Elements Of Data Science - S2022

Week 7: Model Evaluation and Hyperparameter Tuning

3/1/2022

TODOs

- Readings:
    - **PDSH Chapter 5: In-Depth: Decision Trees and Random Forests**
    - HOML: Chapter 6
    - HOML: Chapter 7
    - **PDSH Chapter 5: Feature Engineering**

- **Quiz 7**, due **Monday March 7th, 11:59pm ET**
- **HW2**, out this week **Fri March 11th, 11:59pm ET**
- **Project**
    - March 22nd presentation
    - Details will be released on Canvas

Today

- Model Evaluation and Selection
- Hyperparameter Tuning
- Regularization

Questions?

Environment Setup

In [1]:

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

from mlxtend.plotting import plot_decision_regions

sns.set_style('darkgrid')

%matplotlib inline
```

Model Evaluation and Hyperparameter Tuning

- How well are any of our models working?
- How can we compare different models?
- How do we decide on hyperparameter settings?
- How can we keep our models from "overfitting"?
- How do we do all this both for Regression and Classification?

How well are our models performing?

Regression

- Mean Squared Error (MSE) and Root Mean Squared Error (RMSE)
- R^2 or `R^2`
- (Adjusted R^2 - will talk about during Feature Selection)

Classification

- Accuracy
- Precision/Recall/F1
- ROC Area Under the Curve (AUC)

Data Setup for Regression

In [2]:

```
zscore = lambda x: (x - x.mean()) / x.std()

df_wine = pd.read_csv('../data/wine_dataset.csv',
                      usecols=['alcalinity_of_ash','magnesium','alcohol','ash','proline','hue','class'])
numeric_cols = ['alcalinity_of_ash','magnesium','alcohol','ash','proline','hue']

df_wine[numeric_cols] = df_wine[numeric_cols].apply(zscore)  # standardize numeric feature cols

X = df_wine[['proline','hue','ash']]

y_r = df_wine['alcohol']                                      # regression target
```

In [3]:

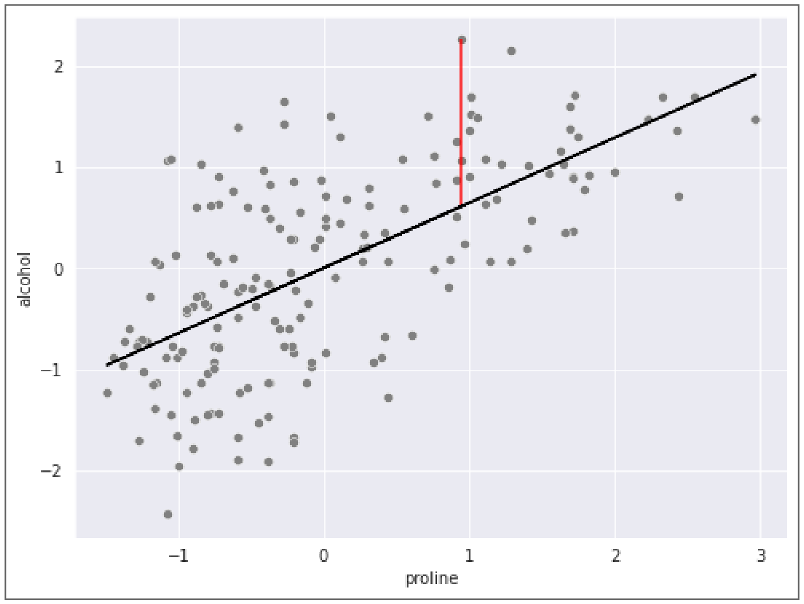
```
df_wine.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 178 entries, 0 to 177
Data columns (total 7 columns):
 #   Column             Non-Null Count  Dtype  
---  ------             --------------  -----  
 0   alcohol            178 non-null    float64
 1   ash                178 non-null    float64
 2   alcalinity_of_ash  178 non-null    float64
 3   magnesium          178 non-null    float64
 4   hue                  178 non-null    float64
 5   proline              178 non-null    float64
 6   class                178 non-null    int64
dtypes: float64(6), int64(1)
memory usage: 9.9 KB
```

Regression with Simple Linear Model

In [4]:

```
from sklearn.linear_model import LinearRegression

lr = LinearRegression().fit(X[['proline']],y_r)
argmax_y_r = np.argmax(y_r)
y_pred = lr.predict(X[['proline']])

fig,ax = plt.subplots(1,1,figsize=(8,6))
sns.scatterplot(x=X.proline, y=y_r, color='grey');
ax.plot(X.proline,y_pred,color='k');
ax.vlines(X.proline.iloc[argmax_y_r],y_r.iloc[argmax_y_r],y_pred[argmax_y_r],color='r');
```



How Good is This Fit? MSE and RMSE

- **Mean Squared Error:** $\frac{1}{n}\sum_i (y_i - \hat{y}_i)^2$

In [5]:

```
from sklearn.metrics import mean_squared_error

lr_mse = mean_squared_error(y_r,y_pred)
print(f'{lr_mse = :0.2f}')
```

```
lr_mse = 0.58
```

- But this is the squared error! (alcohol^2)
- **Root Mean Squared Error:** $\sqrt{\frac{1}{n}\sum_i (y_i - \hat{y}_i)^2}$

In [6]:

```
def root_mean_squared_error(y_true, y_pred):
    return np.sqrt(mean_squared_error(y_true,y_pred))

lr_rmse = root_mean_squared_error(y_r,y_pred)
print(f'{lr_rmse = :0.2f}')
```

```
lr_rmse = 0.76
```

Is this good? Need a Baseline Comparison

- What's a baseline to compare against?
- Simple one for Regression: always predict the mean of the targets

In [7]:

```
from sklearn.dummy import DummyRegressor

dummyr = DummyRegressor(strategy='mean') # default strategy
dummyr.fit(X[['proline']],y_r)

dummy_rmse = root_mean_squared_error(y_r,dummyr.predict(X[['proline']]))

print(f'{dummy_rmse = :0.2f}')
```

```
dummy_rmse = 1.00
```

Comparing against the mean: R^2

- the proportion of variance explained by the model

$$R^2 = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2}$$

- maximum value of 1
- a value below 0 means the model is predicting worse than just predicting the mean
- sklearn uses R^2 as the default for regression scoring

In [8]:

```
r2_lr = lr.score(X[['proline']],y_r)
r2_dummyr = dummyr.score(X[['proline']],y_r)

print(f'{r2_dummyr = :0.2f}\n{r2_lr     = :0.2f}')
```

```
r2_dummyr = 0.00
r2_lr     = 0.41
```

Can we do better?

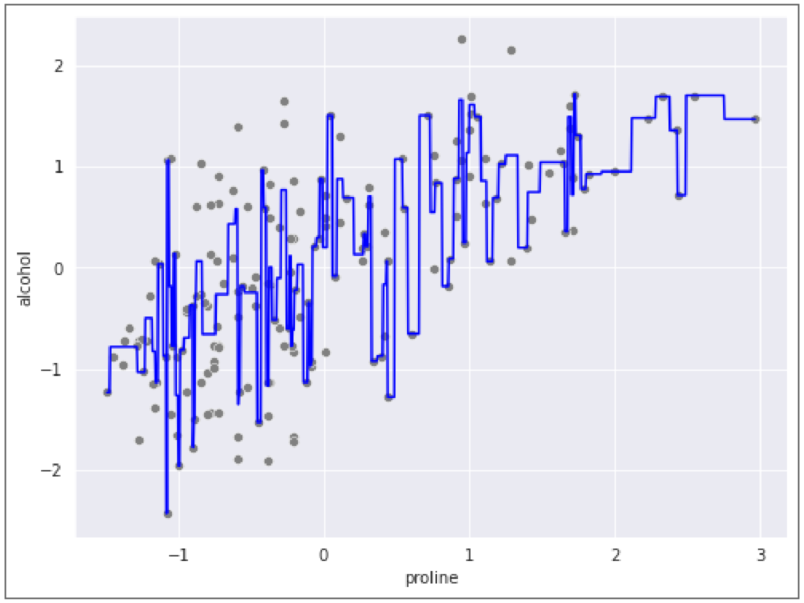
In [9]:

```
from sklearn.tree import DecisionTreeRegressor

dtr = DecisionTreeRegressor(max_depth=10)
dtr.fit(X[['proline']],y_r)
r2_dtr = dtr.score(X[['proline']],y_r)
print(f'{r2_lr  = :0.2f}\n{r2_dtr = :0.2f}')
```

```
r2_lr  = 0.41
r2_dtr = 0.76
```

In [10]:

```
X_proline_sorted = X[['proline']].sort_values(by='proline').values
X_query = np.linspace(X_proline_sorted.min(),X_proline_sorted.max(),1000).reshape(-1,1)
y_pred = dtr.predict(X_query)
fig,ax = plt.subplots(1,1,figsize=(8,6))
sns.scatterplot(x=X.proline, y=y_r,color='gray');
ax.plot(X_query,y_pred,color='b');
```


alcohol
proline
2
1
0
−1
−2
−1
0
1
2
3

But is this what we want? Interpretation vs Prediction

Always good to ask:

- do we want our model to very closely fit our data for interpretation?
- do we want our model to predict well on new, unseen data?

Generalization:

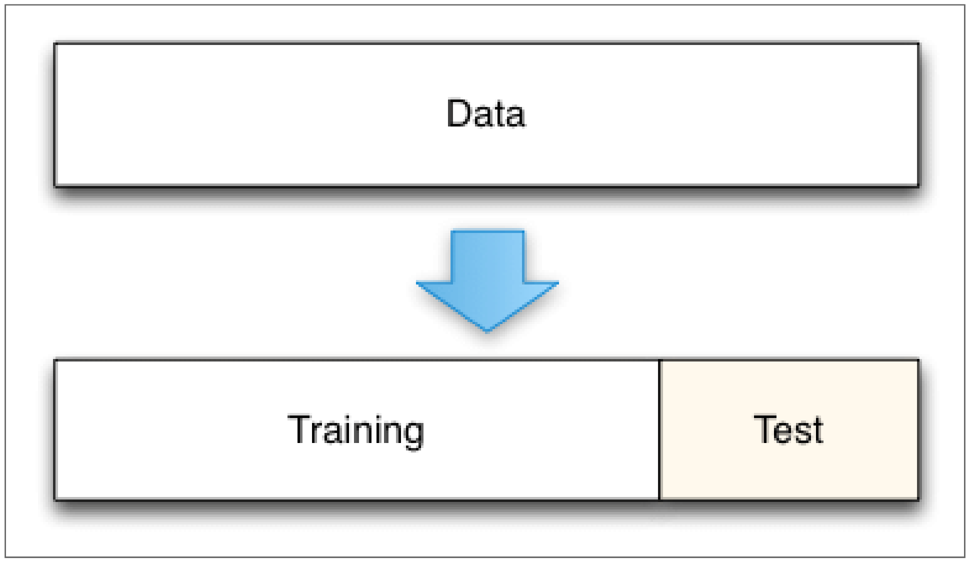
- how well will model predict on data that it hasn't seen yet?

But we used all of our data to train?

- Need to do a **Train/Test Split** to create a held-aside set

Train/Test Split

- **Training Set:** portion of dataset used for training
- **Test/Held-Aside/Out of sample:** portion of dataset used for evaluation
- Want the test set to reflect the same distribution as training



From https://www.researchgate.net/figure/Train-Test-Data-Split_fig6_325870973

Train/Test split with Sklearn

In [11]:

