Elements Of Data Science - F2020

Week 7: Model Evaluation and Hyperparameter Tuning

10/26/2020

TODOs

- Readings:
    - PDSH Chapter 5: Feature Engineering
    - (Recommended) PML Chapter 4
- HW2, Out this week?
- Answer and submit Quiz 7, **Sunday Nov 8th, 11:59pm ET**
- **Midterm**
    - Release **Monday Oct 26th, 11:59pm ET**
    - Due **Saturday Oct 31st, 11:59pm ET**
    - Have 24hrs after starting exam to finish
    - 30 questions (fill in the blank/multiple choice/short answer)
    - Online via Gradescope
    - Questions asked/answered **privately** via Piazza
    - Open-book, open-note, open-python

Generating Predictions for a Single Value

In [2]:
```
from sklearn.linear_model import LogisticRegression
```

In [3]:
```
X = np.random.rand(5,2)
y = (np.random.rand(5) > .5).astype(int)

lr = LogisticRegression().fit(X,y)

# use reshape(1,-1) when generating a single prediction
# recall that sklearn expects X to be two dimensional
lr.predict(np.array([.2,.3]).reshape(1,-1))
```

Out[3]:
```
array([0])
```

In [4]:
```
# Note: this is different from when training on a single feature: .reshape(-1,1)
lr.fit(X[:,0].reshape(-1,1),y)

lr.predict(np.array(.2).reshape(1,-1))
```

Out[4]:
```
array([0])
```

Today

- Model Evaluation and Selection
- Hyperparameter Tuning
- Regularization

Questions?

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
- Adjusted R^2

Classification

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

Data Setup for Regression

In [5]:
```
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_r = df_wine[['proline','hue','ash']]                       # multiple features for regression task

X_1d = X_r.proline.values.reshape(-1,1)                      # create single feature vector using reshape

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

In [6]:
```
df_wine
```

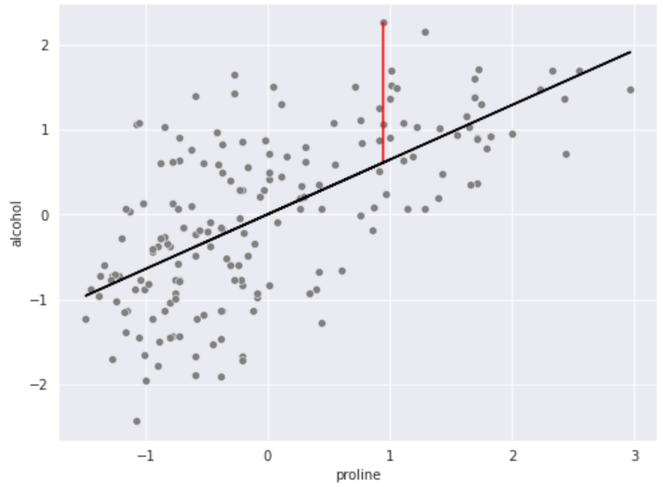
Out[6]:

	alcohol	ash	alcalinity_of_ash	magnesium	hue	proline	class
0	1.514341	0.231400	-1.166303	1.908522	0.361158	1.010159	0
1	0.245597	-0.825667	-2.483841	0.018094	0.404908	0.962526	0
2	0.196325	1.106214	-0.267982	0.088110	0.317409	1.391224	0
3	1.686791	0.486554	-0.806975	0.928300	-0.426341	2.328007	0
4	0.294868	1.835226	0.450674	1.278379	0.361158	-0.037767	0
...	...	...	...	...	...	...	...
173	0.873810	0.304301	0.300954	-0.331985	-1.388840	-0.021890	2
174	0.491955	0.413653	1.049555	0.158126	-1.126341	0.009866	2
175	0.331822	-0.388260	0.151234	1.418411	-1.607590	0.279786	2
176	0.208643	0.012696	0.151234	1.418411	-1.563840	0.295664	2
177	1.391162	1.361368	1.498716	-0.261969	-1.520090	-0.593486	2

178 rows × 7 columns

Regression with Simple Linear Model

In [7]:
```
from sklearn.linear_model import LinearRegression

lr = LinearRegression().fit(X_1d,y_r)
argmax_y_r = np.argmax(y_r)
y_pred = lr.predict(X_1d)

fig,ax = plt.subplots(1,1,figsize=(8,6))
sns.scatterplot(x=X_r.proline, y=y_r, color='grey');
ax.plot(X_1d,y_pred,color='k');
ax.vlines(X_1d[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:** $\sum_i (y_i - \hat{y}_i)^2$

In [8]:
```
from sklearn.metrics import mean_squared_error

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

Out[8]:
```
'lr_mse = 0.58'
```

- But this is the squared error! (alcohol^2)

- **Root Mean Squared Error:** $\sqrt{\sum_i (y_i - \hat{y}_i)^2}$

In [9]:
```
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)
f'{lr_rmse = :0.2f}'
```

Out[9]:
```
'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 [10]:
```
from sklearn.dummy import DummyRegressor

dummyr = DummyRegressor(strategy='mean') # default strategy
dummyr.fit(X_1d,y_r)

dummy_rmse = root_mean_squared_error(y_r,dummyr.predict(X_1d))

f'{dummy_rmse = :0.2f}'
```

Out[10]:
```
'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 [11]:
```
r2_lr = lr.score(X_1d,y_r)
r2_dummyr = dummyr.score(X_1d,y_r)

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

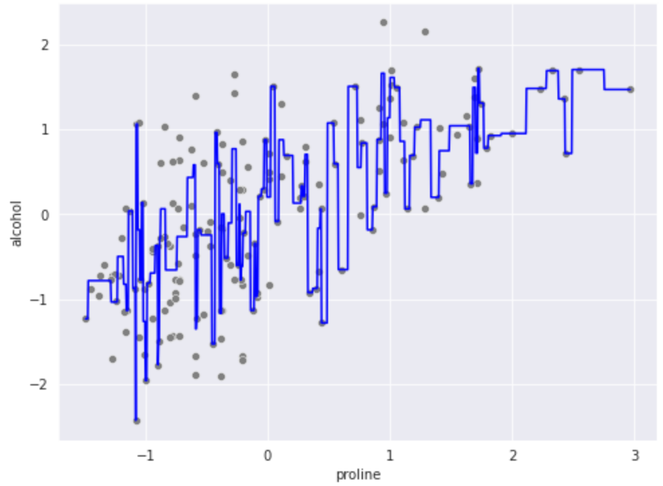
```
r2_dummyr = 0.00
r2_lr     = 0.41
```

Can we do better?

