Lecture 3: Model Selection

Can I trust you?

Joaquin Vanschoren, Eindhoven University of Technology

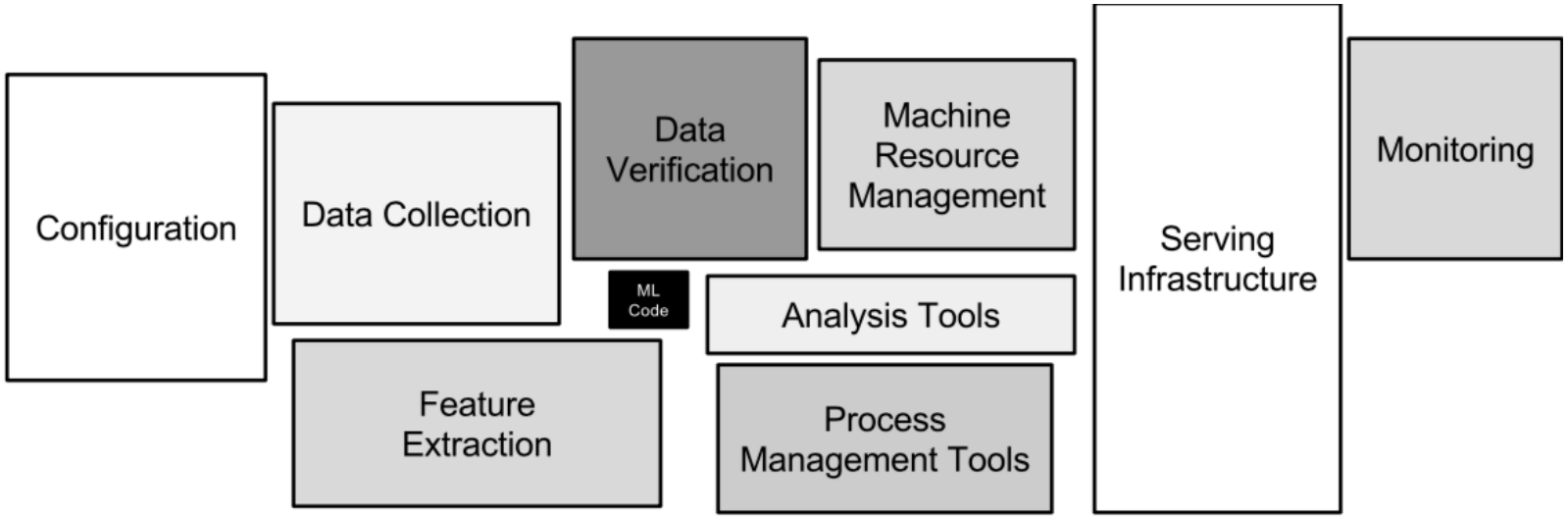
Evaluation

- To know whether we can *trust* our method or system, we need to evaluate it.
- If you cannot measure it, you cannot improve it.
- Model selection: choose between different models in a data-driven way.
- Convince others that your work is meaningful
    - Peers, leadership, clients, yourself(!)
- Keep evaluating relentlessly, adapt to changes

Designing Machine Learning systems

- Just running your favourite algorithm is usually not a great way to start
- Consider the problem at large
    - Do you want to understand phenomena or do black box modelling?
    - How to define and measure success? Are there costs involved?
    - Do you have the right data? How can you make it better?
- Build prototypes early-on to evaluate the above.

- Analyze your model's mistakes
    - Should you collect more, or additional data?
    - Should the task be reformulated?
    - Often a higher payoff than endless finetuning
- Technical debt: creation-maintenance trade-off
    - Very complex machine learning systems are hard/impossible to put into practice
    - See 'Machine Learning: The High Interest Credit Card of Technical Debt'



Only a small fraction of real-world ML systems is composed of the ML code

Real world evaluations

- Evaluate predictions, but also how outcomes improve *because of them*
- Feedback loops: predictions are fed into the inputs, e.g. as new data, invalidating models
    - Example: a medical recommendation model may change future measurements
- The signal your model found may just be an artifact of your biased data
    - When possible, try to *interpret* what your model has learned
    - See 'Why Should I Trust You?' by Marco Ribeiro et al.

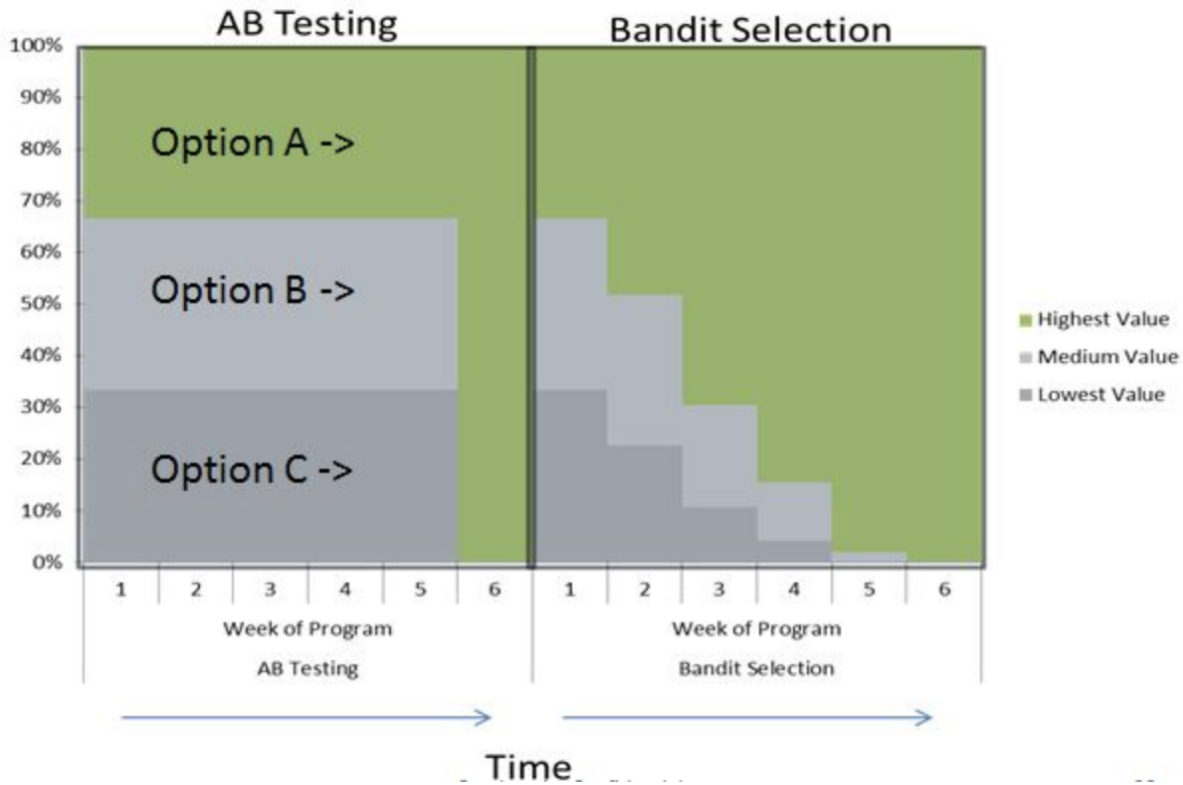
(a) Husky classified as wolf

(b) Explanation

- Adversarial situations (e.g. spam filtering) can subvert your predictions
- Do A/B testing (or bandit testing) to evaluate algorithms in the wild

A/B and bandit testing

- Test a single innovation (or choose between two models)
- Have most users use the old system, divert small group to new system
- Evaluate and compare performance
- Bandit testing: smaller time intervals, direct more users to currently winning system

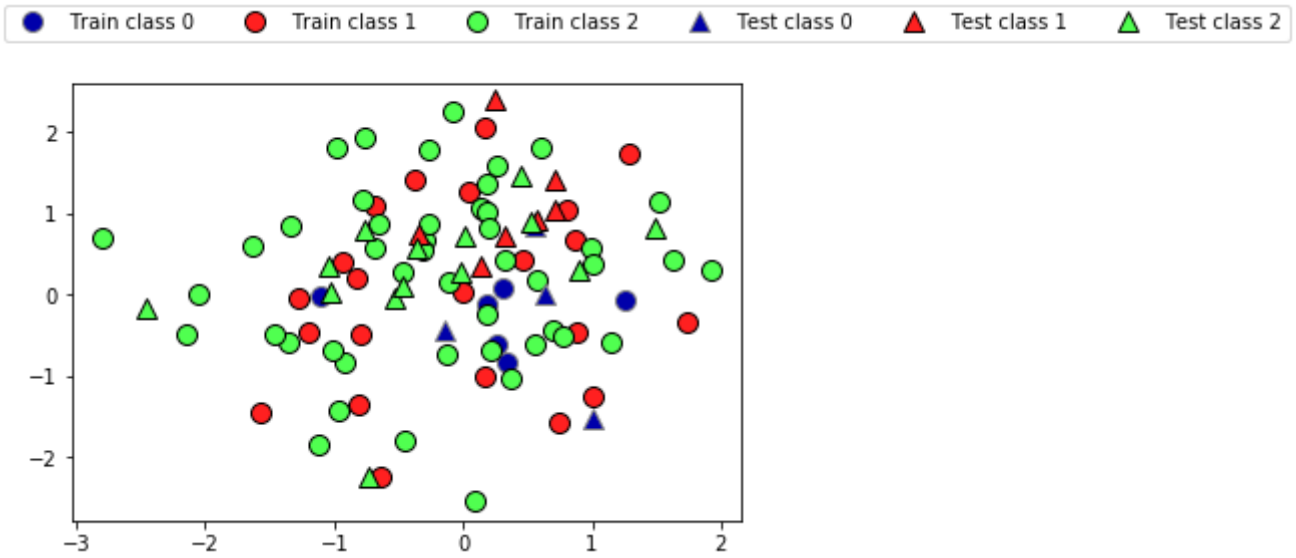


Performance estimation techniques

- We do not have access to future observations
- Always evaluate models *as if they are predicting the future*
- Set aside data for objective evaluation
    - How?

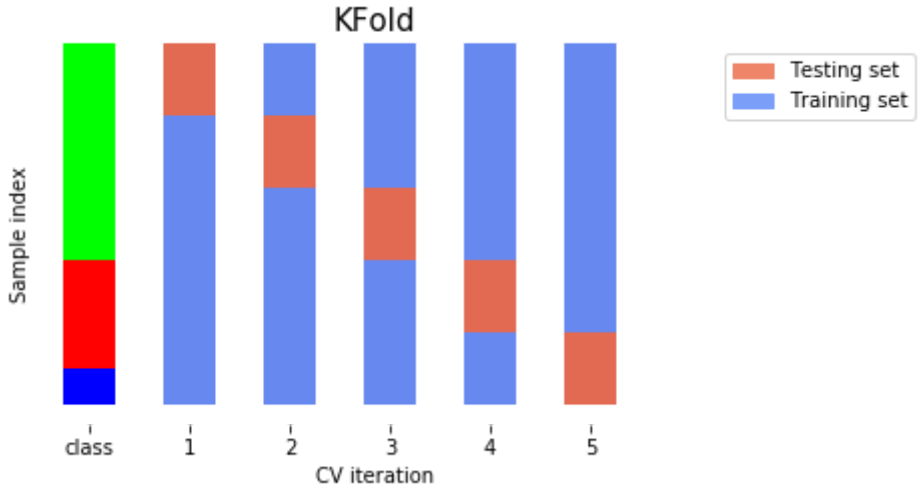
The holdout (simple train-test split)

- *Randomly* split data (and corresponding labels) into training and test set (e.g. 75%-25%)
- Train (fit) a model on the training data, score on the test data



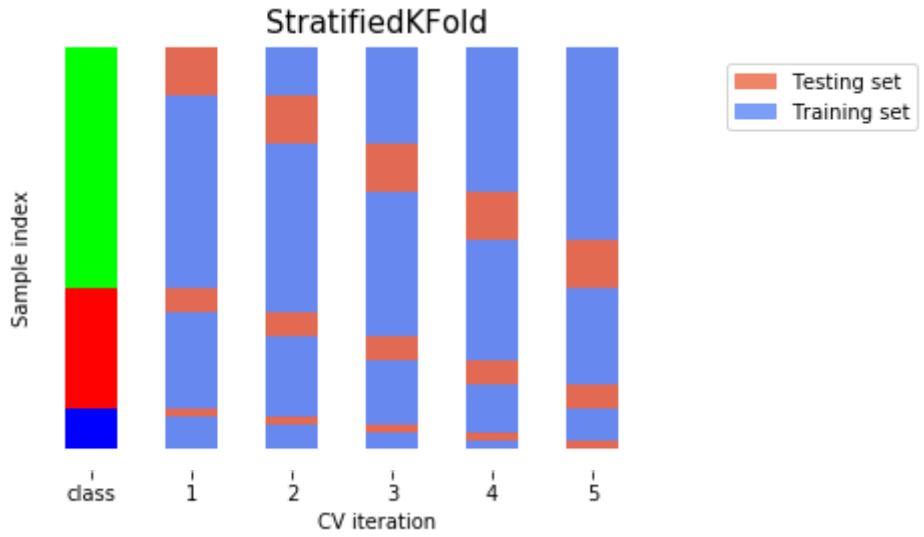
K-fold Cross-validation

- Each random split can yield very different models (and scores)
    - e.g. all easy (of hard) examples could end up in the test set
- Split data (randomly) into *k* equal-sized parts, called *folds*
    - Create *k* splits, each time using a different fold as the test set
- Compute *k* evaluation scores, aggregate afterwards (e.g. take the mean)
- Examine the score variance to see how *sensitive* (unstable) models are
- Reduces sampling bias by testing on every point exactly once
- Large *k* gives better estimates (more training data), but is expensive



Stratified K-Fold cross-validation

- If the data is *unbalanced*, some classes have many fewer samples
- Likely that some classes are not present in the test set
- Stratification: *proportions* between classes are conserved in each fold
    - Order examples per class
    - Separate the samples of each class in k sets (strata)
    - Combine corresponding strate into folds



Can you explain this result?

```
kfold = KFold(n_splits=3)
print("Cross-validation scores KFold(n_splits=3):\n{}".format(
      cross_val_score(logreg, iris.data, iris.target, cv=kfold)))
```

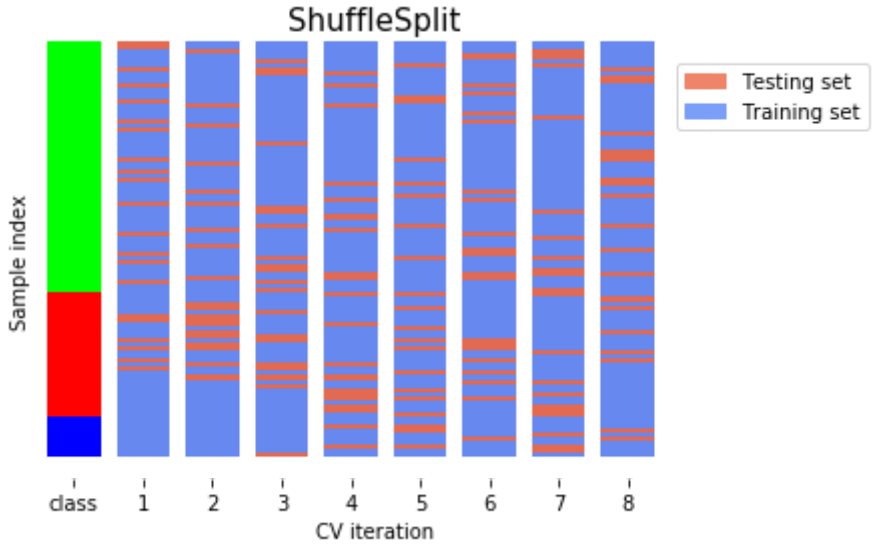
```
Cross-validation scores KFold(n_splits=3):
[0. 0. 0.]
```

Leave-One-Out cross-validation

- *k* fold cross-validation with *k* equal to the number of samples
- Completely unbiased (in terms of data splits), but computationally expensive
- But: generalizes *less* well towards unseen data
    - The training sets are correlated (overlap heavily)
    - Overfits on the data used for (the entire) evaluation
    - A different sample of the data can yield different results
- Recommended only for small datasets

Shuffle-Split cross-validation

- Additionally shuffles the data (only do this when the data is not ordered)
- Samples a number of samples (`train_size`) randomly as the training set
- Can also use a smaller (`test_size`), handy when using very large datasets

