Model Selection

Evaluating and selecting algorithms and hyperparameters.

[2]:
```
# 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:

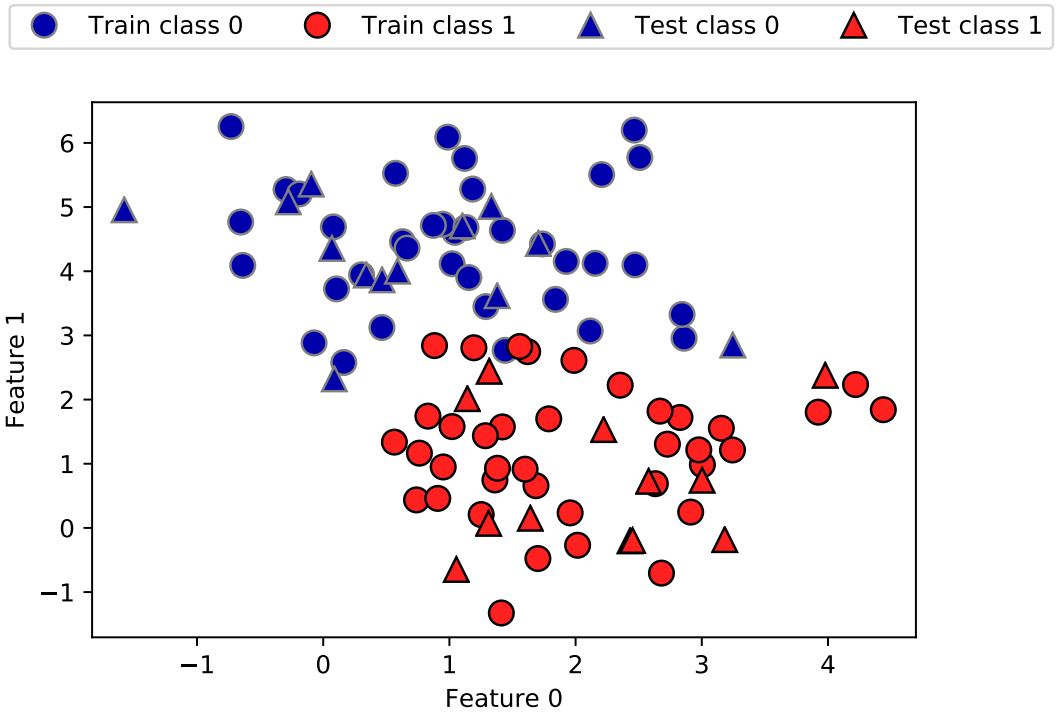
- Split data into training and test set (75%-25%)
  - In sklearn we split in training and test predictors (X_train, X_test) and labels (y_train, y_test)
- Train (fit) a model on the training data
- Score a model on the test data (comparing predicted and true labels)
  - We are interested in how well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

[3]:
```
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

```
[4]: 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));
```



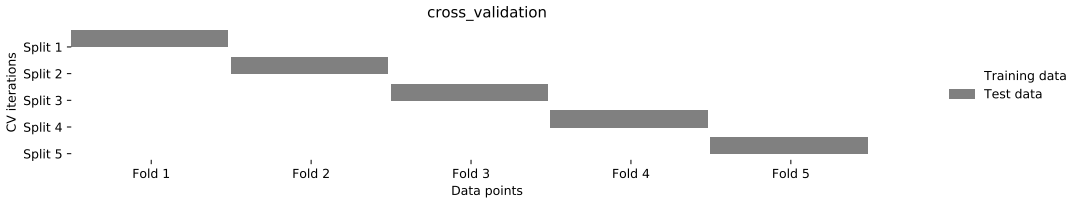
Limitations to this approach:

- 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)

```
[5]: 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

```
[6]: 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

```
[7]: 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*

```
[8]: print("Average cross-validation score: {:.2f}".format(scores.mean()))
     print("Variance in cross-validation score: {:.4f}".format(np.var(scores)))
```

```
Average cross-validation score: 0.96
Variance in cross-validation score: 0.0015
```

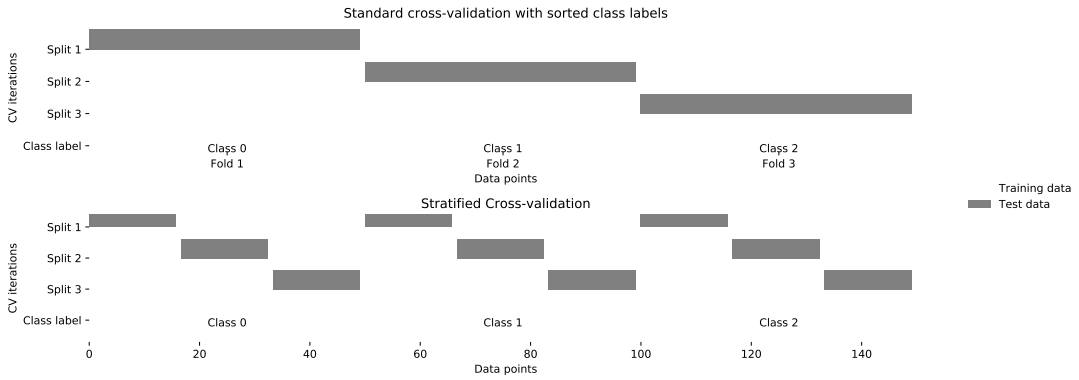
Benefits of cross-validation

- 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

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



- scikit-learn (e.g. `cross_val_score`) will use:
  - stratified cross-validation by default for classification
  - normal cross-validation for regression
  - both are non-randomized (samples are not shuffled beforehand)
    - ordered data (e.g. time series) should never be randomized
- You can build folds manually with `KFold`
  - randomizable (`shuffle` parameter), non-stratified (!)
- Or `StratifiedKFold`

- randomizable (`shuffle` parameter), stratified

```
[76]: from sklearn.model_selection import KFold, StratifiedKFold
      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.    0.7   0.    0.967 0.   ]
```

```
[77]: # 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.]
```

```
[79]: kfold = KFold(n_splits=3, shuffle=True, random_state=0)
      print("Cross-validation scores (shuffled, not stratified):\n{}".format(
          cross_val_score(logreg, iris.data, iris.target, cv=kfold)))
      skfold = StratifiedKFold(n_splits=3, shuffle=True, random_state=0)
      print("Cross-validation scores (shuffled, stratified):\n{}".format(
          cross_val_score(logreg, iris.data, iris.target, cv=skfold)))
      print("Cross-validation scores (default: stratified, not shuffled):\n{}".f
          cross_val_score(logreg, iris.data, iris.target, cv=3)))
```

