# Model Selection

Evaluating and selecting algorithms and hyperparameters.

```
[1]: # Global imports and settings
     from preamble import *
     %matplotlib inline
     plt.rcParams['savefig.dpi'] = 100 # Use 300 for PDF, 100 for slides
     # InteractiveShell.ast_node_interactivity = "all"
     HTML('''<style>html, body{overflow-y: visible !important} .CodeMirror{min-w
```

```
<IPython.core.display.HTML object>
```

## Evaluating models

To know whether we can *trust* what our algorithm has learned, we need to evaluate it.
We will focus on supervised methods (classification and regression) - With the labels we can objectively evaluate models - There are still many ways to do this
In unsupervised learning (e.g. clustering) we don't know what the 'right' output should be - We can only optimize for certain properties (e.g. cluster purity) - Ultimately, we need to inspect results manually (or create an external evaluation measure)

### The holdout (simple train-test split)

We've already seen the most basic form of evaluation:

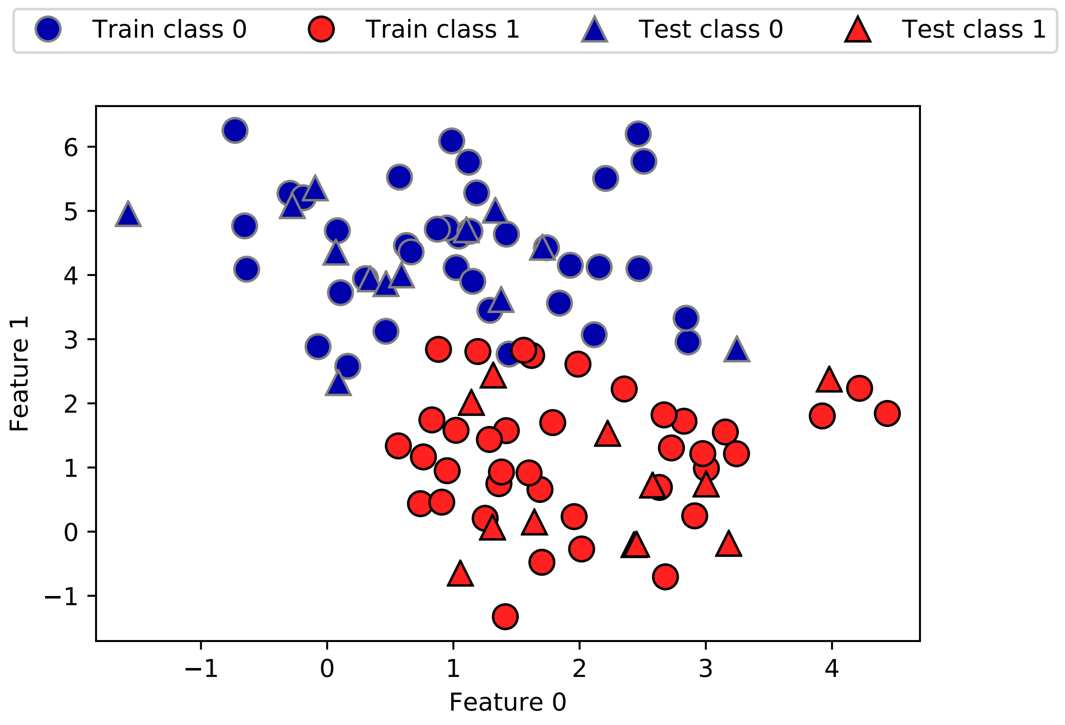
- Split data into training and test set (75%-25%)
  - In sklearn we split in training and test predictors (X_train, X_test) and labels (y_train, y_test)
- Train (fit) a model on the training data
- Score a model on the test data (comparing predicted and true labels)
  - We are interested in how well the model *generalizes* to new (test) data

```
[7]: from sklearn.datasets import make_blobs
     from sklearn.linear_model import LogisticRegression
     from sklearn.model_selection import train_test_split

     # create a synthetic dataset
     X, y = make_blobs(centers=2, random_state=0)
     # split data and labels into a training and a test set
     X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
     # Instantiate a model and fit it to the training set
     lr = LogisticRegression().fit(X_train, y_train)
     # evaluate the model on the test set
     print("Test set score: {:.2f}".format(lr.score(X_test, y_test)))
```

```
Test set score: 0.92
```

Visualized

```
[8]: fig = plt.figure()
     ax = fig.add_subplot(111)

     mglearn.discrete_scatter(X_train[:, 0], X_train[:, 1], y_train,
                              markers='o', ax=ax)
     mglearn.discrete_scatter(X_test[:, 0], X_test[:, 1], y_test,
                              markers='^', ax=ax)
     ax.set_xlabel("Feature 0")
     ax.set_ylabel("Feature 1")
     ax.legend(["Train class 0", "Train class 1", "Test class 0",
                "Test class 1"], ncol=4,  loc=(-0.1, 1.1));
```



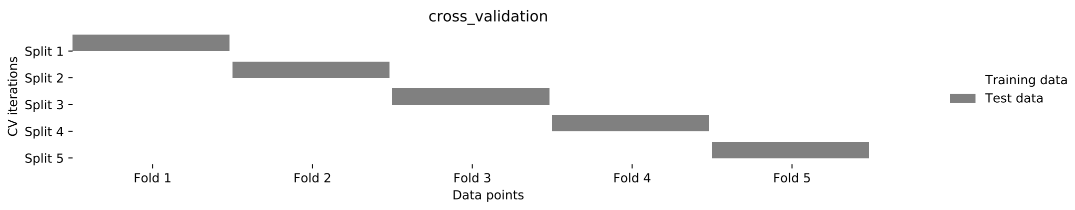
Limitations to this approach:

- Why 75%? Are there better ways to split?
- What if one random split yields different models (and scores) than another?
- What if all examples of one class all end up in the training/test set?

## Cross-validation

- More stable, thorough way to estimate generalization performance
- *k-fold cross-validation* (CV): split (randomized) data into *k* equal-sized parts, called *folds*
  - First, fold 1 is the test set, and folds 2-5 comprise the training set
  - Then, fold 2 is the test set, folds 1,3,4,5 comprise the training set
  - Compute *k* evaluation scores, aggregate afterwards (e.g. take the mean)

```
[9]: mglearn.plots.plot_cross_validation()
```



### Cross-validation in scikit-learn

- `cross_val_score` function with learner, training data, labels
- Returns list of all scores
    - Does 3-fold CV by default
    - Default scoring measures are accuracy (classification) or $R^2$ (regression)
- Even though models are built internally, they are not returned

```
[10]: from sklearn.model_selection import cross_val_score
      from sklearn.datasets import load_iris
      from sklearn.linear_model import LogisticRegression

      iris = load_iris()
      logreg = LogisticRegression()

      scores = cross_val_score(logreg, iris.data, iris.target)
      print("Cross-validation scores: {}".format(scores))
```

```
Cross-validation scores: [ 0.961  0.922  0.958]
```

- Change the number of folds with `cv` parameter
- Note that there can be quite some *variance* in the results
    - Depends on the stability of the model and the amount of training data
    - Typically, the more training data, the more stable the models

```
[11]: scores = cross_val_score(logreg, iris.data, iris.target, cv=5)
      print("Cross validation scores: {}".format(scores))
```

```
Cross validation scores: [ 1.     0.967  0.933  0.9    1.   ]
```

- Aggregate the scores yourself (e.g. mean)
- This means that the model is 96% accurate *on average*

```
[12]: print("Average cross-validation score: {:.2f}".format(scores.mean()))
```

```
Average cross-validation score: 0.96
```

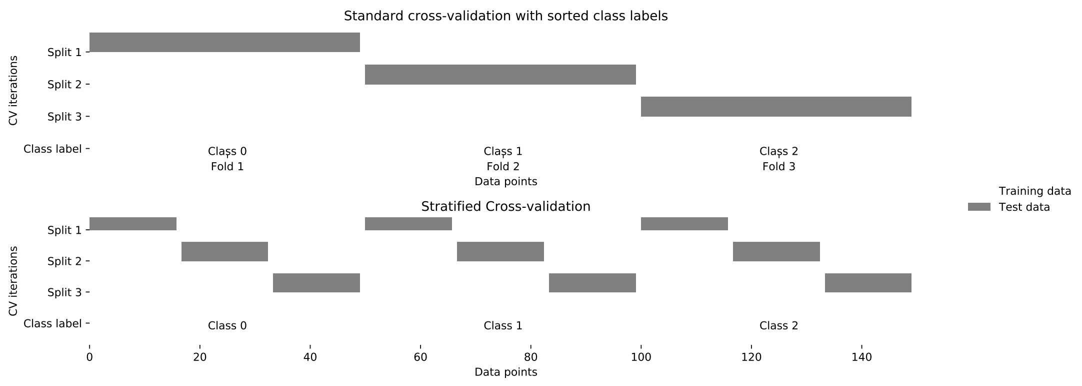
### Benefits of cross-validation

- More robust: every training example will be in a test set exactly once
  - Model is evaluated on all samples, needs to do well on all
  - With a train-test split, we can be
    - 'lucky': all easy examples in test set
    - 'unlucky: all hard examples in test set
- Shows how *sensitive* the model is to the exact training set
- Better estimation of true performance
  - 10-fold CV uses 90% of all data for training (vs 75% for holdout)
  - The higher $k$, the more accurate the estimation
- Disadvantage: computational cost, roughly $k$ times slower than holdout

### 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: make sure that *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

```
[13]: mglearn.plots.plot_stratified_cross_validation()
```



- scikit-learn will use:
  - stratified cross-validation by default for classification
  - normal cross-validation for regression
  - both are non-randomized (samples are not shuffled beforehand)
- You can build folds manually with `KFold`
  - non-randomized, non-stratified

```
[14]: from sklearn.model_selection import KFold
      kfold = KFold(n_splits=5)
      print("Cross-validation scores:\n{}".format(
            cross_val_score(logreg, iris.data, iris.target, cv=kfold)))
```

```
Cross-validation scores:
[ 1.     0.933  0.433  0.967  0.433]
```

```
[15]: # Can you explain this result?
      kfold = KFold(n_splits=3)
      print("Cross-validation scores:\n{}".format(
            cross_val_score(logreg, iris.data, iris.target, cv=kfold)))
```

```
Cross-validation scores:
[ 0.  0.  0.]
```

```
[16]: kfold = KFold(n_splits=3, shuffle=True, random_state=0)
      print("Cross-validation scores:\n{}".format(
          cross_val_score(logreg, iris.data, iris.target, cv=kfold)))
```

```
Cross-validation scores:
[ 0.9   0.96  0.96]
```

