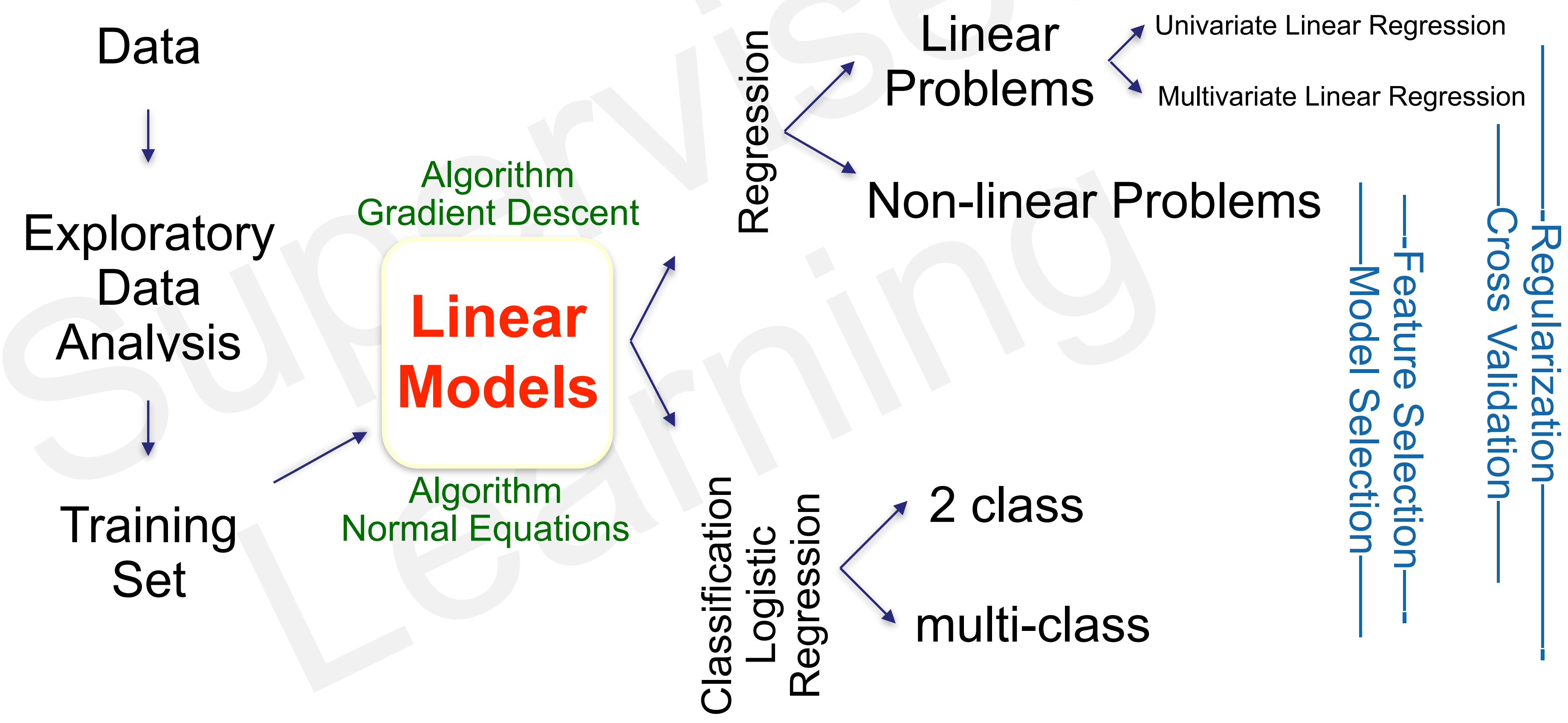
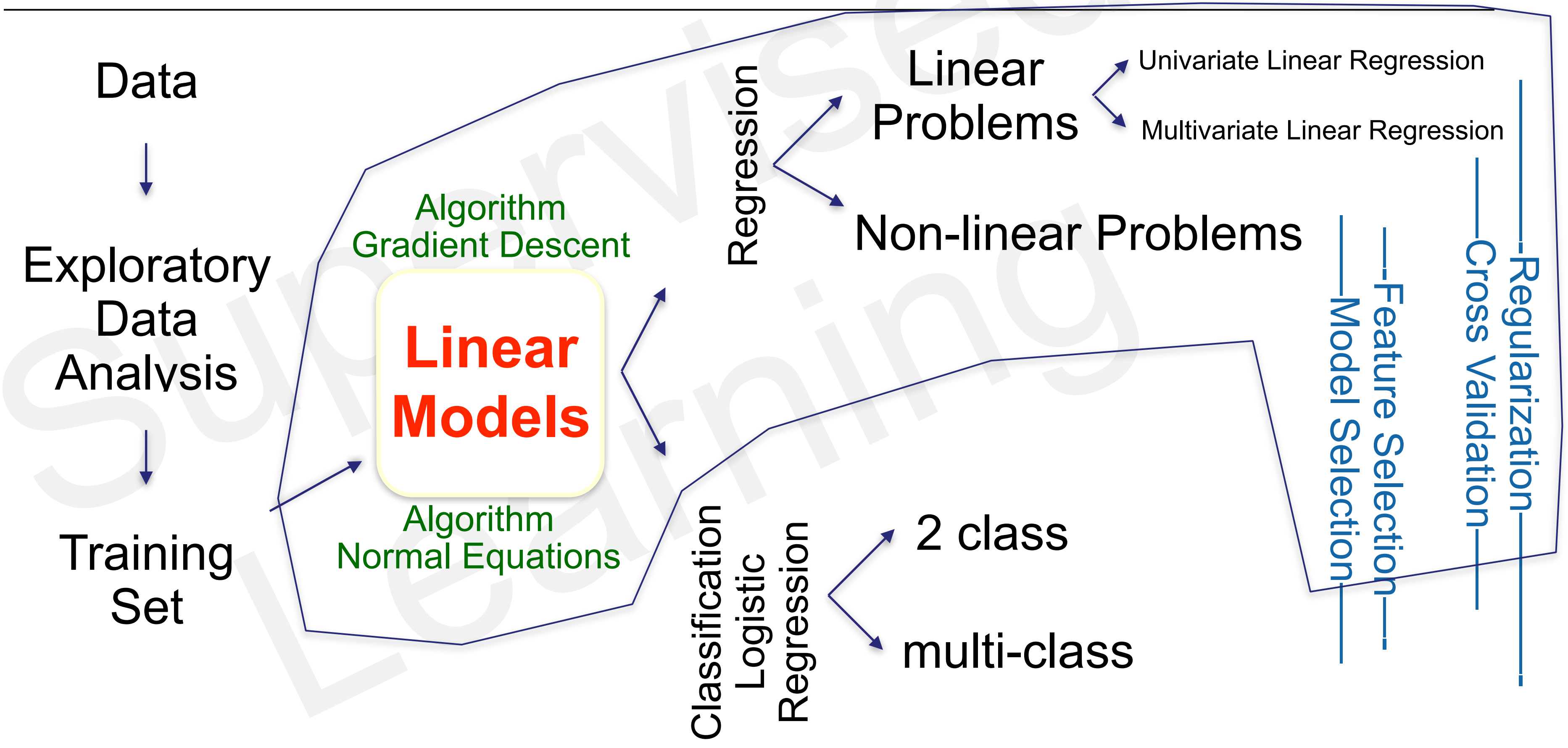
GENERAL ASSEMBLY

INTRO TO DATA SCIENCE
LECTURE 7: FEATURE SELECTION, MODEL SELECTION, REGULARIZATION

WHERE ARE WE ON THE DATA SCIENCE ROAD-MAP?



