Supervised Machine Learning

Part One: Regression

DistrictDataLabs

Agenda

- Overview of Supervised Learning
- Regression Models - Linear Regression
    - OLS
    - LASSO
    - Ridge
    - ElasticNet
- Model Evaluation
    - Pipelines & Feature Selection (GridSearchCV)
- Model Selection

Supervised Learning

Definition

Supervised learning is the machine learning task of inferring a function from labeled training data. The training data consist of a set of training examples. In supervised learning, each example is a pair consisting of an input object (typically a vector) and a desired output value (also called the supervisory signal). A supervised learning algorithm analyzes the training data and produces an inferred function, which can be used for mapping new examples.

https://en.wikipedia.org/wiki/Supervised_learning

Important Points

1. Labeled training data
2. Desired output
3. Produces an inferred function
4. Used for novel examples

Approaches

1. Classification
2. Regression

Regression Models

Regression Models

- Supervised learning algorithms that estimate the relationship among variables.
- Focus is on the relationship between a dependent variable (target) and 1(+) independent variables (predictor)
- Does the dependent variable change when the independent variable(s) change?
- Common algorithms
  - Generalized linear models

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 $y = X\beta + \epsilon$

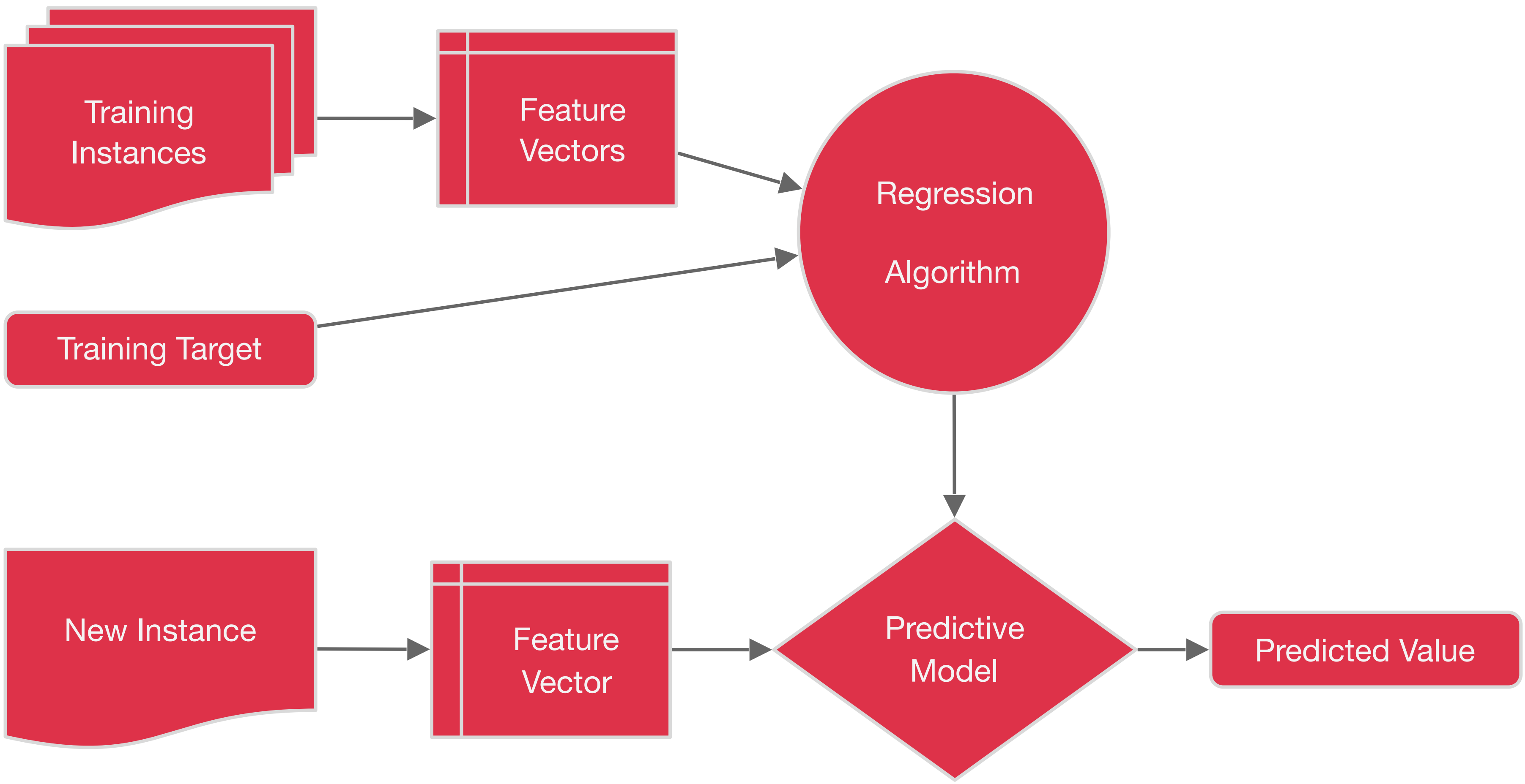
(2) Objective function $\min_{w} \sum (Xw - y)^2$

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

Notation:

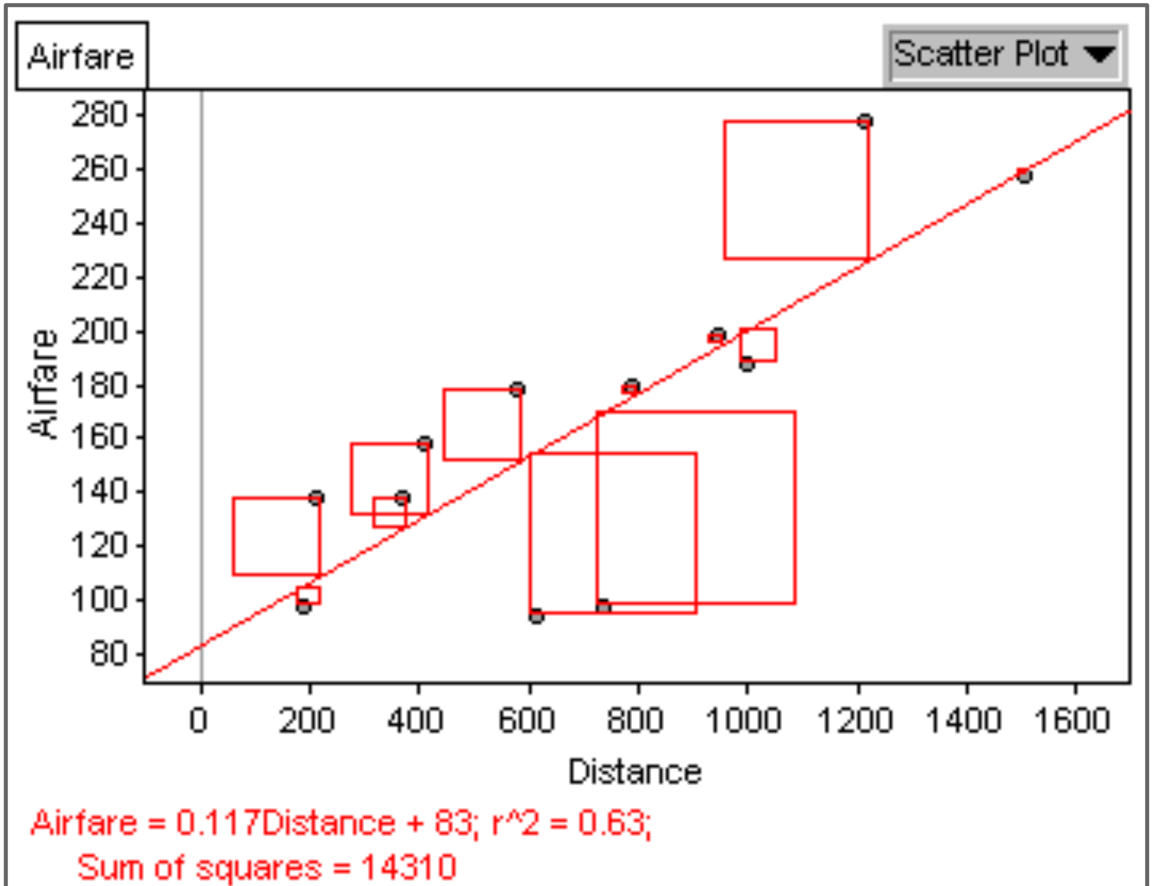
- y is the observed value
- x is the input variables
- β is the set of coefficients
- ε is noise or randomness in observation
- w is the set of weights
- w_0 is the ability to adjust the plane in space
- $\hat{y}$ is the predicted value