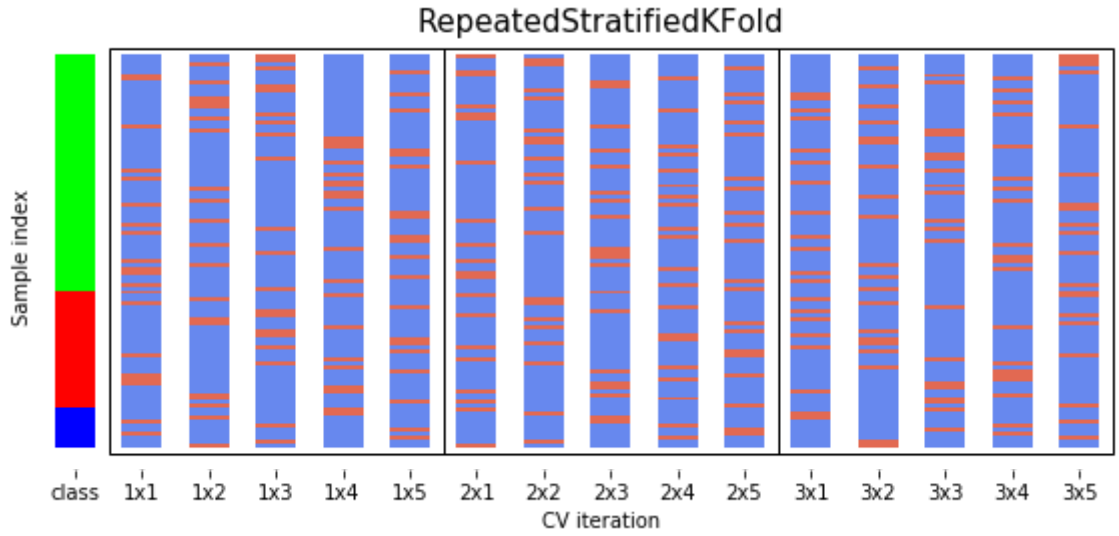


Note: this is related to *bootstrapping*:

- Sample n (total number of samples) data points, with replacement, as training set (the bootstrap)
- Use the unsampled (out-of-bootstrap) samples as the test set
- Repeat `n_iter` times, obtaining `n_iter` scores
- Not supported in scikit-learn, only approximated
    - Use Shuffle-Split with `train_size=0.66`, `test_size=0.34`
    - You can prove that bootstraps include 66% of all data points on average

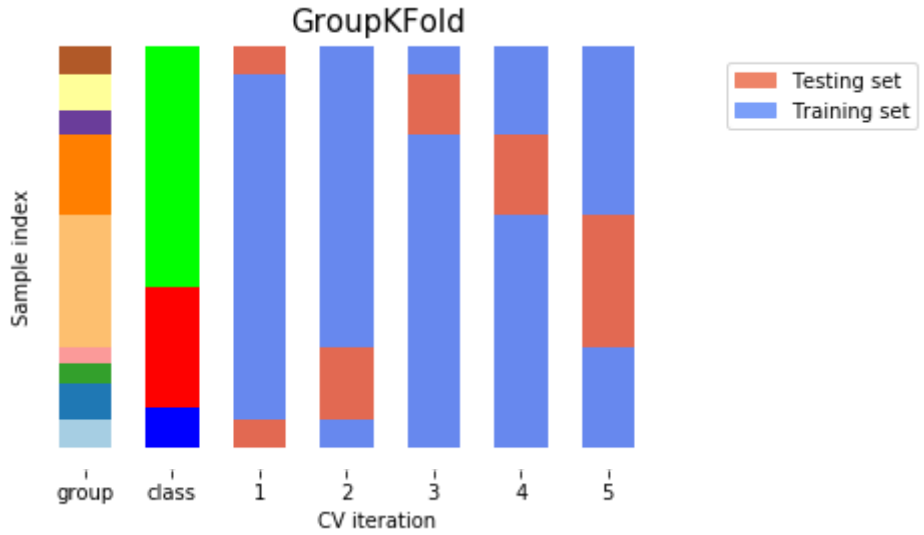
Repeated cross-validation

- Cross-validation is still biased in that the initial split can be made in many ways
- Repeated, or n-times-k-fold cross-validation:
    - Shuffle data randomly, do k-fold cross-validation
    - Repeat n times, yields n times k scores
- Unbiased, very robust, but n times more expensive



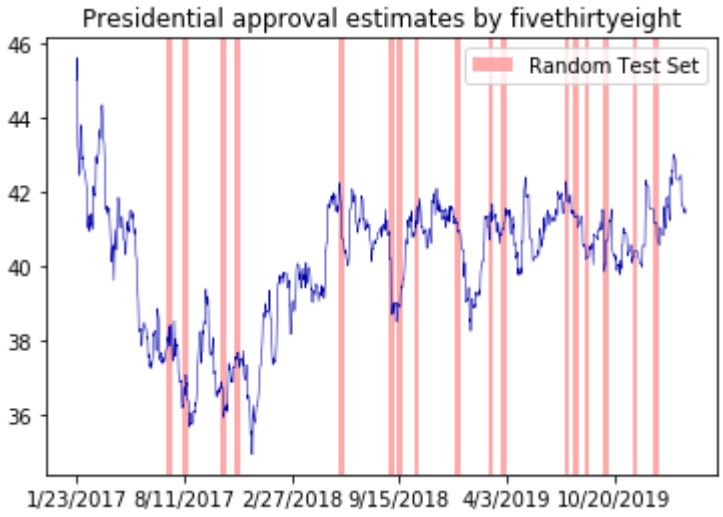
Cross-validation with groups

- Sometimes the data contains inherent groups:
  - Multiple samples from same patient, images from same person,...
- With normal cross-validation, data from the same person may end up in the training *and* test set
- We want to measure how well the model generalizes to *other* people
- Make sure that data from one person are in *either* the train or test set
  - This is called *grouping* or *blocking*
  - Leave-one-subject-out cross-validation: test set for each subject



Time series

When the data is ordered, random test sets are not a good idea



Time series

- Test-then-train (prequential evaluation)
  - Every new sample is evaluated on once, then added to the training set
  - Can also be done in batches (of n samples at a time)
- `TimeSeriesSplit`
  - In the kth split, the first k folds are used as the train set and the (k+1)th fold as the test set
  - Can also be done with a maximum training set size: more robust against concept drift

Choosing a performance estimation procedure

No strict rules, only guidelines:

- Always use stratification for classification (sklearn does this by default)
- Use holdout for very large datasets (e.g. >1.000.000 examples)
    - Or when learners don't always converge (e.g. deep learning)
- Choose *k* depending on dataset size and resources
    - Use leave-one-out for small datasets (e.g. <500 examples)
    - Use cross-validation otherwise
        - Most popular (and theoretically sound): 10-fold CV
        - Literature suggests 5x2-fold CV is better
- Use grouping or leave-one-subject-out for grouped data
- Use train-then-test for time series

Evaluation Metrics and scoring

Keep the end-goal in mind

Evaluation vs Optimization

- Each algorithm optimizes a given objective function (on the training data)
    - E.g. remember L2 loss in Ridge regression

$$\mathcal{L}_{ridge} = \sum_i (y_i - \sum_j x_{i,j} w_j)^2 + \alpha \sum_i w_i^2$$

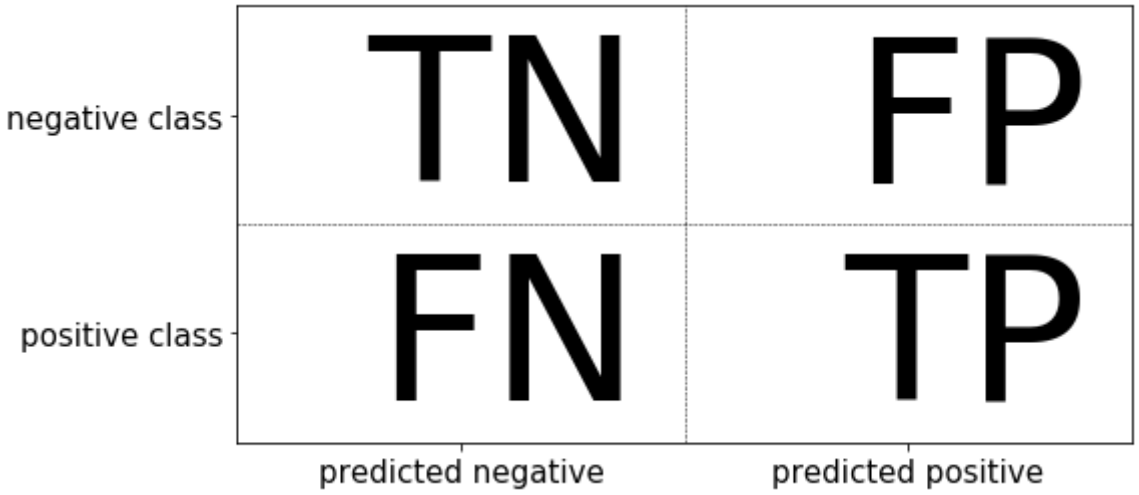
- The choice of function is limited by what can be efficiently optimized
    - E.g. gradient descent requires a differentiable loss function
- However, we *evaluate* the resulting model with a score that makes sense **in the real world**
    - E.g. percentage of correct predictions (on a test set)
- We also tune the algorithm's hyperparameters to maximize that score

Binary classification

- We have a positive and a negative class
- 2 different kind of errors:
    - False Positive (type I error): model predicts positive while the true label is negative
    - False Negative (type II error): model predicts negative while the true label is positive
- They are not always equally important
    - Which side do you want to err on for a medical test?

Confusion matrices

- We can represent all predictions (correct and incorrect) in a confusion matrix
    - n by n array (n is the number of classes)
    - Rows correspond to true classes, columns to predicted classes
    - Each entry counts how often a sample that belongs to the class corresponding to the row was classified as the class corresponding to the column.
    - For binary classification, we label these true negative (TN), true positive (TP), false negative (FN), false positive (FP)



Predictive accuracy

- Accuracy is one of the measures we can compute based on the confusion matrix:

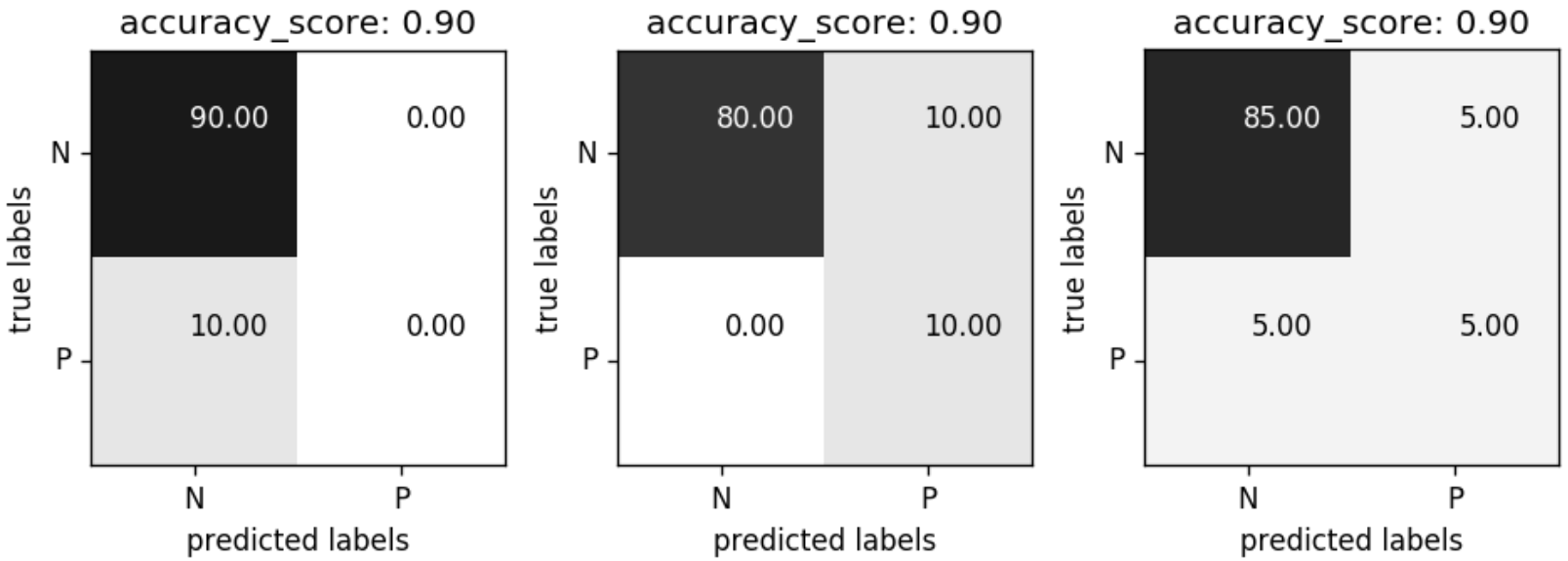
$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}}$$

- In sklearn: use `confusion_matrix` and `accuracy_score` from `sklearn.metrics`.
- Accuracy is also the default evaluation measure for classification

```
confusion_matrix(y_test, y_pred):
 [[48  5]
 [ 5 85]]
accuracy_score(y_test, y_pred):  0.9300699300699301
model.score(X_test, y_test):  0.9300699300699301
```

The problem with accuracy: imbalanced datasets

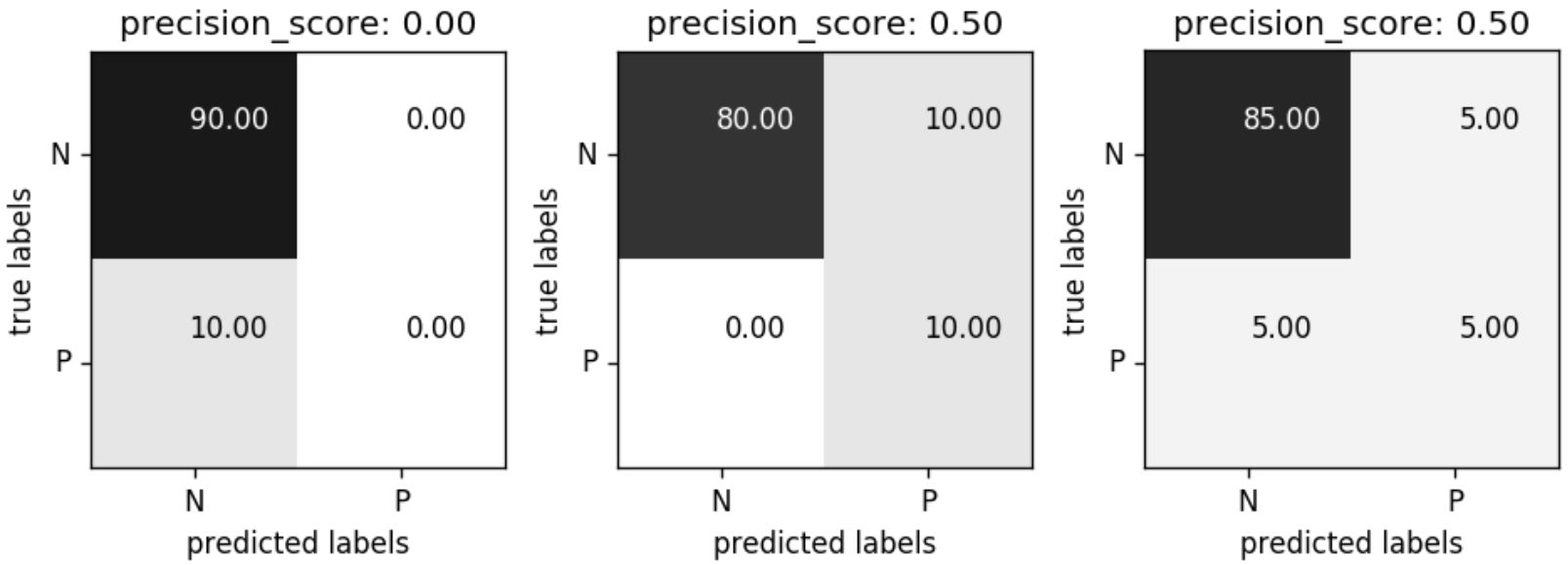
- The type of error plays an even larger role if the dataset is imbalanced
  - One class is much more frequent than the other, e.g. credit fraud
  - Is a 99.99% accuracy good enough?
- Are these three models really equally good?



