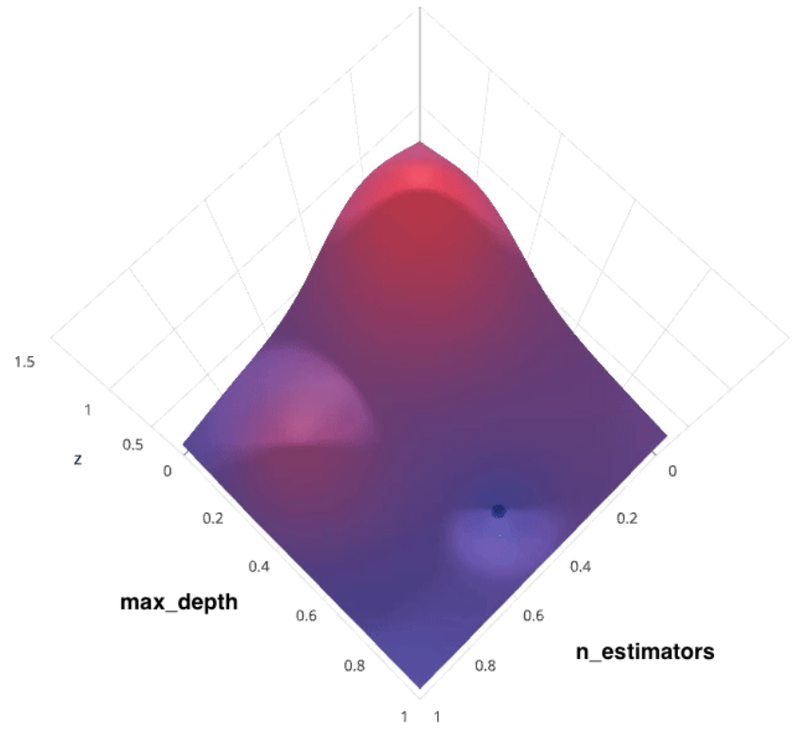
- Ideally, we would want to have an **analytical** expression of the model performance as a function of the **hyperparameters** and use a gradient descent algorithm



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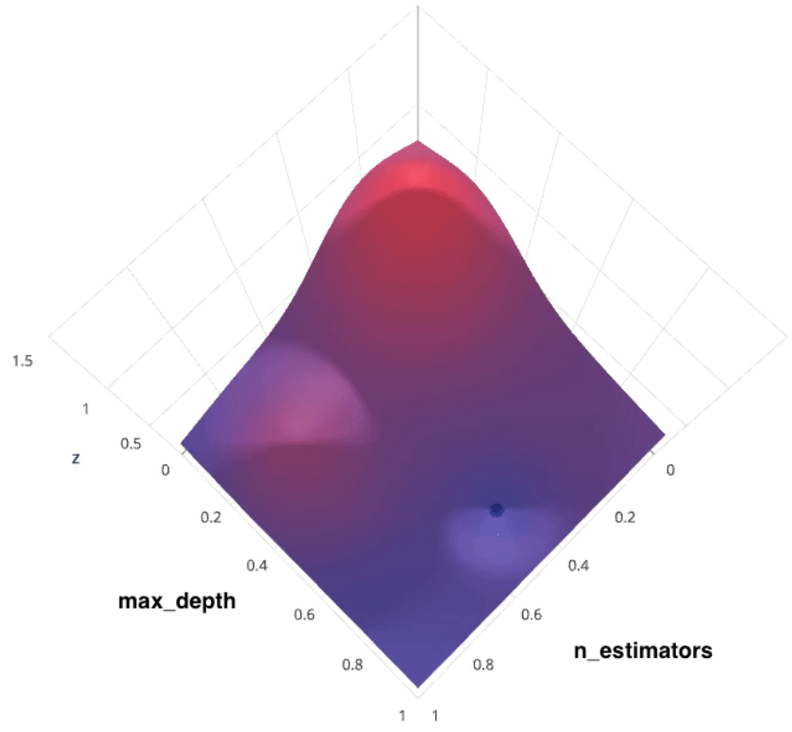

- The choice would be trivial. But we can’t have this kind of function, unless we evaluate the performance of each **possible combination**

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  - We select the **best** combination

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- Example: Random Forest Grid Search

Nb Estimators \ Max Depth	5	7	9
10	(10, 5)	(10, 7)	(10, 9)
20	(20, 5)	(20, 7)	(20, 9)
30	(30, 5)	(30, 7)	(30, 9)