In [12]:
```
from sklearn.tree import DecisionTreeRegressor

dtr = DecisionTreeRegressor(max_depth=10)
dtr.fit(X_1d,y_r)
r2_dtr = dtr.score(X_1d,y_r)
print(f'{r2_lr  = :0.2f}\n{r2_dtr = :0.2f}')
```

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

In [13]:
```
X_1d_sorted = np.sort(X_1d.flatten()).reshape(-1,1)
X_query = np.linspace(X_1d.min(),X_1d.max(),1000).reshape(-1,1)
y_pred = dtr.predict(X_query)
fig,ax = plt.subplots(1,1,figsize=(8,6))
sns.scatterplot(x=X_r.proline, y=y_r,color='gray');
ax.plot(X_query,y_pred,color='b');
```



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?

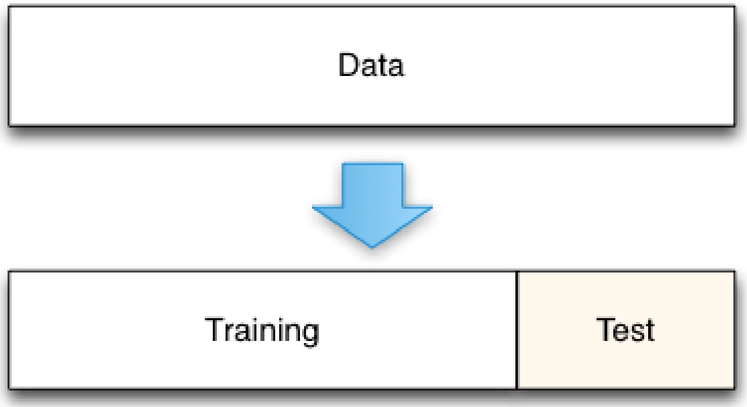
But we used all of our data to train?

- Need to do a **Train/Test Split**

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 [14]:
```
from sklearn.model_selection import train_test_split

X_train_r,X_test_r,y_train_r,y_test_r = train_test_split(X_1d,
                                                         y_r,
                                                         test_size=.25, #default
                                                         random_state=123)

print(X_1d.shape[0])
print(X_train_r.shape[0])
print(X_test_r.shape[0])
```

```
178
133
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 [15]:
```
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!

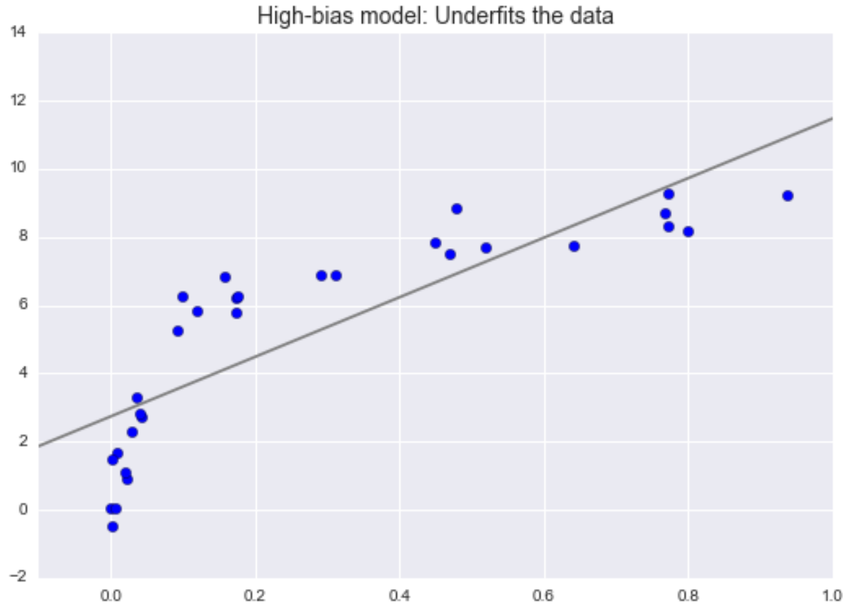
Overfitting and Underfitting

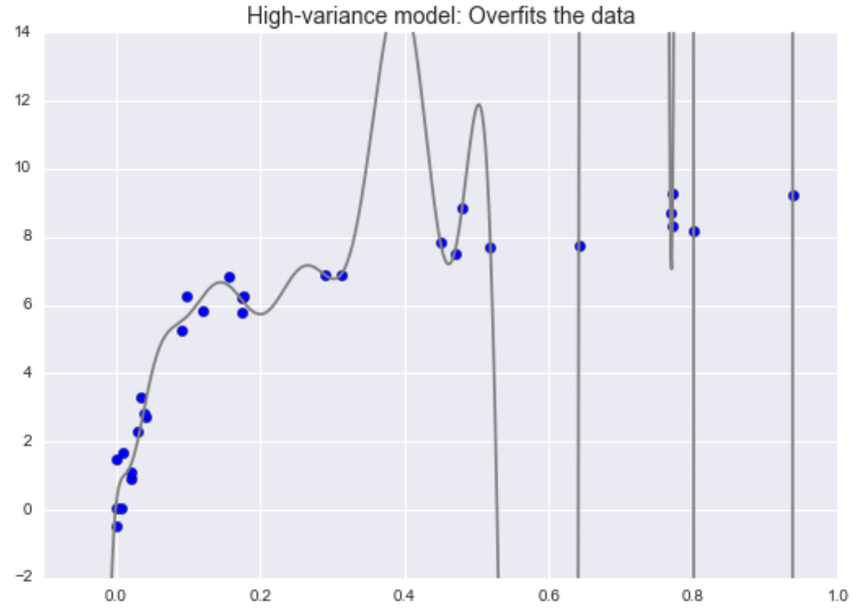
- **Overfitting:** poor generalization due to complexity
    - learning noise in training data

