In [1]:

```
# My standard magic !  You will see this in almost all my notebooks.

from IPython.core.interactiveshell import InteractiveShell
InteractiveShell.ast_node_interactivity = "all"

# Reload all modules imported with %aimport
%load_ext autoreload
%autoreload 1

%matplotlib inline
```

Becoming a successful Data Scientist

As of now, you should know

- how to construct models (the "recipe")
- how to use them for prediction
- some simple metrics on how they perform

But, to a degree, this knowledge is purely knowing the mechanics. Perhaps having answers to the following questions is *the most important* topic from this course

- How can you *improve* your models ?
- How can you tell if your model's predictions "make sense"
- How can I be most productive ?

In this module, the topics to be covered provide answers:

- model diagnostics and interpretation
    - What is the model fit telling you ?
        - need to understand model math
    - What should you do about it
        - Transformations
- data cleaning, munging

We will illustrate this with a running example: MNIST digit classification

We will *illustrate* many points using the `LinearRegression` and `LogisticRegression` models.

- you presumably have at least some (i.e., more than other models) exposure/understanding
- "Classical ML" has a well-developped statistical background

The goal is **not** to make you an expert in Regression. These are only illustrations; many concepts carry over to other models.

Model diagnostics

- Beyond summary statistics
    - for classification
    - for regression
- What is a "good" value for the summary statistic

Classification: Beyond accuracy

Recall that we previewed the "confusion matrix" in the previous lecture.

This is how we explore model errors for **classification** problems.

Let's re-run the MNIST problem and examine measures of error more detailed than accuracy

In [2]:

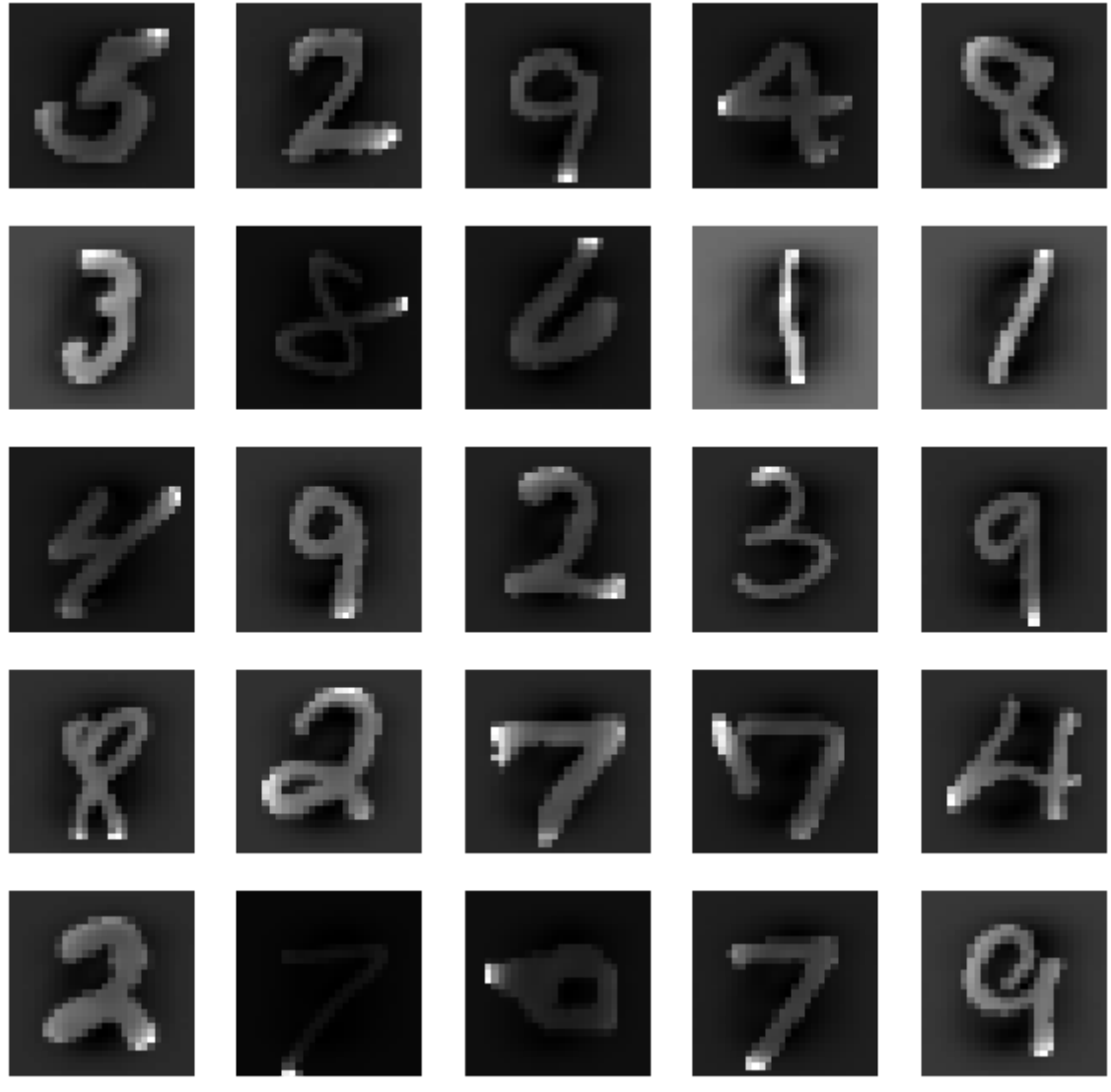
```
# %load mnist_1.py
import time
import matplotlib.pyplot as plt
import numpy as np

import os

from sklearn.datasets import fetch_openml
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.utils import check_random_state

from sklearn import datasets, svm, metrics

import os

def fetch_mnist_784():
    # The fetch from the remote site is SLOW b/c the data is so big
    # Try getting it from a local cache
    cache_dir = "cache/mnist_784"
    (X_file, y_file) = [ "{c}/{f}.npy".format(c=cache_dir, f=fn) for fn in ["X"
, "y"] ]

    if os.path.isfile(X_file) and os.path.isfile(y_file):
        print("Retrieving MNIST_784 from cache")
        X = np.load(X_file)
        y = np.load(y_file)
    else:
        print("Retrieving MNIST_784 from remote")
        # Load data from hiittps://www.openml.org/d/554
        X, y = fetch_openml('mnist_784', version=1, return_X_y=True)

        # Cache it !
        os.makedirs(cache_dr, exist_ok=True)
        np.save(X_file, X)
```

```
        np.save(y_file, y)

    return X,y


# Author: Arthur Mensch <arthur.mensch@m4x.org>
# License: BSD 3 clause

# Turn down for faster convergence
train_samples = 5000

# Fetch the data
X, y = fetch_mnist_784()

random_state = check_random_state(0)
permutation = random_state.permutation(X.shape[0])
X = X[permutation]
y = y[permutation]
X = X.reshape((X.shape[0], -1))

X_train, X_test, y_train, y_test = train_test_split(
    X, y, train_size=train_samples, test_size=10000)

scaler = StandardScaler()
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)
```

```
Retrieving MNIST_784 from cache
```

In [3]:

```
# %load mnist_vis_train.py
fig = plt.figure(figsize=(10,10))
(num_rows, num_cols) = (5, 5)
for i in range(0, num_rows * num_cols):
    img = X_train[i].reshape(28, 28)

    ax  = fig.add_subplot(num_rows, num_cols, i+1)
    _ = ax.set_axis_off()

    _ = plt.imshow(img, cmap="gray")
```



In [4]:
```
# %load mnist_train.py
X_train.shape, y_train.shape

# Turn up tolerance for faster convergence
mnist_lr_clf = LogisticRegression(C=50. / train_samples,  # n.b. C is 1/(regular
ization penalty)
                          multi_class='multinomial',
                          # penalty='l1',   # n.b., "l1" loss: sparsity (number o
f non-zero) >> "l2" loss (dafault)
                          solver='saga', tol=0.1)

t0 = time.time()

# Fit the model
mnist_lr_clf.fit(X_train, y_train)

run_time = time.time() - t0
print('Example run in %.3f s' % run_time)
```

Out[4]:
```
((5000, 784), (5000,))
```

Out[4]:
```
LogisticRegression(C=0.01, class_weight=None, dual=False, fit_intercept=True,
          intercept_scaling=1, max_iter=100, multi_class='multinomial',
          n_jobs=None, penalty='l2', random_state=None, solver='saga',
          tol=0.1, verbose=0, warm_start=False)

Example run in 3.726 s
```

In [5]:

```
# How many zero coefficients were forced by the penalty ?
sparsity = np.mean(mnist_lr_clf.coef_ == 0) * 100
score = mnist_lr_clf.score(X_test, y_test)
# print('Best C % .4f' % clf.C_)

print("Sparsity with {p} penalty: {s:.2f}.".format(p=mnist_lr_clf.penalty, s=spa
rsity) )
print("Test score with {p} penalty:{s:.4f}".format(p=mnist_lr_clf.penalty, s=sco
re) )
```

```
Sparsity with l2 penalty: 15.69.
Test score with l2 penalty:0.8724
```

Aside: Cross-validated score

87% accuracy.

- Are we done ?
    - Is 87% "good"

In [8]:

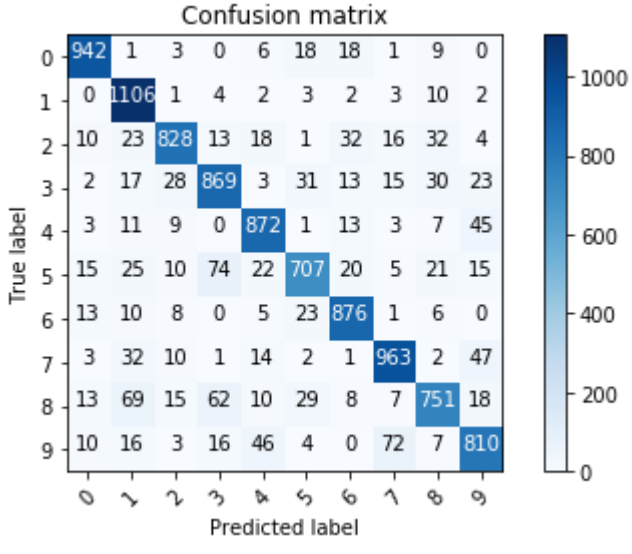
```
# %load mnist_plot_confusion.py
import itertools

def plot_confusion_matrix(cm, classes,
                          normalize=False,
                          title='Confusion matrix',
                          cmap=plt.cm.Blues):
    """
    This function prints and plots the confusion matrix.
    Normalization can be applied by setting `normalize=True`.
    """
    if normalize:
        # Normalize by row sums
        cm_pct = cm.astype('float') / cm.sum(axis=1)[:, np.newaxis]
        cm = np.around( 100 * cm_pct, decimals=0).astype(int)

        print("Normalized confusion matrix")
    else:
        print('Confusion matrix, without normalization')

    plt.imshow(cm, interpolation='nearest', cmap=cmap)
    plt.title(title)
    plt.colorbar()
    tick_marks = np.arange(len(classes))
    plt.xticks(tick_marks, classes, rotation=45)
    plt.yticks(tick_marks, classes)

    fmt = '.2f' if normalize else 'd'
    fmt = 'd'
    thresh = cm.max() / 2.
    for i, j in itertools.product(range(cm.shape[0]), range(cm.shape[1])):
        # Plot coordinate system has origin in upper left corner
        # -  coordinates are (horizontal offset, vertical offset)
        # -  so cm[i,j] should appear in plot coordinate (j,i)
        plt.text(j, i, format(cm[i, j], fmt),
                 horizontalalignment="center",
```

```
                color="white" if cm[i, j] > thresh else "black")

    plt.ylabel('True label')
    plt.xlabel('Predicted label')
    plt.tight_layout()
```

Here is the confusion matrix, both in count and percent.

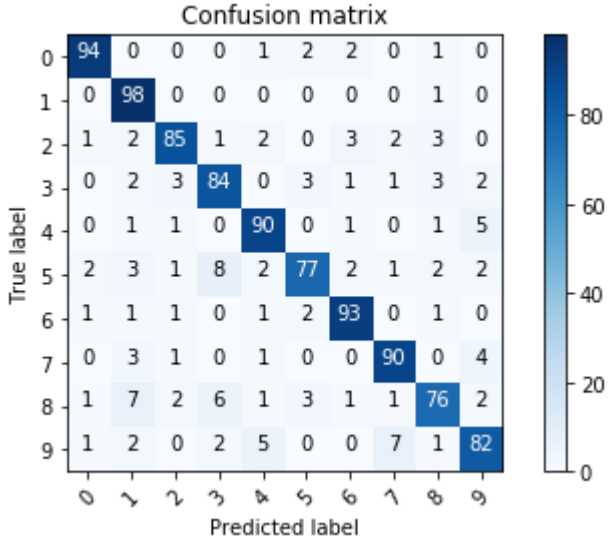
In [9]:
```
plot_confusion_matrix(confusion_mat, range(10))
```

```
Confusion matrix, without normalization
```



In [10]:
```
plot_confusion_matrix(confusion_mat, range(10), normalize=True)
```

Normalized confusion matrix



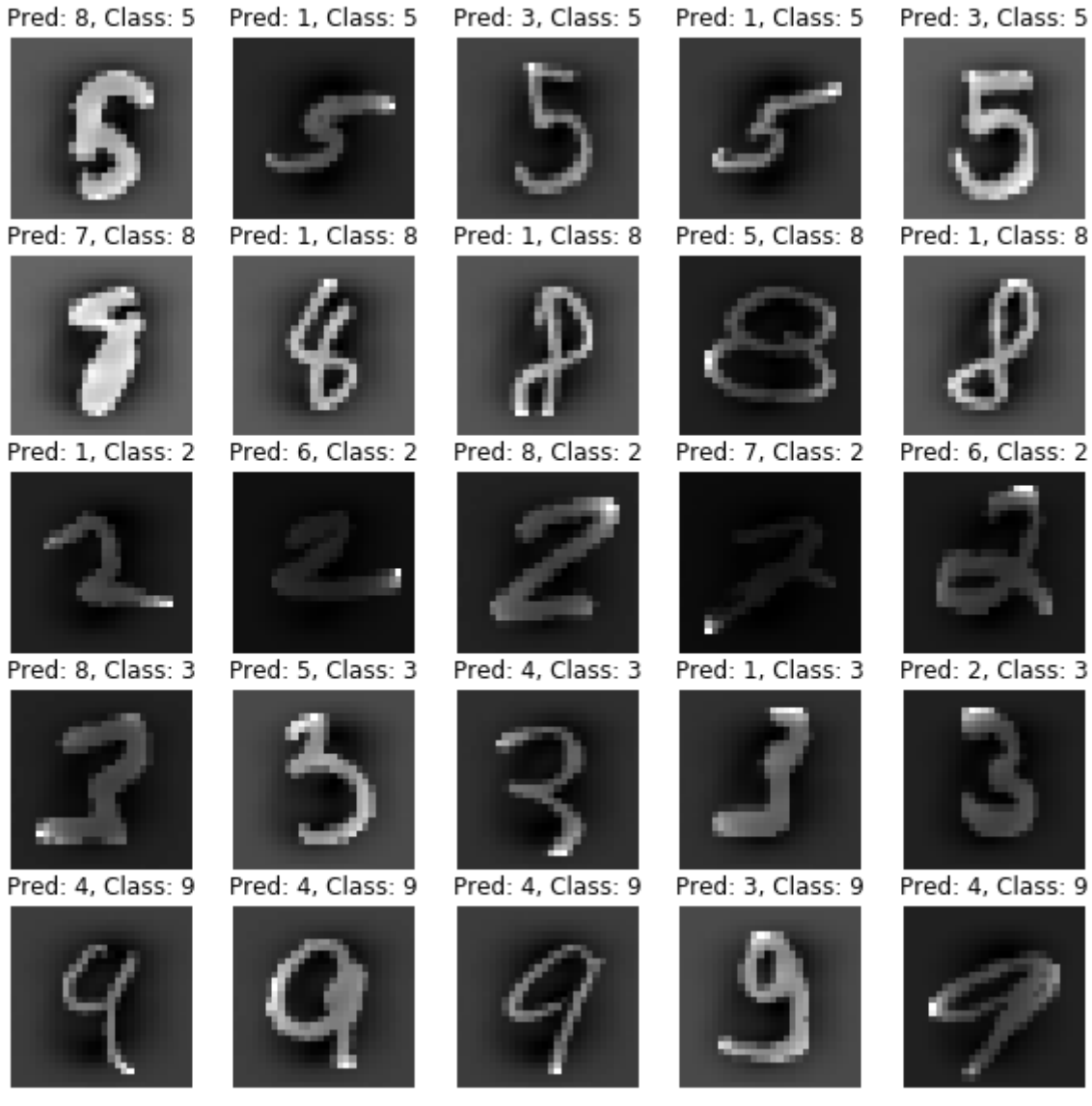
- You can see that we didn't do equally well for all digits
    - "5", "8": below 80% correctly classified
    - "2", "3", "9": 80%-90% correctly classified
- Questions:
    - Are the errors acceptable ?
    - What can we do about the errors ?

In [11]:

```
problem_digits = [ '5', '8', '2', '3', '9' ]

def plot_problem_digits(problem_digits):
    """
    Plot mis-classified digits

    Parameters
    ----------
    problem_digits: List of characters.  Each element of list is a digit

    For each digit T in list: find the test set examples where true label is T b
ut is classified otherwise.
    Plot the mis-classified test examples
    """
    # Dimensions of plot grid
    num_rows, num_cols = len(problem_digits), 5
    fig = plt.figure(figsize=(2*num_cols, 2*num_rows))

    # Plot examples for each problem digit
    for i, digit in enumerate(problem_digits):
        # Find the mis-classified test obsevations for this digit
        mask = (expected == digit) & (expected != predicted)
        X_misclassified = X_test[mask]
        y_misclassified = predicted[mask]
        num_misclassified = X_misclassified.shape[0]

        # Plot the mis-classified instance of digit
        plot_num = num_cols * i
        for j in range(0, min(num_cols, num_misclassified)):
            # Get the X, y for the mis-classified image
            img = X_misclassified[j].reshape(28,28)
            pred =   y_misclassified[j]

            # Plot the image
            ax = fig.add_subplot(num_rows, num_cols, plot_num + j +1)
            _ = ax.set_axis_off()
```

```
            _ = plt.imshow(img, cmap="gray")
            _ = ax.set_title("Pred: {c:s}, Class: {t:s}".format(c=pred, t=digit
))
```

In [12]:
```
plot_problem_digits( problem_digits )
```



- Now that you can visualize the "problems", can you think of ways to improve the prediction ?

Detailed metrics for clasification

Note For simplicity we will illustrate with binomial classification.

To expand to multinomial: just consider "one versus all" binary classifiers.

Accuracy, the fraction of correct predictions.

$$\text{Accuracy} = \frac{\text{number of correct predictions}}{\text{number of predictions}}$$

We can categorize our predictions by comparing actual target with predicted target:

- Correct predictions (Actual == Predicted)
    - for each class (classes called "Positive" and "Negative")
    - True positives (TP)
    - True negatives (TN)
- Incorrect predictions (Actual != Predicted) for each class
    - False Positive (FP)
    - False Negatives(FN)

In pictures:

		Predicted	
		P	**N**
Actual	**P**	*TP*	*FN*
	N	*FP*	*TN*

So

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

- Create a binary classifier for a single MNIST digit

In [13]:
```
def make_binary(digit, y_train, y_test):
    """
    Turn multinomial target into binary target

    Parameters
    ----------
    digit: Character.  Value of digit on which to make target binary: "Is digi
t"/"Is NOT digit"
    y_train, y_test: ndarrays.  Train/test target values

    Returns
    -------
    Tuple (y_train, y_test)
    """
    y_train_d = ( y_train == digit)
    y_test_d  = ( y_test  == digit)

    return  y_train_d, y_test_d

digit = '5'
y_train_d, y_test_d = make_binary(digit, y_train, y_test)
```

In [14]:
```
# Fit the model
mnist_lr_clf.fit(X_train, y_train_d)
cross_val_score(mnist_lr_clf, X_train, y_train_d, cv=3, scoring="accuracy")

from sklearn.model_selection import cross_val_predict

y_train_pred = cross_val_predict(mnist_lr_clf, X_train, y_train_d, cv=3)
```

Out[14]:
```
LogisticRegression(C=0.01, class_weight=None, dual=False, fit_intercept=True,
          intercept_scaling=1, max_iter=100, multi_class='multinomial',
          n_jobs=None, penalty='l2', random_state=None, solver='saga',
          tol=0.1, verbose=0, warm_start=False)
```

Out[14]:
```
array([0.94961008, 0.9280144 , 0.93037215])
```

In [15]:
```
y_scores = cross_val_predict(mnist_lr_clf, X_train, y_train_d, cv=3,
                             method="decision_function")
```

Precision

A metric to tell you the fraction of your Positive predictions that were correct.

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

There is a degenerate case of perfect precision:

- predict "Positive" for only a single, known actual positive
- 100% precision, but you fail to correctly predict most actual positives

Recall, True Positive Rate

aka, Sensitivity

Fraction of Actual Positives that are classified as Positive

$$\text{Recall} = \text{TPR} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

This pushes against Precision by trying to predict more actual positives.

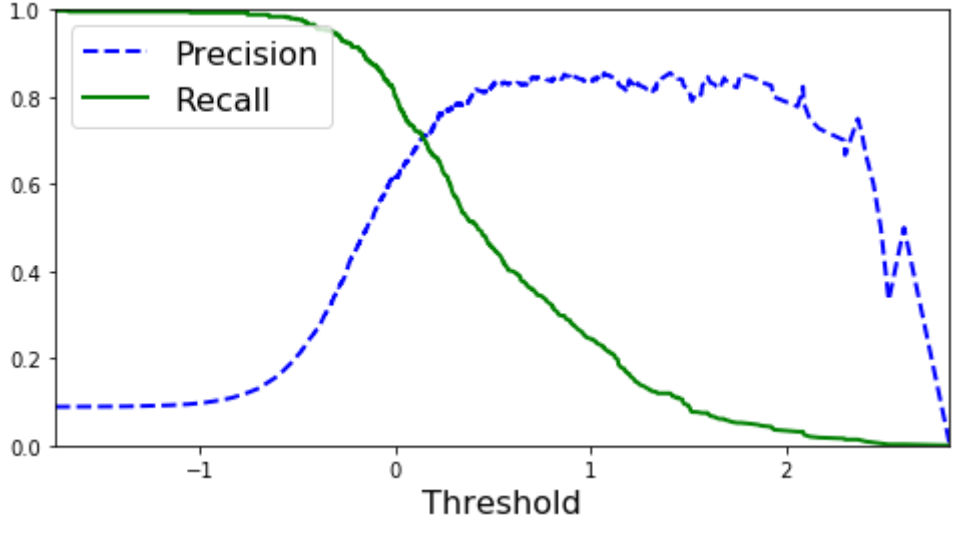
Precison/Recall Tradeoff

In [16]:

```
from sklearn.metrics import precision_recall_curve

precisions, recalls, thresholds = precision_recall_curve(y_train_d, y_scores)

def plot_precision_recall_vs_threshold(precisions, recalls, thresholds):
    _ = plt.plot(thresholds, precisions[:-1], "b--", label="Precision", linewidt
h=2)
    _ = plt.plot(thresholds, recalls[:-1], "g-", label="Recall", linewidth=2)
    _ = plt.xlabel("Threshold", fontsize=16)
    _ = plt.legend(loc="upper left", fontsize=16)
    _ = plt.ylim([0, 1])
```

In [17]:

```
_ = plt.figure(figsize=(8, 4))
plot_precision_recall_vs_threshold(precisions, recalls, thresholds)
_ = plt.xlim([ thresholds.min(), thresholds.max()])

_ = plt.show()
```



Precision vs Recall: which one to favor ?

- Depending on the context, you may favor Precision over Recall, or vice-versa:
    - Favor Precision when a False Positive is undesirable
        - FP: mistakenly tell someone they are in trouble
    - Favor Recall when False Negative is undesirable
        - FN: mistakenly fail to identify a highly-communicable disease

F_1: Another way to combine Precision and Recall

Combines Precision and Recall

$$F_1 = \frac{TP}{TP + \frac{FN+FP}{2}}$$

ROC: Motivation

Recall that, the `LogisticRegression` based classifier converted a score into a probability using the sigmoid function (σ), and based our prediction on whether the probability was above/below a threshhold of 50%:

$$h_\theta(x) = \sigma(s)$$

Probability

$$\hat{p} = h_\theta(x) = \sigma(s)$$

Prediction

$$\hat{y} = \begin{cases} 0 & \text{if } \hat{p} < 0.5 \\ 1 & \text{if } \hat{p} \geq 0.5 \end{cases}$$

- What if we lowered the threshhold ?
    - We would classify more observations as Positive
        - May increase TP (recall) but also FP (decrease precision)
- What if we raised the threshhold ?
    - We would classify fewer observations as Positive
        - May decrease TP (recall) but also FP (increase precision)
        - Degenerate case: identify only a single TP so perfect precision but hardly any recall !

A few more bits of jargon (unfortunate, but ultimately used in the ROC)

Specificity, True Negative Rate

$$\text{Specificity} = \text{TNR} = \frac{\text{TN}}{\text{TN} + \text{FP}}$$

False Positive Rate

$$\begin{aligned} \text{FPR} &= \frac{\text{FP}}{\text{FP+TN}} \\ &= 1 - \text{Sensitivity} \end{aligned}$$

The **ROC** plots the TPR versus the FPR.

We illustrate the ROC by converting the mult-digit MNIST classifier into a binary classifier for a single digit.

- Create a binary classifier for a single MNIST digit
- Plot the ROC

ROC

Plot TPR vs FPR

- Vary the $\hat{p}$ cut-off
    - Compute True Positive Rate and False Positive Rate
    - plot the trade-off
    - 45 degrees line is equal trade-off; want to be above the line
    - ROC curve is the plot of the trade-off

In [18]:

```
from sklearn.metrics import roc_curve

fpr_lr, tpr_lr, thresholds = roc_curve(y_train_d, y_scores)

def plot_roc_curve(ax, fpr, tpr, label=None):
    _ = ax.plot(fpr, tpr, linewidth=2, label=label)
    _ = ax.plot([0, 1], [0, 1], 'k--')
    _ = ax.axis([0, 1, 0, 1])
    _ = ax.set_xlabel('False Positive Rate', fontsize=16)
    _ = ax.set_ylabel('True Positive Rate', fontsize=16)
```

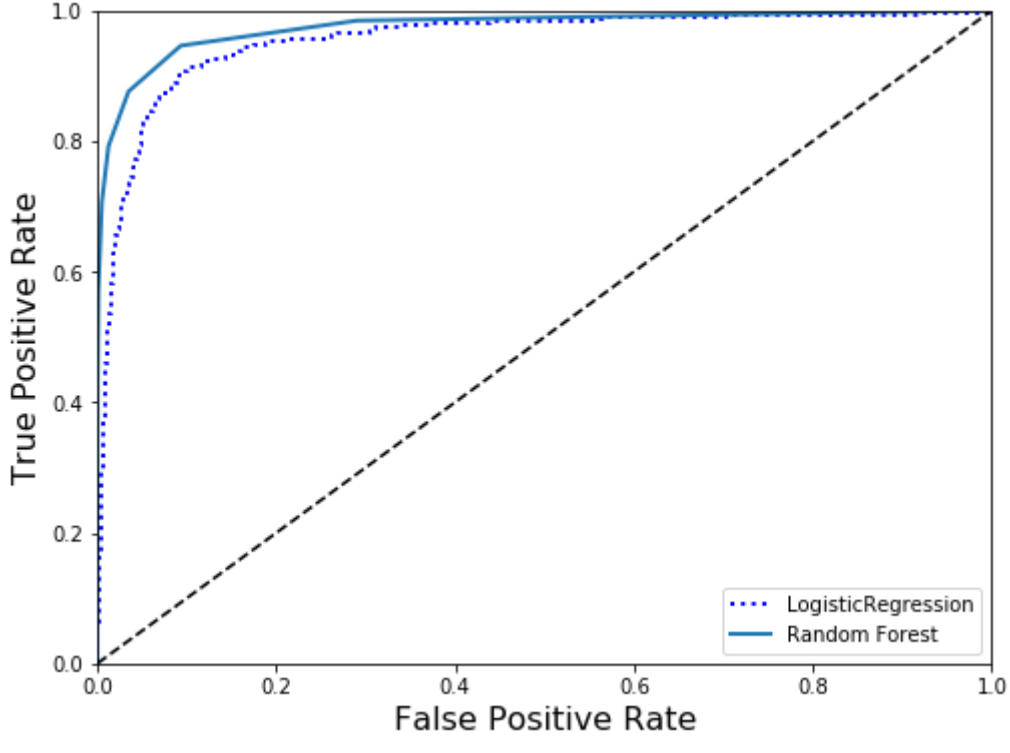
- Let's create a second model for binary classification so we can compare two models
- We will plot the ROC for each model so we can compare
- Goal: High TPR, Low FPR

In [19]:

```
from sklearn.ensemble import RandomForestClassifier
forest_clf = RandomForestClassifier(n_estimators=10, random_state=42)
y_probas_forest = cross_val_predict(forest_clf, X_train, y_train_d, cv=3,
                                    method="predict_proba")

y_scores_forest = y_probas_forest[:, 1] # score = proba of positive class
fpr_forest, tpr_forest, thresholds_forest = roc_curve(y_train_d,y_scores_forest)
```

In [20]:

```
fig = plt.figure(figsize=(8, 6))
ax  = fig.add_subplot(1,1,1)
_ = ax.plot(fpr_lr, tpr_lr, "b:", linewidth=2, label="LogisticRegression")

plot_roc_curve(ax, fpr_forest, tpr_forest, "Random Forest")
_ = ax.legend()
```



AUC

- Compare the ROC curves for two models
- Area under curve: the higher the better
    - choose model with higher AUC (absent any constraints on trade-off)

You can see from the pair of ROC plots that Random Forest has slightly greater AUC

Regression: beyond RMSE/R^2

What is the Regression analog of the confusion matrix for examining errors ?

Examining the residuals.

The assumptins of Linear Regression is that the residuals:

- are normally distributed
- constant variance
- no pattern

Let's go back to our old example from a previous lecture: fitting a straight line to curvy data.

A simple plot of the residuals will show the problem.

n.b., A quantile-quantile (quantile of residual vs quantile of a normal distribution) plot can also be used

In [21]:

```
# %load recipe_regress.py
def plot_fit(X, y, ax=ax, on_idx=0):
    """
    Plot the fit

    Parameters
    ----------
    X: ndarray of features
    y: ndarray of targets
    ax: a matplotlib axes pbject (matplotlib.axes._subplots.AxesSubplot)

    Optional
    --------
    on_idx: Integer.  Which column of X to use for the horizontal axis of the pl
ot

    """
    sort_idx = X[:, on_idx].argsort()
    X_sorted = X[ sort_idx,:]
    y_sorted = y[ sort_idx,:]

    _ = ax.plot(X_sorted[:, on_idx] , y_sorted, color="red")

def transform(X):
    """
    Add a column to X with squared values

    Parameters
    ----------
    X: ndarray of features
    """
    X_p2 = np.concatenate( [X, X **2], axis=1)
    return X_p2

def run_regress(X,y, run_transforms=False):
    """
```

```
    Do the full pipeline of the regression of y on X

    Parameters
    ----------
    X: ndarray of features
    y: ndarray of targets

    Optional
    --------
    runTransforms: Boolean.  If True, run additional data transformations to cre
ate new features
    """
    X_train, X_test, y_train, y_test = split(X,y)

    # Transform X's
    if (run_transforms):
        X_train = transform(X_train)
        X_test  = transform(X_test)

    # Create linear regression object
    regr = linear_model.LinearRegression()

    # Train the model using the training sets
    _ = regr.fit(X_train, y_train)

    # The coefficients
    print('Coefficients: \n', regr.intercept_, regr.coef_)
    # Lots of predictions: predict on entire test set
    y_pred = regr.predict(X_test)

    # Explained variance score: 1 is perfect prediction
    print("R-squared (test): {:.2f}".format(r2_score(y_test, y_pred)) )

    y_pred_train = regr.predict(X_train)
    print("R-squared (train): {:.2f}".format(r2_score(y_train, y_pred_train)) )

    # Plot predicted ylabel (red) and true label (black)
    fig = plt.figure()
```

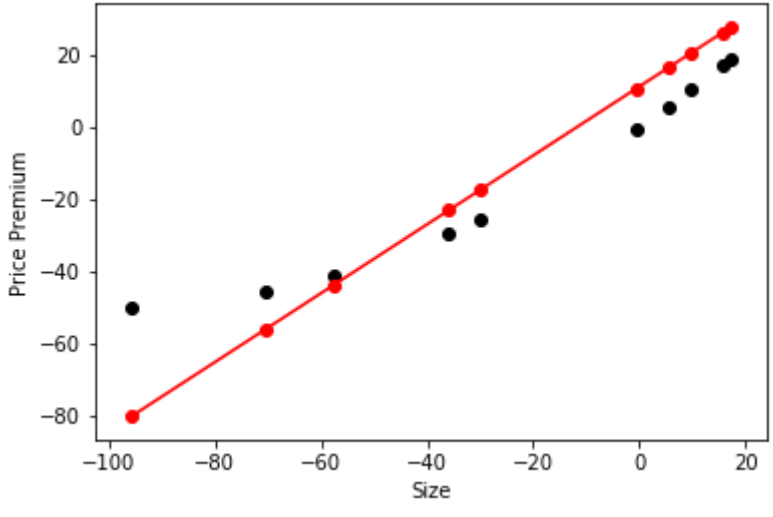
```
    ax  = fig.add_subplot(1,1,1)

    _ = ax.scatter(X_test[:,0], y_test, color='black')
    _ = ax.scatter(X_test[:,0], y_pred, color="red")

    # _ = ax.plot(X_test[:,0], y_pred, color="red")
    plot_fit(X_test, y_pred, ax=ax, on_idx=0)
    _ = ax.set_xlabel(xlabel)
    _ = ax.set_ylabel(ylabel)

    return

def plot_resid(X, y, y_pred):
    resid_curve = y - y_pred
    fig = plt.figure()
    ax  = fig.add_subplot(1,1,1)
    ax.scatter(X, resid_curve)
    _ = ax.set_xlabel(xlabel)
    _ = ax.set_ylabel("Residual")
```

In [22]:

```
from sklearn import datasets, linear_model
from sklearn.metrics import mean_squared_error, r2_score

import gen_data as gd
%aimport gen_data

(xlabel, ylabel) = ("Size", "Price Premium")
v1, a1 = 1, .005
v2, a2 = v1, a1*2
X_curve, y_curve = gd.gen_data(num=50, v=v2, a=a2)

from sklearn.model_selection import train_test_split
X_curve_train, X_curve_test, y_curve_train, y_curve_test = train_test_split(X_cu
rve, y_curve,
                                                                             test
_size=0.20, random_state=42)

# Create linear regression object
regr = linear_model.LinearRegression()

# Train the model using the training sets
_ = regr.fit(X_curve_train, y_curve_train)

# The coefficients
print('Coefficients: \n', regr.intercept_, regr.coef_)
# Lots of predictions: predict on entire test set
y_curve_pred = regr.predict(X_curve_test)

# Explained variance score: 1 is perfect prediction
print("R-squared (test): {:.2f}".format(r2_score(y_curve_test, y_curve_pred)) )

y_curve_pred_train = regr.predict(X_curve_train)
print("R-squared (train): {:.2f}".format(r2_score(y_curve_train, y_curve_pred_tr
ain)) )

# Plot predicted ylabel (red) and true label (black)
```

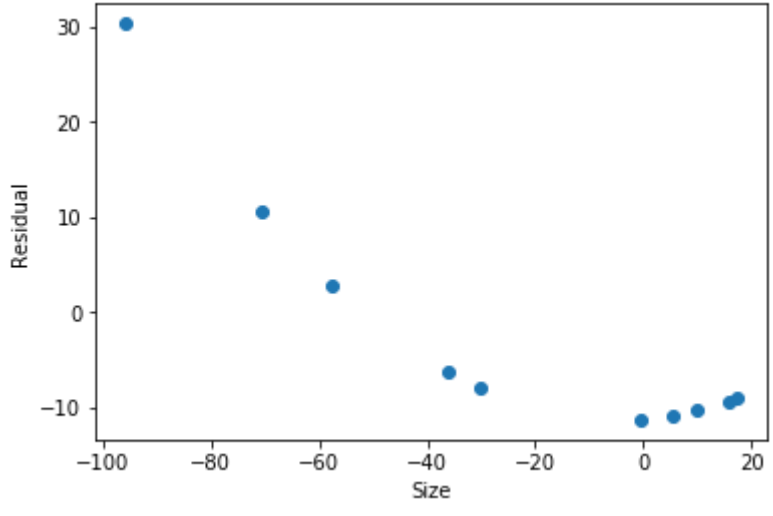
```
fig = plt.figure()
ax  = fig.add_subplot(1,1,1)

_ = ax.scatter(X_curve_test[:,0], y_curve_test, color='black')
_ = ax.scatter(X_curve_test[:,0], y_curve_pred, color="red")

# _ = ax.plot(X_test[:,0], y_pred, color="red")
plot_fit(X_curve_test, y_curve_pred, ax=ax, on_idx=0)
_ = ax.set_xlabel(xlabel)
_ = ax.set_ylabel(ylabel)
```

```
Coefficients:
 [11.25338949] [[0.95652077]]
R-squared (test): 0.75
R-squared (train): 0.92
```



Let's plot the residuals of fitting a straight line to curvy data

In [23]:
```
plot_resid(X_curve_test, y_curve_test, y_curve_pred)
```



Not good !

- clear pattern: errors increase in the tails
- not constant variance

Recall that our conclusion was that there was a missing feature: a higher order x^2 term.

Once we added that term, the target became linear in

$$\Theta^T \cdot X = \beta_1 * x + \beta_2 * x^2$$

What is a ”good” value for the performance metric

Consider the Accuracy Performance Metric applied to the MNIST classification problem

- Is 50% accuracy good for the 10-digit classifier ?
- Is 50% accuracy good for a single-digit (binary) classifier ?

One way to evaluate our model is to set up an extremely simple model as our "baseline" and compare our model's statistics to the baseline model.

Some baseline models for classification

Most baseline classifiers choose a value from the Train target dataset `y_train` as the prediction. The choice depends on the strategy

- Uniform
    - choose target from `y_train` using uniform random
- Most Frequent
    - choose target from `y_train`that occurs with highest frequency
- Stratified
    - choose target from `y_train` using distribution of `y_train`
- Constant
    - ignore `y_train`; return a constant

In [24]:

```
from sklearn.dummy import DummyClassifier

strats = { "stratified": {},
           "uniform": {},
           "constant": {"constant": True}
         }

plt_num = 1

# Compute Accuracy for various baseline classifiers
for strat, args in strats.items():
    dmy_clf = DummyClassifier(strategy=strat, **args)
    acc_scores_dmy = cross_val_score(dmy_clf, X_train, y_train_d, cv=3, scoring=
"accuracy")

    print("{s}: Accuracy = {a:.2f}".format(s=strat, a=acc_scores_dmy.mean()))
```

```
stratified: Accuracy = 0.84
uniform: Accuracy = 0.50
constant: Accuracy = 0.09
```

Digression: R^2 and the mean baseline model

$$
\begin{aligned}
R^2 &= 1 - \left(\frac{\sum_{i=1}^{m} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{m} (y_i - \bar{y}_i)^2} \right) \\
&= 1 - \left(\frac{m \cdot \text{RMSE}(\hat{y}, y)^2}{\sum_{i=1}^{m} (y_i - \bar{y}_i)^2} \right)
\end{aligned}
$$

Compares the MSE Performance Metric of a model to a baseline model that makes a constant prediction of the mean, $\bar{y}$

Fixing/Improving a model

A deeper look at individual errors may have revealed a problem.

- What can we do ?
    - Throw away the model
    - Add features
    - Transform features
    - don't try to fit a square peg (non-linear target) into a round hole (linear model)

Adding features

LinearRegression on our ”curvy” data set: adding a polynomial feature

Examining the errors of `LinearRegression` on the "curvy" data set showed a pattern and suggested a fix

- add polynomial features

Lessons

- Don't try to fit a square peg in a round hole
    - Simple linear model doesn't fit curvy data
    - Adding a feature makes the data linear (explain) in the new features

The plot of residual errors also revealed an even bigger problem: *Violation of assumptions* of Linear Regression

- residuals are normal
- residuals are homeskedatic: constant variance
    - bigger residuals in tails

So forcing a square peg into a round hole is not only not productive, it can be just plain wrong !

Lesson Understand the requirements of your model and use it appropriately.

This is *not* a course on linear regression (highly recommend that you learn though !) But it is a "go-to" model so we will try to find time to do a deeper dive on Linear Regression in the next lesson.

Cross Features

- categorical
    - for each observation, create a True/False depending on pairs of features

Transforming data (preview)

Another way to fix/improve your model is by data transformations.

There are many transformations and we will introduce a few in the next section.

But, as motivation:

- For a Linear model:
    - can you take a relationship that is not completely linear and make it more linear ?
        - Titanic: is survival probability linear in Age ?
- For a model that wants normality
    - if the data is log-normal: take the log the the data
        - e.g. returns in Finance

Right now you only know 2 types of Regression models. We'll digress and introduce another model, which is useful in its own right, but will also motivate one type of transformation.

-

K Nearest Neighbors: you are known by the company you keep

K Nearest Neighbors is a model that can be used for both Classification and Regression problems. The concept is very simple: to make a prediction for feature vector x:

- Rank each observation in the Training Set by how "similar" its features are to x
- Choose the k closest observations
- Prediction for x: the average of the targets for the k observations closest to x
    - Classification: most frequent target among the k targets
    - Regression: average across the k targets

- Manifold Hypothesis
    - you are known by the neighbors you keep
- Applies even if you don't understand the features
- To predict given an observation with feature vector x:
    - compute "distance" between x and each $x^{(i)}$ in the training set X
        - let $d^{(i)}$ denote distance between x and $x^{(i)}$
    - Let C be the sequence of observations $(x^{(i)}, y^{(i)})$ in increasing order of $d^{(i)}$
    - prediction: the average of $\{y^{(i)} | i \in C[0:k]\}$

Measures of similarity

Euclidean distance

$$||A||^2 = A \cdot A$$

so

$$||A|| = \sqrt{A \cdot A}$$

$$\text{dist}(A, B) = A \cdot B$$

Cosine similarity of two vectors

$$\text{sim}(A, B) = \cos(\theta) = \frac{A \cdot B}{||A|| \times ||B||}$$

So cosine similarity is distance of normalized $A = \frac{A}{||A||}$ and normalized $B = \frac{B}{||B||}$

The difference between Euclidean and Cosine similarity is analagous to the difference between Covariance and Correlation from statistics

- Covariance is unscaled
- Correlation is normalized
- Correlation can be shown to be the covariance of standardized variables

For zero mean A, B:

$$\begin{aligned}
\operatorname{cov}(A, B) &= \frac{1}{m} \times A \cdot B \\
\operatorname{corr}(A, B) &= \frac{\frac{1}{m} \times A \cdot B}{\frac{1}{\sqrt{m}} \times ||A|| \times \frac{1}{\sqrt{m}} \times ||B||} \\
&= \frac{A \cdot B}{||A|| \times ||B||}
\end{aligned}$$

Note In the above, A, B are *vectors* (one point in m dimensions) whereas below, A, B are each *sequences* of m scalars (i.e, m one-dimensional points)

So $\mathrm{corr}(A, B)$ is covariance of normalized $A = \frac{A}{||A||}$ and normalized $B = \frac{B}{||B||}$

And

$$\mathrm{corr}(A, B) = \cos(\theta)$$

see (http://people.sju.edu/~pklingsb/dot.cov.pdf)

Example

In [25]:
```
def stretch_ds(ds, mag):
    """
    Stretch a dataset by scaling the features

    Parameters
    ----------
    ds: Tuple (X,y)
    - X are the features, y are the targets
    -- X: ndarray.   Two dimensional

    mag: ndarray. One dimensional.  Length matches second dimension of X

    Returns
    --------
    Xprime: ndarray
    - same dimension as X
    - each column of X is multiplied by the corresponding magnitude in mag

    """
    (X, y) = ds
    Xprime = X * mag

    return (Xprime, y)
```

In [26]:

```
# Code source: Gaël Varoquaux
#              Andreas Müller
# Modified for documentation by Jaques Grobler
# License: BSD 3 clause

import numpy as np
import matplotlib.pyplot as plt
from matplotlib.colors import ListedColormap
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.datasets import make_moons, make_circles, make_classification
from sklearn.neural_network import MLPClassifier
from sklearn.neighbors import KNeighborsClassifier
from sklearn.svm import SVC
from sklearn.gaussian_process import GaussianProcessClassifier
from sklearn.gaussian_process.kernels import RBF
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import RandomForestClassifier, AdaBoostClassifier
from sklearn.naive_bayes import GaussianNB
from sklearn.discriminant_analysis import QuadraticDiscriminantAnalysis

h = .02  # step size in the mesh

names = ["Nearest Neighbors",
         "Decision Tree", "Random Forest"]

classifiers = [
    KNeighborsClassifier(3),
    DecisionTreeClassifier(max_depth=5),
    RandomForestClassifier(max_depth=5, n_estimators=10, max_features=1),
    ]

cm = plt.cm.RdBu
cm_bright = ListedColormap(['#FF0000', '#0000FF'])

def plot_scatter(ax, X, X_train, X_test,  y_train, y_test, ds_cnt):
```

```
    x_min, x_max = X[:, 0].min() - .5, X[:, 0].max() + .5
    y_min, y_max = X[:, 1].min() - .5, X[:, 1].max() + .5

    xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                         np.arange(y_min, y_max, h))

    # just plot the dataset first

    if ds_cnt == 0:
        ax.set_title("Input data")

    # Plot the training points
    _= ax.scatter(X_train[:, 0], X_train[:, 1], c=y_train, cmap=cm_bright,
               edgecolors='k')
    # Plot the testing points
    _= ax.scatter(X_test[:, 0], X_test[:, 1], c=y_test, cmap=cm_bright, alpha=
0.6,
               edgecolors='k')
    _= ax.set_xlim(xx.min(), xx.max())
    _= ax.set_ylim(yy.min(), yy.max())
    #_= ax.set_xticks(())
    #_= ax.set_yticks(())

    _ = ax.set_xlabel("Feature 1")
    _ = ax.set_ylabel("Feature 2")

    return (xx, yy)

def plot_countour(ax, Z, X_train, X_test, y_train, y_test, xx, yy, name, score,
ds_cnt):
    # Put the result into a color plot
    Z = Z.reshape(xx.shape)
    _= ax.contourf(xx, yy, Z, cmap=cm, alpha=.8)

    # Plot the training points
    _= ax.scatter(X_train[:, 0], X_train[:, 1], c=y_train, cmap=cm_bright,
               edgecolors='k')
    # Plot the testing points
```

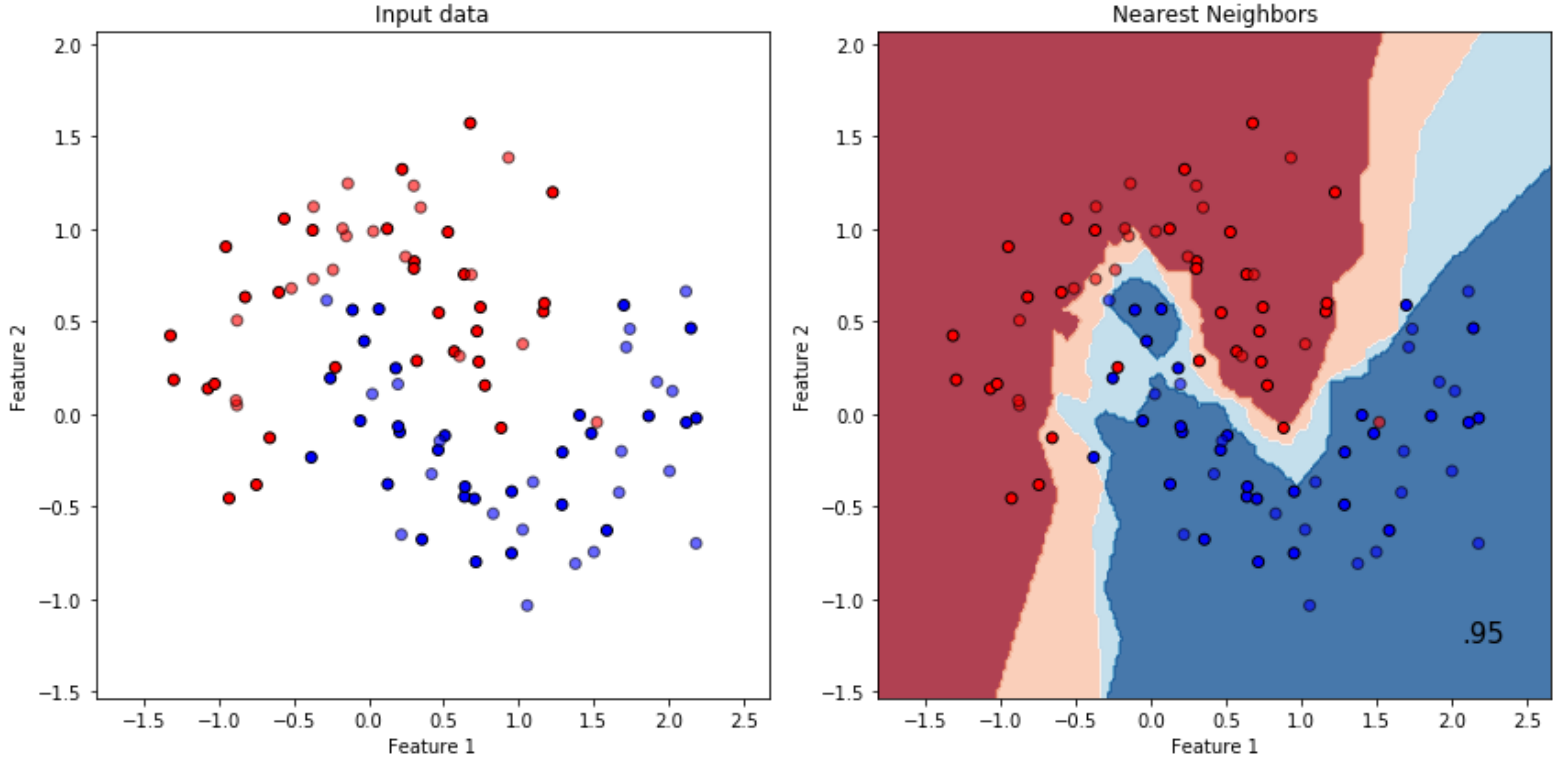
```
    _= ax.scatter(X_test[:, 0], X_test[:, 1], c=y_test, cmap=cm_bright,
               edgecolors='k', alpha=0.6)

    _= ax.set_xlim(xx.min(), xx.max())
    _= ax.set_ylim(yy.min(), yy.max())
    #_= ax.set_xticks(())
    #_= ax.set_yticks(())

    _ = ax.set_xlabel("Feature 1")
    _ = ax.set_ylabel("Feature 2")

    if ds_cnt == 0:
        _= ax.set_title(name)
    _= ax.text(xx.max() - .3, yy.min() + .3, ('%.2f' % score).lstrip('0'),
            size=15, horizontalalignment='right')
```

In [27]:

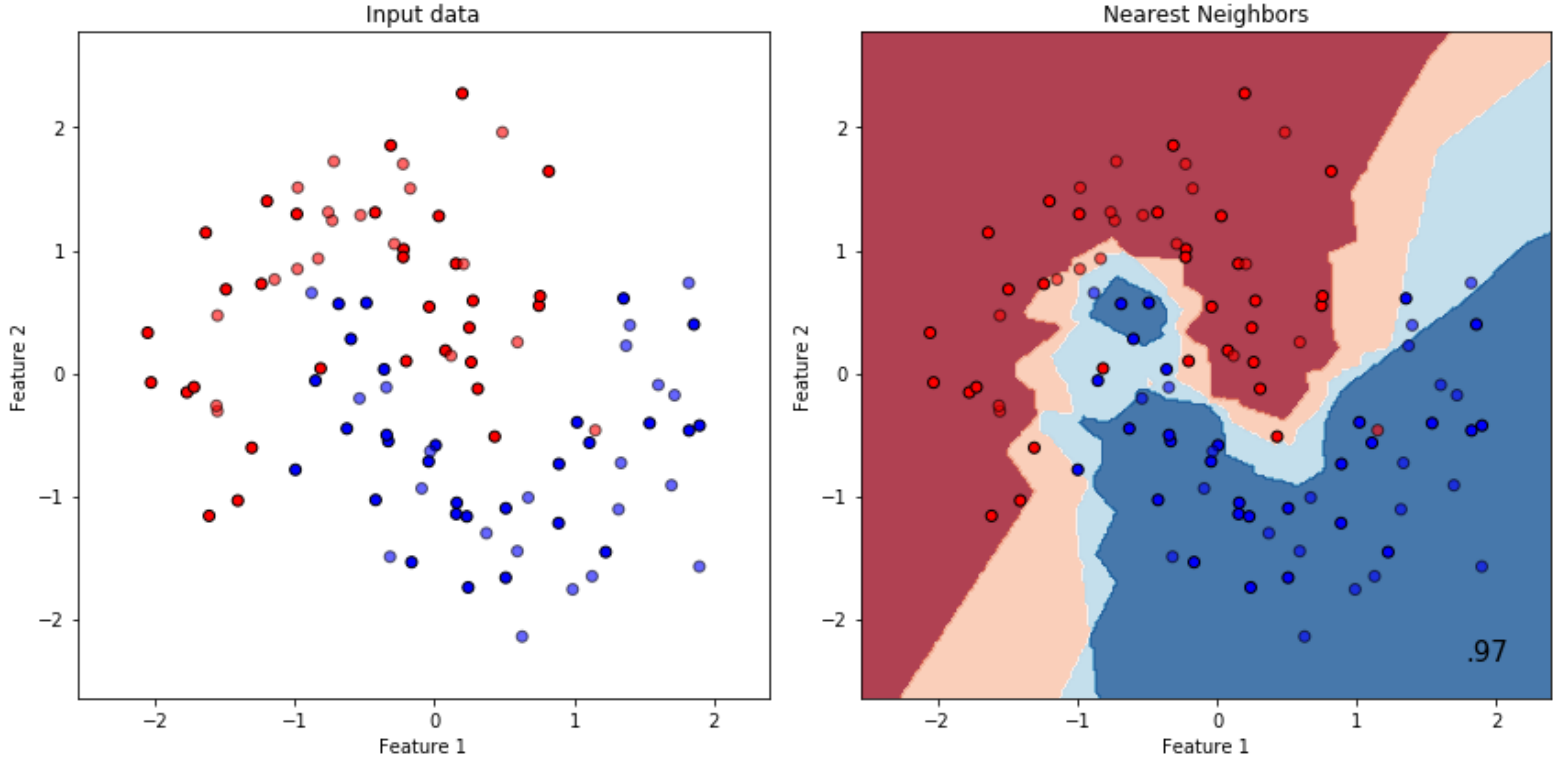
```
def plot_classifiers(names, classifiers, num_samples=100, scale=True, num_ds=1):
    X, y = make_classification(n_features=2, n_redundant=0, n_informative=2,
                               random_state=1, n_clusters_per_class=1)
    rng = np.random.RandomState(2)
    X += 2 * rng.uniform(size=X.shape)
    linearly_separable = (X, y)

    moons_ds = make_moons(noise=0.3, random_state=0, n_samples=num_samples)

    datasets = [ moons_ds,
                 stretch_ds(moons_ds, np.array([10,1])),
                 make_circles(noise=0.2, factor=0.5, random_state=1, n_samples=nu
m_samples),
                 linearly_separable
                 ]

    # Short version: limit classifiers and datasets to num_ds
    names, classifiers, datasets = [ a[:num_ds] for a in [names, classifiers, d
atasets] ]
    figure = plt.figure(figsize=(12,6))
    i = 1
    # iterate over datasets
    for ds_cnt, ds in enumerate(datasets):
        ax = plt.subplot(len(datasets), len(classifiers) + 1, i)

        # preprocess dataset, split into training and test part
        X, y = ds

        # CHEATING ALERT: scaling BEFORE train/test split so info from test leak
s into train
        if scale:
            X = StandardScaler().fit_transform(X)

        X_train, X_test, y_train, y_test = \
            train_test_split(X, y, test_size=.4, random_state=42)
```

```
        xx, yy = plot_scatter(ax, X, X_train, X_test,  y_train, y_test, ds_cnt)
        i += 1

        # iterate over classifiers
        for name, clf in zip(names, classifiers):
            ax = plt.subplot(len(datasets), len(classifiers) + 1, i)
            clf.fit(X_train, y_train)
            score = clf.score(X_test, y_test)

            # Plot the decision boundary. For that, we will assign a color to ea
ch
            # point in the mesh [x_min, x_max]x[y_min, y_max].
            if hasattr(clf, "decision_function"):
                Z = clf.decision_function(np.c_[xx.ravel(), yy.ravel()])
            else:
                Z = clf.predict_proba(np.c_[xx.ravel(), yy.ravel()])[:, 1]

            plot_countour(ax, Z, X_train, X_test, y_train, y_test, xx, yy, name
, score, ds_cnt)
            i += 1

    plt.tight_layout()
    return (names, classifiers, datasets)
```

In [28]:
```
_= plot_classifiers(names, classifiers, scale=False)
```

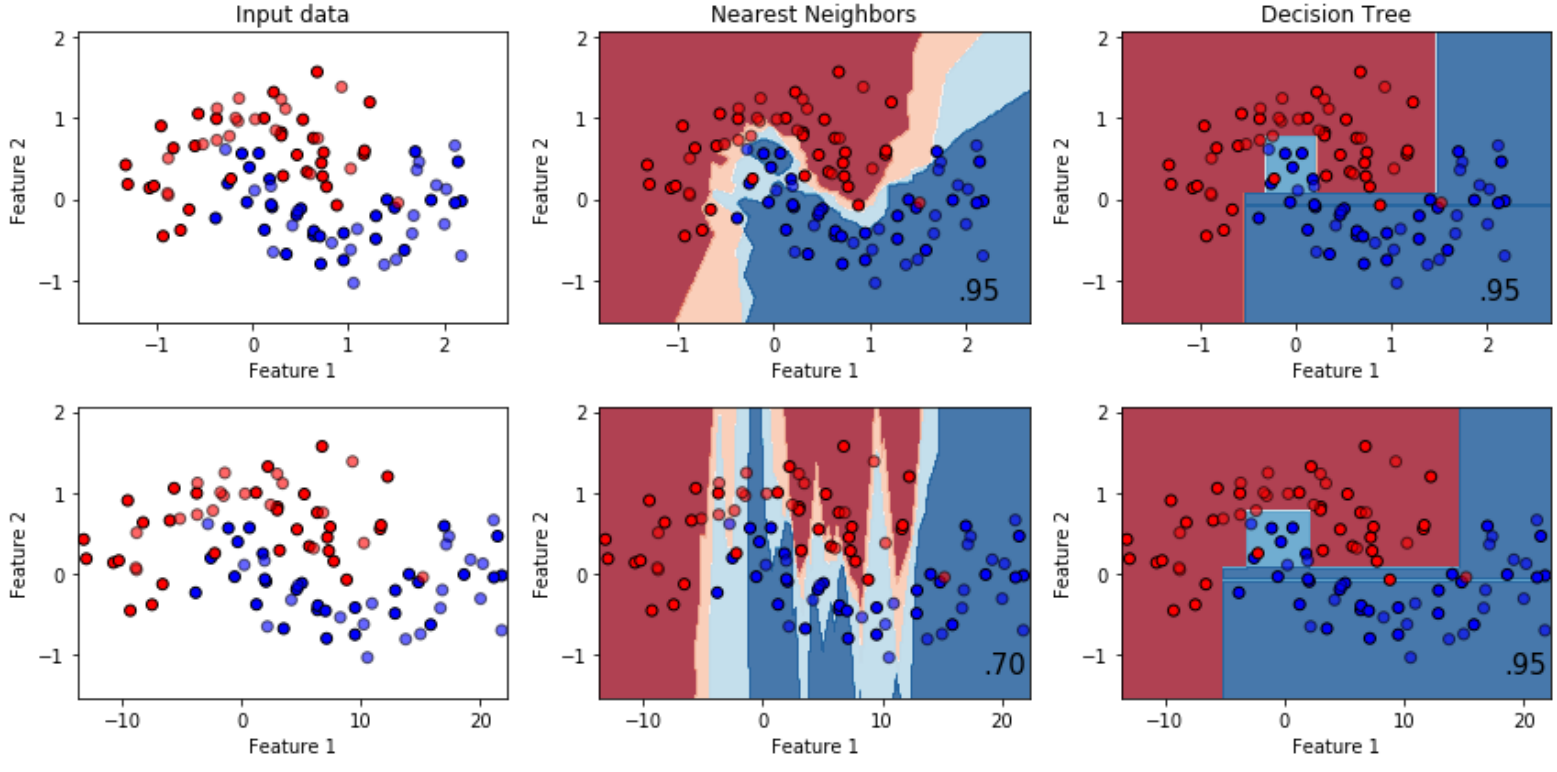


In [29]:
```
_ = plot_classifiers(names, classifiers, scale=True)
```



- What happens if the two features are **not** on the same scale
- Why do the plots of the unstretched/stretched datasets look the same ?
    - plot package is scaling the axis to improve display !
- Drastically different KNN classification
    - score decreases quite a bit
- Decision tree classifier doesn't seem to care

In [30]:
```
_ = plot_classifiers(names, classifiers, scale=False, num_ds=2)
```



- Why did stretching Feature 1 matter for KNN with no scaling ?
    - Look at Euclidean distance measure
    - What did scaling accomplish ?

Transformations

Having seen the effect of features with different scales on one classifier (KNN), we have sufficient motivation for our first class of transformations

Note that transformations may be applied

- to features
- to targets
- to both features and targets

Caveats on transformations

- **Remember** If you scale the Train data, you must apply the same transformation to Test data
    - fit on *train only*
- If you transform the target
    - the prediction will be in "transformed" space
    - need a reverse transformation to put transformed target back into "raw" space

Rransformations in sklearn can be

- fit once (to train)
- applied (via the `transform` method) to test
- reversed (via the `inverse_transfoorm` method)

Feature Scaling

Put features on similar scale

- some models are sensitive to feature magnitude

Example KNN

See above. Compare the fit when features are normalized versus when they are not normalized.

Example: Regularization penalty

- if $x_1 \approx 10x_2$, then $\beta_{x_1} = .1\beta_{x_2}$
    - does that make x_1 "less important" because of smaller beta ?
- $\beta_i = \frac{\partial(y)}{\partial x_i}$
    - $\beta_i = y(x+1) - y(x)$
        - a move of 1 is huge for small range x and tiny for huge range x

[Ridge Regression (external/PythonDataScienceHandbook/notebooks/05.06-Linear-Regression.ipynb#Ridge-regression-%28L_2-Regularization%29)]

Penalty is: sum (over parameters) of squared paramter value

$$P = \alpha \sum_{n=1}^{N} \theta_n^2$$

Also known as L_2 regularizer. This tends to push parameters θ_n towards smaller values.

[Lasso Regression (external/PythonDataScienceHandbook/notebooks/05.06-Linear-Regression.ipynb#Lasso-regression-(L_1-regularization))]

Penalty is: sum (over parameters) of parameter's absolute value

$$P = \alpha \sum_{n=1}^{N} |\theta_n|$$

Also know as the L_1 regularizer.

Centering

Transforming a feature to have mean 0.

$$\hat{x}^{(i)} = x^{(i)} - \bar{x}$$

- star rating
- some algos (PCA) need centered data

Normalization

Motivation, examples

- Centering
    - 5 star ratings
        - 1 star very negative, 5 very positive
            - uncentered (1 to 5) makes coefficients harder to interpret (intercept has to handle the centering)
    - incremental effect vs total effect

Standardize (z-score)

$$\hat{x}^{(i)} = \frac{x^{(i)} - \bar{x}}{\sigma_x}$$

MinMax

Covert to $[0, 1]$ range.

$$\hat{x}^{(i)} = \frac{x^{(i)} - \min_x}{\max_x - \min_x}$$

Ratio

- Pooling
    - more than putting on same numeric scale: put on same *logical* scale
    - Put on same basis vs time
        - time-varying data
        - pre/post split
        - drifting data: Price or Income levels (normalize by GDP, Deflator)
    - Put on same basis vs, e.g. units, like currency
        - convert to same currency

- Pooling (continued)
    - Put on same basis vs cross-section
    - Price to return
    - Price/income levels across multiple countries
        - just converting to common currency not enough
        - normalize to GDP, etc

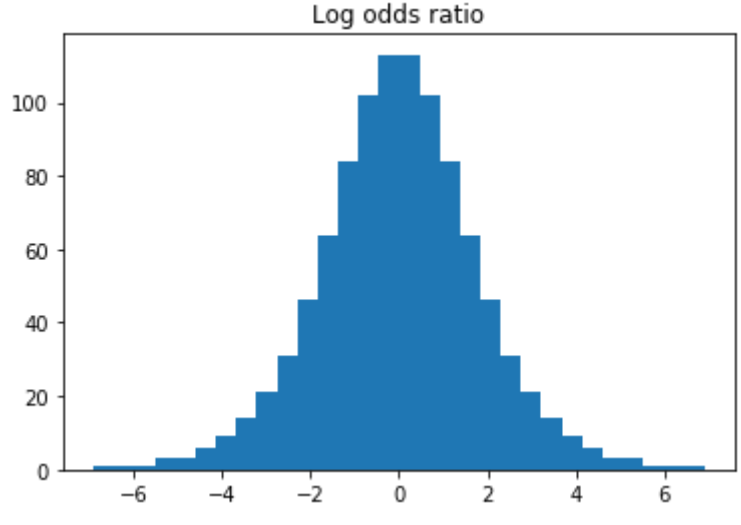
Log transformation

Logistic Regression as Linear Regression with a Log Transformation

- Log of the odds ratio is normally distributed
- So errors are normally distributed and satisfy the assumptions of `LinearRegression`

In [31]:
```
p = np.linspace(0,1, 1000)

# Note: add epsilon to denominator to prevent division by 0
eps = 1e-6
odds = p/(1-p + eps)
log_odds = np.log( odds )

fig, axes = plt.subplots(nrows=1, ncols=1)
ax = axes

# Drop the first/last points b/c they are infinite
_ = ax.hist( np.log(odds)[1:-1], bins=30 )
_ = ax.set_title("Log odds ratio")
```

```
/home/kjp/anaconda3/lib/python3.6/site-packages/ipykernel_launcher.py:6: Runti
meWarning: divide by zero encountered in log

/home/kjp/anaconda3/lib/python3.6/site-packages/ipykernel_launcher.py:12: Runt
imeWarning: divide by zero encountered in log
  if sys.path[0] == '':
```



$$
\begin{aligned}
\frac{\hat{p}}{1-\hat{p}} &= \frac{\frac{1}{1+e^{-s}}}{1-\frac{1}{1+e^{-s}}} \\
&= \frac{\frac{1}{1+e^{-s}}}{\frac{1+e^{-s}-1}{1+e^{-s}}} \\
&= \frac{1}{e^{-s}} \\
&= e^{s}
\end{aligned}
$$

So `LogisticRegression` is really just a `LinearRegression` with a transformed target

$$\log(\frac{\hat{p}}{1 - \hat{p}}) = \Theta^T \cdot x$$

Bucketing/Binning

- Target may be linear in a feature only in broad ranges of the feature
    - income vs age
        - very young (below working age) all income is identical (0)
        - very old (above retirement) - no job related income
    - Latitude/Longitude
        - small changes matter MUCH less than big changes
- Converts numerical feature into categorical
    - or numeric using center of bin

- Equal spaced buckets
- Equal quantile buckets

Lesson Don't fit a square peg (non-linear response) into a round hole (linear model)

Outliers

Pull in extreme values to reduce their influence on the fit.

- Clipping, Winsorization

Missing Values

What can we do about missing values among the features in the Train and Test data sets ?

- Drop the entire observation
    - Loses potentially useful data
- Drop the feature from the entire dataset
    - Lose even more data
- Create a substitute value for the missing feature in an observation

We will explore the latter.

There are some subtitutions that are better than others. Consider the following possible substitutes

- Awful
    - -9999, i.e, some visually outstanding value
    - 0
- Naive
    - mean
    - median
- Predictive

In order to evaluate our options, let's articulate some goals

- Univariate
    - substitute value plausible relative to the distribution of values for the feature
        - mean, median
- Multivariate
    - substitute is plausible in the context of the values for the other features in the observation
        - consider two perfectly negatively correlated features
        - a subsitute that ignores this is less than ideal
- Don't bias the prediction

Your goal is to create a substitute so that you can get *some* value out of the observation without influencing the prediction too much.

Naive methods

Suppose our ML algorithm works (like KNN) using a distance metric.

The following example shows the difference in cosine similarity using 3 different approaches for substitution:

- zero
- mean
- centering, followed by 0

Data:

- Each row is a student
- Each column is the student's rating of a professor (scale 0 to 5)
- KNN will ultimately use the filled-in data to measure similarity of students, based on their ratings

In [32]:

```
import pandas as pd
import numpy as np

S1 = pd.Series( { "a": 4,                "d": 5, "e":1 })
S2 = pd.Series( { "a": 5, "b":5, "c": 4})
S3 = pd.Series( {                        "d": 2, "e": 4, "f": 5})

df = pd.DataFrame( [S1, S2, S3], index=["A", "B", "C"])
df

A = df.loc["A",:]
B = df.loc["B",:]
C = df.loc["C",:]


def sim(A, B):
    """
    Compute cosine similarity of vectors A and B

    Parameters
    -----------
    A, B: ndarrays of same length
    """
    return (A * B).sum()/( np.sqrt( (A*A).sum() ) * np.sqrt( (B*B).sum() ) )

def compare_subs(X, Y):
    """
    Compare various ways of filling in missing values

    Parameters
    ----------
    X, Y: ndarrays of equal length
    """
    (Xp, Yp) = (X.fillna(0), Y.fillna(0))
    print("\tSubstitute 0: similarity= {s:0.2f}".format(s= sim( Xp, Yp )) )
```

```
    # Substitute mean of each student
    (Xp, Yp) = (X.fillna( X.mean() ), Y.fillna( Y.mean() ))
    print("\tSubstitute respective mean: similarity= {s:0.2f}".format(s= sim( Xp
, Yp  )) )

    # Center data, then substitute 0
    # Centered mean tells a different story (b/c of magnitudes of entries ?)
    # n.Y., Cov(X,Y) = E(X*Y) - E(X)E(Y) so is X, Y not centered, dot product is
not Cov(X,Y)
    (Xp, Yp) = ( (X - X.mean()).fillna(0), (Y - Y.mean()).fillna(0) )
    print("\tCenter, then Substitute 0: similarity= {s:0.2f}".format(s= sim( Xp,
Yp  )) )
```

Out[32]:

	a	d	e	b	c	f
A	4.0	5.0	1.0	NaN	NaN	NaN
B	5.0	NaN	NaN	5.0	4.0	NaN
C	NaN	2.0	4.0	NaN	NaN	5.0

In [33]:

```
print("A vs B")
compare_subs(A,B)

print("A vs C")
compare_subs(A,C)
```

```
A vs B
        Substitute 0: similarity= 0.38
        Substitute respective mean: similarity= 0.94
        Center, then Substitute 0: similarity= 0.09
A vs C
        Substitute 0: similarity= 0.32
        Substitute respective mean: similarity= 0.87
        Center, then Substitute 0: similarity= -0.56
```

- A versus B
    - missing values are paired against relatively high values
        - Substituting 0 (a low value) reduces similarity
        - Substituting mean (a relatively high value) increase similarity
            - A is a tougher rater: A.mean() < B.mean()
    - in the end, A and B had only a *single* true point of comparison ("a")
        - you made up the similarity
- A versus C:
    - *NO* professors in common !
    - But at least A and B are closer than A and C for some substitutions

Cosine similarity assumes centered data !

- $Cov(X, Y) = E(X * Y) - E(x) * E(Y)$
- Formula for cosine similarity assumes $E(X) = E(Y) = 0$

Predictive methods for missing values

Prediction from other features that are present

How do we get a substitute value for a feature that is consistent with the values for the other features in the observation ?

Use Machine Learning !

- Create a model to predict a feature x_i from all the other (non-missing) features $\{x_j | j \neq i\}$
    - Regression
    - Clustering (KNN again)

Clustering observations

- create a "distance metric" to measure the proximity of one feature vector to another
    - based on features that are present in both vectors
- to predict the i^{th} feature of observation A (feature $x_i^{(A)}$) that is missing
    - drop feature i from all feature vectors in Train set
    - measure distance from $x^{(A)}$ to all other $x^{(j)}, j \neq A$
    - the k nearest observations to A are it's cohort
        - use an aggregate value for feature i from the cohort as the substitue for $x_i^{(A)}$

Prediction from external featuers

- Create a model to predict a feature x_i from external features that are correlated
- Now-casting
    - derive higher frequency values for low frequency data
        - intra-year GDP
        - intra-month Economic statistics: Employment, Manufacturing
    - National Manufacturing employment may be highly correlated to Employment in a few states
        - state-level employment may be published
            - at higher frequency
            - earlier date
    - Many of these low frequency features are *composites* of other features
        - some elements of the composite are released before others
            - may predict the whole
        - Now-casting site (https://www.now-casting.com/home)

Data Augmentation

In [34]:

```
print("Done")
```

Done