Session 13:

Supervised learning, part 2

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Agenda

Vaaaamos

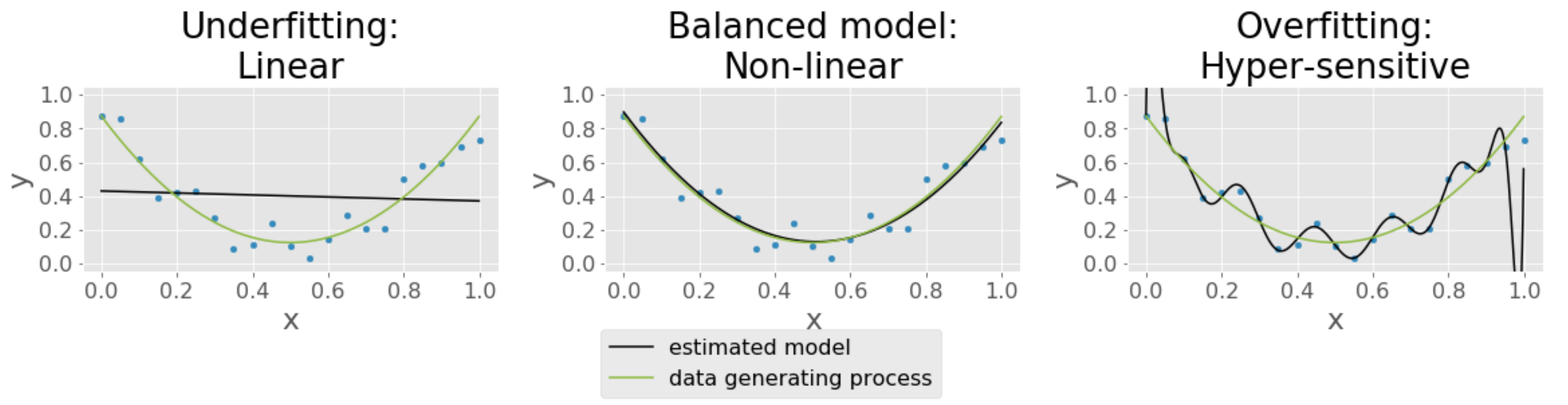
In [15]:
```python
import warnings
from sklearn.exceptions import ConvergenceWarning
warnings.filterwarnings(action='ignore', category=ConvergenceWarning)

import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
import seaborn as sns
```

Supervised problems (1)

What is the tradeoff for making supervised regression models?

```
In [63]: f_bias_var['regression'][2]
```

```
Out[63]:
```



Supervised problems (2)

What was a remedy to overfitting in linear models? How do we measure overfitting?

Regularization

- Too many irrelevant features - solved by L1 regularization ~ lasso
- Exploding coefficients - solved by L2 regularization ~ ridge

Model building

Model pipelines (1)

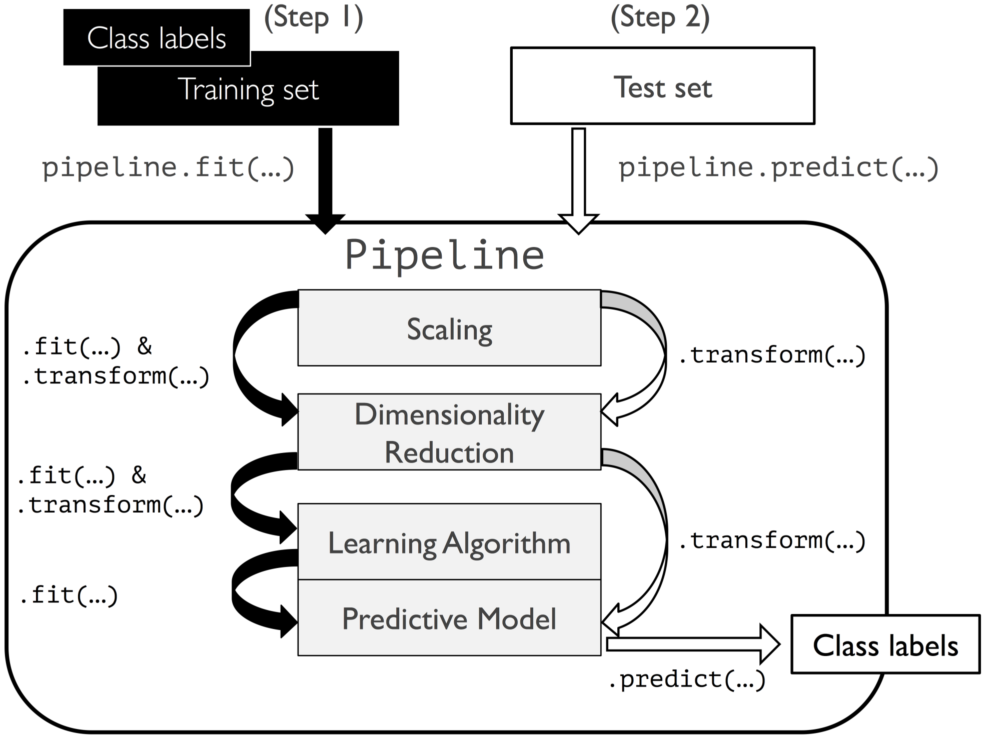
Is there a smart way to build ML models?