- **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**

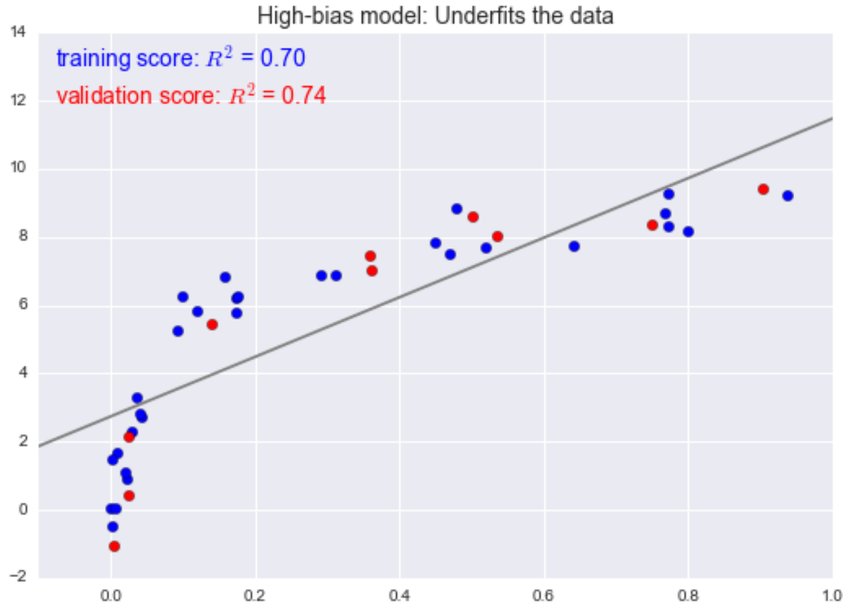
Bias-Variance Tradeoff

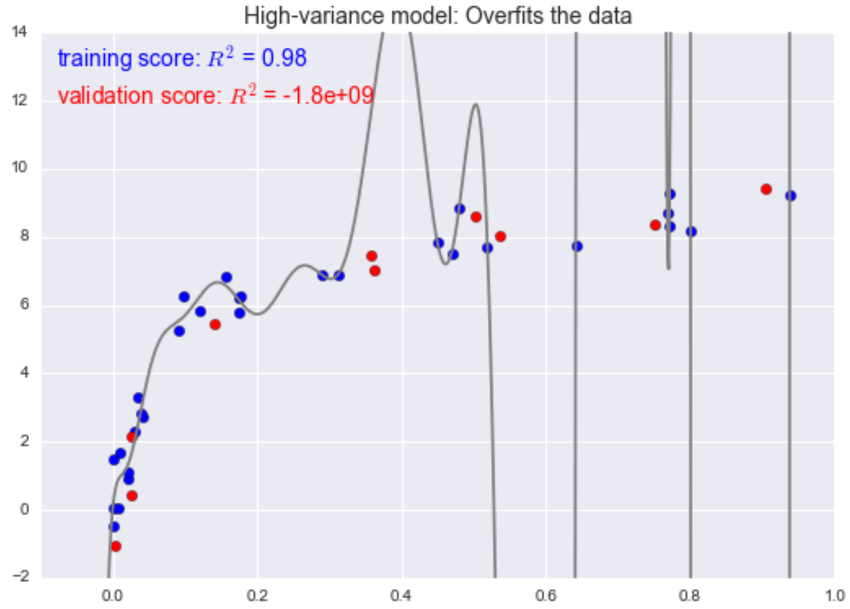




From PDSH

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?

