Lecture 4: Model Selection

Can I trust you?

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Evaluation

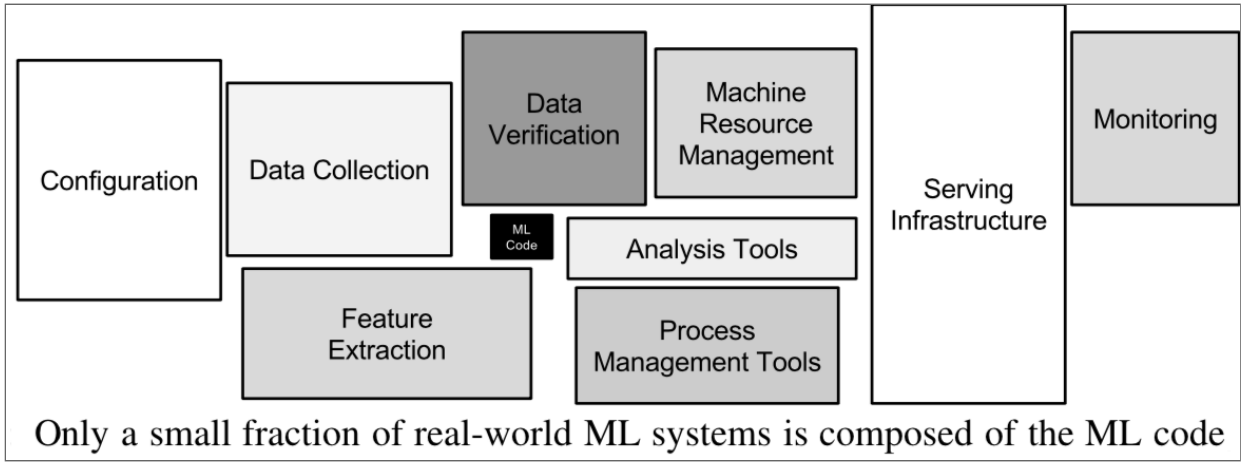
- To know whether we can *trust* our method or system, we need to evaluate it.
- Model selection: choose between different models in a data-driven way.
    - If you cannot measure it, you cannot improve it.
- Convince others that your work is meaningful
    - Peers, leadership, clients, yourself(!)
- When possible, try to *interpret* what your model has learned
    - The signal your model found may just be an artifact of your biased data
    - See 'Why Should I Trust You?' by Marco Ribeiro et al.

(a) Husky classified as wolf

(b) Explanation

Designing Machine Learning systems

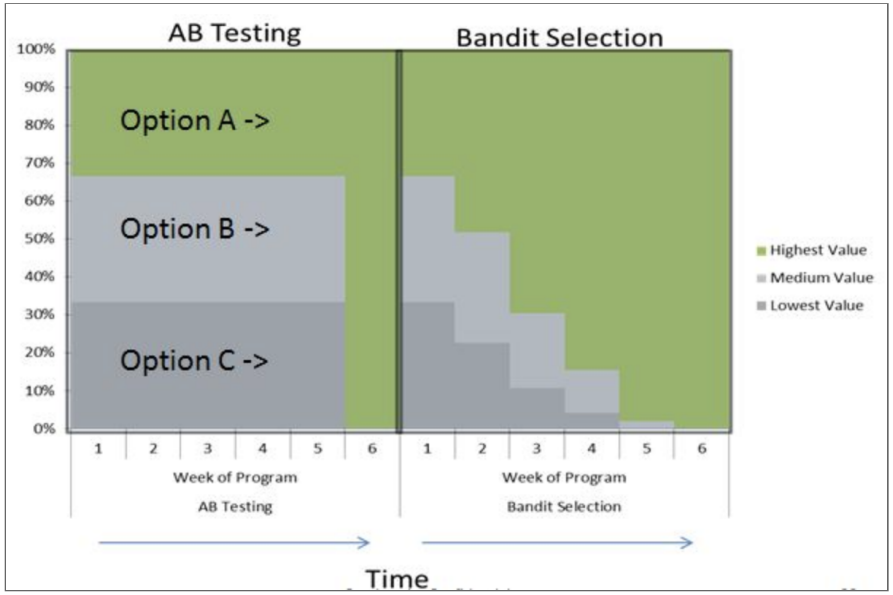
- Just running your favourite algorithm is usually not a great way to start
- Consider the problem: How to measure success? Are there costs involved?
    - Do you want to understand phenomena or do black box modelling?
- Analyze your model's mistakes. Don't just finetune endlessly.
    - Build early prototypes. Should you collect more, or additional data?
    - Should the task be reformulated?
- Overly complex machine learning systems are hard to maintain
    - See 'Machine Learning: The High Interest Credit Card of Technical Debt'



Real world evaluations

- Evaluate predictions, but also how outcomes improve *because of them*
- Beware of feedback loops: predictions can influence future input data
    - Medical recommendations, spam filtering, trading algorithms,...
- Evaluate algorithms *in the wild*.
    1. A/B testing: split users in groups, test different models in parallel
    2. Bandit testing: gradually direct more users to the winning system

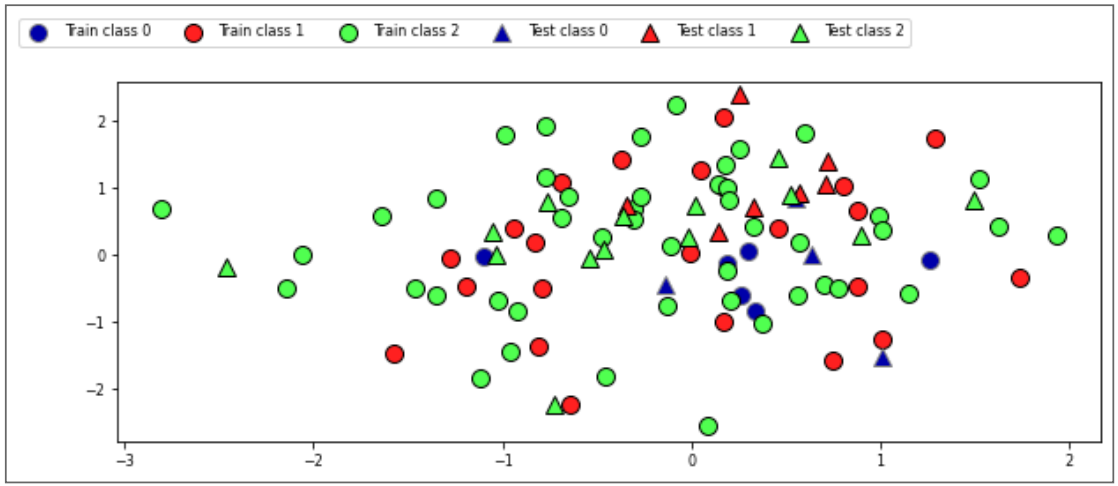
means here data we see



Example:
At least 10 links should be interesting->Recall
Not missing naything->Precision

Performance estimation techniques

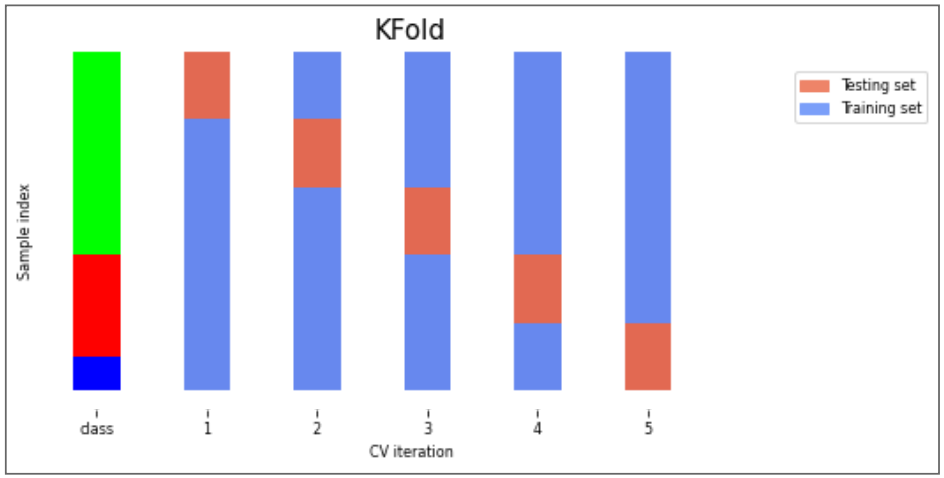
- Always evaluate models *as if they are predicting future data*
- We do not have access to future data, so we pretend that some data is hidden
- Simplest way: the *holdout* (simple train-test split)
    - *Randomly* split data (and corresponding labels) into training and test set (e.g. 75%-25%) one of the pitfall is that it introduces bias, and may sometimes mix up train test data
    - Train (fit) a model on the training data, score on the test data



K-fold Cross-validation

since the splits are completely independent so the ques of data independence does not arrise

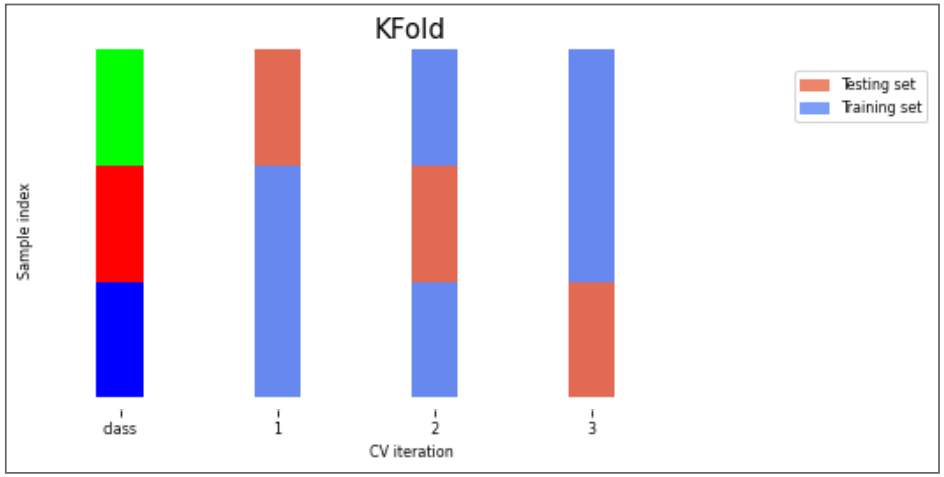
- Each random split can yield very different models (and scores)
    - e.g. all easy (of hard) examples could end up in the test set
- Split data into *k* equal-sized parts, called *folds*
    - Create *k* splits, each time using a different fold as the test set
- Compute *k* evaluation scores, aggregate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



Can you explain this result?

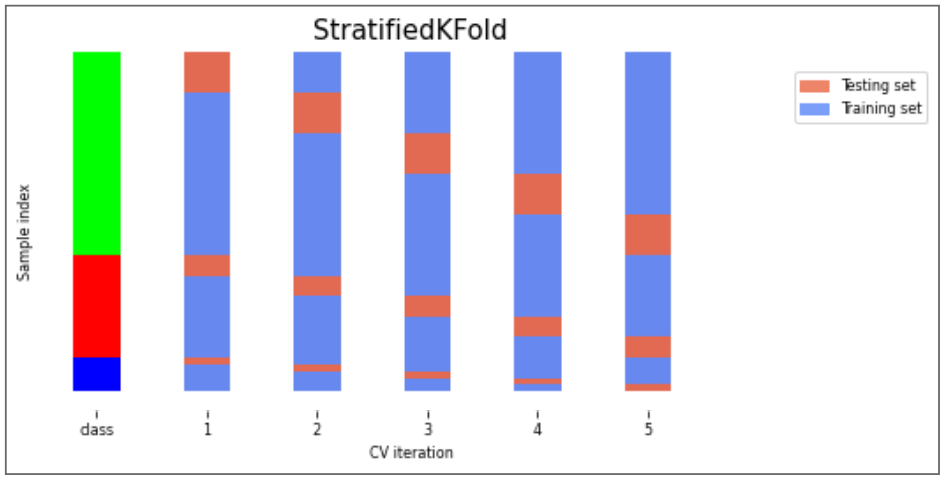
```
kfold = KFold(n_splits=3)
cross_val_score(logistic_regression, iris.data, iris.target, cv=kfold)
```

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



Stratified K-Fold cross-validation

- If the data is unbalanced, some classes have only few 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 strata into folds

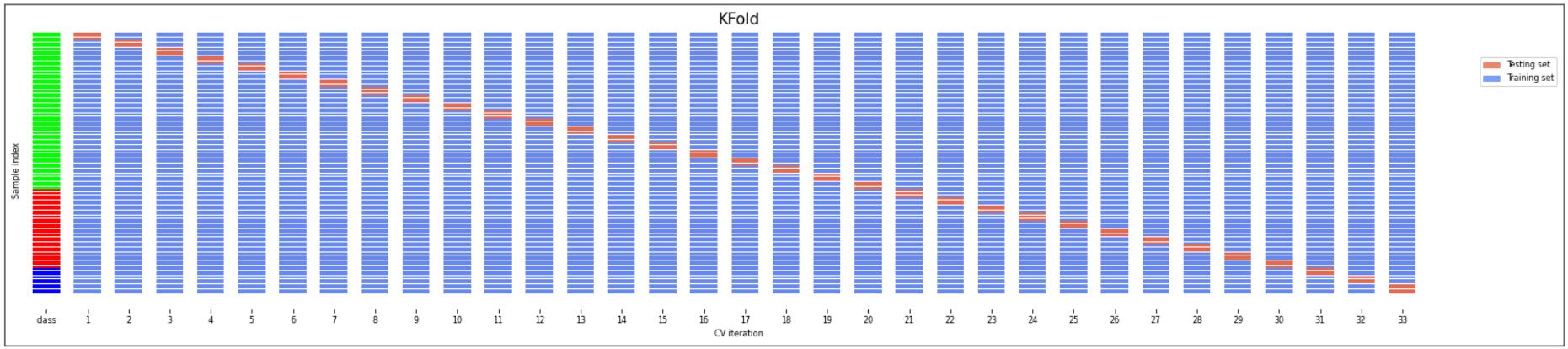


it is likely for every set same proportion of blue, red and green classes is distributed acroos the five. Blue->1/5. Red->1/5, Green ->1/5

also in this retraining five times does not occur but individual training occurs for 5 models independently