Precision is used when the goal is to limit FPs

- Clinical trails: you only want to test drugs that really work
- Search engines: you want to avoid bad search results

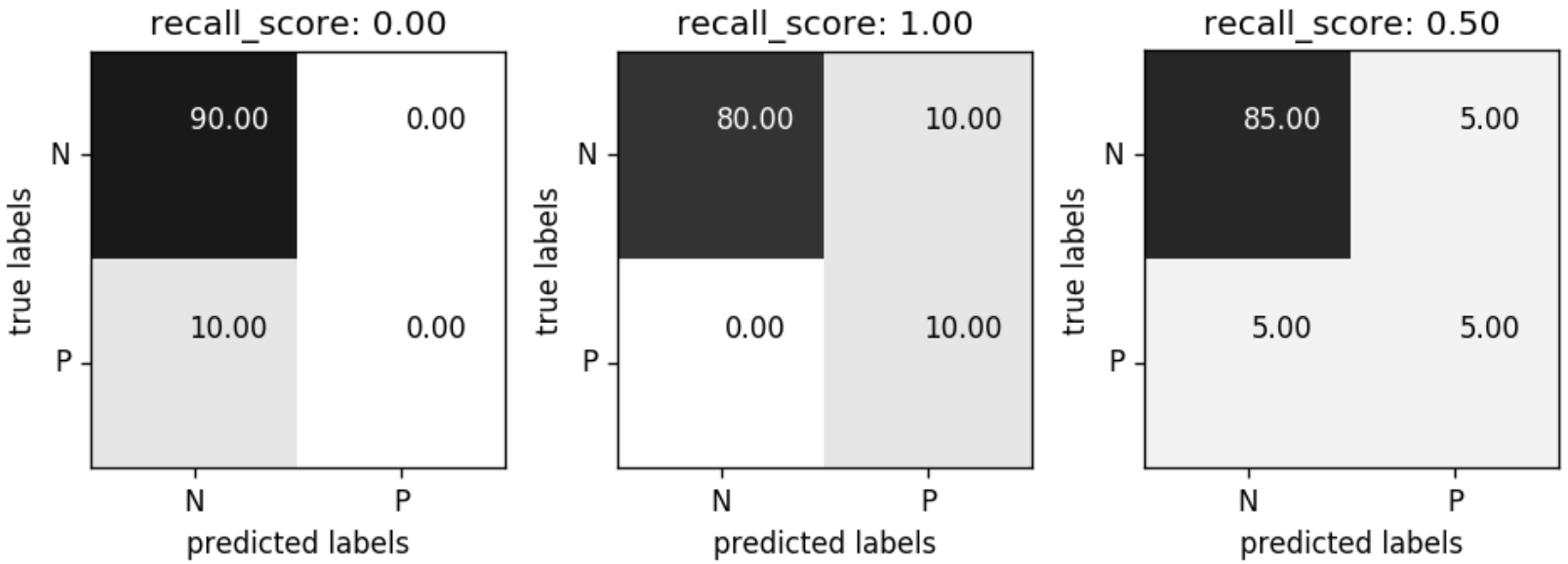
$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$



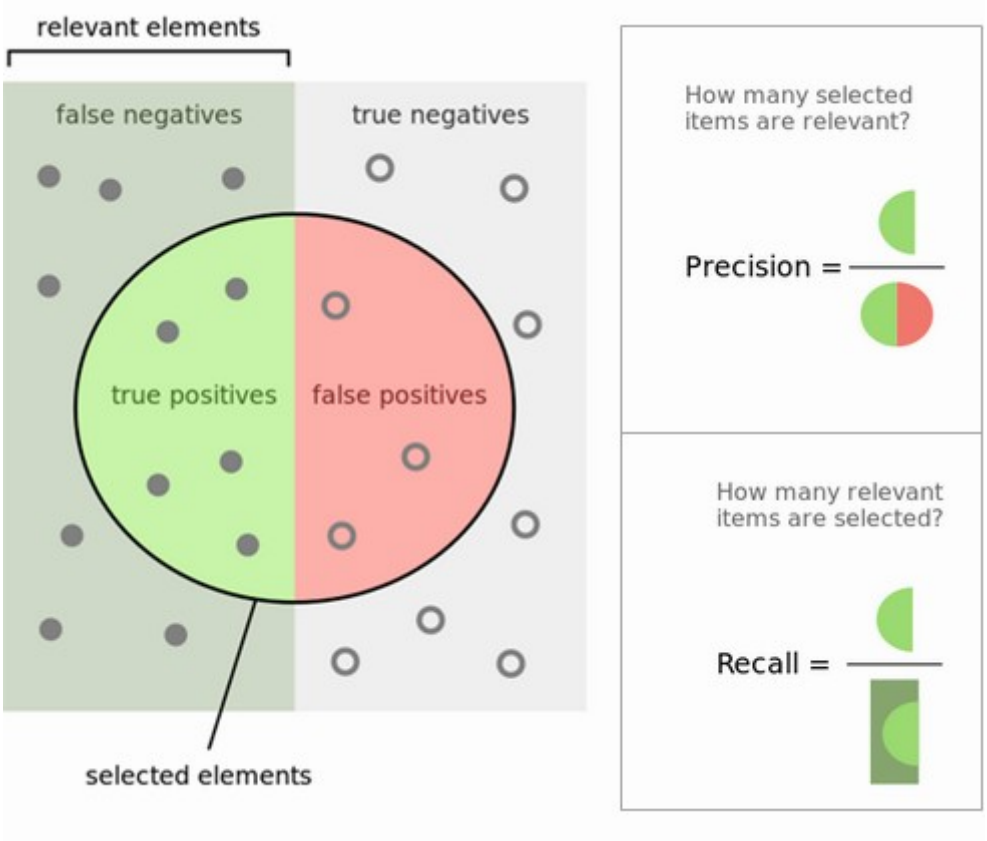
Recall is used when the goal is to limit FNs

- Cancer diagnosis: you don't want to miss a serious disease
- Search engines: You don't want to omit important hits
- Also know as sensitivity, hit rate, true positive rate (TPR)

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

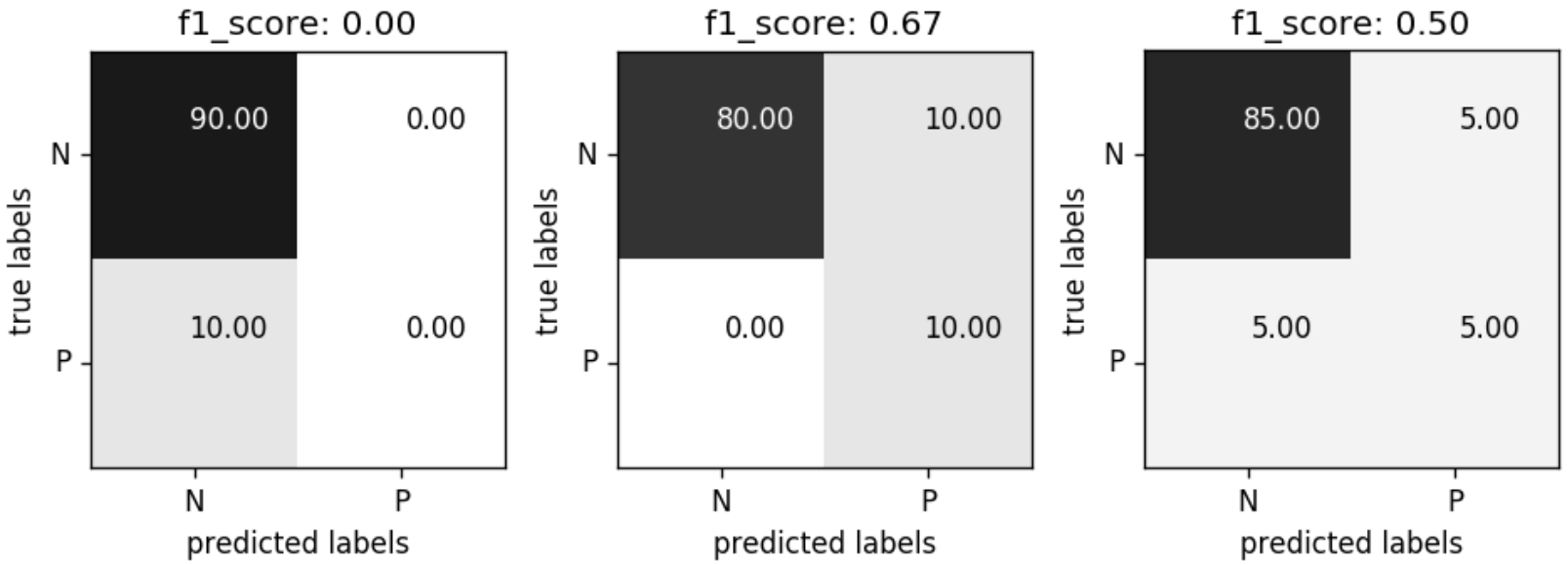


Comparison


relevant elements
false negatives
true negatives
true positives
false positives
selected elements
How many selected items are relevant?
Precision =
How many relevant items are selected?
Recall =

F1-score or F1-measure trades off precision and recall:

$$\mathrm{F1} = 2 \cdot \frac{\mathrm{precision} \cdot \mathrm{recall}}{\mathrm{precision} + \mathrm{recall}}$$



Classification measure Zoo

		True condition				
	Total population	Condition positive	Condition negative	Prevalence = $\frac{\Sigma \text{ Condition positive}}{\Sigma \text{ Total population}}$	Accuracy (ACC) = $\frac{\Sigma \text{ True positive} + \Sigma \text{ True negative}}{\Sigma \text{ Total population}}$	
Predicted condition	Predicted condition positive	**True positive**, Power	**False positive**, Type I error	Positive predictive value (PPV), Precision = $\frac{\Sigma \text{ True positive}}{\Sigma \text{ Predicted condition positive}}$	False discovery rate (FDR) = $\frac{\Sigma \text{ False positive}}{\Sigma \text{ Predicted condition positive}}$	
	Predicted condition negative	**False negative**, Type II error	**True negative**	False omission rate (FOR) = $\frac{\Sigma \text{ False negative}}{\Sigma \text{ Predicted condition negative}}$	Negative predictive value (NPV) = $\frac{\Sigma \text{ True negative}}{\Sigma \text{ Predicted condition negative}}$	
		True positive rate (TPR), Recall, Sensitivity, probability of detection = $\frac{\Sigma \text{ True positive}}{\Sigma \text{ Condition positive}}$	False positive rate (FPR), Fall-out, probability of false alarm = $\frac{\Sigma \text{ False positive}}{\Sigma \text{ Condition negative}}$	Positive likelihood ratio (LR+) = $\frac{\text{TPR}}{\text{FPR}}$	Diagnostic odds ratio (DOR) = $\frac{\text{LR+}}{\text{LR−}}$	F_1 score = $\frac{2}{\frac{1}{\text{Recall}} + \frac{1}{\text{Precision}}}$
		False negative rate (FNR), Miss rate = $\frac{\Sigma \text{ False negative}}{\Sigma \text{ Condition positive}}$	Specificity (SPC), Selectivity, True negative rate (TNR) = $\frac{\Sigma \text{ True negative}}{\Sigma \text{ Condition negative}}$	Negative likelihood ratio (LR−) = $\frac{\text{FNR}}{\text{TNR}}$		

https://en.wikipedia.org/wiki/Precision_and_recall (https://en.wikipedia.org/wiki/Precision_and_recall)

Averaging scores per class

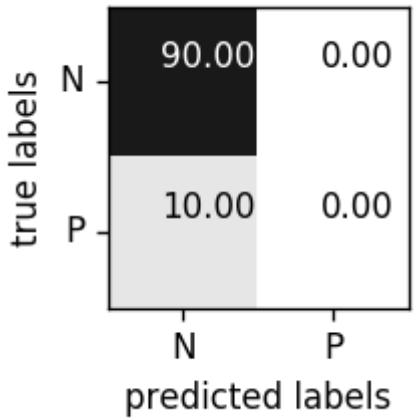
- Study the scores *by class* (in scikit-learn: `classification_report`)
  - One class viewed as positive, other(s) als negative
  - Support: number of samples in each class
  - Last line: weighted average over the classes (weighted by number of samples in each class)
- Averaging for scoring measure R across C classes (also for multiclass):
  - micro: count total number of TP, FP, TN, FN
  - macro

$$\frac{1}{C}\sum_{c\in C} R(y_c, \hat{y}_c)$$

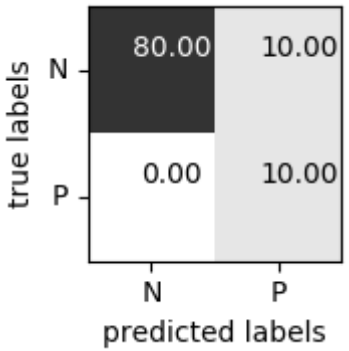
  - weighted (w_c: ratio of examples of class c)

$$\sum_{c\in C} w_c R(y_c, \hat{y}_c)$$

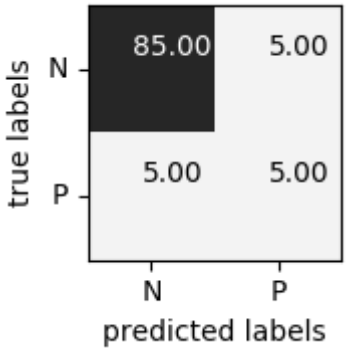
	precision	recall	f1-score	support
0	0.90	1.00	0.95	90
1	0.00	0.00	0.00	10
accuracy			0.90	100
macro avg	0.45	0.50	0.47	100
weighted avg	0.81	0.90	0.85	100



	precision	recall	f1-score	support
0	1.00	0.89	0.94	90
1	0.50	1.00	0.67	10
accuracy			0.90	100
macro avg	0.75	0.94	0.80	100
weighted avg	0.95	0.90	0.91	100



	precision	recall	f1-score	support
0	0.94	0.94	0.94	90
1	0.50	0.50	0.50	10
accuracy			0.90	100
macro avg	0.72	0.72	0.72	100
weighted avg	0.90	0.90	0.90	100



Uncertainty estimates from classifiers

- Classifiers can often provide uncertainty estimates of predictions.
- Remember that linear models actually return a numeric value.
    - When $\hat{y} < 0$, predict class -1, otherwise predict class +1

$$\hat{y} = w_0 * x_0 + w_1 * x_1 + \ldots + w_p * x_p + b$$

- In practice, you are often interested in how certain a classifier is about each class prediction (e.g. cancer treatments).

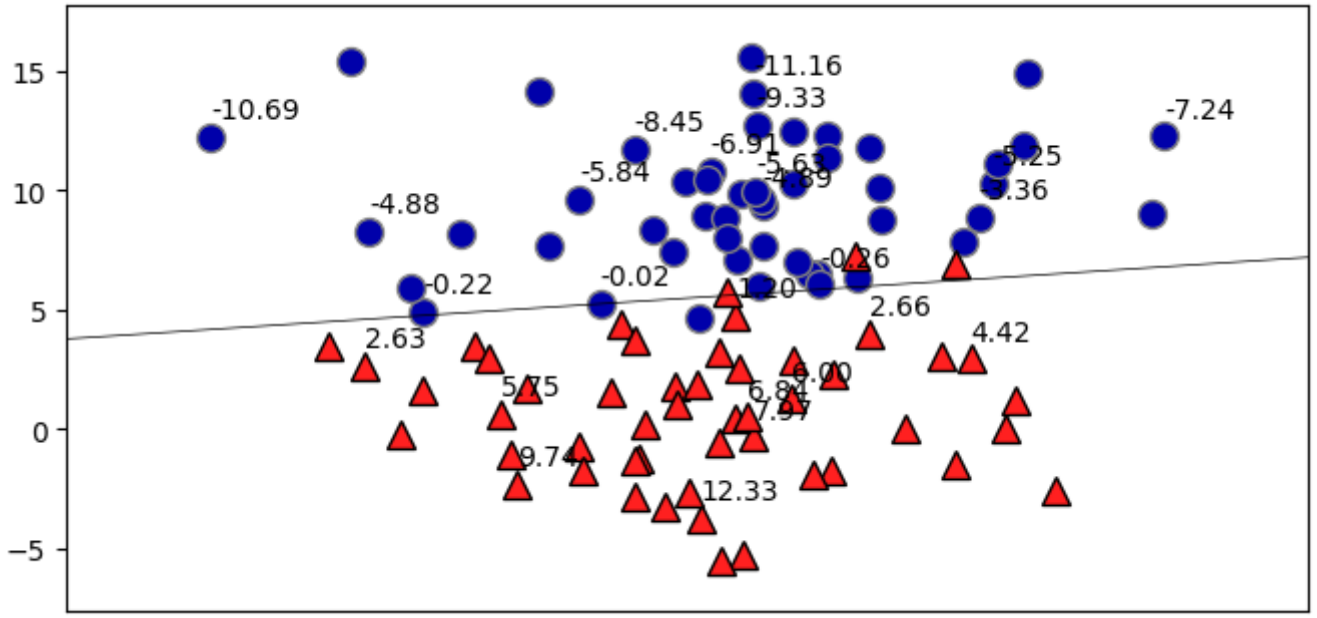
Scikit-learn offers 2 functions. Often, both are available for every learner, but not always.

- decision_function: returns floating point value for each sample
- predict_proba: return probability for each class

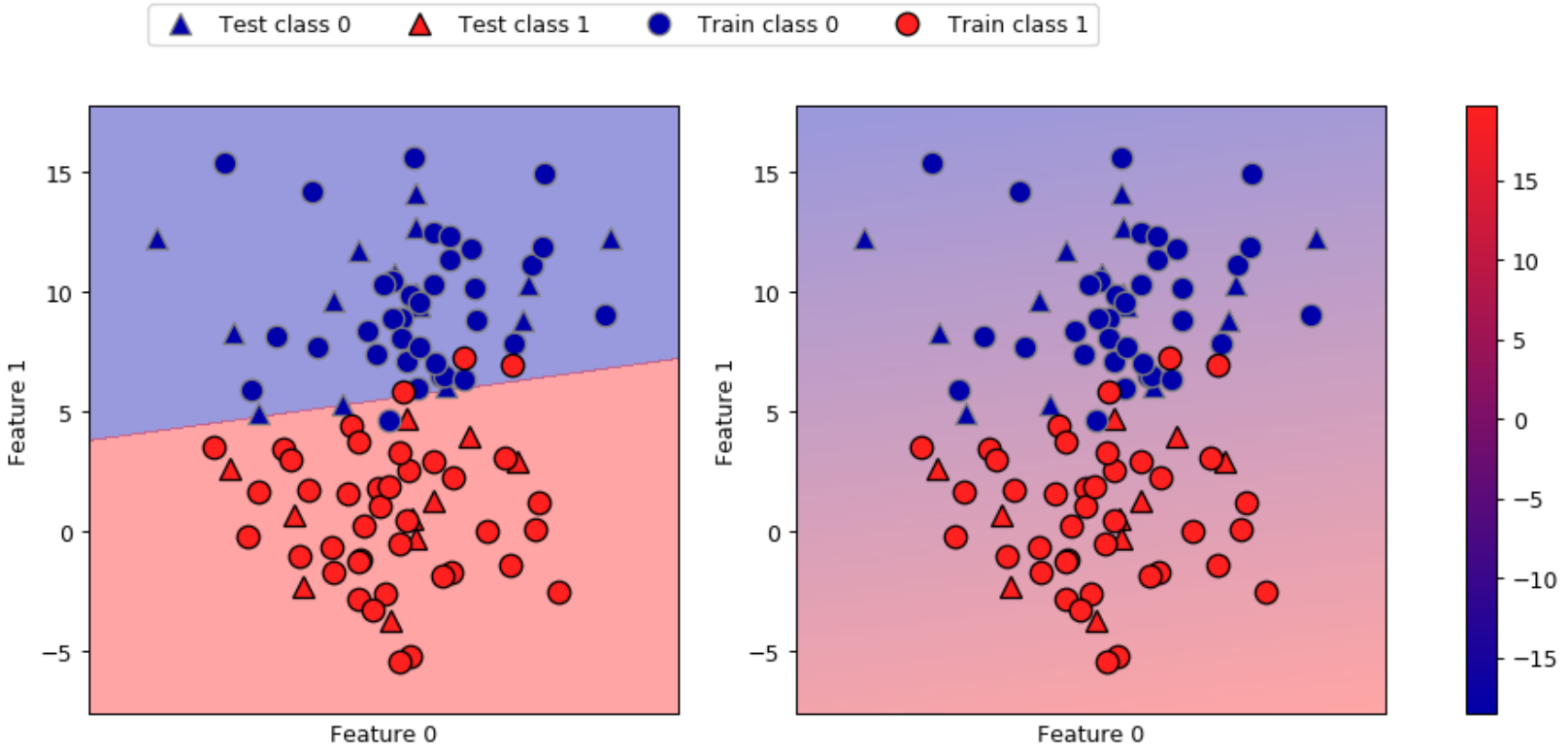
The Decision Function

In the binary classification case, the return value of decision_function encodes how strongly the model believes a data point to belong to the “positive” class.