Regression Pipeline



Ordinary Least Squares

- Method for estimating unknown parameters in a linear regression model
- 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
280
260
240
220
200
180
160
140
120
100
80
Airfare
0
200
400
600
800
1000
1200
1400
1600
Distance
Airfare = 0.117Distance + 83; r^2 = 0.63;
Sum of squares = 14310

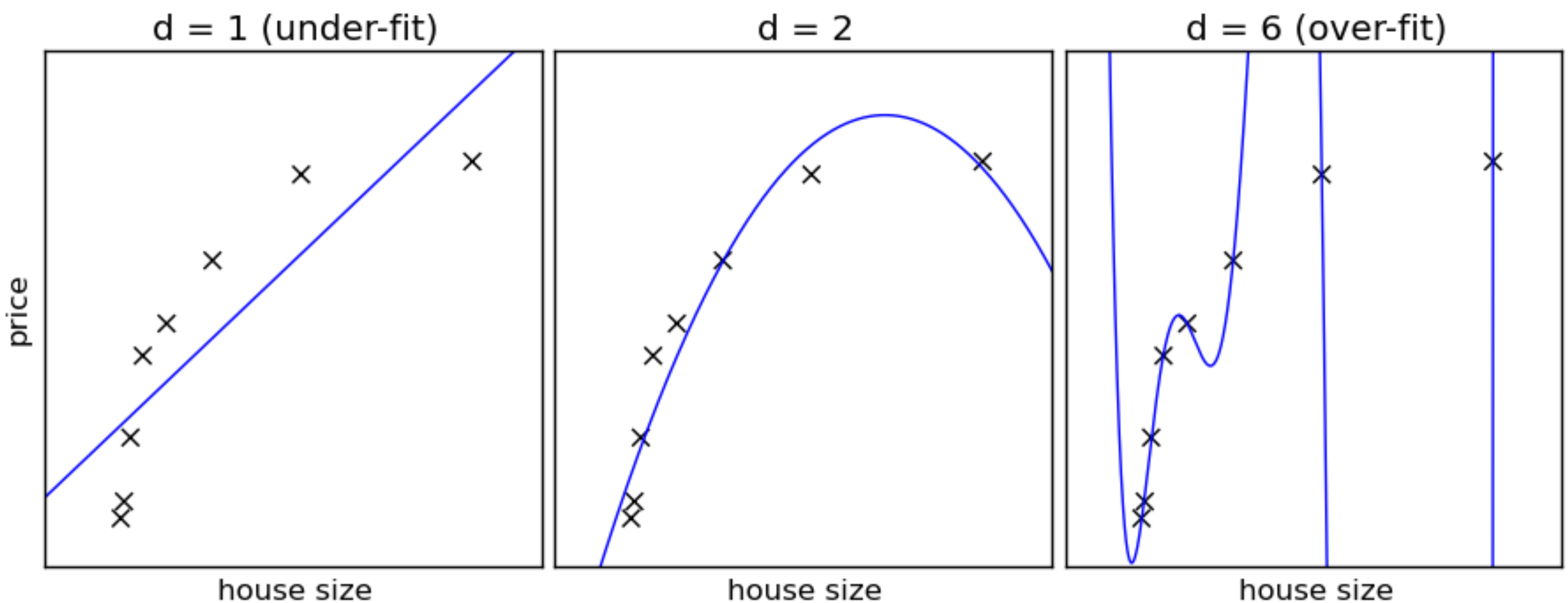
Simple Regression with OLS

```
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))
0.92521397739317868
```

Lab: Linear Regression

Sklearn & MLlib

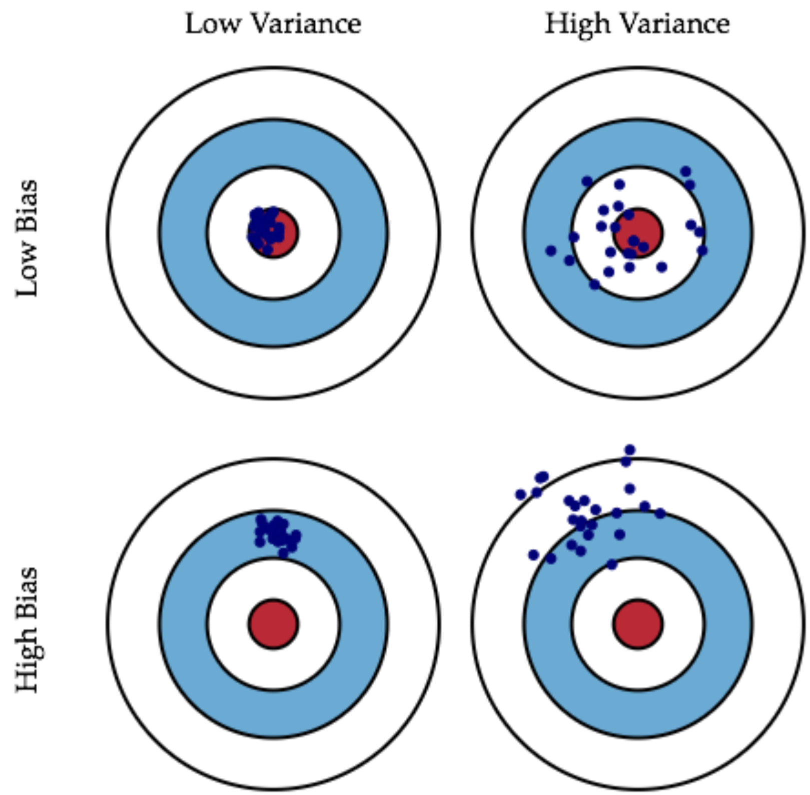
What Can Go Wrong With Simple Linear Models?