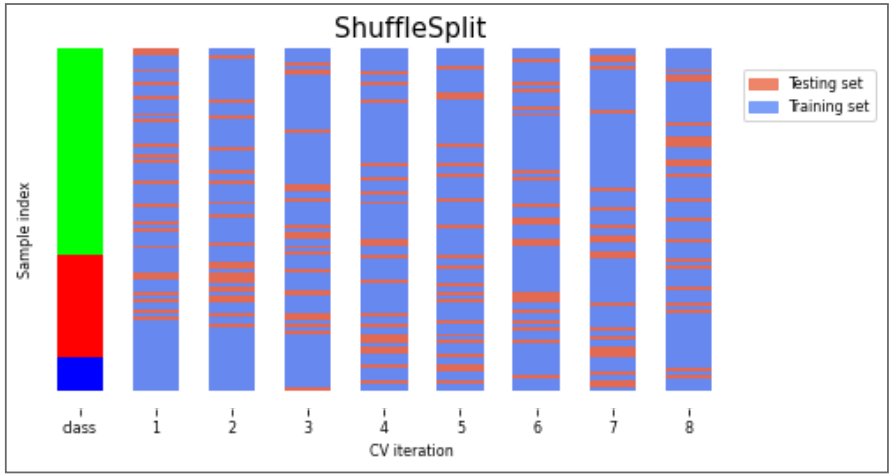
Leave-One-Out cross-validation

- *k* fold cross-validation with *k* equal to the number of samples
- Completely unbiased (in terms of data splits), but computationally expensive
- Actually 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



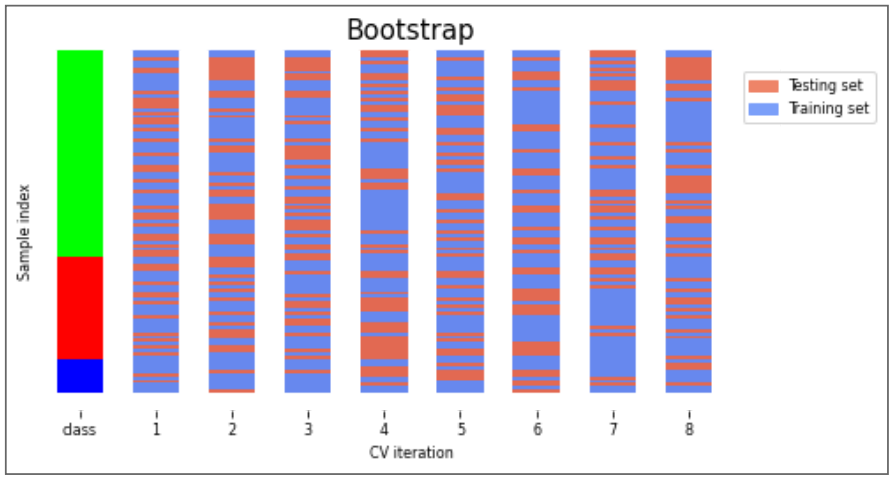
Shuffle-Split cross-validation

- Shuffles the data, samples (`train_size`) points randomly as the training set
- Can also use a smaller (`test_size`), handy with very large datasets
- Never use if the data is ordered (e.g. time series)



The Bootstrap possible to take same point twice

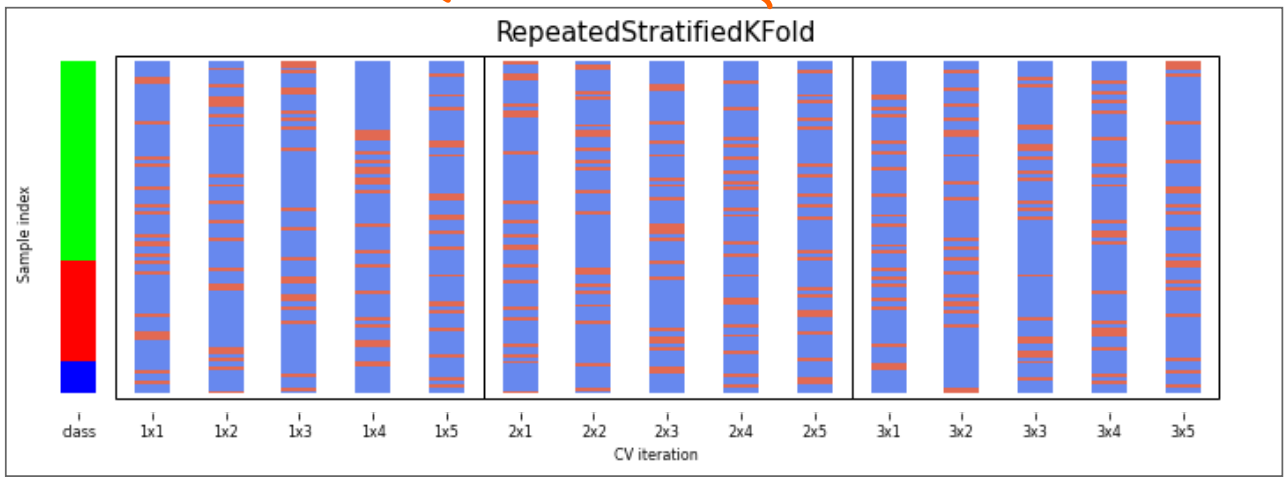
- Sample *n* (dataset size) data points, with replacement, as training set (the bootstrap)
    - On average, bootstraps include 66% of all data points (some are duplicates)
- Use the unsampled (out-of-bootstrap) samples as the test set
- Repeat k times to obtain k scores
- Similar to Shuffle-Split with `train_size=0.66`, `test_size=0.34` but without duplicates



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

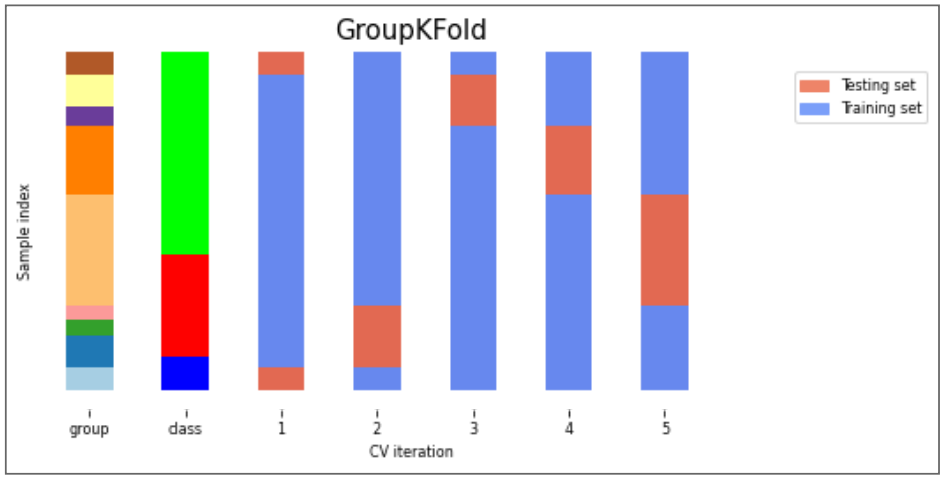
shuffle after every k iterations for a split



Cross-validation with groups

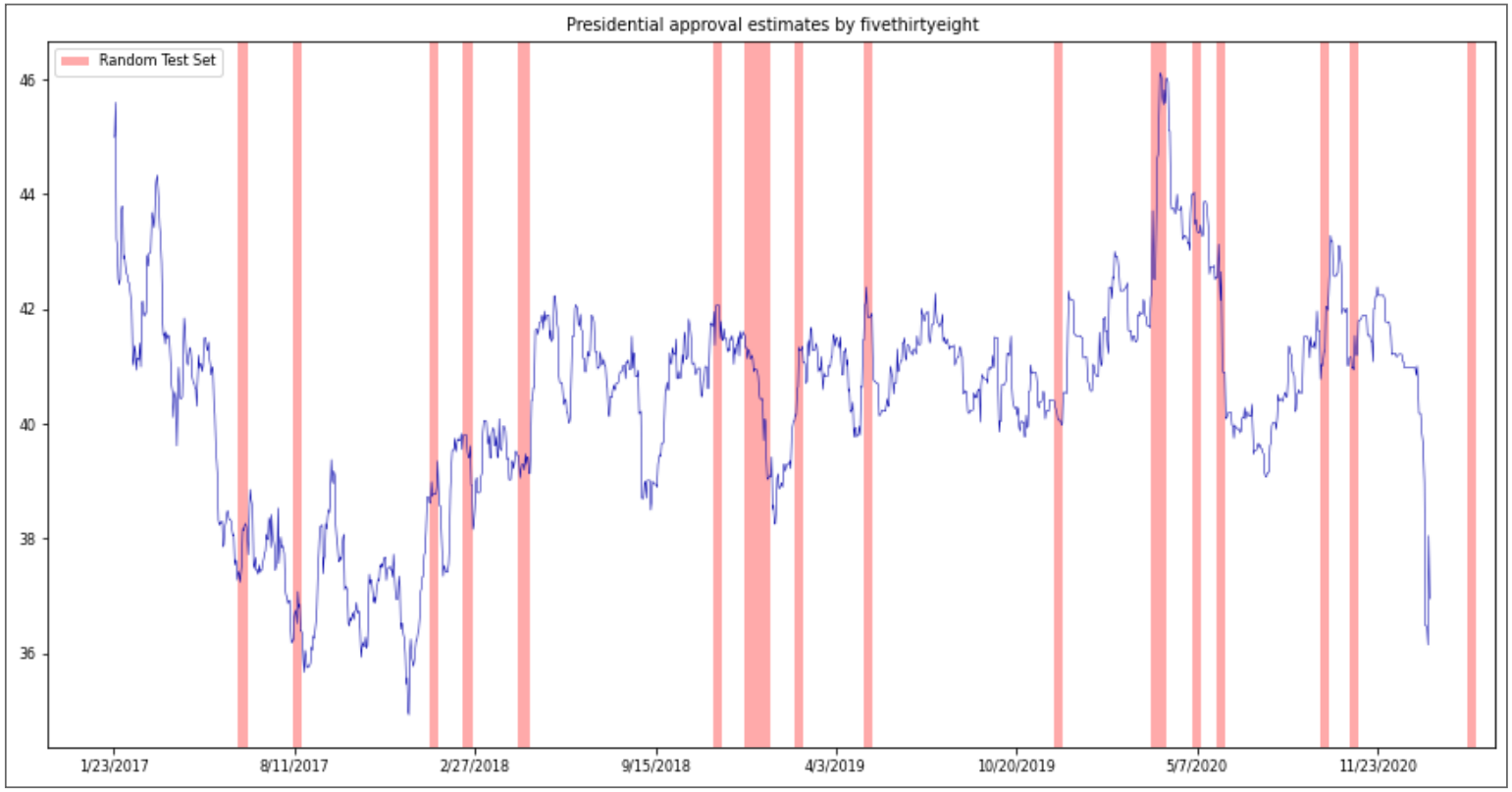
- Sometimes the data contains inherent groups:
  - Multiple samples from same patient, images from same person,...
- Data from the same person may end up in the training *and* test set
- We want to measure how well the model generalizes to *other* people
- Make sure that data from one person are in *either*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

to avoid shortcuts in training
we do not want data of same person en
ing in test and train set; this mayhamper
whether model generalises properly or not
.Ex-Model may pick upon weird ears



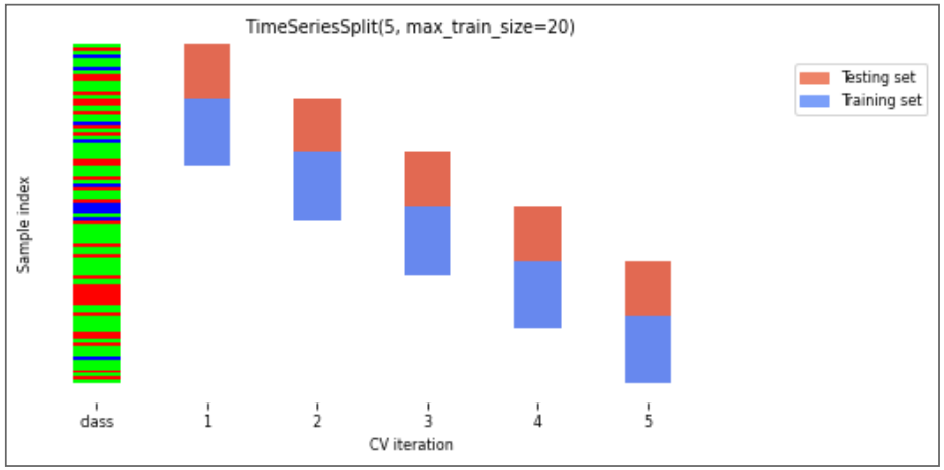
Time series

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



Test-then-train (prequential evaluation)

- Every new sample is evaluated only 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 the train set and the (k+1)th fold as the test set
    - Often, a maximum training set size (or window) is used
        - more robust against concept drift (change in data over time)



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 very small datasets (e.g. <100 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 for Classification