Yes, we build a pipeline:

- Preprocessing data
    - Standard: adding polynomials, imputation, rescaling
    - Unsupervised learning (more info..)
- Supervised learning

Model pipelines (2)

How does the pipeline look?



Model pipelines (3)

What are the advantages of using a pipeline?

- Ensures good practice - we only fit on training data.
    - No leakage of data from train to test!
- Much less code!

Applying a model pipeline (1)

What would this look like in Python?

In [7]:
```
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import PolynomialFeatures, StandardScaler

pipe_preproc = make_pipeline(PolynomialFeatures(),
                             StandardScaler())

print(pipe_preproc.steps[0])
print(pipe_preproc.steps[1])
```

```
('polynomialfeatures', PolynomialFeatures(degree=2, include_bias=True, interaction_on
ly=False))
('standardscaler', StandardScaler(copy=True, with_mean=True, with_std=True))
```

Applying a model pipeline (2)

Does this remind you of something?

YES!

Method chaining from Pandas

Applying a model pipeline (3)

Let's some load Boston house price data

```
In [5]: from sklearn.datasets import load_boston
        boston = load_boston()
        print(boston['DESCR'])
        # print('\n'.join(load_boston()['DESCR'].split('\n')[12:26]))
```

Applying a model pipeline (4)

And how do I apply the pipe on the data?

```
In [9]: pipe_preproc = make_pipeline(PolynomialFeatures(),
                                     StandardScaler()) # apply preproc - fit on train
        pipe_preproc.fit(X_train) # fit to training
        X_train_prep = pipe_preproc.transform(X_train) # transform training data
        X_test_prep = pipe_preproc.transform(X_test) # transform test data
```

Applying a model pipeline (5)

What would it like look if we did use the pipe..?

The more steps we have, the more code we save.

In [10]:
```
poly_trans = PolynomialFeatures()
scaler = StandardScaler()

# we call both transformations twice on both test and train
X_train_poly = poly_trans.fit_transform(X_train)
X_test_poly = poly_trans.fit_transform(X_test)
scaler.fit(X_train_poly)
X_train_prep_alt = scaler.transform(X_train_poly)
X_test_prep_alt = scaler.transform(X_test_poly)
```

Model selection

Measuring the problem

Does machine learning work out of the box?

- In some cases ML works quite well out of the box.
- Often ML requires making careful choices.
    - Note that automated machine learning packages and services exist.
    - E.g. AutoML - this a hot research topic

Which choices are to be made?

- We need to pick model building **hyperparameters**.
- E.g. λ for Lasso, Ridge.

Model validation (1)

How do we measure our model's performance for different hyperparameters?

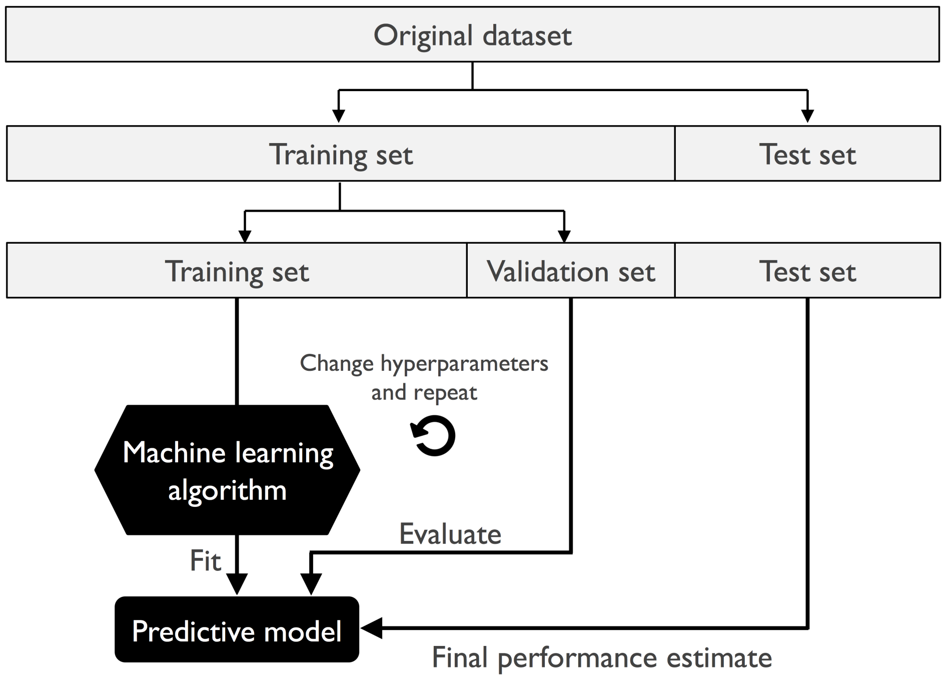
- Remember we cannot use the test set.

