Regression Analysis

CEB Day 3: January 12, 2017

DistrictDataLabs

What makes Scikit-Learn Special?

The Scikit-Learn API

Object-oriented interface centered around the concept of an Estimator:

“An estimator is any object that learns from data; it may be a classification, regression or clustering algorithm or a transformer that extracts/filters useful features from raw data.”

- Scikit-Learn Tutorial

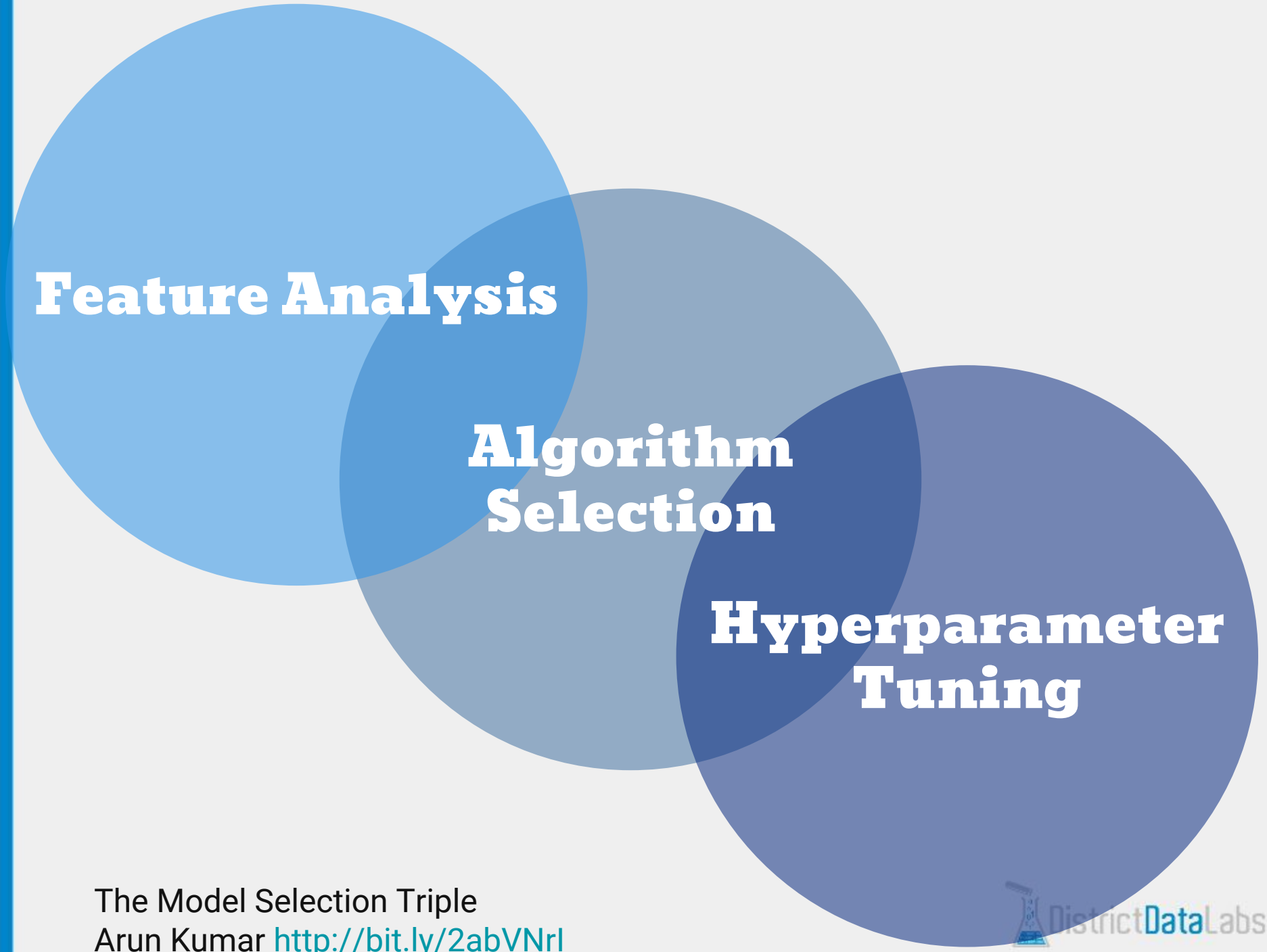
The Scikit-Learn API

```
class Estimator(object):

    def fit(self, X, y=None):
        """
        Fits estimator to data.
        """
        # set state of self
        return self

    def predict(self, X):
        """
        Predict response of X
        """
        # compute predictions pred
        return pred
```

```
class Transformer(Estimator):

    def transform(self, X):
        """
        Transforms the input data.
        """
        # transform X to X_prime
        return X_prime
```

```
class Pipeline(Transfomer):

    @property
    def named_steps(self):
        """
        Returns a sequence of estimators
        """
        return self.steps

    @property
    def _final_estimator(self):
        """
        Terminating estimator
        """
        return self.steps[-1]
```

Buitinck, Lars, et al. "API design for machine learning software: experiences from the scikit-learn project." arXiv preprint arXiv:1309.0238 (2013).



The Model Selection Triple
Arun Kumar http://bit.ly/2abVNrI

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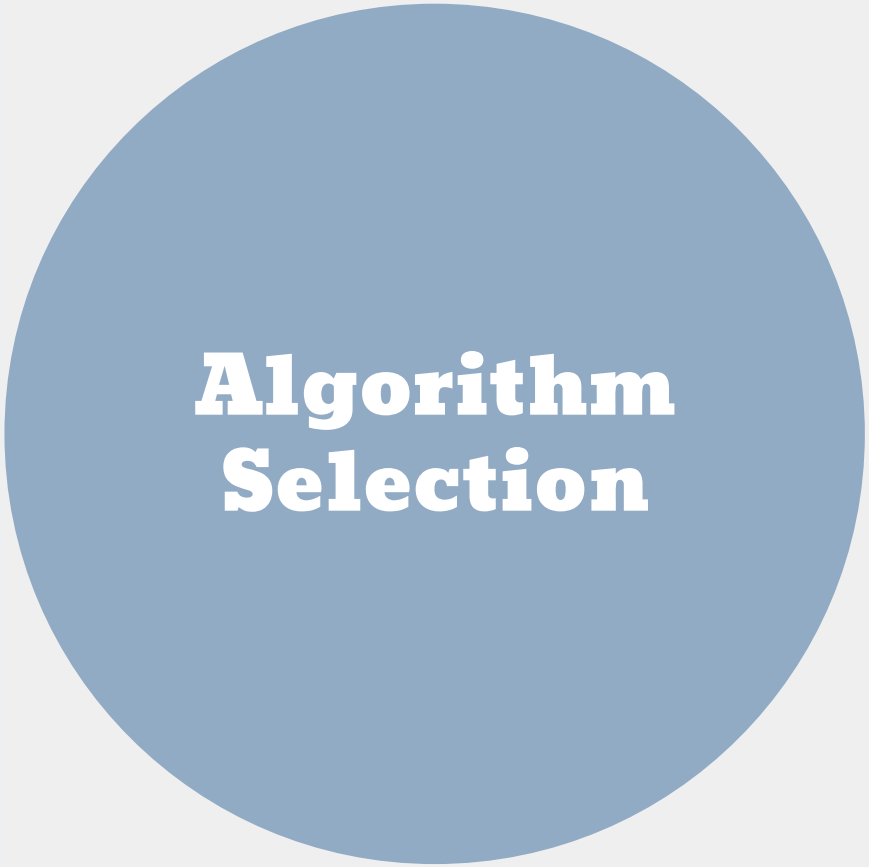
The Model Selection Triple

- Define a bounded, high dimensional feature space that can be effectively modeled.
- Transform and manipulate the space to make modeling easier.
- Extract a feature representation of each instance in the space.