WHERE ARE WE ON THE DATA SCIENCE ROAD-MAP?



KEY CONCEPTS - FEATURE SELECTION

- Choosing the inputs to your model
- Depending on the number of features you have you might decide to adopt a ‘brute force’ approach
- e.g. africa soil inputs

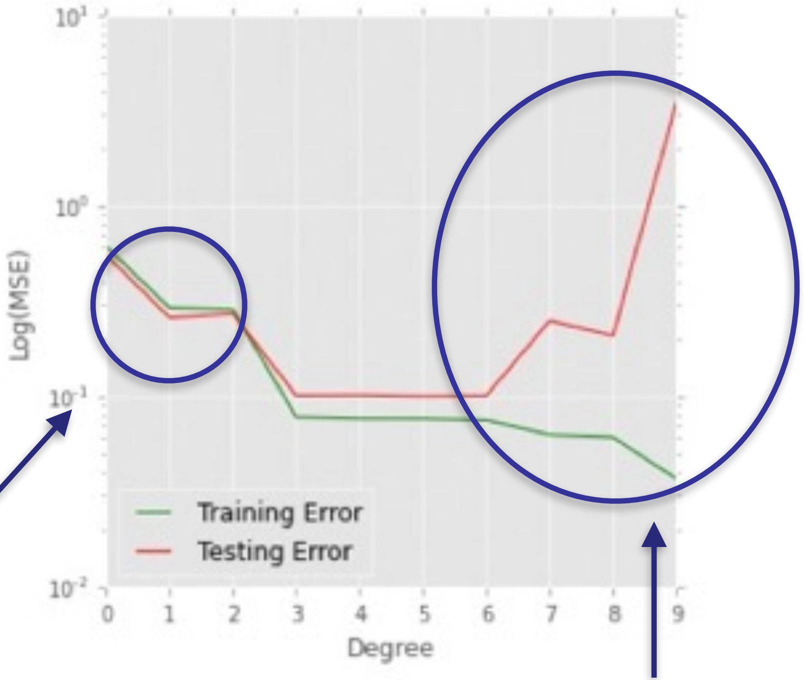
KEY CONCEPTS - MODEL SELECTION & FEATURE SELECTION

- Both Feature Selection and Model Selection need to be optimized
- The mechanism by which you choose which features to use and how complex the model should be is a matter of judgement. If the search space is large then brute force is not really an option
- Validation is the mechanism by which you optimize over a set of features and models

Linear models are prone to:

- under-fitting (bias), and
- over-fitting (variance)

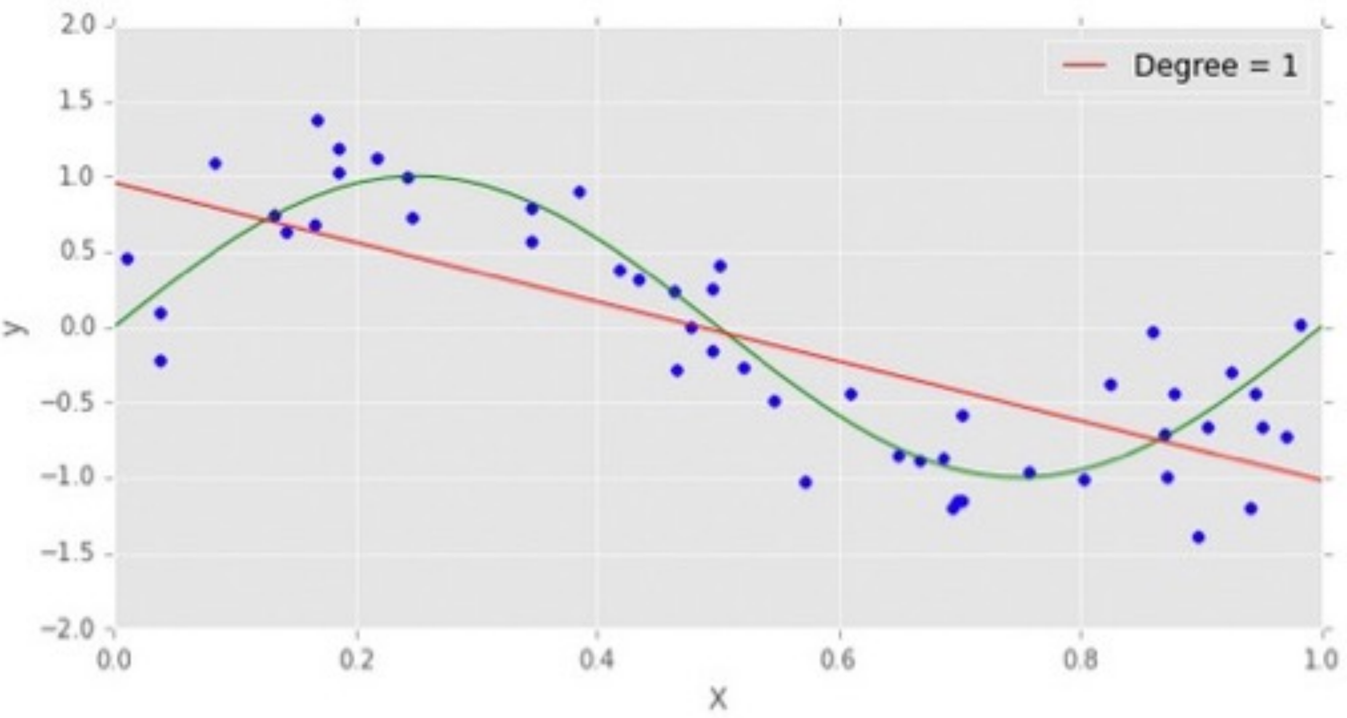
What does this actually look like?