### Leave-One-Out cross-validation

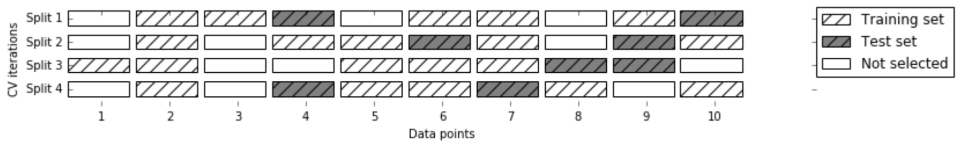
- *k* fold cross-validation with *k* equal to the number of samples
- Completely unbiased, but computationally expensive
- Recommended for small datasets

```
[17]: from sklearn.model_selection import LeaveOneOut
      loo = LeaveOneOut()
      scores = cross_val_score(logreg, iris.data, iris.target, cv=loo)
      print("Number of cv iterations: ", len(scores))
      print("Mean accuracy: {:.2f}".format(scores.mean()))
```

```
Number of cv iterations:  150
Mean accuracy: 0.95
```

### Shuffle-Split cross-validation

- Samples a number of samples (`train_size`) randomly as the training set, and a disjoint number of samples (`test_size`) as the test set
- Repeat this procedure `n_iter` times, obtaining `n_iter` scores
- Typically, the whole dataset is used each iteration (except for large datasets)
- Example with `train_size` = 10, `test_size` = 2, `n_iter` = 4



shuffle_split

- In scikit-learn, `train_size` and `test_size` can be absolute numbers or a percentage of the total dataset
- Stratified variant: 'StratifiedShuffleSplit' (recommended for classification)

```
[18]: from sklearn.model_selection import ShuffleSplit
      shuffle_split = ShuffleSplit(test_size=.5, train_size=.5, n_splits=10)
      scores = cross_val_score(logreg, iris.data, iris.target, cv=shuffle_split)
      print("Cross-validation scores:\n{}".format(scores))
```

```
Cross-validation scores:
[ 0.987  0.907  0.96   0.92   0.933  0.773  0.987  0.787  1.     0.92 ]
```

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, use Shuffle-Split instead. - With `train_size=0.66`, `test_size=0.34` - You can prove that bootstraps include 66% of all data points on average

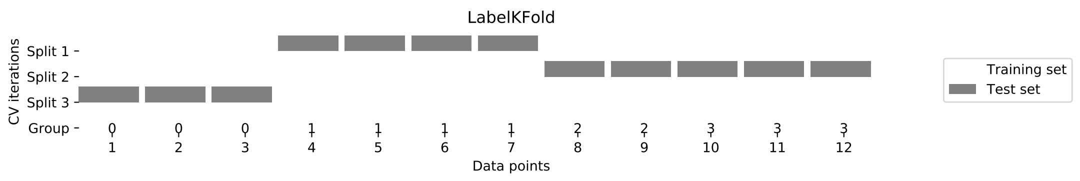
### Repeated cross-validation

- 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:
  - Blood analysis results on specific patients
  - Facial expressions of specific people
- With normal cross-validation, data from the same persion may end up in the training *and* test set
- If we want to measure how well the model generalizes to *other* people, this is undesirable
- We want to make sure that data points fom one person are in *either* the training or test set
  - This is called *grouping* or *blocking*
  - Leave-one-subject-out cross-validation: create test set for each user individually

```
[19]: mglearn.plots.plot_group_kfold()
```



- In scikit-learn, this is supported by `GroupKFold`
  - Add an array with group membership to `cross_val_scores`
  - Use `GroupKFold` with the number of groups as CV procedure

```
[20]: from sklearn.model_selection import GroupKFold
      # create synthetic dataset
      X, y = make_blobs(n_samples=12, random_state=0)
      # assume the first three samples belong to the same group,
      # then the next four etc.
      groups = [0, 0, 0, 1, 1, 1, 1, 2, 2, 3, 3, 3]
      scores = cross_val_score(logreg, X, y, groups, cv=GroupKFold(n_splits=3))
      print("Cross-validation scores:\n{}".format(scores))
```

```
Cross-validation scores:
[ 0.75   0.8    0.667]
```

### Choosing a performance estimation procedure

No strict rules, only guidelines:

- Always use stratification for classification
- 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

## 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 bias for variance through (de)regularization
  - The challenge is to find the right trade-off (minimizing total error)
- Useful to understand how to tune or adapt learning algorithm
- Sadly, this is not yet supported by scikit-learn

- How to measure bias and variance (for regression):
  - Take 100 or more bootstraps (or shuffle-splits)
  - For each data point x:
    - $bias(x) = (x_{true} - mean(x_{predicted}))^2$
    - $variance(x) = var(x_{predicted})$
  - Total bias: $\sum_x bias(x) * w_x$, with $w_x$ the ratio of x occuring in the test set
  - Total variance: $\sum_x variance(x) * w_x$

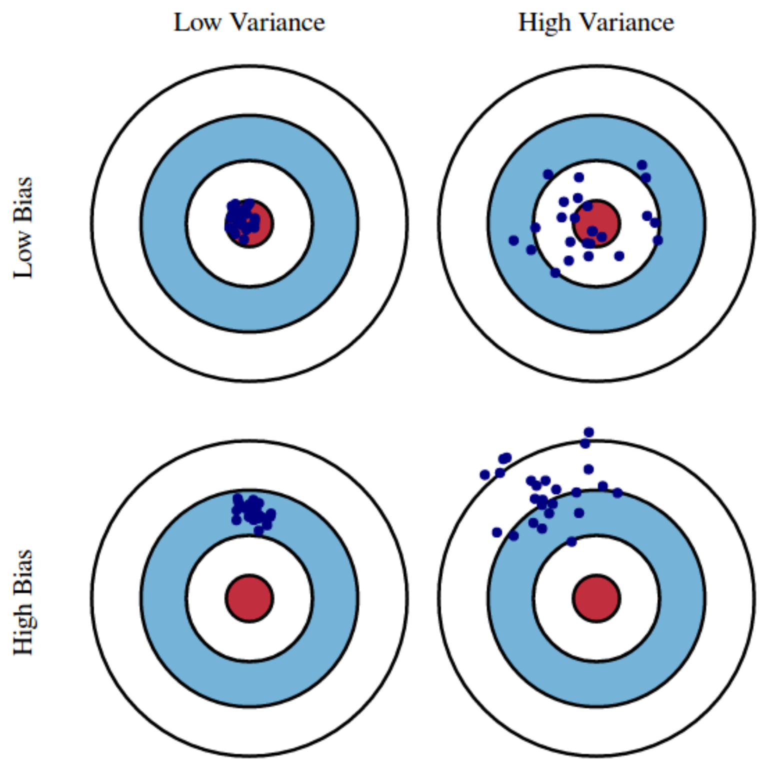


Fig. 1 Graphical illustration of bias and variance.

Bias-variance

- General procedure for (binary) classification:
  - Take 100 or more bootstraps (or shuffle-splits)
  - Bias for any point x = misclassification ratio
    - If misclassified 50% of the time: $bias(x) = 0.5$
  - Variance for any point x is $(1 - (P(class_1)^2 + P(class_2)^2))/2$
    - $P(class_i)$ is ratio of class $i$ predictions
    - When each class predicted half of the time: $variance(x) = (1-(0.5^2+0.5^2))/2 = 0.25$
  - Total bias: $\sum_x bias(x)^2 * w_x$, with $w_x$ the ratio of x occuring in the test data
  - Total variance: $\sum_x variance(x) * w_x$

```
[34]: # Data and classifier
      X, y = make_blobs(centers=2, n_samples=1000, random_state=0)
      clf = LogisticRegression()

      # Bootstraps
      n_repeat = 100
      shuffle_split = ShuffleSplit(test_size=0.33, n_splits=n_repeat)

      # Store sample predictions
      y_all_pred = [[] for _ in range(len(y))]

      # Train classifier on each bootstrap and score predictions
      for i, (train_index, test_index) in enumerate(shuffle_split.split(X)):
          # Train and predict
          clf.fit(X[train_index], y[train_index])
          y_pred = clf.predict(X[test_index])

          # Store predictions
          for i,index in enumerate(test_index):
              y_all_pred[index].append(y_pred[i])

      # Compute bias, variance, error
      bias_sq = sum([ (1 - x.count(y[i])/len(x))**2 * len(x)/n_repeat
                  for i,x in enumerate(y_all_pred)])
      var = sum([((1 - ((x.count(0)/len(x))**2 + (x.count(1)/len(x))**2))/2) * l
                 for i,x in enumerate(y_all_pred)])
      error = sum([ (1 - x.count(y[i])/len(x)) * len(x)/n_repeat
                  for i,x in enumerate(y_all_pred)])

      print("Bias squared: %.2f, Variance: %.2f, Total error: %.2f" % (bias_sq,
```

```
Bias squared: 14.23, Variance: 0.75, Total error: 14.98
```

- High bias means that you are likely underfitting
  - Do less regularization
  - Use a more flexible/complex model (another algorithm)
  - Use a bias-reduction technique (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 (bagging)
- Boosting and Bagging will be explained later

### Hyperparameter tuning

Now that we know how to evaluate models, we can improve them by tuning their hyperparameters

We can basically use any optimization technique to optimize hyperparameters:

- **Grid search**
- **Random search**
- Local search
- Racing algorithms
- **Model-based optimization**
- Multi-armed bandits
- Genetic algorithms

### Grid Search

- For each hyperparameter, create a list of interesting/possible values
  - E.g. For kNN: k in [1,3,5,7,9,11,33,55,77,99]
- Evaluate all possible combination of hyperparameter values
  - E.g. using cross-validation
- Select the hyperparameter values yielding the best results

A naive approach would be to just loop over all combinations
Note: we've seen the `C` parameter of SVMs, we'll see the `gamma` parameter later.

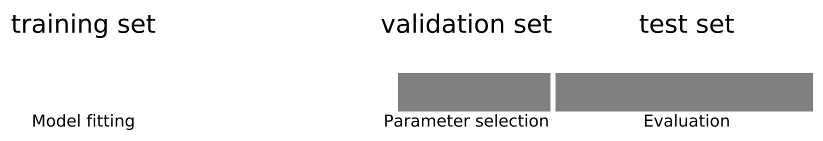
```
[35]: # naive grid search implementation
      from sklearn.svm import SVC
      X_train, X_test, y_train, y_test = train_test_split(iris.data, iris.target
                                                           random_state=0)
      print("Size of training set: {}   size of test set: {}".format(
             X_train.shape[0], X_test.shape[0]))

      best_score = 0

      for gamma in [0.001, 0.01, 0.1, 1, 10, 100]:
          for C in [0.001, 0.01, 0.1, 1, 10, 100]:
              # for each combination of parameters
              # train an SVC
              svm = SVC(gamma=gamma, C=C);
              svm.fit(X_train, y_train);
              # evaluate the SVC on the test set
              score = svm.score(X_test, y_test)
              # if we got a better score, store the score and parameters
              if score > best_score:
                  best_score = score
                  best_parameters = {'C': C, 'gamma': gamma}

      print("Best score: {:.2f}".format(best_score))
      print("Best parameters: {}".format(best_parameters))
```

```
Size of training set: 112   size of test set: 38
Best score: 0.97
Best parameters: {'gamma': 0.001, 'C': 100}
```

### Overfitting the parameters and the validation set

- Simply taking the best performing model yields optimistic results
- We've already used the test data to evaluate each hyperparameter setting
- Hence, we don't have an independent test set to evaluate these hyperparameter settings
  - Information 'leaks' from test set into the final model
- Solution: 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

```
[36]: mglearn.plots.plot_threefold_split()
```



```
[37]: from sklearn.svm import SVC
      # split data into train+validation set and test set
      X_trainval, X_test, y_trainval, y_test = train_test_split(
          iris.data, iris.target, random_state=0)
      # split train+validation set into training and validation set
      X_train, X_valid, y_train, y_valid = train_test_split(
          X_trainval, y_trainval, random_state=1)
      print("Size of training set: {}   size of validation set: {}   size of tes
             " {}\n".format(X_train.shape[0], X_valid.shape[0], X_test.shape[0]))

      best_score = 0

      for gamma in [0.001, 0.01, 0.1, 1, 10, 100]:
          for C in [0.001, 0.01, 0.1, 1, 10, 100]:
              # for each combination of parameters
              # train an SVC
              svm = SVC(gamma=gamma, C=C)
              svm.fit(X_train, y_train)
              # evaluate the SVC on the test set
              score = svm.score(X_valid, y_valid)
              # if we got a better score, store the score and parameters
              if score > best_score:
                  best_score = score
                  best_parameters = {'C': C, 'gamma': gamma}

      # rebuild a model on the combined training and validation set,
      # and evaluate it on the test set
      svm = SVC(**best_parameters)
      svm.fit(X_trainval, y_trainval)
      test_score = svm.score(X_test, y_test)
```

```
print("Best score on validation set: {:.2f}".format(best_score))
print("Best parameters: ", best_parameters)
print("Test set score with best parameters: {:.2f}".format(test_score))
```

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

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

#### Grid-search with cross-validation

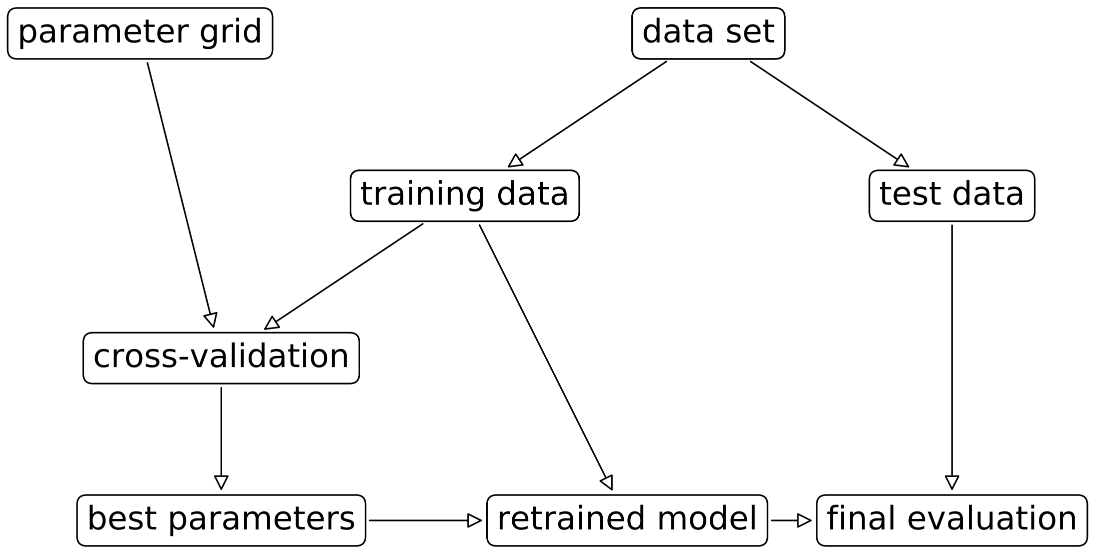
- Same problem as before: the way that we split the data into training, validation, and test set may have a large influence on estimated performance
- We need to use cross-validation again, instead of a single split
- Expensive. Often, 5-fold CV is enough, or a shuffle_split with `n_iter=1`

```
[38]: # reference: manual_grid_search_cv
      for gamma in [0.001, 0.01, 0.1, 1, 10, 100]:
          for C in [0.001, 0.01, 0.1, 1, 10, 100]:
              # for each combination of parameters
              # train an SVC
              svm = SVC(gamma=gamma, C=C)
              # perform cross-validation
              scores = cross_val_score(svm, X_trainval, y_trainval, cv=5)
              # compute mean cross-validation accuracy
              score = np.mean(scores)
              # if we got a better score, store the score and parameters
              if score > best_score:
                  best_score = score
                  best_parameters = {'C': C, 'gamma': gamma}
      # rebuild a model on the combined training and validation set
      svm = SVC(**best_parameters)
      svm.fit(X_trainval, y_trainval)
```

```
SVC(C=100, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma=0.01, kernel='rbf',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)
```

Overall process

```
[39]: mglearn.plots.plot_grid_search_overview()
```



### Grid search in scikit-learn

- Create a parameter grid as a dictionary
  - Keys are parameter names
  - Values are lists of hyperparameter values

```
[40]: param_grid = {'C': [0.001, 0.01, 0.1, 1, 10, 100],
                    'gamma': [0.001, 0.01, 0.1, 1, 10, 100]}
      print("Parameter grid:\n{}".format(param_grid))
```

```
Parameter grid:
{'gamma': [0.001, 0.01, 0.1, 1, 10, 100], 'C': [0.001, 0.01, 0.1, 1, 10, 100]}
```

- `GridSearchCV`: like a classifier that uses CV to automatically optimize its hyperparameters internally
  - Input: (untrained) model, parameter grid, CV procedure
  - Output: optimized model on given training data
  - Should only have access to trinaing data

```
[41]: from sklearn.model_selection import GridSearchCV
      from sklearn.svm import SVC
      grid_search = GridSearchCV(SVC(), param_grid, cv=5)
      X_train, X_test, y_train, y_test = train_test_split(
              iris.data, iris.target, random_state=0)
      grid_search.fit(X_train, y_train)
```

```
GridSearchCV(cv=5, error_score='raise',
       estimator=SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma='auto', kernel='rbf',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False),
       fit_params={}, iid=True, n_jobs=1,
       param_grid={'gamma': [0.001, 0.01, 0.1, 1, 10, 100], 'C': [0.001, 0.01, 0
       pre_dispatch='2*n_jobs', refit=True, return_train_score=True,
       scoring=None, verbose=0)
```

The optimized test score and hyperparameters can easily be retrieved:

```
[42]: print("Test set score: {:.2f}".format(grid_search.score(X_test, y_test)))
```

```
Test set score: 0.97
```

```
[43]: print("Best parameters: {}".format(grid_search.best_params_))
      print("Best cross-validation score: {:.2f}".format(grid_search.best_score_
```

```
Best parameters: {'gamma': 0.01, 'C': 100}
Best cross-validation score: 0.97
```

```
[44]: # Not really necessary because grid_search can also predict and score
      print("Best estimator:\n{}".format(grid_search.best_estimator_))
```

```
Best estimator:
SVC(C=100, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma=0.01, kernel='rbf',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)
```

**Visualizing hyperparameter impact** We can retrieve and visualize the cross-validation resulst to better understand the impact of hyperparameters

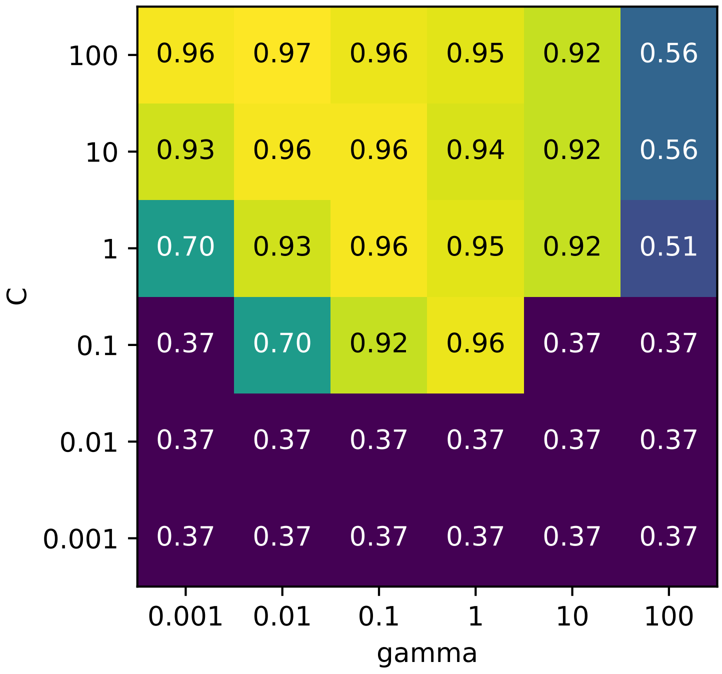
```
[45]: import pandas as pd
      # convert to Dataframe
      results = pd.DataFrame(grid_search.cv_results_)
      # Show the first 5 rows
      display(results.head())
```

```
   mean_fit_time  mean_score_time  mean_test_score  mean_train_score  \
0       1.62e-03         8.03e-04             0.37              0.37
1       1.72e-03         8.86e-04             0.37              0.37
2       9.09e-04         3.46e-04             0.37              0.37
3       7.22e-04         2.69e-04             0.37              0.37
4       7.34e-04         2.76e-04             0.37              0.37

        ...         std_fit_time std_score_time std_test_score  std_train_score
0       ...             1.41e-03       9.17e-04           0.01         2.85e-03
```

```
1        ...            5.46e-04          5.14e-04             0.01           2.85e-03
2        ...            4.05e-04          1.39e-04             0.01           2.85e-03
3        ...            1.20e-04          2.90e-05             0.01           2.85e-03
4        ...            4.36e-05          1.19e-05             0.01           2.85e-03

[5 rows x 22 columns]
```

Visualize as a heatmap

```
[46]: scores = np.array(results.mean_test_score).reshape(6, 6)
      # plot the mean cross-validation scores
      mglearn.tools.heatmap(scores, xlabel='gamma', xticklabels=param_grid['gamm
                            ylabel='C', yticklabels=param_grid['C'], cmap="virid
```



When hyperparameters depend on other parameters, we can use lists of dictionaries to define the hyperparameter space

```
[47]: param_grid = [{'kernel': ['rbf'],
                     'C': [0.001, 0.01, 0.1, 1, 10, 100],
                     'gamma': [0.001, 0.01, 0.1, 1, 10, 100]},
                    {'kernel': ['linear'],
                     'C': [0.001, 0.01, 0.1, 1, 10, 100]}]
      print("List of grids:\n{}".format(param_grid))
```

```
List of grids:
[{'gamma': [0.001, 0.01, 0.1, 1, 10, 100], 'kernel': ['rbf'], 'C': [0.001, 0.01,
```

### 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

```
[48]: scores = cross_val_score(GridSearchCV(SVC(), param_grid, cv=5),
                              iris.data, iris.target, cv=5)
      print("Cross-validation scores: ", scores)
      print("Mean cross-validation score: ", scores.mean())
```

```
Cross-validation scores:  [ 0.967  1.     0.9    0.967  1.   ]
Mean cross-validation score:  0.966666666667
```

### Parallelizing cross-validation and grid-search

- On a practical note, it is easy to parallellize CV and grid search
- `cross_val_score` and `GridSearchCV` have a `n_jobs` parameter defining the number of cores it can use.
  - set it to `n_jobs=-1` to use all available cores.

### Random Search

- Grid Search has a few downsides:
  - Optimizing many hyperparameters creates a combinatorial explosion
  - You have to predefine a grid, hence you may jump over optimal values
- Random Search:
  - Picks `n_iter` random parameter values
  - Scales better, you control the number of iterations
  - Often works better in practice, too
    - not all hyperparameters interact strongly
    - you don't need to explore all combinations
- Executing random search in scikit-learn:
  - `RandomizedSearchCV` works like `GridSearchCV`
  - Has `n_iter` parameter for the number of iterations
  - Search grid can use distributions instead of fixed lists

```
[49]: from sklearn.model_selection import RandomizedSearchCV
      from scipy.stats import expon

      param_grid = {'C': expon(scale=100),
                    'gamma': expon(scale=.1)}
      random_search = RandomizedSearchCV(SVC(), param_distributions=param_grid,
                                         n_iter=20)
      X_train, X_test, y_train, y_test = train_test_split(
              iris.data, iris.target, random_state=0)
      random_search.fit(X_train, y_train)
```

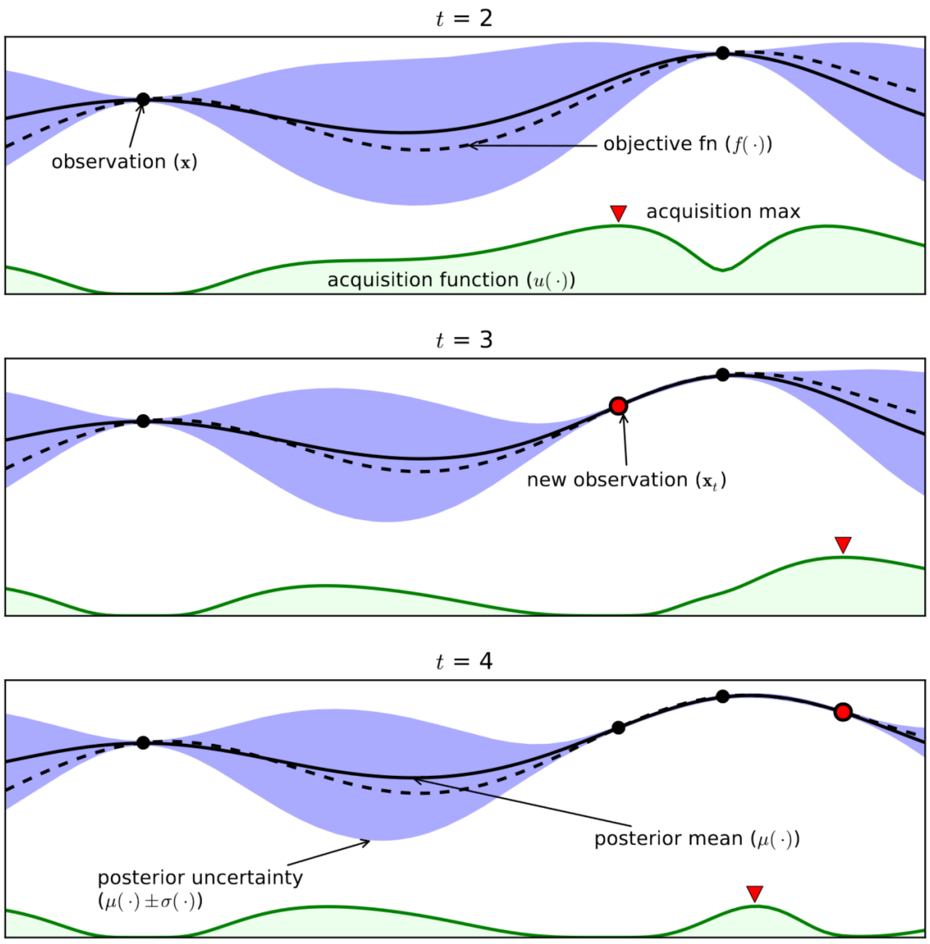
```
RandomizedSearchCV(cv=None, error_score='raise',
          estimator=SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma='auto', kernel='rbf',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False),
          fit_params={}, iid=True, n_iter=20, n_jobs=1,
          param_distributions={'gamma': <scipy.stats._distn_infrastructure.rv_fr
          pre_dispatch='2*n_jobs', random_state=None, refit=True,
          return_train_score=True, scoring=None, verbose=0)
```

## Model-based optimization

- After a number of random search iterations we know more about the performance of hyperparameter settings on the given dataset
- We can use this data to train a model, and predict which other hyperparameter values might be useful
- This is often a probabilistic (e.g. Bayesian) model that predicts confidence intervals for all hyperparameter settings

Example: Bayesian optimization (see figure):

- Consider only 1 continuous hyperparameter (X-axis)
- Y-axis shows cross-validation performance
- Evaluate a number of random hyperparameter settings (black dots)
  - Sometimes an initialization design is used
- Train a model, and predict the expected performance of other (unseen) hyperparameter values
  - Mean value (black line) and distribution (blue band)
- An *acquisition function* (green line) trades off maximal expected performace and maximal uncertainty
  - Exploitation vs exploration
- Optimal value of the asquisition function is the next hyperparameter setting to be evaluated
- Repeat a fixed number of times, or until time budget runs out


$t$ = 2
observation ($\mathbf{x}$)
objective fn ($f(\cdot)$)
acquisition max
acquisition function ($u(\cdot)$)
$t$ = 3
new observation ($\mathbf{x}_t$)
$t$ = 4
posterior mean ($\mu(\cdot)$)
posterior uncertainty
($\mu(\cdot) \pm \sigma(\cdot)$)

BayesOpt

## Evaluation Metrics and scoring

Keep the end-goal in mind

### Metrics for binary classification

- The most common (and simple) application of machine learning in practive
- We have a positive and a negative class
- 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
- Which side do you want to err on for a medical test?

### 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
  - This is often typical of real world data
  - E.g. credit card fraud detection
- Is a 99.99% accuracy good enough?
- Let's create an imbalanced dataset from the handwritten digits dataset by classifying the digit 9 against all others.
- Is 90% accuracy still good? Can we do better?

```
[50]: from sklearn.datasets import load_digits

      digits = load_digits()
      y = digits.target == 9

      X_train, X_test, y_train, y_test = train_test_split(
          digits.data, y, random_state=0)
```

```
[51]: from sklearn.dummy import DummyClassifier
      from sklearn.linear_model import LogisticRegression

      # Always predicts majority class
      dummy = DummyClassifier(strategy='most_frequent').fit(X_train, y_train)
      pred_dummy = dummy.predict(X_test)
      print("dummy score: {:.2f}".format(dummy.score(X_test, y_test)))
```

```
dummy score: 0.90
```

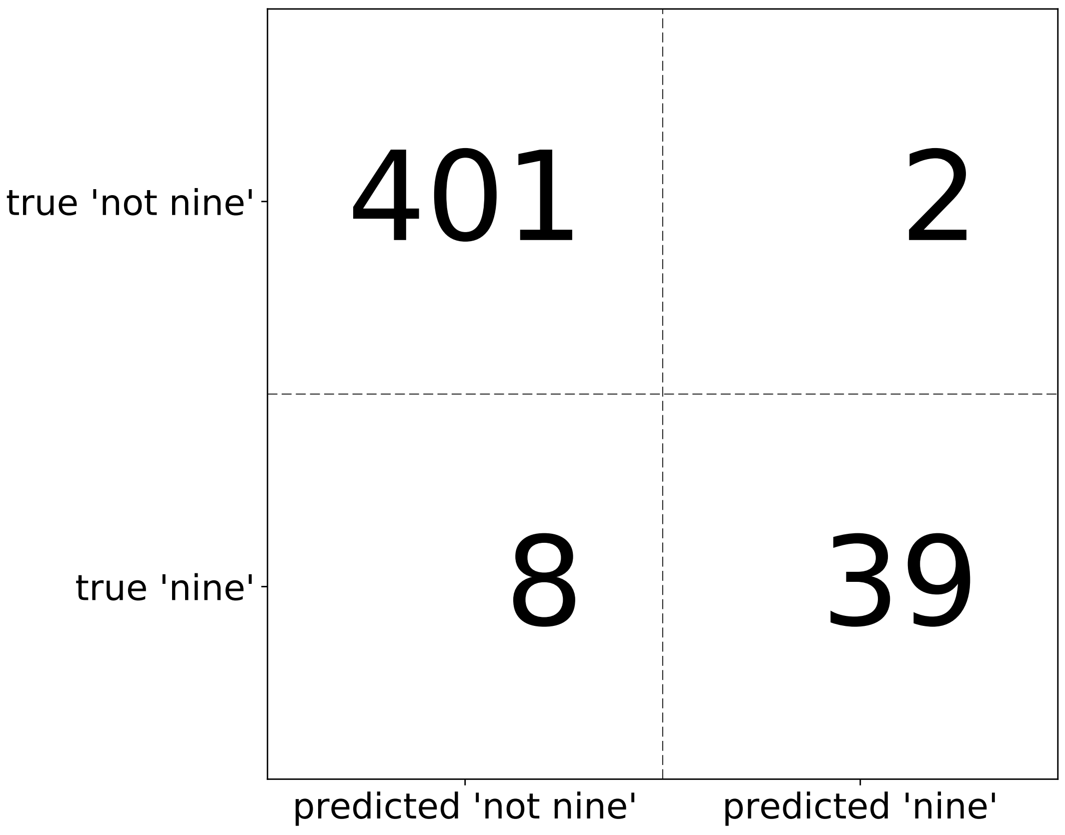
```
[52]: logreg = LogisticRegression(C=0.1).fit(X_train, y_train)
      pred_logreg = logreg.predict(X_test)
      print("logreg score: {:.2f}".format(logreg.score(X_test, y_test)))
```

```
logreg score: 0.98
```

### 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 the true classes
  - Columns correspond to the 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.

```
[53]: mglearn.plots.plot_confusion_matrix_illustration()
```



The confusion matrix can be constructed from the true labels and predcitions as follows:

```
[54]: from sklearn.metrics import confusion_matrix

      confusion = confusion_matrix(y_test, pred_logreg)
      print("Confusion matrix:\n{}".format(confusion))
```

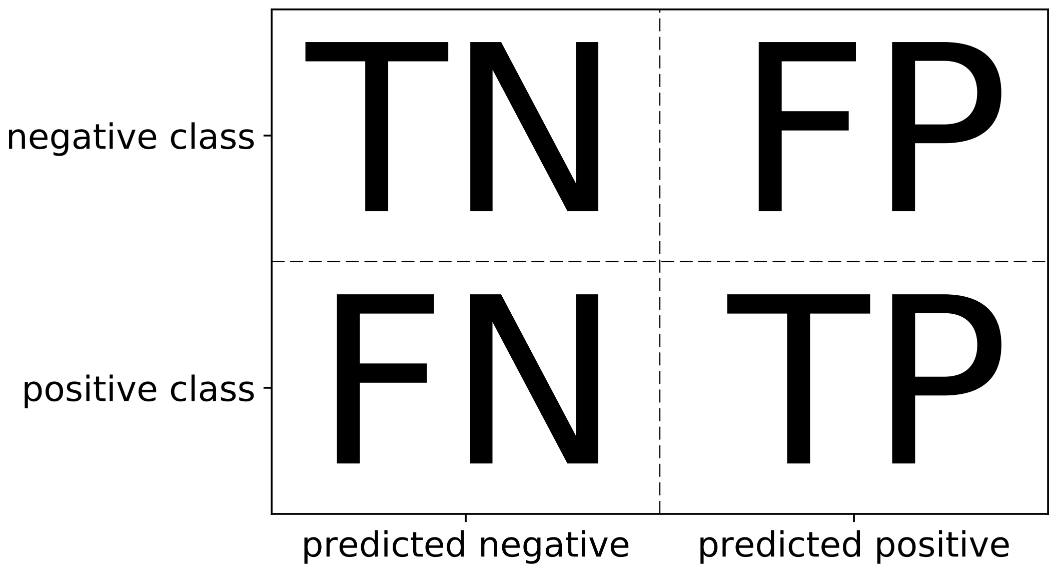
```
Confusion matrix:
[[401   2]
 [  8  39]]
```

For binary classification, we use the following terms:

- True Negative (TN)

- False Positive (FP)
- False Negative (FN)
- True Positive (TP)

```
[55]: mglearn.plots.plot_binary_confusion_matrix()
```



It's often useful to compare the confusion matrices of classifiers: - The dummy classifier always predicts the same class, produces a large number of FNs. - Logistic regression produces more FPs, but much fewer FNs.

```
[56]: print("Most frequent class:")
      print(confusion_matrix(y_test, pred_dummy))
      print("\nLogistic Regression")
      print(confusion_matrix(y_test, pred_logreg))
```

```
Most frequent class:
[[403   0]
 [ 47   0]]

Logistic Regression
[[401   2]
 [  8  39]]
```

The results of the confusion matrix can be summarized in several ways

- We already know accuracy:

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}} \tag{0.1}$$

**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

$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}} \tag{0.2}$$

**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)

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}} \tag{0.3}$$

**F1-score** or F1-measure trades of precision and recall:

$$\text{F} = 2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}} \tag{0.4}$$

```
[57]: from sklearn.metrics import f1_score
      print("f1 score most frequent: {:.2f}".format(
          f1_score(y_test, pred_dummy)))
      print("f1 score logistic regression: {:.2f}".format(
          f1_score(y_test, pred_logreg)))
```

```
f1 score most frequent: 0.00
f1 score logistic regression: 0.89
```

- To study all of them at once, use `classification_report`
  - Support: number of samples in each class
  - Last line: weighted average over the classes (weighted by number of smaples in each class)

```
[58]: from sklearn.metrics import classification_report
      print(classification_report(y_test, pred_dummy,
                                  target_names=["not nine", "nine"]))
```

```
             precision    recall  f1-score   support

   not nine       0.90      1.00      0.94       403
       nine       0.00      0.00      0.00        47

avg / total       0.80      0.90      0.85       450
```

```
[59]: print(classification_report(y_test, pred_logreg,
                                  target_names=["not nine", "nine"]))
```

```
             precision    recall  f1-score   support

   not nine       0.98      1.00      0.99       403
       nine       0.95      0.83      0.89        47

avg / total       0.98      0.98      0.98       450
```

### Taking uncertainty into account

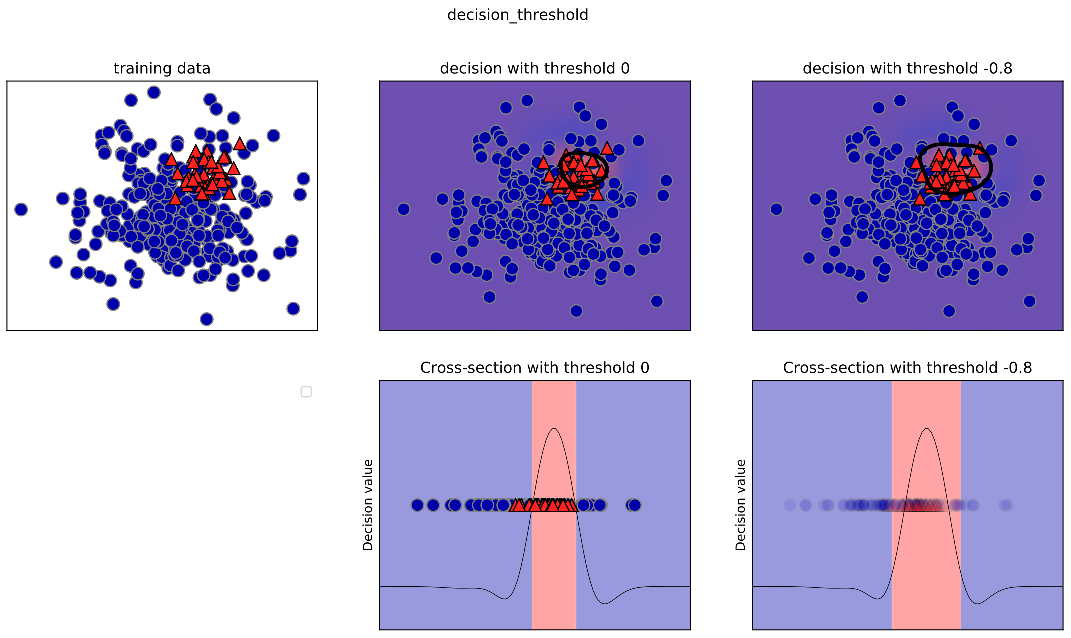
- Remember that many classifiers actually return a probability per class
    - We can retrieve it with `decision_function` and `predict_proba`
- For binary classification, we threshold at 0 for `decision_function` and 0.5 for `predict_proba` by default
- However, depending on the evaluation measure, 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*

#### Visualization

- Imagine that we want to avoid misclassifying a red point
- The black line shows the threshold: points within are classified positive (red)
- By changing the decision treshold, more points will be classified positive

```
[60]: from mglearn.datasets import make_blobs
      X, y = make_blobs(n_samples=(400, 50), centers=2, cluster_std=[7.0, 2],
                        random_state=22)
      X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
      svc = SVC(gamma=.05).fit(X_train, y_train)
```

```
[61]: mglearn.plots.plot_decision_threshold()
```



- 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

```
[62]: print(classification_report(y_test, svc.predict(X_test)))

                 precision    recall  f1-score   support

              0       0.97      0.89      0.93       104
              1       0.35      0.67      0.46         9

    avg / total       0.92      0.88      0.89       113
```

```
[63]: y_pred_lower_threshold = svc.decision_function(X_test) > -.8
      print(classification_report(y_test, y_pred_lower_threshold))

                 precision    recall  f1-score   support

              0       1.00      0.82      0.90       104
              1       0.32      1.00      0.49         9

    avg / total       0.95      0.83      0.87       113
```

#### Precision-Recall curves

- The right threshold depends on your application, should be driven by business goals.
- You can have arbitrary high recall, but you often want reasonable precision, too.
- It is not clear beforehand where the optimale trade-off (or *operating point*) will be, so it is useful to look at all possible thresholds
- Plotting precision against recall for all thresholds yields a **precision-recall curve**

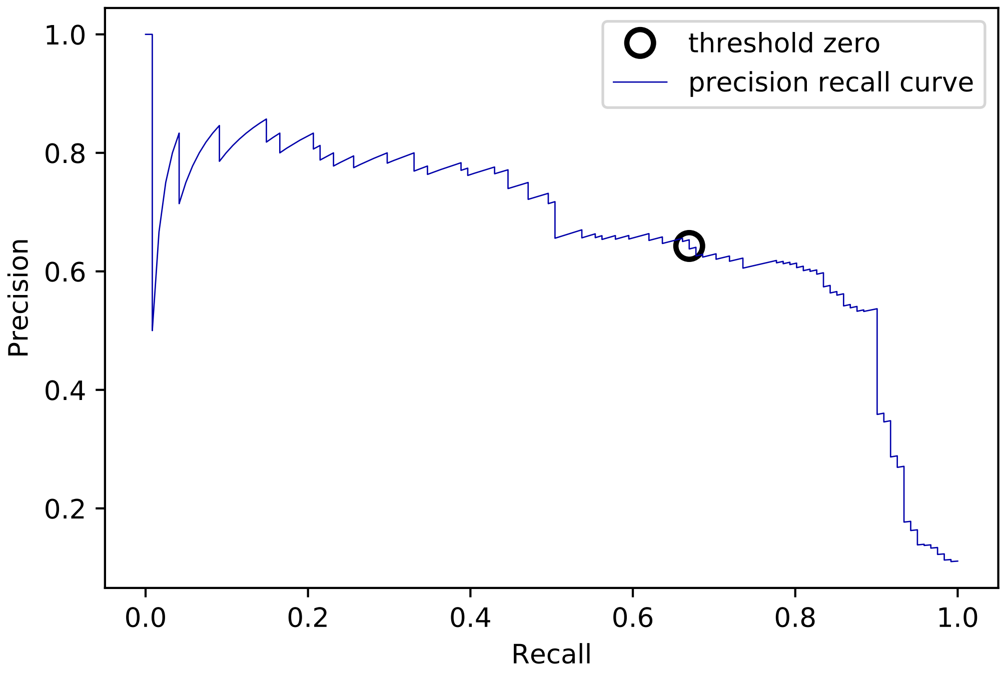
- In scikit-learn, this is included in the `sklearn.metrics` module
- Returns all precision and recall values for all thresholds

```
[64]: from sklearn.metrics import precision_recall_curve
      precision, recall, thresholds = precision_recall_curve(
          y_test, svc.decision_function(X_test))
```

- Now we can plot the curve. The default tradeoff (chosen by the `predict` method) is indicated as *threshold zero*.
- The closer the curve stays to the upper-right corner, the better
  - High precision and high recall
- Here, it is possible to still get a precision of 0.5 with high recall

```
[65]: # create a similar dataset as before, but with more samples
      # to get a smoother curve
      X, y = make_blobs(n_samples=(4000, 500), centers=2, cluster_std=[7.0, 2],
                        random_state=22)
      X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
```

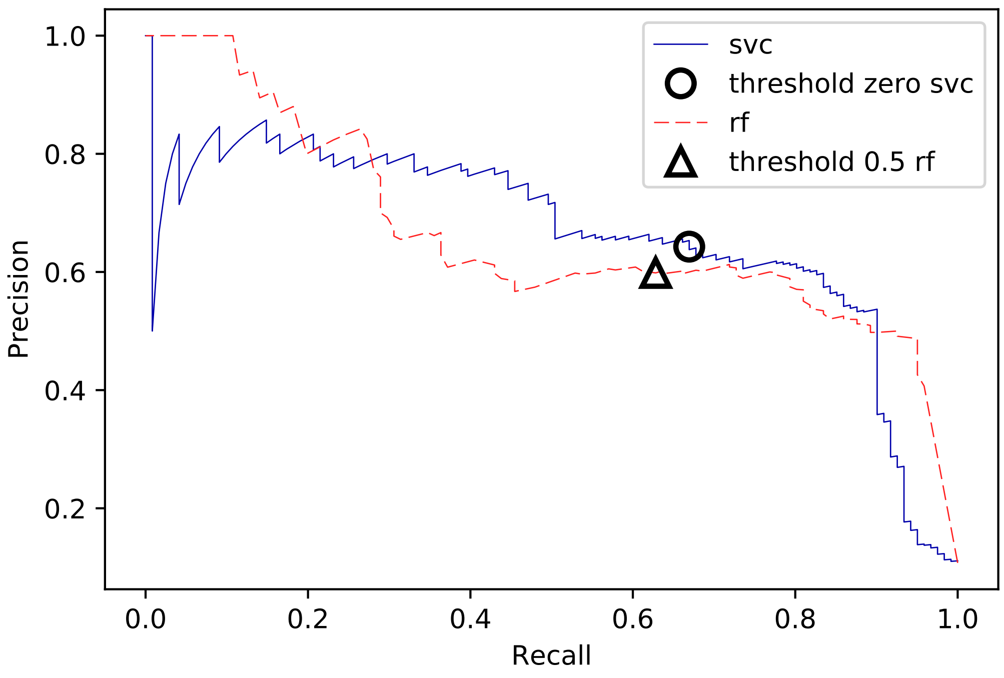
```
svc = SVC(gamma=.05).fit(X_train, y_train)

precision, recall, thresholds = precision_recall_curve(
    y_test, svc.decision_function(X_test))
# find threshold closest to zero:
close_zero = np.argmin(np.abs(thresholds))
plt.plot(recall[close_zero], precision[close_zero], 'o', markersize=10,
         label="threshold zero", fillstyle="none", c='k', mew=2)

plt.plot(recall, precision, label="precision recall curve")
plt.ylabel("Precision")
plt.xlabel("Recall")
plt.legend(loc="best");
```



**Model selection**

- Different classifiers work best in different parts of the curve (at different operating points)
- Let's compare two classifiers (we'll see both soon)
- The RandomForest (in red) performs better at the extremes
- The area under the precision-recall curve (AUPRC) is often used as a general evaluation measure

```
[66]: from sklearn.ensemble import RandomForestClassifier

      rf = RandomForestClassifier(n_estimators=100, random_state=0, max_features
      rf.fit(X_train, y_train)

      # RandomForestClassifier has predict_proba, but not decision_function
      # Only pass probabilities for the positive class
      precision_rf, recall_rf, thresholds_rf = precision_recall_curve(
          y_test, rf.predict_proba(X_test)[:, 1])

      plt.plot(recall, precision, label="svc")

      plt.plot(recall[close_zero], precision[close_zero], 'o', markersize=10,
               label="threshold zero svc", fillstyle="none", c='k', mew=2)

      plt.plot(recall_rf, precision_rf, label="rf")

      close_default_rf = np.argmin(np.abs(thresholds_rf - 0.5))
      plt.plot( recall_rf[close_default_rf], precision_rf[close_default_rf], '^'
               markersize=10, label="threshold 0.5 rf", fillstyle="none", mew=2)
      plt.ylabel("Precision")
      plt.xlabel("Recall")
      plt.legend(loc="best");
```



Note that the F1-measure completely misses these subtleties

```
[67]: print("f1_score of random forest: {:.3f}".format(
                f1_score(y_test, rf.predict(X_test))))
      print("f1_score of svc: {:.3f}".format(f1_score(y_test, svc.predict(X_test
```

```
f1_score of random forest: 0.610
f1_score of svc: 0.656
```

- The area under the precision-recall curve is returned by the `average_precision_score` measure

  - It’s actually a close approximation of the actual area

- This is a good automatic measure, but also hides the subtleties

```
[68]: from sklearn.metrics import average_precision_score
      ap_rf = average_precision_score(y_test, rf.predict_proba(X_test)[:, 1])
      ap_svc = average_precision_score(y_test, svc.decision_function(X_test))
      print("Average precision of random forest: {:.3f}".format(ap_rf))
      print("Average precision of svc: {:.3f}".format(ap_svc))
```

```
Average precision of random forest: 0.666
Average precision of svc: 0.663
```

### Receiver Operating Characteristics (ROC) and AUC

- There is another trade-off between recall (true positive rate, TPR) and the false positive rate (FPR).
- The 2D space created by TPR and FPR is called the Receiver Operating Characteristics (ROC) space
- A model will be at one point in this ROC space

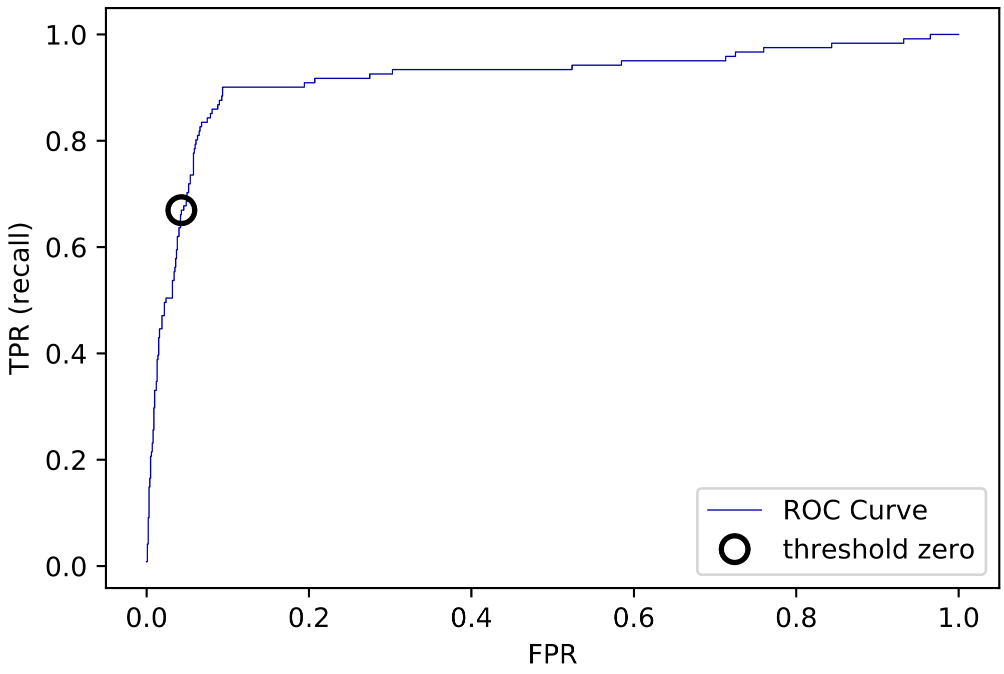
$$\text{TPR} = \frac{\text{TP}}{\text{TP} + \text{FN}} \tag{0.5}$$

$$\text{FPR} = \frac{\text{FP}}{\text{FP} + \text{TN}} \tag{0.6}$$

- Varying the decision threshold yields the ROC curve
- It can be computed with the `roc_curve` function
- Ideal is close to the top left: high recall, low FPR
- Inspect the curve to find the preferred calibration

  - Here, we can get much higher recall with slightly worse FPR

```
[69]: from sklearn.metrics import roc_curve
      fpr, tpr, thresholds = roc_curve(y_test, svc.decision_function(X_test))

      plt.plot(fpr, tpr, label="ROC Curve")
      plt.xlabel("FPR")
      plt.ylabel("TPR (recall)")
      # find threshold closest to zero:
      close_zero = np.argmin(np.abs(thresholds))
      plt.plot(fpr[close_zero], tpr[close_zero], 'o', markersize=10,
               label="threshold zero", fillstyle="none", c='k', mew=2)
      plt.legend(loc=4);
```



### Visualization

- Imagine 2 overlapping distributions (positive red class, negative blue class)
- All points to the right of the threshold are predicted positive, others negative
- As we increase the threshold, we'll get fewer FPs, more FNs
  - Perfect classifier would perfectly separate the classes
  - For a random classifier, the distributions overlap completely

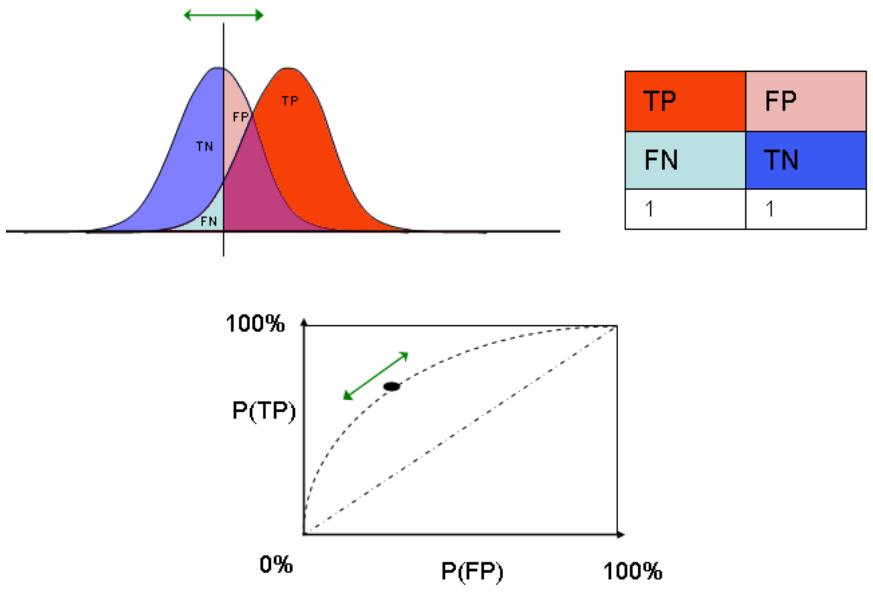
### ROC Isometrics

- Different *costs* can be involved for FP and 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 in minimal
  - If a FP and FN are weigthed equally, cost lines follow the diagonal (blue line)
  - If a FP is 10 times worse than a FN: pink line
  - IF a FN is 10 times worse than a FP: red line