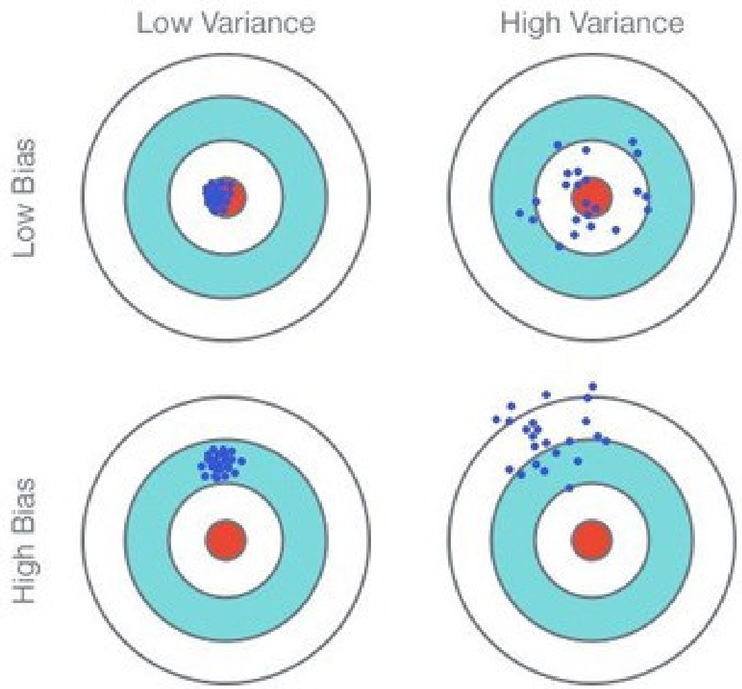
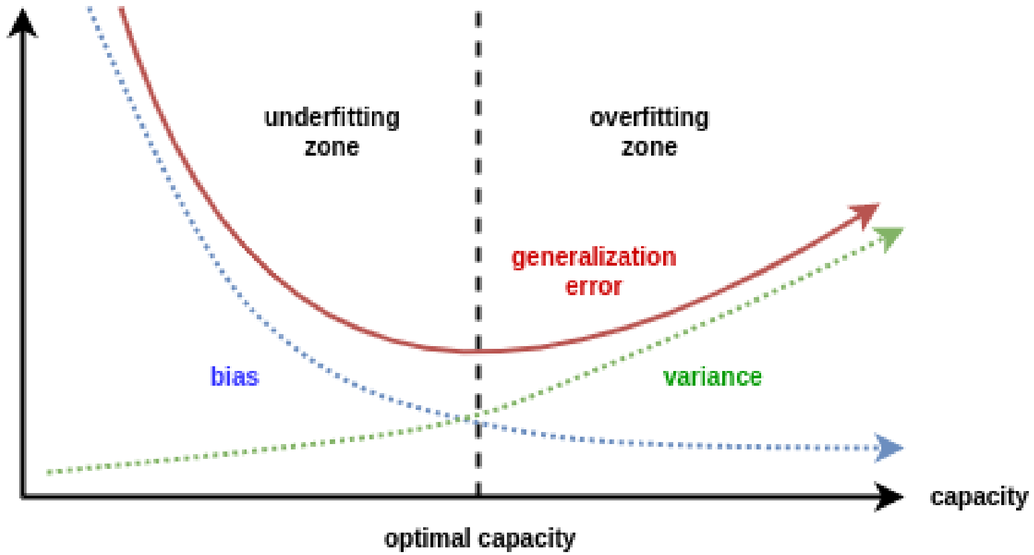


Fig. 1: Graphical Illustration of bias-variance trade-off , Source: Scott Fortmann-Roe., Understanding Bias-Variance Trade-off

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**

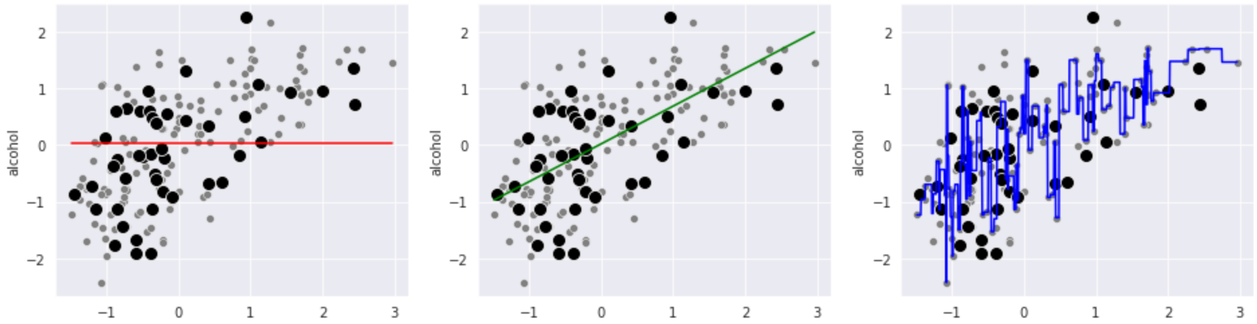
Overfitting/Underfitting Revisited

- **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

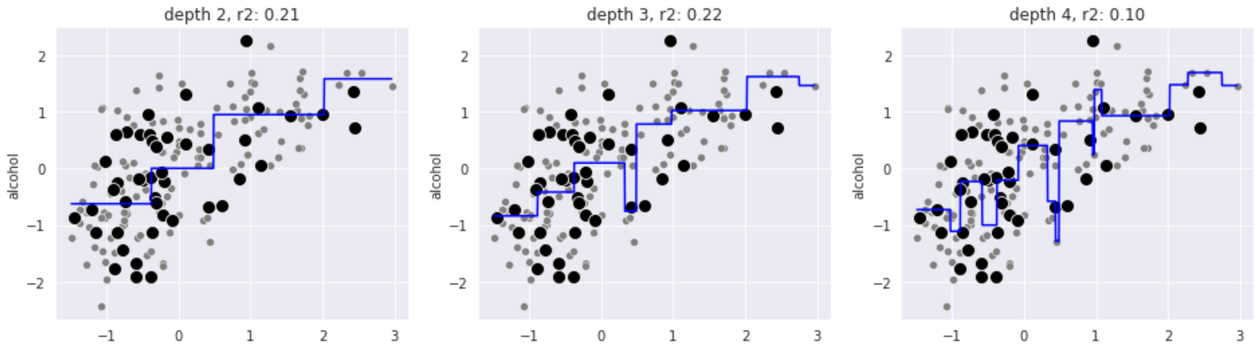
- Never train and evaluate on the same set of data!
    - train test split
    - **cross-validation**
- Keep the model as simple as possible (Occom's Razor)