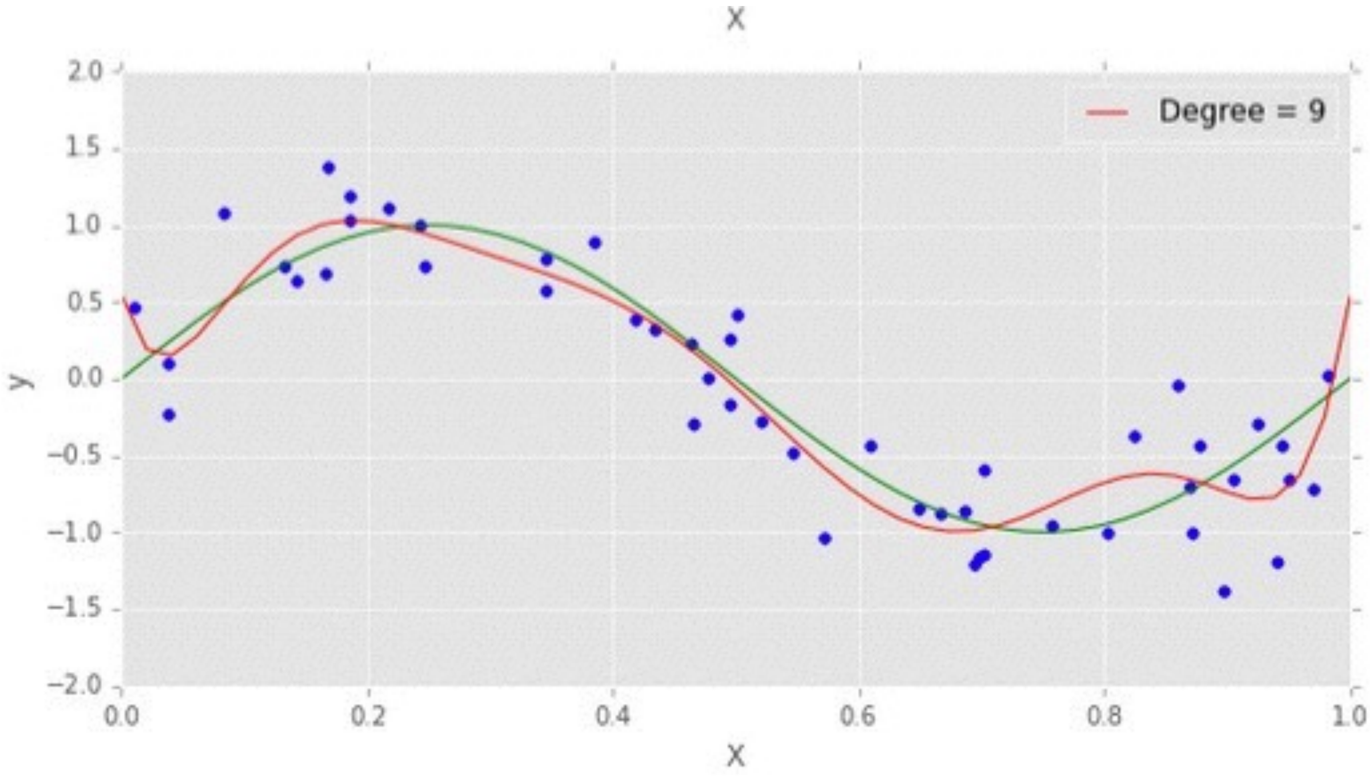
Under-fit
High Bias

Over-fit
High Variance

Key Concepts - High Bias - Under-fitting



KEY CONCEPTS - HIGH VARIANCE - OVER-FITTING



KEY CONCEPTS - OVER-FITTING

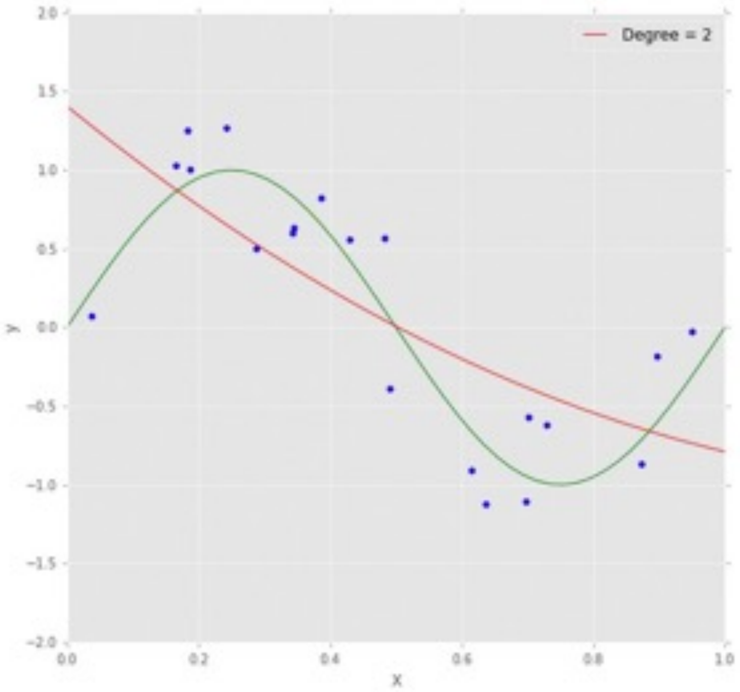
- Too many features and/or too complex a model can cause over-fitting
- While it may be tempting to reduce the complexity of a model and/or reduce the number of features over-fitting can be controlled by regularization
- In general the complexity of your features (number and kind) should be determined by the complexity of the problem you are trying to solve AND NOT by a desire to get the model to fit the data

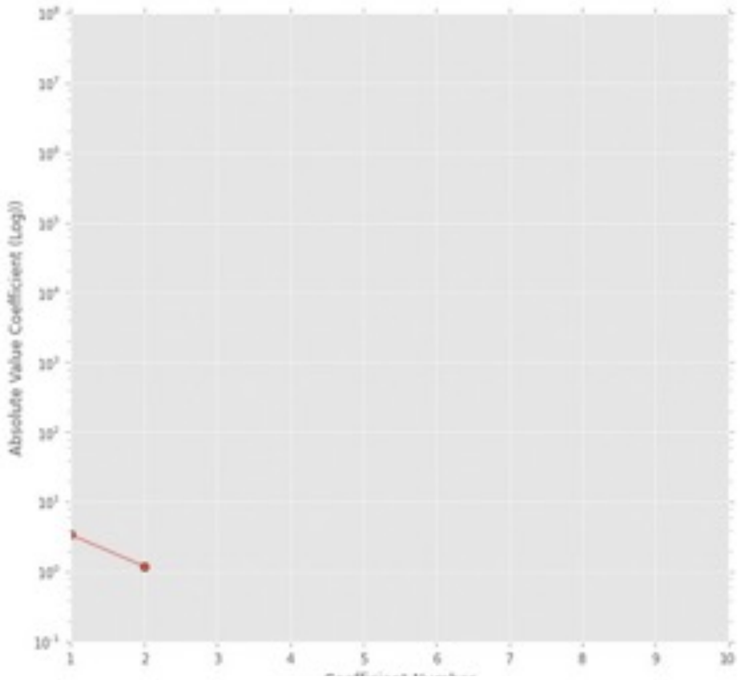
KEY CONCEPTS - REGULARIZATION

- Once features have been chosen - number and type, then fitting the model is controlled by regularization
- Linear models should always be regularized
- To see what regularization achieves let’s examine the size of our model parameters (θ) as over-fitting occurs
- Understanding this will suggest a solution to the problem

KEY CONCEPTS - UNDER & OVER-FITTING

Here we have a simple model that is under-fitting the training data (blue points)
The magnitude of the model parameters is between 1 and 10