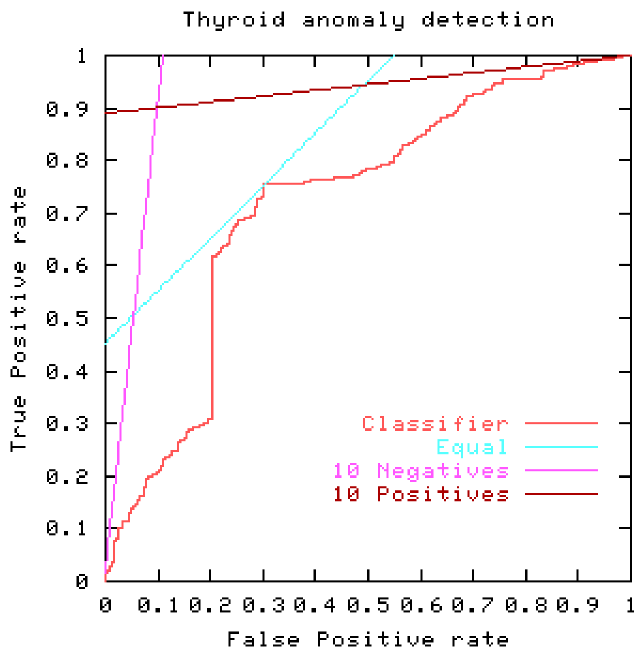
### Model selection

- 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.

```
[70]: from sklearn.metrics import roc_curve
      fpr_rf, tpr_rf, thresholds_rf = roc_curve(y_test, rf.predict_proba(X_test)
```

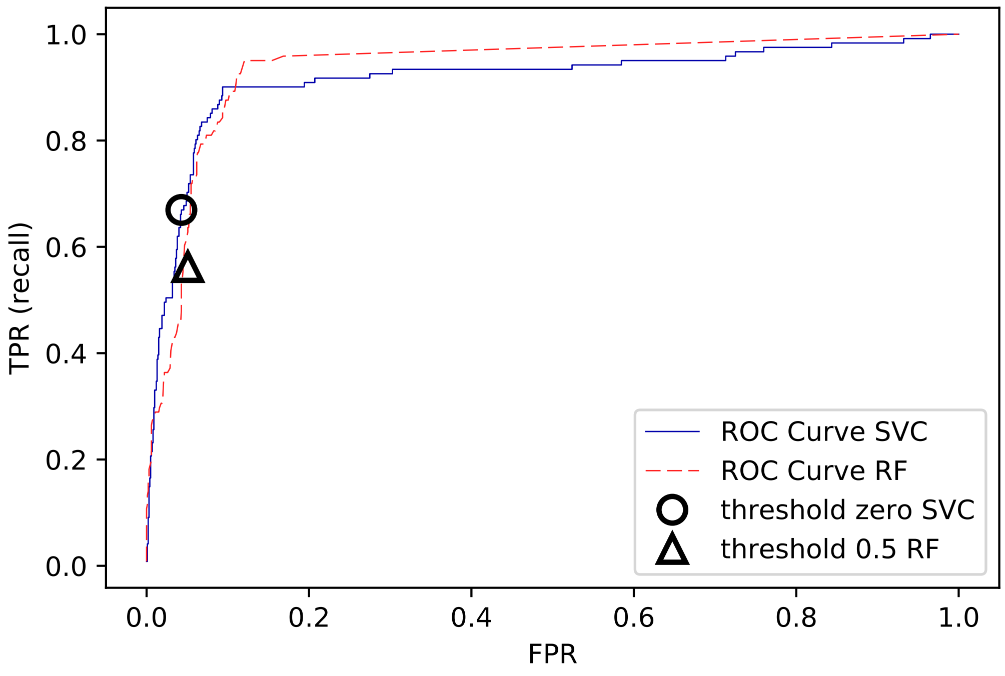


roc



ROC cost curves

```
plt.plot(fpr, tpr, label="ROC Curve SVC")
plt.plot(fpr_rf, tpr_rf, label="ROC Curve RF")

plt.xlabel("FPR")
plt.ylabel("TPR (recall)")
plt.plot(fpr[close_zero], tpr[close_zero], 'o', markersize=10,
         label="threshold zero SVC", fillstyle="none", c='k', mew=2)
close_default_rf = np.argmin(np.abs(thresholds_rf - 0.5))
plt.plot(fpr_rf[close_default_rf], tpr[close_default_rf], '^', markersize=
         label="threshold 0.5 RF", fillstyle="none", c='k', mew=2)

plt.legend(loc=4);
```



### Area under the ROC curve

- A good summary measure is the area under the ROC curve (AUROC or AUC)
- Compute using the `roc_auc_score`
  - Don't use `auc`

```
[71]: from sklearn.metrics import roc_auc_score
      rf_auc = roc_auc_score(y_test, rf.predict_proba(X_test)[:, 1])
      svc_auc = roc_auc_score(y_test, svc.decision_function(X_test))
      print("AUC for Random Forest: {:.3f}".format(rf_auc))
      print("AUC for SVC: {:.3f}".format(svc_auc))
```

```
AUC for Random Forest: 0.937
AUC for SVC: 0.916
```

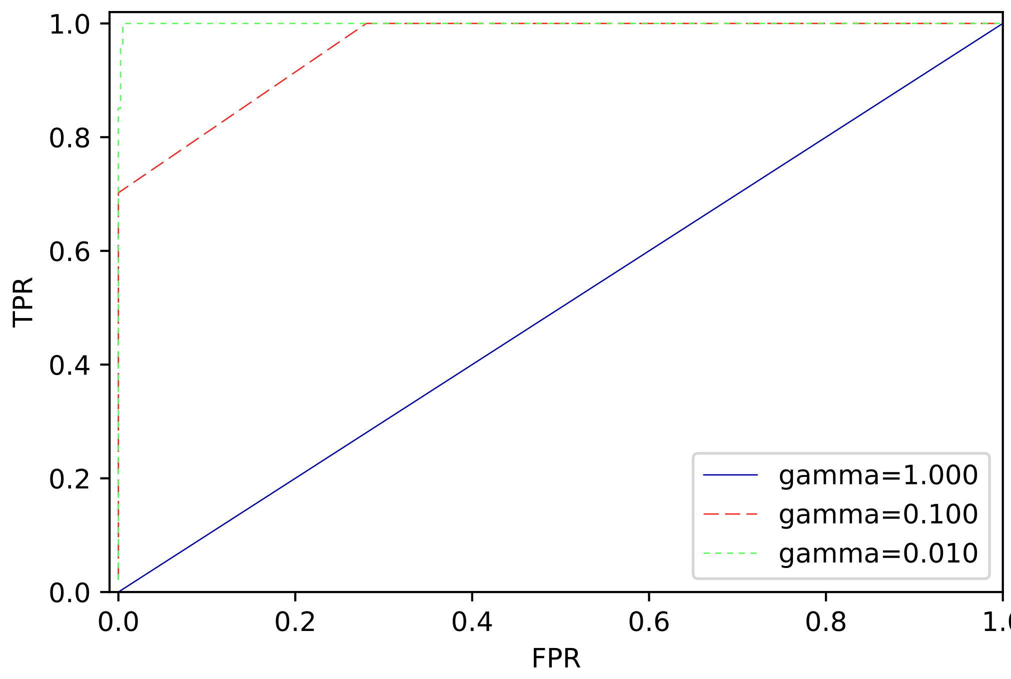
### Imbalanced classes

- AUC is popular because it is insensitive to class imbalance
  - Random guessing yields TPR=FPR no matter what the class imbalance is
  - All points are on the diagonal line, hence an AUC of 0.5
  - Hint: use the visualization of TPR,FPR to see this
- Example: unbalanced digits
  - 3 models, ACC is the same, AUC not
  - If we optimize for ACC, our model could be just random guessing

```
[72]: y = digits.target == 9

      X_train, X_test, y_train, y_test = train_test_split(
          digits.data, y, random_state=0)

      plt.figure()

      for gamma in [1, 0.1, 0.01]:
          svc = SVC(gamma=gamma).fit(X_train, y_train)
          accuracy = svc.score(X_test, y_test)
          auc = roc_auc_score(y_test, svc.decision_function(X_test))
          fpr, tpr, _ = roc_curve(y_test , svc.decision_function(X_test))
          print("gamma = {:.3f}  accuracy = {:.2f}  AUC = {:.4f}".format(
                  gamma, accuracy, auc))
          plt.plot(fpr, tpr, label="gamma={:.3f}".format(gamma))
      plt.xlabel("FPR")
      plt.ylabel("TPR")
      plt.xlim(-0.01, 1)
      plt.ylim(0, 1.02)
      plt.legend(loc="best")
```

```
gamma = 1.000  accuracy = 0.90  AUC = 0.5000
gamma = 0.100  accuracy = 0.90  AUC = 0.9582
gamma = 0.010  accuracy = 0.90  AUC = 0.9995
```

```
<matplotlib.legend.Legend at 0x11253c6d8>
```



### Take home message

- AUC is highly recommended, especially on imbalanced data
- Remember to calibrate the threshold to your needs

### Multi-class classification

- Multiclass metrics are derived from binary metrics, averaged over all classes
- Let's consider the full (10-class) handwritten digit recognition data

Confusion matrix

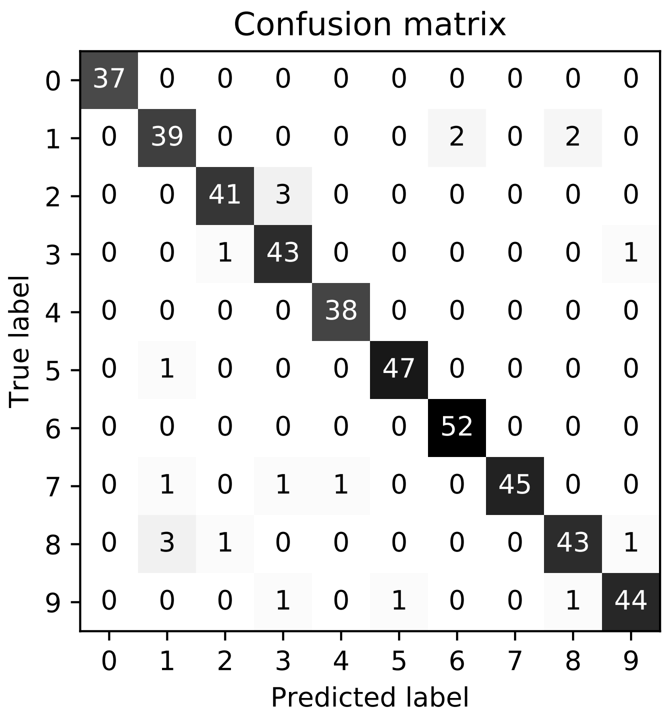
```
[73]: from sklearn.metrics import accuracy_score
      digits = load_digits()
      X_train, X_test, y_train, y_test = train_test_split(
          digits.data, digits.target, random_state=0)
      lr = LogisticRegression().fit(X_train, y_train)
      pred = lr.predict(X_test)
      print("Accuracy: {:.3f}".format(accuracy_score(y_test, pred)))
      print("Confusion matrix:\n{}".format(confusion_matrix(y_test, pred)))
```

```
Accuracy: 0.953
Confusion matrix:
[[37  0  0  0  0  0  0  0  0  0]
 [ 0 39  0  0  0  0  2  0  2  0]
 [ 0  0 41  3  0  0  0  0  0  0]
 [ 0  0  1 43  0  0  0  0  0  1]
 [ 0  0  0  0 38  0  0  0  0  0]
 [ 0  1  0  0  0 47  0  0  0  0]
 [ 0  0  0  0  0  0 52  0  0  0]
 [ 0  1  0  1  1  0  0 45  0  0]
 [ 0  3  1  0  0  0  0  0 43  1]
 [ 0  0  0  1  0  1  0  0  1 44]]
```