```
Cross-validation scores (shuffled, not stratified):
[0.66 0.96 0.84]
Cross-validation scores (shuffled, stratified):
[0.784 0.863 0.792]
Cross-validation scores (default: stratified, not shuffled):
[0.804 0.863 0.771]
```

Leave-One-Out cross-validation

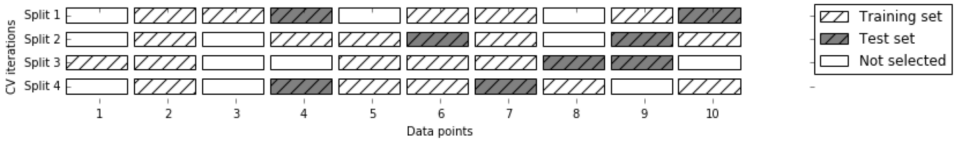
- *k* fold cross-validation with *k* equal to the number of samples
- Completely unbiased (in terms of data splits), but computationally expensive
- But: generalizes *less* well towards unseen data
  - The training sets are correlated (overlap heavily)
  - Overfits on the data used for (the entire) evaluation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

```
[13]: 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` = 5, `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)

```
[14]: 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:
[0.88  0.947 0.973 0.867 0.987 0.96  0.973 0.867 0.933 0.853]
```

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

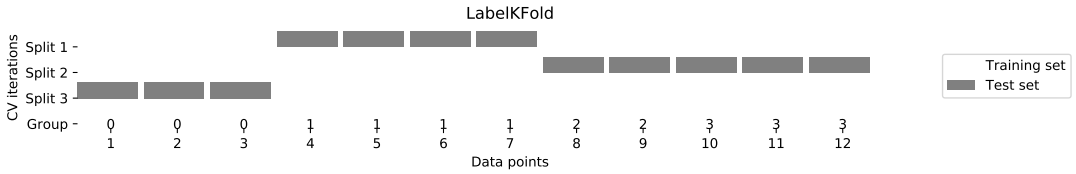
- Cross-validation is still biased in that the initial split can be made in many ways
- Repeated, or n-times-k-fold cross-validation:
  - Shuffle data randomly, do k-fold cross-validation
  - Repeat n times, yields n times k scores
- Unbiased, very robust, but n times more expensive

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

```
[15]: 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

```
[16]: 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: $\sum_x variance(x) * w_x$

- 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: $\sum_x variance(x) * w_x$

[17]:
```
# 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))]
```

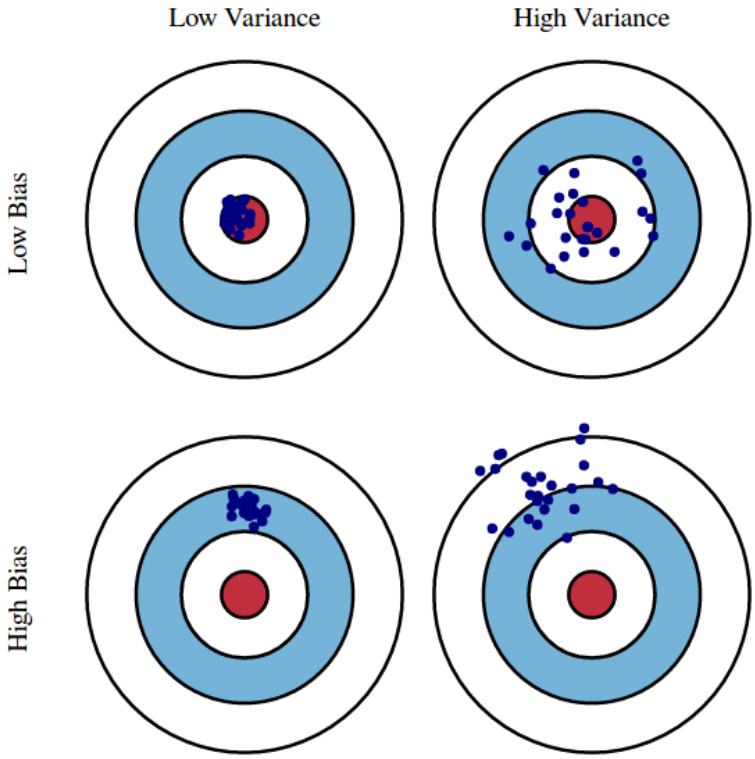


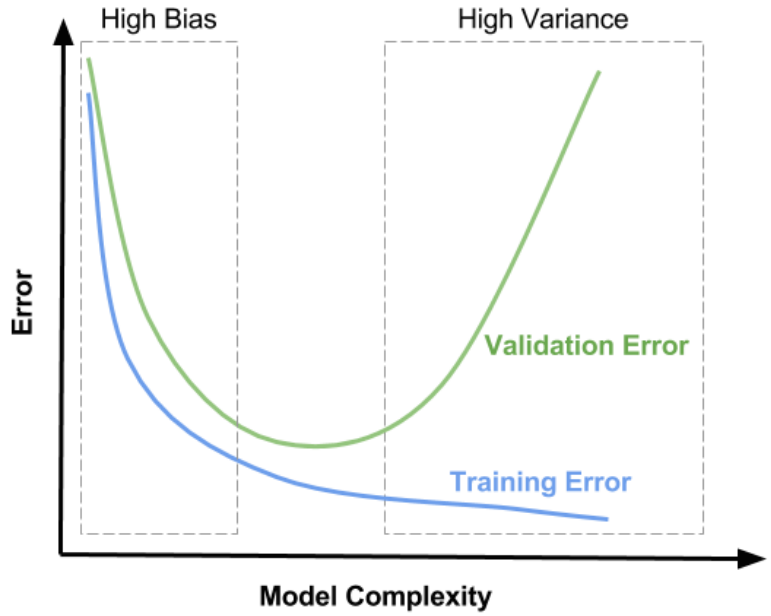
Fig. 1 Graphical illustration of bias and variance.