Could we somehow mimick what we do with test data?

- Yes, we can split the remaining non-test data into training and validation data:
  - we train model for various hyperparameters on training data;
  - pick the hyperparameters which performs best on validation data.

Model validation (2)

The non-test data is split into training and validation



Model validation (3)

What would this look like in Python?

In [94]:
```
# splitting into development (2/3) and test data (1/3)
X_dev, X_test, y_dev, y_test = train_test_split(X, y, test_size=1/3, random_state=1)

# splitting development into train (1/3) and validation (1/3)
X_train, X_val, y_train, y_val = train_test_split(X_dev, y_dev, test_size=1/2, random_st
ate=1)
```

Model validation (4)

Let's train a linear regression model

In [95]:
```
from sklearn.linear_model import Lasso, LinearRegression
pipe_lr = make_pipeline(PolynomialFeatures(include_bias=False),
                        StandardScaler(),
                        LinearRegression())

pipe_lr.fit(X_dev, y_dev)
```

Out[95]:
```
Pipeline(memory=None,
     steps=[('polynomialfeatures', PolynomialFeatures(degree=2, include_bias=False, i
nteraction_only=False)), ('standardscaler', StandardScaler(copy=True, with_mean=True,
with_std=True)), ('linearregression', LinearRegression(copy_X=True, fit_intercept=Tru
e, n_jobs=None,
         normalize=False))])
```

Model validation (5)

Let's find the Lasso model which performs best in the validation set

```
In [96]: from sklearn.metrics import mean_squared_error as mse

         perform = []
         lambdas = np.logspace(-4, 4, 33)
         for lambda_ in lambdas:
             pipe_lasso = make_pipeline(PolynomialFeatures(include_bias=False),
                                        StandardScaler(),
                                        Lasso(alpha=lambda_, random_state=1))
             pipe_lasso.fit(X_train, y_train)
             y_pred = pipe_lasso.predict(X_val)
             perform.append(mse(y_pred, y_val))

         hyperparam_perform = pd.Series(perform,index=lambdas)

         optimal = hyperparam_perform.nsmallest(1)
         print('Optimal alpha:', optimal.index[0])
         print('Validation MSE: %.3f' % optimal.values[0])
```

```
Optimal alpha: 0.01
Validation MSE: 18.421
```

Model validation (6)

Let's compare the performance of the Lasso vs. Linear Regression

```
In [97]: pipe_lasso = make_pipeline(PolynomialFeatures(include_bias=False),
                                    StandardScaler(),
                                    Lasso(alpha=optimal.index[0]))

         pipe_lasso.fit(X_dev,y_dev)
         print('Lasso', round(mse(pipe_lasso.predict(X_test),y_test), 3))
         print('LinReg', round(mse(pipe_lr.predict(X_test),y_test), 3))
```

```
Lasso 12.399
LinReg 17.802
```

Bias and variance (1)

How do we describe the modelling error?

From [Wikipedia (https://en.wikipedia.org/wiki/Bias%E2%80%93variance_tradeoff)](https://en.wikipedia.org/wiki/Bias%E2%80%93variance_tradeoff) yesterday:

- model **bias**: *an error from erroneous assumptions in the learning algorithm*
    - high bias can cause an algorithm to miss the relevant relations between features and target outputs (**underfitting**)
- model **variance**: *an error from sensitivity to small fluctuations in the training set*
    - high variance can cause an algorithm to model the random noise in the training data, rather than the intended outputs (**overfitting**).

Bias and variance (2)

So what is overfitting?