```
from sklearn.model_selection import train_test_split

X_train_r,X_test_r,y_train_r,y_test_r = train_test_split(X[['proline']],
                                                         y_r,
                                                         train_size=.75,  #default (only need one of train/test)
                                                         test_size=.25,   #default
                                                         random_state=123)
print(f"n_total = {X[['proline']].shape[0]}")
print(f'n_train = {X_train_r.shape[0]}')
print(f'n_test  = {X_test_r.shape[0]}')
```

```
n_total = 178
n_train = 133
n_test  = 45
```

- How big should test be?
  - Large enough to capture variance of dataset.
  - Depends on the dataset and the models being trained

Training and Evaluate on Different Data

In [12]:

```
dummyr = DummyRegressor().fit(X_train_r,y_train_r)
lr = LinearRegression().fit(X_train_r,y_train_r)
dtr = DecisionTreeRegressor(max_depth=10).fit(X_train_r,y_train_r)

r2_dummyr = dummyr.score(X_test_r,y_test_r)
r2_lr     = lr.score(X_test_r,y_test_r)
r2_dtr    = dtr.score(X_test_r,y_test_r)

print(f'{r2_dummyr = : 0.2f}\n{r2_lr     = : 0.2f}\n{r2_dtr    = : 0.2f}')
```

```
r2_dummyr = -0.03
r2_lr     =  0.28
r2_dtr    = -0.31
```

- DecisionTree model is doing worse than the Dummy model on the test set!

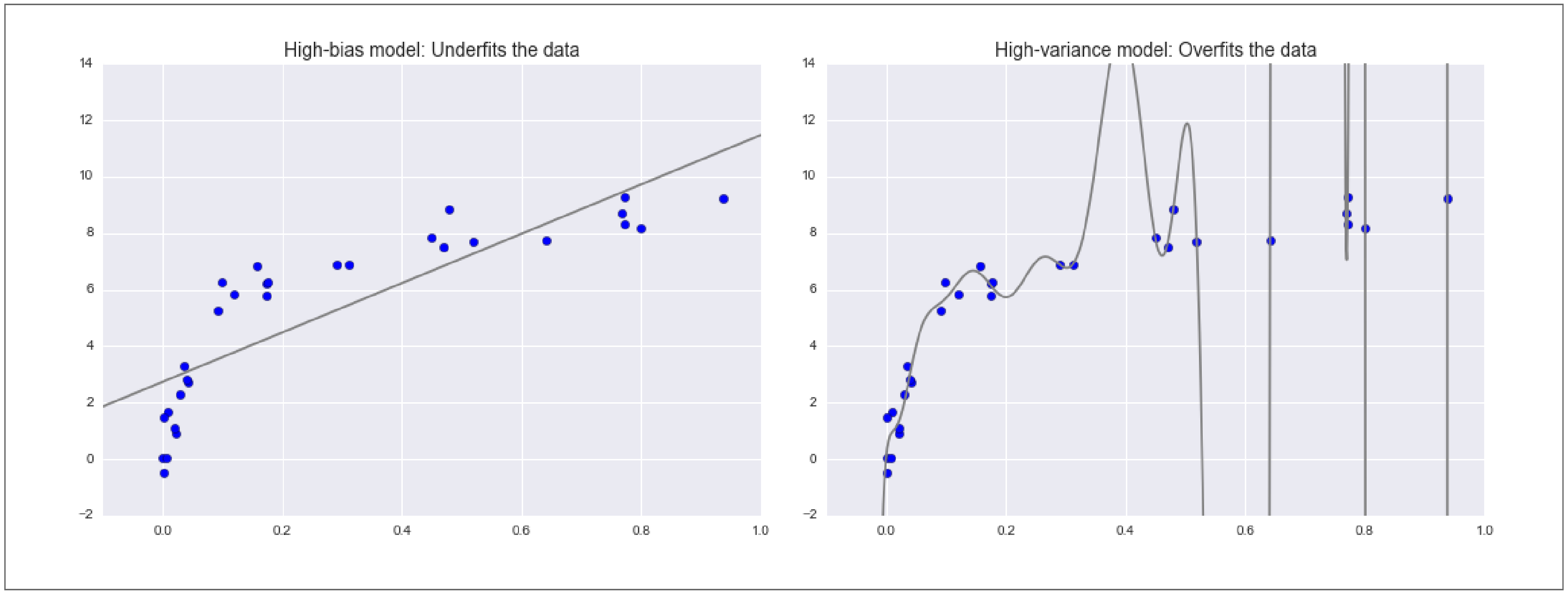
Overfitting and Underfitting

- **Overfitting:** poor generalization due to complexity
    - learning noise in training data

- **Underfitting:** poor generalization due to simplicity
    - not flexibile enough to learn concept

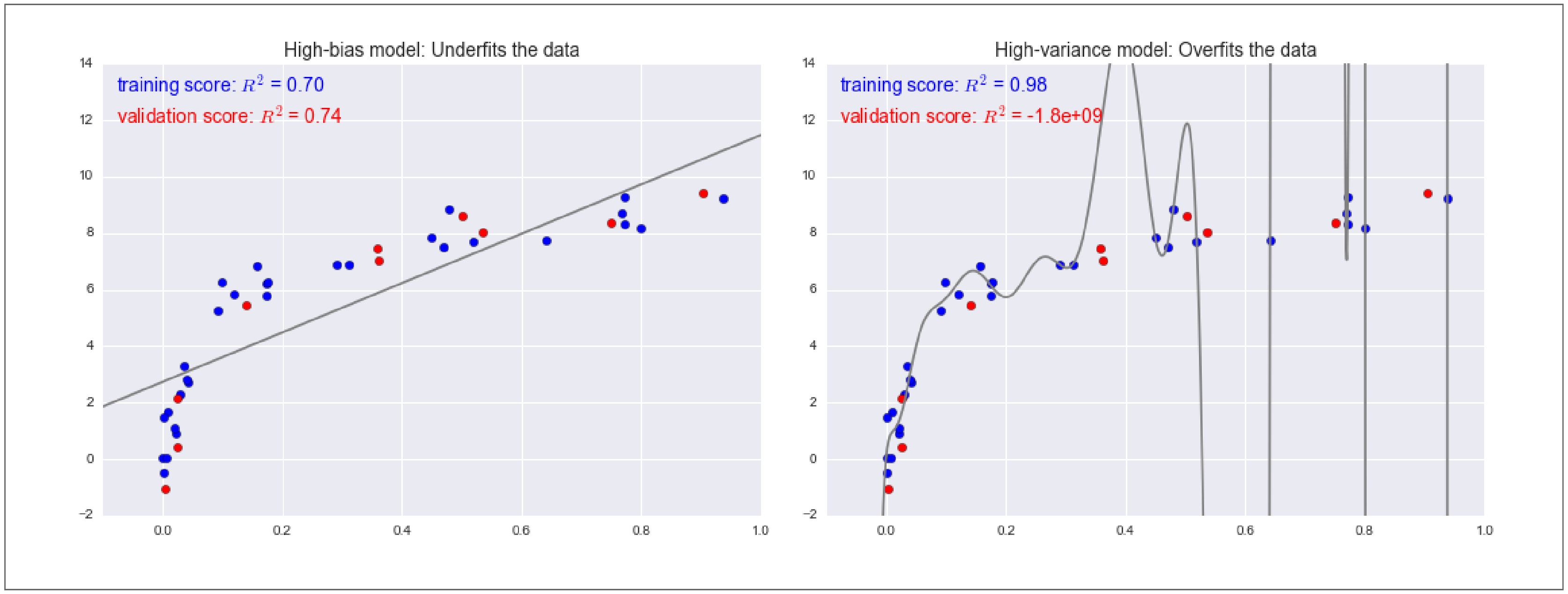
- Need to find a balance between simplicity and complexity