Bias-variance

```
        # 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: 14.35, Variance: 0.75, Total error: 15.10
```

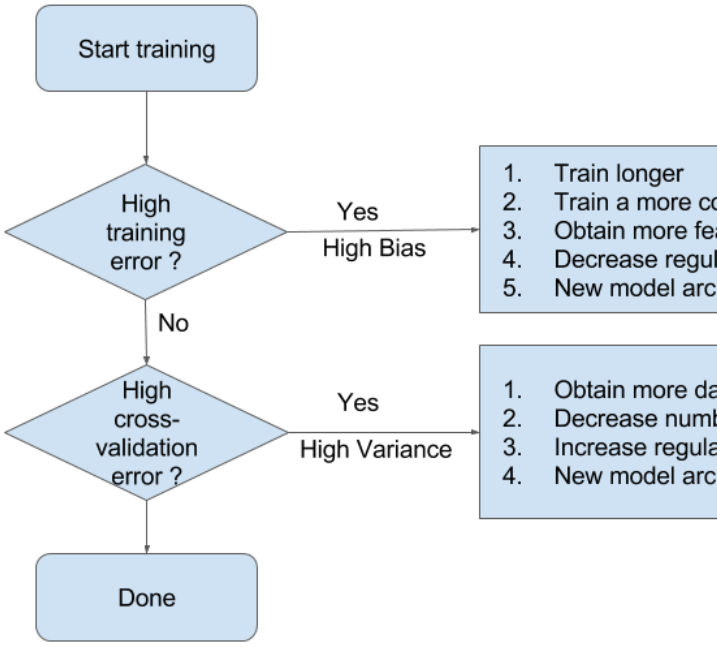
Bias-variance and overfitting



Bias-variance-tradeoff

- 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



Bias-Variance Flowchart (Andrew Ng, Coursera)

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.

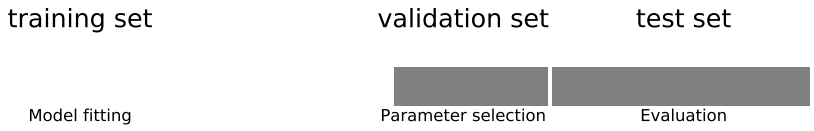
```
[18]: # naive grid search implementation
      from sklearn.svm import SVC
      X_train, X_test, y_train, y_test = train_test_split(iris.data, iris.target
                                                          random_state=0)
      print("Size of training set: {}   size of test set: {}".format(
            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: {'C': 100, 'gamma': 0.001}
```

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

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



```
[20]: 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:  {'C': 10, 'gamma': 0.001}
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`

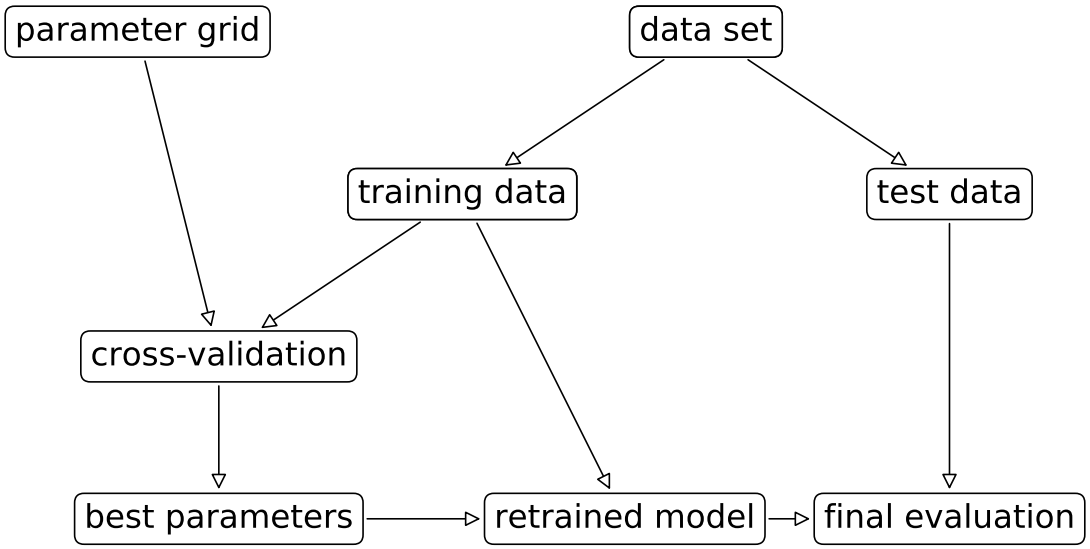
```
[21]: # manual grid search cv
      for gamma in [0.001, 0.01, 0.1, 1, 10, 100]:
```

```
            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='ovr', degree=3, gamma=0.01, kernel='rbf',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)
```

Overall process

[69]:
```
plt.rcParams['savefig.dpi'] = 75 # Avoid overlapping boxes
mglearn.plots.plot_grid_search_overview()
```



[70]:
```
plt.rcParams['savefig.dpi'] = 100 # Back to normal
```

Grid search in scikit-learn

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

```
[23]: 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:
{'C': [0.001, 0.01, 0.1, 1, 10, 100], 'gamma': [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

```
[24]: 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='ovr', degree=3, gamma='auto', kernel='rbf',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False),
       fit_params=None, iid=True, n_jobs=1,
       param_grid={'C': [0.001, 0.01, 0.1, 1, 10, 100], 'gamma': [0.001, 0.01, 0
       pre_dispatch='2*n_jobs', refit=True, return_train_score='warn',
       scoring=None, verbose=0)
```

The optimized test score and hyperparameters can easily be retrieved:

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

```
Test set score: 0.97
```

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

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

```
[27]: # 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='ovr', degree=3, gamma=0.01, kernel='rbf',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)
```