Overfitting is: low bias / high variance

- traning our model captures all patterns but we also find some irrelevant
- reacts too much to training sample errors
    - some errors are just noise, and thus we find too many spurious relations
- examples of causes:
    - too much polynomial expansion of variables (`PolynomialFeatures`)
    - non-linear/logistic without properly tuned hyperparameters:
        - Decision Trees, Support Vector Machines or Neural Networks

Bias and variance (3)

So what is underfitting?

Underfitting is: high bias / low variance

- oversimplification of models, cannot approximate all patterns found
- examples of causes:
    - linear and logistic regression (without polynomial expansion)

Bias and variance (4)

Not so fast.. OLS is unbiased, right?

Yes, OLS is unbiased. But...?

- But .. only by assumption..
    - Requires we know the true form of the model.
        - However, we never know do..

What happens if we introduce regularization?

- Then model is no longer unbiased.
    - (if we assume the model is true)

Smarter validation

Is this approach the smartest way for deciding on choice of hyperparameters?

NO

Our model choice depends a lot on which sample we pick. Could we use more of the data?

Cross validation

The holdout method

How do we got the more out of the data?

We reuse the data in the development set repeatedly

- We test on all the data
- Rotate which parts of data is used for test and train.

Leave-one-out CV

How do we got the most of the data?

The most robust approach

- Each single observation in the training data we use the remaining data to train.
- Makes number of models equal to the number of observations
- Very computing intensive - does not scale! LOOCV

K fold method (1)

How do balance computing time vs. overfitting?

We split the sample into K even sized test bins.

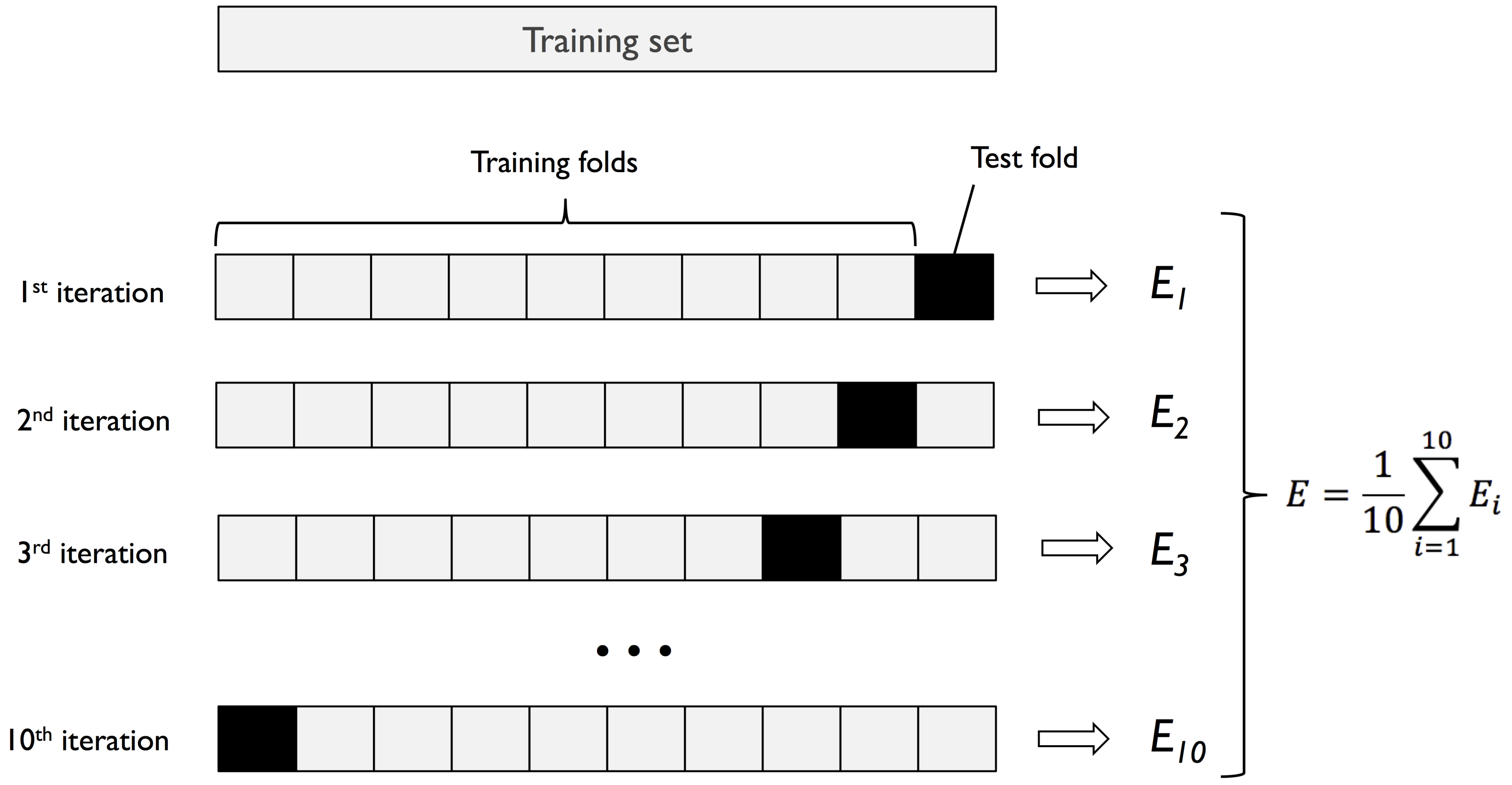
- For each test bin k we use the remaining data for training.