- Positive values indicate a preference for the "positive" class
- Negative values indicate a preference for the "negative" (other) class



- The range of decision_function can be arbitrary, and depends on the data and the model parameters. This makes it sometimes hard to interpret.
- We can visualize the decision function as follows, with the actual decision boundary left and the values of the decision boudaries color-coded on the right.
- Note how the test examples are labeled depending on the decision function.

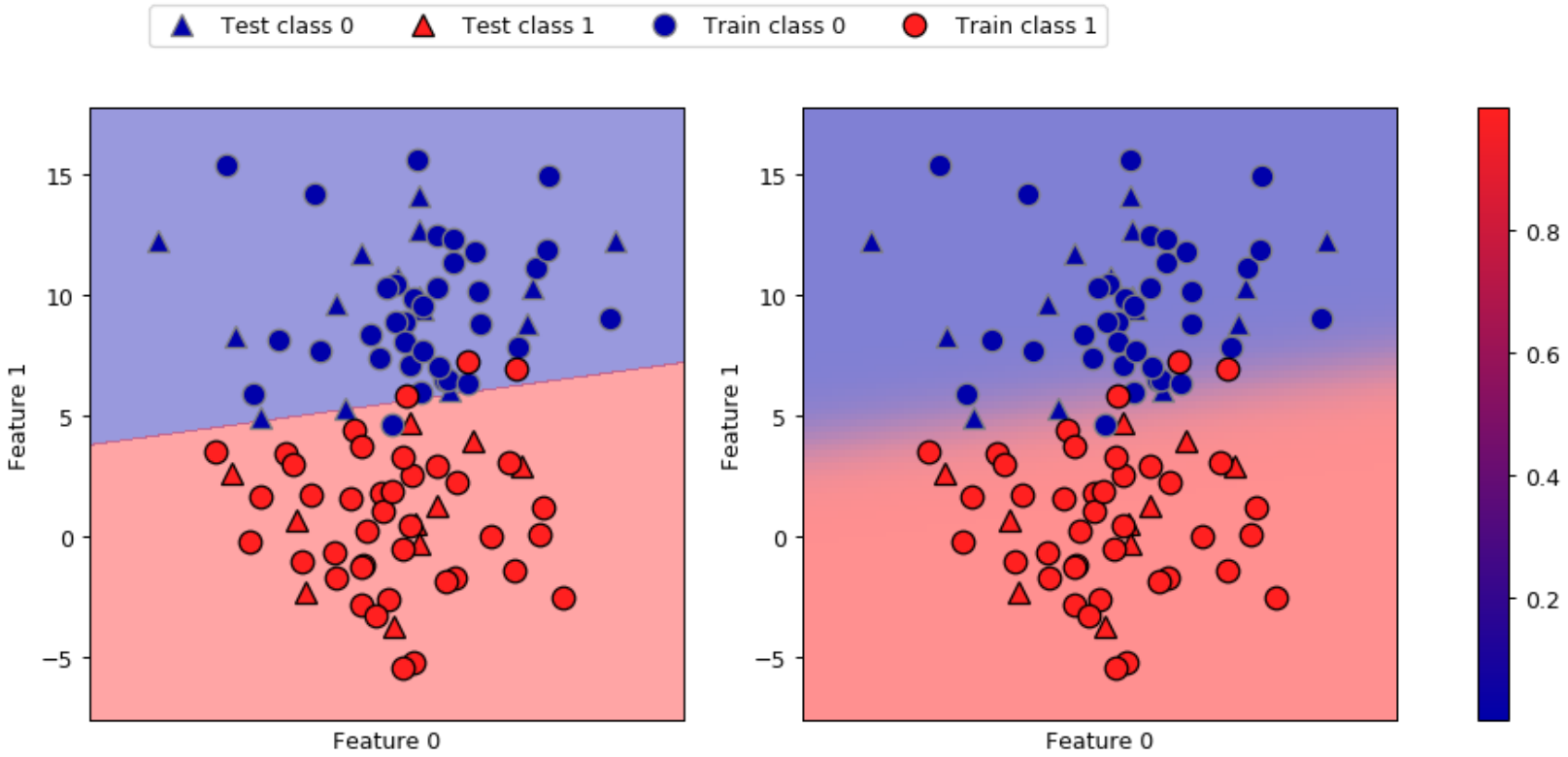


Predicting probabilities

The output of predict_proba is a *probability* for each class, with one column per class. They sum up to 1.

```
Shape of probabilities: (25, 2)
Predicted probabilities:
[[0.232 0.768]
 [0.002 0.998]
 [0.    1.   ]
 [0.003 0.997]
 [0.001 0.999]
 [1.    0.   ]]
```

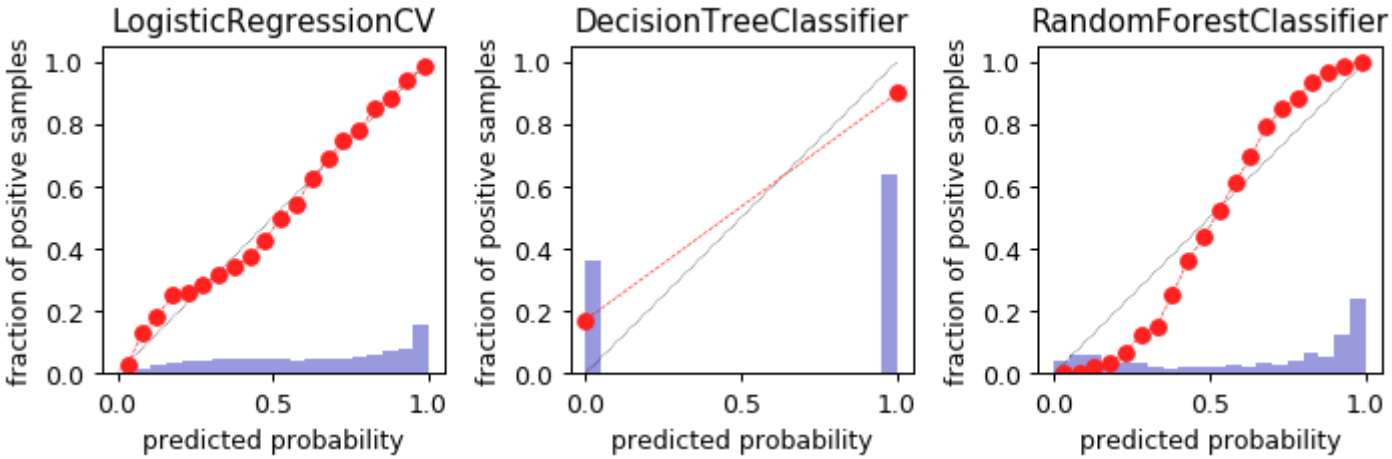
We can visualize them again. Note that the gradient looks different now.



Interpreting probabilities

- The class with the highest probability is predicted.
- How well the uncertainty actually reflects uncertainty in the data depends on the model and the parameters.
    - An overfitted model tends to make more certain predictions, even if they might be wrong.
    - A model with less complexity usually has more uncertainty in its predictions.
- A model is called *calibrated* if the reported uncertainty actually matches how correct it is — A prediction made with 70% certainty would be correct 70% of the time.
    - LogisticRegression returns well calibrated predictions by default as it directly optimizes log-loss
    - Linear SVM are not well calibrated. They are *biased* towards points close to the decision boundary.
- Calibration techniques (http://scikit-learn.org/stable/modules/calibration.html) can calibrate models in post-processing.

Model calibration



Model calibration

- Build another model, mapping classifier probabilities to better probabilities!
- 1d model! (or more for multi-class)

$$f_{calib}(s(x)) \approx p(y)$$

- s(x) is score given by model, usually
- Can also work with models that don't even provide probabilities! Need model for f_{calib}, need to decide what data to train it on.
- Can train on training set, causes overfit
- Can train using cross-validation, slower

Platt Scaling

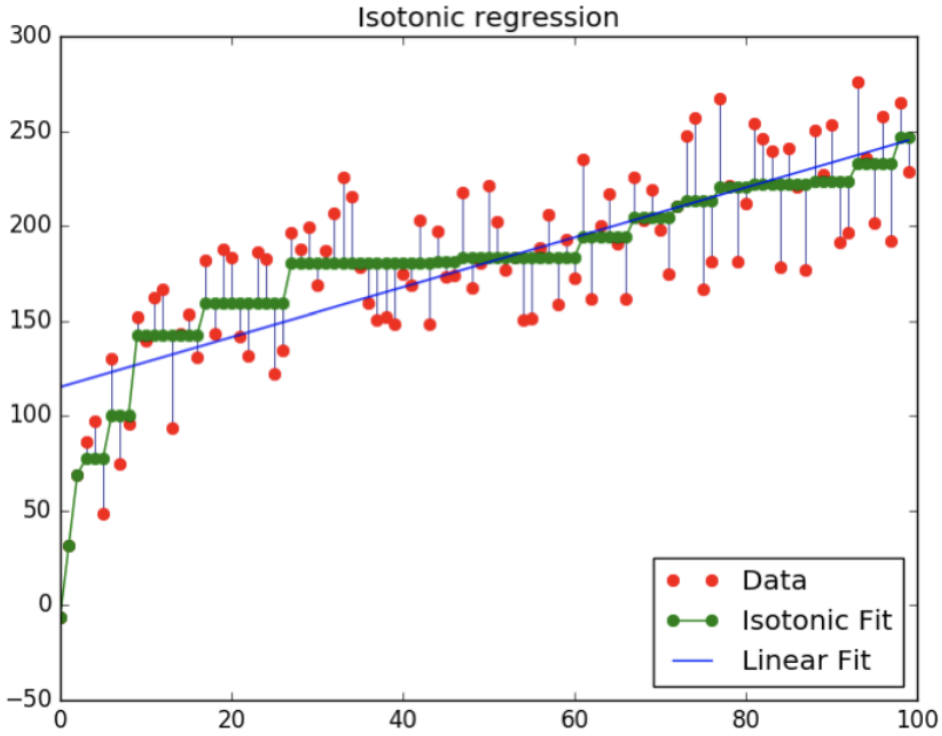
- Use a logistic sigmoid for f_{calib}

$$f_{platt} = \frac{1}{1 + \exp(-ws(x) - b)}$$

- Basically learning a 1d logistic regression (+ some tricks)
- Works well for SVMs

Isotonic regression

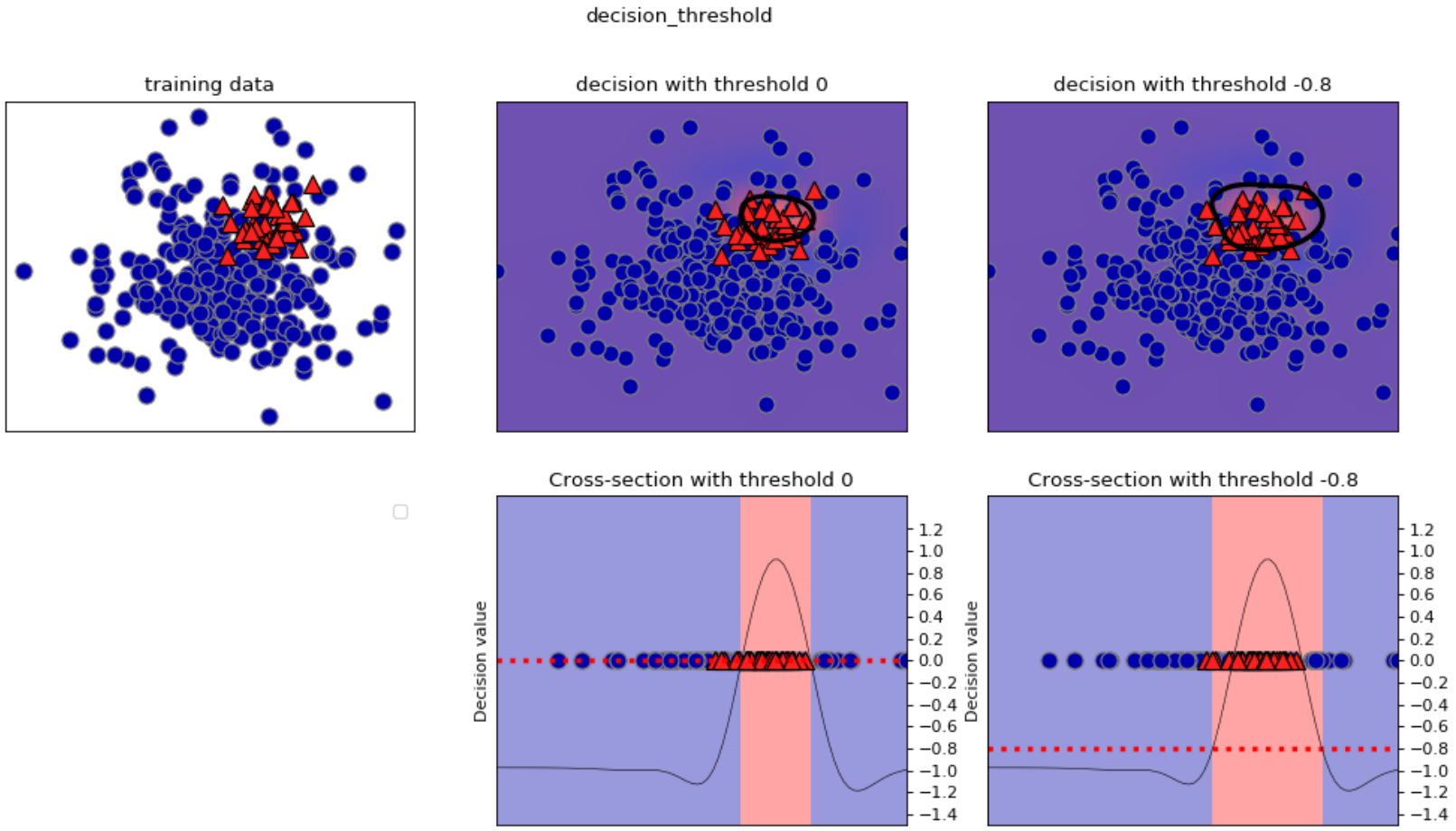
- Very flexible way to specify $f_{calib}
- Learns arbitrary monotonically increasing step-functions in 1d.
- Groups data into constant parts, steps in between.
- Optimum monotone function on training data (wrt MSE)



Threshold calibration

- Remember that many classifiers actually return a probability per class
    - We can retrieve it with `decision_function` and `predict_proba`
- For binary classification, we threshold at 0 for `decision_function` and 0.5 for `predict_proba` by default
- However, depending on the evaluation measure, you may want to threshold differently to fit your goals
    - For instance, when a FP is much worse than a FN
    - This is called *threshold calibration*

- Imagine that we want to avoid misclassifying a positive (red) point
- Points within decision boundary (black line) are classified positive
- Lowering the decision treshold (bottom figure): fewer FN, more FP