Visualized as a heatmap

- Which digits are easy to predict? Which ones are confused?

```
[74]: scores_image = mglearn.tools.heatmap(
          confusion_matrix(y_test, pred), xlabel='Predicted label',
          ylabel='True label', xticklabels=digits.target_names,
          yticklabels=digits.target_names, cmap=plt.cm.gray_r, fmt="%d")
      plt.title("Confusion matrix")
      plt.gca().invert_yaxis()
```



|  | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 37 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1 | 0 | 39 | 0 | 0 | 0 | 0 | 2 | 0 | 2 | 0 |
| 2 | 0 | 0 | 41 | 3 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | 0 | 0 | 1 | 43 | 0 | 0 | 0 | 0 | 0 | 1 |
| 4 | 0 | 0 | 0 | 0 | 38 | 0 | 0 | 0 | 0 | 0 |
| 5 | 0 | 1 | 0 | 0 | 0 | 47 | 0 | 0 | 0 | 0 |
| 6 | 0 | 0 | 0 | 0 | 0 | 0 | 52 | 0 | 0 | 0 |
| 7 | 0 | 1 | 0 | 1 | 1 | 0 | 0 | 45 | 0 | 0 |
| 8 | 0 | 3 | 1 | 0 | 0 | 0 | 0 | 0 | 43 | 1 |
| 9 | 0 | 0 | 0 | 1 | 0 | 1 | 0 | 0 | 1 | 44 |

Precision, recall, F1-score

- Now yield 10 per-class scores

```
[75]: print(classification_report(y_test, pred))
```

```
              precision    recall  f1-score   support

           0       1.00      1.00      1.00        37
           1       0.89      0.91      0.90        43
           2       0.95      0.93      0.94        44
           3       0.90      0.96      0.92        45
```

```
              4       0.97      1.00      0.99        38
              5       0.98      0.98      0.98        48
              6       0.96      1.00      0.98        52
              7       1.00      0.94      0.97        48
              8       0.93      0.90      0.91        48
              9       0.96      0.94      0.95        47

avg / total       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, them 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

```
[76]: print("Micro average f1 score: {:.3f}".format(f1_score(y_test, pred, avera
      print("Weighted average f1 score: {:.3f}".format(f1_score(y_test, pred, av
      print("Macro average f1 score: {:.3f}".format(f1_score(y_test, pred, avera
```

```
Micro average f1 score: 0.953
Weighted average f1 score: 0.953
Macro average f1 score: 0.954
```

## Regression metrics

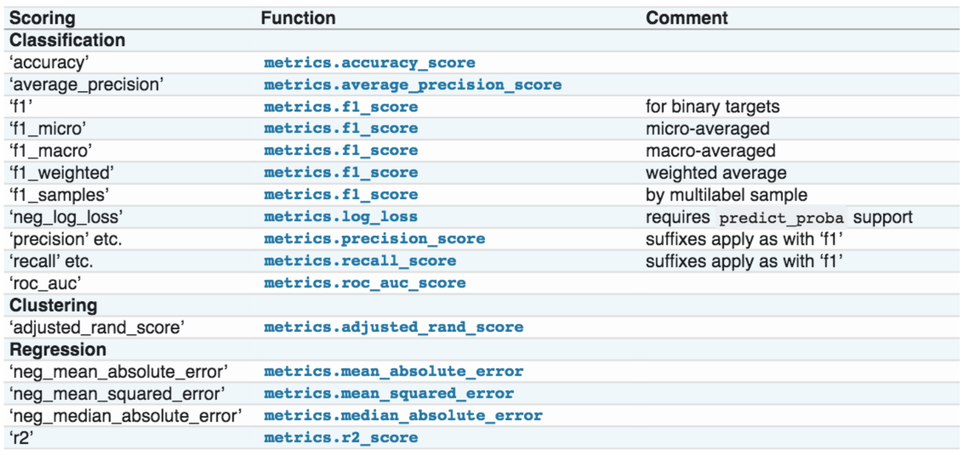
Most commonly used are - (root) mean squared error: $\frac{\sum_i (y_{pred_i} - y_{actual_i})^2}{n}$ - mean absolute error: $\frac{\sum_i |y_{pred_i} - y_{actual_i}|}{n}$ - Less sensitive to outliers and large errors - R squared (r2) - Ratio of variation explained by the model / total variation - Always between 0 and 1, easier to interpret (higher is better) - Does not measure bias. Look at the residuals to make sure.

## Using evaluation metrics in model selection

- You typically want to use AUC or other relevant measures in `cross_val_score` and `GridSearchCV` instead of the default accuracy.
- scikit-learn makes this easy through the `scoring` argument
  - But, you need to need to look the mapping between the scorer and the metric

Or simply look up like this:

```
[77]: from sklearn.metrics.scorer import SCORERS
      print("Available scorers:\n{}".format(sorted(SCORERS.keys())))
```



| Scoring | Function | Comment |
|---|---|---|
| **Classification** | | |
| 'accuracy' | metrics.accuracy_score | |
| 'average_precision' | metrics.average_precision_score | |
| 'f1' | metrics.f1_score | for binary targets |
| 'f1_micro' | metrics.f1_score | micro-averaged |
| 'f1_macro' | metrics.f1_score | macro-averaged |
| 'f1_weighted' | metrics.f1_score | weighted average |
| 'f1_samples' | metrics.f1_score | by multilabel sample |
| 'neg_log_loss' | metrics.log_loss | requires `predict_proba` support |
| 'precision' etc. | metrics.precision_score | suffixes apply as with 'f1' |
| 'recall' etc. | metrics.recall_score | suffixes apply as with 'f1' |
| 'roc_auc' | metrics.roc_auc_score | |
| **Clustering** | | |
| 'adjusted_rand_score' | metrics.adjusted_rand_score | |
| **Regression** | | |
| 'neg_mean_absolute_error' | metrics.mean_absolute_error | |
| 'neg_mean_squared_error' | metrics.mean_squared_error | |
| 'neg_median_absolute_error' | metrics.median_absolute_error | |
| 'r2' | metrics.r2_score | |

scorers

```
Available scorers:
['accuracy', 'adjusted_rand_score', 'average_precision', 'f1', 'f1_macro', 'f1_m
```

Cross-validation with accuracy and AUC

```
[80]: # default scoring for classification is accuracy
      print("Default scoring: {}".format(
            cross_val_score(SVC(), digits.data, digits.target == 9)))
      # providing scoring="accuracy" doesn't change the results
      explicit_accuracy =  cross_val_score(SVC(), digits.data, digits.target ==
                                           scoring="accuracy")
      print("Explicit accuracy scoring: {}".format(explicit_accuracy))
      roc_auc =  cross_val_score(SVC(), digits.data, digits.target == 9,
                                 scoring="roc_auc")
      print("AUC scoring: {}".format(roc_auc))
```

```
Default scoring: [ 0.9   0.9   0.9]
Explicit accuracy scoring: [ 0.9   0.9   0.9]
AUC scoring: [ 0.994   0.99    0.996]
```

Grid Search with accuracy and AUC

- With accuracy, gamma=0.0001 is selected
- With AUC, gamma=0.01 is selected
  - Actually has better accuracy on the test set

```
[81]: X_train, X_test, y_train, y_test = train_test_split(
          digits.data, digits.target == 9, random_state=0)

      # we provide a somewhat bad grid to illustrate the point:
      param_grid = {'gamma': [0.0001, 0.01, 0.1, 1, 10]}
      # using the default scoring of accuracy:
      grid = GridSearchCV(SVC(), param_grid=param_grid)
      grid.fit(X_train, y_train)
```

```
print("Grid-Search with accuracy")
print("Best parameters:", grid.best_params_)
print("Best cross-validation score (accuracy)): {:.3f}".format(grid.best_s
print("Test set AUC: {:.3f}".format(
        roc_auc_score(y_test, grid.decision_function(X_test))))
print("Test set accuracy: {:.3f}".format(grid.score(X_test, y_test)))

# using AUC scoring instead:
grid = GridSearchCV(SVC(), param_grid=param_grid, scoring="roc_auc")
grid.fit(X_train, y_train)
print("\nGrid-Search with AUC")
print("Best parameters:", grid.best_params_)
print("Best cross-validation score (AUC): {:.3f}".format(grid.best_score_)
print("Test set AUC: {:.3f}".format(
        roc_auc_score(y_test, grid.decision_function(X_test))))
print("Test set accuracy: {:.3f}".format(grid.score(X_test, y_test)))
```

```
Grid-Search with accuracy
Best parameters: {'gamma': 0.0001}
Best cross-validation score (accuracy)): 0.970
Test set AUC: 0.992
Test set accuracy: 0.973

Grid-Search with AUC
Best parameters: {'gamma': 0.01}
Best cross-validation score (AUC): 0.997
Test set AUC: 1.000
Test set accuracy: 1.000
```

## Summary

- k-fold Cross-validation
  - Choose k depending on how much data you have
    - Larger k is slower, but allows more training data
    - 10-fold, 5-fold, 5x2-fold most popular
  - Always use stratification for (imbalanced) classification
  - Train-test split and Shuffle-split: useful for large datasets
  - Use grouping when you want to generalize over groups
- Model selection
  - Don't aggregate over test scores: those have seen the test data
  - Use validation sets to choose algorithms/hyperparameters first
- Optimization
  - Grid Search: exhaustive but simple
  - Random Search: scales better
  - Model-based optimization: more efficient, scales better
- Evaluation measures

- High accuracy is seldom the true goal
- Choose metric depending on how you will use the model
- Real world data is often imbalanced, has different costs for FP, FN