- Need to find a balance between **bias** and **variance**

Bias-Variance Tradeoff



From PDSH

Bias-Variance Tradeoff



From PDSH

Bias-Variance Tradeoff Continued

- How close is the model to the underlying concept?
- How sensitive is the model to the training set?

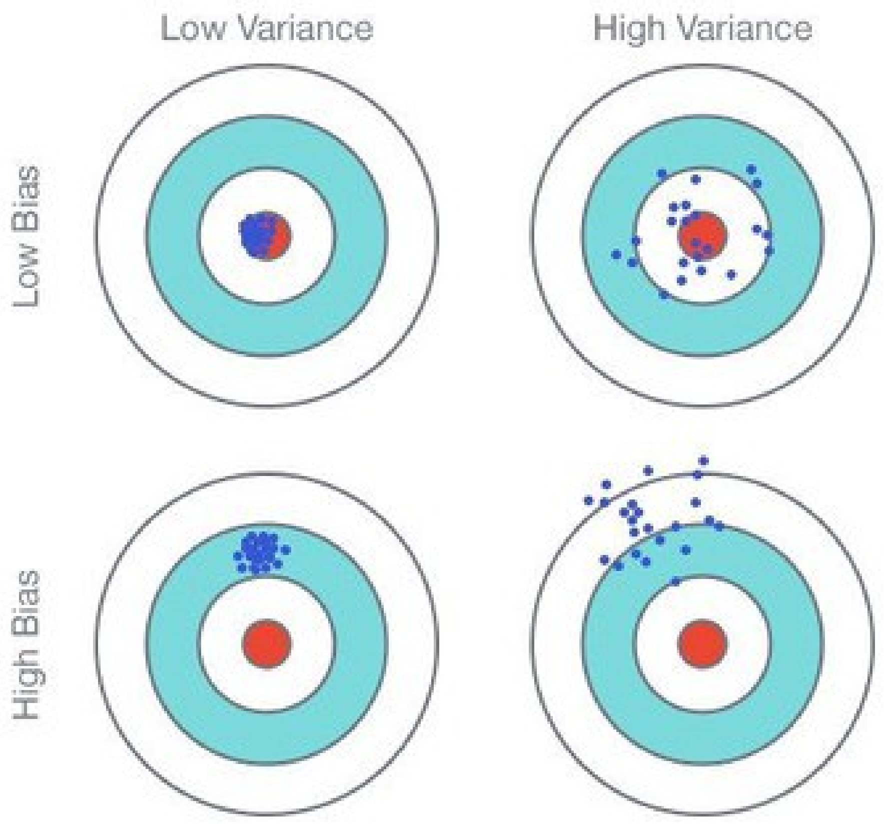
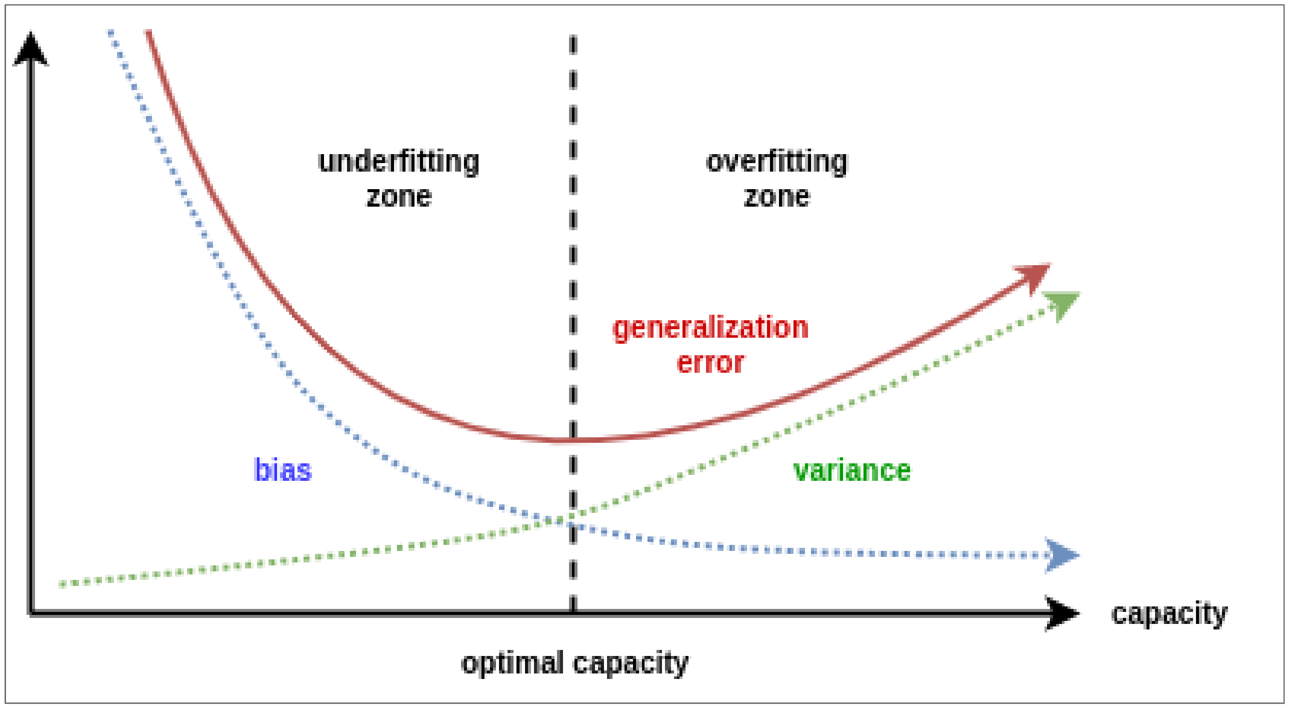


Fig. 1: Graphical Illustration of bias-variance trade-off , Source: Scott Fortmann-Roe., Understanding Bias-Variance Trade-off

Bias-Variance Tradeoff Continued



- We'd like to:
  - reduce the Bias (use a model complex enough to capture the concept)
  - without introducing too much Variance (overfit the data)
  - all in order to minimize **Generalization Error**

Overfitting/Underfitting Revisited

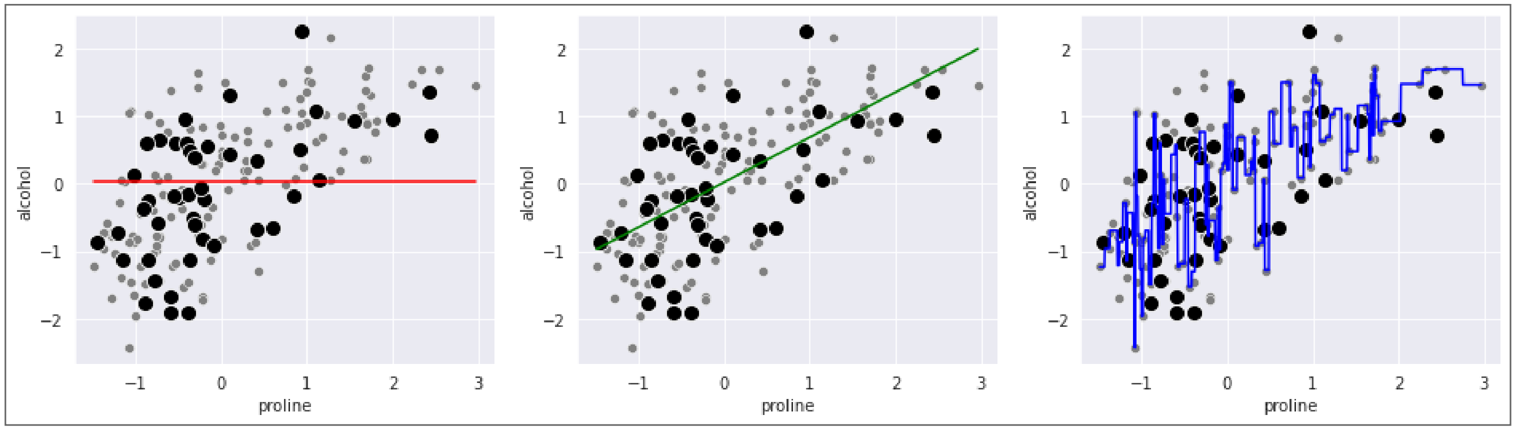
- **Overfitting:** poor generalization due to complexity
    - learning noise in training data
    - model has **high variance and low bias**
- **Underfitting:** poor generalization due to simplicity
    - not flexibile enough to learn concept
    - model has **high bias and low variance**

Avoiding Overfitting/Underfitting

- Never train and evaluate on the same set of data!
    - train test split
    - **cross-validation**
- Keep the model as simple as possible (Occom's Razor)

In [13]:

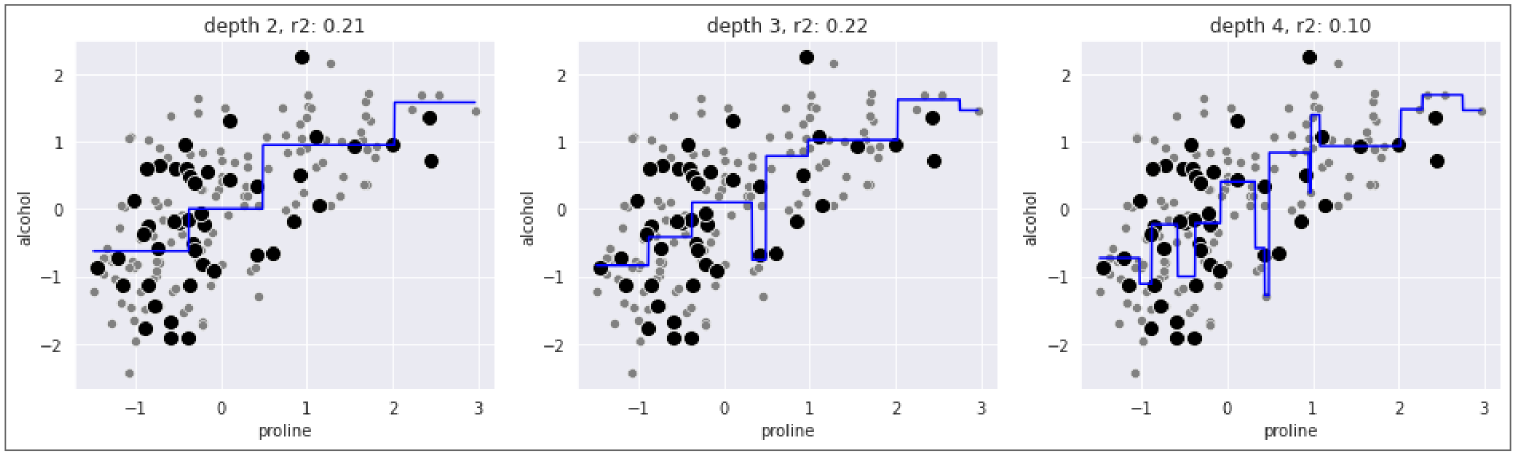
```
fig,ax = plt.subplots(1,3,figsize=(16,4))
for i in range(3):
    sns.scatterplot(x=X_train_r.proline,y=y_train_r,color="gray",ax=ax[i])
    sns.scatterplot(x=X_test_r.proline,y=y_test_r,color="black",s=100,ax=ax[i]);
ax[0].plot(X_query,dummyr.predict(X_query),color='r');
ax[1].plot(X_query,lr.predict(X_query),color='g');
ax[2].plot(X_query,dtr.predict(X_query),color='b');
```



Overfitting? Simplify the model

In [14]:

```
max_depths = [2,3,4]
fig,ax = plt.subplots(1,3,figsize=(16,4))
for i in range(3):
    dtr = DecisionTreeRegressor(max_depth=max_depths[i]).fit(X_train_r,y_train_r)
    sns.scatterplot(x=X_train_r.proline,y=y_train_r,color="gray",ax=ax[i])
    sns.scatterplot(x=X_test_r.proline,y=y_test_r,color="black",s=100,ax=ax[i]);
    ax[i].plot(X_query,dtr.predict(X_query),color='b');
    ax[i].set_title(f'depth {max_depths[i]}, r2: {dtr.score(X_test_r,y_test_r):0.2f}')
```



- But now we might be overfitting on the test set!
- How to choose hyperparameters: **Cross-Validation**

Aside: Hyperparameters

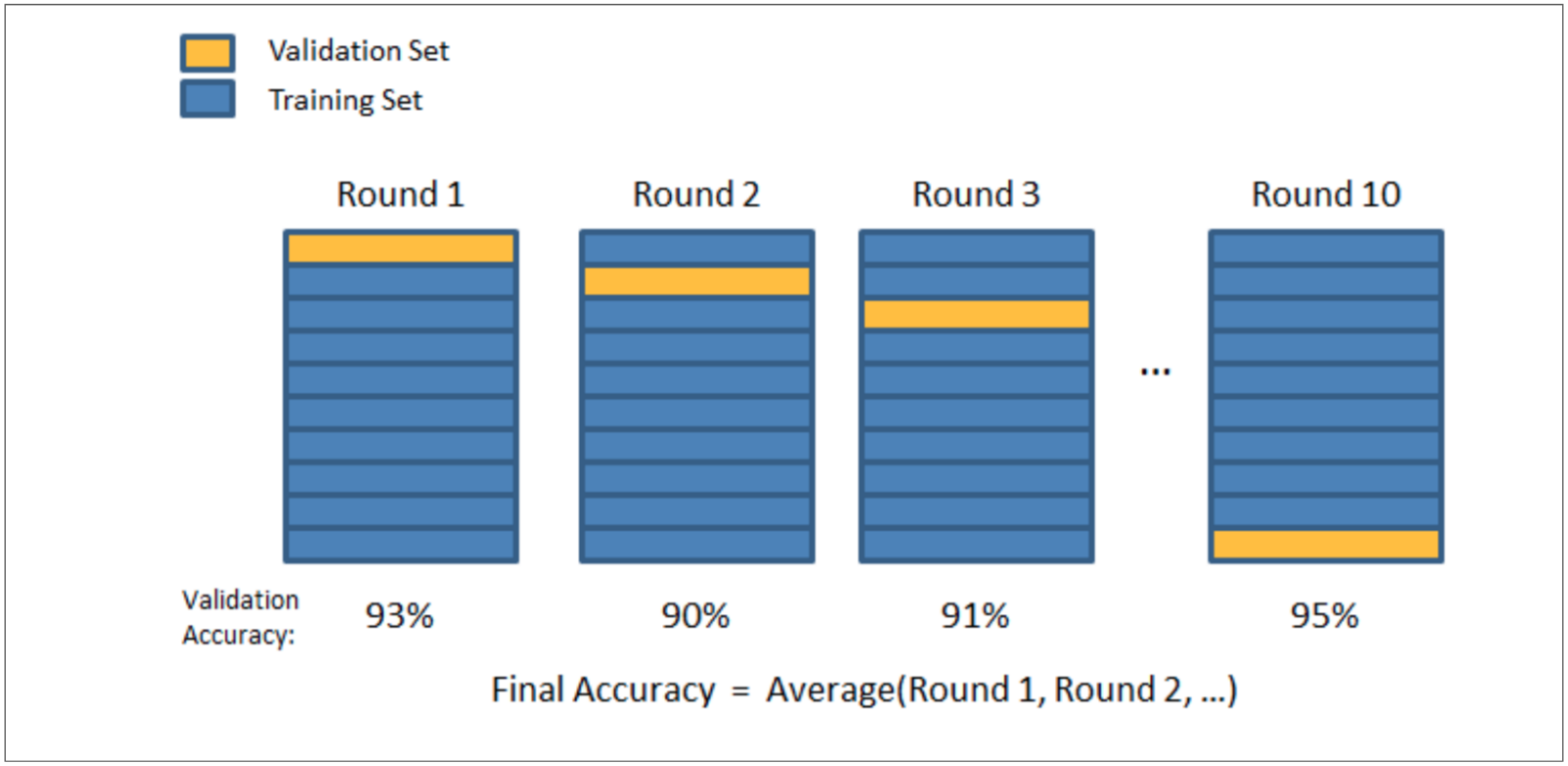
- **parameter:** something learned by the model itself (eg. coefficient in linear model)
- **hyperparameter:** something we set by hand (eg. decision tree max depth)

k-Fold Cross-Validation

1. split dataset into k equal sized subsets (folds)
2. for each subset (fold)
    - train on the other $k-1$ subsets combined
    - test on this subset to get a score
3. average across all scores

- Result is a set of samples of model performance
- Can use to set hyperparameters without overfitting on train or test
- Can also use to estimate range of generalization performance

Example: 10-Fold Cross-Validation



k-Fold Cross-Validation Continued

- Can be used for:
  - tuning hyperparameters
  - model selection
  - any time we need estimate of model performance

- **Issue:** each fold requires training the model
  - Training time can be an issue for large k

- What values can k take?
  - min: 2
  - max: n, the size of the dataset (aka Leave-One-Out CV)

k-Fold Cross-Validation in sklearn

In [15]:

```
from sklearn.model_selection import cross_val_score

scores = cross_val_score(DecisionTreeRegressor(max_depth=2),
                         X_train_r,
                         y_train_r,
                         cv=5) #default
scores
```

Out[15]:

```
array([0.41853032, 0.37075208, 0.45405394, 0.2588269 ,
0.22799476])
```

In [16]:

```
print(f'{np.mean(scores) :0.2f} +- {2*np.std(scores) :0.2f}')
```

```
0.35 +- 0.18
```

Tuning Hyperparameters with CV

In [17]:

```
mean_scores = []

for depth in [1, 2, 3, 5, 10]:
    dtr = DecisionTreeRegressor(max_depth=depth)
    scores = cross_val_score(dtr,X_train_r,y_train_r,cv=5)
    mean_scores.append( (depth,scores.mean().round(3)) )

for depth,mean_score in mean_scores:
    print(f'{depth = :2d} : {mean_score: 0.3f}')
```

```
depth =  1 :  0.289
depth =  2 :  0.346
depth =  3 :  0.341
depth =  5 :  0.050
depth = 10 : -0.142
```

In [18]:

```
# find the depth that gives best score (highest R^2)
sorted(mean_scores, key=lambda x:x[1],reverse=True)[0] # sorted is ascending by default
```

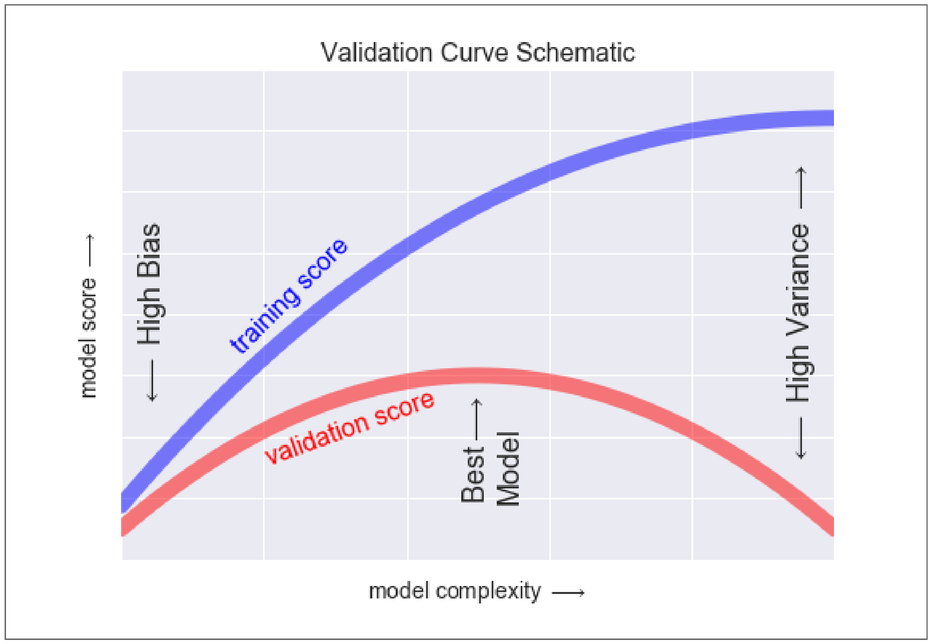
Out[18]:

```
(2, 0.346)
```

Visualize Tuning: Validation Curve

Validation Curve

- Show model complexity vs model performance on both train and test/validation
- Want to find point where performance on validation set begins to decline (overfitting)



From PDSH

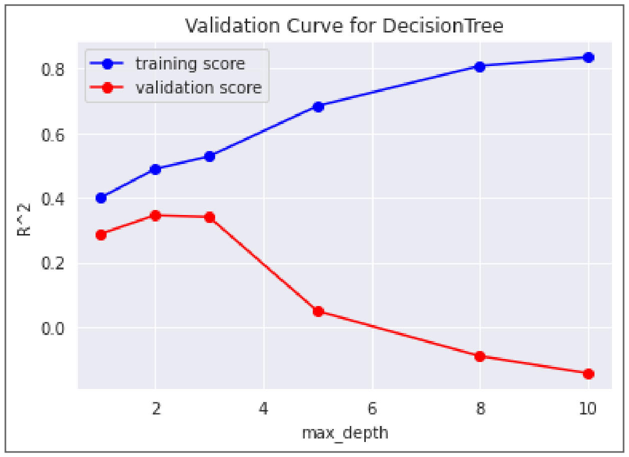
Validation Curve in sklearn

In [19]:

```python
from sklearn.model_selection import validation_curve

depth = [1,2,3,5,8,10]
train_scores,test_scores = validation_curve(DecisionTreeRegressor(),
                                            X_train_r, y_train_r,
                                            param_name='max_depth',
                                            param_range=depth,
                                            cv=5)
mean_train_scores = np.mean(train_scores,axis=1) # take the mean across columns
mean_test_scores = np.mean(test_scores,axis=1)
```

In [20]:

```python
fig,ax = plt.subplots(1,1)
ax.plot(depth, mean_train_scores, 'o-', color='b',label='training score');
ax.plot(depth, mean_test_scores, 'o-', color='r', label='validation score');
ax.set_xlabel('max_depth'), ax.set_ylabel('R^2'); ax.set_title('Validation Curve for DecisionTree');
ax.legend();
```



More Than One HyperParameter? Grid Search

Grid Search: Search over a 'grid' of hyperparameter settings
Example: KNN "number of neighbors" and "distance metric"

In [21]:

```
distance_metrics = ['euclidean','manhattan']
n_neighbors = [1,3,5]

grid = []
for d in distance_metrics:
    for k in n_neighbors:
        print([d,k])
```

```
['euclidean', 1]
['euclidean', 3]
['euclidean', 5]
['manhattan', 1]
['manhattan', 3]
['manhattan', 5]
```

Grid Search in sklearn

In [22]:

```
from sklearn.model_selection import GridSearchCV
from sklearn.neighbors import KNeighborsRegressor

params = {'n_neighbors':[1,2,3,5,10],
          'metric':['euclidean','manhattan']}
gscv = GridSearchCV(KNeighborsRegressor(),
                    param_grid=params,     # grid of size 10
                    cv=3,       # do 3-fold CV at every grid point
                    refit=True) # refit True trains one more time on the entire training set

gscv.fit(X_train_r,y_train_r)       # How many times are we training a model here? (2*5*3 + 1 = 31)

print(gscv.best_params_)
```

```
{'metric': 'euclidean', 'n_neighbors': 5}
```

In [23]:

```
scores = cross_val_score(gscv.best_estimator_,X_train_r,y_train_r,cv=5)

print(f'{np.mean(scores):0.2f} +- {2*np.std(scores):0.2f}')
```

```
0.35 +- 0.21
```

Review So Far

- Regression Metrics
    - MSE and RMSE
    - R^2
- Model Selection
    - Comparison to Baseline Model
    - Underfitting/Overfitting, Bias/Variance
    - Train/Test Split
- Hyperparameter Tuning
    - Cross-Validation
    - Grid Search
    - Validation Curve

Data Setup for Classification

In [24]:

```
idx_binary = df_wine['class'].isin([0,1])              # reduce to binary classification

X_bc = df_wine.loc[idx_binary,['alcalinity_of_ash','magnesium']]         # only 2 features for ease of plotting
y_bc = df_wine.loc[idx_binary,'class']                  # pull out classification target [0,1]

X_train_bc,X_test_bc,y_train_bc,y_test_bc = train_test_split(X_bc,
                                                              y_bc,
                                                              stratify=y_bc, # maintain label proportions
                                                              random_state=0
                                                             )

pd.DataFrame({'train':y_train_bc.value_counts(),'test':y_test_bc.value_counts()}).sort_index()
```

Out[24]:

	train	test
0	44	15
1	53	18

In [25]:

```
X_mc = df_wine.loc[:,['alcalinity_of_ash', 'magnesium']]      # multiple features for multiclass classification task
y_mc = df_wine.loc[:,'class']                                # pull out classification target [0,1,2]
X_train_mc,X_test_mc,y_train_mc,y_test_mc = train_test_split(X_mc,
                                                              y_mc,
                                                              stratify=y_mc, # maintain label proportions
                                                              random_state=123
                                                             )
pd.DataFrame({'train':y_train_mc.value_counts(),'test':y_test_mc.value_counts()}).sort_values(by="train")
```

Out[25]:

	train	test

	train	test
2	36	12
0	44	15
1	53	18

Default Metric in Classification: Accuracy

- **Accuracy**: out of all the observations, how many did I get right?

In [26]:

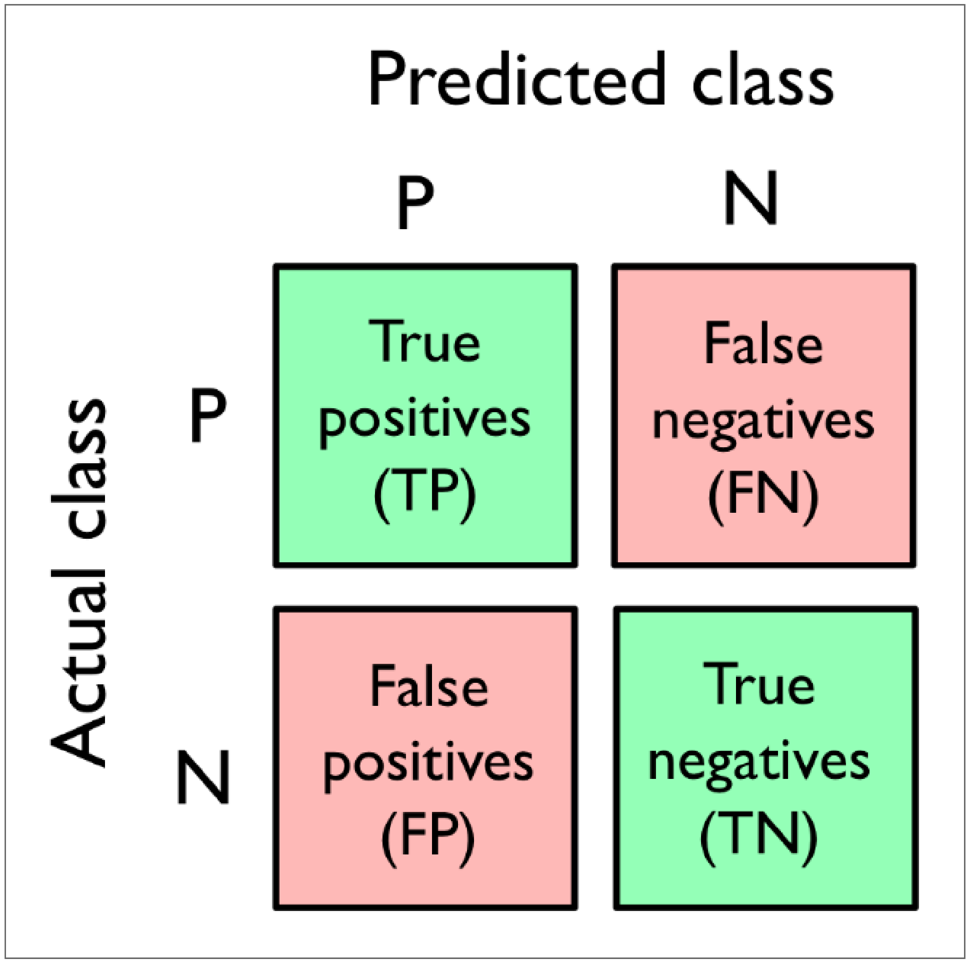
```
from sklearn.dummy import DummyClassifier
from sklearn.tree import DecisionTreeClassifier
dummyc = DummyClassifier(strategy='prior').fit(X_train_bc,y_train_bc) # works like 'most-frequent'
dtc = DecisionTreeClassifier(max_depth=2).fit(X_train_bc,y_train_bc)

print(f'{dummyc.score(X_test_bc,y_test_bc) = :0.2f}') # default classification score is accuracy
print(f'{dtc.score(X_test_bc,y_test_bc)    = :0.2f}')
```

```
dummyc.score(X_test_bc,y_test_bc) = 0.55
dtc.score(X_test_bc,y_test_bc)    = 0.79
```

- But what if the cost of calling a negative a positive is different from calling a positive a negative?
- Examples:
    - disease testing
    - medical product failures
    - incarceration

Errors in Classification

- There are different kinds of error in classification

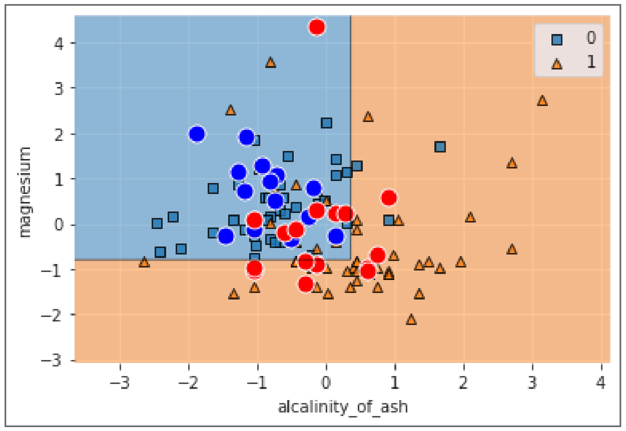


From PML

Visualizing Errors with a Confusion Matrix

In [27]:

```
fig,ax = plt.subplots(1,1,figsize=(6,4));
plot_decision_regions(X_train_bc.values,y_train_bc.values,dtc,ax=ax);
sns.scatterplot(x=X_bc.columns[0],y=X_bc.columns[1],data=X_test_bc[y_test_bc == 0],color="blue",s=120);
sns.scatterplot(x=X_bc.columns[0],y=X_bc.columns[1],data=X_test_bc[y_test_bc == 1],color="red",s=120);
```



In [28]:

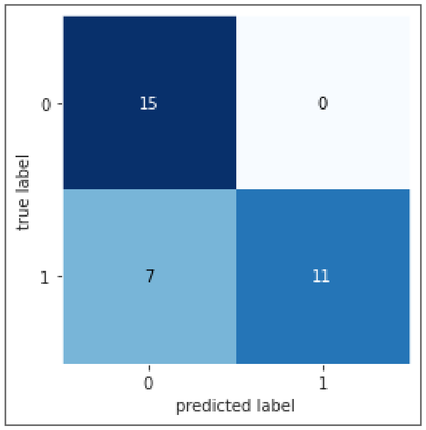
```
from sklearn.metrics import confusion_matrix

print('training set error\n', confusion_matrix(y_train_bc,dtc.predict(X_train_bc)))
print()
print('test set error\n', confusion_matrix(y_test_bc,dtc.predict(X_test_bc)))
```