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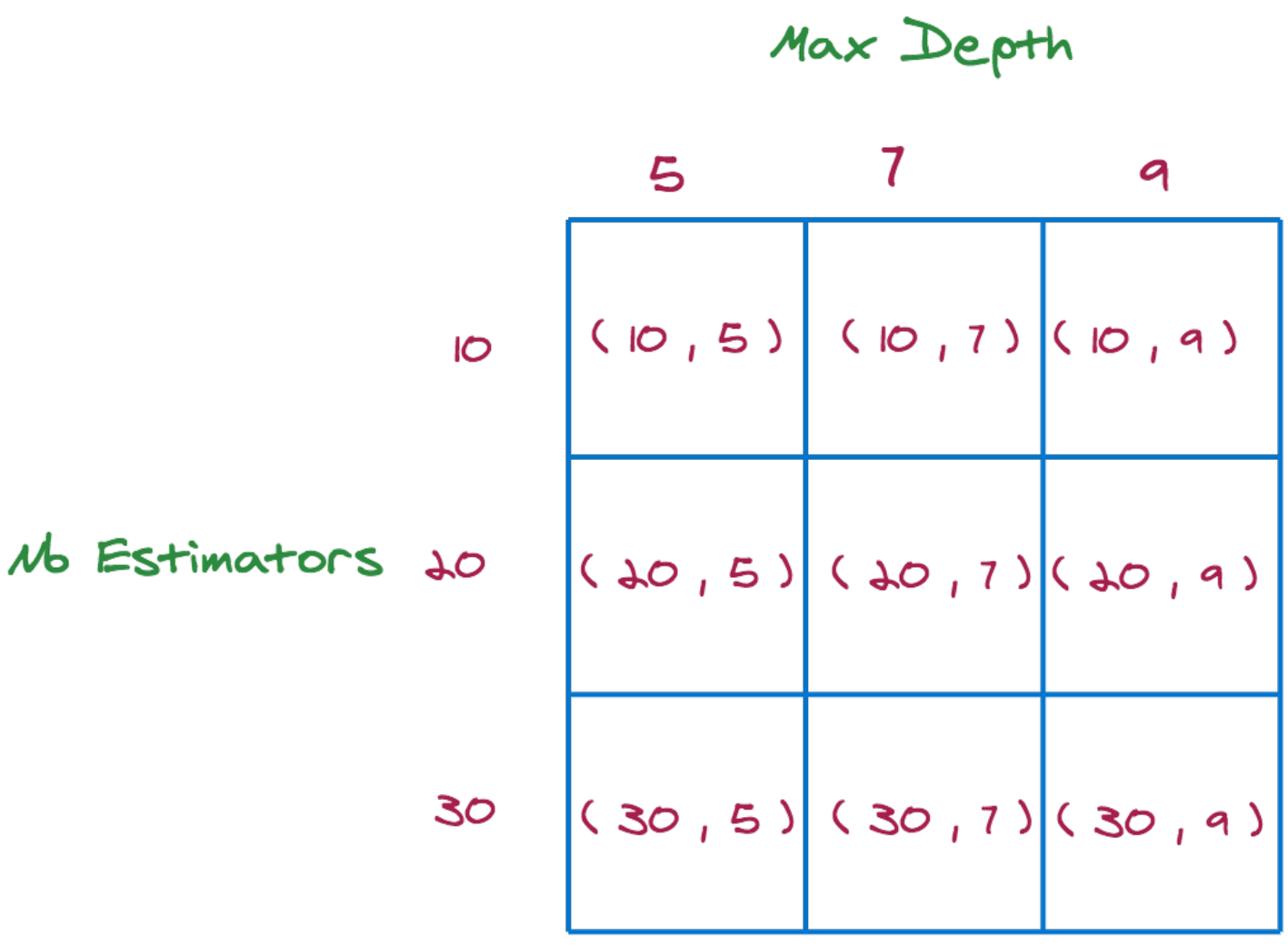
- Example: Random Forest Grid Search



- We will train and evaluate 9 models: one for each parameters' combination
- We will keep the best performing one

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Bengio & Bergstra, 2012

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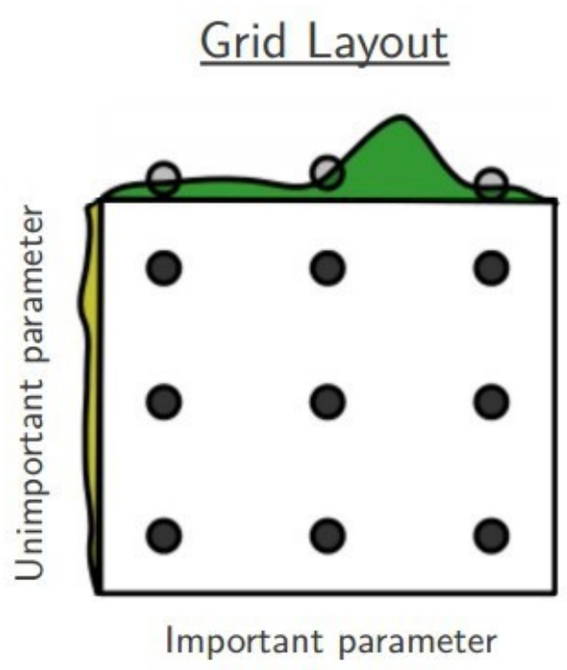

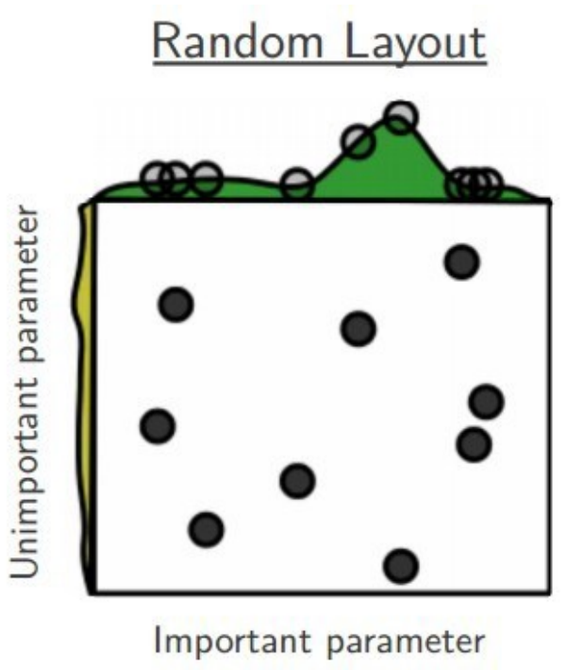

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- The major drawback is that there are **no guarantee of finding a local minimum** except if the space is thoroughly searched
- There are some **smarter** algorithms that can yield better results through **intelligent sampling**, but this is out of the scope of this class