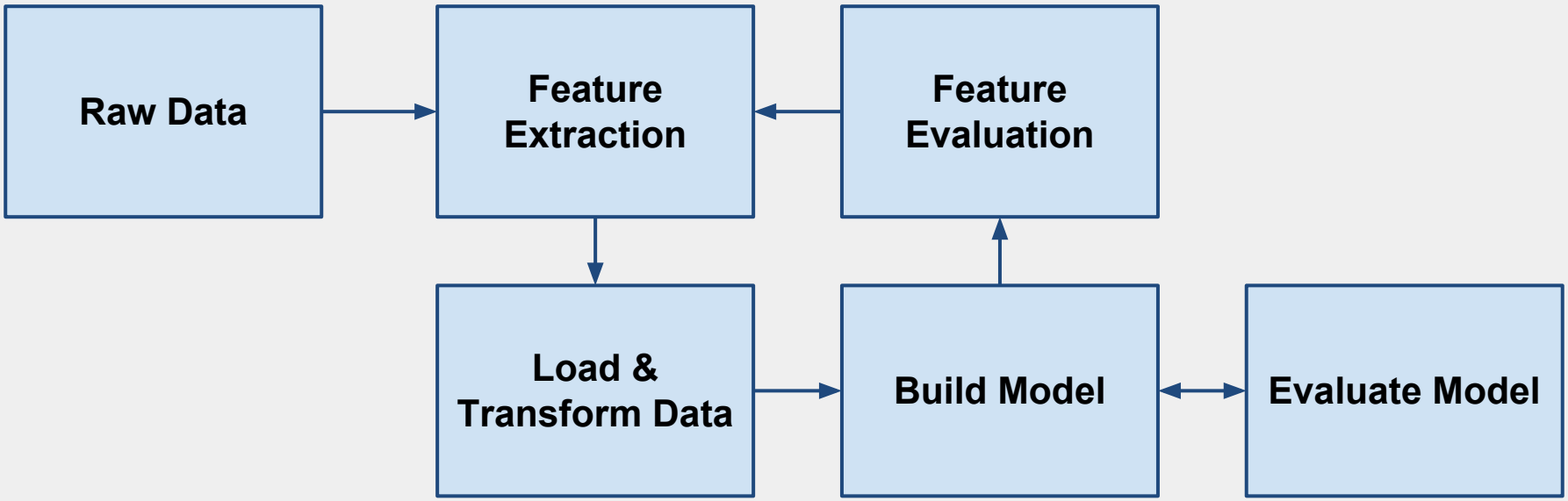
The Model Selection Triple



- Select a model family that best/correctly defines the relationship between the variables of interest.
- Define a model form that specifies exactly how features interact to make a prediction.
- Train a fitted model by optimizing internal parameters to the data.

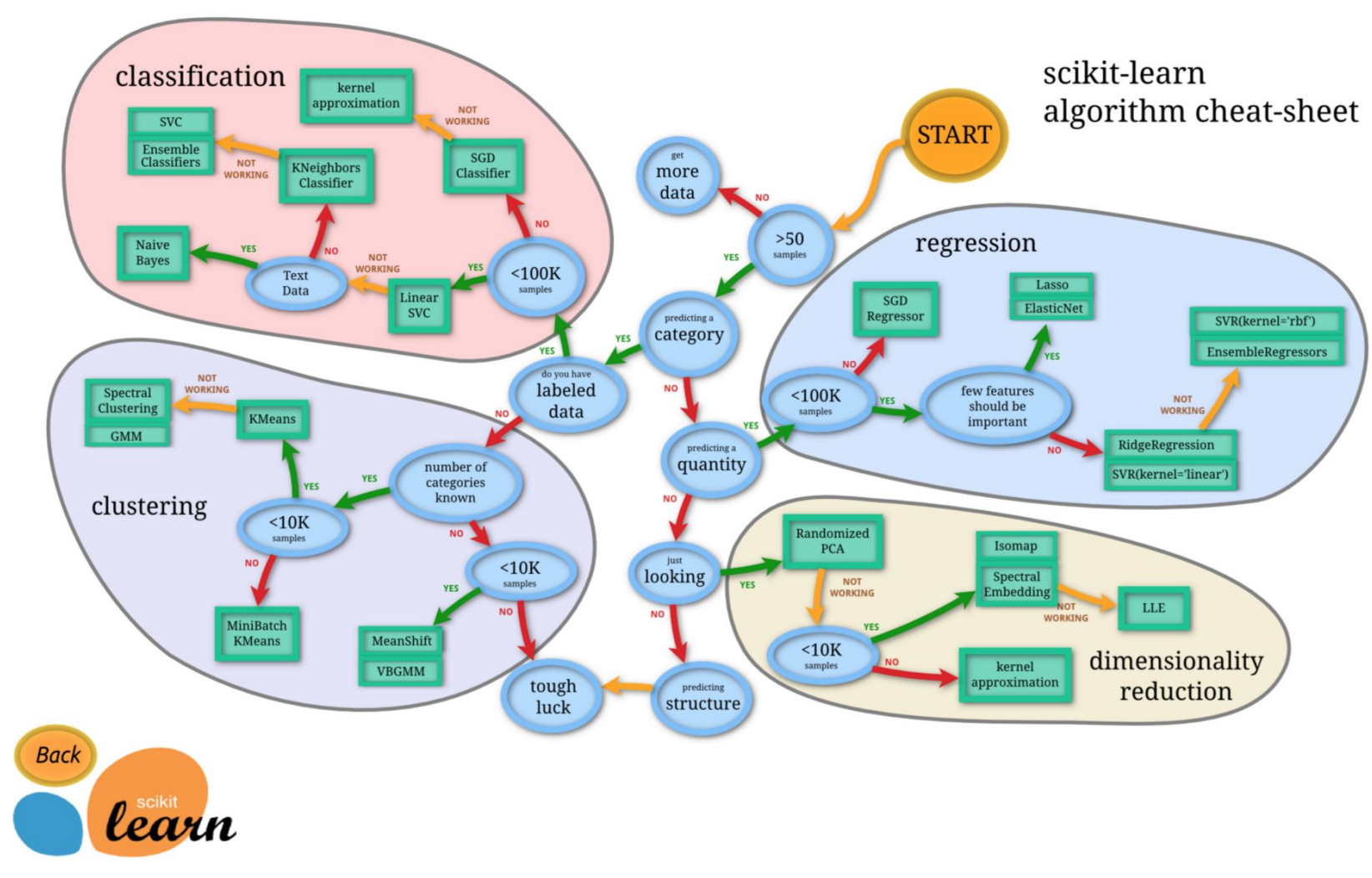
The Model Selection Triple

- Evaluate how the model form is interacting with the feature space.
- Identify hyperparameters (parameters that affect training or the prior, not prediction)
- Tune the fitting and prediction process by modifying these params.



Preliminary Workflow

Choosing the Right Estimator



Scikit-Learn

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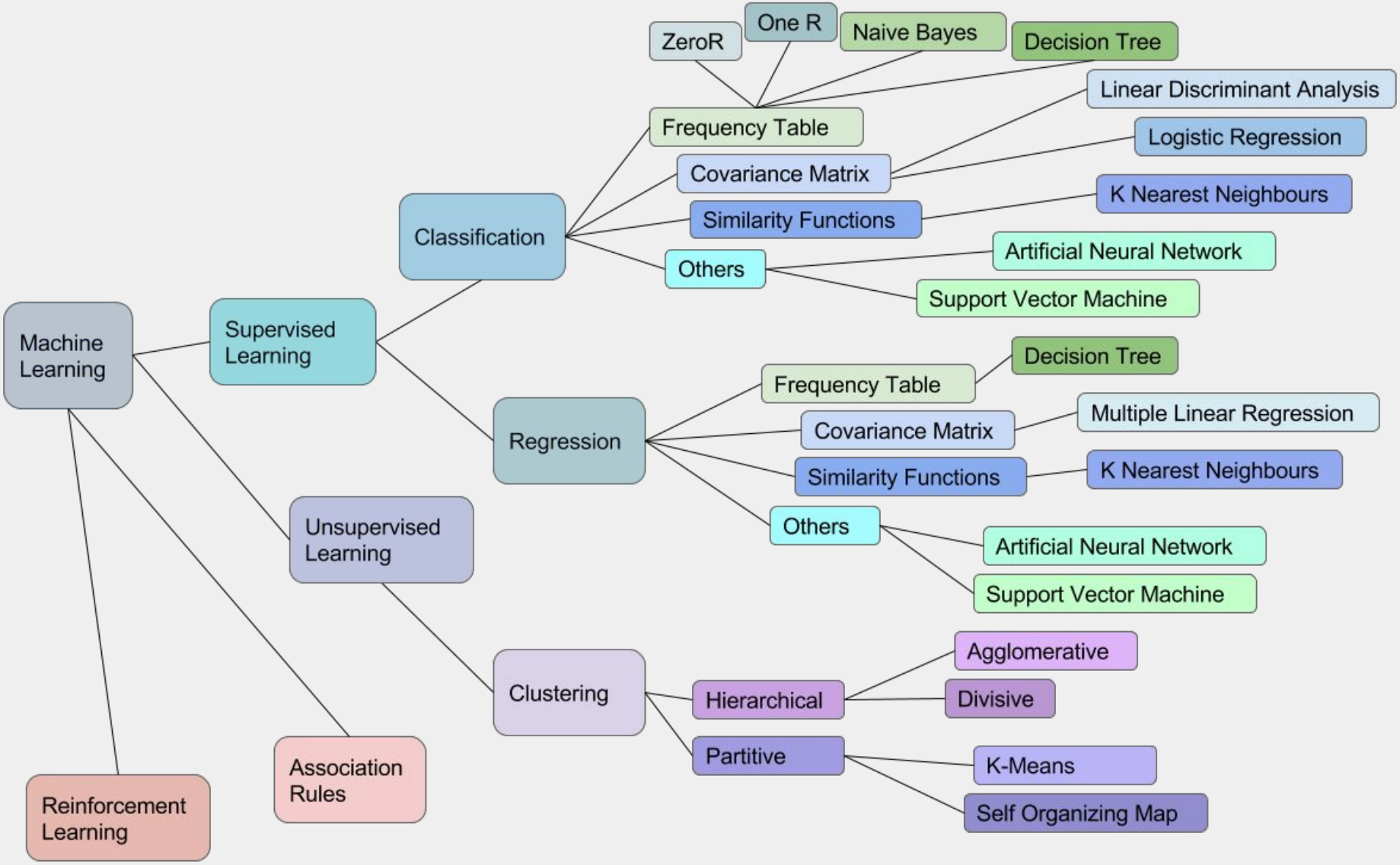