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.

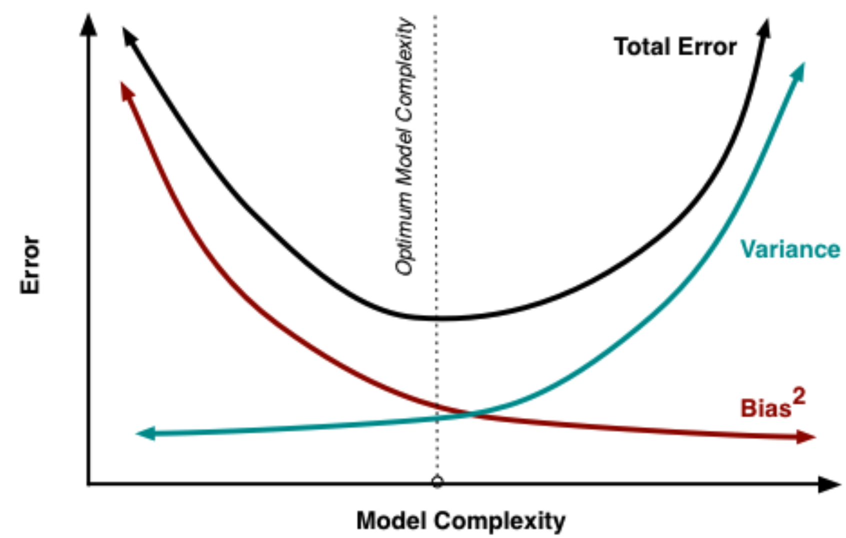


http://scott.fortmann-roe.com/docs/BiasVariance.html

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.



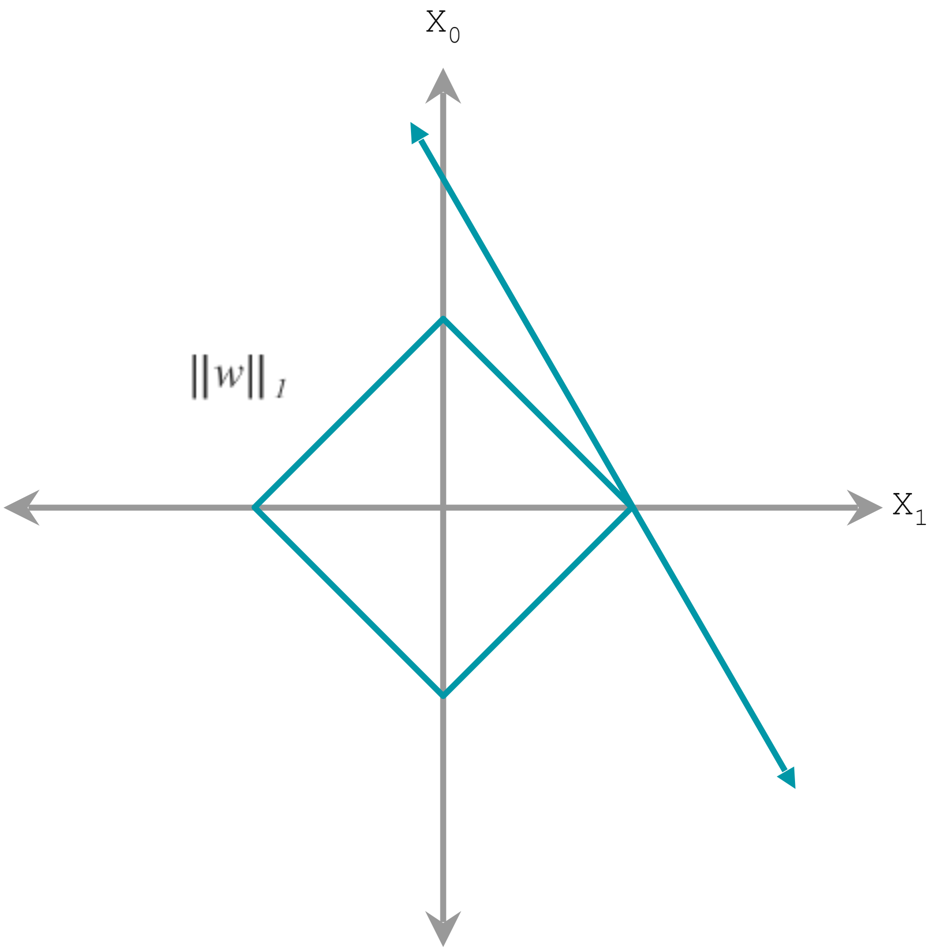
Sources of complexity:

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

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

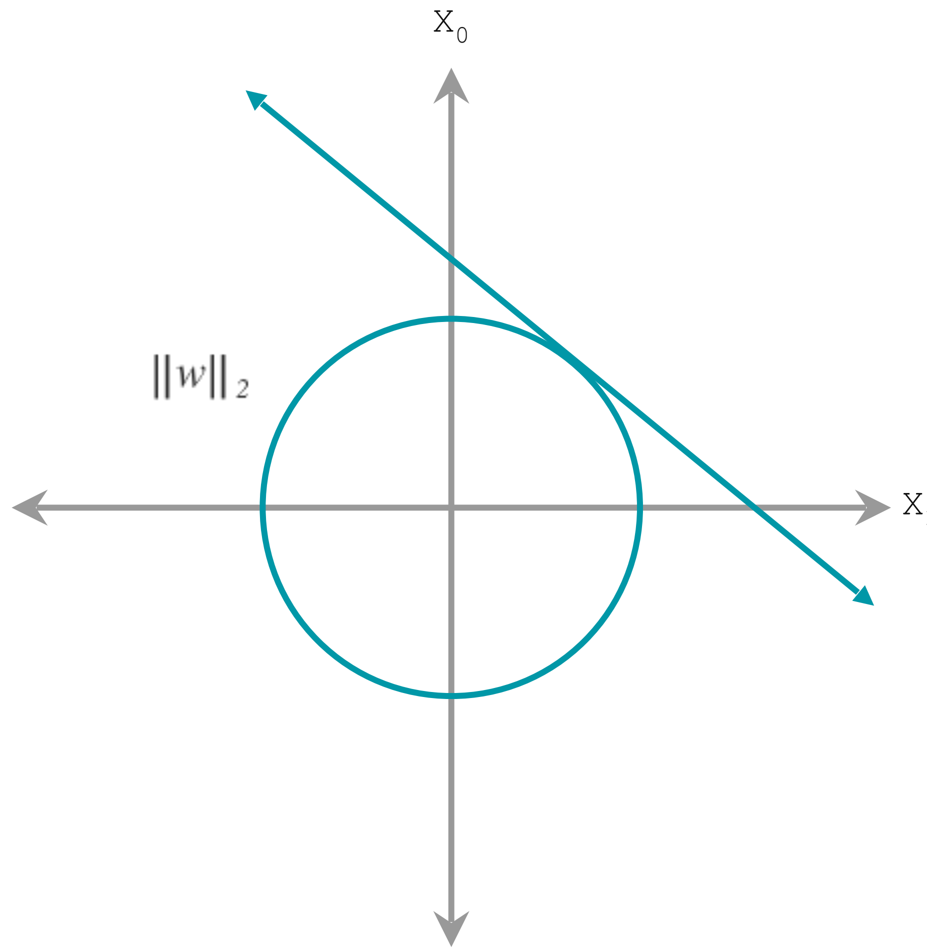
Regularization

- As we increase the complexity of the model we reduce bias but increase variance, which can lead to overfitting.
- Regularization introduces a parameter to penalize the magnitude of coefficients of features and minimize the error between predicted and actual observations.
  - Generally, the size (magnitude) of coefficients increases exponentially with an increase in model complexity, which leads to overfitting.
- OLS does not include regularization



L1 Regularization

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



L2 Regularization

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

Lasso

- Uses L1 regularization
- Prefers fewer parameters attempting to reduce the number of variables the solution depends on.

Lasso Regression

```
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)
0.8287049176334194 7
```

Lab: Lasso Regression

Sklearn & MLlib

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 $\alpha > 0$ 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.

Ridge Regression

```
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
```

Lab: Ridge Regression

Sklearn & MLlib

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)
0.92542477512171173
```

Error As a Function of Alpha

```
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()
```

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)

ElasticNet

- Combines L1 and L2 regularization
- Works well with a large number of features
- Forms a group of independent, correlated variables. If any of the variables are a strong predictor, EN includes the entire group in model building.

Lab: ElasticNet Regression

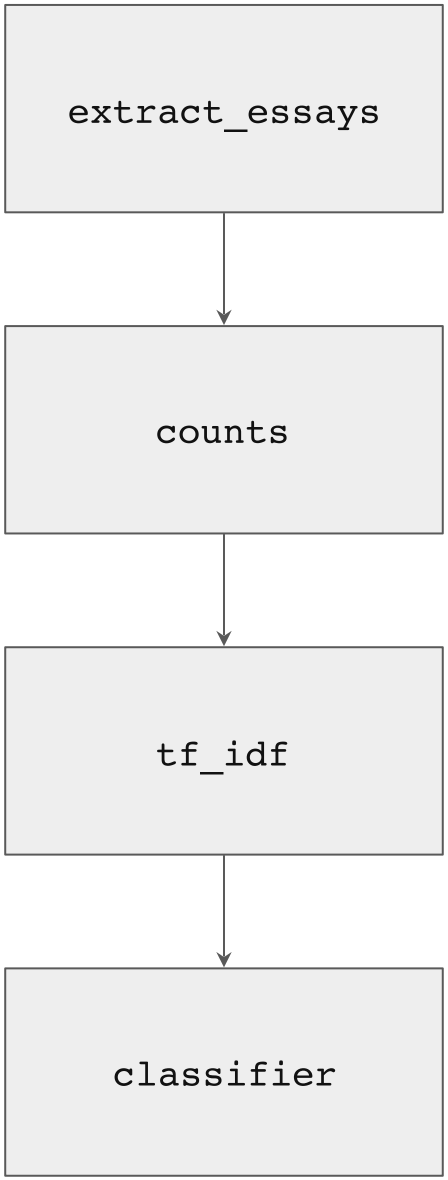
Sklearn & MLlib

Pipelines (Steps)

`sklearn.pipeline.Pipeline`

- 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.

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

pipeline = Pipeline([
    ('extract_essays', EssayExtractor()),
    ('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)))
```