In [16]:
```
fig,ax = plt.subplots(1,3,figsize=(16,4))
for i in range(3):
    sns.scatterplot(x=X_train_r.flatten(),y=y_train_r,color="gray",ax=ax[i])
    sns.scatterplot(x=X_test_r.flatten(),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 [17]:
```
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.flatten(),y=y_train_r,color="gray",ax=ax[i])
    sns.scatterplot(x=X_test_r.flatten(),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}')
```



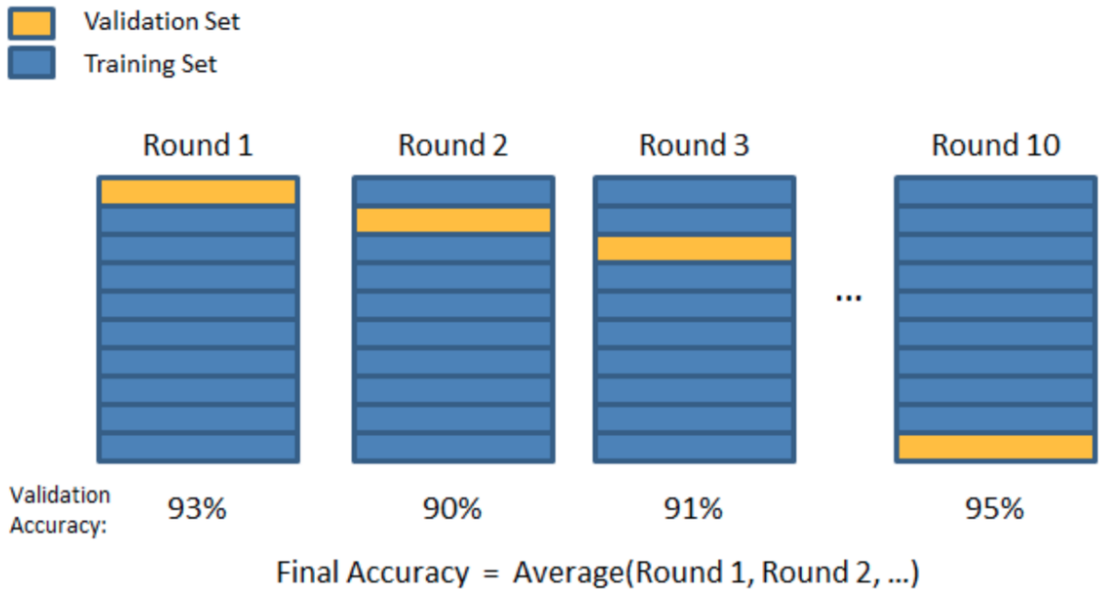
- But now we might be overfitting on the test set!
- How to choose hyperparameters: **Cross-Validation**

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 [18]:
```
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[18]:
```
array([0.41853032, 0.37075208, 0.45405394, 0.2588269 , 0.22799476])
```

In [19]:
```
print(f'{np.mean(scores) :0.2f} +- {2*np.std(scores) :0.2f}')
```

```
0.35 +- 0.18
```

Tuning Hyperparameters with CV

In [20]:
```
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()) )

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
```

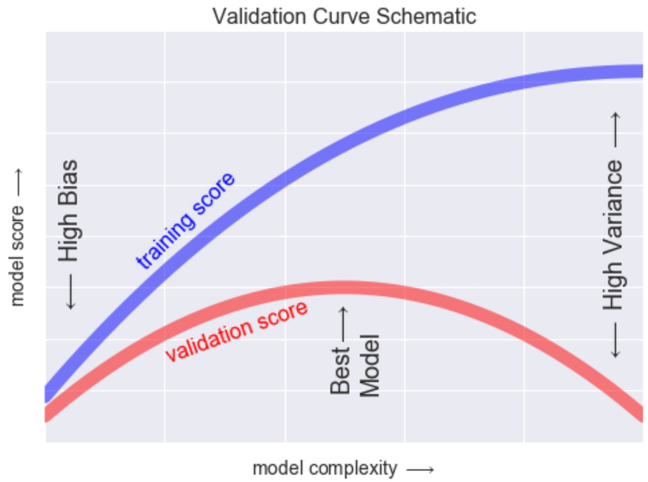
In [22]:
```
# find the depth that gives best score (highest R^2)
sorted(mean_scores, key=lambda x:x[1],reverse=True)[0] # sorted is ascending by default
```

Out[22]:
```
(2, 0.3460316005269502)
```

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)

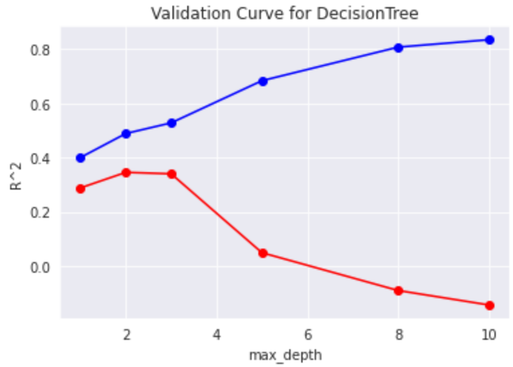


From PDSH

Validation Curve in sklearn

In [23]:
```
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 [24]:
```
plt.plot(depth, mean_train_scores, 'o-', color='b',label='training score');
plt.plot(depth, mean_test_scores, 'o-', color='r', label='validation score');
plt.xlabel('max_depth'), plt.ylabel('R^2'); plt.title('Validation Curve for DecisionTree');
```



More Than One HyperParameter? Grid Search

Grid Search: Search over a 'grid' of hyperparameter settings

Example: KNN "number of neighbors" and "distance metric"

In [25]:
```
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 [26]:
```
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 [27]:
```
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 [28]:
```
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[28]:

	train	test
0	44	15
1	53	18

In [29]:
```
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[29]:

	train	test
2	36	12
0	44	15

Default Metric in Classification: Accuracy

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

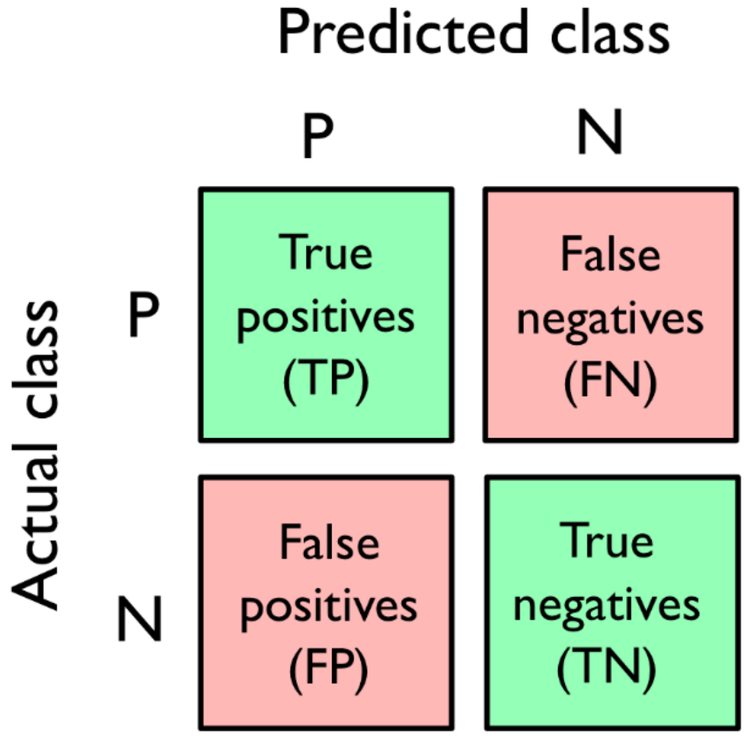
In [30]:
```
from sklearn.dummy import DummyClassifier
from sklearn.tree import DecisionTreeClassifier
dummyc = DummyClassifier(strategy='prior').fit(X_train_bc,y_train_bc) # works like 'most-frequent'
dtc = DecisionTreeClassifier(max_depth=2).fit(X_train_bc,y_train_bc)

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

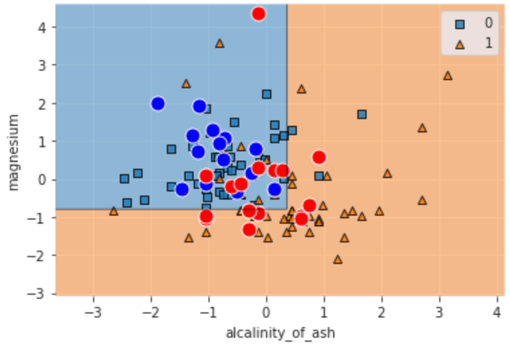
- There are different kinds of error in classification



From PML

Visualizing Errors with a Confusion Matrix

In [31]:
```
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);
```

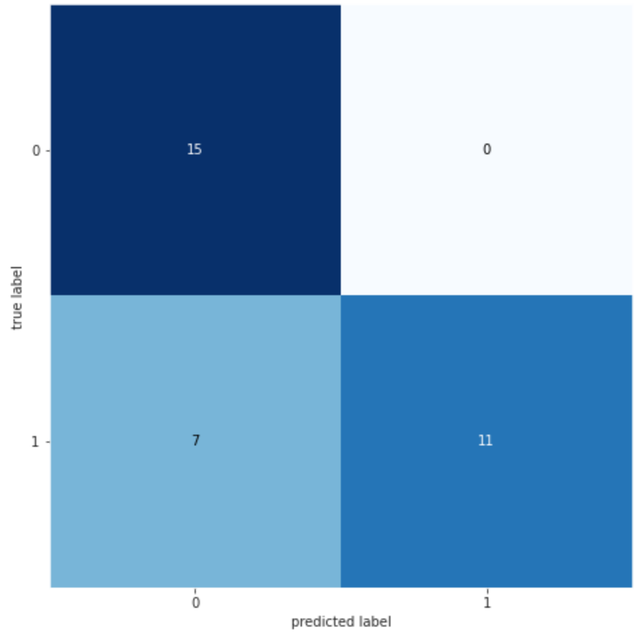


In [32]:
```
from sklearn.metrics import confusion_matrix

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 [33]:
```
from mlxtend.plotting import plot_confusion_matrix

fig,ax = plt.subplots(1,1,figsize=(8,8))
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)?

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

Recall

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

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

Using Other Measures in sklearn

In [34]:
```
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 [35]:
```
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 [36]:
```
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
```

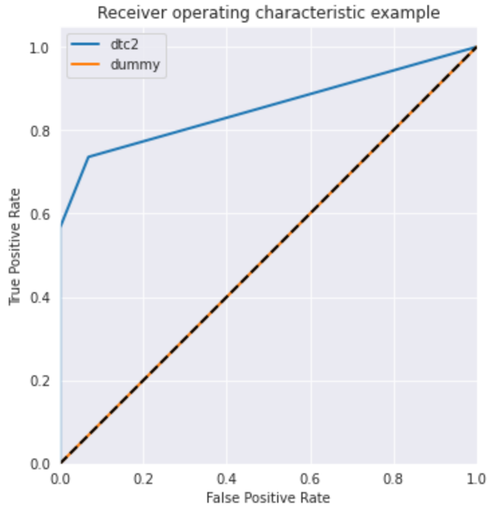
Out[36]:
```
(array([0.        , 0.        , 0.06818182, 1.        ]),
 array([0.        , 0.56603774, 0.73584906, 1.        ]))
```

Plotting ROC Curves

In [37]:
```
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()
```

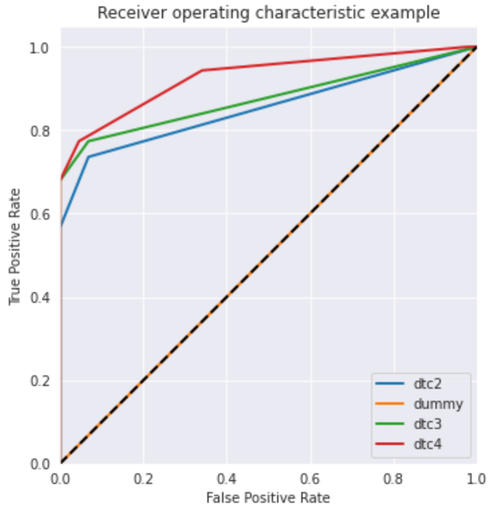
Plotting ROC Curves

In [38]:
```
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 [39]:
```
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_
    curves.append((fpr,tpr,'dtc'+str(depth)))
plot_roc(curves);
```