Advantages:

- We use all our data for testing.
- Training is done with 100-(100/K) pct. of the data, i.e. 90 pct. for K=10.

K fold method (2)

In K-fold cross validation we average the errors.



K fold method (3)

How would we use K-fold cross validation to select our model?

We compute MSE for every lambda and every fold (nested for loop)

In [98]:
```python
from sklearn.model_selection import KFold
kfolds = KFold(n_splits=10)

# outer loop: lambdas
mseCV = []
for lambda_ in lambdas:
    # inner loop: folds
    mseCV_ = []
    for train_idx, val_idx in kfolds.split(X_dev, y_dev):
        # train model and compute MSE on test fold
        pipe_lassoCV = make_pipeline(PolynomialFeatures(degree=3, include_bias=False),
                                     StandardScaler(),
                                     Lasso(alpha=lambda_, random_state=1))
        X_train, y_train, = X_dev[train_idx], y_dev[train_idx]
        X_val, y_val = X_dev[val_idx], y_dev[val_idx]
        pipe_lassoCV.fit(X_train, y_train)
        mseCV_.append(mse(pipe_lassoCV.predict(X_val), y_val))

    # store result
    mseCV.append(mseCV_)

# convert to DataFrame
lambdaCV = pd.DataFrame(mseCV, index=lambdas)
```

K fold method (4)

Training the model with optimal hyperparameters and compare MSE

In [99]:
```
# choose optimal hyperparameters
optimal_lambda = lambdaCV.mean(axis=1).nsmallest(1)

# retrain model using optimal hyperparameters
pipe_lassoCV = make_pipeline(PolynomialFeatures(include_bias=False),
                             StandardScaler(),
                             Lasso(alpha=optimal_lambda.index[0], random_state=1))
pipe_lassoCV.fit(X_dev,y_dev)

# compare performance
models = {'Lasso': pipe_lasso, 'Lasso CV': pipe_lassoCV, 'LinReg': pipe_lr}
for name, model in models.items():
    score = mse(model.predict(X_test),y_test)
    print(name, round(score, 2))
```

```
Lasso 12.4
Lasso CV 12.4
LinReg 17.8
```