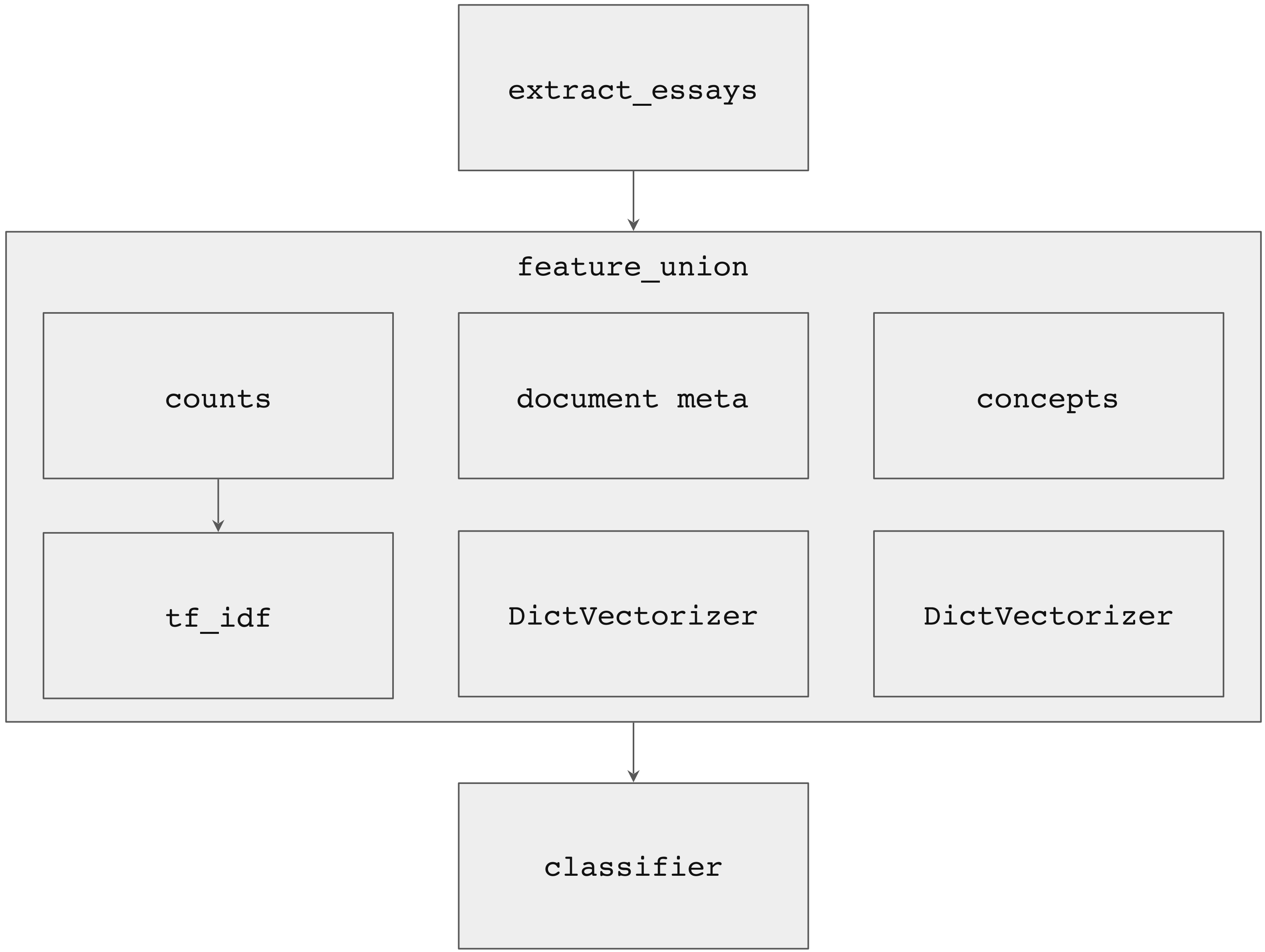


http://zacstewart.com/2014/08/05/pipelines-of-featureunions-of-pipelines.html

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

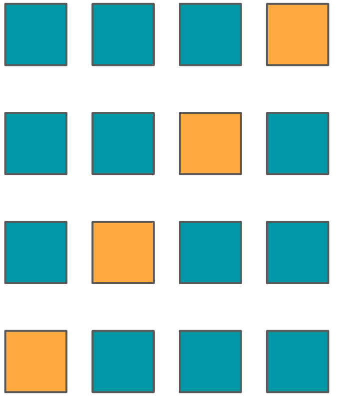
Model Evaluation

Cross-Validation and Evaluation

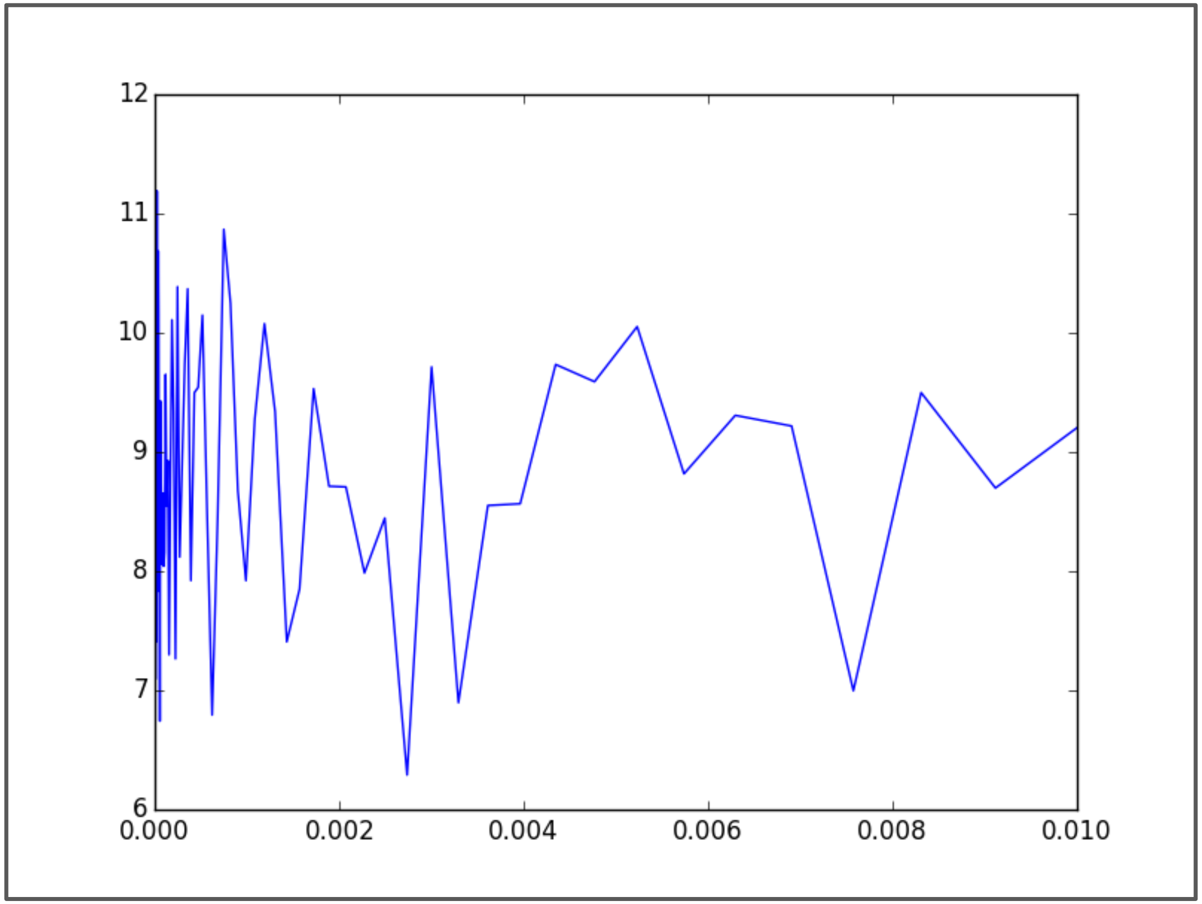
- In regressions we can determine how well the model fits by computing the mean square error and the coefficient of determination.
  - MSE = np.mean((predicted-expected)**2)
  - R^2 is a predictor of "goodness of fit" and is a value $\in [0,1]$ where 1 is perfect fit.

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.



Resulting Plot



How to pick the right parameters?

Search/Tuning

Search Requires

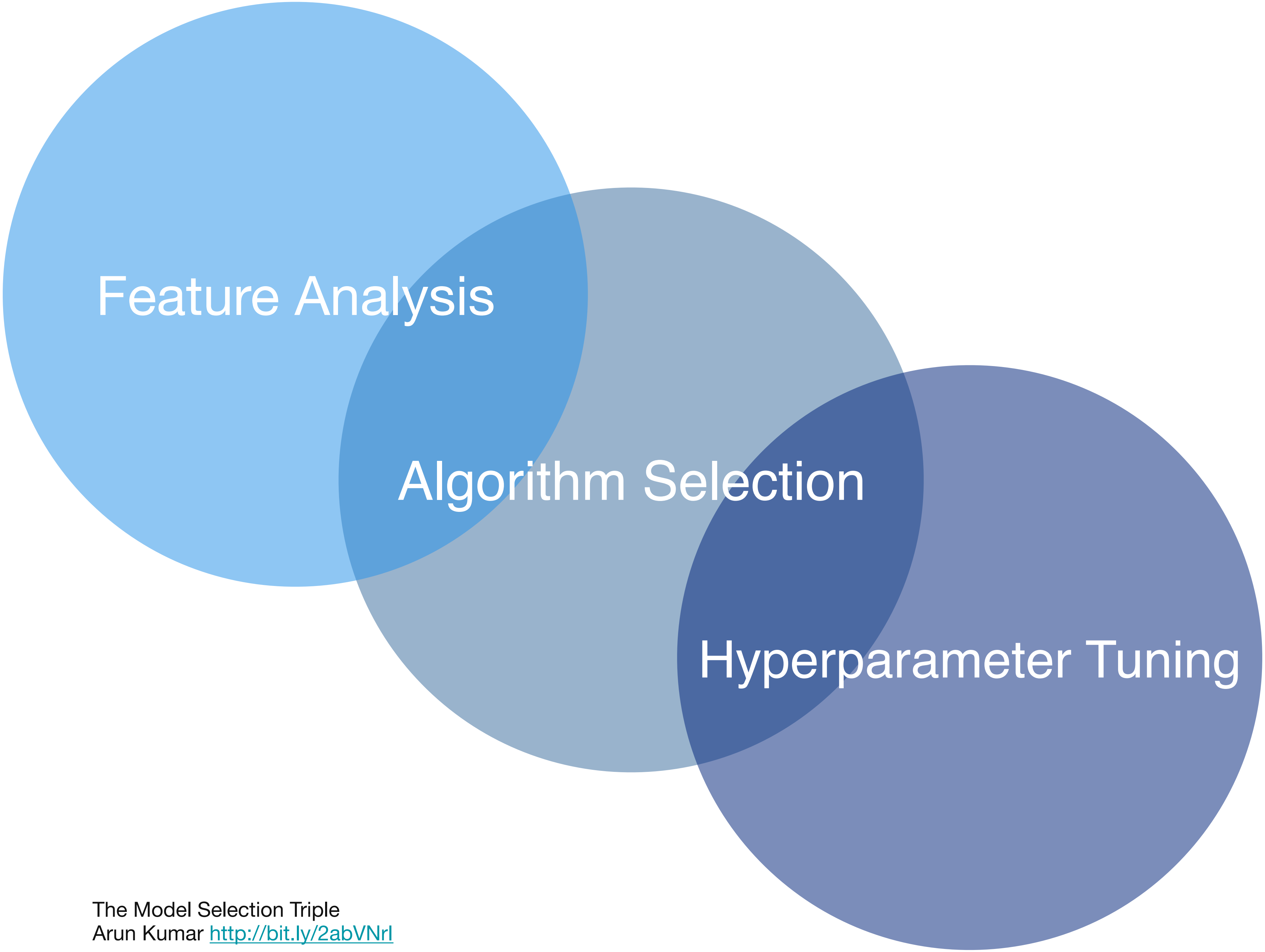
- Estimator
- Parameter Space
- Method for sampling
- Cross validation scheme
- A score function

Search Types

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

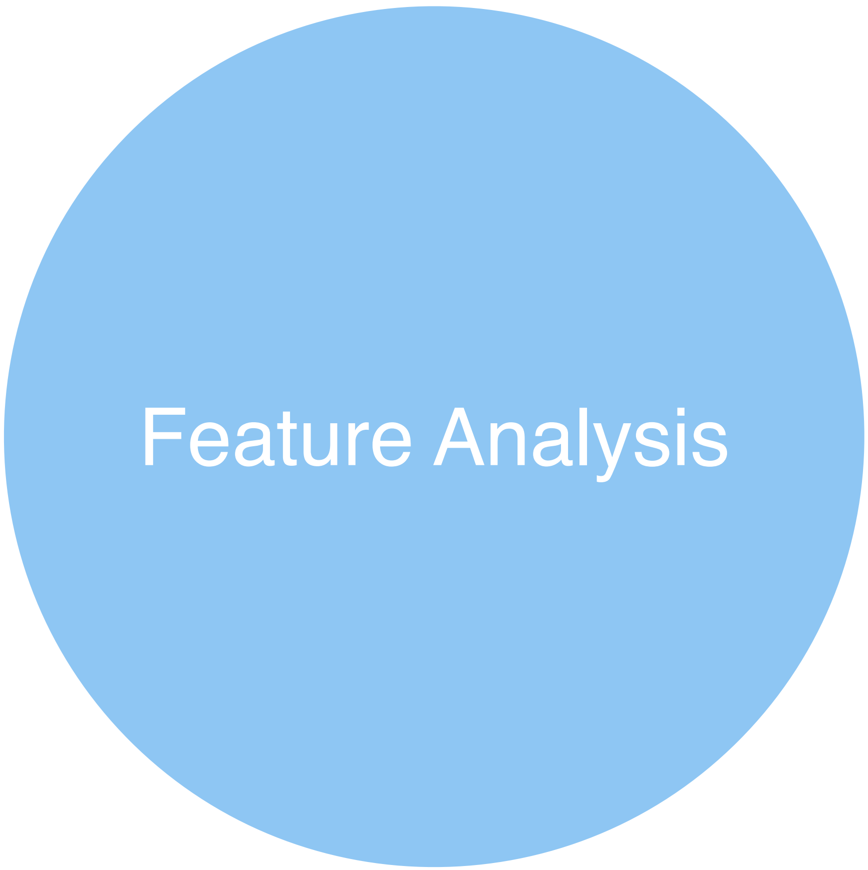
Lab: Pipelines & Feature Extraction with Sklearn

Model Selection



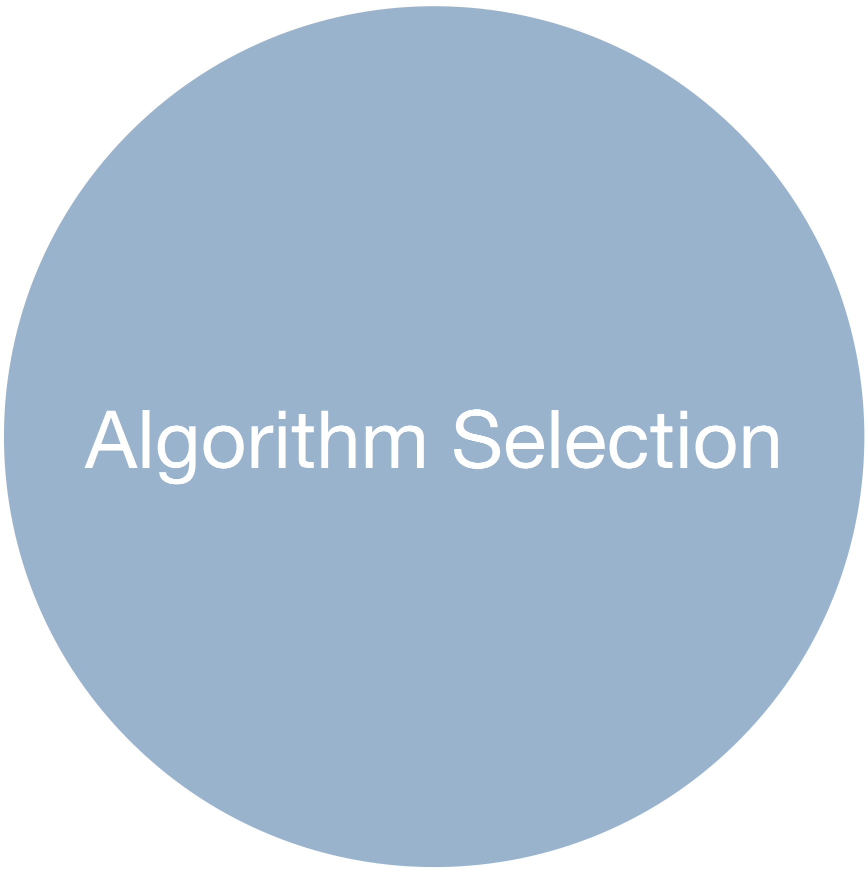
The Model Selection Triple
Arun Kumar http://bit.ly/2abVNrl

The Model Selection Triple



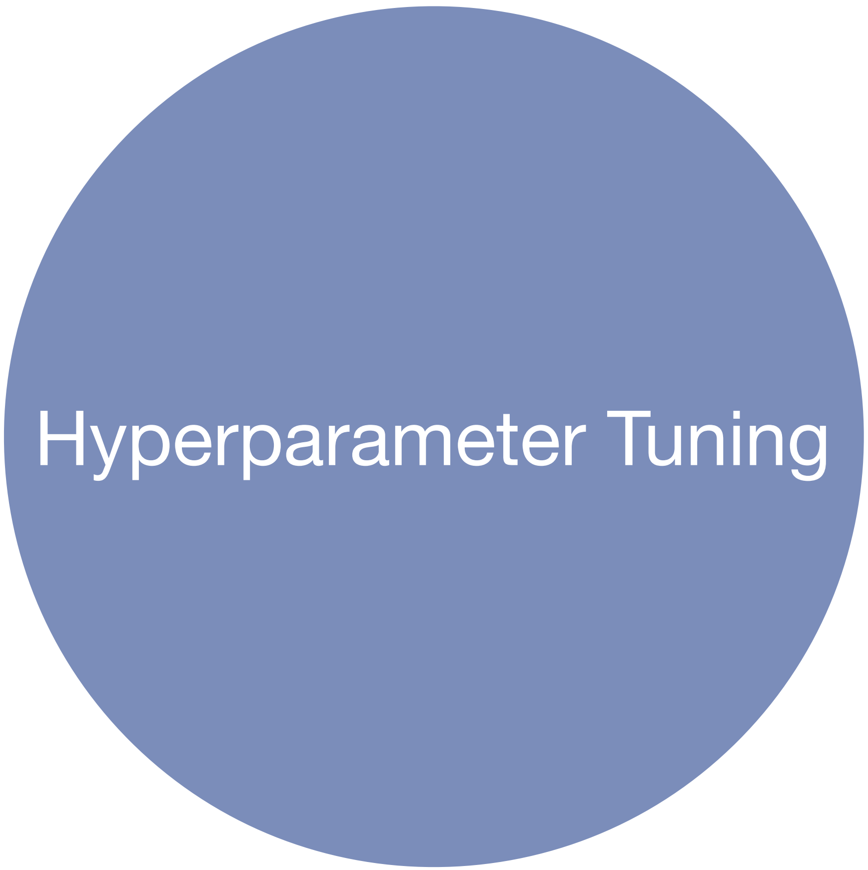
- Define a bounded, high dimensional feature space that can be effectively modeled.
- Transform and manipulate the space to make modeling easier.
- Extract a feature representation of each instance in the space.

The Model Selection Triple



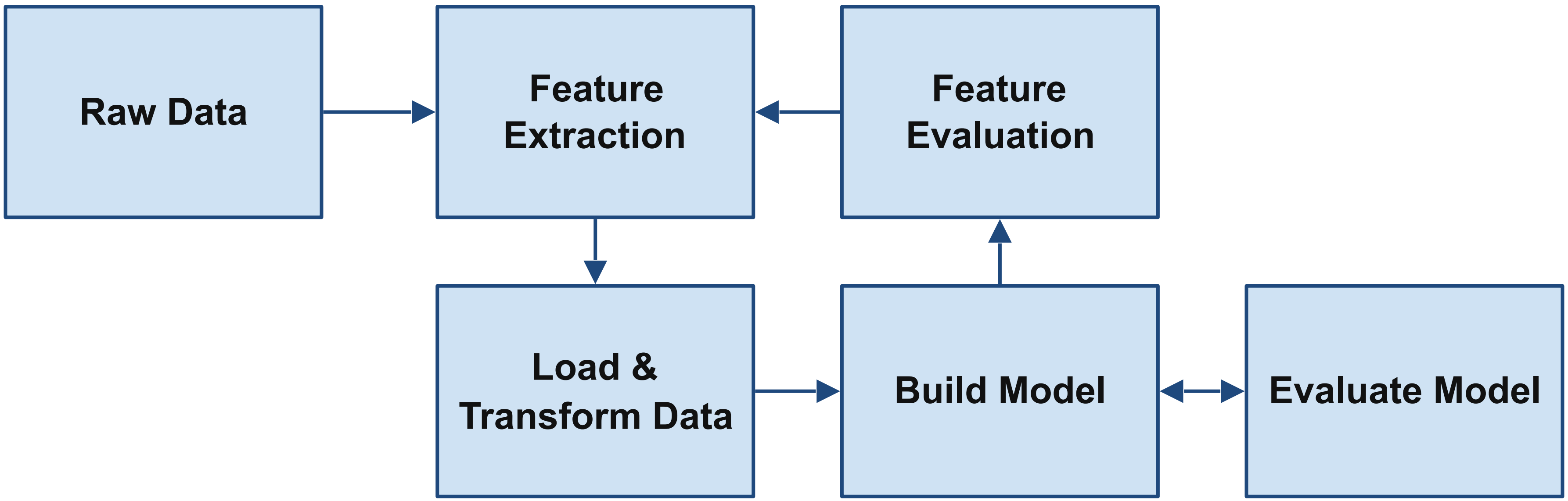
- Select a model family that best/correctly defines the relationship between the variables of interest.
- Define a model form that specifies exactly how features interact to make a prediction.
- Train a fitted model by optimizing internal parameters to the data.

The Model Selection Triple

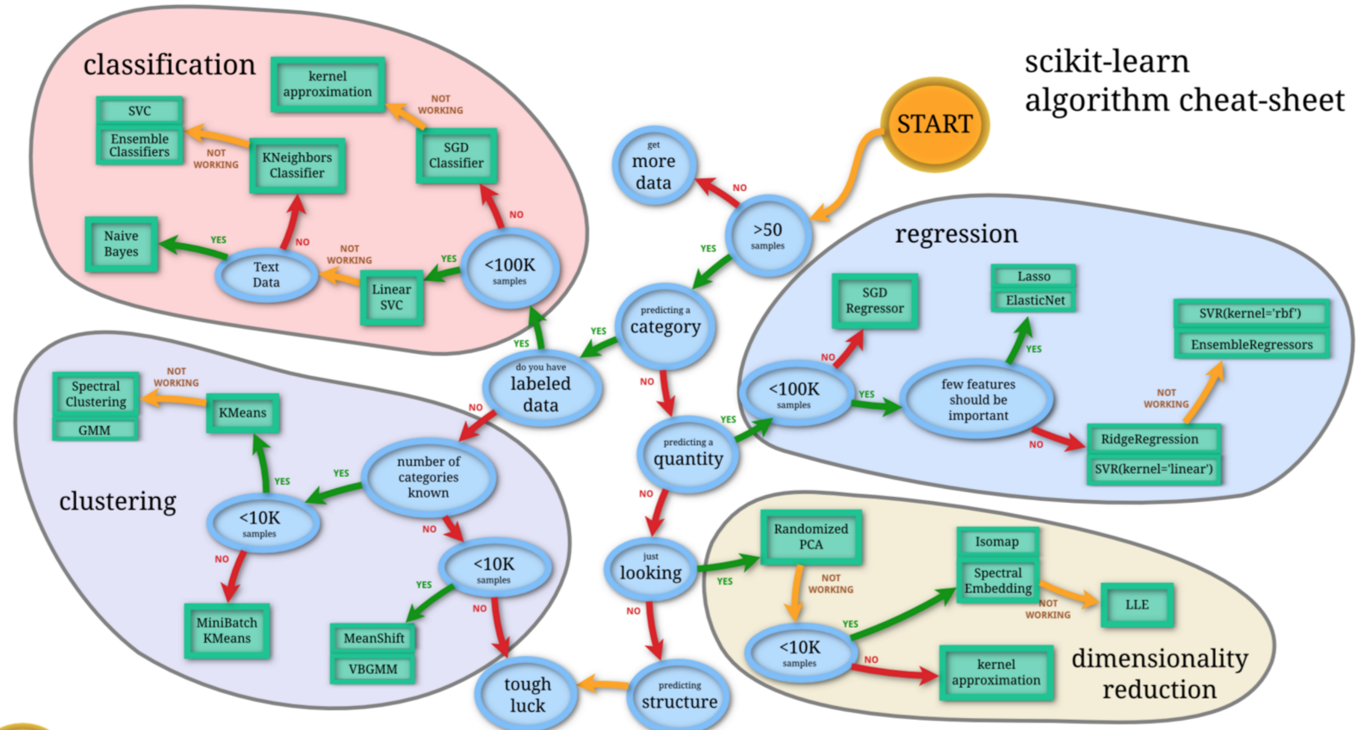


- Evaluate how the model form is interacting with the feature space.
- Identify hyperparameters (parameters that affect training or the prior, not prediction)
- Tune the fitting and prediction process by modifying these params.

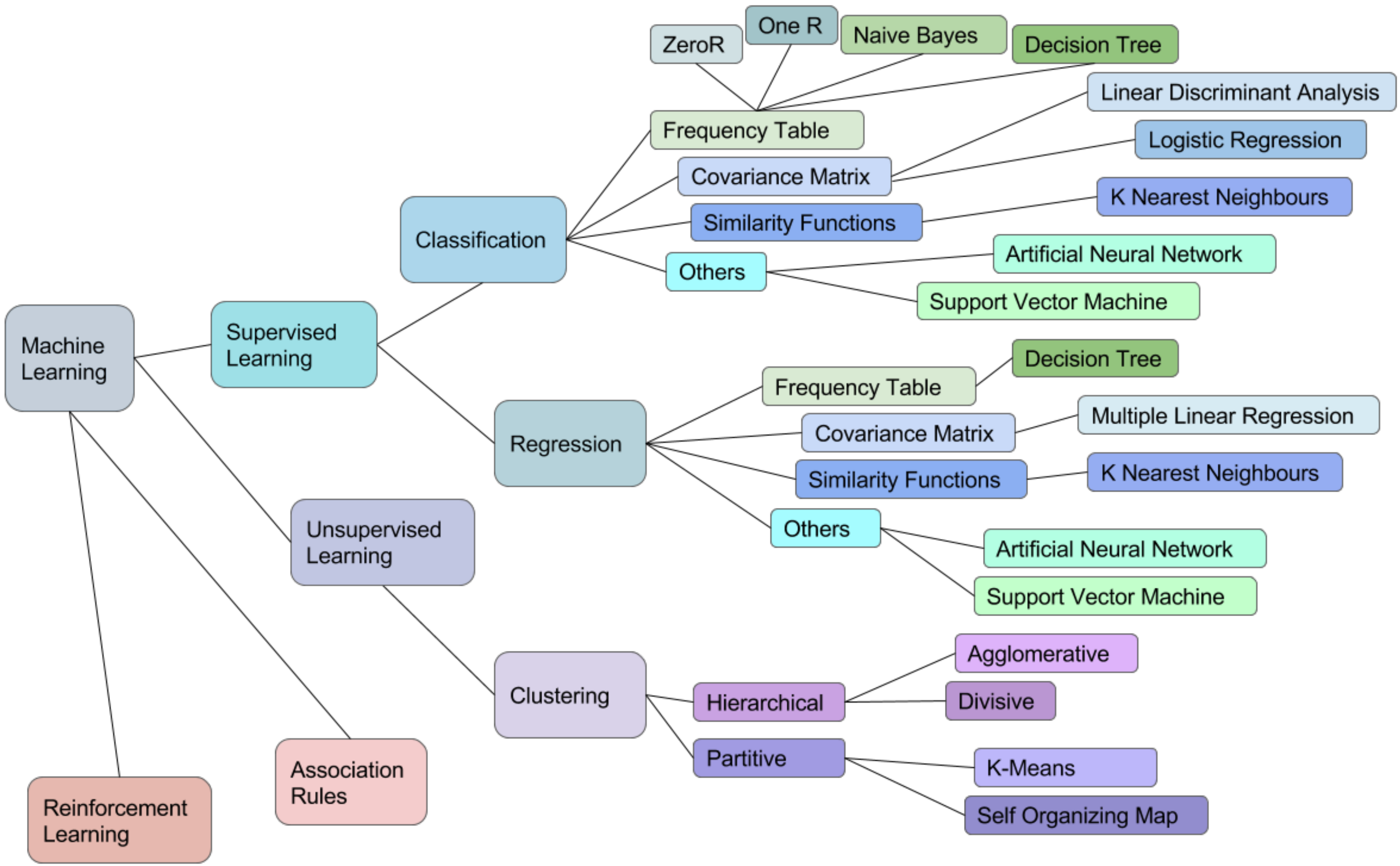
Preliminary Workflow



Choosing the Right Estimator



Back


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