Evaluation vs Optimization

we cannot do that job with only loss

maybe utilising only accuracy

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

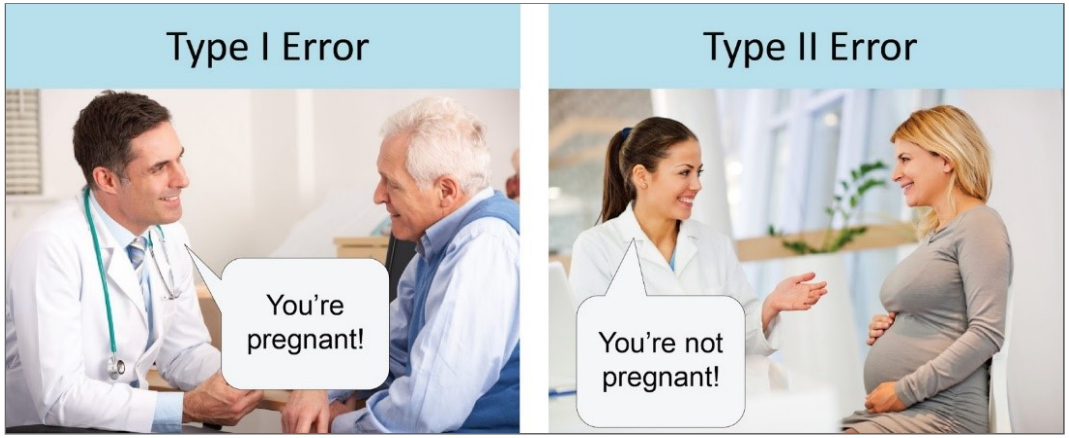
$$\mathcal{L}_{Ridge} = \sum_{n=1}^{N}(y_n - (\mathbf{wx_n} + w_0))^2 + \alpha \sum_{i=0}^{p} w_i^2$$

- The choice of function is limited by what can be efficiently optimized
- However, we *evaluate* the resulting model with a score that makes sense **in the real world**
    - Percentage of correct predictions (on a test set)
    - The actual cost of mistakes (e.g. in money, time, lives,...)
- 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 true label is negative
    - False Negative (type II error): model predicts negative while true label is positive
- They are not always equally important
    - Which side do you want to err on for a medical test?

fn more lethal, predicting no cancer when person has cencer



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
    - Count how often samples belonging to a class C are classified as C or any other class.
    - For binary classification, we label these true negative (TN), true positive (TP), false negative (FN), false positive (FP)

	Predicted Neg	Predicted Pos
Actual Neg	TN	FP
Actual Pos	FN	TP

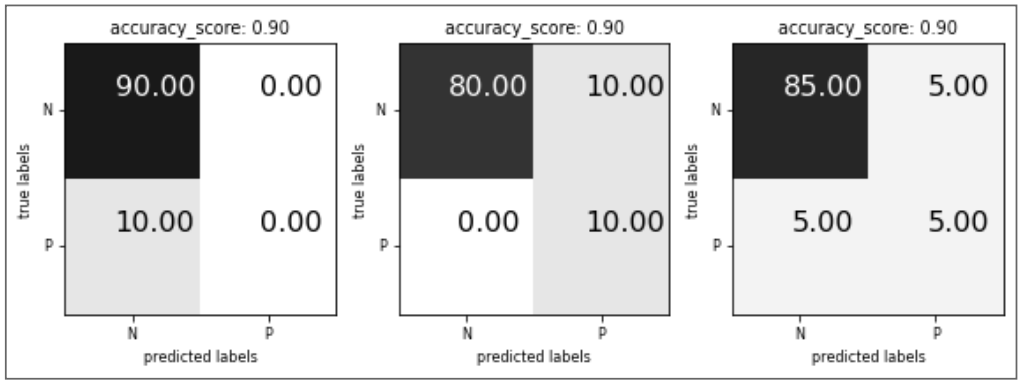
```
confusion_matrix(y_test, y_pred):
 [[48  5]
 [ 5 85]]
```

Predictive accuracy

- Accuracy can be computed based on the confusion matrix
- Not useful if the dataset is very imbalanced
    - E.g. credit card fraud: is 99.99% accuracy good enough?

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}} \tag{1}$$

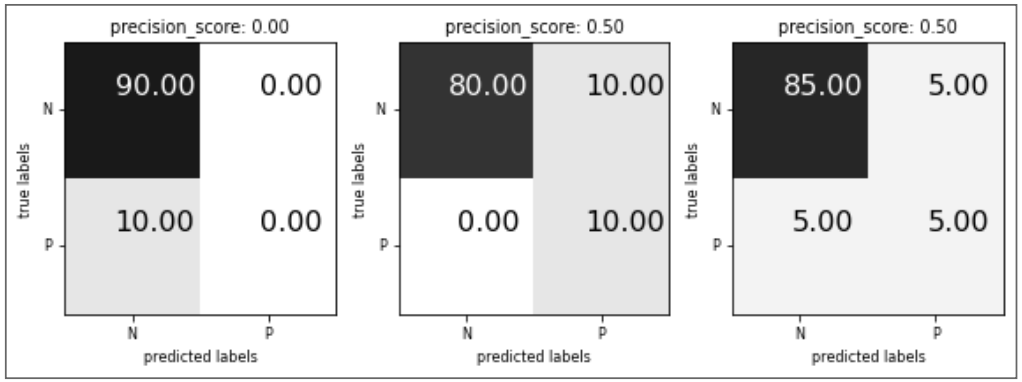
- 3 models: very different predictions, same accuracy:



Precision

- Use 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

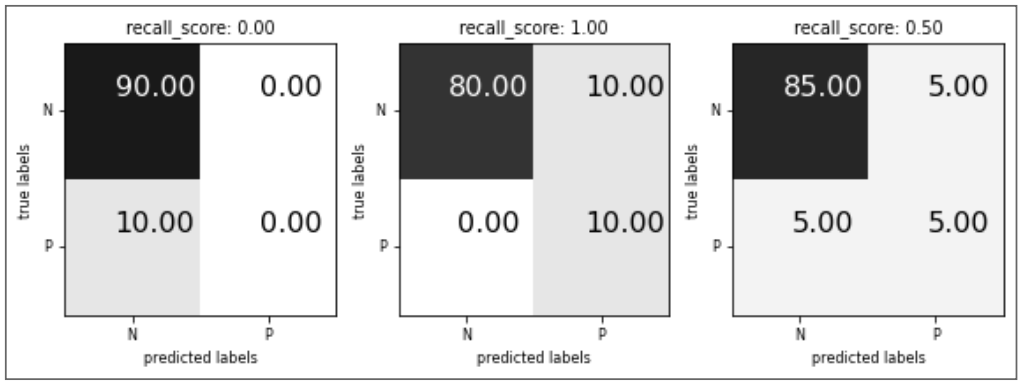
$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}} \tag{2}$$



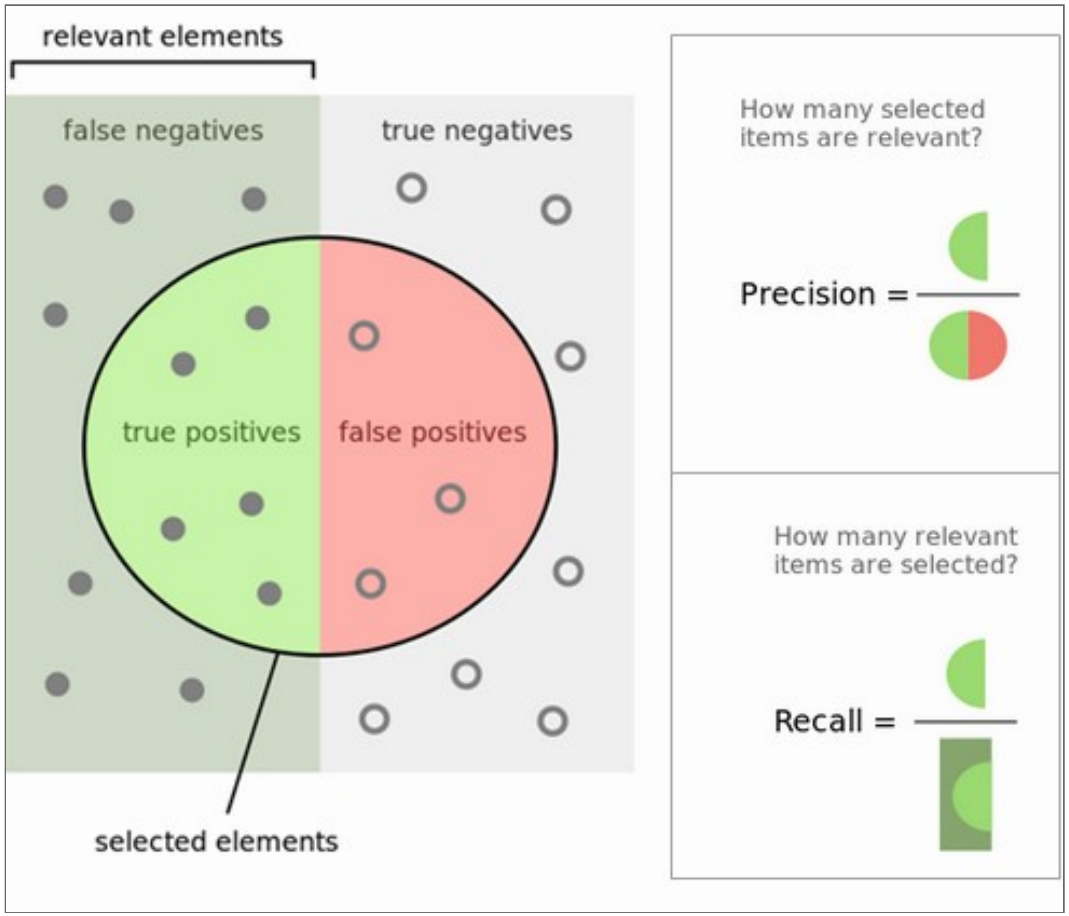
Recall

- Use 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)

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}} \tag{3}$$



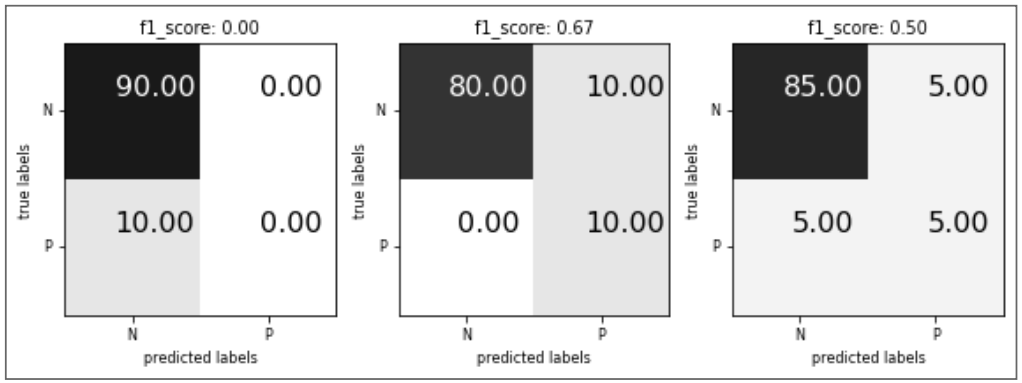
Comparison


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

- Trades off precision and recall:

$$\mathrm{F1} = 2 \cdot \frac{\mathrm{precision} \cdot \mathrm{recall}}{\mathrm{precision} + \mathrm{recall}} \tag{4}$$



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

Multi-class classification

- Train models *per class* : one class viewed as positive, other(s) als negative, then average
  - micro-averaging: count total TP, FP, TN, FN (every sample equally important) ?

example theft

    - micro-precision, micro-recall, micro-F1, accuracy are all the same

$$\text{Precision:} \frac{\sum_{c=1}^{C} \text{TP}_c}{\sum_{c=1}^{C} \text{TP}_c + \sum_{c=1}^{C} \text{FP}_c} \xrightarrow{c=2} \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}}$$

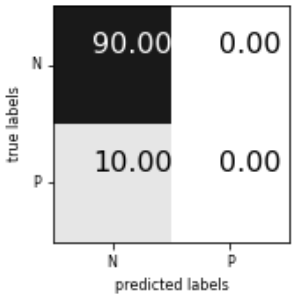
  - macro-averaging: average of scores $R(y_c, \hat{y}_c)$ obtained on each class

recommend books

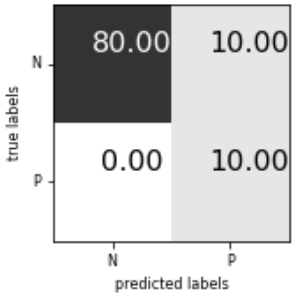
    - Preferable for imbalanced classes (if all classes are equally important) ?
    - macro-averaged recall is also called *balanced accuracy*

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

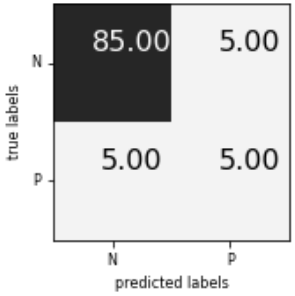
  - weighted averaging (w_c: ratio of examples of class c, aka support):
    $\sum_{c=1}^{C} w_c R(y_c, \hat{y}_c)$



	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

Other useful classification metrics

- Cohen's Kappa
  - Measures 'agreement' between different models (aka inter-rater agreement)
  - To evaluate a single model, compare it against a model that does random guessing
    - Similar to accuracy, but taking into account the possibility of predicting the right class by chance
  - Can be weighted: different misclassifications given different weights
  - 1: perfect prediction, 0: random prediction, negative: worse than random
  - With p_0 = accuracy, and p_e = accuracy of random classifier:

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

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- Matthews correlation coefficient
  - Corrects for imbalanced data, alternative for balanced accuracy or AUROC
  - 1: perfect prediction, 0: random prediction, -1: inverse prediction

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

Probabilistic evaluation

- 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

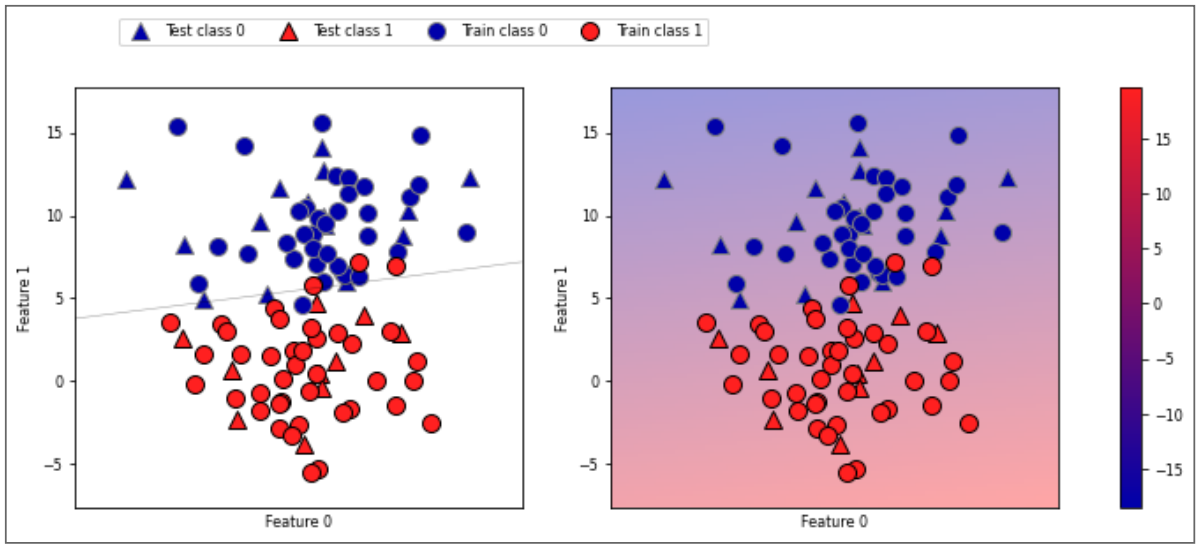
$$\hat{y} = w_0 * x_0 + w_1 * x_1 + \ldots + w_p * x_p + b$$

- In practice, you are often interested in how certain a classifier is about each class prediction (e.g. cancer treatments).
- Most learning methods can return at least one measure of *confidence* in their predicions.
    - Decision function: floating point value for each sample (higher: more confident)
    - Probability: estimated probability for each class

The decision function

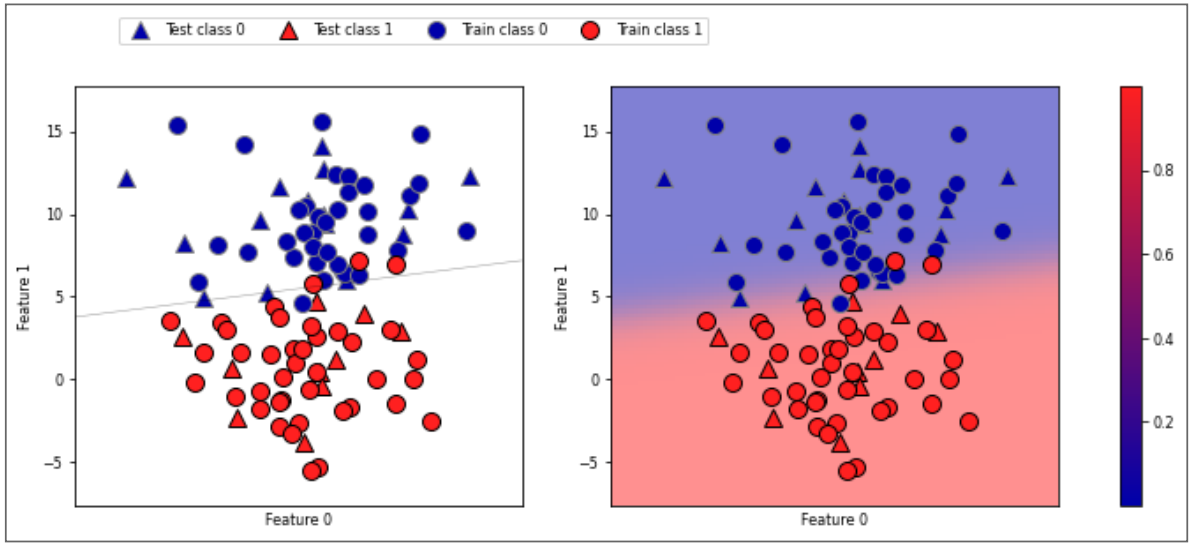
In the binary classification case, the return value of the decision function encodes how strongly the model believes a data point belongs to the “positive” class.

- Positive values indicate preference for the positive class.
- The range can be arbitrary, and can be affected by hyperparameters. Hard to interpret.



Predicting probabilities

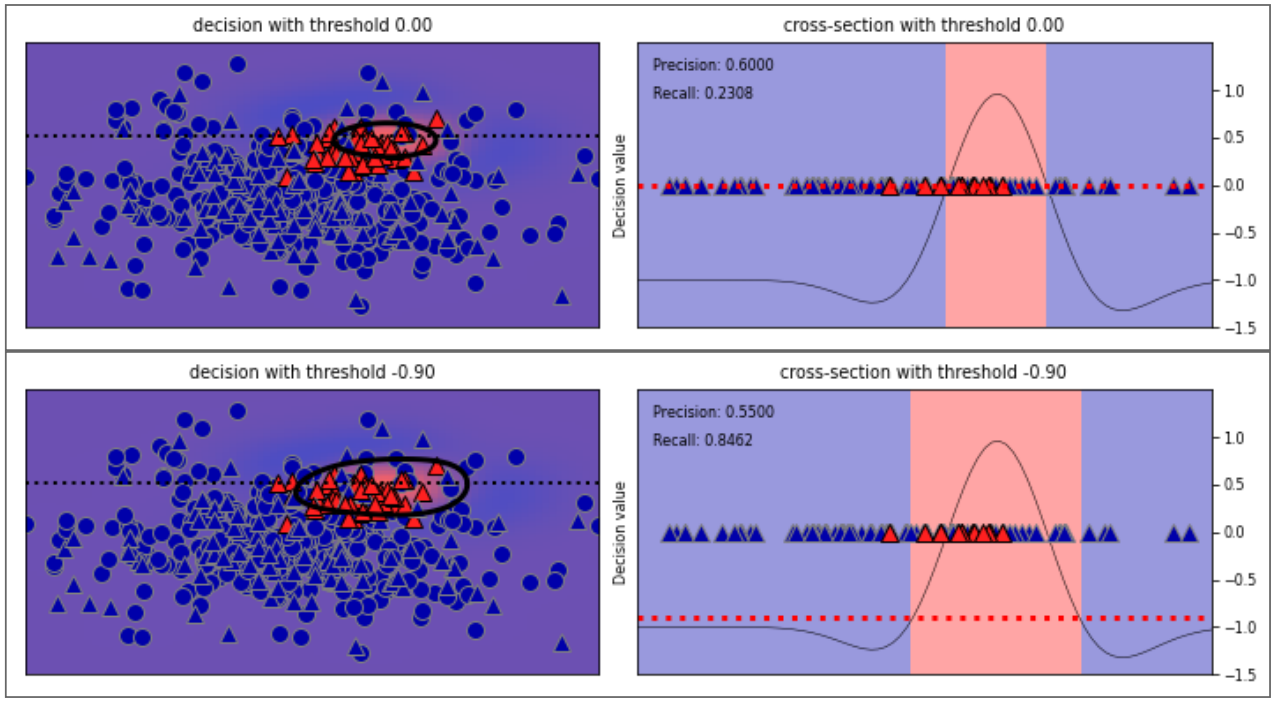
Some models can also return a *probability* for each class with every prediction. These sum up to 1. We can visualize them again. Note that the gradient looks different now.



Threshold calibration

- By default, we threshold at 0 for `decision_function` and 0.5 for `predict_proba`
- Depending on the application, you may want to threshold differently
    - Lower threshold yields fewer FN (better recall), more FP (worse precision), and vice-versa

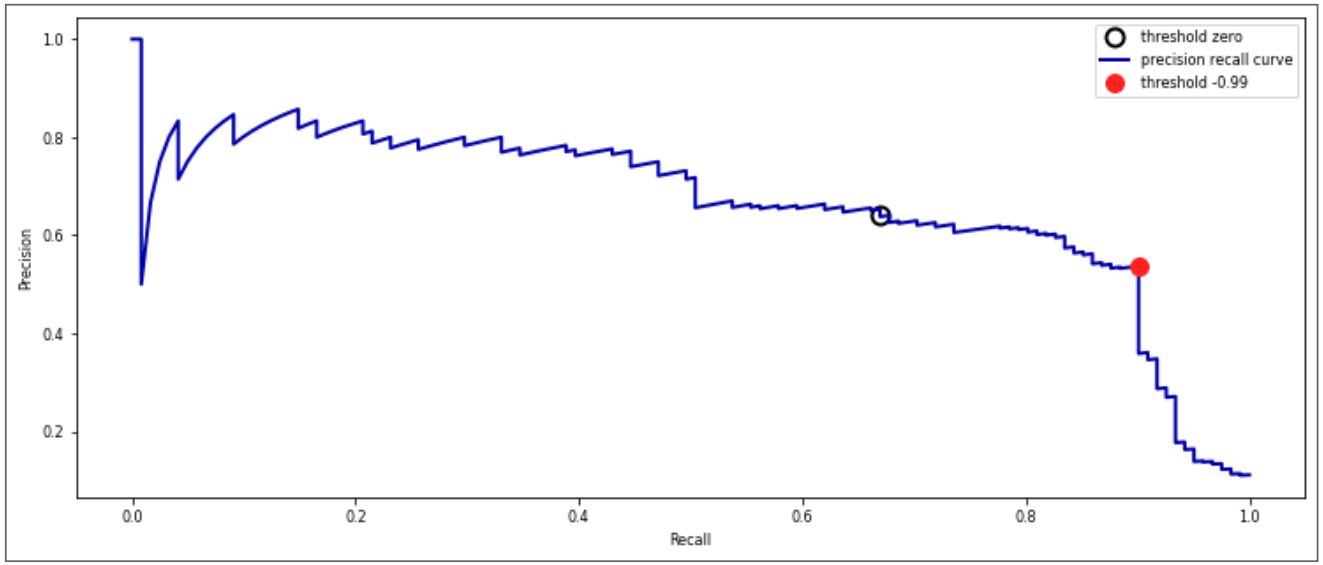
inside points red outside points blue



SVC

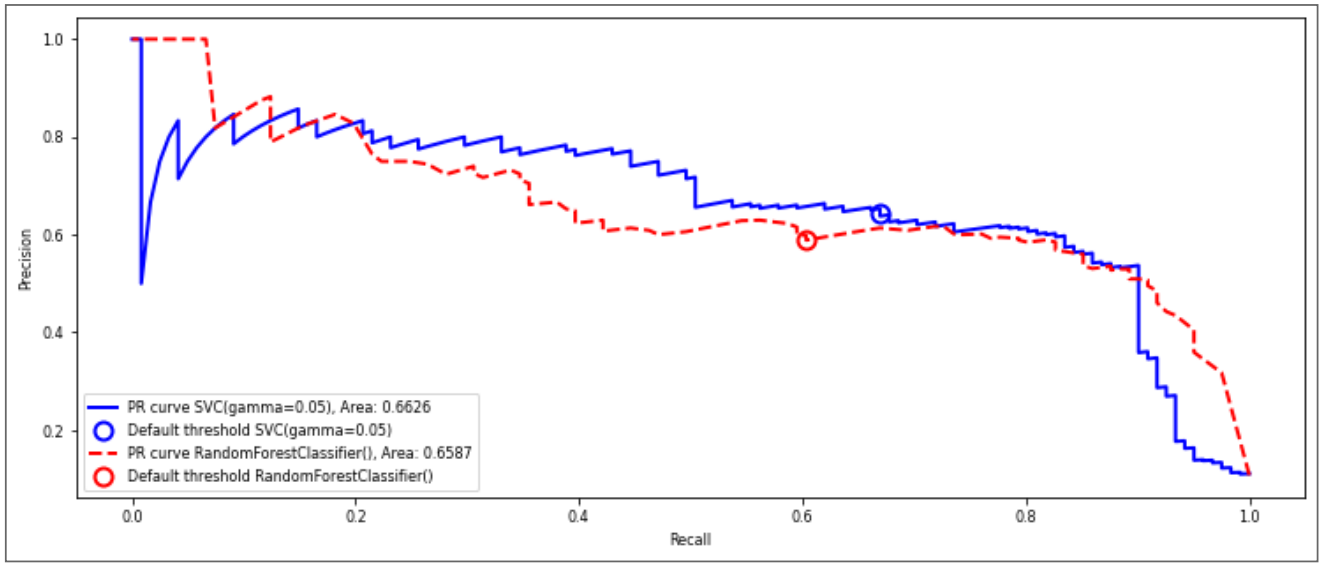
Precision-Recall curve

- The best trade-off between precision and recall depends on your application
    - 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**
    - Change the treshold until you find a sweet spot in the precision-recall trade-off
    - Often jagged at high thresholds, when there are few positive examples left



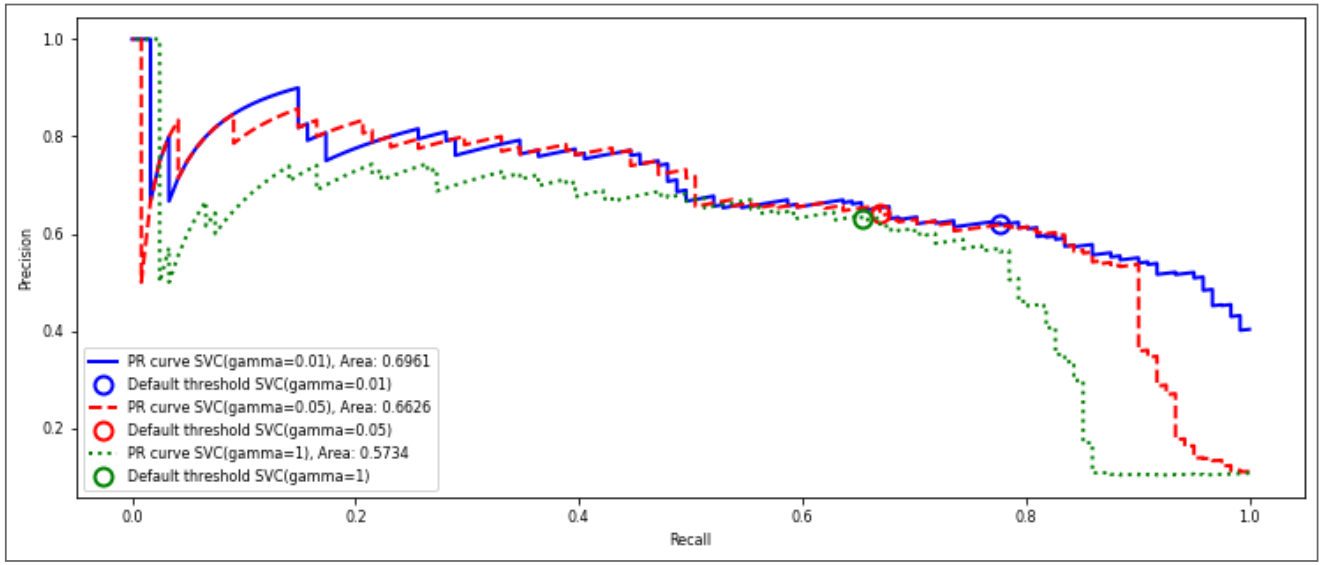
Model selection

- Some models can achieve trade-offs that others can't
- Your application may require very high recall (or very high precision)
    - Choose the model that offers the best trade-off, given your application
- The area under the PR curve (AUPRC) gives the *best overall* model



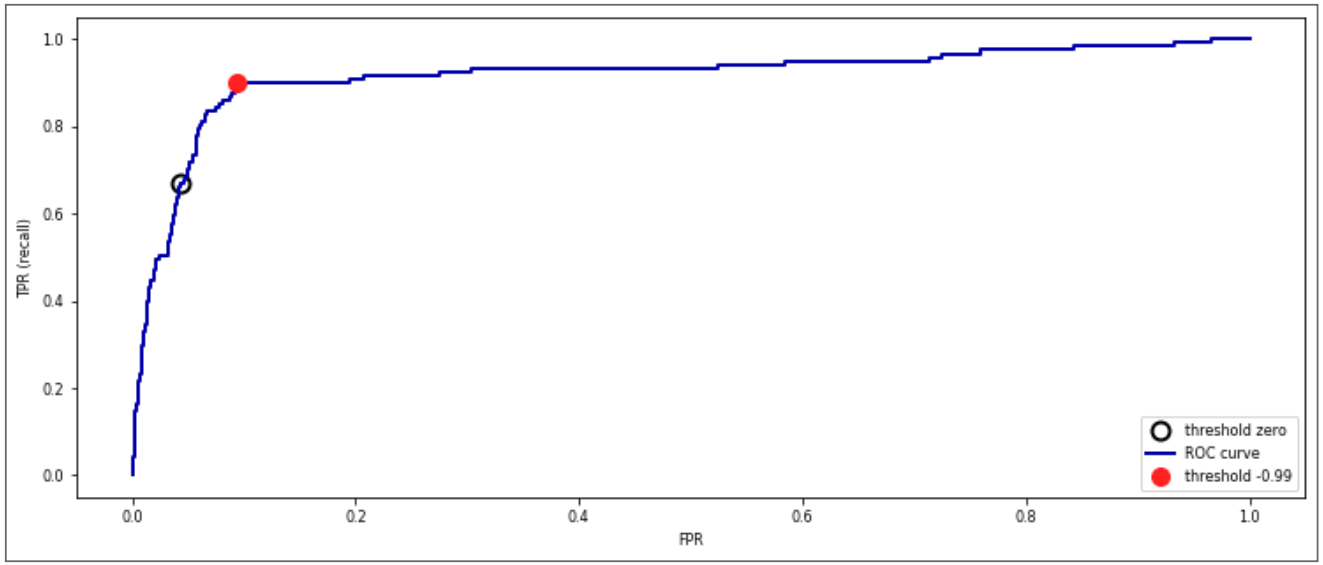
Hyperparameter effects

Of course, hyperparameters affect predictions and hence also the shape of the curve



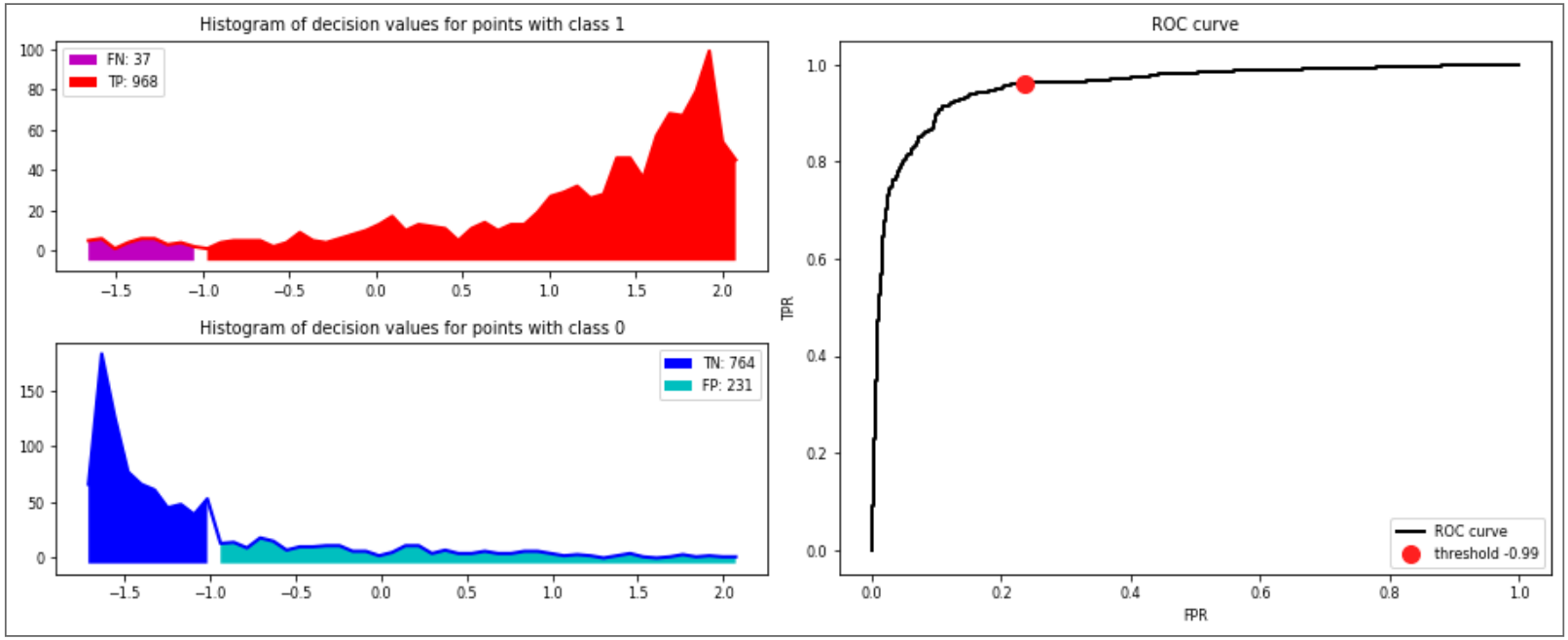
Receiver Operating Characteristics (ROC)

- Trade off *true positive rate* $TPR = \frac{TP}{TP+FN}$ with *false positive rate* $FPR = \frac{FP}{FP+TN}$
- Plotting TPR against FPR *for all possible thresholds* yields a *Receiver Operating Characteristics curve*
    - Change the treshold until you find a sweet spot in the TPR-FPR trade-off
    - Lower thresholds yield higher TPR (recall), higher FPR, and vice versa



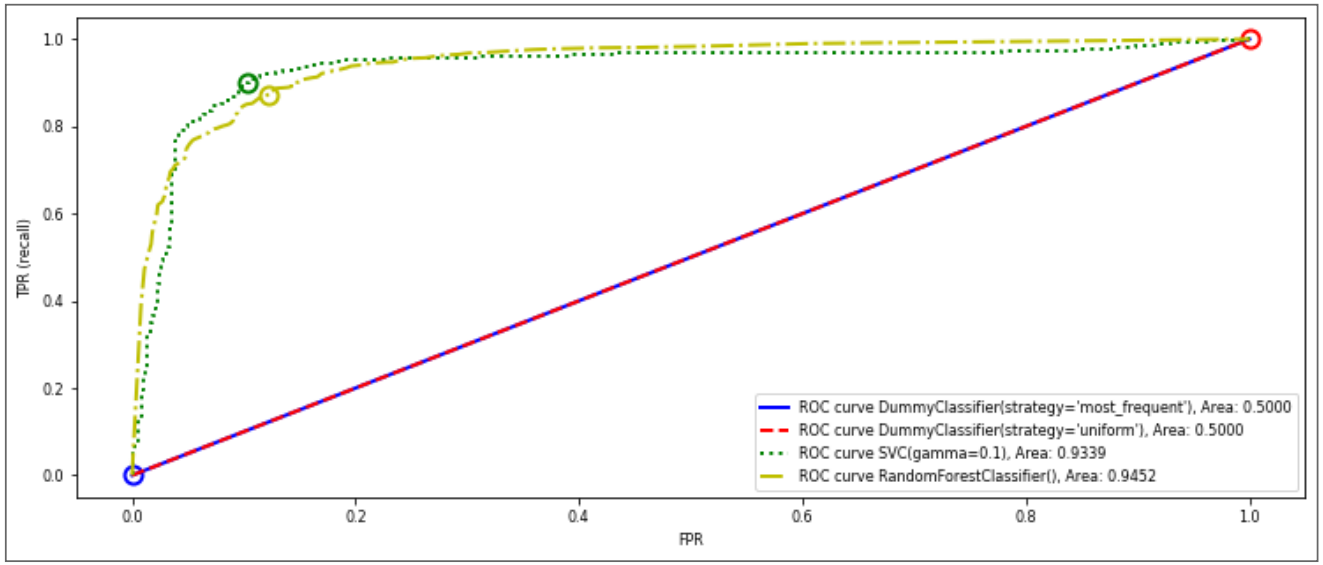
Visualization

- Histograms show the amount of points with a certain decision value (for each class)
- $TPR = \frac{TP}{TP+FN}$ can be seen from the positive predictions (top histogram)
- $FPR = \frac{FP}{FP+TN}$ can be seen from the negative predictions (bottom histogram)



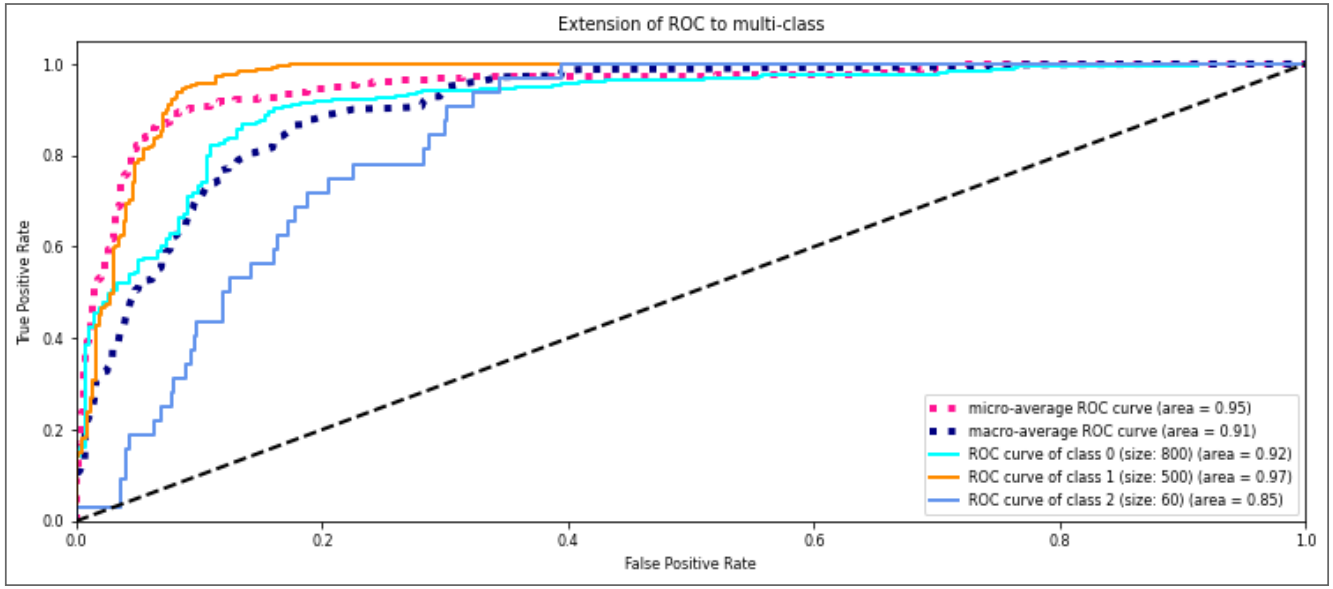
Model selection

- Again, some models can achieve trade-offs that others can't
- Your application may require minizing FPR (low FP), or maximizing TPR (low FN)
- The area under the ROC curve (AUROC or AUC) gives the *best overall* model
    - Frequently used for evaluating models on imbalanced data
    - Random guessing (TPR=FPR) or predicting majority class (TPR=FPR=1): 0.5 AUC



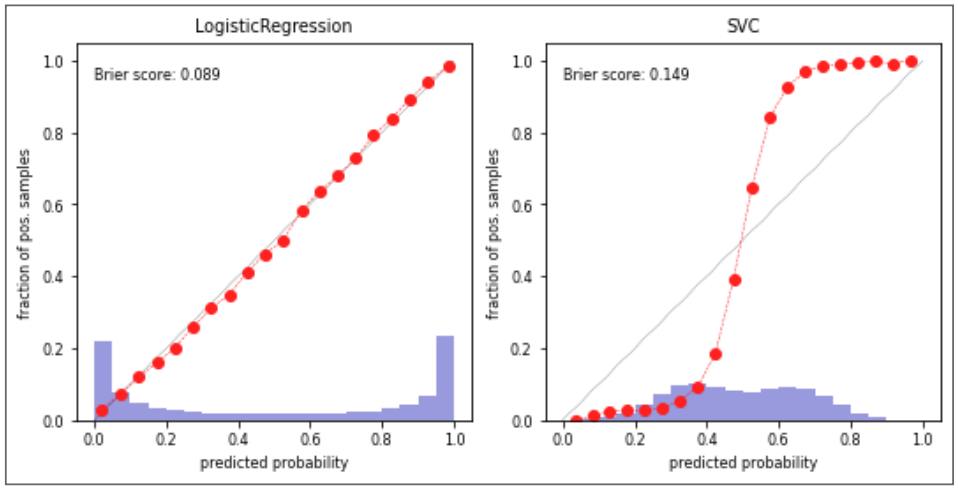
Multi-class AUROC (or AUPRC)

- We again need to choose between micro- or macro averaging TPR and FPR.
  - Micro-average if every sample is equally important (irrespective of class)
  - Macro-average if every class is equally important, especially for imbalanced data



Model calibration

- For some models, the *predicted* uncertainty does not reflect the *actual* uncertainty
    - If a model is 90% sure that samples are positive, is it also 90% accurate on these?
- A model is called *calibrated* if the reported uncertainty actually matches how correct it is
    - Overfitted models also tend to be over-confident
    - LogisticRegression models are well calibrated since they learn probabilities
    - SVMs are not well calibrated. *Biased* towards points close to the decision boundary.



Brier score

- You may want to select models based on how accurate the class confidences are.
- The **Brier score loss**: squared loss between predicted probability $\hat{p}$ and actual outcome y
    - Lower is better

$$\mathcal{L}_{Brier} = \frac{1}{n}\sum_{i=1}^{n}(\hat{p}_i - y_i)^2$$

```
Logistic Regression Brier score loss: 0.0322
SVM Brier score loss: 0.0795
```

Model calibration techniques

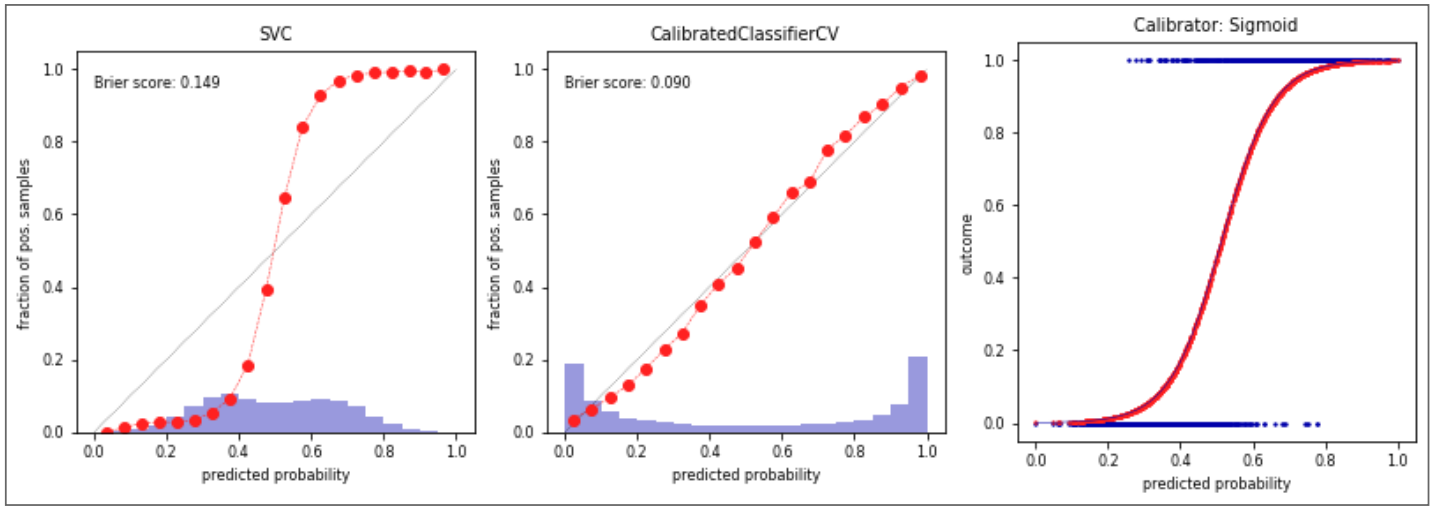
- We can post-process trained models to make them more calibrated.
- Fit a regression model (a calibrator) to map the model's outcomes $f(x)$ to a calibrated probability in [0,1]
    - $f(x)$ returns the decision values or probability estimates
    - f_{calib} is fitted on the training data to map these to the correct outcome
        - Often an internal cross-validation with few folds is used
    - Multi-class models require one calibrator per class

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

Platt Scaling

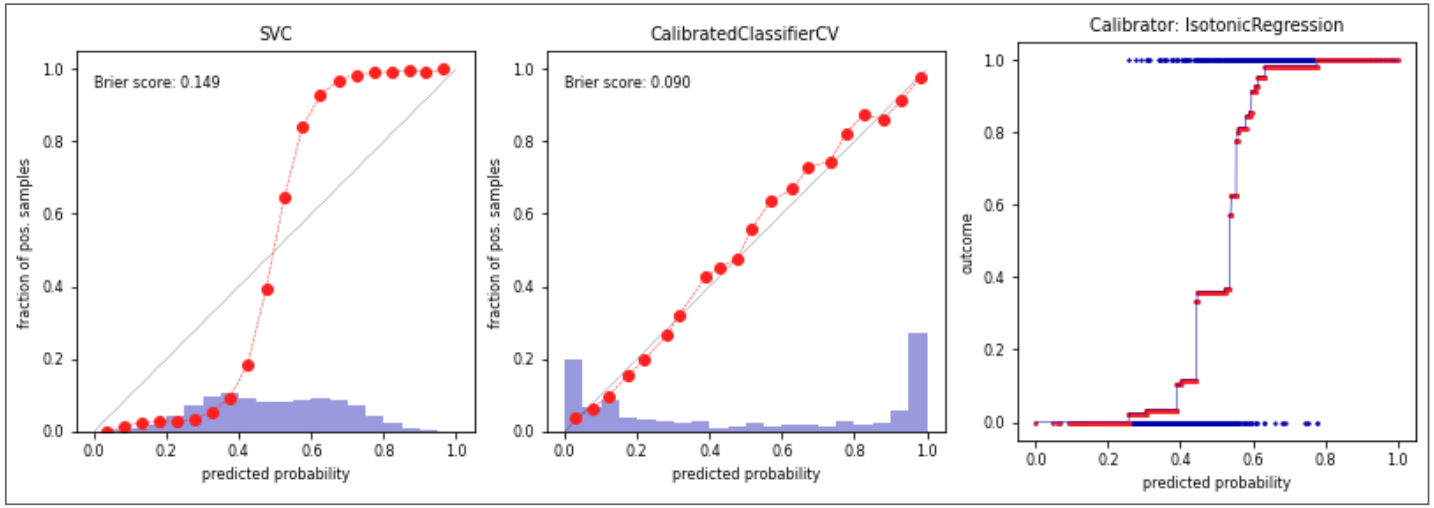
- Calibrator is a logistic (sigmoid) function:
  - Learn the weight w_1 and bias w_0 from data

$$f_{platt} = \frac{1}{1 + \exp(-w_1 f(x) - w_0)}$$



Isotonic regression

- Maps input x_i to an output $\hat{y}_i$ so that $\hat{y}_i$ increases monotonically with x_i and minimizes loss $\sum_i^n (y_i - \hat{y}_i)$
    - Predictions are made by interpolating the predicted $\hat{y}_i$
- Fit to minimize the loss between the uncalibrated predictions $f(x)$ and the actual labels
- Corrects any monotonic distortion, but tends to overfit on small samples



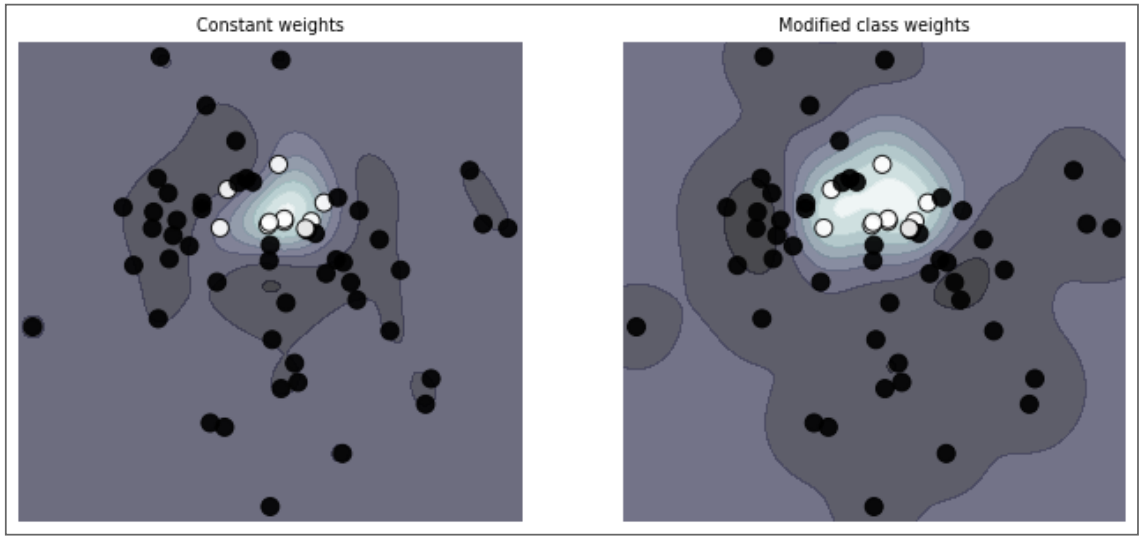
Cost-sensitive classification (dealing with imbalance)

- In the real worlds, different kinds of misclassification can have different costs
    - Misclassifying certain classes can be more costly than others
    - Misclassifying certain samples can be more costly than others
- Cost-sensitive resampling: resample (or reweight) the data to represent real-world expectations
    - oversample minority classes (or undersample majority) to 'correct' imbalance
    - increase weight of misclassified samples (e.g. in boosting)
    - decrease weight of misclassified (noisy) samples (e.g. in model compression)

Class weighting

- If some classes are more important than others, we can give them more weight
    - E.g. for imbalanced data, we can give more weight to minority classes
- Most classification models can include it in their loss function and optimize for it
    - E.g. Logistic regression: add a class weight w_c in the log loss function

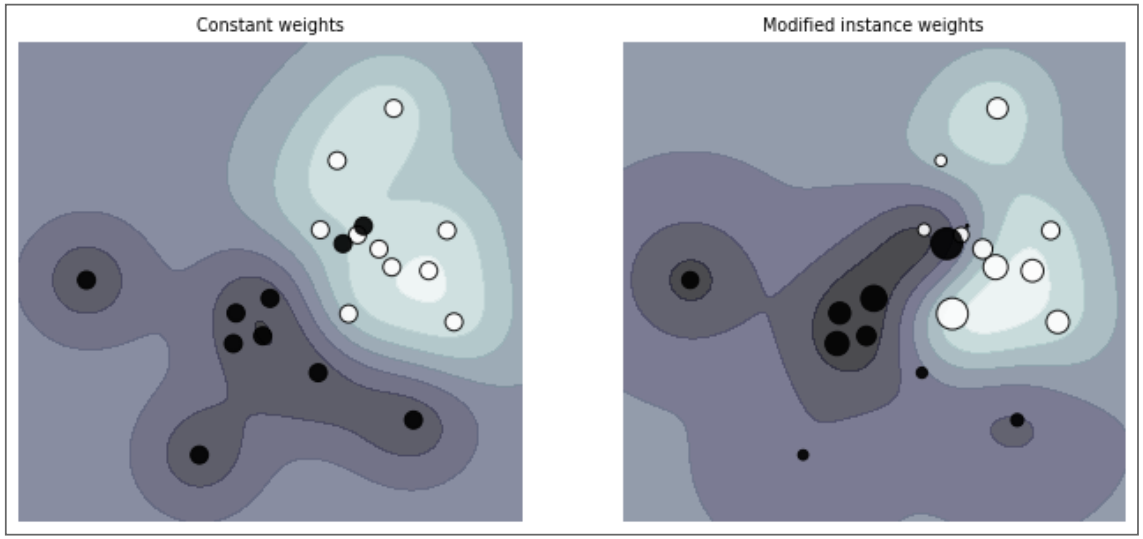
$$\mathcal{L}_{log}(\mathbf{w}) = -\sum_{c=1}^{C} w_c \sum_{n=1}^{N} p_{n,c} log(q_{n,c})$$



