

Supervised Learning

Fitting a response to data

Classification

- Training data: (point, class)
- Ex: Reading digits (image, {0, 1, ...9})

Regression

- Training data: (point, value)
- Ex: Predict salary (characteristics, salary)

Building a supervised model

True relationship between x and y represented by a function \mathbf{f} :

$$X \rightarrow \mathbf{f}(x) = y$$

You want to build a model \mathbf{f}' :

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Neural Networks can, in theory, represent any function.

Training and testing a model

Workflow

- **TRAINING:** Consider some of the data (training data):
 - Build a model f' which works well on it
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 - Check how f' is performing on that

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The test data is necessarily distinct from the training data in order to assess how your model generalises

Train-test split

- Usually around 70%-30% split
- Randomised for representativity
- Can be stratified if the data is imbalanced

When doing one hot encoding, what if the test set has new labels? Common source of bugs!

Evaluating a model

Loss function: Measure of performance of a specific model evaluated on a given set of points S (usually training/test points)

E.g.: Mean Squared Error (MSE) for regression:

$$L_{\text{MSE}}(\hat{f}) = \sum_{i \in S} (\hat{f}(x_i) - y_i)^2$$

Training a model = Minimising the loss

Consider a parametric model \mathbf{f}' defined by a vector of parameters β

Best β is such that the loss is minimised

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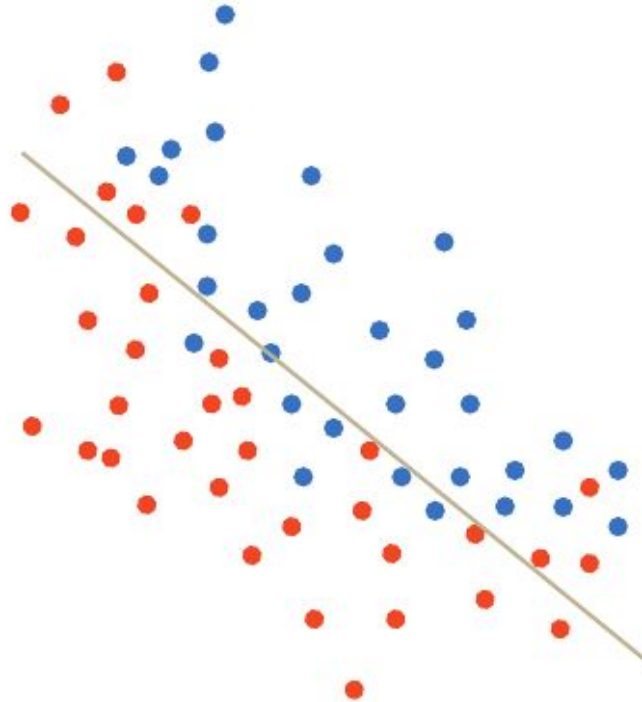
Training problem:

$$\text{Find } \beta^* \in \arg \min L(f')$$

Training and testing: the cases

- Poor on training: **underfitting**

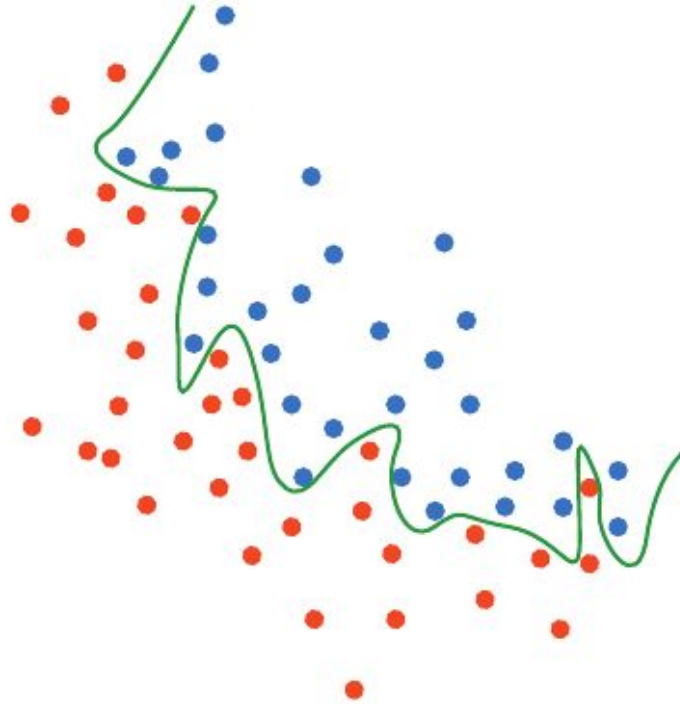
Underfitting



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Overfitting

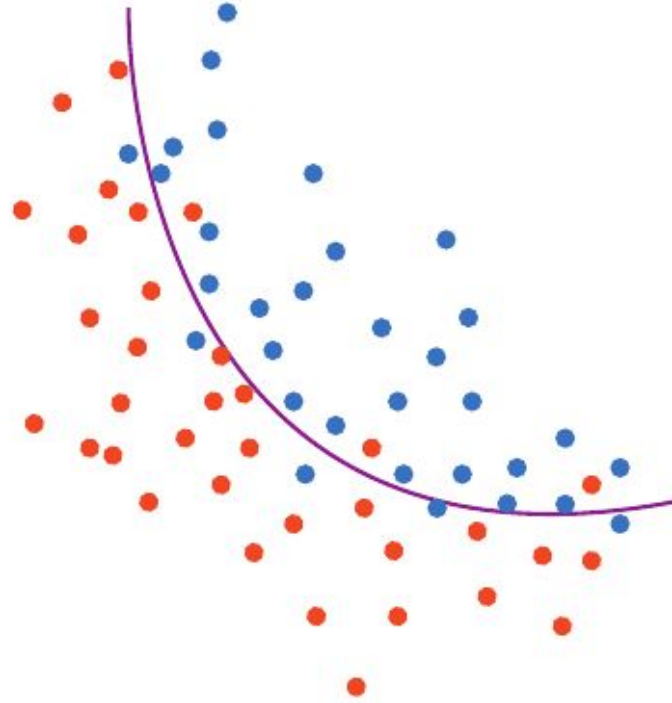


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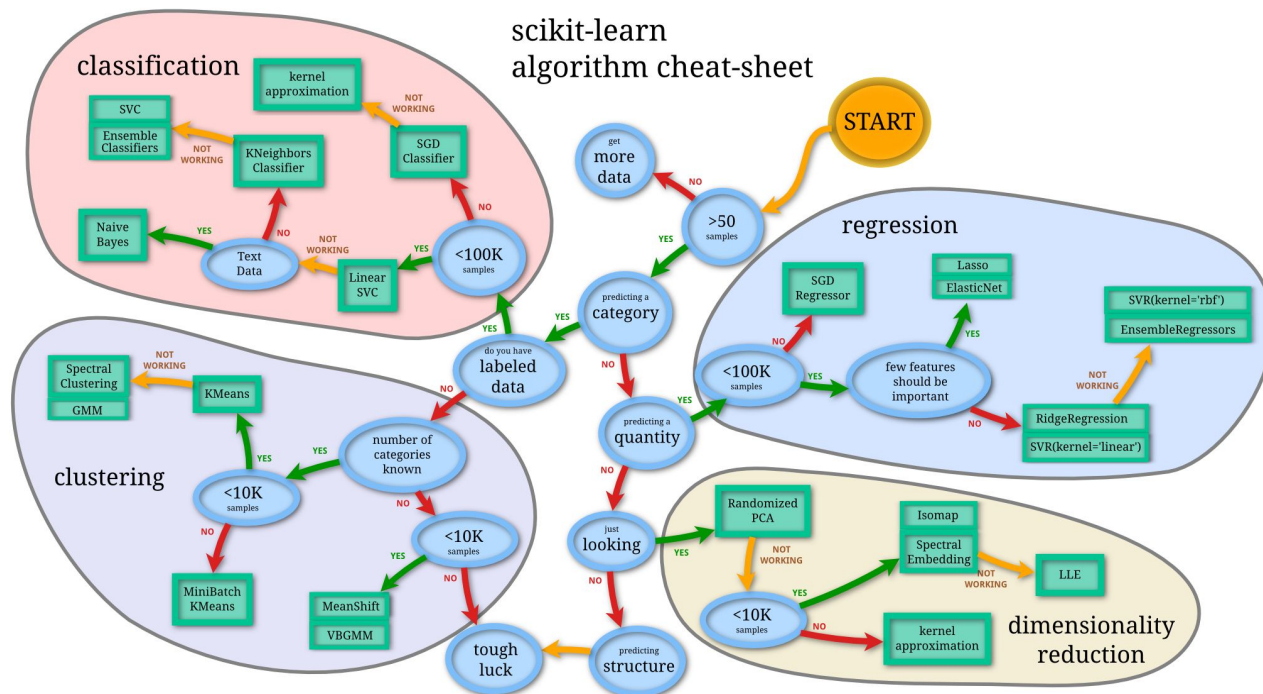
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- Good on training but poor on testing: **overfitting**
- Good on training and good on testing: **job done**

More about this later, now how do you build a model in Python?