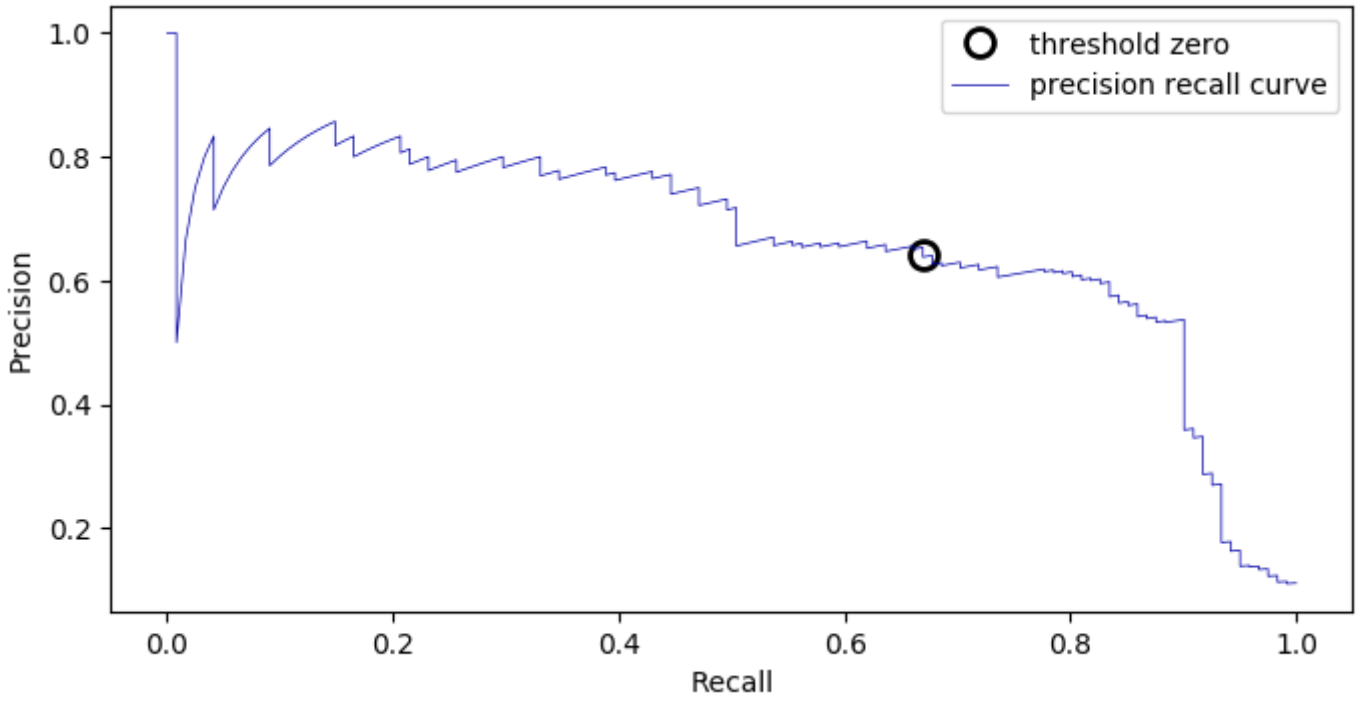
- Studying the classification report, we see that lowering the threshold yields:
    - higher recall for class 1 (we risk more FPs in exchange for more TP)
    - lower precision for class 1
- We can often trade off precision for recall

```
Threshold 0
              precision    recall  f1-score   support

           0       0.91      0.96      0.93        96
           1       0.67      0.47      0.55        17

    accuracy                           0.88       113
   macro avg       0.79      0.71      0.74       113
weighted avg       0.87      0.88      0.88       113


Threshold -0.8
              precision    recall  f1-score   support

           0       0.98      0.92      0.95        96
           1       0.65      0.88      0.75        17

    accuracy                           0.91       113
   macro avg       0.81      0.90      0.85       113
weighted avg       0.93      0.91      0.92       113
```

Precision-Recall curves

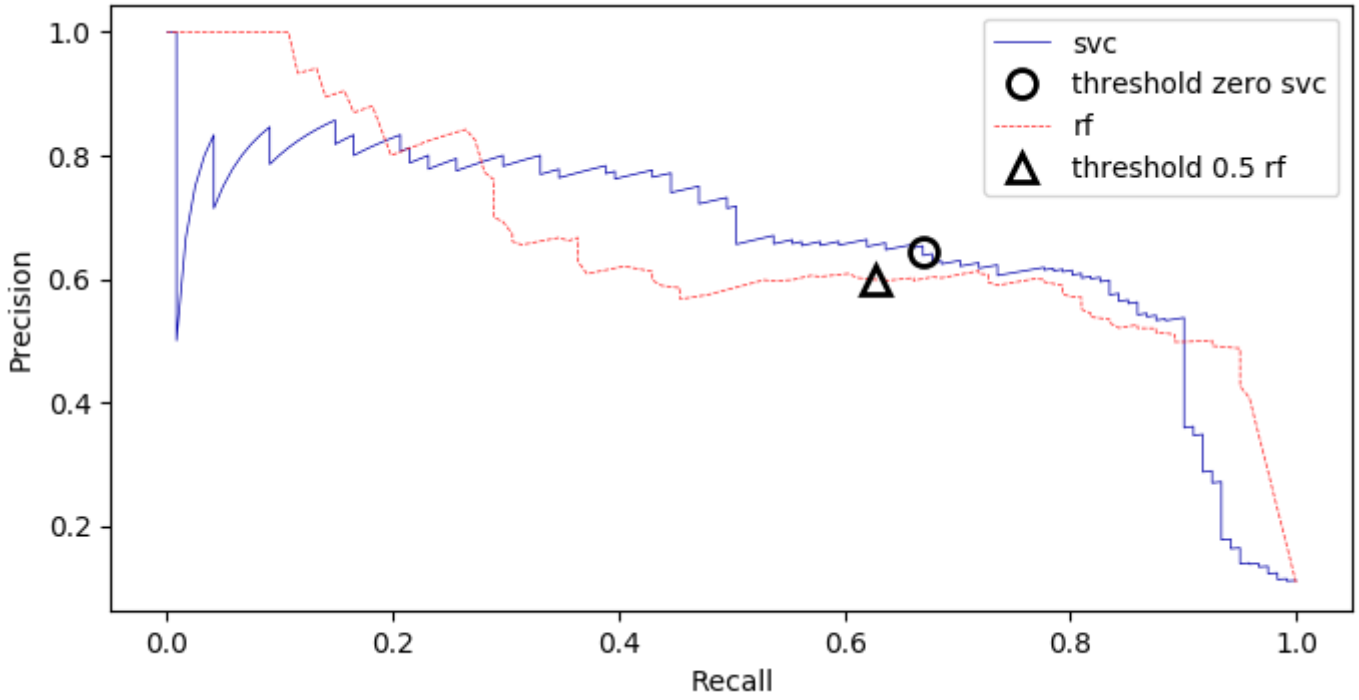
- As we've seen, you can trade off precision for recall by changing the decision threshold
- The best trade-off depends on your application, driven by real-world goals.
    - You can have arbitrary high recall, but you often want reasonable precision, too.
- Plotting precision against recall for all possible thresholds yields a **precision-recall curve**
- It helps answer multiple questions:
    - Threshold calibration: what's the best achievable precision-recall tradeoff?
    - How much more precision can I gain without losing too much recall?
    - Which models offer the best trade-offs?

- The default threshold (*threshold zero*) gives a certain precision and recall
  - Lower the threshold to gain higher recall (move right)
  - Increase the threshold to gain higher precision (move left)
- The curve is often jagged: increasing the threshold leaves fewer and fewer positive predictions, so precision ($\frac{TP}{TP+FP}$) can change dramatically
- The closer the curve stays to the upper-right corner, the better
- Here, it is possible to still get a precision of 0.55 with recall 0.9



Model selection

- Different classifiers offer different trade-offs
- RandomForest (in red) performs better at the extremes, SVM better in center
- In applications we may only care about a specific region (e.g. very high recall)



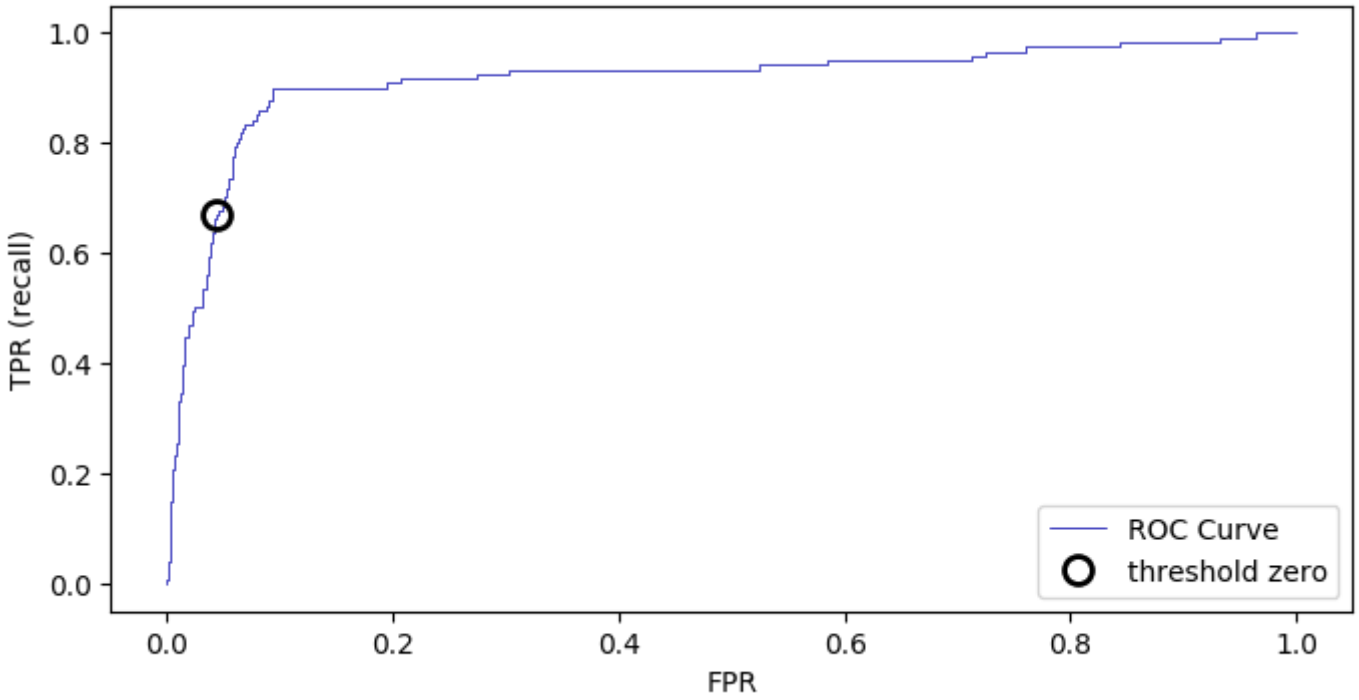
AUPRC

- The area under the precision-recall curve (AUPRC) is often used as a general evaluation measure
- This is a good general measure, but also hides the subtleties we saw in the curve

```
Average precision of random forest: 0.660
Average precision of svc: 0.666
```

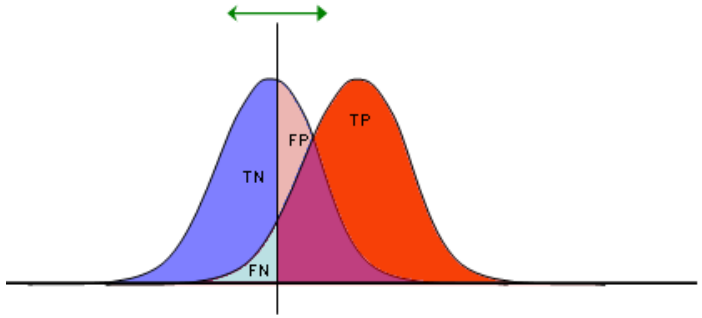
Receiver Operating Characteristics (ROC)

- We can also trade off recall (or true positive rate) $TPR = \frac{TP}{TP+FN}$ with *false positive rate* $FPR = \frac{FP}{FP+TN}$
- Varying the decision threshold yields the ROC curve
  - Lower the threshold to gain more recall (move right)
  - Increase the threshold to reduce FPs (move left)

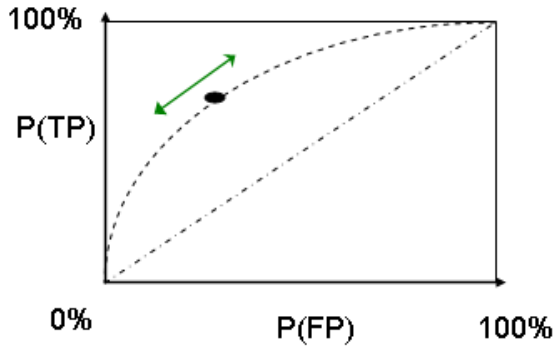


Visualization

- Horizontal axis represents the decision function. Every predicted point is on it.
- The blue probability density shows the actual negative points. The red one is for the positive points.
- Vertical line is the decision threshold: every point to the left is predicted negative (TN or FN) and vice versa (TP or FP).
- Increase threshold: fewer FP and TP: point on ROC curve moves leftward

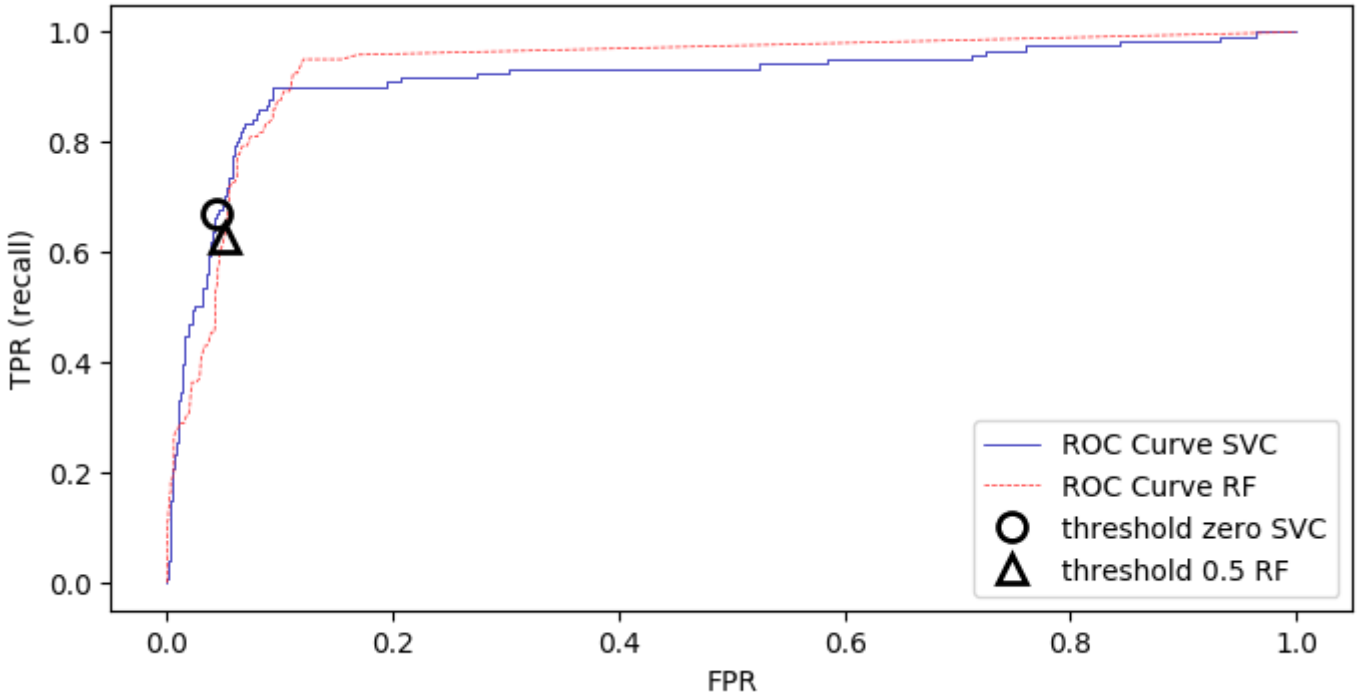


TP	FP
FN	TN
1	1



Model selection

- Again, we can compare multiple models by looking at the ROC curves
- We can calibrate the threshold depending on whether we need high recall or low FPR
- We can select between algorithms (or hyperparameters) depending on the involved *costs*