Instance weighting

- If some *training instances* are important to get right, we can give them more weight
    - E.g. when some examples are from groups underrepresented in the data
- These are passed during training (fit), and included in the loss function
    - E.g. Logistic regression: add a instance weight w_n in the log loss function

$$\mathcal{L}_{log}(\mathbf{w}) = -\sum_{c=1}^{C}\sum_{n=1}^{N} w_n p_{n,c} log(q_{n,c})$$



Cost-sensitive algorithms

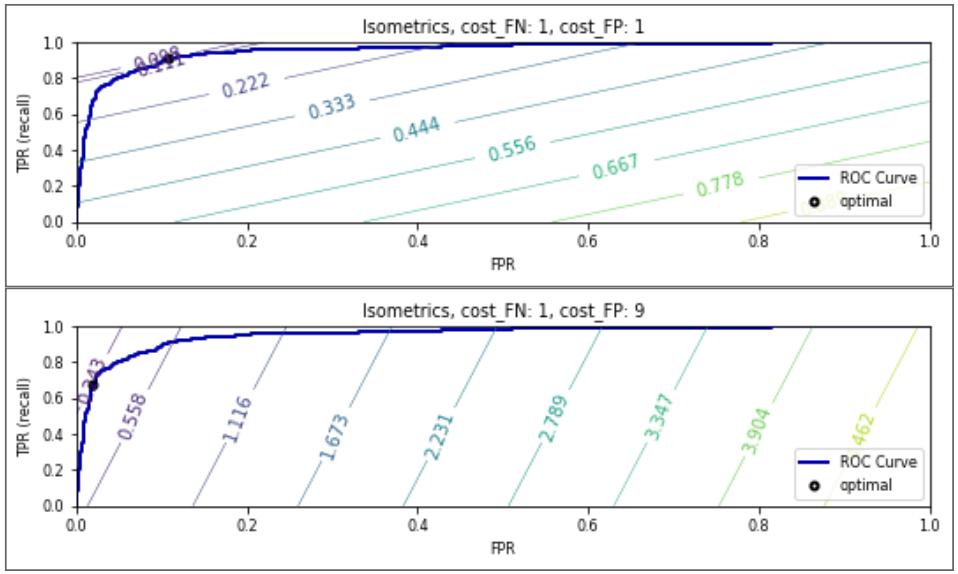
- Cost-sensitive algorithms
  - If misclassification cost of some classes is higher, we can give them higher weights
  - Some support *cost matrix* C: costs $c_{i,j}$ for every possible type of error
- Cost-sensitive ensembles: convert cost-insensitive classifiers into cost-sensitive ones
  - MetaCost: Build a model (ensemble) to learn the class probabilities $P(j|x)$
    - Relabel training data to minimize expected cost: $\operatorname{argmin}_i \sum_j P_j(x) c_{i,j}$
    - Accuracy may decrease but cost decreases as well.
  - AdaCost: Boosting with reweighting instances to reduce costs

Tuning the decision threshold

- If every FP or FN has a certain cost, we can compute the total cost for a given model:

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

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



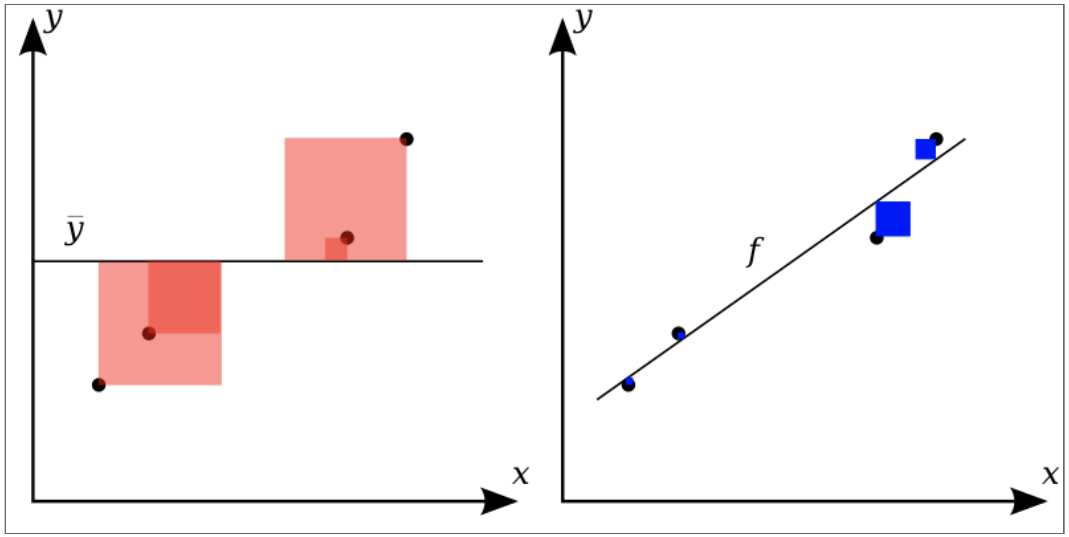
Regression metrics

Most commonly used are

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

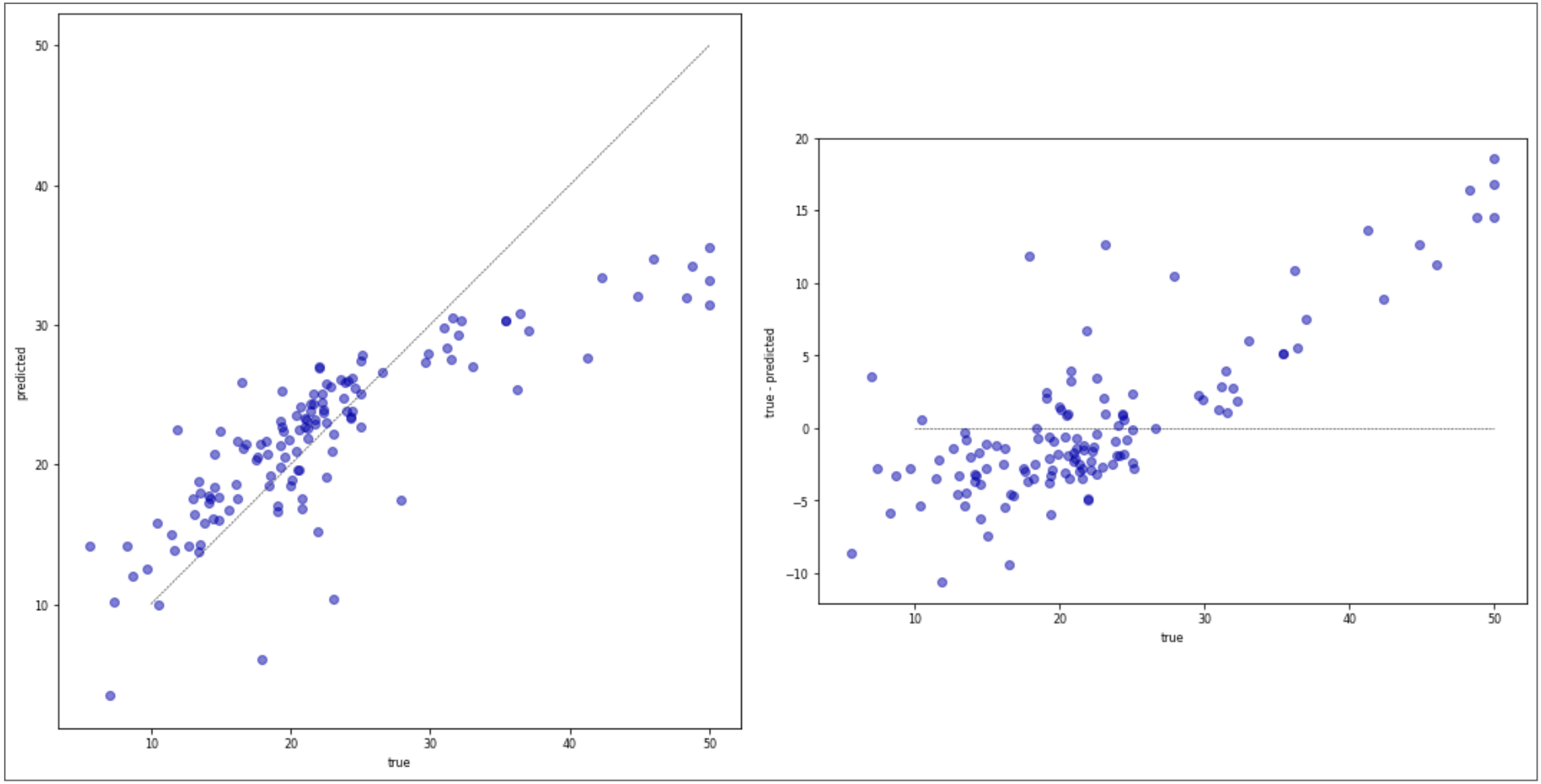
R squared

- $R^2 = 1 - \frac{\sum_i (y_{pred_i} - y_{actual_i})^2}{\sum_i (y_{mean} - y_{actual_i})^2}$
  - 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 regression 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



Bias-Variance decomposition

- Evaluate the same algorithm multiple times on different random samples of the data
- Two types of errors can be observed:
    - Bias error: systematic error, independent of the training sample
        - These points are predicted (equally) wrong every time
    - Variance error: error due to variability of the model w.r.t. the training sample
        - These points are sometimes predicted accurately, sometimes inaccurately

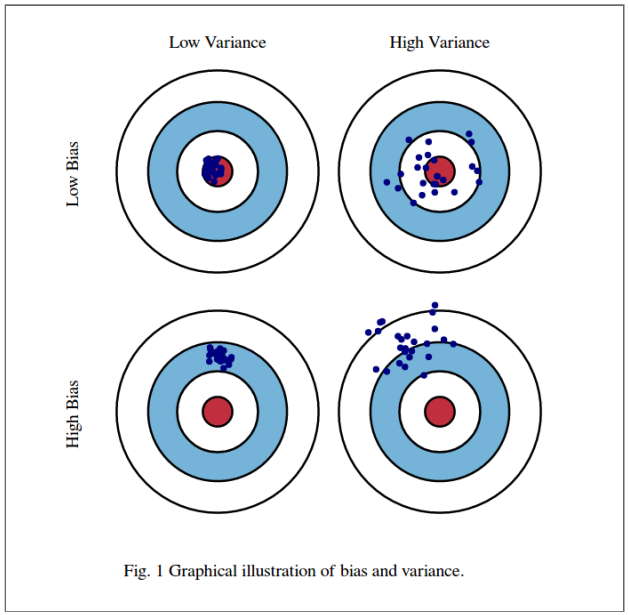


Fig. 1 Graphical illustration of bias and variance.

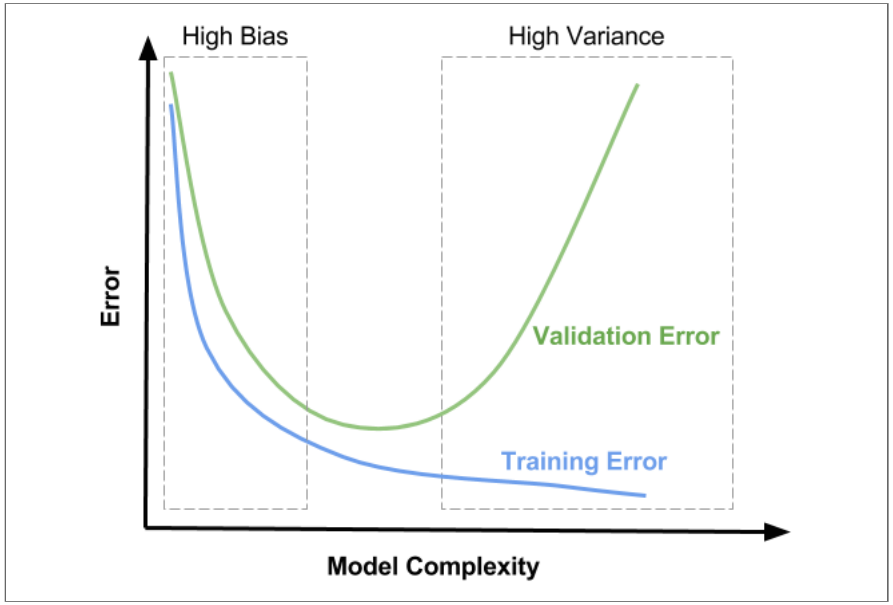
Computing bias and variance error

- 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: $\sum_x bias(x)^2 * w_x$ w_x: the percentage of times x occurs in the test sets
- Total variance: $\sum_x variance(x) * w_x$