Machine Learning
Supervised Learning
Classification
ZeroR
One R
Naive Bayes
Decision Tree
Frequency Table
Linear Discriminant Analysis
Logistic Regression
Covariance Matrix
K Nearest Neighbours
Similarity Functions
Artificial Neural Network
Others
Support Vector Machine
Regression
Frequency Table
Decision Tree
Multiple Linear Regression
Covariance Matrix
K Nearest Neighbours
Similarity Functions
Artificial Neural Network
Others
Support Vector Machine
Unsupervised Learning
Clustering
Hierarchical
Agglomerative
Divisive
Partitive
K-Means
Self Organizing Map
Association Rules
Reinforcement Learning

Generalized Linear Models

Linear Models

Linear Regression fits a linear model to the data by adjusting a set of coefficients *w* to minimize the residual sum of squares between observed responses & prediction.

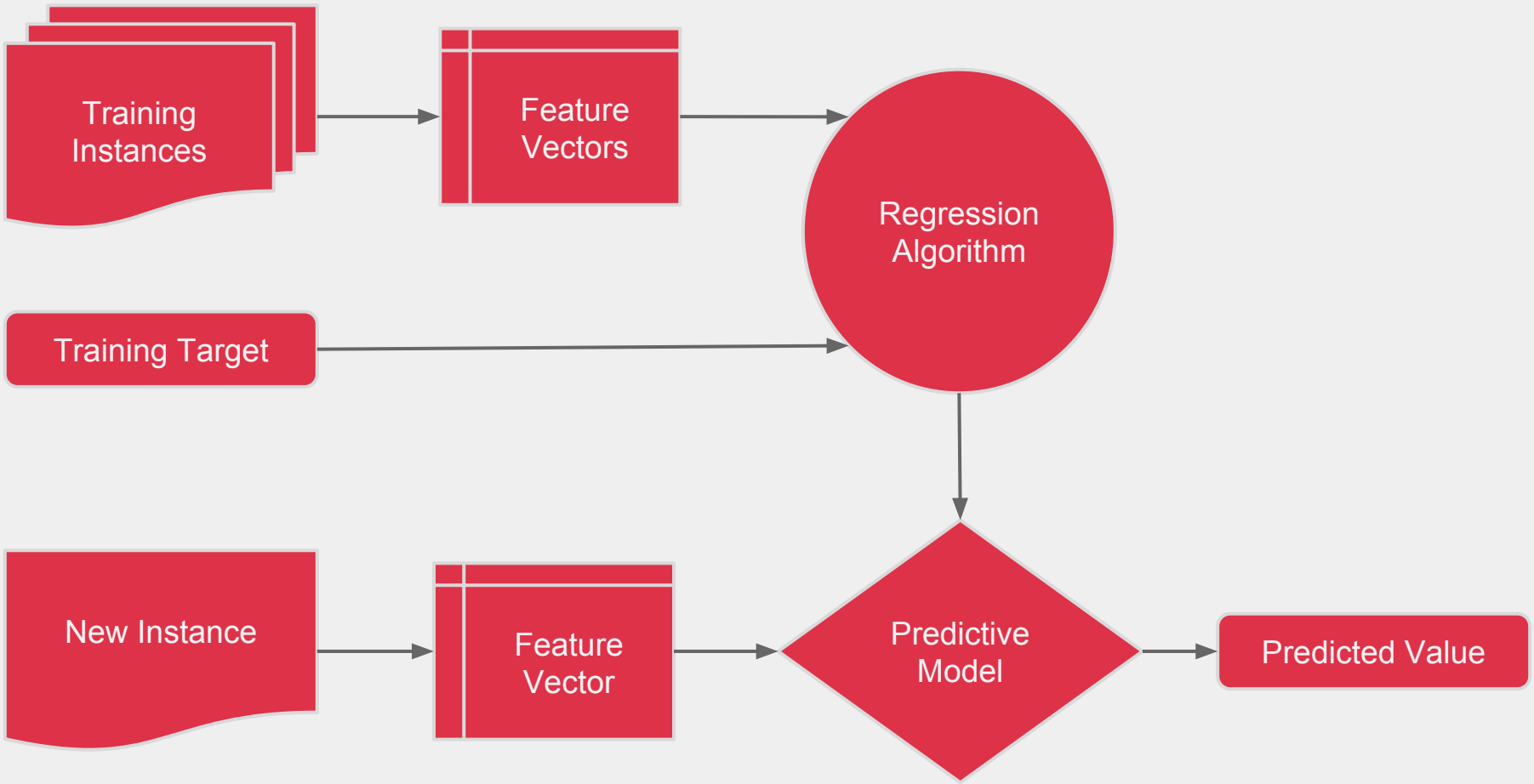
(1) Linear model $$y = X\beta + \epsilon$$

(2) Objective function $$\min_{w} \sum (Xw - y)^2$$

(3) Predictive model $$\hat{y}(w, x) = w_0 + w_1 x_1 + \ldots + w_p x_p$$

Notation:

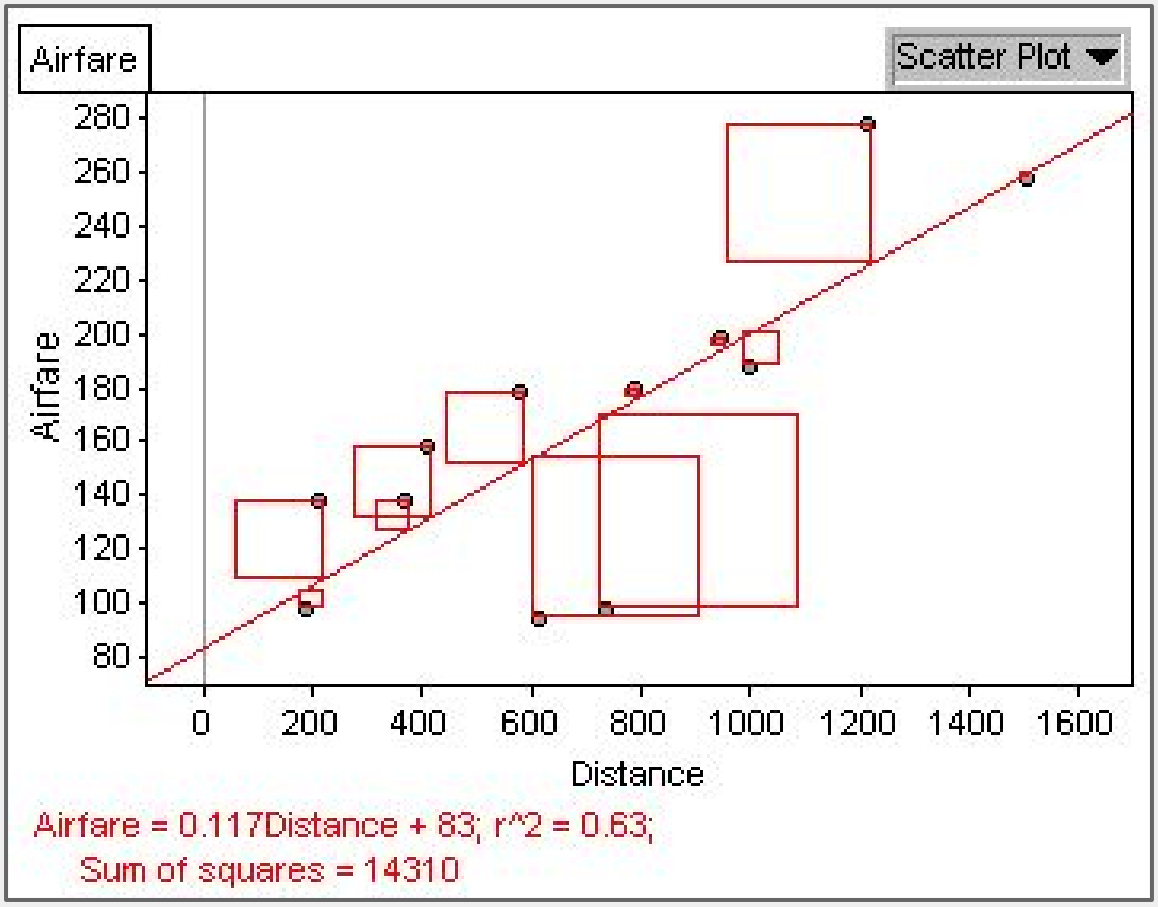
- y is the observed value
- X is the input variables
- β is the set of coefficients
- ε is noise or randomness in observation
- w is the set of weights
- w_0 is the ability to adjust the plane in space
- ŷ is the predicted value



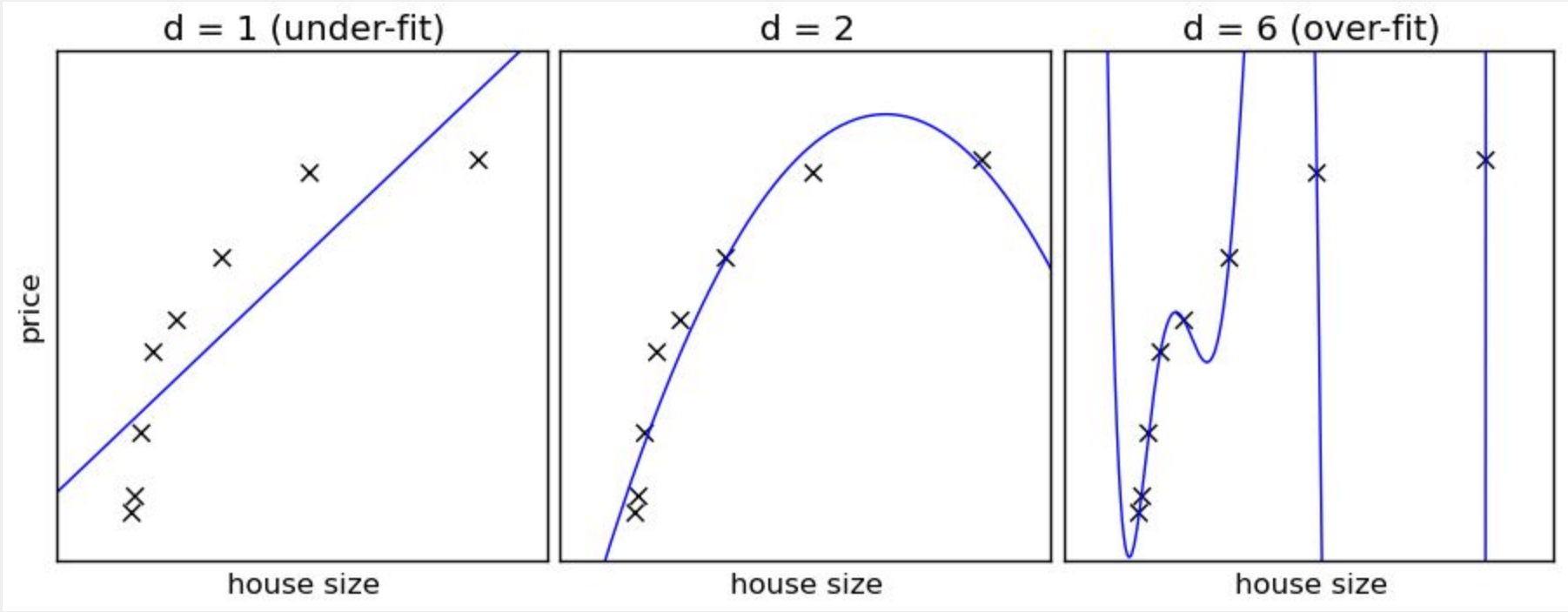
Regression Pipeline

Ordinary Least Squares

- Keep adjusting parameters until minimum squared residuals (e.g. minimize some cost function).
- Relies on the independence of the model terms
- *multicollinearity*: two or more predictor variables in a multiple regression model are highly correlated, one can be linearly predicted from the others
- If this happens, the estimate becomes sensitive to error.


Airfare
Scatter Plot
Airfare
280
260
240
220
200
180
160
140
120
100
80
0
200
400
600
800
1000
1200
1400
1600
Distance
Airfare = 0.117Distance + 83; r^2 = 0.63;
Sum of squares = 14310

```
>>> from sklearn import linear_model
>>> from sklearn.metrics import mean_squared_error, r2_score
>>> regr = linear_model.LinearRegression()
>>> regr.fit(X_train, y_train)
LinearRegression(copy_X=True, fit_intercept=True, normalize=False)

>>> print regr.coef_
[ -6.02985639e+01  -3.02367158e+11   3.02367158e+11   6.04734316e+11
   4.17860883e+00  -3.41060763e-02   2.03234971e+01   2.15758256e-01]

>>> print regr.intercept_
76.9490920195

>>> print mean_squared_error(y_test, regr.predict(X_test))
7.92744075579

>>> regr.score(X_test, y_test)  # r2_score(y_test, regr.predict(X_test))
0.925213977393178 68
```



What can go wrong with simple linear models?

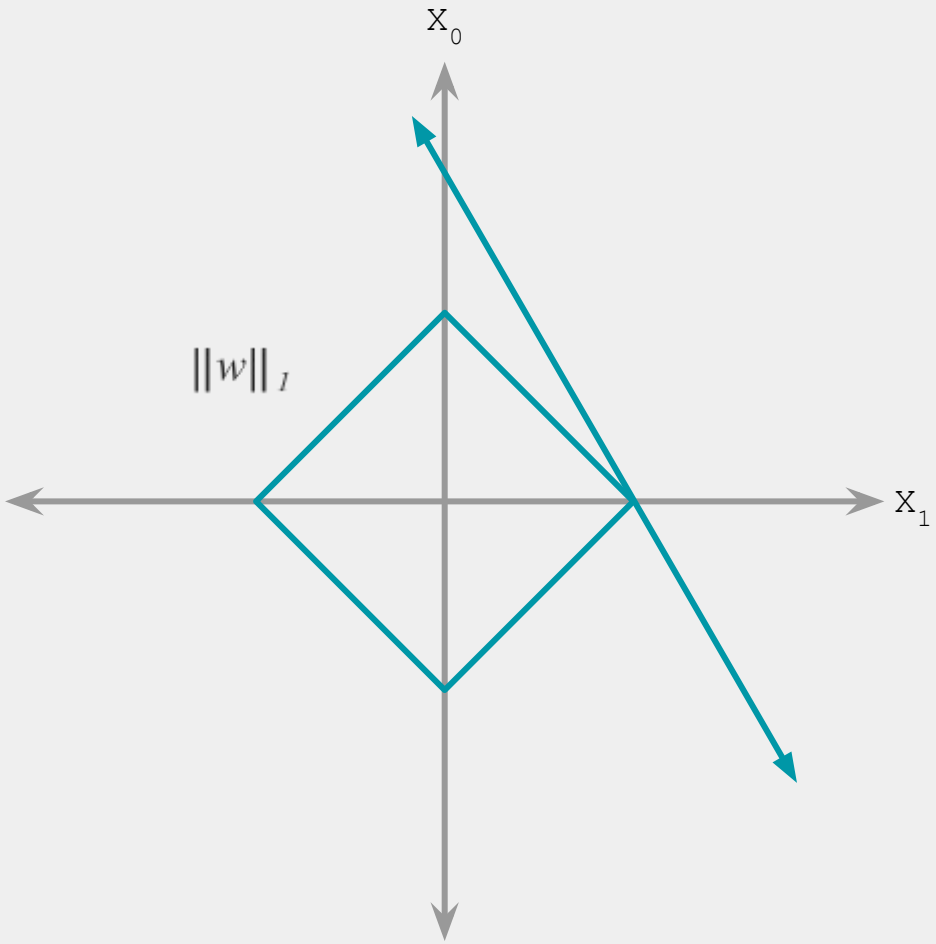
Regularization

- As we increase the complexity of the model we reduce the bias but increase the variance of the model.
- Variance: the tendency for the model to fit to noise (randomness) -- overfit.
- Introduce a parameter to penalize complexity in the function being minimized.