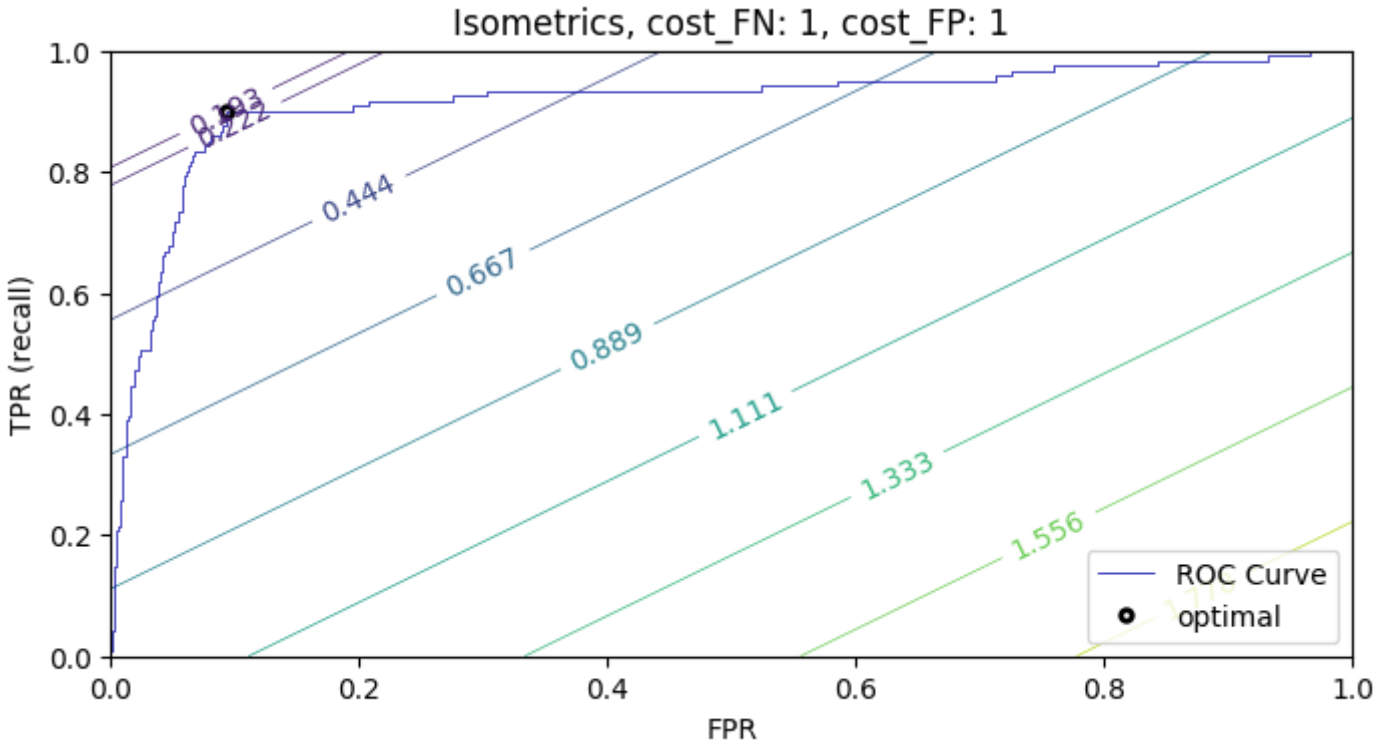


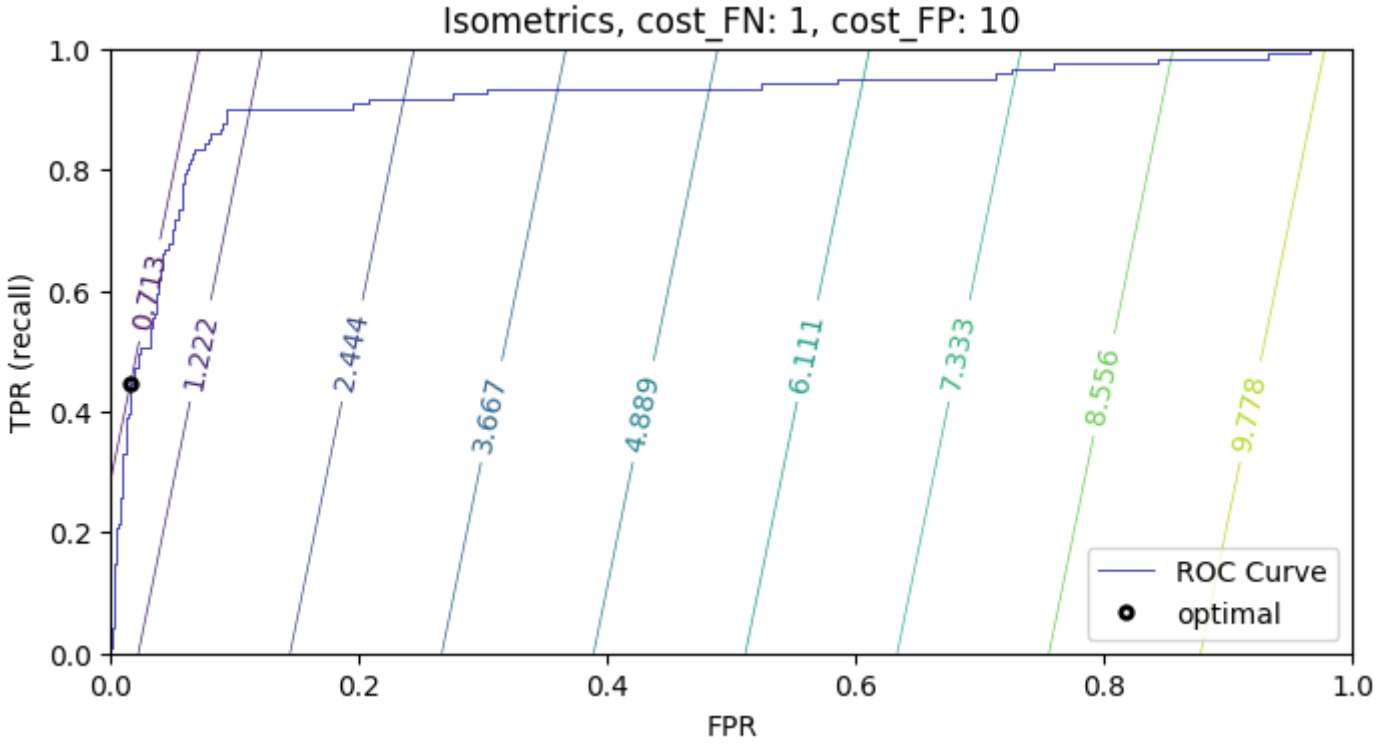
Calculating costs

- A certain amount of FP and FN can be translated to a *cost*:

$$\text{total cost} = \text{FPR} * cost_{FP} + (1 - \text{TPR}) * cost_{FN}$$

- This yields different *isometrics* (lines of equal cost) in ROC space
- The optimal threshold is the point on the ROC curve where the cost is minimal


Isometrics, cost_FN: 1, cost_FP: 1
TPR (recall)
FPR
0.0
0.2
0.4
0.6
0.8
1.0
0.444
0.667
0.889
1.111
1.333
1.556
ROC Curve
optimal


Isometrics, cost_FN: 1, cost_FP: 10
TPR (recall)
FPR
0.0
0.2
0.4
0.6
0.8
1.0
0.713
1.222
2.444
3.667
4.889
6.111
7.333
8.556
9.778
ROC Curve
optimal

Area under the ROC curve

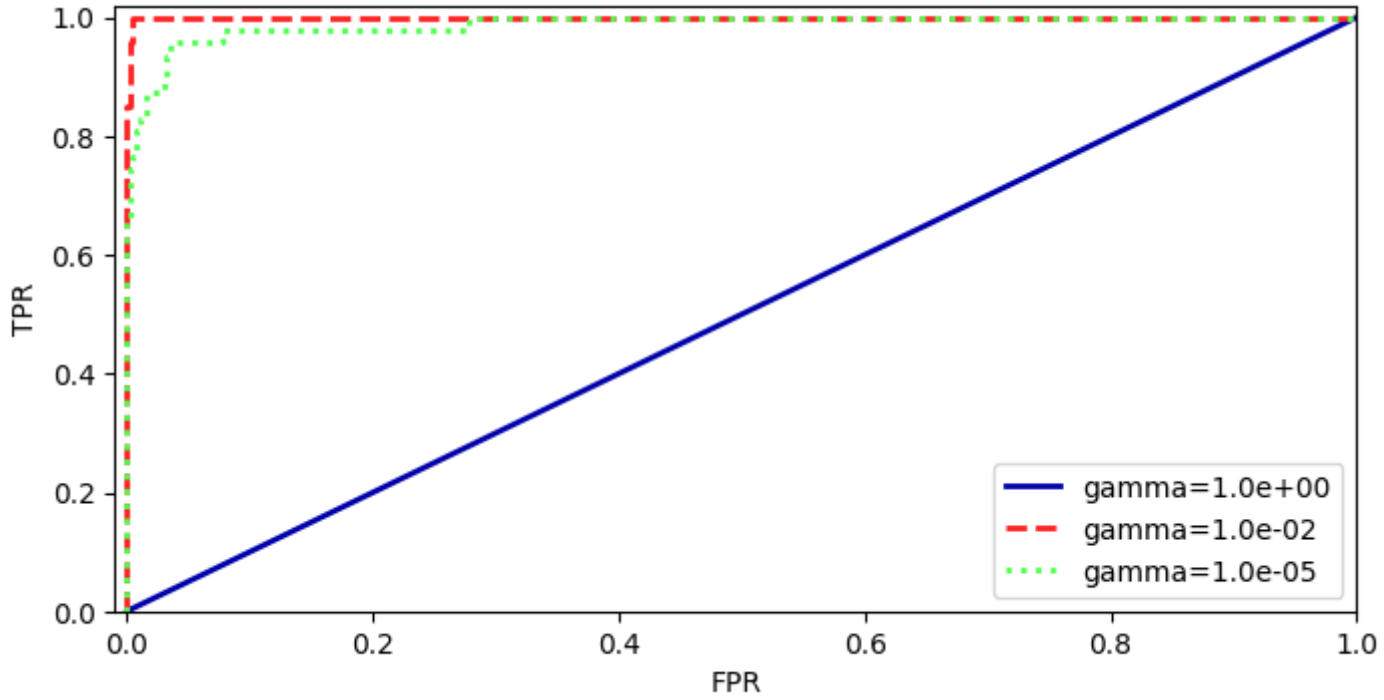
- A useful summary measure is the area under the ROC curve (AUROC or AUC)
- Key benefit: 'sensitive' to class imbalance
    - Random guessing always yields TPR=FPR
    - All points are on the diagonal line, hence an AUC of 0.5

```
AUC for Random Forest: 0.937
AUC for SVC: 0.916
AUC for dummy classifier: 0.498
```

Example: unbalanced dataset (10% positive, 90% negative):

- 3 models: overfitting ($\gamma = 1.0$), good ($\gamma = 0.01$), underfitting (γ=1e-5)
- ACC is the *same* (we might be random guessing), AUC is more informative

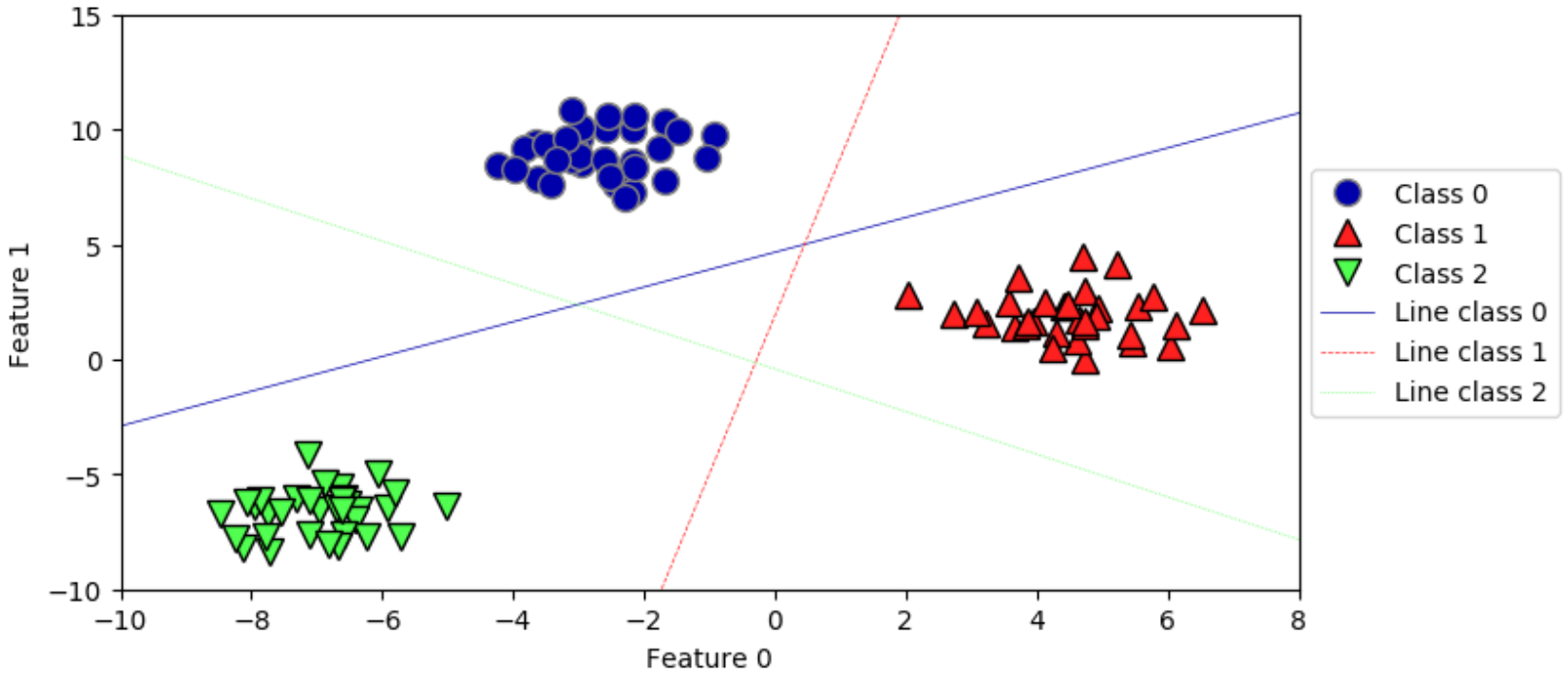
```
gamma = 1.0e+00   ACC = 0.90   AUC = 0.5000
gamma = 1.0e-02   ACC = 0.90   AUC = 0.9995
gamma = 1.0e-05   ACC = 0.90   AUC = 0.9882
```



Multiclass classification

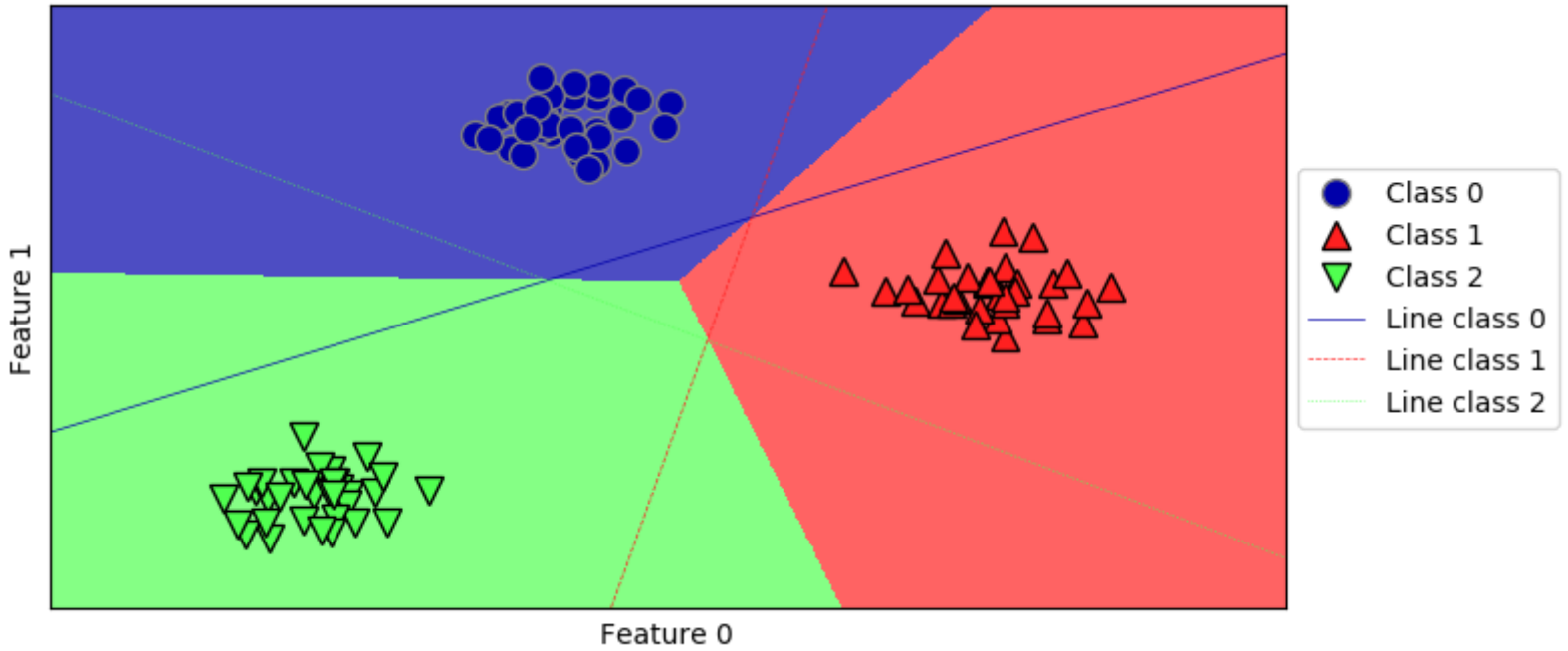
Common technique: one-vs-rest approach:

- A binary model is learned for each class vs. all other classes
- Creates as many binary models as there are classes



Every binary classifiers makes a prediction

- The confidence (decision score) of that prediction is the confidence in that class
- The class with the highest decision score (>0) wins
- Decision boundaries visualized below