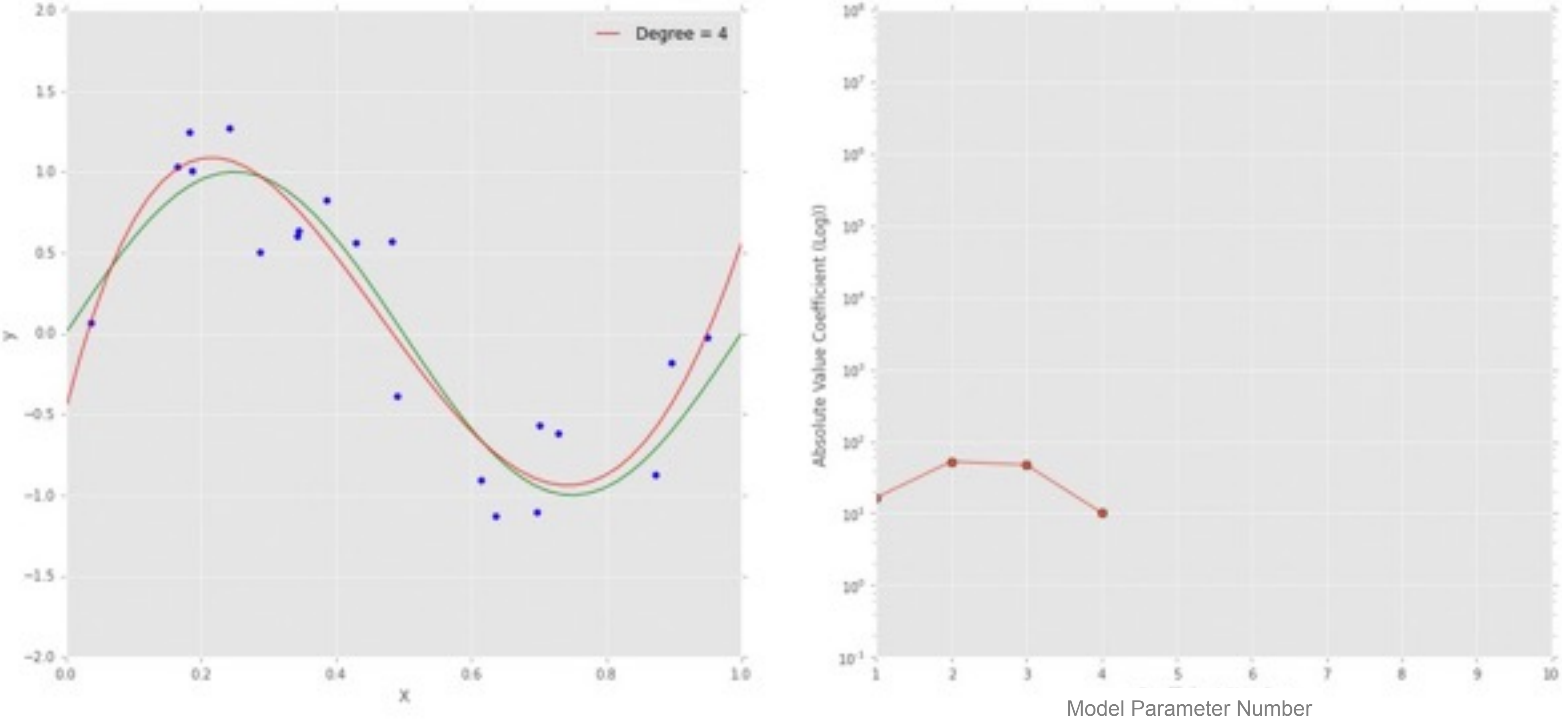


Model Parameter Number

KEY CONCEPTS - UNDER & OVER-FITTING

A more complex model that fits well.

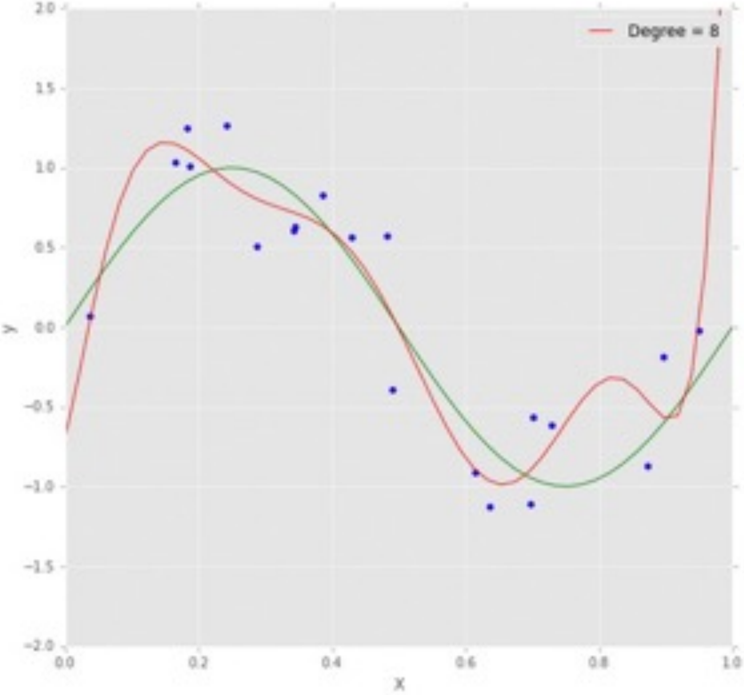
The magnitude of the model parameters is between 10 and 100

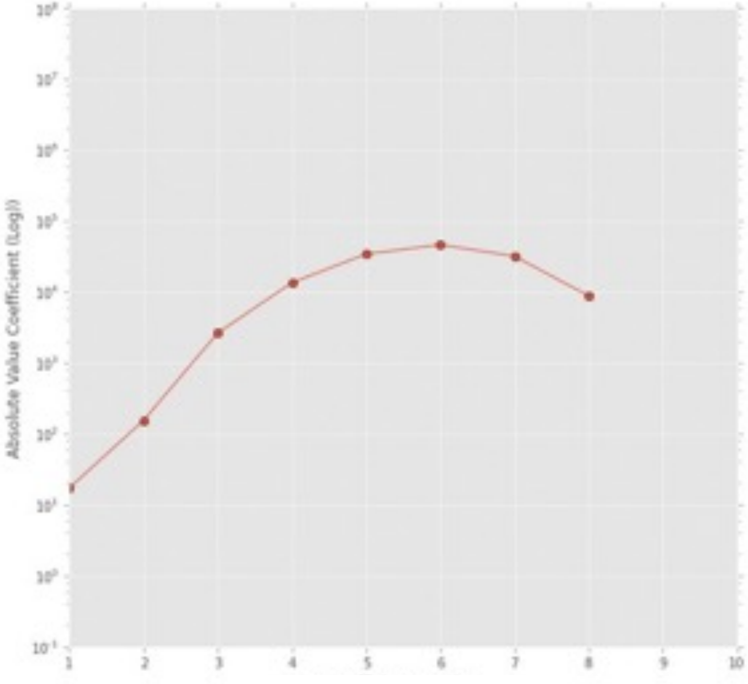


KEY CONCEPTS - UNDER & OVER-FITTING

This model is over-fitting the training data

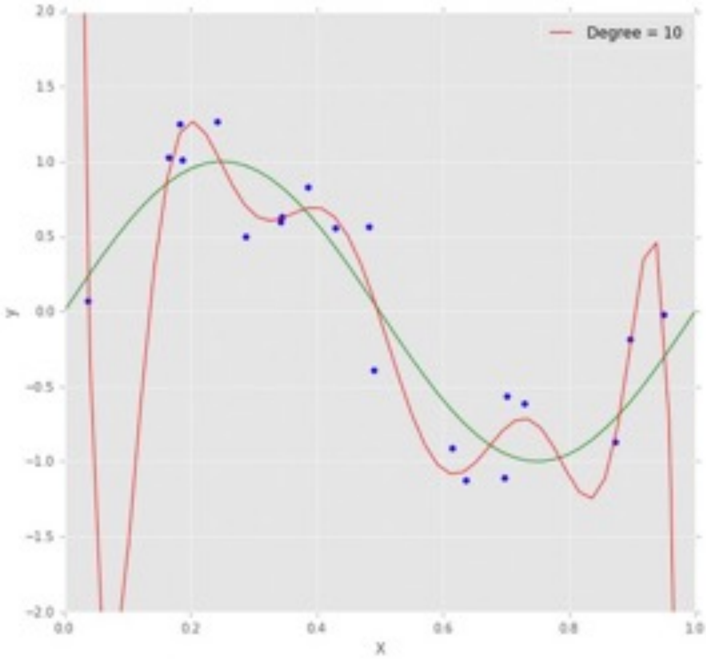
The magnitude of the model parameters is between 10 and 100000!