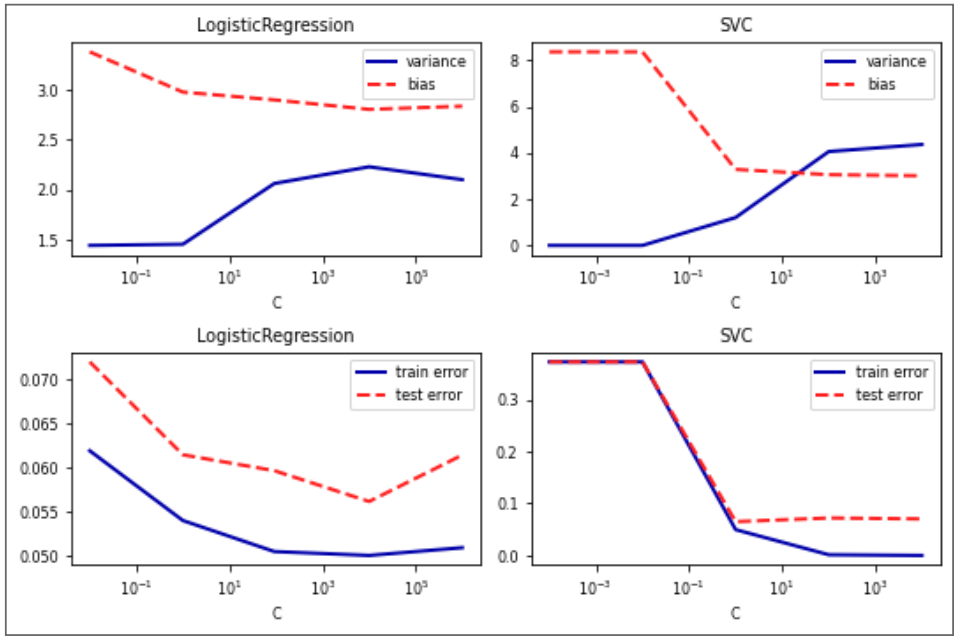
Bias and variance, underfitting and overfitting

- High variance means that you are likely overfitting
    - Use more regularization or use a simpler model
- High bias means that you are likely underfitting
    - Do less regularization or use a more flexible/complex model
- Ensembling techniques (see later) reduce bias or variance directly
    - Bagging (e.g. RandomForests) reduces variance, Boosting reduces bias

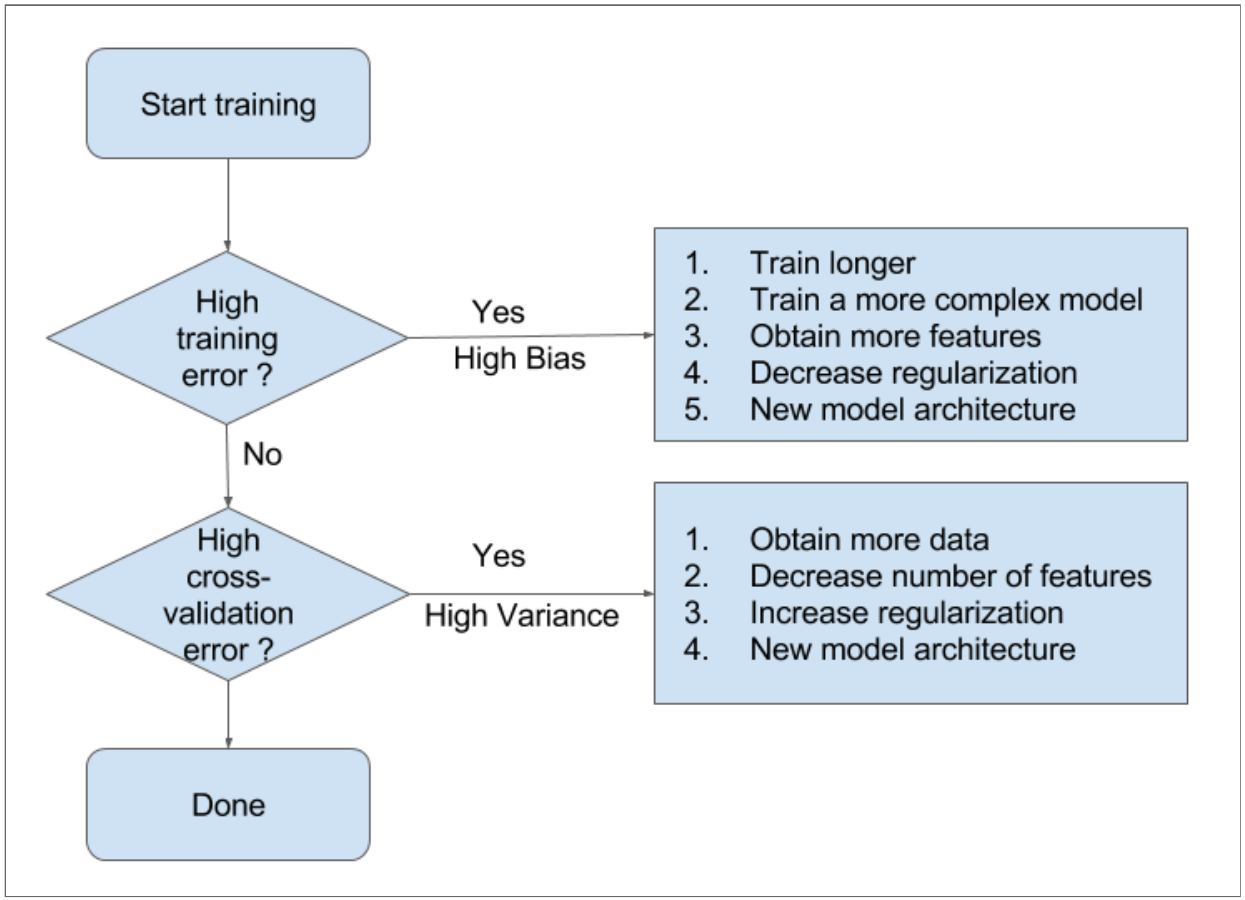


Understanding under- and overfitting

- Regularization reduces variance error (increases stability of predictions)
    - But too much increases bias error (inability to learn 'harder' points)
- High regularization (left side): Underfitting, high bias error, low variance error
    - High training error and high test error
- Low regularization (right side): Overfitting, low bias error, high variance error
    - Low training error and higher test error

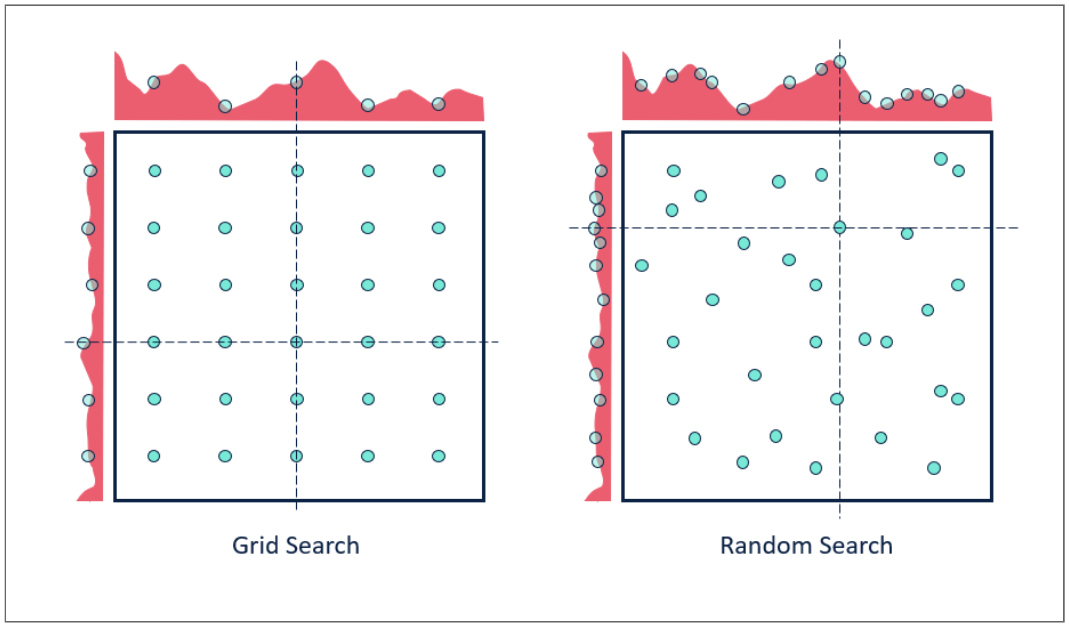


Summary Flowchart (by Andrew Ng)

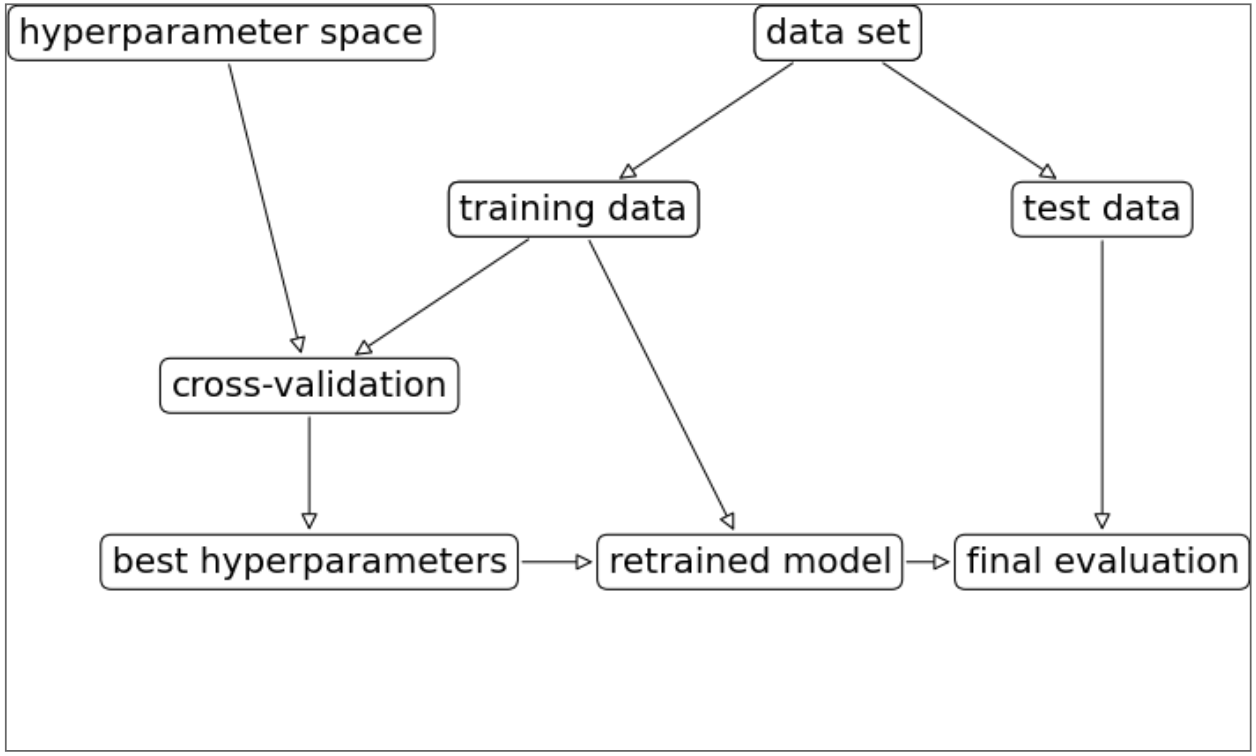


Hyperparameter tuning

- There exists a huge range of techniques to tune hyperparameters. The simplest:
    - Grid search: Choose a range of values for every hyperparameter, try every combination
        - Doesn't scale to many hyperparameters (combinatorial explosion)
    - Random search: Choose random values for all hyperparameters, iterate n times
        - Better, especially when some hyperparameters are less important
- Many more advanced techniques exist, see lecture on Automated Machine Learning



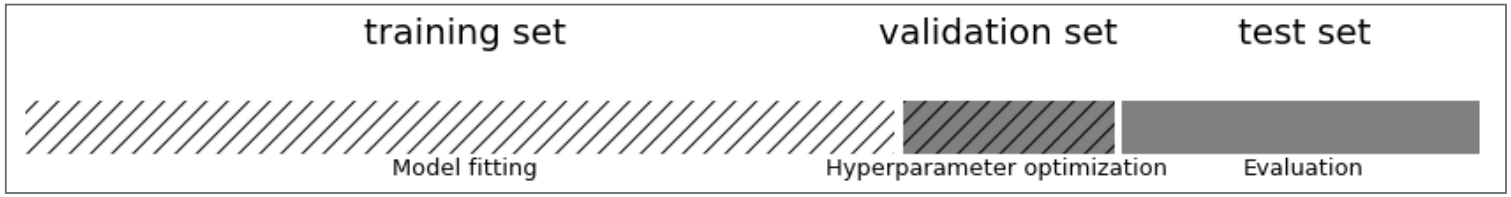
- First, split the data in training and test sets (outer split)
- Split up the training data again (inner cross-validation)
    - Generate hyperparameter configurations (e.g. random/grid search)
    - Evaluate all configurations on all inner splits, select the best one (on average)
- Retrain best configurations on full training set, evaluate on held-out test data



Nested cross-validation

- Simplest approach: single outer split and single inner split (shown below)
- Risk of over-tuning hyperparameters on specific train-test split
    - Only recommended for very large datasets
- Nested cross-validation:
    - Outer loop: split full dataset in k_1 training and test splits
    - Inner loop: split training data into k_2 train and validation sets
- This yields k_1 scores for k_1 possibly different hyperparameter settings
    - Average score is the expected performance of the tuned model
- To use the model in practice, retune on the **entire** dataset

```
hps = {'C': expon(scale=100), 'gamma': expon(scale=.1)}
scores = cross_val_score(RandomizedSearchCV(SVC(), hps, cv=3), X, y, cv=5)
```



Summary

- Split the data into training and test sets according to the application
    - Holdout only for large datasets, cross-validation for smaller ones
    - For classification, always use stratification
    - Grouped or ordered data requires special splitting
- Choose a metric that fits your application
    - E.g. precision to avoid false positives, recall to avoid false negatives
- Calibrate the decision threshold to fit your application
    - ROC curves or Precision-Recall curves can help to find a good tradeoff
- If possible, include the actual or relative costs of misclassifications
    - Class weighting, instance weighting, ROC isometrics can help
    - Be careful with imbalanced or unrepresentative datasets
- When using the predicted probabilities in applications, calibrate the models
- Always tune the most important hyperparameters
    - Manual tuning: Use insight and train-test scores for guidance
    - Hyperparameter optimization: be careful not to over-tune