Good fit



Scikit-learn algorithm map





Hands-on session

01-supervised_learning.ipynb
Part 1: Preparing the data

A simple classifier: K-Nearest-Neighbours

Basic Idea:

- Consider the K training points closest to a test point
- Majority vote over which class the point should belong to

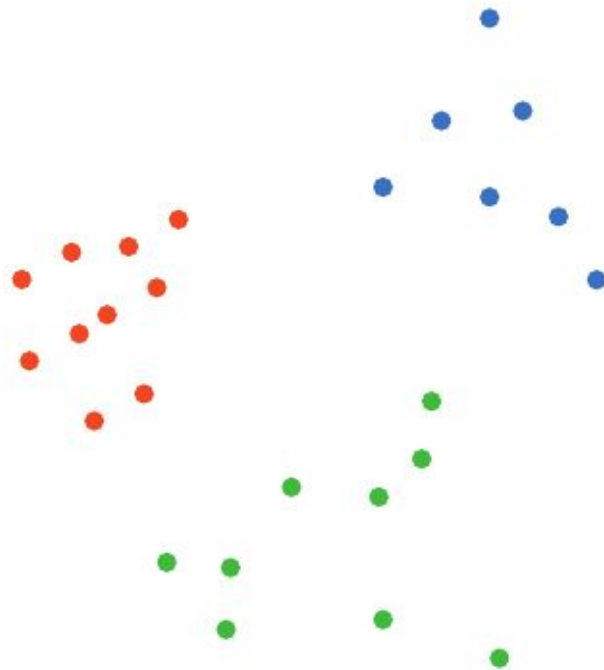
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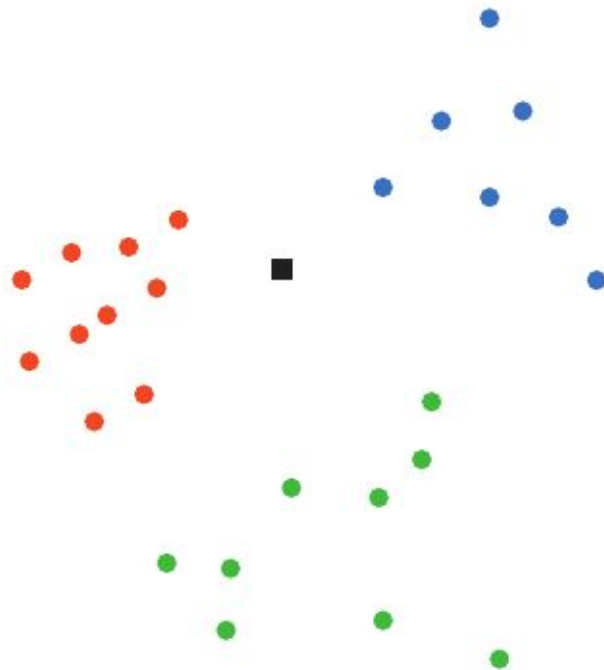
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Let's see...

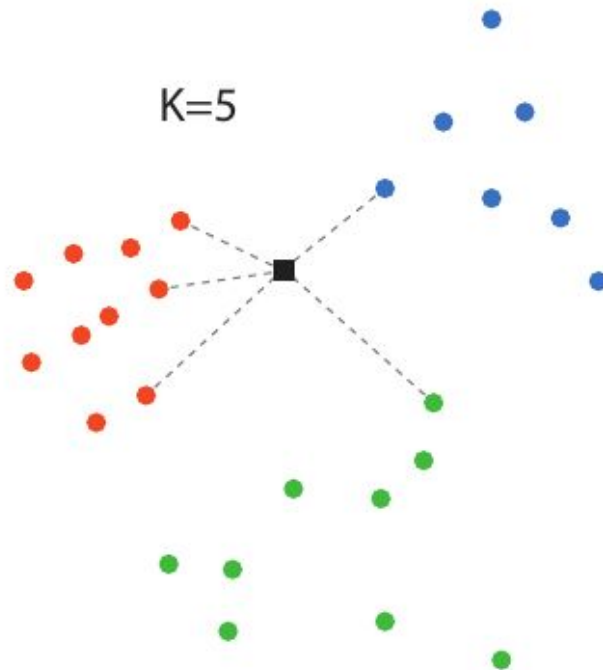
K-Nearest-Neighbours



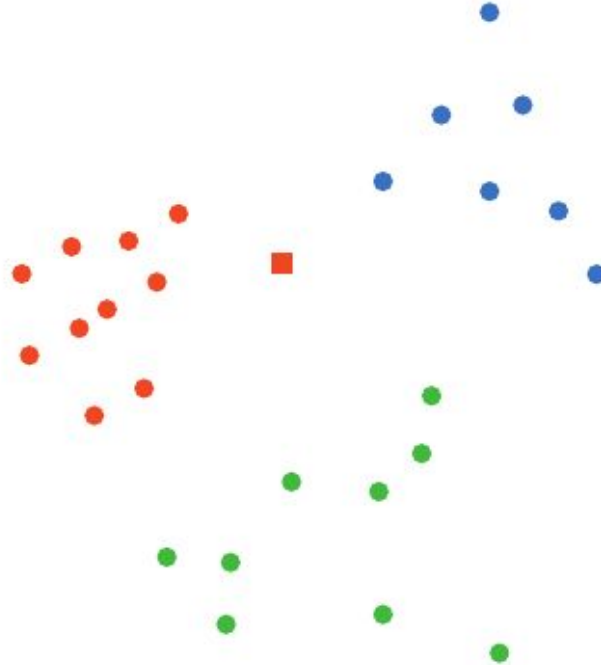
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You should only use the test set for a final assessment of the model...



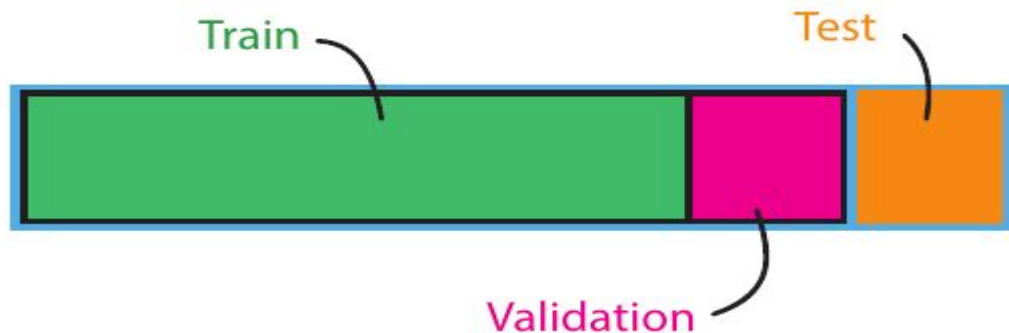
Training-Validation-Testing



1. Take a slice of the training data -> validation set
2. Apply the same procedure as before to adjust the model but using the smaller training set and validation set
3. Report performance on the untouched test set

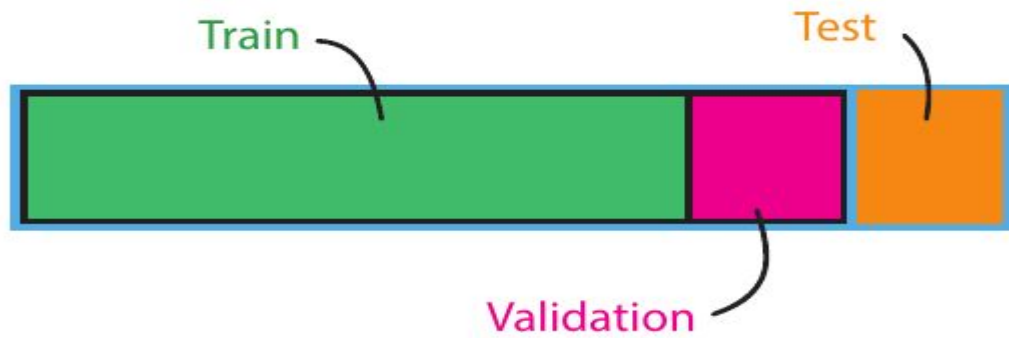
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Nice but we're not using the whole training data...

From validation to cross-validation

We would like to:

- Use something like validation to tune our model without looking at the test set
- Exploit all the data from the initial training set

WARNING: There will be a lot of K's in the following slides, those are **not** referring to the k in kNN but for k -fold cross validation.

K-fold cross validation

1. Shuffle the training set and slice it in k batches

For each model to train and evaluate:

2. Pick one slice s of the k batches
3. Use the rest of the batches to train the model
4. Compute accuracy on slice s (validation)

K-fold cross validation

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For each model to train and evaluate:

2. Pick one slice s of the k batches
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4. Compute accuracy on slice s (validation)
5. Go back to 2) and repeat for all slices
6. Report the average accuracy

Pick the model with the highest average accuracy

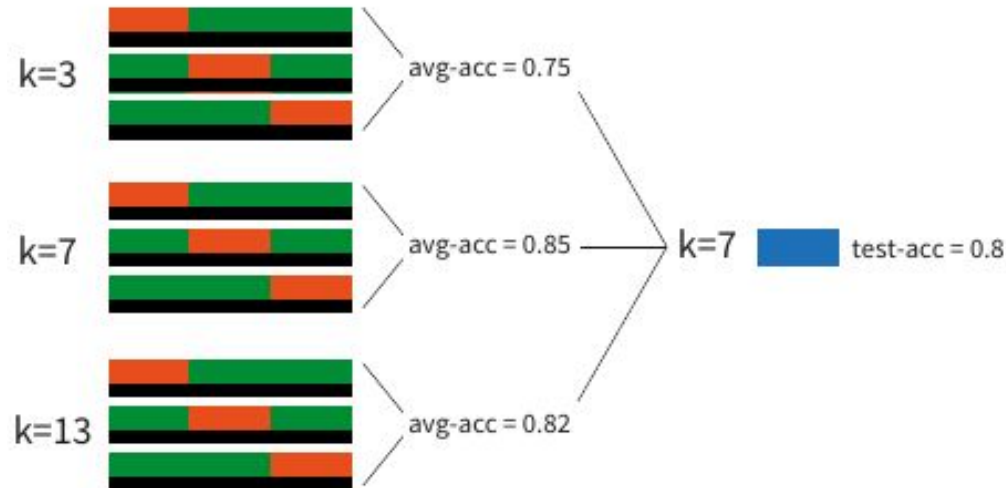
K-fold cross validation

Train-test split: 

Training (kNN)

Selection

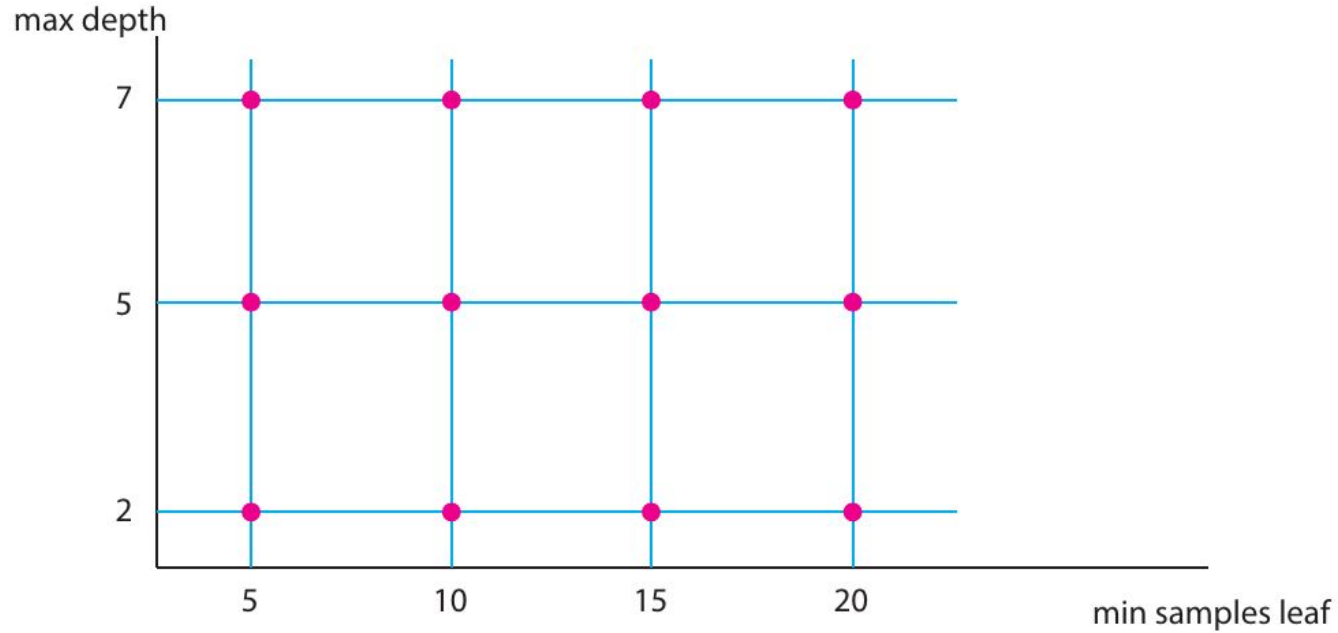
Testing



K-fold cross validation

Now that we have a way to evaluate models with different parameters, how do we choose the parameters we want to test?

Grid Search



Testing a binary classifier

On the test data, compare the predicted responses $y' = f'(x)$ to the actual response y .

		PREDICTED	
		Positive	Negative
ACTUAL	Positive	TP	FN
	Negative	FP	TN

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- Predicted Jargon from clinical trials, positive/negative defined by context
- This is the confusion matrix

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Accuracy: $(TP + TN) / N$

Sensitivity/Recall: $TP / (TP + FN)$

Precision: $TP / (TP + FP)$

The metric of importance is usually dictated by context.

Example: Fraud

- Flagging a clean transaction as fraudulent (OK)
- Not flagging a fraudulent transaction (bad)

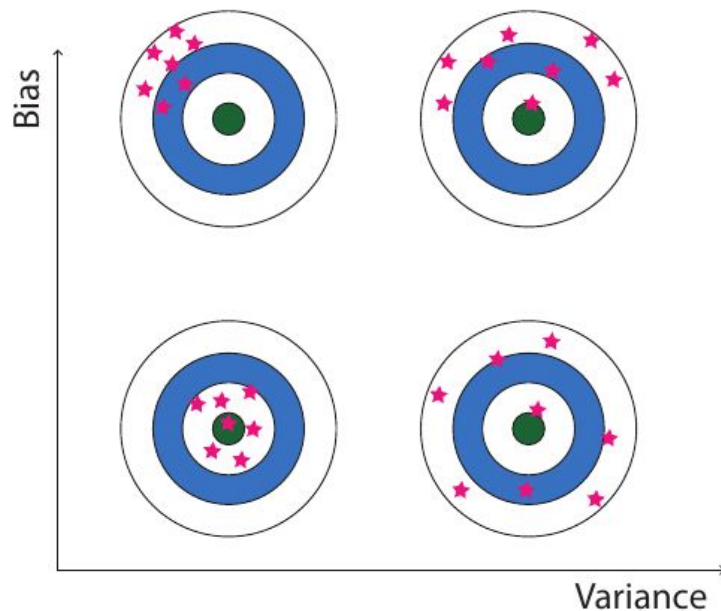


Hands-on session

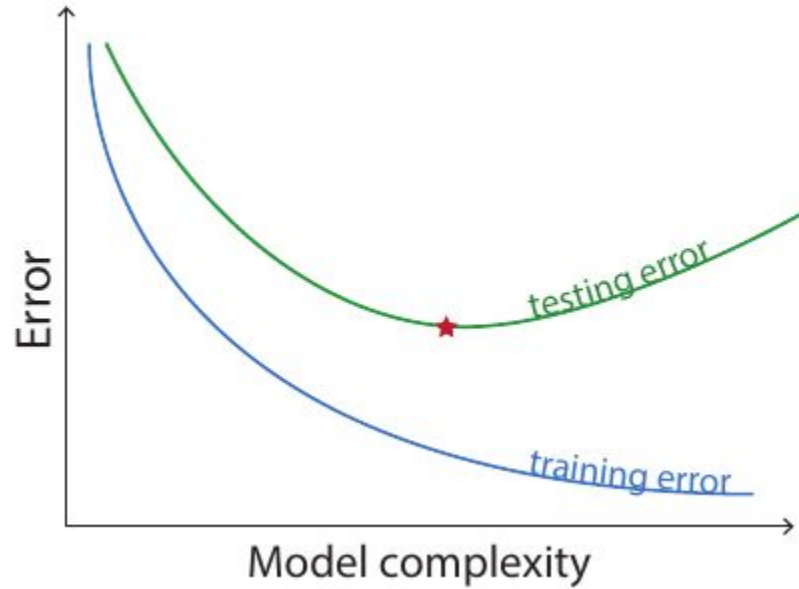
02-supervised_learning.ipynb
Part 2: Training a model

Bias and Variance

One way of visualising the performances achieved by a model is to imagine that it corresponds to a dart thrower.



Bias-Variance Tradeoff



Bias-Variance Tradeoff