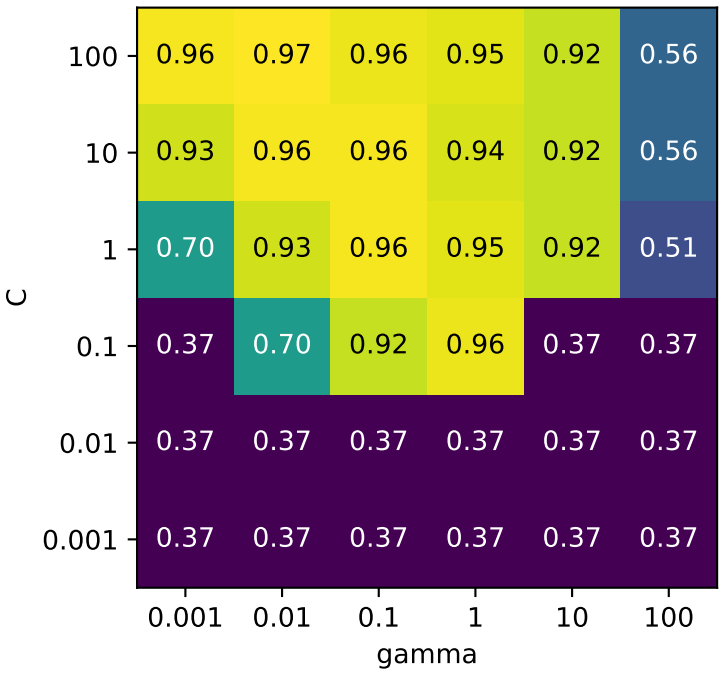
Visualizing hyperparameter impact We can retrieve and visualize the cross-validation resulst to better understand the impact of hyperparameters

```
[28]: 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       6.84e-04         2.75e-04             0.37              0.37
1       5.68e-04         2.36e-04             0.37              0.37
2       5.16e-04         2.12e-04             0.37              0.37
3       5.17e-04         2.11e-04             0.37              0.37
4       5.01e-04         2.05e-04             0.37              0.37

        ...        std_fit_time std_score_time std_test_score  std_train_score
0       ...            2.48e-04       8.84e-05           0.01         2.85e-03
1       ...            4.18e-05       2.65e-05           0.01         2.85e-03
2       ...            8.66e-06       2.95e-06           0.01         2.85e-03
3       ...            1.94e-05       2.88e-06           0.01         2.85e-03
4       ...            9.35e-06       1.39e-06           0.01         2.85e-03

[5 rows x 22 columns]
```

Visualize as a heatmap

```
[29]: 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

```
[30]: 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:
[{'kernel': ['rbf'], 'C': [0.001, 0.01, 0.1, 1, 10, 100], 'gamma': [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

```
[31]: 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:  0.9666666666666668
```

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

```
[32]: 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='ovr', degree=3, gamma='auto', kernel='rbf',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False),
          fit_params=None, iid=True, n_iter=20, n_jobs=1,
```

```
param_distributions={'C': <scipy.stats._distn_infrastructure.rv_frozen
pre_dispatch='2*n_jobs', random_state=None, refit=True,
return_train_score='warn', 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):

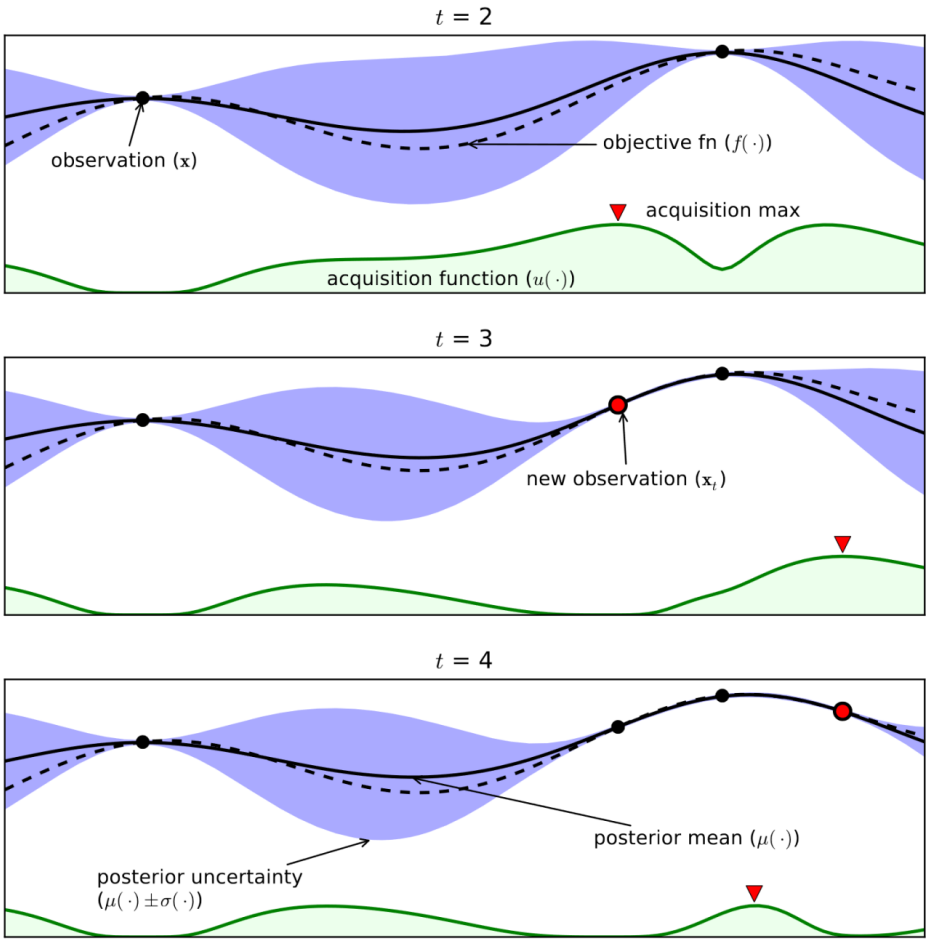
- Consider only 1 continuous hyperparameter (X-axis)
- Y-axis shows cross-validation performance
- Evaluate a number of random hyperparameter settings (black dots)
  - Sometimes an initialization design is used
- Train a model, and predict the expected performance of other (unseen) hyperparameter values
  - 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

Evaluation Metrics and scoring

Keep the end-goal in mind

Metrics for binary classification

- The most common (and simple) application of machine learning in practice
- 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?


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

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?

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

      digits = load_digits()
      y = digits.tar get == 9

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

```
[83]: 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 (accuracy): {:.2f}".format(dummy.score(X_test, y_test))
```