```
training set error
 [[41  3]
 [14 39]]

test set error
 [[15  0]
 [ 7 11]]
```

Plot Confusion Matrix with mlxtend

In [29]:

```
from mlxtend.plotting import plot_confusion_matrix

fig,ax = plt.subplots(1,1,figsize=(4,4))
plot_confusion_matrix(confusion_matrix(y_test_bc,dtc.predict(X_test_bc)),axis=ax);
```



Weighing Errors: Precision vs. Recall

Precision

- Out of the observations I predicted positive (TP+FP), how many are truly positive (TP)?

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

Recall

- Out of the truly positive (TP+FN), how many obsersevations did I predict positive (TP)?

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

Using Other Measures in sklearn

In [30]:

```
dummyc_precision_scores = cross_val_score(dummyc,X_train_bc,y_train_bc,cv=5,scoring='precision')
dummyc_recall_scores    = cross_val_score(dummyc,X_train_bc,y_train_bc,cv=5,scoring='recall')

print(f'dummy precision: {np.mean(dummyc_precision_scores):0.2f} +- {2*np.std(dummyc_precision_scores):0.2f}')
print(f'dummy recall   : {np.mean(dummyc_recall_scores):0.2f} +- {2*np.std(dummyc_recall_scores):0.2f}')
print()

dtc_precision_scores = cross_val_score(dtc,X_train_bc,y_train_bc,cv=5,scoring='precision')
dtc_recall_scores    = cross_val_score(dtc,X_train_bc,y_train_bc,cv=5,scoring='recall')

print(f'dtc precision  : {np.mean(dtc_precision_scores):0.2f} +- {2*np.std(dtc_precision_scores):0.2f}')
print(f'dtc recall     : {np.mean(dtc_recall_scores):0.2f} +- {2*np.std(dtc_recall_scores):0.2f}')
```

```
dummy precision: 0.55 +- 0.04
dummy recall   : 1.00 +- 0.00

dtc precision  : 0.85 +- 0.36
dtc recall     : 0.66 +- 0.38
```

How do we decide if something is positive or negative?

Usually set a threshold :

$$\hat{y}_i = \begin{cases} 1 & \text{if } P(y_i = 1|x_i) > \text{threshold}, \\ 0 & \text{o.w.} \end{cases}$$

Usually, threshold = .5, but it doesn't have to be.
What happens if we change it?

- High threshold → High Precision, Low Recall
- Low threshold → High Recall, Low Precision

Combining Precision and Recall: F_1-score

Usually, we just want one number to optimize

F_1**-score:** harmonic mean of precision and recall

- eg. weighted average of the precision and recall

$$F_1 = 2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$$

Note that F_1 ignores True Negatives!

In [31]:

```
dummyc_f1_scores = cross_val_score(dummyc,X_train_bc,y_train_bc,cv=5,scoring='f1')
dtc_f1_scores = cross_val_score(dtc,X_train_bc,y_train_bc,cv=5,scoring='f1')
print(f'dummyc f1 = {np.mean(dummyc_f1_scores):0.2f} +- {2*np.std(dummyc_f1_scores):0.2f}')
print(f'dtc f1    = {np.mean(dtc_f1_scores):0.2f} +- {2*np.std(dtc_f1_scores):0.2f}')
```

```
dummyc f1 = 0.71 +- 0.03
dtc f1    = 0.72 +- 0.31
```

Paying attention to True Negatives: ROC

Receiver **O**perating **C**haracteristic

- displays FPR vs TPR

False Positive Rate (FPR) = $\frac{\text{FP}}{\text{FP+TN}} = \frac{\text{negatives we got wrong}}{\text{all negatives}}$

True Positive Rate (TPR) = Recall = $\frac{\text{TP}}{\text{TP+FN}} = \frac{\text{positives we got right}}{\text{all positives}}$

How do these change as we move our threshold?

In [32]:

```
from sklearn.metrics import roc_curve
fpr_dtc, tpr_dtc, _ = roc_curve(y_train_bc, dtc.predict_proba(X_train_bc)[:,-1])

fpr_dtc,tpr_dtc
```

Out[32]:

```
(array([0.        , 0.        , 0.06818182, 1.        ]),
 array([0.        , 0.56603774, 0.73584906, 1.        ]))
```

Plotting ROC Curves

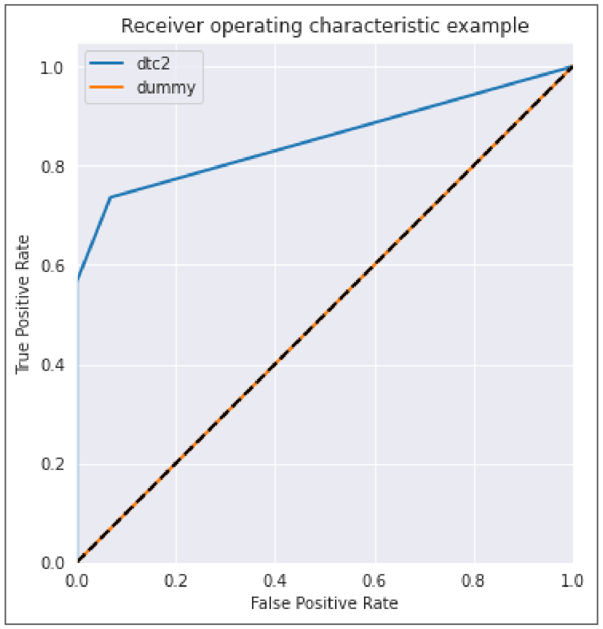
In [33]:

```
def plot_roc(curves):
    fig,ax = plt.subplots(1,1,figsize=(6,6))
    lw = 2
    for fpr,tpr,model_name in curves:
        l1, = ax.plot(fpr, tpr, lw=lw, label=model_name)
    ax.plot([0, 1], [0, 1], color='k', lw=lw, linestyle='--')
    ax.set_xlim([0.0, 1.0])
    ax.set_ylim([0.0, 1.05])
    ax.set_xlabel('False Positive Rate')
    ax.set_ylabel('True Positive Rate')
    ax.set_aspect('equal', 'box')
    ax.set_title('Receiver operating characteristic example')
    ax.legend()
```

Plotting ROC Curves

In [34]:

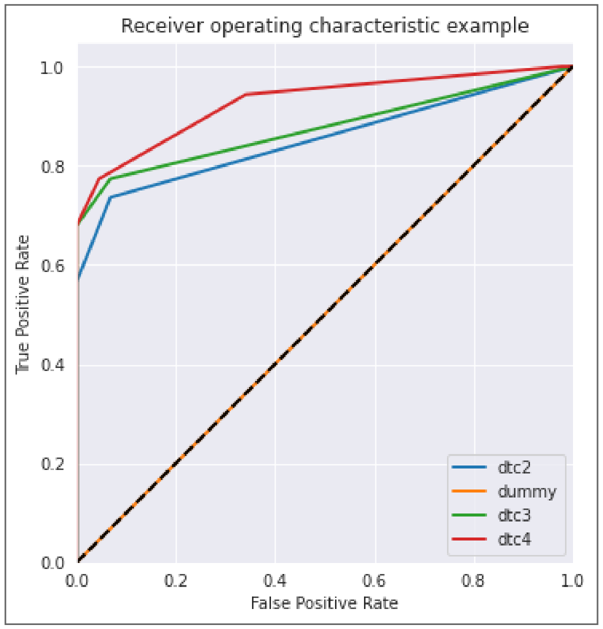
```
curves = [(fpr_dtc,tpr_dtc,'dtc2')]
fpr_dummyc, tpr_dummyc, _ = roc_curve(y_train_bc, dummyc.predict_proba(X_train_bc)[:,1]) # Compare dummy
curves.append((fpr_dummyc,tpr_dummyc,'dummy'));
plot_roc(curves);
```



Plotting ROC Curves

In [35]:

```
for depth in [3,4]:
    fpr, tpr, _ = roc_curve(y_train_bc,DecisionTreeClassifier(max_depth=depth).fit(X_train_bc,y_train_bc).predict_proba(X_train_bc)[:,1]
    curves.append((fpr,tpr,'dtc'+str(depth)))
plot_roc(curves);
```



ROC AUC

- But again, we'd like one number to optimize
- ROC **A**rea **U**nder the **C**urve
    - How much area falls under the ROC curve?

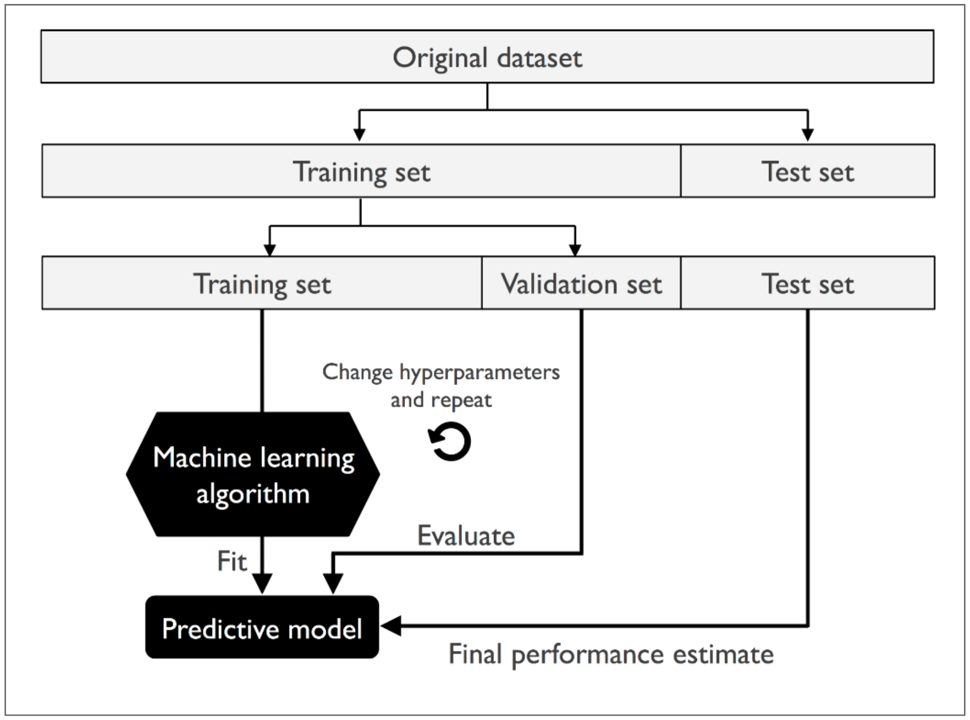
In [36]:

```
dummyc_rocauc_scores = cross_val_score(dummyc,X_train_bc,y_train_bc,cv=5,scoring='roc_auc')
dtc_rocauc_scores = cross_val_score(dtc,X_train_bc,y_train_bc,cv=5,scoring='roc_auc')

print(f'dummyc rocauc = {np.mean(dummyc_rocauc_scores):0.2f} +- {2*np.std(dummyc_rocauc_scores):0.2f}')
print(f'dtc rocauc    = {np.mean(dtc_rocauc_scores):0.2f} +- {2*np.std(dtc_rocauc_scores):0.2f}')
```

```
dummyc rocauc = 0.50 +- 0.00
dtc rocauc    = 0.78 +- 0.22
```

Review: Steps to Choosing a Model

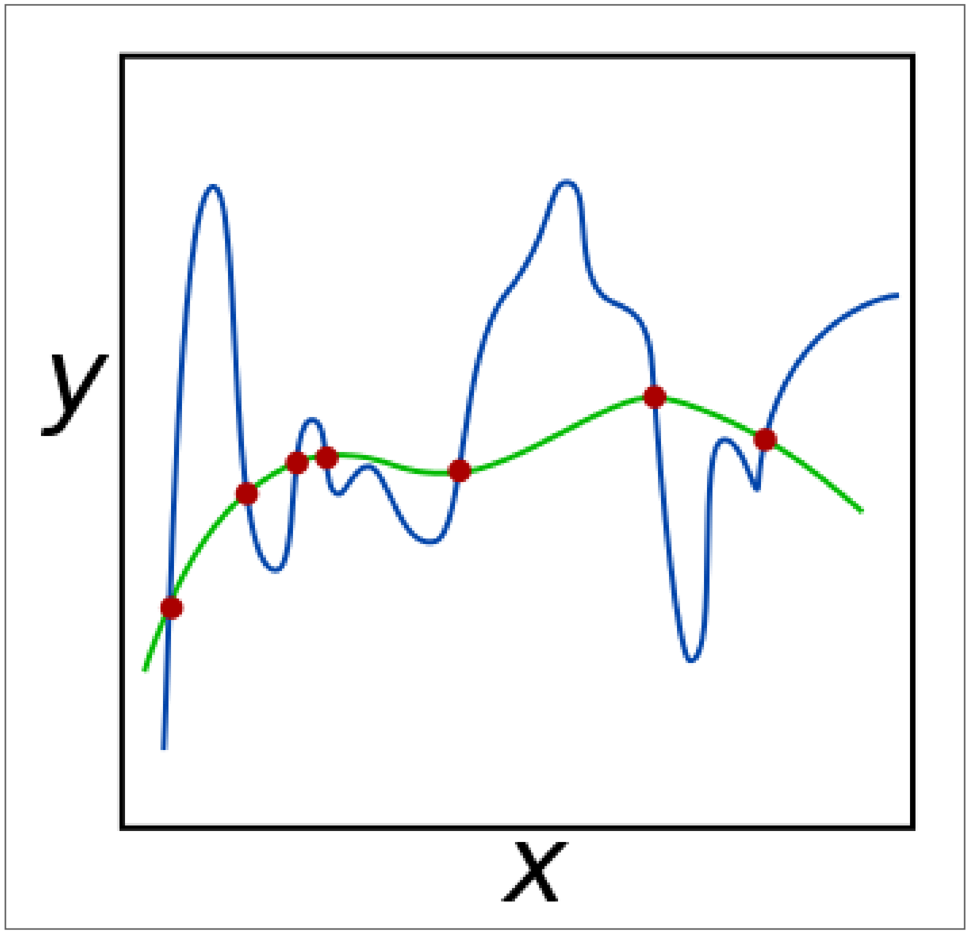
1. Create Held-Aside Set (Train/Test Split)
2. Determine Metric (or combination of metrics)
3. Get a Baseline for comparison
4. Use Cross-Validation to fit Hyperparameters and Choose Model
5. Evaluate Chosen Model on Held-Aside Set



From PML

Avoiding Overfitting in Linear Models: Regularization

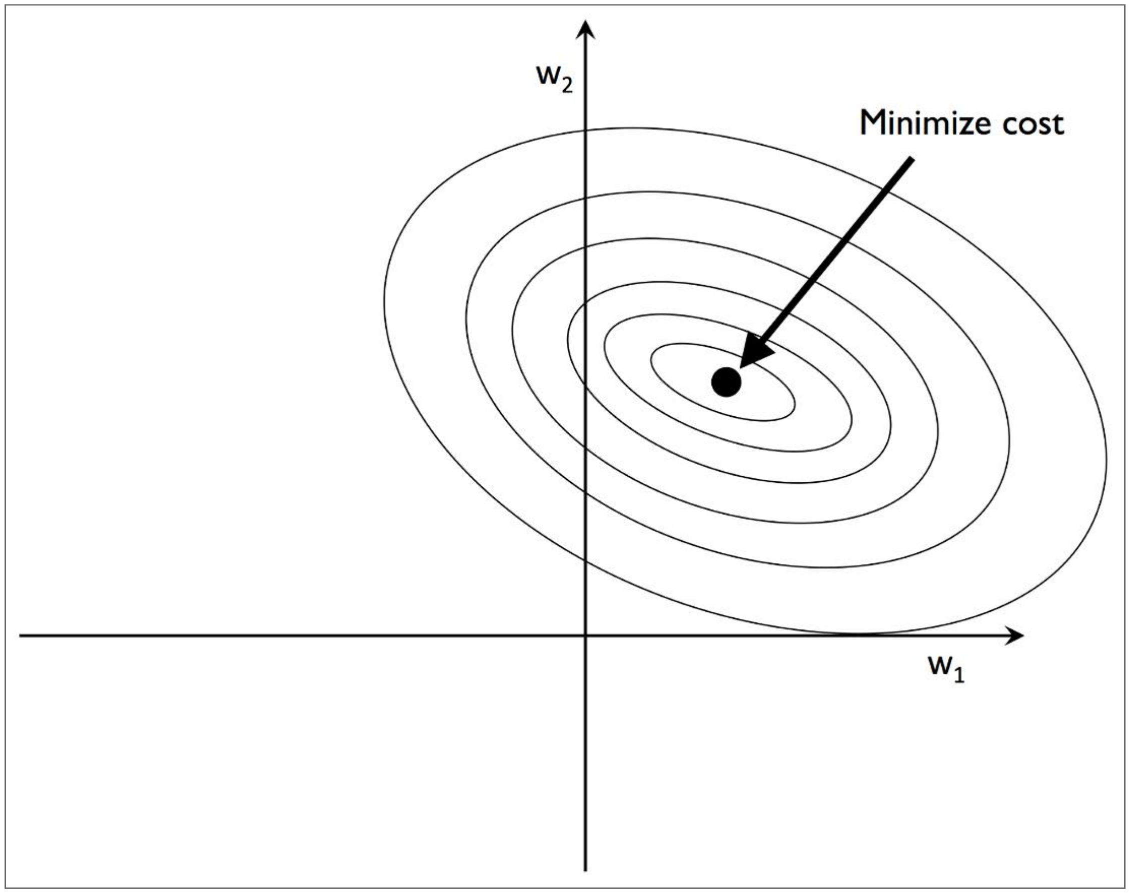
- Use to avoid overfitting in linear models
- Idea: can we reduce complexity of our linear model by minimizing weights?



From **https://www.wikiwand.com/en/Regularization_(mathematics)**

Regression: Finding the Weights

- Linear models learn by finding weights that minimize a cost.
- Can we get close to the solution while still keeping weights small (simpler model)?



From PML

Regularization: Add a cost for large weights

Penalizing extreme weights (w)
If the original cost function looks like:

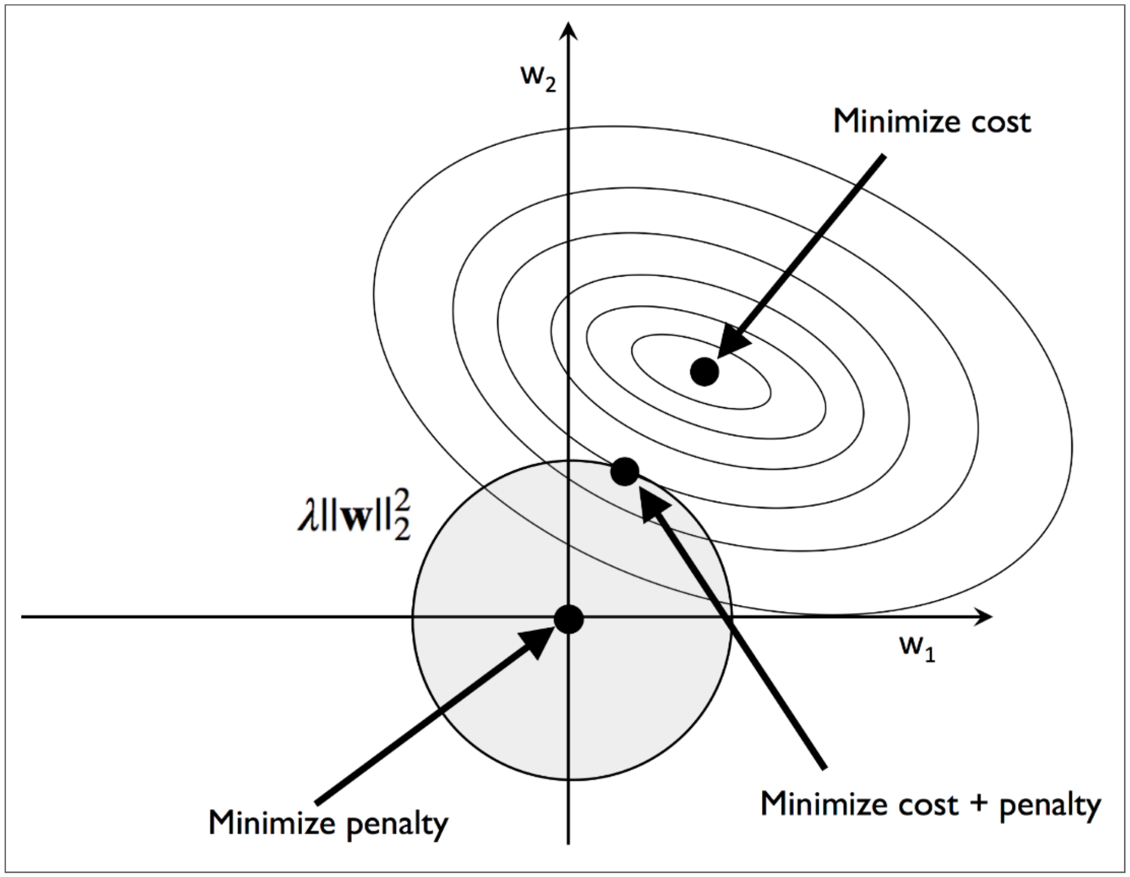
$$\arg\min_w C(f(w, x), y)$$

we can add a **regularization term**:

$$\arg\min_w C(f(w, x), y) + \lambda g(w)$$

Regularization: Ridge

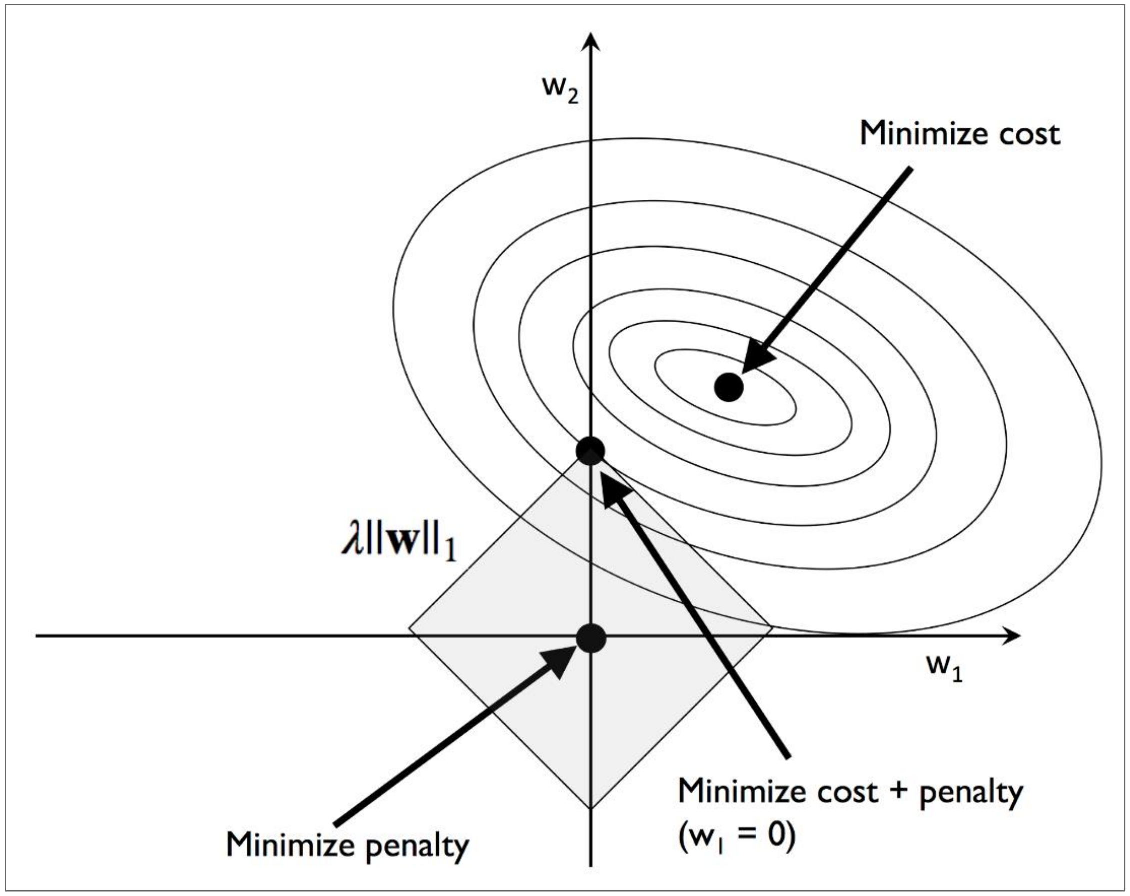
- Coefficients are encouraged to be "small"
- Uses L_2 norm: $\|w\|_2 = \sqrt{\sum_{j=1}^{m} w_j^2}$



From PML

Regularization: LASSO

- Coefficients are (likely) driven to zero
- Uses L_1 norm: $\|w\|_1 = \sum_{j=1}^{m} | w_j|$



From PML

Regularization: ElasticNet

- Mixture of L_1 and L_2
- $\alpha L_1 + (1 - \alpha) L_2$
- introduces a new hyperparameter α or `l1_ratio`
- $l1\_ratio = 1$ is LASSO (L_1)
- $l1\_ratio = 0$ is Ridge (L_2)

Regularization in sklearn

In [37]:

```
from sklearn.linear_model import LogisticRegression

logr = LogisticRegression(penalty='l2', # default
                          C=1.0,        # weight on regularization, 1/lambda above
                          l1_ratio=None # only used when penalty is 'elasticnet'
                         )
```

In [38]:

```
for C in [.001,.1,1,10,1000]:
    logr = LogisticRegression(penalty='l2', # default
                              C=C,          # weight on regularization, 1/lambda above
                             ).fit(X_train_bc,y_train_bc)
    print(f'{str(C):5s} : {logr.coef_[0].round(2)}')
```

```
0.001 : [ 0.02 -0.02]
0.1   : [ 0.69 -0.57]
1     : [ 1.09 -0.93]
10    : [ 1.19 -1.02]
1000  : [ 1.2  -1.03]
```

In [39]:

```
for C in [.001,.1,1,10,1000]:
    logr = LogisticRegression(penalty='l1',
                              C=C,          # weight on regularization, 1/lambda above
                              solver='liblinear'
                             ).fit(X_train_bc,y_train_bc)
    print(f'{str(C):5s} : {logr.coef_[0].round(2)}')
```

```
0.001 : [0. 0.]
0.1   : [ 0.5  -0.37]
1     : [ 1.08 -0.92]
10    : [ 1.19 -1.02]
1000  : [ 1.2  -1.03]
```

GridSearchCV with Regularization

In [40]:

```
param_grid = {'l1_ratio':[0,.5,1],
              'C': [.001,.01,1,10]}
logr_gscv = GridSearchCV(estimator=LogisticRegression(penalty='elasticnet',solver='saga'),
                         param_grid=param_grid,
                         cv=3,
                         n_jobs=-1).fit(X_train_bc,y_train_bc)

print(f'best parameter setting found: {logr_gscv.best_params_}')
print(f'best coefficients found     : {logr_gscv.best_estimator_.coef_[0]}')
print(f'best training score found   : {logr_gscv.best_score_.round(3)}')

logr_gscv_test_score = logr_gscv.score(X_test_bc,y_test_bc)
logr_noreg_test_score = (LogisticRegression(penalty='none')
                         .fit(X_train_bc,y_train_bc)
                         .score(X_test_bc,y_test_bc)
                        )
print()
print(f'logr_gscv test score  : {logr_gscv_test_score.round(3)}')
print(f'logr noreg test score : {logr_noreg_test_score.round(3)}')
```

```
best parameter setting found: {'C': 1, 'l1_ratio': 1}
best coefficients found     : [ 1.09869298 -0.9278305
8]
best training score found   : 0.825

logr_gscv test score  : 0.818
logr noreg test score : 0.818
```

ElasticNetCV

In [41]:

```
from sklearn.datasets import make_regression
from sklearn.linear_model import ElasticNetCV

X_synth,y_synth = make_regression(n_samples=100,
                                  n_features=200,
                                  n_informative=10,
                                  random_state=123
                                 )
X_synth_train,X_synth_test,y_synth_train,y_synth_test = train_test_split(X_synth, y_synth, random_state=123)

dummy_synth = DummyRegressor(strategy='mean').fit(X_synth_train,y_synth_train)
lr_synth = LinearRegression().fit(X_synth_train,y_synth_train)
en_synth = ElasticNetCV(alphas=[.01,.1,1,100]).fit(X_synth_train,y_synth_train)

print(f'found alpha: {en_synth.alpha_}, found l1_ratio: {en_synth.l1_ratio_}\n')
print(f'{dummy_synth.score(X_synth_train,y_synth_train) = : 0.2f}')
print(f'{lr_synth.score(X_synth_train,y_synth_train)    = : 0.2f}')
print(f'{en_synth.score(X_synth_train,y_synth_train)    = : 0.2f}\n')
print(f'{dummy_synth.score(X_synth_test,y_synth_test)   = : 0.2f}')
print(f'{lr_synth.score(X_synth_test,y_synth_test)      = : 0.2f}')
print(f'{en_synth.score(X_synth_test,y_synth_test)      = : 0.2f}')
```

```
found alpha: 1.0, found l1_ratio: 0.5

dummy_synth.score(X_synth_train,y_synth_train) =  0.00
lr_synth.score(X_synth_train,y_synth_train)    =  1.00
en_synth.score(X_synth_train,y_synth_train)    =  0.95
```

```
dummy_synth.score(X_synth_test,y_synth_test)   = -0.00
lr_synth.score(X_synth_test,y_synth_test)      =  0.16
en_synth.score(X_synth_test,y_synth_test)      =  0.24
```

Questions?