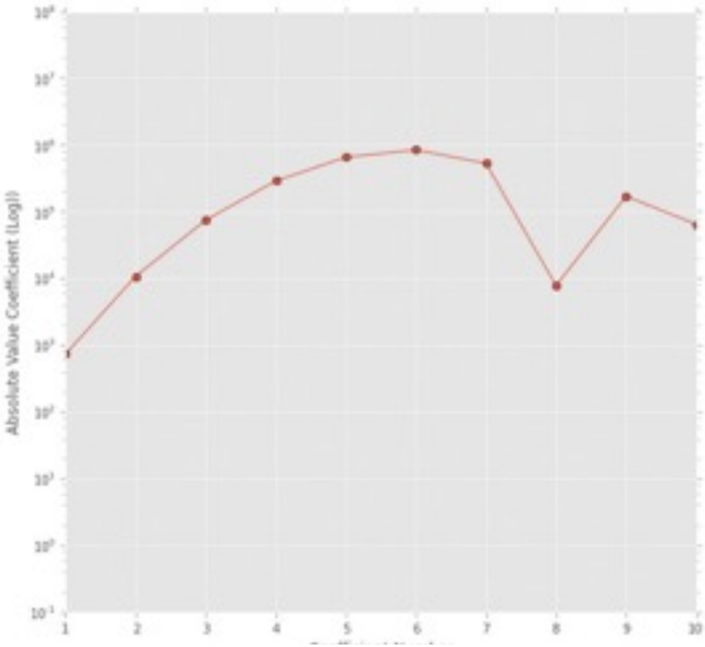




KEY CONCEPTS - UNDER & OVER-FITTING

Severe over-fitting
The magnitude of the model parameters is between 100 and 1000000!!





Model Parameter Number

- Over-fitting is associated with larger model parameter magnitudes

- Therefore, one solution might be to penalize large parameters while fitting the model

- This is our original cost function - minimizing sum of squares

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (y_i - \hat{y}_i)^2$$

- What would happen to the magnitudes of the model parameters if we modified the cost function like this:

$$J(\theta) = \frac{1.0}{2m}\left[\sum_{i=1}^{m}(y_i - \hat{y}_i)^2 + 1000 * \theta_3 + 1000 * \theta_4\right]$$

- Not only would this minimize the sum of squared errors but the two model parameters would also be constrained. Large model parameter values would be penalized

- In general, therefore, we modify the cost function to be:

$$J(\theta) = \frac{1.0}{2m}\left[\sum_{i=1}^{m}(y_i - \hat{y}_i)^2 + \lambda \sum_{j}^{N} \theta_j\right]$$

- λ is called the regularization parameter. The bigger λ is the more the magnitudes of θ will be penalized

- The story doesn't end there, however. The exact mathematical form of the regularization parameters can be altered to penalize the model parameters in different ways.

$$J(\theta) = \frac{1.0}{2m}\left[\sum_{i=1}^{m}(y_i - \hat{y}_i)^2 + \lambda \sum_{j}^{N} \theta_j\right]$$

Key Concepts - Ridge Regression, Lasso Regression

- Ridge Regression and Lasso Regression are two forms of regression where the regularization formulae differ
- Both accept regularizing parameters
- But the resulting models returned by these algorithms are significantly different

Key Concepts - Ridge Regression, Lasso Regression

- Ridge (Tikhonov regularization) = L2-norm = Euclidean norm of the sum of the parameters, θ, of the model = $\lambda||\theta||^2$

  -As the penalty is increased (λ) ALL parameters shrink, while still remaining non-zero

- Lasso (Least Absolute Shrinkage and Selection Operator) = L1-norm = Least Absolute Deviation = $\lambda||\theta||$

  -As the penalty is increased MORE of the parameters will shrink to zero

  -This can discard features

http://www.chioka.in/differences-between-the-l1-norm-and-the-l2-norm-least-absolute-deviations-and-least-squares/

KEY CONCEPTS - ELASTICNET

- Elastic Net is a linear combination of the Ridge and Lasso regularizers

http://scikit-learn.org/stable/modules/generated/sklearn.linear_model.Ridge.html

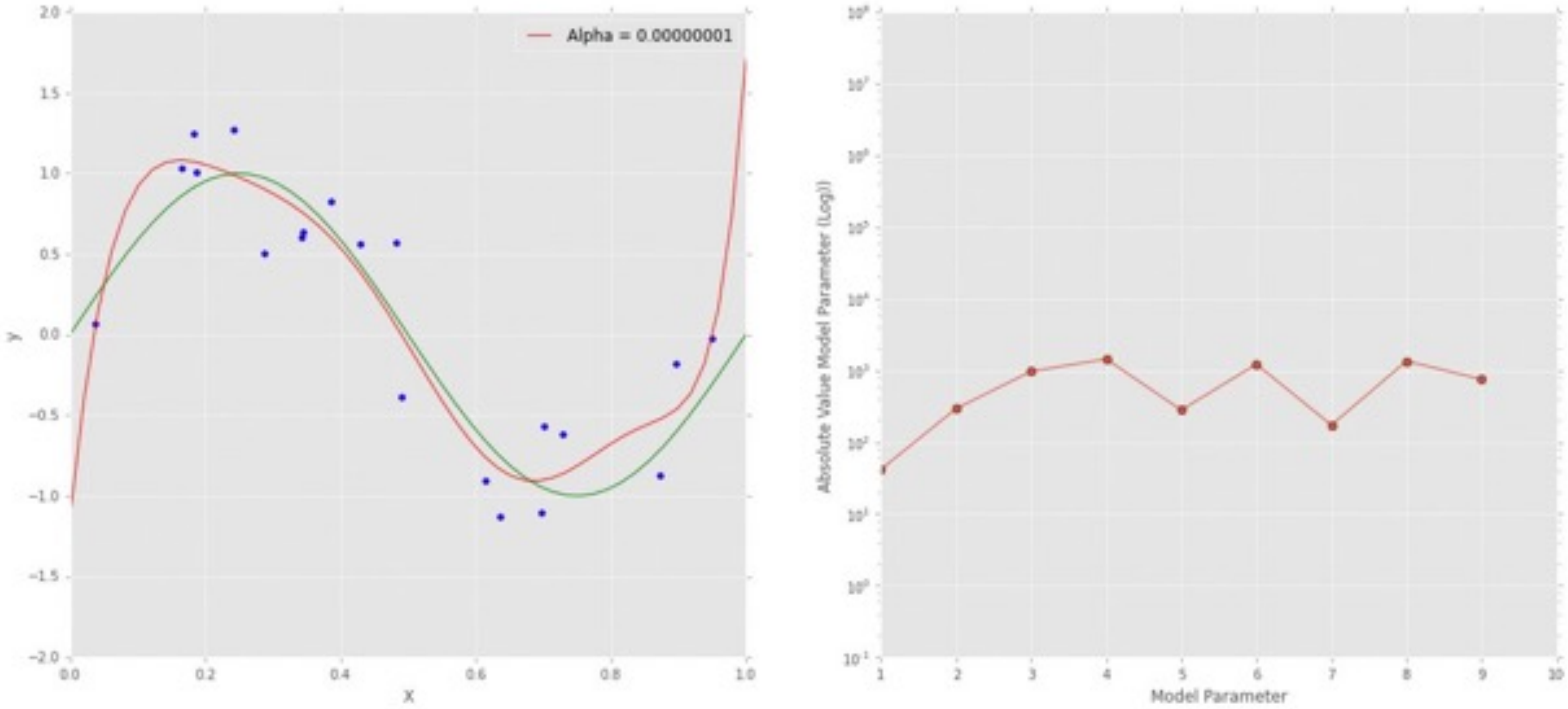
http://scikit-learn.org/0.11/modules/generated/sklearn.linear_model.Lasso.html

http://scikit-learn.org/stable/modules/generated/sklearn.linear_model.ElasticNet.html