```
dummy score (accuracy): 0.90
```

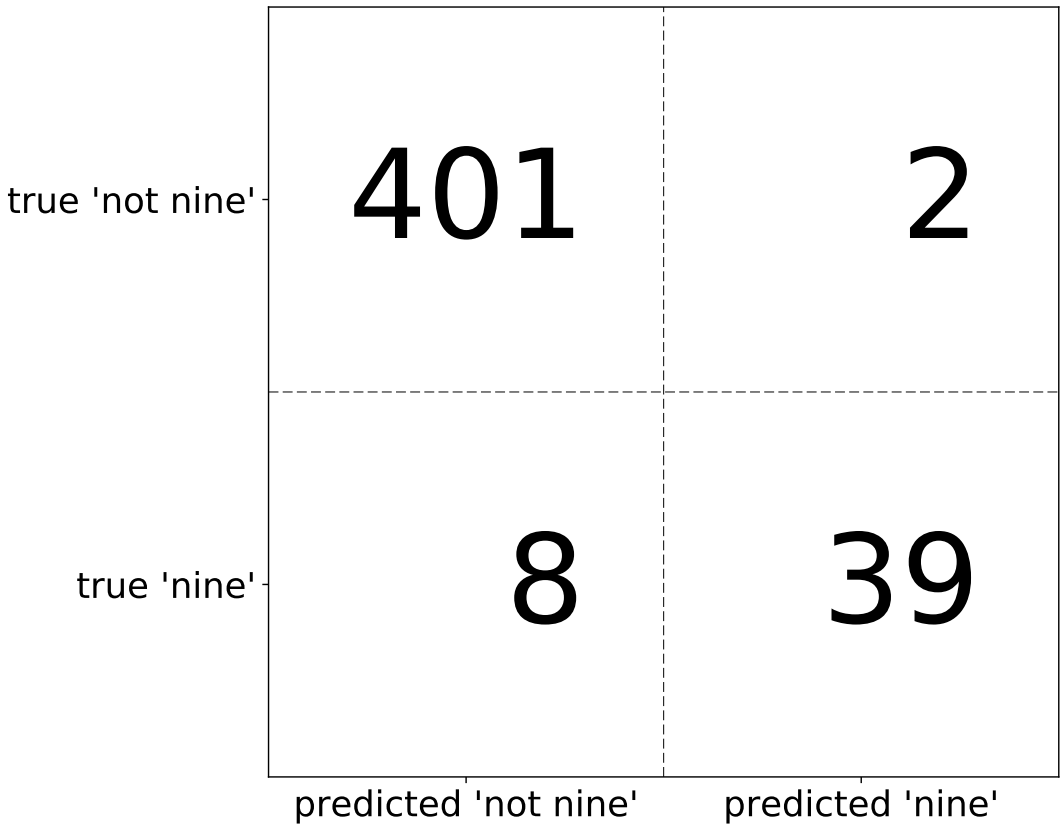
```
[84]: logreg = LogisticRegression(C=0.1).fit(X_train, y_train)
      pred_logreg = logreg.predict(X_test)
      print("logreg score (accuracy): {:.2f}".format(logreg.score(X_test, y_test
```

```
logreg score (accuracy): 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.

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



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

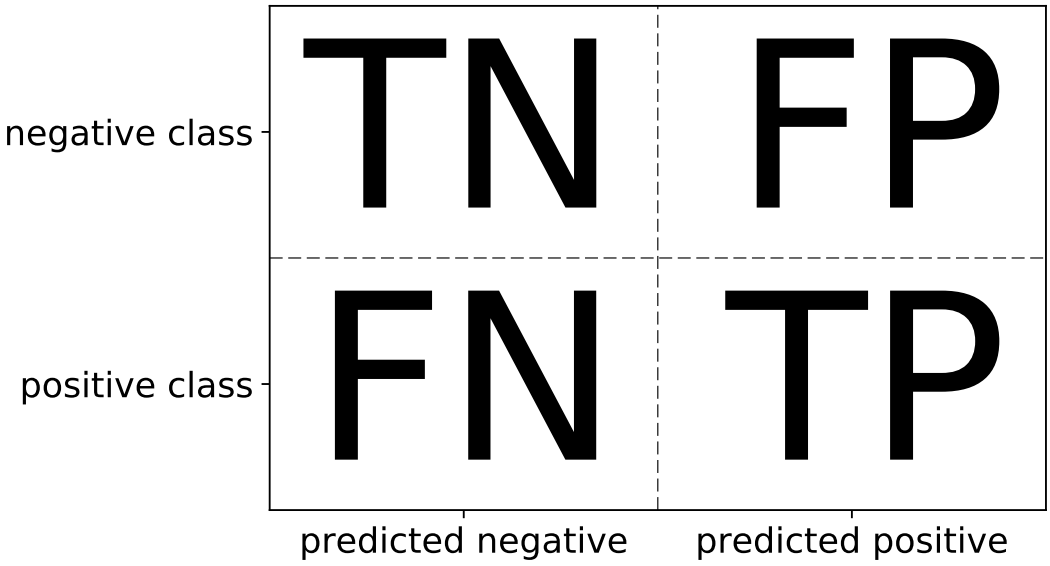
[37]:
```
from sklearn.metrics import confusion_matrix

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)

[38]:
```
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.

```
[39]: 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

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

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

```
precision score most frequent: 0.00
precision score logistic regression: 0.95
```

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)

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

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

```
recall score most frequent: 0.00
recall score logistic regression: 0.83
```

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

$$\text{F1} = 2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}} \tag{0.4}$$

```
[40]: 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 the scores *by class*, use `classification_report`
  - One class viewed as positive, others als negative
  - Support: number of samples in each class
  - Last line: weighted average over the classes (weighted by number of samples in each class)

```
[85]: 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
```

```
[42]: 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
```

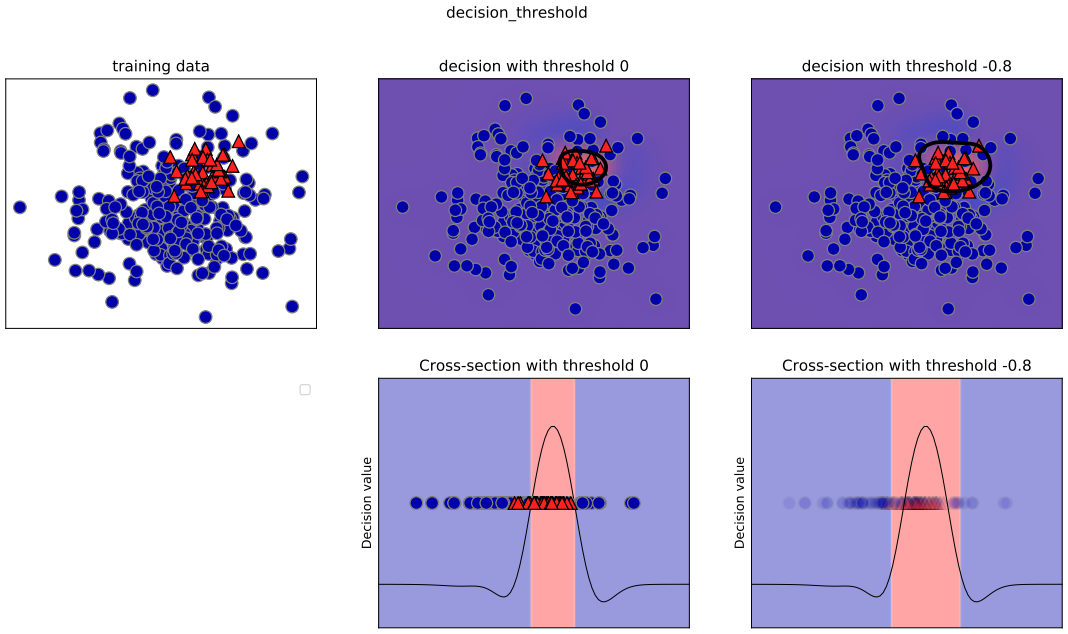
Taking uncertainty into account

- 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

```
[43]: 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)

[44]: 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