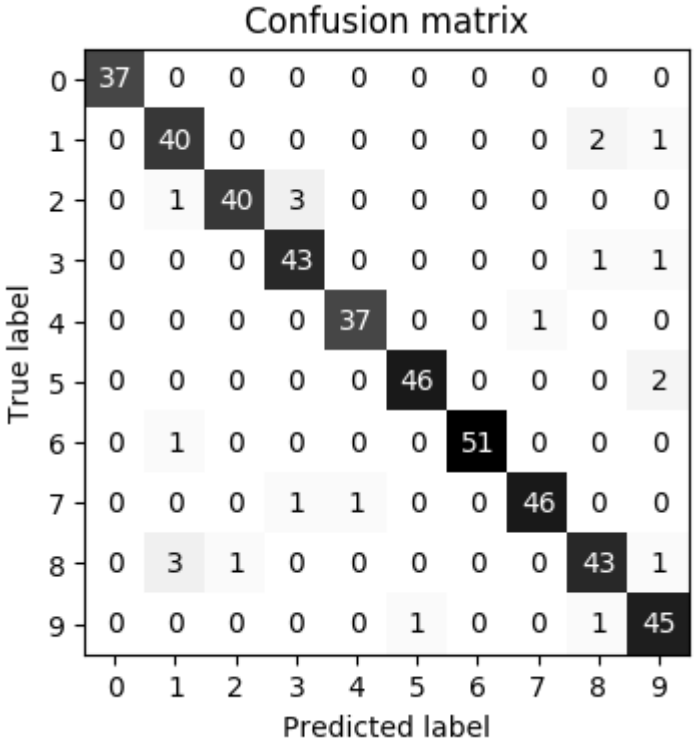
Uncertainty in multi-class classification

- `decision_function` and `predict_proba` also work in the multiclass setting
- always have shape (n_samples, n_classes)
- Example on the Iris dataset, which has 3 classes:

```
Decision function:
[[ -3.035   2.294   0.741]
 [  5.919   3.091  -9.01 ]
 [-10.052   1.875   8.177]
 [ -2.733   2.036   0.697]
 [ -3.737   2.476   1.262]
 [  6.036   3.035  -9.07 ]]
Predicted probabilities:
[[0.004 0.822 0.174]
 [0.944 0.056 0.   ]
 [0.    0.002 0.998]
 [0.007 0.787 0.206]
 [0.002 0.77  0.229]
 [0.953 0.047 0.   ]]
```

Multi-class metrics

- Multiclass metrics are derived from binary metrics, averaged over all classes
- Example: handwritten digit recognition (MNIST)



Precision, recall, F1-score now yield 10 per-class scores

	precision	recall	f1-score	support
0	1.00	1.00	1.00	37
1	0.89	0.93	0.91	43
2	0.98	0.91	0.94	44
3	0.91	0.96	0.93	45
4	0.97	0.97	0.97	38
5	0.98	0.96	0.97	48
6	1.00	0.98	0.99	52
7	0.98	0.96	0.97	48
8	0.91	0.90	0.91	48
9	0.90	0.96	0.93	47
accuracy			0.95	450
macro avg	0.95	0.95	0.95	450
weighted avg	0.95	0.95	0.95	450

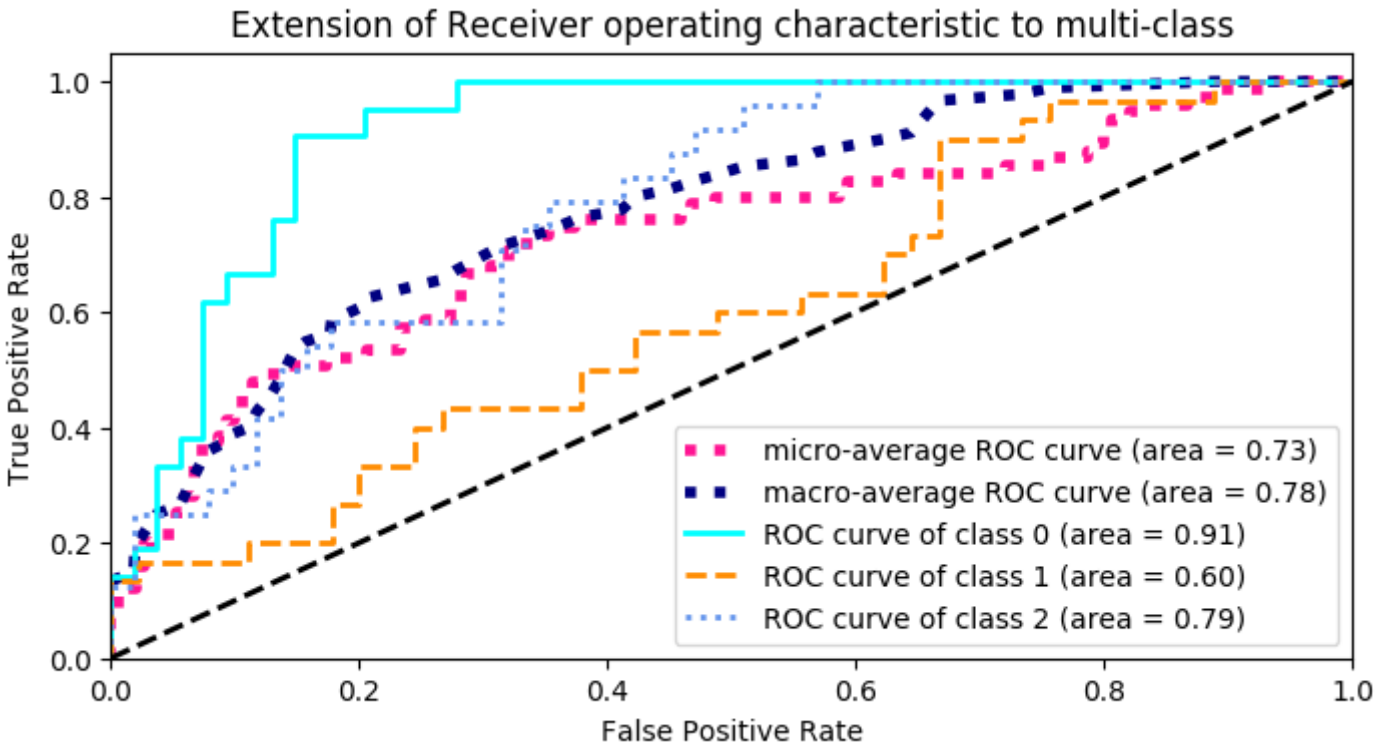
Different ways to compute average

- macro-averaging: computes unweighted per-class scores: $\frac{\sum_{i=0}^{n} score_i}{n}$
    - Use when you care about each class equally much
- weighted averaging: scores are weighted by the relative size of the classes (support): $\frac{\sum_{i=0}^{n} score_i weight_i}{n}$
    - Use when data is imbalanced
- micro-averaging: computes total number of FP, FN, TP over all classes, then computes scores using these counts: $recall = \frac{\sum_{i=0}^{n} TP_i}{\sum_{i=0}^{n} TP_i + \sum_{i=0}^{n} FN_i}$
    - Use when you care about each sample equally much

```
Micro average f1 score: 0.951
Weighted average f1 score: 0.951
Macro average f1 score: 0.952
```

Multi-class ROC

- To use AUC in a multi-class setting, you need to choose whether you use a micro- or macro average TPR and FPR.
- Depends on the application: is every class equally important?
    - SKlearn currently doesn't have a default option

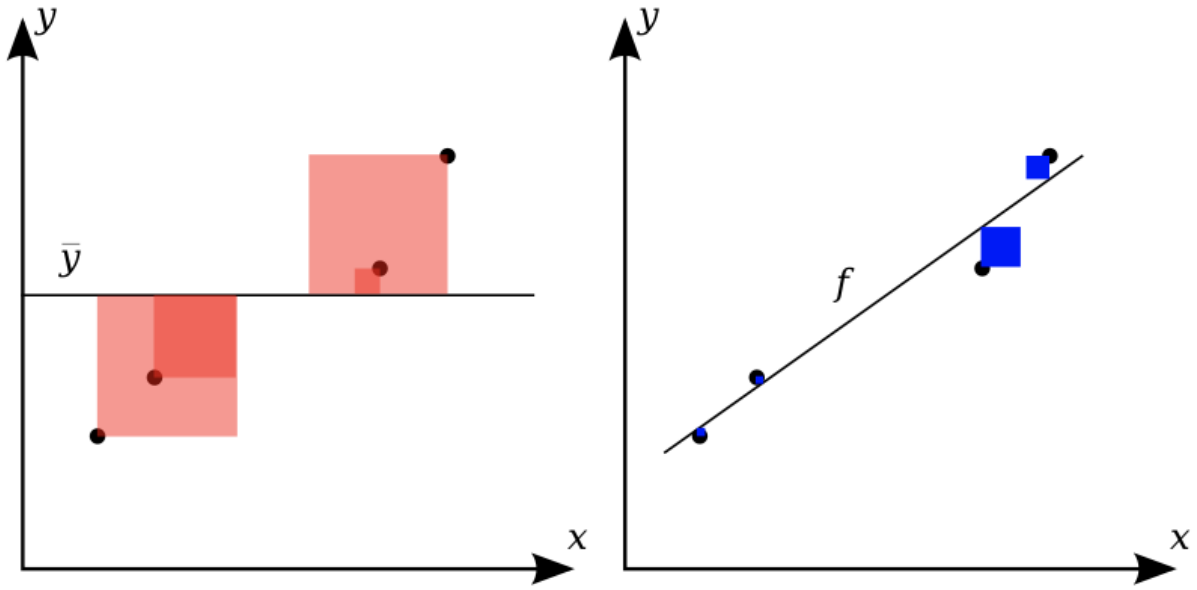


Regression metrics

Most commonly used are

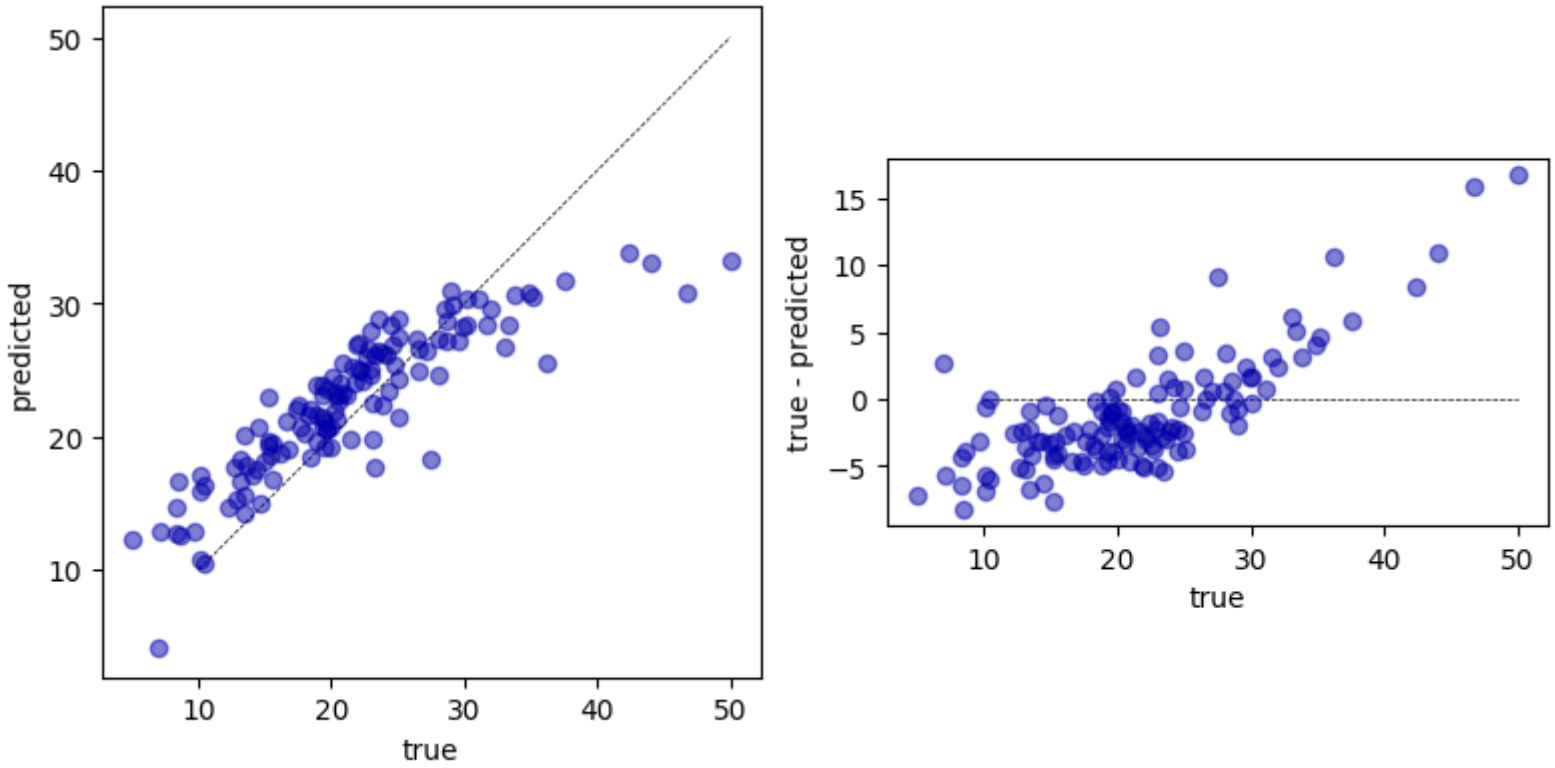
- (root) mean squared error: $\frac{\sum_i (y_{pred_i} - y_{actual_i})^2}{n}$
- mean absolute error: $\frac{\sum_i |y_{pred_i} - y_{actual_i}|}{n}$
    - Less sensitive to outliers and large errors

- R squared (r2): $1 - \frac{\sum_i (y_{pred_i} - y_{actual_i})^2}{\sum_i (y_{mean} - y_{actual_i})^2}$
  - Ratio of variation explained by the model / total variation
  - Between 0 and 1, but *negative* if the model is worse than just predicting the mean
  - Easier to interpret (higher is better).



Visualizing errors

- Prediction plot (left): predicted vs actual target values
- Residual plot (right): residuals vs actual target values
    - Over- and underpredictions can be given different costs



Other considerations

- There exist techniques to correct label imbalance (see next lecture)
    - Undersample the majority class, or oversample the minority class
    - SMOTE (Synthetic Minority Oversampling TEchnique) adds artificial *training* points by interpolating existing minority class points
        - Think twice before creating 'artificial' training data
- Cost-sensitive classification (not in sklearn)
    - *Cost matrix*: a confusion matrix with a costs associated to every possible type of error
    - Some algorithms allow optimizing on these costs instead of their usual loss function
    - Meta-cost: builds ensemble of models by relabeling training sets to match a given cost matrix
        - Black-box: can make any algorithm cost sensitive (but slower and less accurate)

- There are many more metrics to choose from
    - Balanced accuracy: accuracy where each sample is weighted according to the inverse prevalence of its true class
        - Identical to macro-averaged recall
    - Cohen's Kappa: accuracy, taking into account the possibility of predicting the right class by chance
        - 1: perfect prediction, 0: random prediction, negative: worse than random
        - With p_0 = accuracy, and p_e = accuracy of random classifier:

$$\kappa = \frac{p_o - p_e}{1 - p_e}$$

    - Matthews correlation coefficient: another measure that can be used on imbalanced data
        - 1: perfect prediction, 0: random prediction, -1: inverse prediction

$$MCC = \frac{tp \times tn - fp \times fn}{\sqrt{(tp + fp)(tp + fn)(tn + fp)(tn + fn)}}$$

Bias-Variance decomposition

- When we repeat evaluation procedures multiple times, we can distinguish two sources of errors:
    - Bias: systematic error (independent of the training sample). The classifier always gets certain points wrong
    - Variance: error due to variability of the model with respect to the training sample. The classifier predicts some points accurately on some training sets, but inaccurately on others.
- There is also an intrinsic (noise) error, but there's nothing we can do against that.
- Bias is associated with underfitting, and variance with overfitting
- Bias-variance trade-off: you can often exchange variance for bias through regularization (and vice versa)
    - The challenge is to find the right trade-off (minimizing total error)
- Useful to understand how to tune or adapt learning algorithm

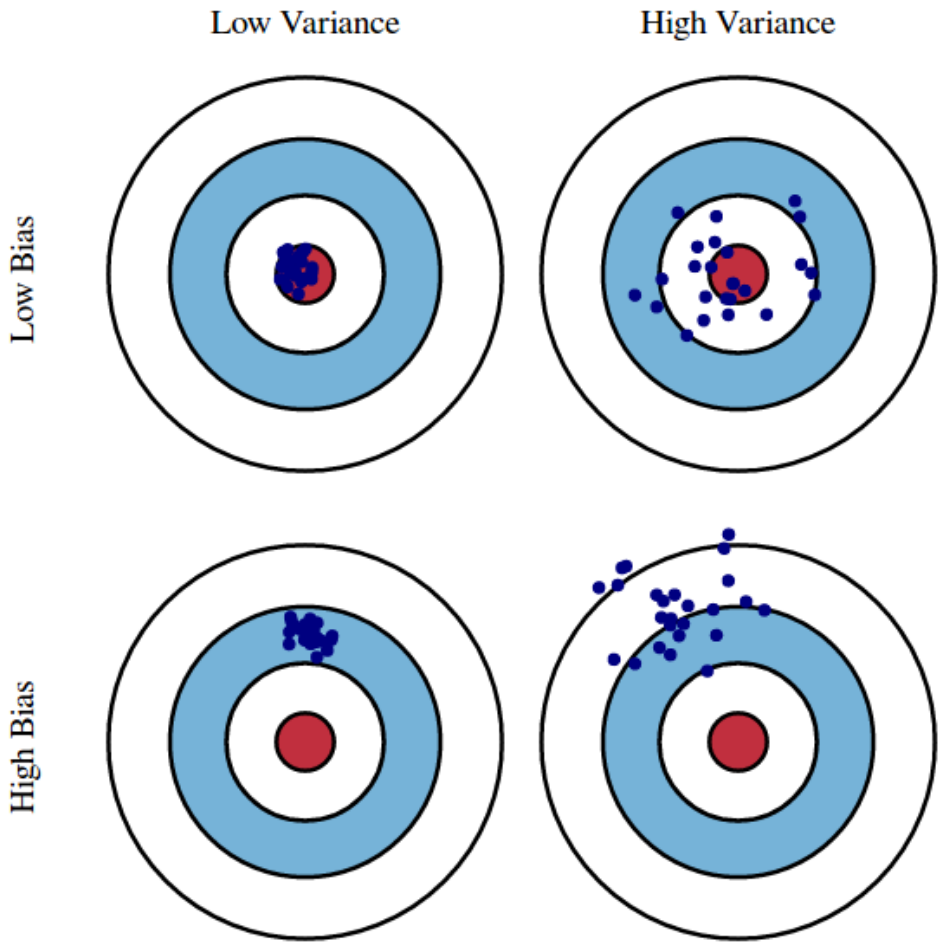


Fig. 1 Graphical illustration of bias and variance.