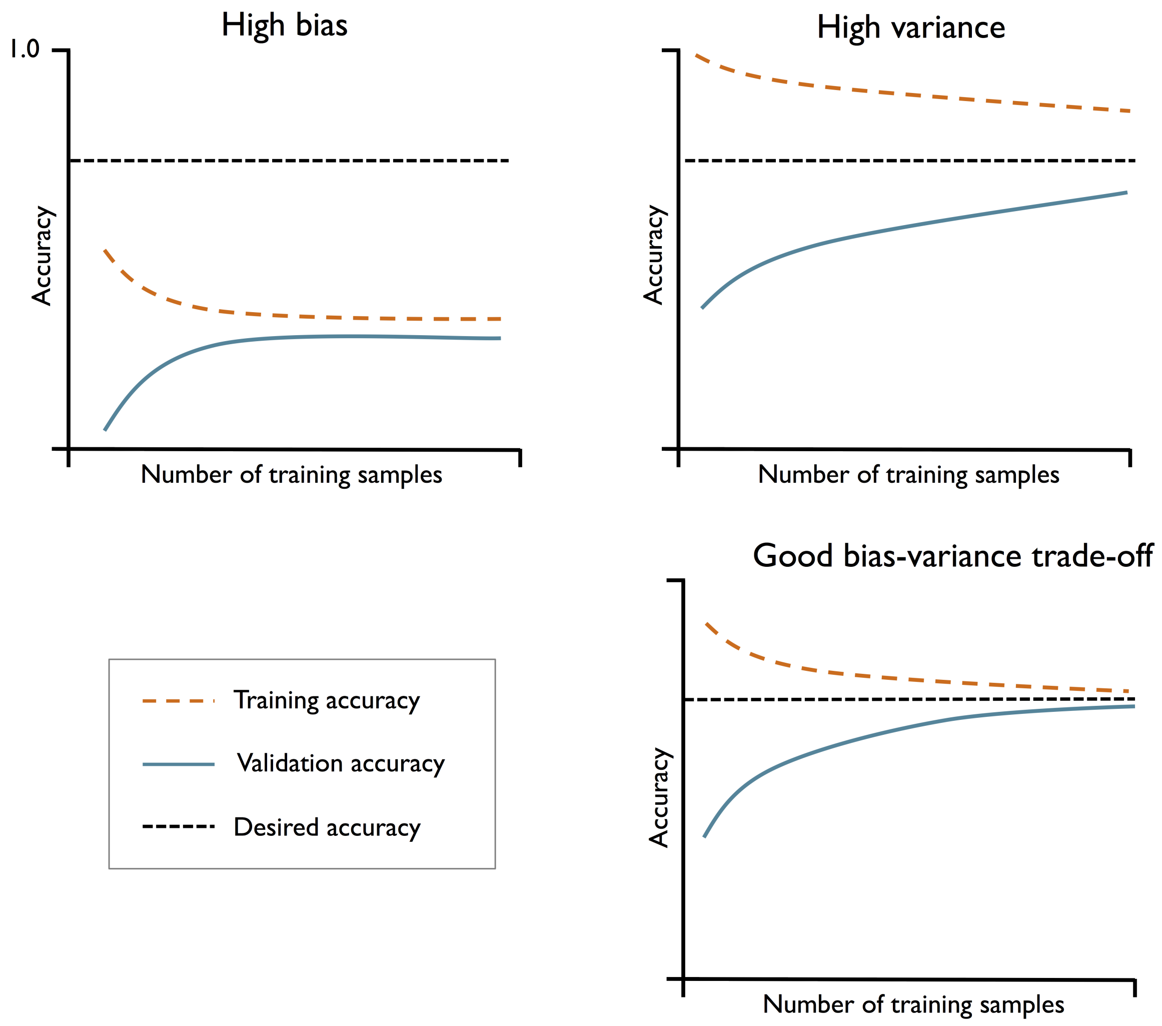
K fold method (5)

What else could we use cross-validation for?

- Getting more evaluations of our model performance.
- We can cross validate at two levels:
    - Outer: we make multiple splits of test and train/dev.
    - Inner: within each train/dev. dataset we make cross validation to choose hyperparameters

Learning curves (1)

What does a balanced model look like?



Learning curves (2)

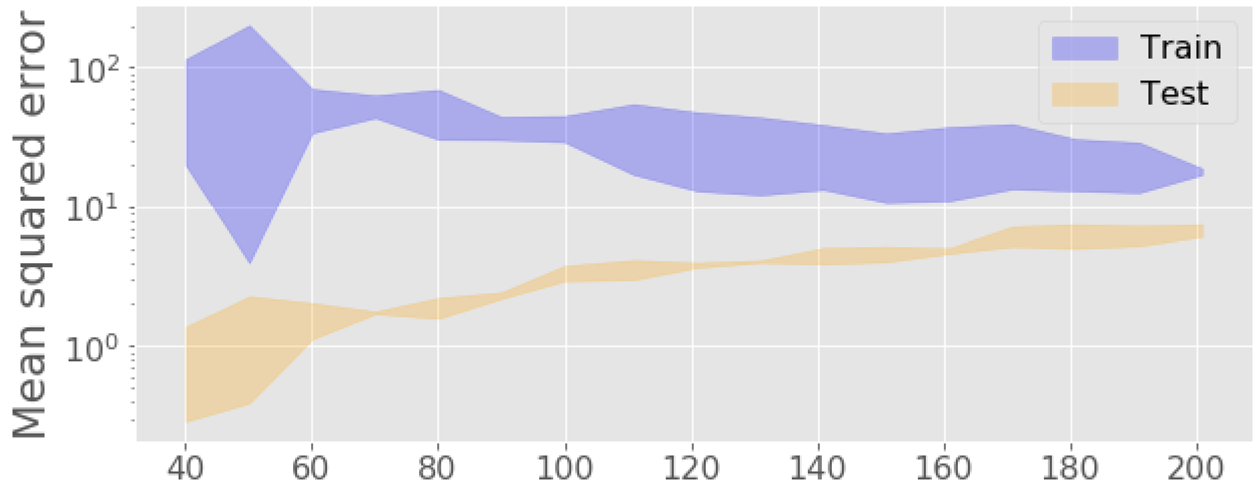
```
In [52]: from sklearn.model_selection import learning_curve

         train_sizes, train_scores, test_scores = \
             learning_curve(estimator=pipe_lasso,
                            X=X_train,
                            y=y_train,
                            train_sizes=np.arange(0.2, 1.05, .05),
                            scoring='neg_mean_squared_error',
                            cv=3)

         mse_ = pd.DataFrame({'Train':-train_scores.mean(axis=1),
                              'Test':-test_scores.mean(axis=1)})\
                 .set_index(pd.Index(train_sizes,name='sample size'))
         print(mse_.head(3))
```

```
                Train        Test
sample size
40           0.836417   67.617824
50           1.343929  103.111180
60           1.592246   52.207788
```