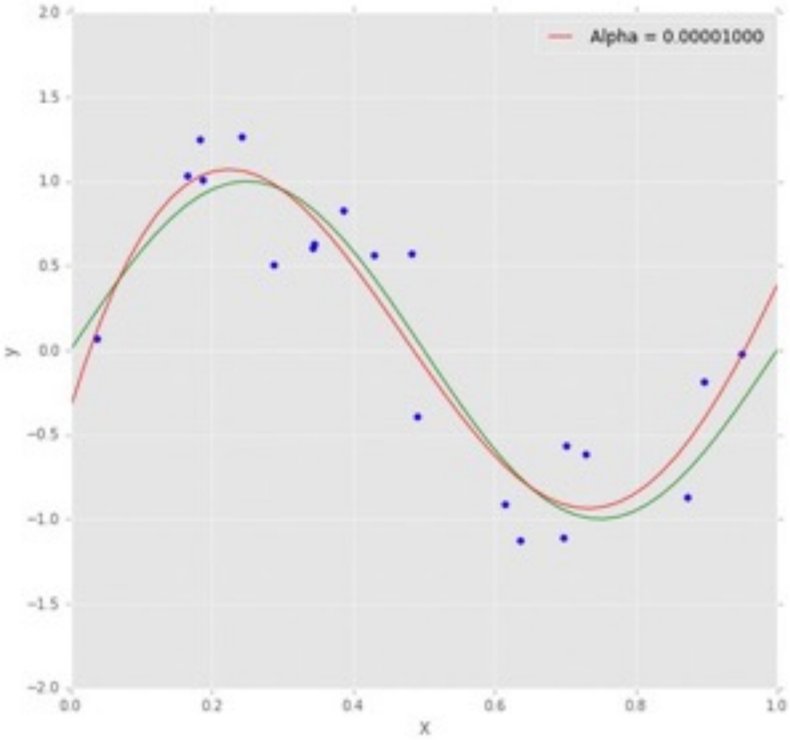
Key Concepts - Ridge Regression, Lasso Regression

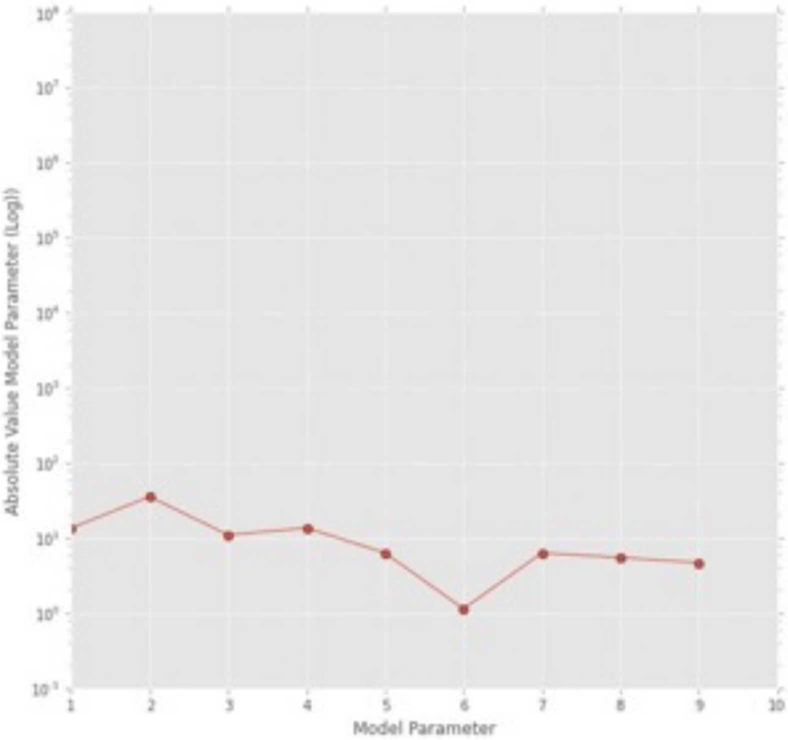
- Sklearn implementation - alpha is the regularizer
- Ridge, Lasso and ElasticNet internally use gradient descent
  -You will notice a ‘maximum iterations’ argument
- In short the algorithms take care of the method and mechanism of optimization for you