Vector Norm

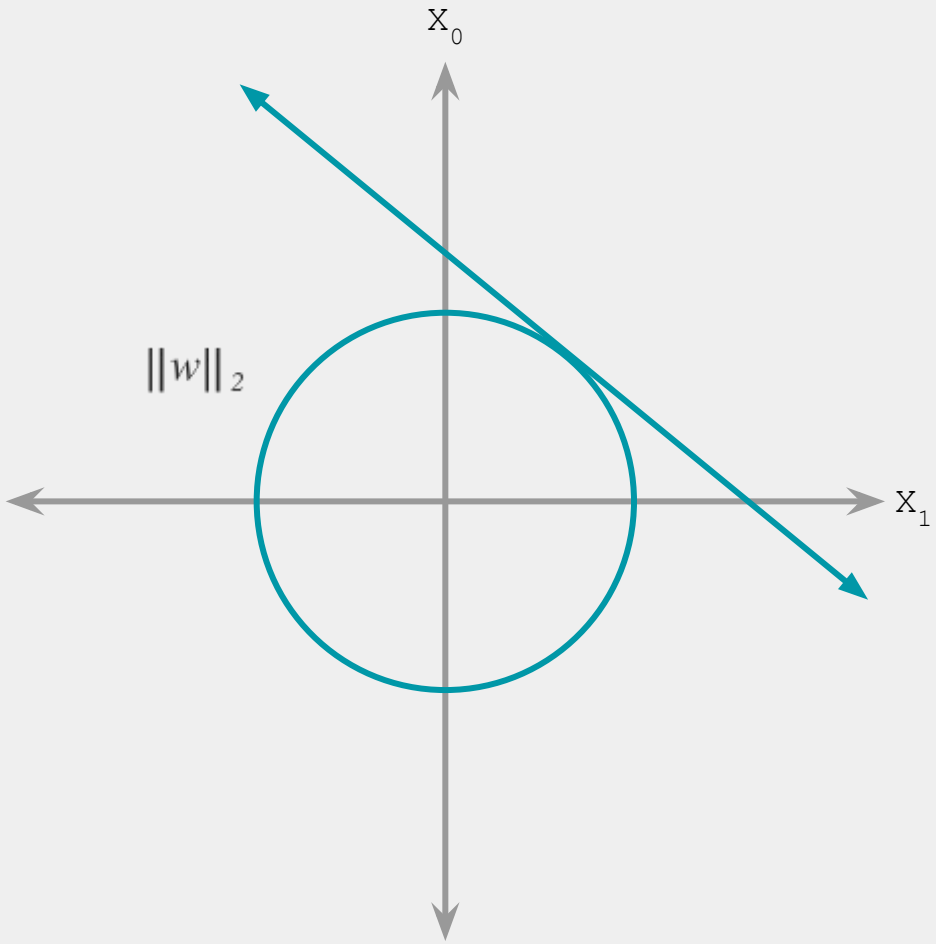
- Describes the length of the vector.
- L1: sum of the absolute values of components
- L2: euclidian distance from the origin
- L∞: maximal absolute value component

```python
import numpy as np
import numpy.linalg as la

vec = np.array([-10, 3, 3, -5, -3, -2, 1, 9, 3, 4, 6, -8])
l1  = la.norm(vec, 1)
# 57.0

l2  = la.norm(vec, 2)
# 19.0525588833

lin = la.norm(vec, 'inf')
# 10
```



L1 Normalization

Possibility that a feature is eliminated by setting its coefficient equal to zero.



L2 Normalization

Features are kept balanced by minimizing the relative change of coefficients during learning.

Ridge Regression

- Prevent overfit/collinearity by penalizing the size of coefficients - minimize the penalized residual sum of squares:
- Said another way, shrink the coefficients to zero.

$$\min_{w} \sum (Xw-y)^2+\alpha \sum w^2$$

- Where α > 0 is complexity parameter that controls shrinkage. The larger α, the more robust the model to collinearity.
- Alpha influences the bias/variance tradeoff: the larger the ridge alpha, the higher the bias and the lower the variance.

```
>>> clf = linear_model.Ridge(alpha=0.5)
>>> clf.fit(X_train, y_train)
Ridge(alpha=0.5, copy_X=True, fit_intercept=True, max_iter=None,
   normalize=False, solver='auto', tol=0.001)

>>> print mean_squared_error(y_test, clf.predict(X_test))
8.34260312032

>>> clf.score(X_test, y_test)
0.92129741176557278
```

Choosing `alpha`

We can search for the best parameter using the `RidgeCV` which is a form of Grid Search, but uses a more efficient form of leave-one-out cross-validation.

```
>>> import numpy as np
>>> n_alphas = 200
>>> alphas = np.logspace(-10, -2, n_alphas)
>>> clf = linear_model.RidgeCV(alphas=alphas)
>>> clf.fit(X_train, y_train)
>>> print clf.alpha_
0.0010843659686896108
>>> clf.score(X_test, y_test)
0.9254247751217173
```

Cross-Validation and Evaluation

In regressions we can determine how well the model fits by computing the mean square error and the coefficient of determination.

MSE = np.mean((predicted-expected)**2)

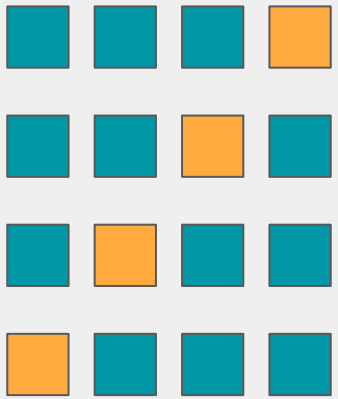
R^2 is a predictor of “goodness of fit” and is a value $\in [0,1]$ where 1 is perfect fit.

Cross-Validation and Evaluation

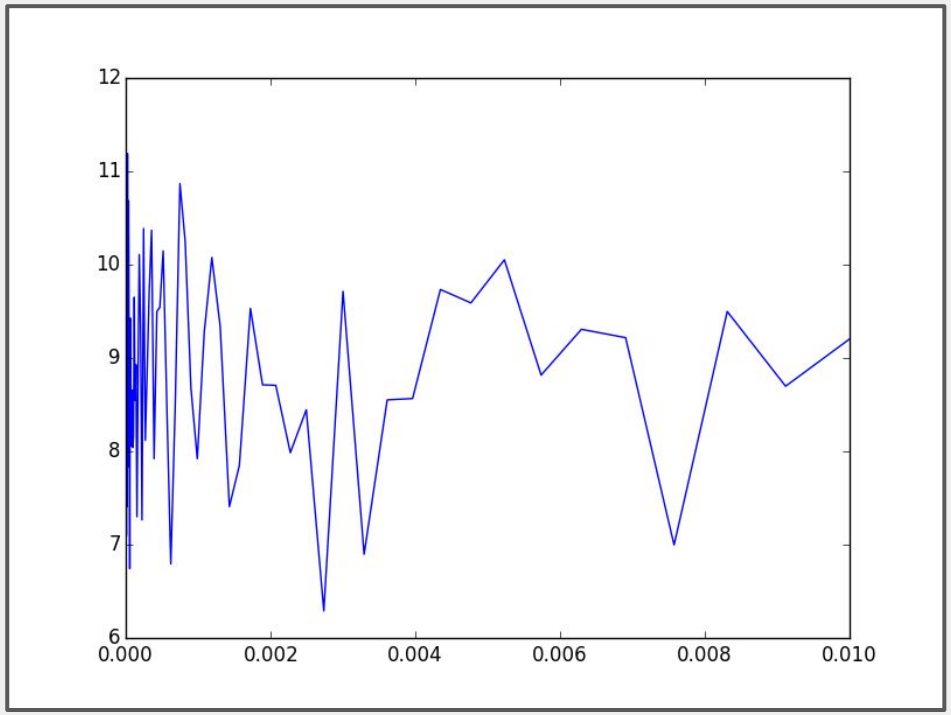
In order to prevent overfit and be assured of generalizability, cross-validation fits the model on a portion of the data set and evaluates it on an unseen portion of the data set.

Shuffle data, split into a large train set and smaller test set.

This can be done K=12 times, and scores averaged.



```
>>> clf = linear_model.Ridge(fit_intercept=False)
>>> errors = []
>>> for alpha in alphas:
...     splits = tts(dataset.data, dataset.target('Y1'), test_size=0.2)
...     X_train, X_test, y_train, y_test = splits
...     clf.set_params(alpha=alpha)
...     clf.fit(X_train, y_train)
...     error = mean_squared_error(y_test, clf.predict(X_test))
...     errors.append(error)
...
>>> axe = plt.gca()
>>> axe.plot(alphas, errors)
>>> plt.show()
```



Error as a function of alpha

How to pick the right parameters?

Search Requires:

- Estimator
- Parameter Space
- Method for sampling
- Cross validation scheme
- A score function

Search Types:

- Exhaustive
- Randomized
- Parallel
- Leave One Out
- Model Specific

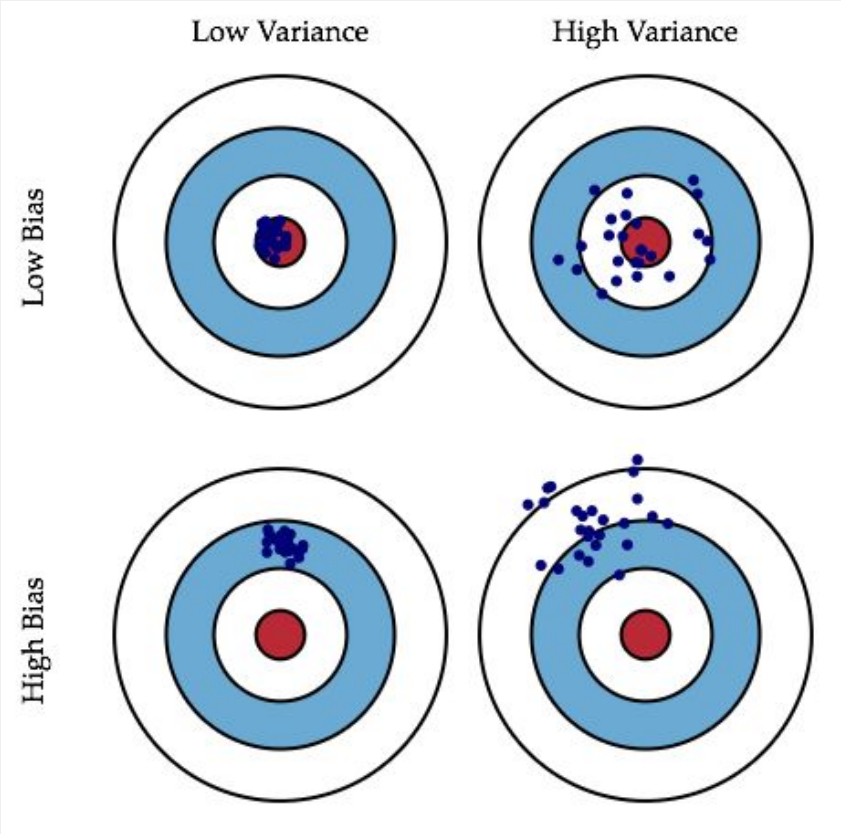
```
from sklearn.svm import SVC
from sklearn.grid_search import GridSearchCV

params = [
  {'C': [1, 10, 100, 1000], 'kernel': ['linear']},
  {'C': [1, 10, 100, 1000], 'gamma': [0.001, 0.0001], 'kernel':
['rbf']},
]

estimator = GridSearchCV(SVC(), params)
estimator.fit(dataset.data, dataset.target)
```

Creating an exhaustive grid search for a classifier.

Error: Bias vs Variance

Bias: the difference between expected (average) prediction of the model and the correct value.

Variance: how the predictions for a given point vary between different realizations for the model.



http://scott.fortmann-roe.com/docs/BiasVariance.html

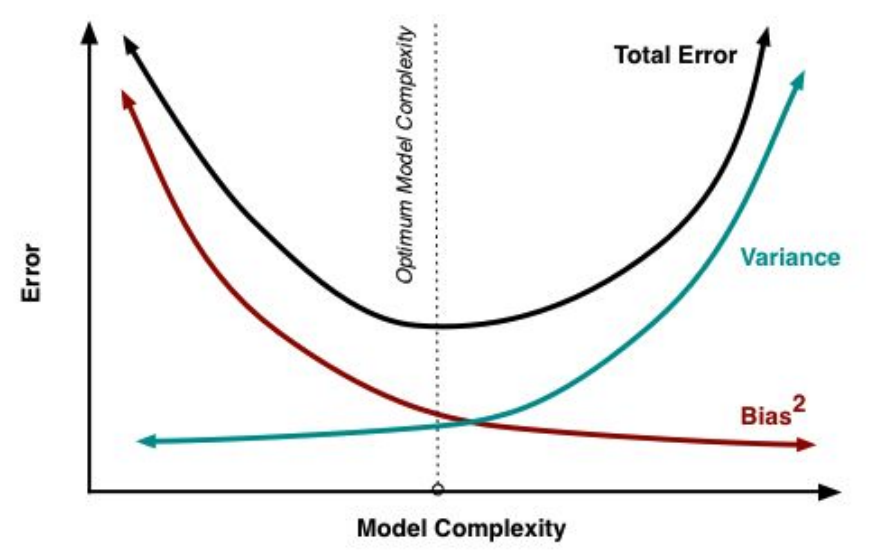
Bias vs. Variance Trade-Off

Related to model complexity:

The more parameters added to the model (the more complex), Bias is reduced, and variance increased.

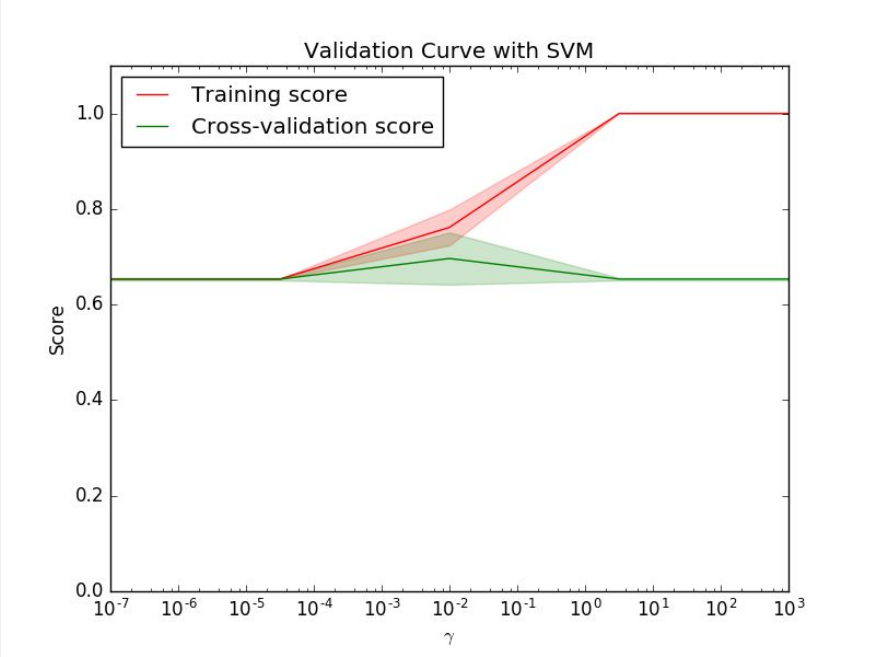
Sources of complexity:

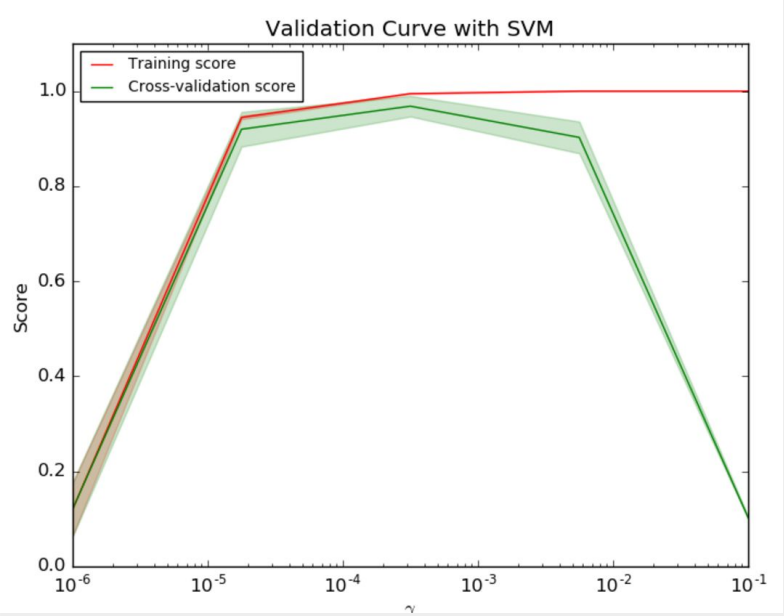
- k (nearest neighbors)
- epochs (neural nets)
- # of features
- learning rate



http://scott.fortmann-roe.com/docs/BiasVariance.html

Visual Parameter Tuning





- 2 different datasets: tic-tac-toe (left) & digits (right)
- Training vs. validation scores of SVM
- Different values of the kernel parameter gamma
- Things to look for:
  - Training score and validation score both low => Underfit
  - Training score high and validation score low => Overfit

Lasso

- Reducing bias is one thing, but what if the coefficients are very sparse? E.g. the more dimensions we add, the more *space* goes into the model.
- Lasso prefers fewer parameters attempting to reduce the number of variables the solution depends on.

$$\min_{w} \frac{1}{2n_{samples}} \left(\sum (Xw - y)^2 \right) + \alpha \|w\|_1$$

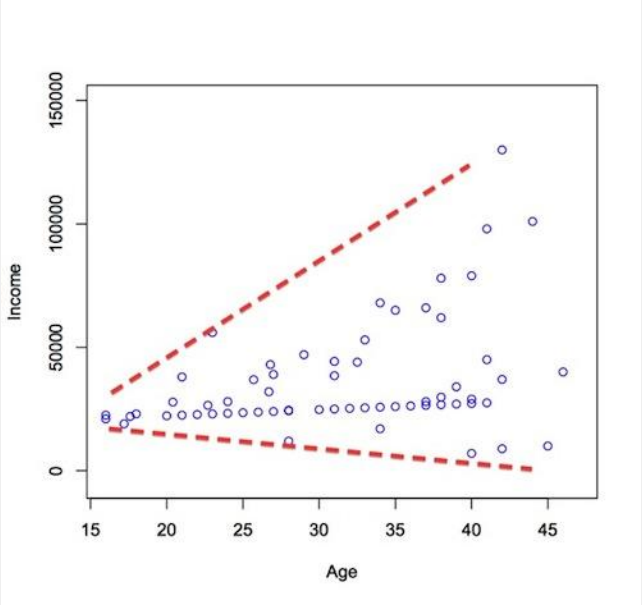
- The term $\alpha \|w\|_1$ is the L1 norm, whereas in ridge we used the L2 norm, $\alpha \|w\|_2^2$.
- See also Least Angle Regression (LARS) as similar.
- Can also use `LassoCV` and `LassoLarsCV`

```
>>> clf = linear_model.Lasso(alpha=0.5)
>>> clf.fit(X_train, y_train)
Lasso(alpha=0.5, copy_X=True, fit_intercept=True, max_iter=1000,
   normalize=False, positive=False, precompute='auto', tol=0.0001,
   warm_start=False)

>>> print mean_squared_error(y_test, clf.predict(X_test))
18.84667821

>>> clf.score(X_test, y_test)
0.82870491763341947
```

Instance Variance

Heteroscedasticity: variability of variable is unequal along range of predicted values.

Homoscedasticity: variance is equal along prediction (assumed in most models).



And More Models

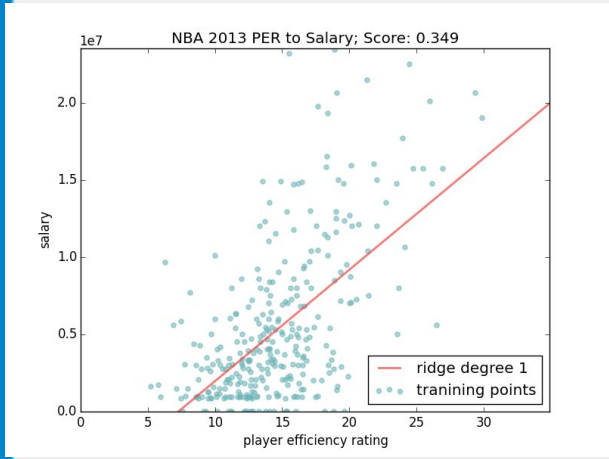
Listed only from the Documentation (not API):

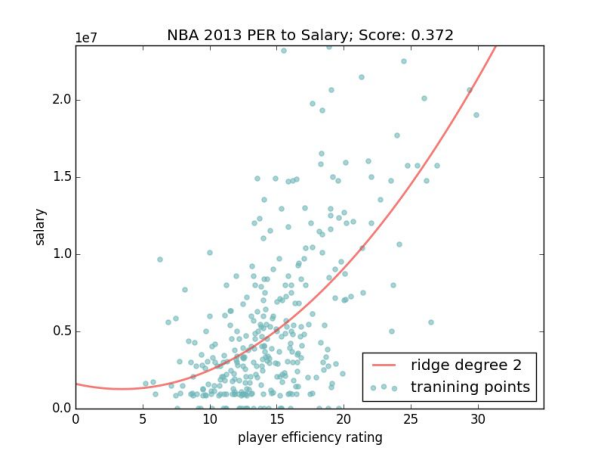
- ElasticNet
- Multi-Task Lasso
- Least Angle Regression
- LARS Lasso
- Orthogonal Matching Pursuit (OMP)
- Bayesian Regression
- Automatic Relevance Determination (ARD)
- Logistic Regression
- Stochastic Gradient Descent
- Perceptron
- Random Sample Consensus (RANSAC)

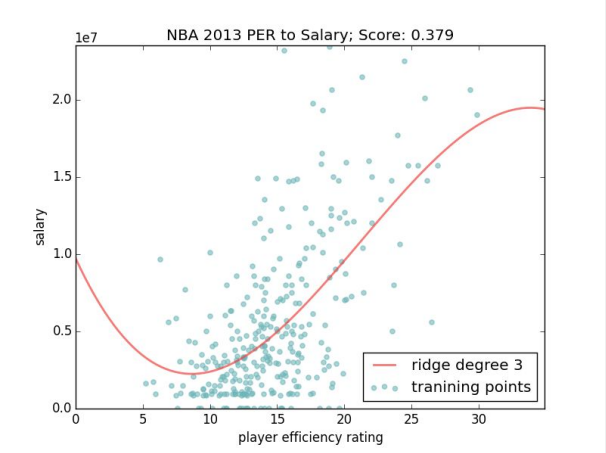
Polynomial Regression

In order to do higher order polynomial regression, we can use *linear models* trained on *nonlinear* functions of data!

- Speed of linear model computation
- Fit a wider range of data or functions
- But remember: polynomials aren't the only functions to fit







Polynomial Regression

The way this works is via *Pipelining*.
Consider the standard linear regression case:

$$\hat{y}(w,x) = w_0 + \sum_{i=1}^{n} w_i x_i$$

The quadratic case (polynomial degree = 2) is:

$$\hat{y}(w,v,x) = w_0 + \sum_{i=1}^{n} w_i x_i + \sum_{i=1}^{n} v_i x_i^2$$

But this can just be seen as a new feature space:

$$z = [x_1, \ldots, x_n, x_1^2, \ldots, x_n^2]$$

And this feature space can be computed in a linear fashion.
We just need some way to add our 2nd degree dimensions.

```
>>> from sklearn.preprocessing import PolynomialFeatures
>>> from sklearn.pipeline import make_pipeline
>>> model = make_pipeline(PolynomialFeatures(2),
linear_model.Ridge())
>>> model.fit(X_train, y_train)
Pipeline(steps=[('polynomialfeatures', PolynomialFeatures(degree=2,
include_bias=True, interaction_only=False)), ('ridge',
Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=None,
   normalize=False, solver='auto', tol=0.001))])

>>> mean_squared_error(y_test, model.predict(X_test))
3.1498887586451594

>>> model.score(X_test, y_test)
0.97090576345108104
```

Pipelined Model

Pipelines

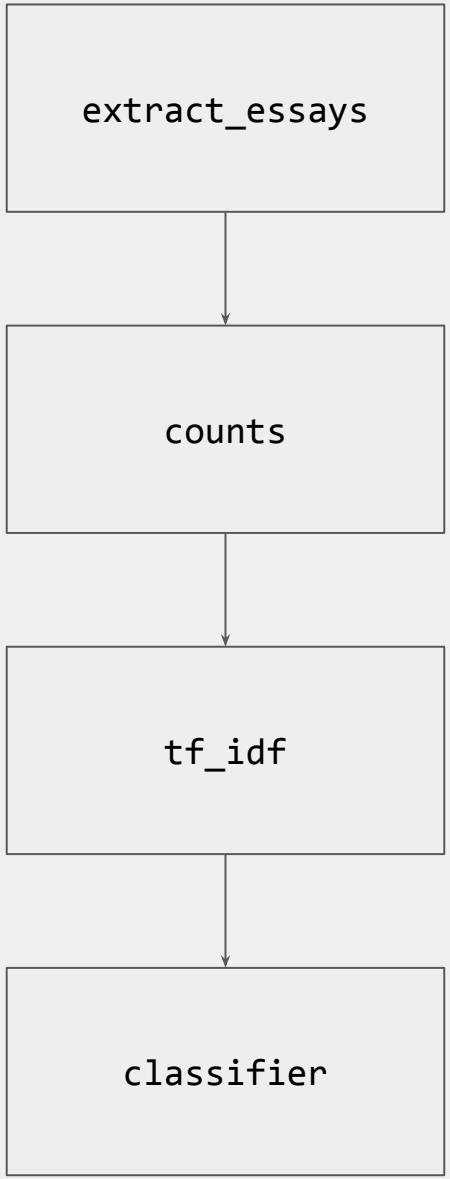
`sklearn.pipeline.Pipeline(steps)`

- Sequentially apply *repeatable* transformations to final estimator that can be validated at every step.
- Each step (except for the last) must implement `Transformer`, e.g. `fit` and `transform` methods.
- Pipeline itself implements both methods of `Transformer` and `Estimator` interfaces.

```
class Transformer(Estimator):

    def transform(self, X):
        """Transforms the input data. """
        # transform ``X`` to ``X_prime``
        return X_prime

from sklearn import preprocessing

Xt = preprocessing.normalize(X) # Normalizer
Xt = preprocessing.scale(X)     # StandardScaler

imputer =Imputer(missing_values='Nan',
                 strategy='mean')
Xt = imputer.fit_transform(X)
```

```
class Estimator(object):

    def fit(self, X, y=None):
        """Fits estimator to data. """
        # set state of ``self``
        return self

    def predict(self, X):
        """Predict response of ``X``. """
        # compute predictions ``pred``
        return pred
```

```python
from sklearn.pipeline import Pipeline
from sklearn.cross_validation import KFold

pipeline = Pipeline([
    ('extract_essays', EssayExractor()),
    ('counts', CountVectorizer()),
    ('tf_idf', TfidfTransformer()),
    ('classifier', MultinomialNB())
])

scores = []
folds = KFold(
     n = dataset.data.shape[0], n_folds=12, shuffle=True
)

for tidx, cidx in folds:
    pipeline.fit(dataset.data[tidx], dataset.target[idx]
    score = pipeline.score(dataset.data[cidx],
dataset.target[cidx])
    scores.append(score)

print("Score: {}".format(np.mean(scores)))
```

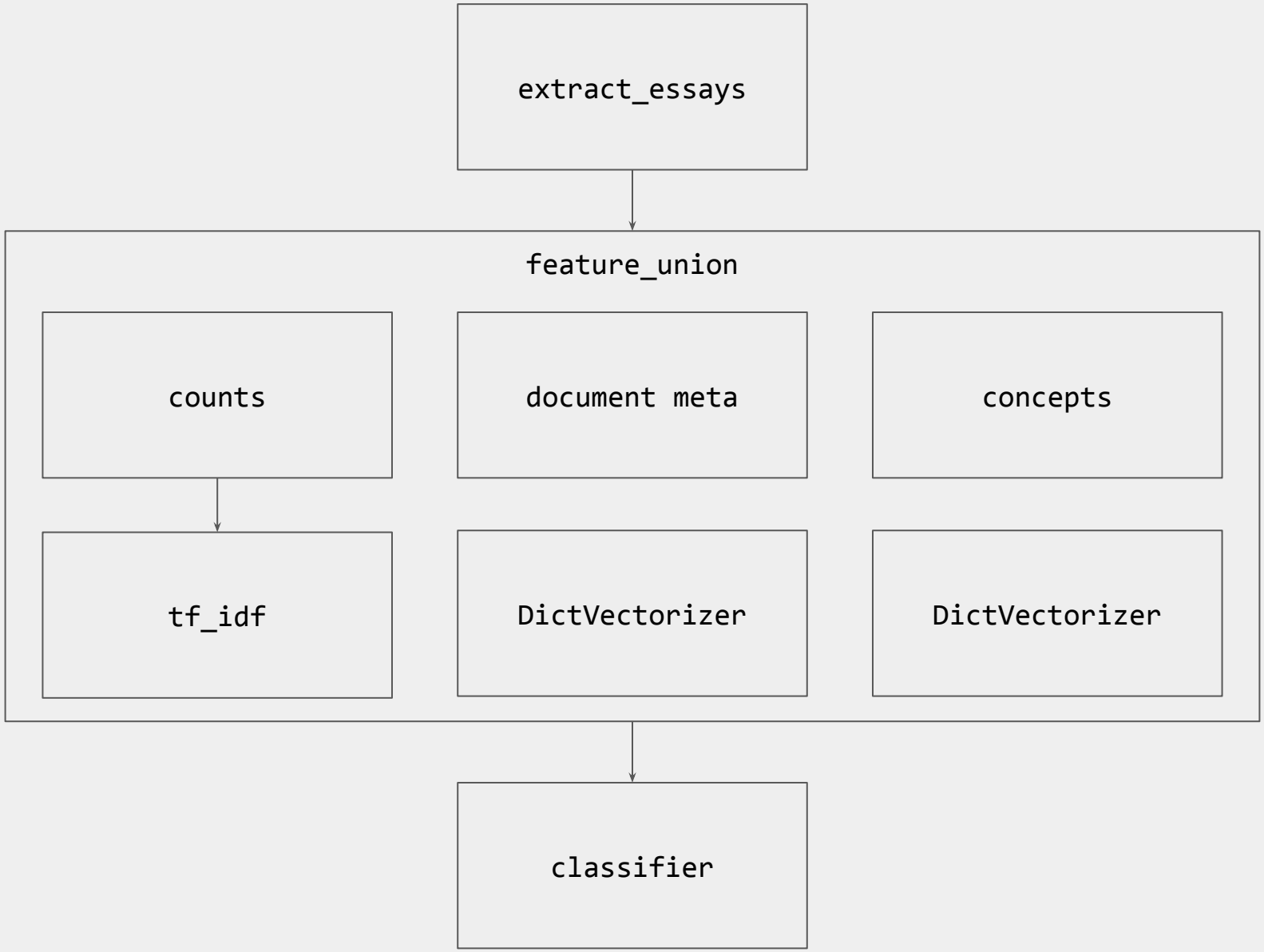


http://zacstewart.com/2014/08/05/pipelines-of-featureunions-of-pipelines.html

Pipelined Feature Extraction

The most common use for the Pipeline is to combine multiple feature extraction methodologies into a single, repeatable processing step.

- `FeatureUnion`
- `SelectKBest`
- `TruncatedSVD`
- `DictVectorizer`



Feature unions example from Zac's post