Learning curves (3)

In [53]:
```
f_learn, ax = plt.subplots(figsize=(10,4))
ax.fill_between(train_sizes,
                -test_scores.mean(1) + test_scores.std(1)*1.96,
                -test_scores.mean(1) - test_scores.std(1)*1.96,
                alpha=0.25, label ='Train', color='blue')

ax.fill_between(train_sizes,
                -train_scores.mean(1) + train_scores.std(1)*1.96,
                -train_scores.mean(1) - train_scores.std(1)*1.96,
                alpha=0.25, label='Test', color='orange')
ax.set_ylabel('Mean squared error')
ax.set_yscale('log')
ax.legend()
```

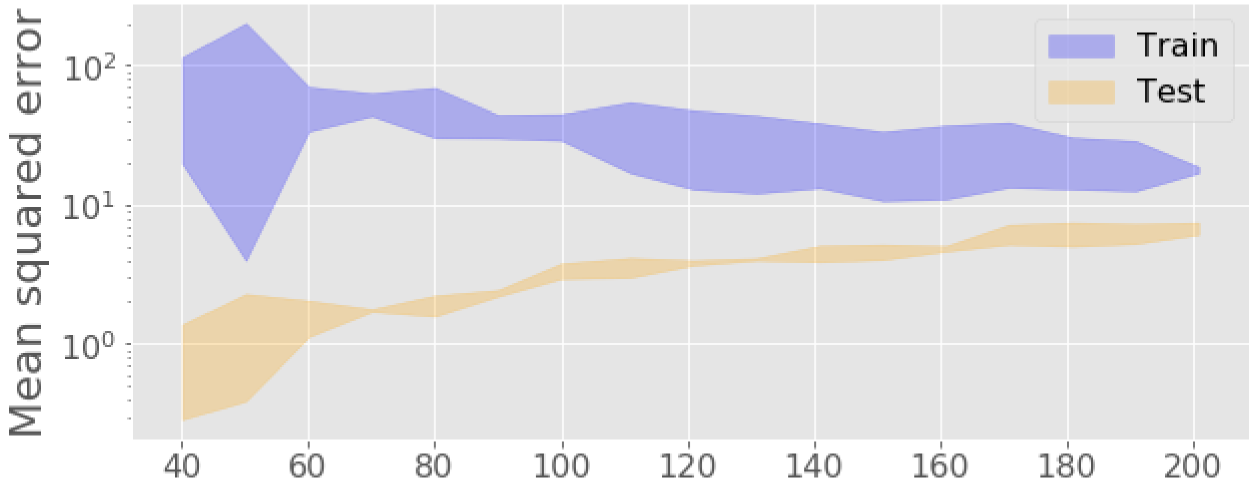
Out[53]:
```
<matplotlib.legend.Legend at 0x23991865ef0>
```