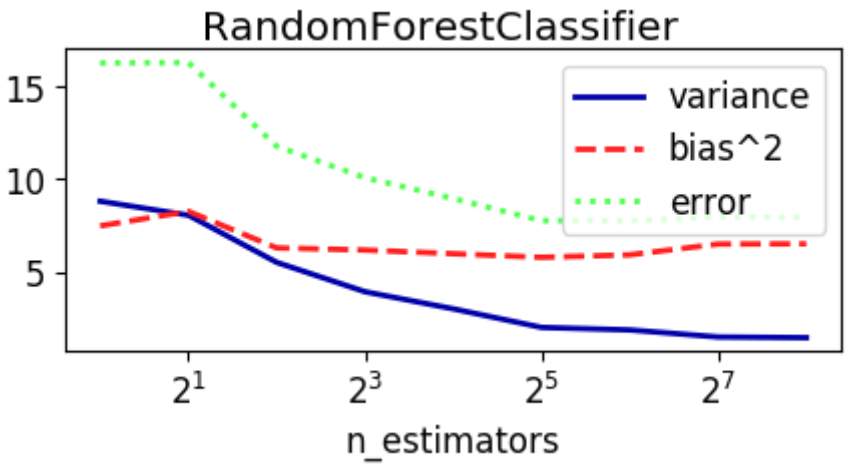
Computing bias-variance

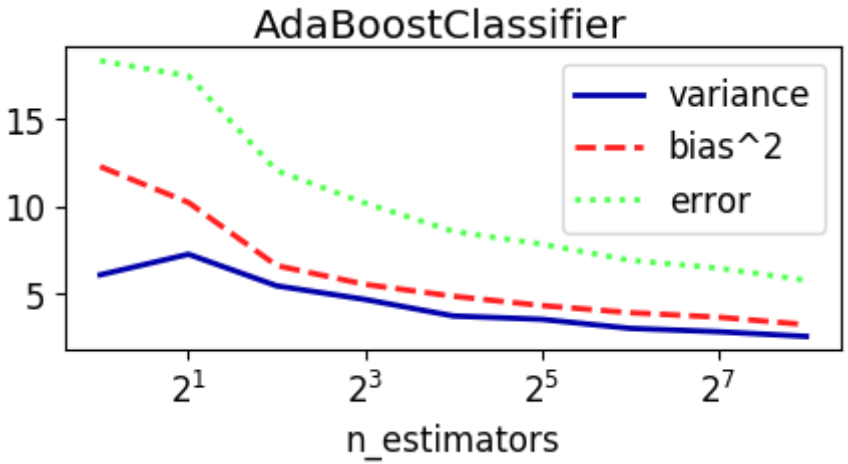
- Take 100 or more bootstraps (or shuffle-splits)
- Regression: for each data point x:
    - $bias(x)^2 = (x_{true} - mean(x_{predicted}))^2$
    - $variance(x) = var(x_{predicted})$
- Classification: for each data point x:
    - $bias(x)$ = misclassification ratio
    - $variance(x)$

      $= (1 - (P(class_1)^2 + P(class_2)^2))/2$
        - $P(class_i)$ is ratio of class i predictions
- Total bias: $\sum_x bias(x)^2 * w_x$, with w_x the ratio of x occuring in the test sets
- Total variance: $\sum_x variance(x) * w_x$

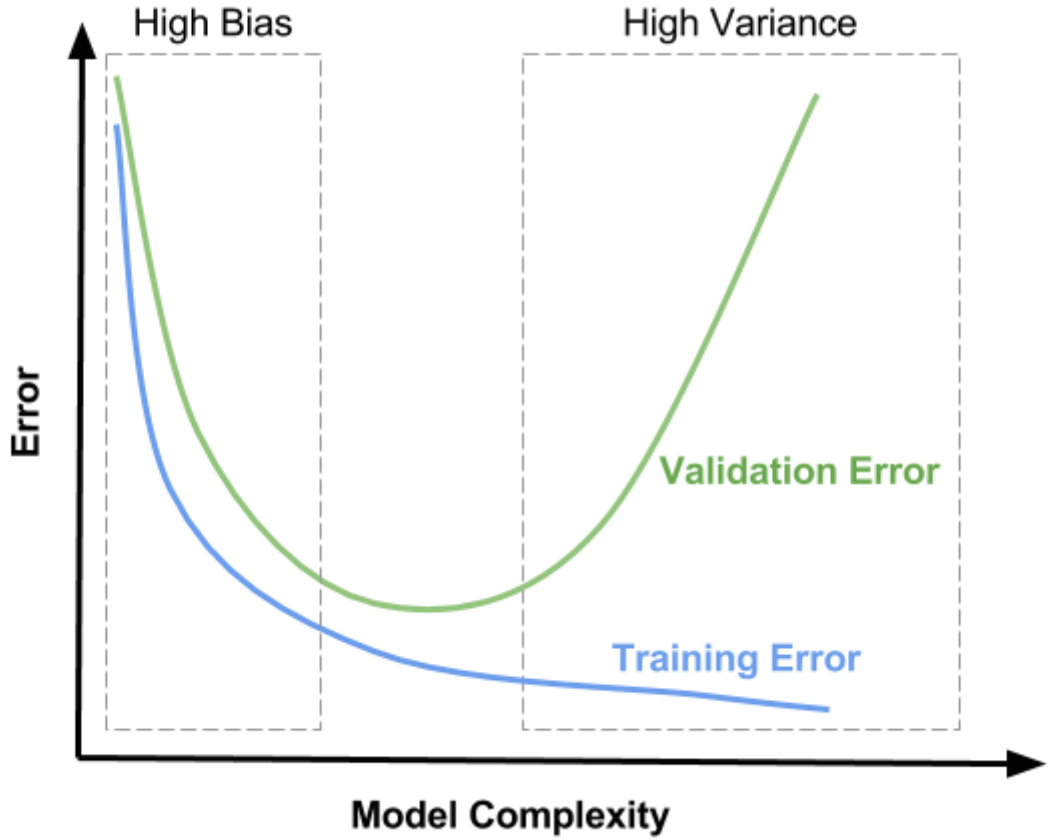
Bias and variance reduction

- Bagging (RandomForests) is a variance-reduction technique
- Boosting is a bias-reduction technique


RandomForestClassifier
15
10
5
variance
bias^2
error
2^1
2^3
2^5
2^7
n_estimators

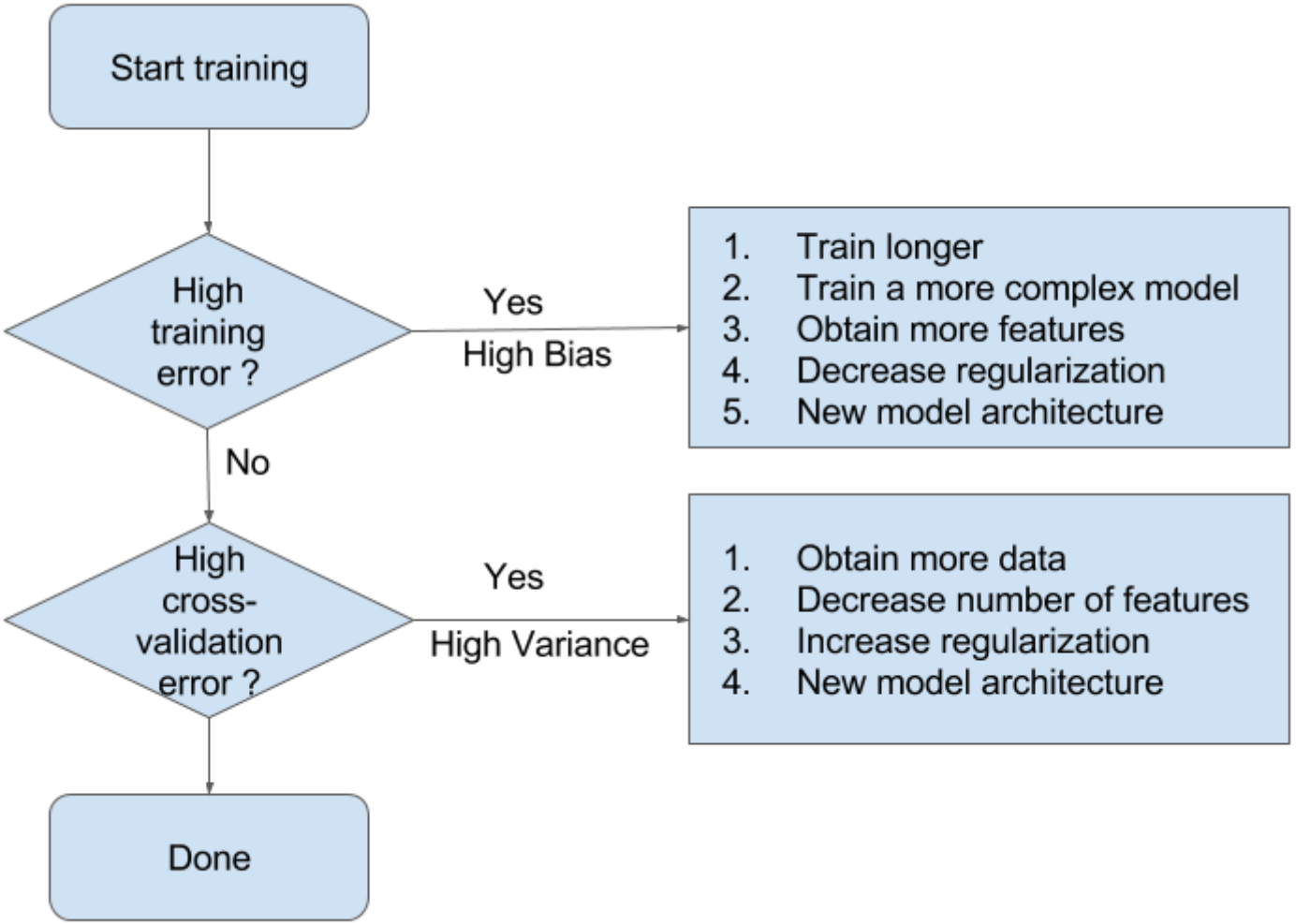

AdaBoostClassifier
15
10
5
variance
bias^2
error
2^1
2^3
2^5
2^7
n_estimators

Bias-variance and overfitting



- High bias means that you are likely underfitting
    - Do less regularization
    - Use a more flexible/complex model (another algorithm)
    - Use a bias-reduction technique (e.g. boosting)
- High variance means that you are likely overfitting
    - Use more regularization
    - Get more data
    - Use a simpler model (another algorithm)
    - Use a variance-reduction techniques (e.g. bagging)

Bias-Variance Flowchart (Andrew Ng, Coursera)



Hyperparameter tuning

We can basically use any optimization technique to optimize hyperparameters:

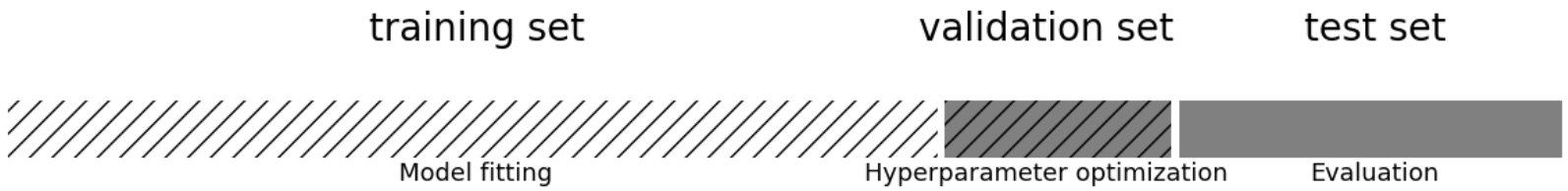
- **Grid search**
- **Random search**

More advanced techniques (see lecture 7):

- Local search
- Racing algorithms
- Model-based optimization (see later)
- Multi-armed bandits
- Genetic algorithms

Overfitting on the test set

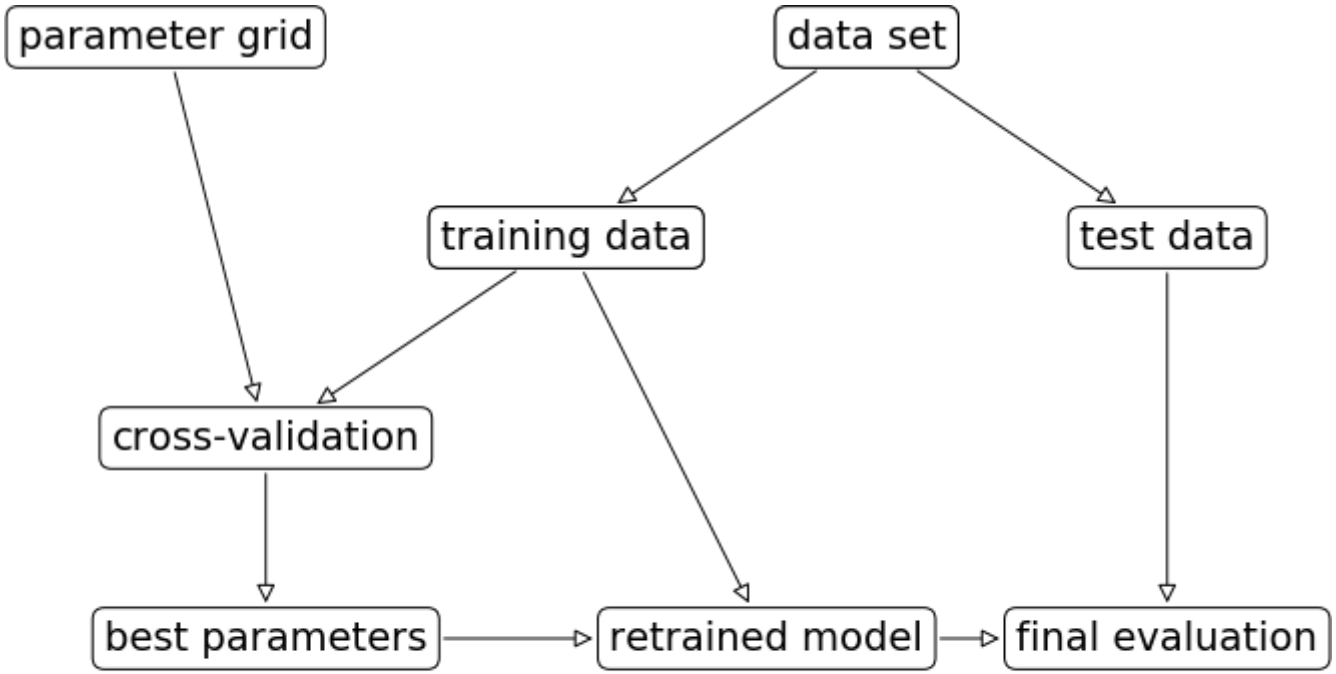
- Simply taking the best performing hyperparameters yields optimistic results
- We've already used the test data to evaluate each hyperparameter setting!
    - Information 'leaks' from test set into the final model
- Set aside part of the training data to evaluate the hyperparameter settings
    - Select best hyperparameters on validation set
    - Rebuild the model on the training+validation set
    - Evaluate optimal model on the test set




```
Size of training set: 84   size of validation set: 28   size of test set:
38

Best score on validation set: 0.96
Best parameters:  {'C': 10, 'gamma': 0.001}
Test set score with best parameters: 0.92
```

Grid-search with cross-validation

- The way that we split the data into training, validation, and test set may have a large influence on estimated performance
- We need to use cross-validation again (e.g. 3-fold CV), instead of a single split



Nested cross-validation

- Note that we are still using a single split to create the outer test set
- We can also use cross-validation here
- Nested cross-validation:
    - Outer loop: split data in training and test sets
    - Inner loop: run grid search, splitting the training data into train and validation sets
- Result is a just a list of scores
    - There will be multiple optimized models and hyperparameter settings (not returned)
- To apply on future data, we need to train `GridSearchCV` on all data again

```
scores = cross_val_score(GridSearchCV(SVC(), param_grid, cv=5),
                         iris.data, iris.target, cv=5)
```