```
[45]: 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
```

```
[46]: 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

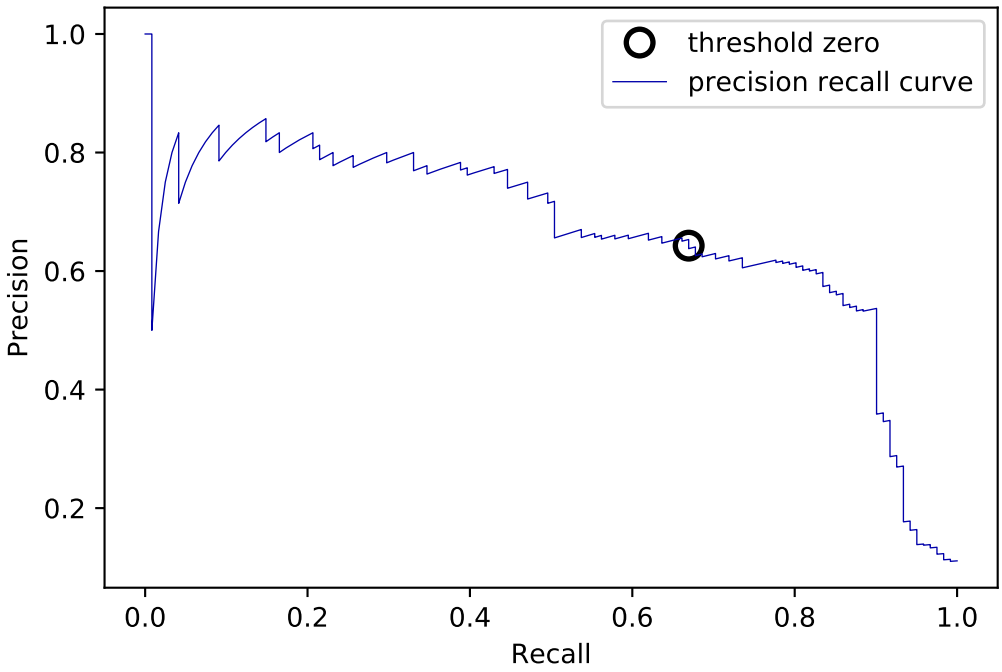
- The right threshold depends on your application, should be driven by business goals.
- You can have arbitrary high recall, but you often want reasonable precision, too.
- It is not clear beforehand where the optimale trade-off (or *operating point*) will be, so it is useful to look at all possible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

[86]:
```
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 shown 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

[87]:
```
plt.rcParams['savefig.dpi'] = 200 # Use 300 for PDF, 100 for slides
# 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");
```

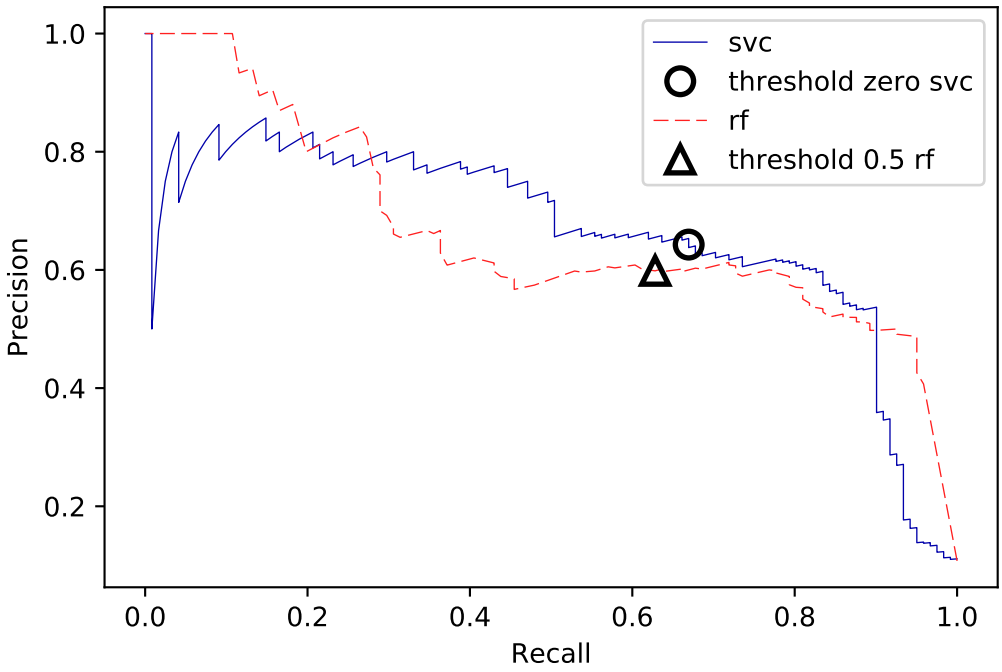


Model selection

- 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

[88]:
```
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

```
[50]: 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