Learning curves (4)

```
In [54]: f_learn
```

```
Out[54]:
```



Tools for model selection

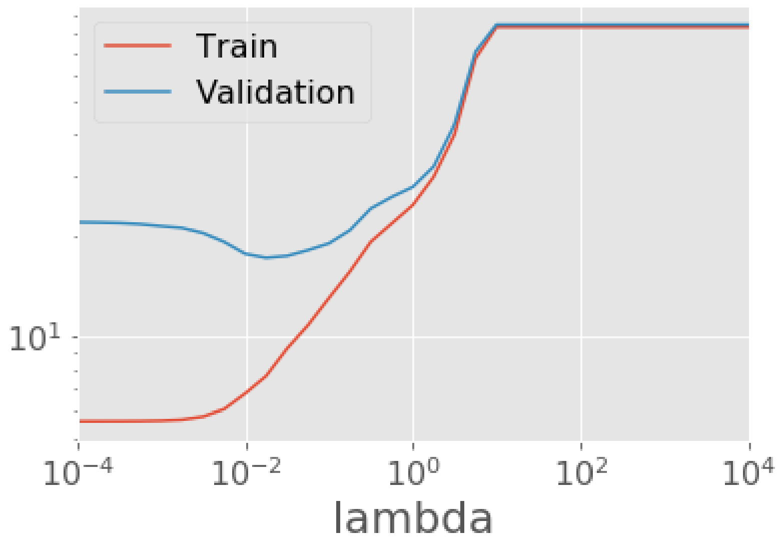
Validation curves (1)

```
In [55]: from sklearn.model_selection import validation_curve

         train_scores, test_scores = \
             validation_curve(estimator=pipe_lasso,
                              X=X_train,
                              y=y_train,
                              param_name='lasso__alpha',
                              param_range=lambdas,
                              scoring='neg_mean_squared_error',
                              cv=3)

         mse_score = pd.DataFrame({'Train':-train_scores.mean(axis=1),
                                   'Validation':-test_scores.mean(axis=1),
                                   'lambda':lambdas})\
                       .set_index('lambda')
         print(mse_score.Validation.nsmallest(1))
```

```
lambda
0.017783    17.207944
Name: Validation, dtype: float64
```

Validation curves (2)

```
In [56]: mse_score.plot(logx=True, logy=True)

Out[56]: <matplotlib.axes._subplots.AxesSubplot at 0x23991b08208>
```



Grid search (1)

How do we search for two or more optimal parameters? (e.g. elastic net)

- Goal: find the optimal parameter combination:
$$\lambda_1^*, \lambda_2^* = \arg\min_{\lambda_1,\lambda_2} MSE^{CV}(X_{train}, y_{train})$$
- Option 1: We can loop over the joint grid of parameters.
    - One level for each parameter.
    - Caveats:
- Option 2: sklearn has `GridSearchCV` has a tool which tests all parameter combinations.

Grid search (2)

How does this look in Python?

In [124]:
```python
from sklearn.model_selection import GridSearchCV
from sklearn.linear_model import ElasticNet
pipe_el = make_pipeline(PolynomialFeatures(include_bias=False),
                        StandardScaler(),
                        ElasticNet())
gs = GridSearchCV(estimator=pipe_el,
                  param_grid={'elasticnet__alpha':np.logspace(-4,4,10)*2,
                              'elasticnet__l1_ratio':np.linspace(0,1,10)},
                  scoring='neg_mean_squared_error',
                  n_jobs=4,
                  iid=False,
                  cv=10)
```

- Notation: double underscore between estimator and hyperparameter, e.g. 'est__hyperparam'
- Scoring: negative MSE as we're maximizing the score ~ minimize MSE.

Grid search (3)

What does the grid search yield?

```
In [ ]: models['ElasicNetCV'] = gs.fit(X_train, y_train)
        for name, model in models.items():
            score = mse(model.predict(X_test),y_test)
            print(name, round(score, 2))
        print()
        print('CV params:', gs.best_params_)
```

Grid search (4)

What if we have 10,000 parameter combinations?

- Option 1: you buy a cluster on Amazon, learn how to parallelize across computers.
- Option 2: you drop some of the parameter values
- Option 3: `RandomizedSearchCV` searches a subset of the combinations.

The end

Return to agenda

In [2]:
```
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
import requests
import seaborn as sns

plt.style.use('ggplot')
%matplotlib inline

SMALL_SIZE = 16
MEDIUM_SIZE = 18
BIGGER_SIZE = 20

plt.rc('font', size=SMALL_SIZE)          # controls default text sizes
plt.rc('axes', titlesize=SMALL_SIZE)     # fontsize of the axes title
plt.rc('axes', labelsize=MEDIUM_SIZE)    # fontsize of the x and y labels
plt.rc('xtick', labelsize=SMALL_SIZE)    # fontsize of the tick labels
plt.rc('ytick', labelsize=SMALL_SIZE)    # fontsize of the tick labels
plt.rc('legend', fontsize=SMALL_SIZE)    # legend fontsize
plt.rc('figure', titlesize=BIGGER_SIZE)  # fontsize of the figure title

plt.rcParams['figure.figsize'] = 10, 4 # set default size of plots
```