KEY CONCEPTS - RIDGE REGRESSION

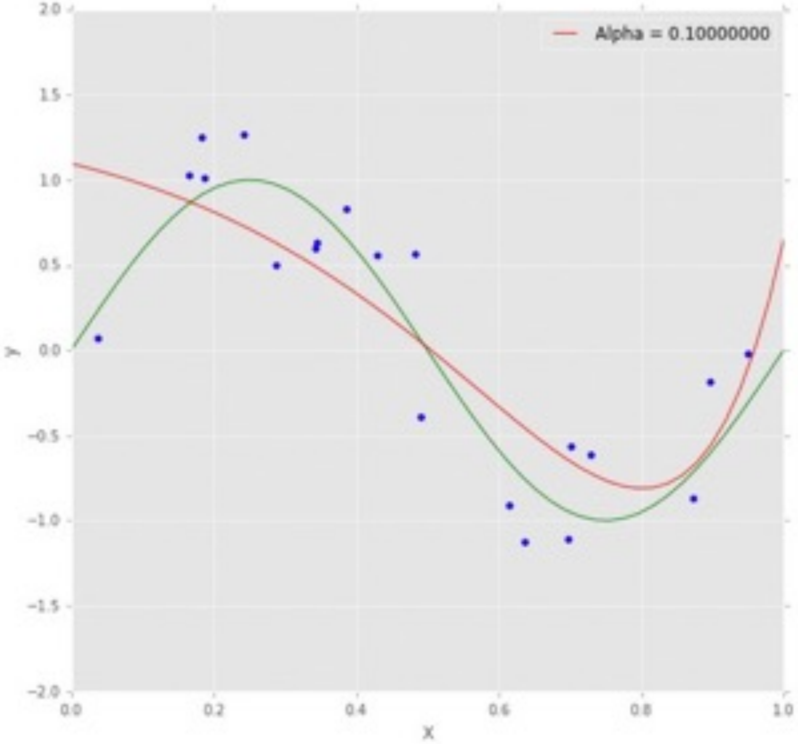


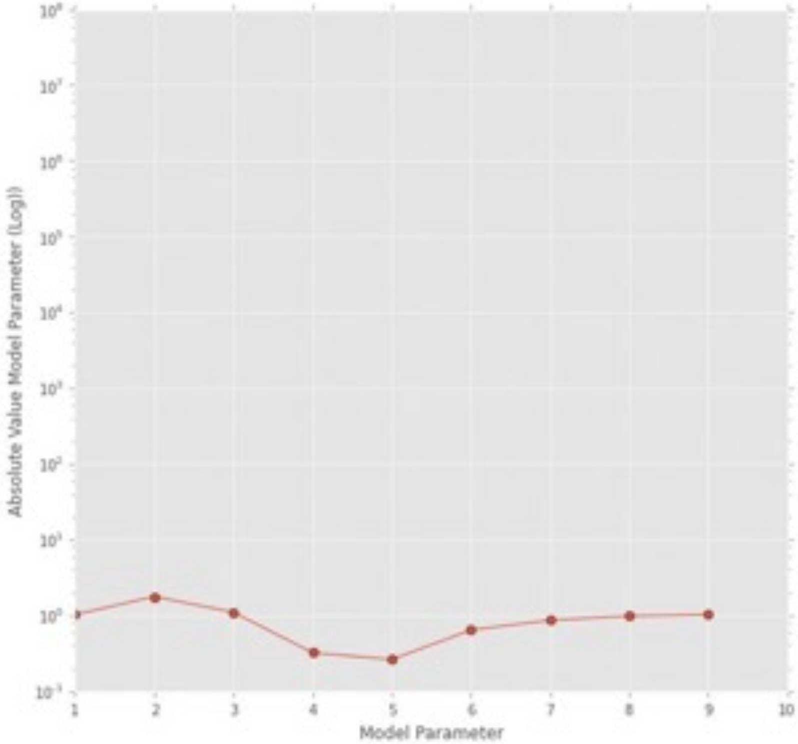
Key Concepts - Ridge Regression



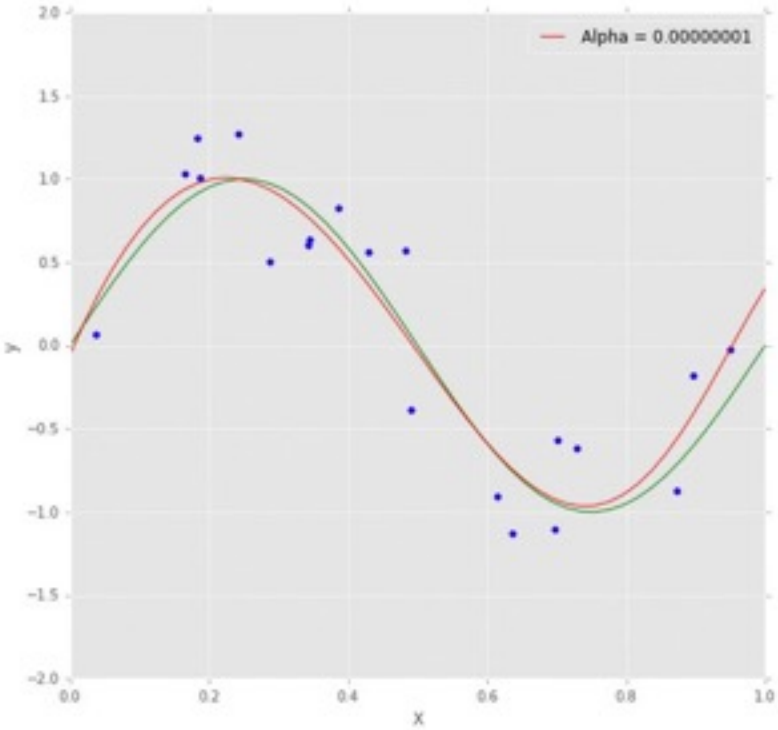


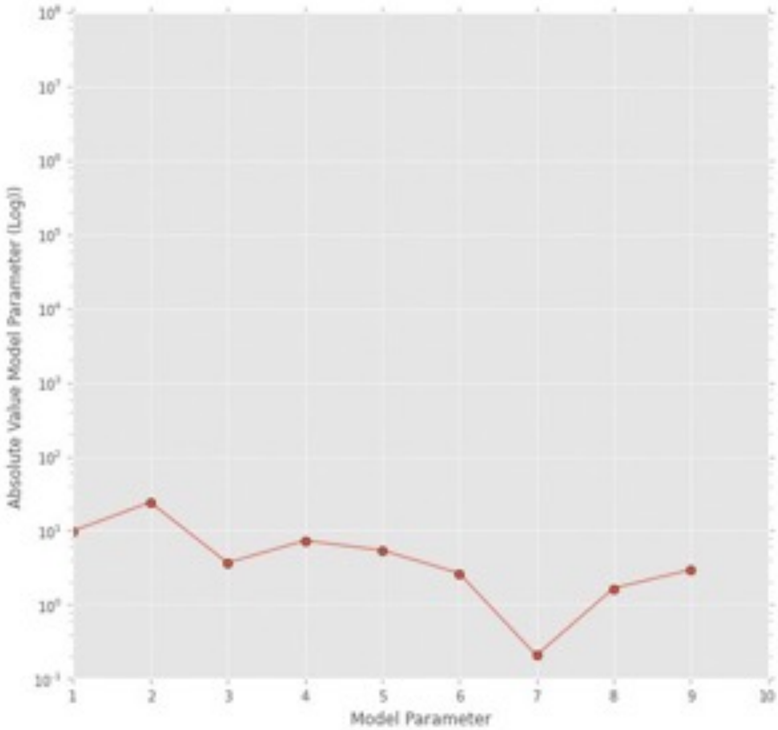
KEY CONCEPTS - RIDGE REGRESSION



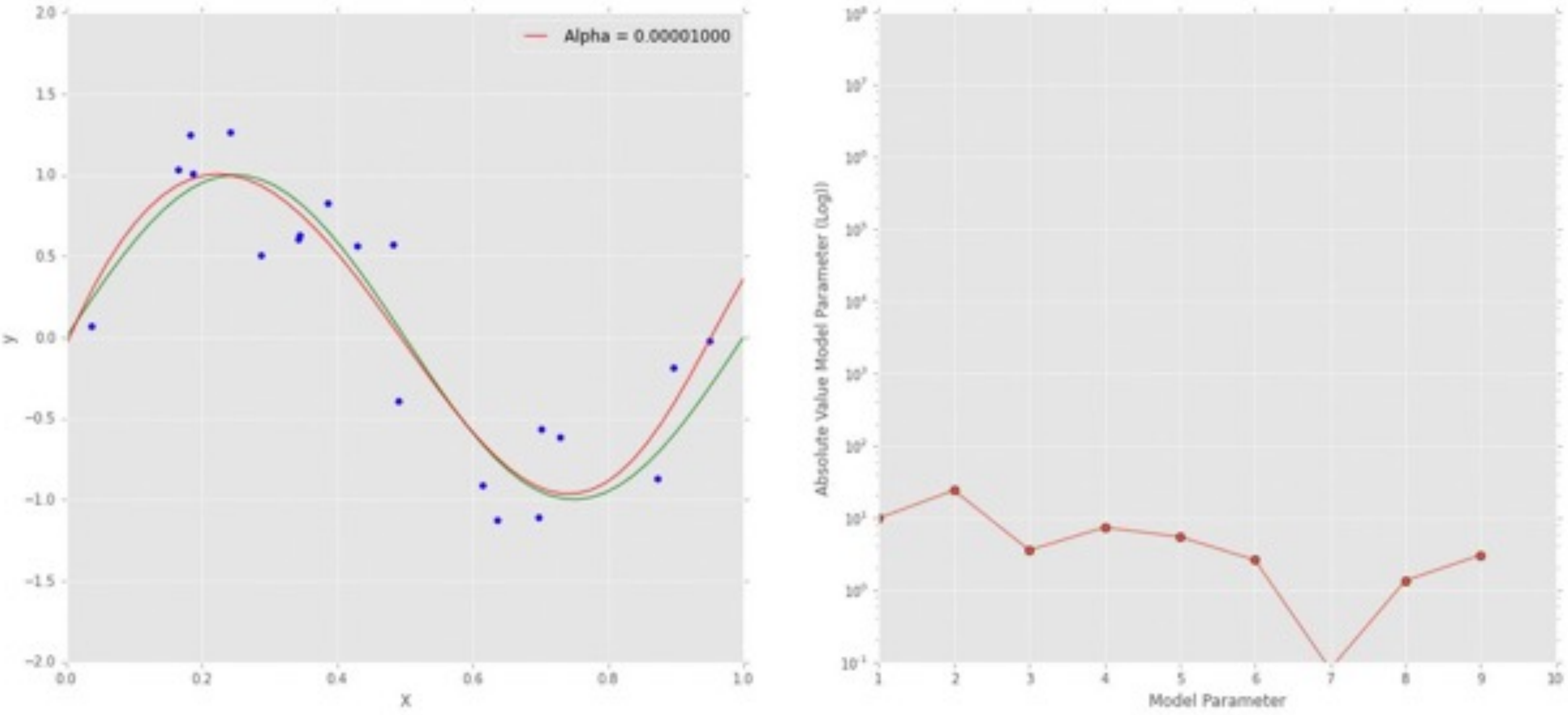


KEY CONCEPTS - LASSO REGRESSION

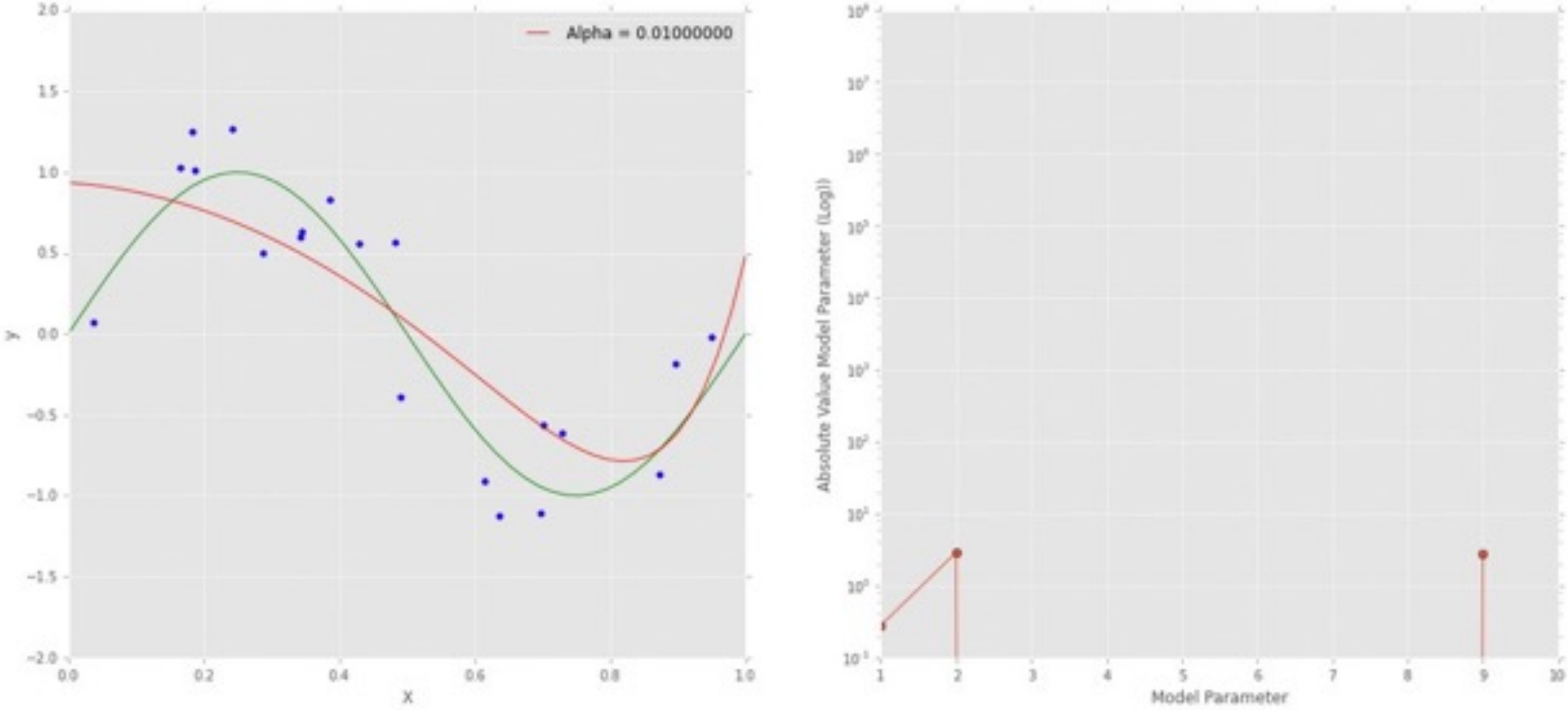




KEY CONCEPTS - LASSO REGRESSION



Key Concepts - Lasso Regression



KEY CONCEPTS - IMPROVING THE PERFORMANCE OF A MACHINE LEARNING ALGORITHM

1. Get more training examples *
2. Try a smaller set of features
3. Try additional features
4. Try different features
5. Try different regularization parameters

* Be careful not to go down a blind avenue. Collecting more data, may, for example, cost a lot of money and cost a lot of time, and may yield not net improvement in the model!

Key Concepts - Diagnostics for a Machine Learning Algorithm

1. Both bias (under-fitting) and variance (over-fitting) result in poor generalization
2. Make sure you split your data
    - use the datasets correctly!
    - 70/30 or 60/20/20 (Equal size is ideal)
    - if data is limited use S-fold cross validation
3. Monitor a metric that will indicate good generalization performance = mse on the validation set

4. Choose the model with the lowest mse on the validation set
5. If you have a test set then use it to report the results of your best model

Key Concepts - Regularization, Bias and Variance

1. Plot the degree of polynomial vs training AND validation error

   -High bias = high training and validation error

   -High variance = low training/high validation error

2. Use regularization to prevent over-fitting
3. Be aware that the values for the regularization of different algorithms differ!! One size does not fit all

KEY CONCEPTS - REGULARIZATION, BIAS AND VARIANCE

1. Plot the regularization parameters vs training error AND validation error

   - High bias = large regularization parameter, high training AND high validation error

   - High Variance = low regularization parameter, low training/ high validation error

1. High Bias:
    - Generally means the model is too simple
        - Try additional features
        - Try different features (higher degree polynomial)
        - Check your regularization parameter (is it too high?)

1. High Variance:
    - Try a smaller set of features
        - Either less number of features or a lower degree polynomial
    - Check your regularization parameter (is it too low?)

Key Concepts - Regularization, Bias and Variance

1. Learning curves may be useful, but often very noisy, messy and inconclusive