```
[51]: 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: 0.660
Average precision of svc: 0.666
```

Receiver Operating Characteristics (ROC) and AUC

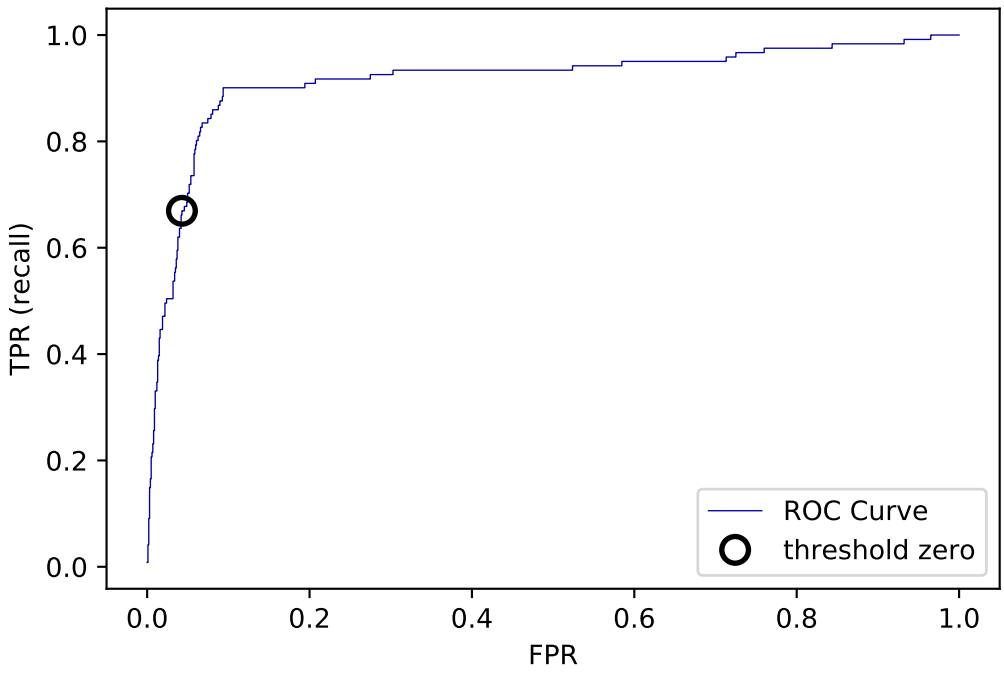
- There is another trade-off between recall (true positive rate, TPR) and the false positive rate (FPR).
- The 2D space created by TPR and FPR is called the Receiver Operating Characteristics (ROC) space
- A model will be at one point in this ROC space

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

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

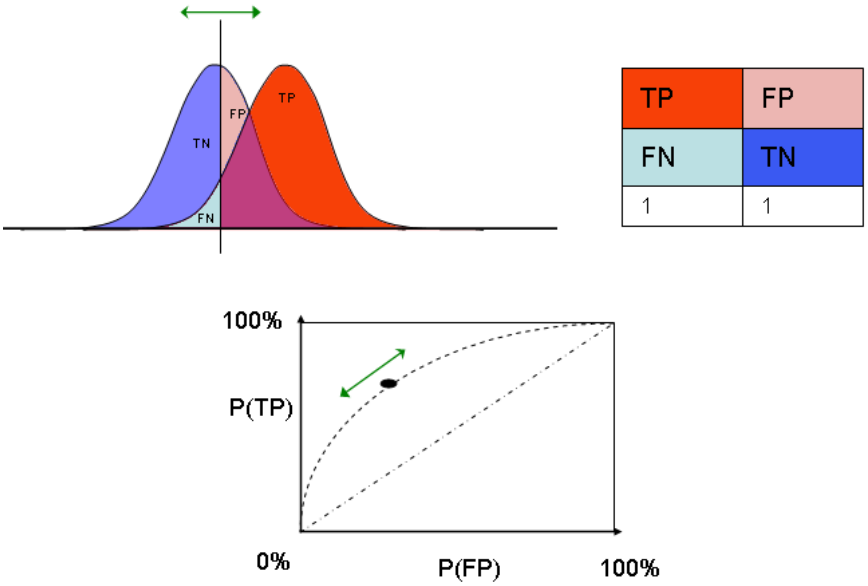
- Varying the decision threshold yields the ROC curve
- It can be computed with the `roc_curve` function
- Ideal is close to the top left: high recall, low FPR
- Inspect the curve to find the preferred calibration
  - Here, we can get much higher recall with slightly worse FPR

[92]:
```
plt.rcParams['savefig.dpi'] = 100 # Use 300 for PDF, 100 for slides
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

- The blue probability density shows the probability p(x) that the model predicts blue if a data point has a certain predicted probability x to be blue. Same for red.
- In a random classifier the probability densities completely overlap.
- All points with a predicted probability higher than the threshold are predicted positive, others negative
- As we increase the threshold, we'll get fewer FPs, more FNs. We move from right to left along the ROC curve.