ROC AUC

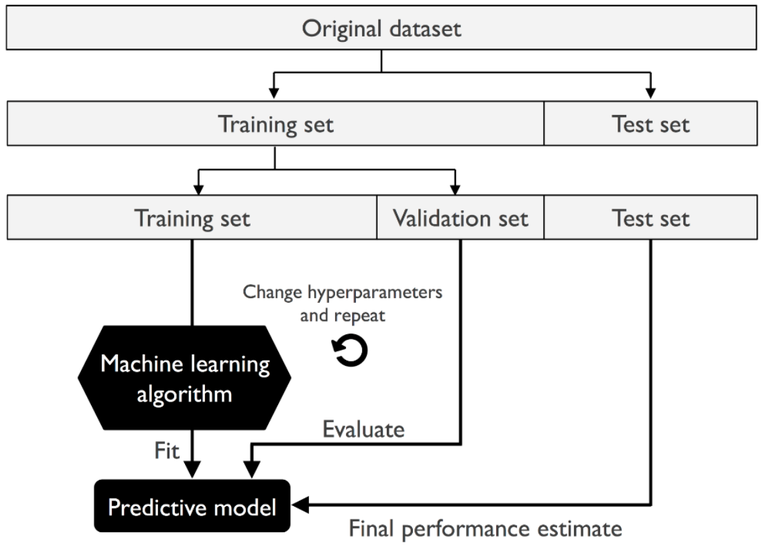
- But again, we'd like one number to optimize
- ROC **A**rea **U**nder the **C**urve
    - How much area falls under the ROC curve?

In [40]:
```
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

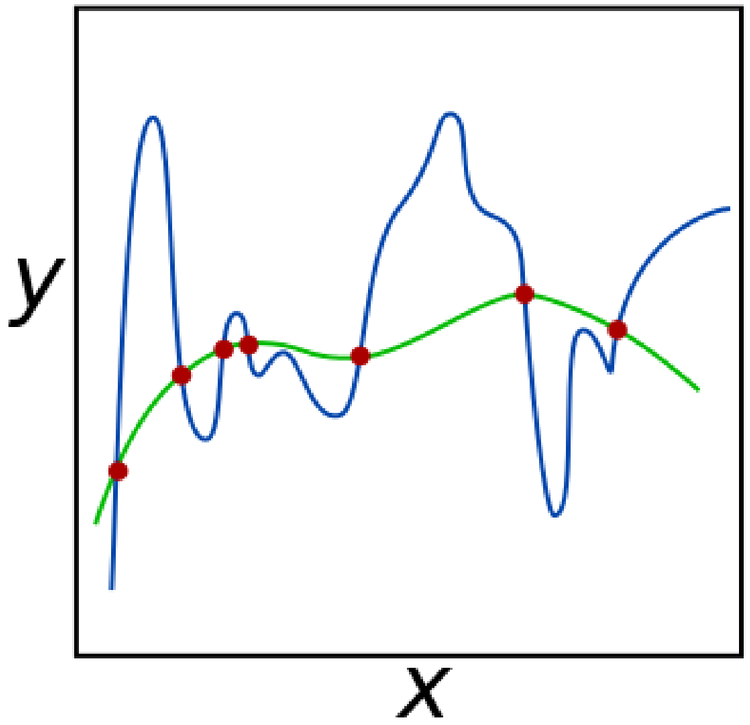
1. Create Held-Aside Set (Train/Test Split)
2. Determine Metric (or combination of metrics)
3. Get a Baseline for comparison
4. Use Cross-Validation to fit Hyperparameters and Choose Model
5. Evaluate Chosen Model on Held-Aside Set



From PML

Avoiding Overfitting in Linear Models: Regularization

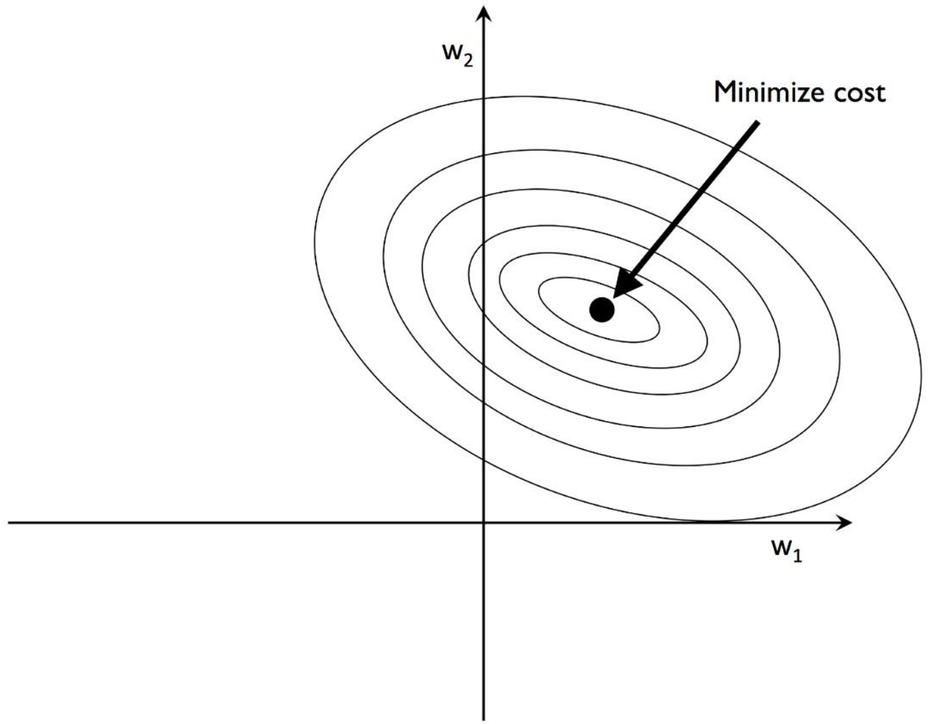
- Use to avoid overfitting in linear models
- Idea: can we reduce complexity of our linear model by minimizing weights?



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:

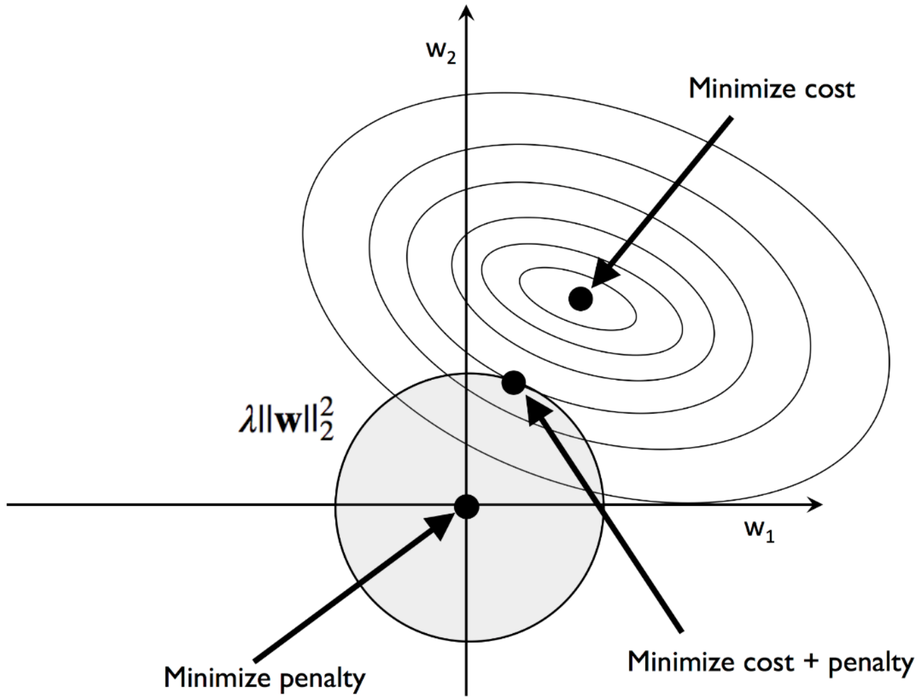
$$\arg\min_w C(f(w, x), y)$$

we can add a **regularization term**:

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

Regularization: Ridge

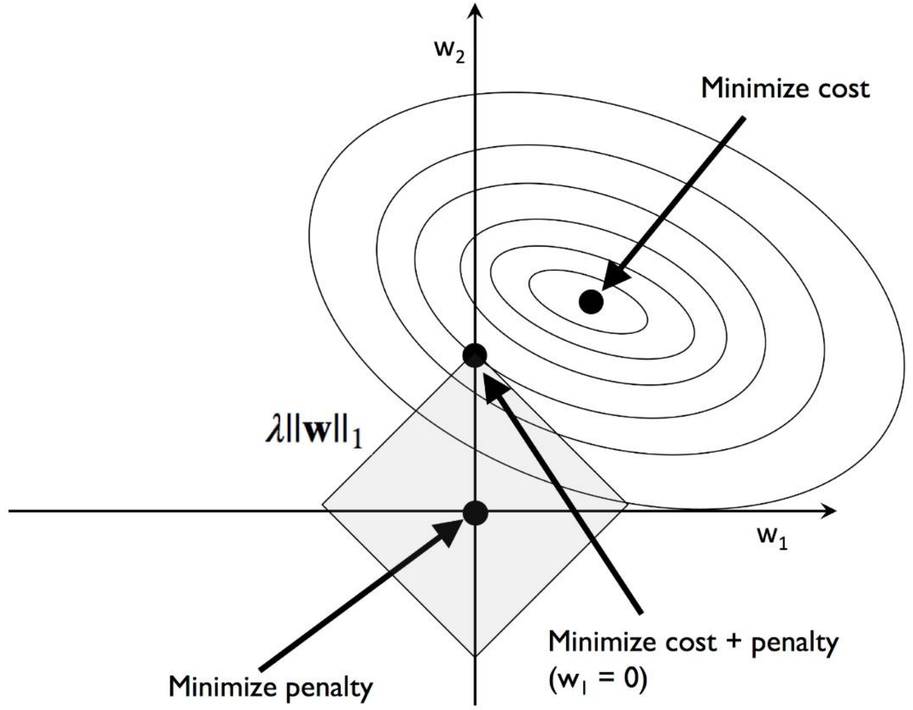
- Coefficients are encouraged to be "small"
- Uses L_2 norm: $\|w\|_2 = \sqrt{\sum_{j=1}^{m} w_j^2}$



From PML

Regularization: LASSO

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



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`
- $\text{l1\_ratio} = 1$ is LASSO (L_1)
- $\text{l1\_ratio} = 0$ is Ridge (L_2)

In [41]:
```
from sklearn.linear_model import LogisticRegression

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