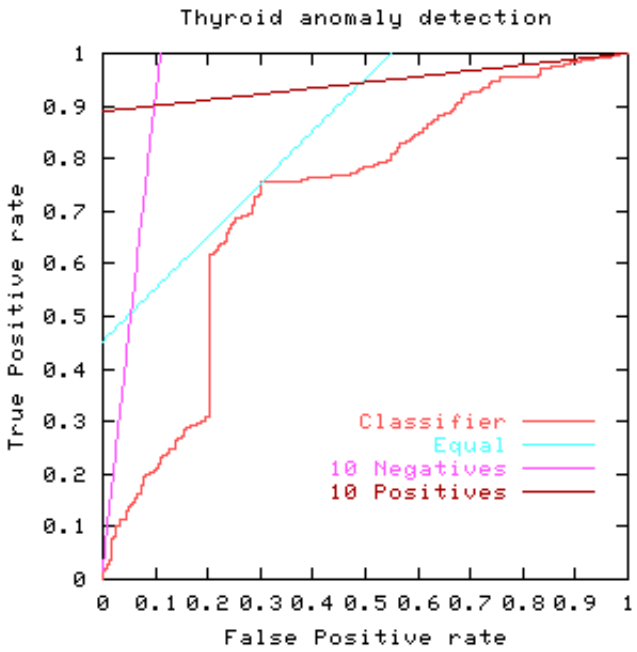
roc

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

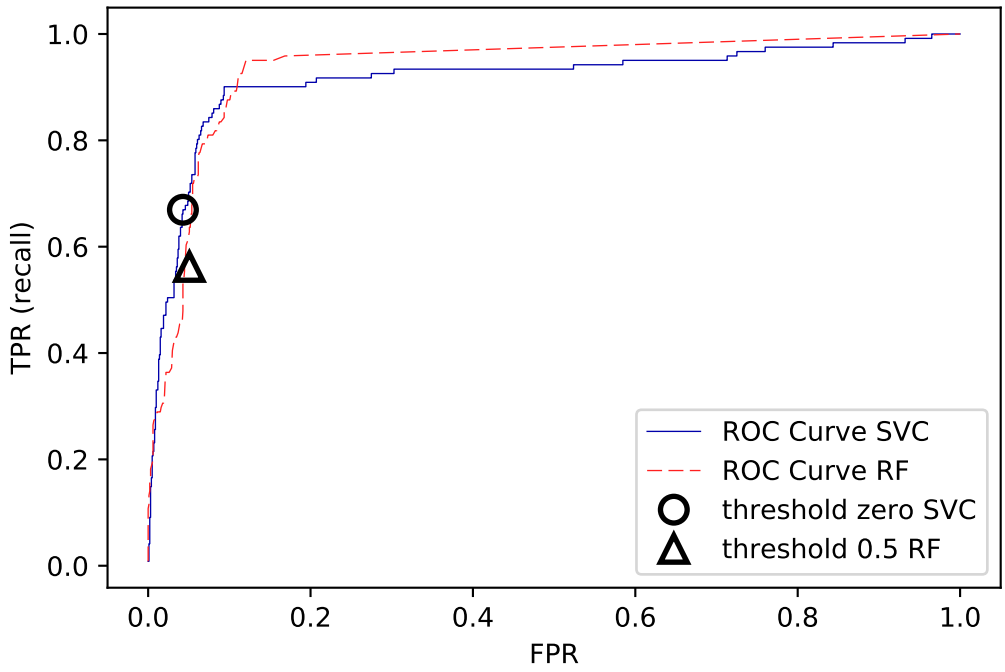
Model selection

- 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.



ROC cost curves

[53]:
```
from sklearn.metrics import roc_curve
fpr_rf, tpr_rf, thresholds_rf = roc_curve(y_test, rf.predict_proba(X_test)

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` (uses less accurate trapezoidal rule)

```
[54]: 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
```

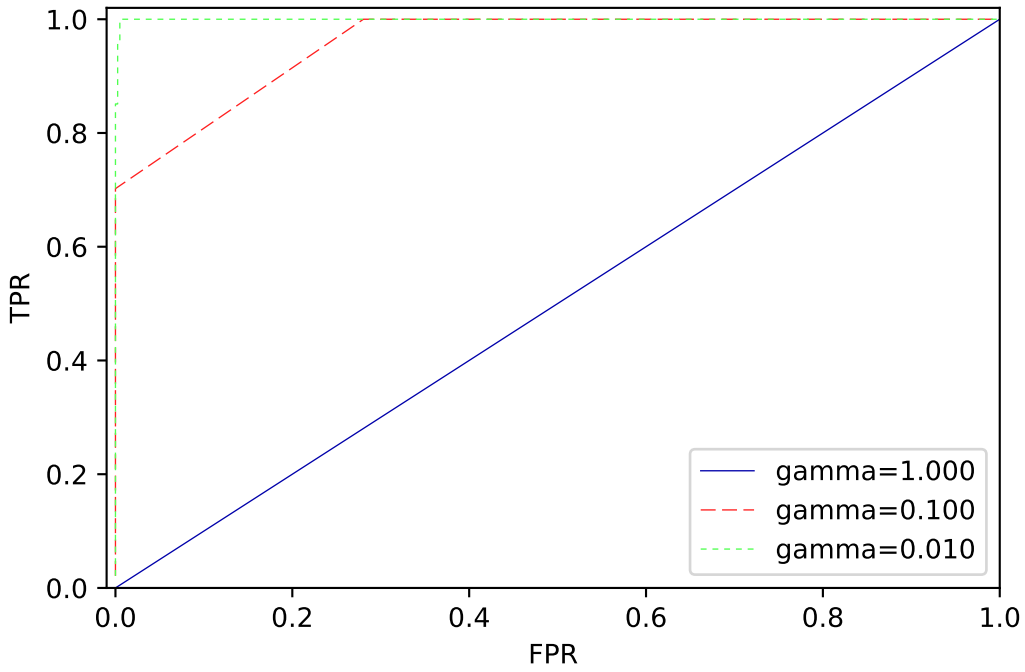
Imbalanced classes

- 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

```
[55]: 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 0x11c4eba58>
```



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

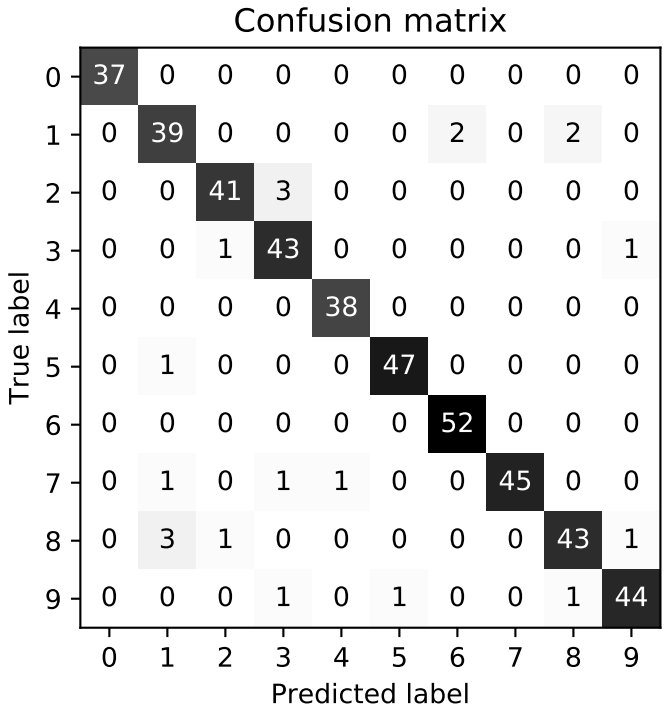
```
[56]: from sklearn.metrics import accuracy_score
      digits = load_digits()
      X_train, X_test, y_train, y_test = train_test_split(
          digits.data, digits.target, random_state=0)
      lr = LogisticRegression().fit(X_train, y_train)
      pred = lr.predict(X_test)
      print("Accuracy: {:.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?

```
[57]: 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()
```



Precision, recall, F1-score

- Now yield 10 per-class scores

```
[58]: 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, then computes scores using these counts: $recall = \frac{\sum_{i=0}^{n} TP_i}{\sum_{i=0}^{n} TP_i + \sum_{i=0}^{n} FN_i}$
  - Use when you care about each sample equally much

```
[59]: 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 (see bias-variance decomposition).

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

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

Or simply look up like this:

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

```
Available scorers:
['accuracy', 'adjusted_mutual_info_score', 'adjusted_rand_score', 'average_preci
```

Cross-validation with accuracy and AUC

```
[61]: # 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

```
[62]: 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

[ ]: