Preventing Overfitting with Ridge and Lasso Regression

Scott O'Hara
TSSG–Data Analytics
Acton Library
03/30/2018

References

Applied Machine Learning in Python
University of Michigan, Prof. Kevin Collins Thompson
https://www.coursera.org/learn/python-machine-learning/home/welcome

Machine Learning: Regression
University of Washington, Profs. Emily Fox & Carlos Guestrin
https://www.coursera.org/learn/ml-regression/home/welcome

CS181 Intelligent Machines: Perception, Learning and Uncertainty
Harvard University, Prof. David Parkes, Spring 2011.

The Machine Learning Problem

One way of looking at machine learning is that we are trying to learn a hidden function in the domain we are interested in so we can make predictions about that domain.

AGENT

$$\overset{\text{Prediction}}{y} = \overset{\text{Learned Function}}{f}(\overset{\text{Features}}{X}) + \overset{\text{Noise}}{\epsilon}$$

$$y_W = F_W(X_W) + \epsilon_W$$

WORLD

Sources of Error in Machine Learning Predictions

$$y = f(X) + \epsilon$$

Reducible Error

- **Bias**
- **Variance**

Irreducible Error

- **Unmeasurable Variables**
- **Unmeasurable Variation**

Bias

Bias is the systematic error in a learning algorithm.

Bias is introduced by approximating a complex domain with a simpler model.

Bias is introduced when the model structure does not “fit” the domain.

No amount of data can fix the bias in a learning algorithm.

EXAMPLE: if your domain is non-linear and you try to represent it with a linear model, then there will be systematic errors.

Restriction Bias

A learning algorithm does not consider all possible classifiers / regressors but restricts the learning to task to a particular kind of solution.

For example:

- <u>Linear Classifier</u> classifies items by partitioning the feature space with a hyperplane.
- <u>Decision Tree</u> classifies items by projecting a tree hierarchy onto the feature space.
- <u>Neural Network</u> classifies items through the ability of features to activate neurons in a hierarchical neural structure.

Preference Bias

Among possible hypotheses that a learning algorithm may consider, prefer some hypotheses over others.

For example:

- Linear Classifier/Regressor: prefer weights on linear equations to be small. (Ridge and Lasso)
- Decision Tree: prefer shallow trees; prefer fewer nodes; prefer leaf nodes to have a minimum size; etc.
- Neural Network prefer fewer hidden units.

Variance

Variance is the error in prediction that can be attributed to the training set.

Classification and regression algorithms require a training set to optimize the parameters of the model it creates.

Different training sets can result in different models and different prediction algorithms.

The more susceptible a machine learning algorithm is to differences in the training set, the more variance it has.

Variance in a High Complexity Model

Assume we fit a high-order polynomial

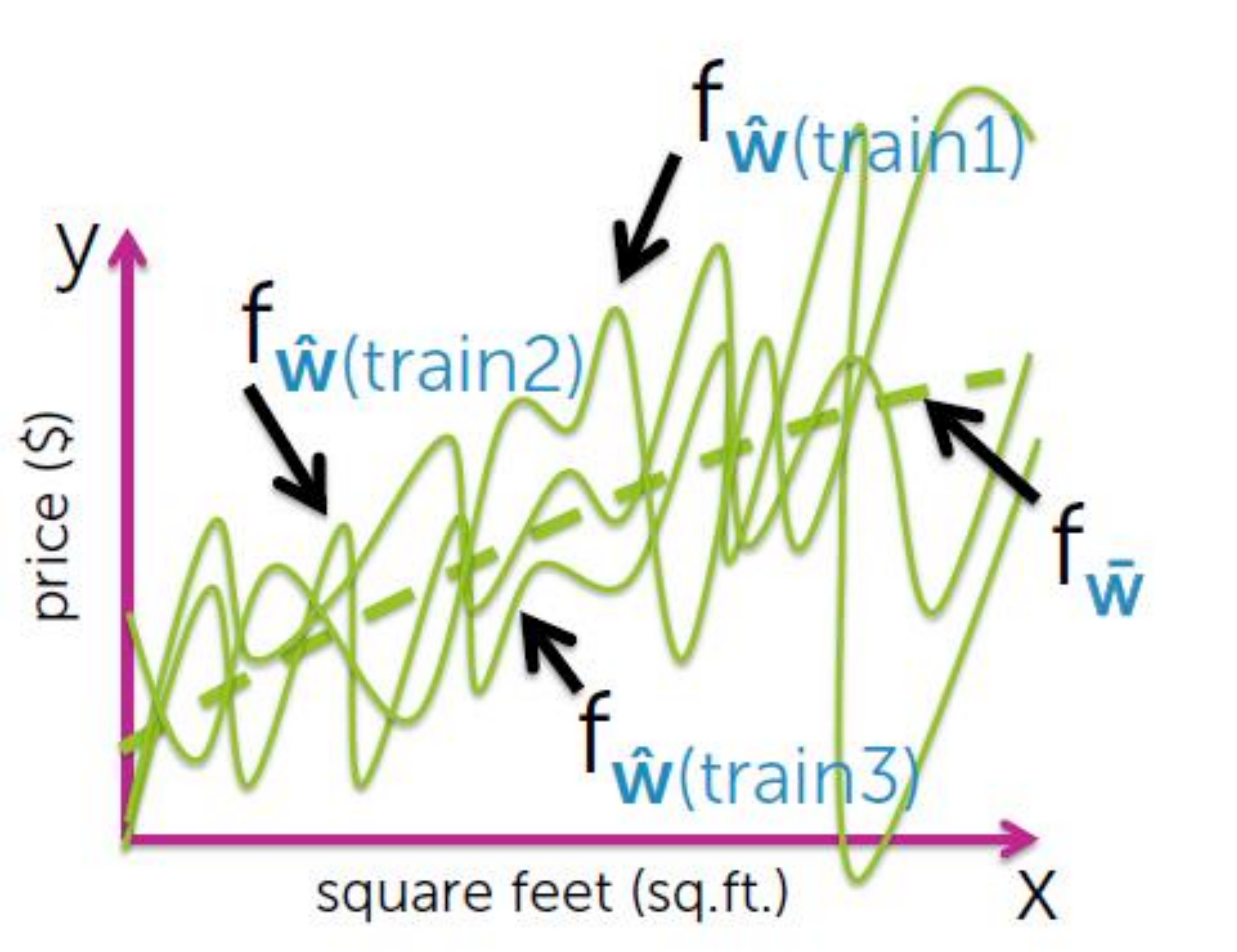
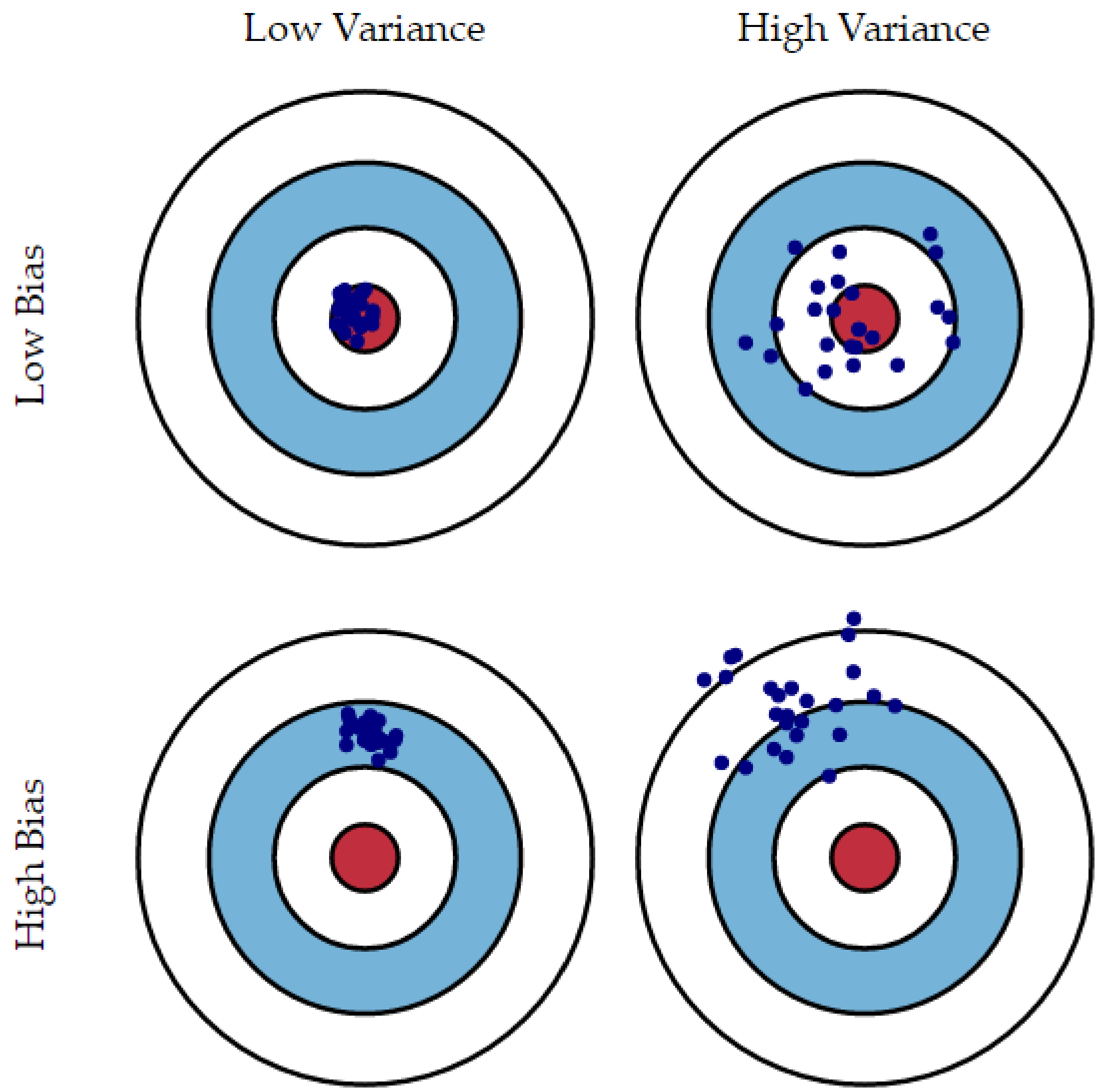


Figure Credit: Emily Fox & Carlos Guestrin, University of Washington

Bias and Variance

Figure Credit : An Introduction to Statistical Learning by Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani



The Bias-Variance Tradeoff

Ideally, to improve a machine learning algorithm, we would like to decrease bias AND decrease variance.

Unfortunately, a decrease in bias often results in an increase in variance and vice-versa.

The Problem of Overfitting

Overfitting is said to occur when the test set error is much greater than the training set error.

The greater the complexity of a model, the more likely it is to fit noise or spurious patterns in the training data.

A simpler model is more immune to noise, but it unable to capture more complex relationships.

So the game becomes finding an optimal balance between bias and variance.

The Bias-Variance Tradeoff

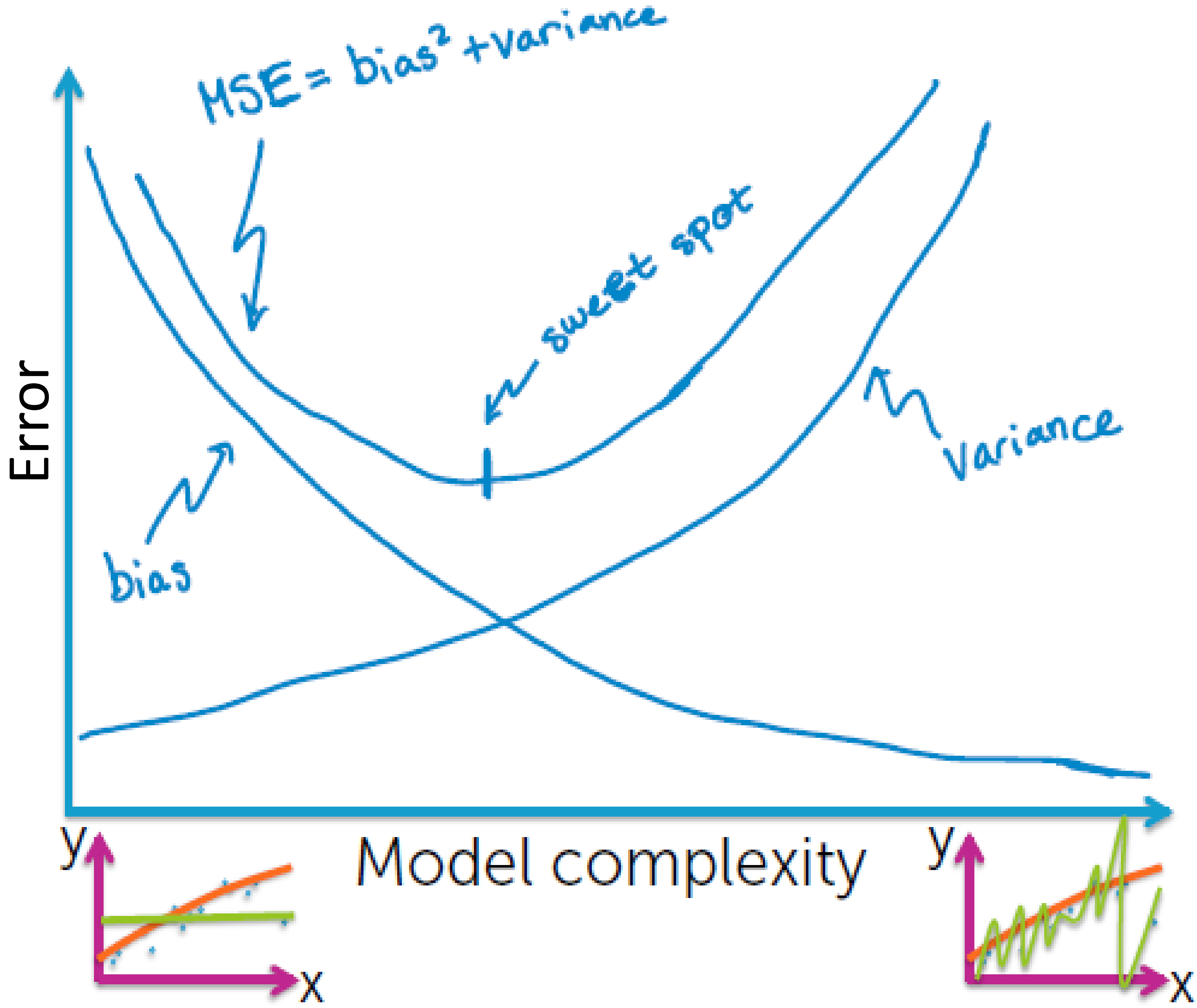


Figure Credit: Emily Fox & Carlos Guestrin, University of Washington, Coursera Machine Learning Specialization.

Ways to Address Overfitting: Avoid it

- **Use More Data:** Need at least 5-10 x data for each additional parameter.
- **Use Cross-Validation:** Make better use of existing data by using cross-validation. This requires greater computation.
- **Use Simpler Models:** *Occam's Razer:* prefer simpler explanations, restrict the classes of models to consider.

Ways to Address Overfitting: Regularization

- Explicitly penalize model complexity.
- Example: Decision Trees: limit tree depth.
- Example: Ridge Regression -$min_W(RMSE) + \lambda w \cdot w$ for suitable a λ.

Simple Linear Regression

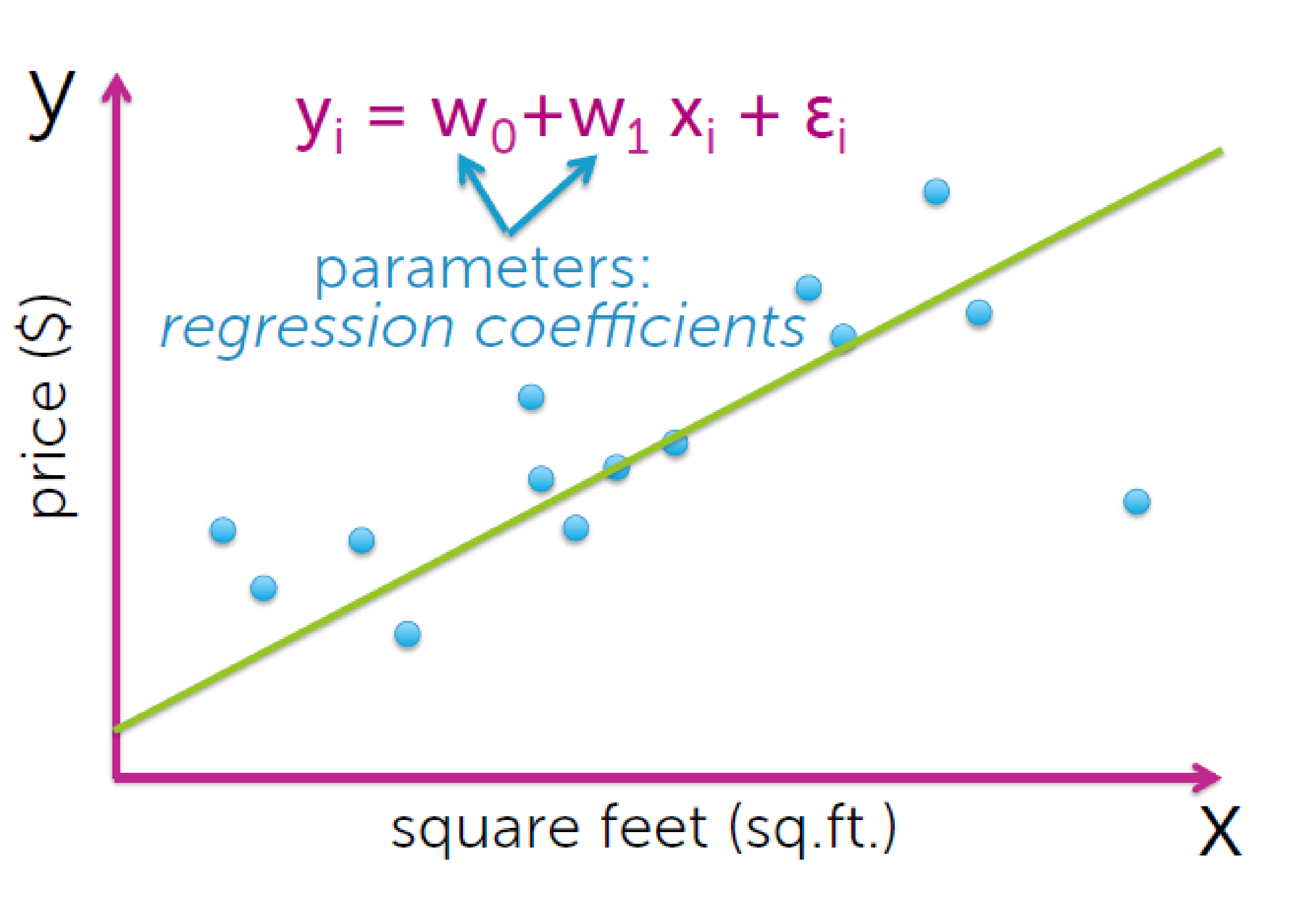


Figure Credit: Emily Fox & Carlos Guestrin, University of Washington

Multiple Linear Regression

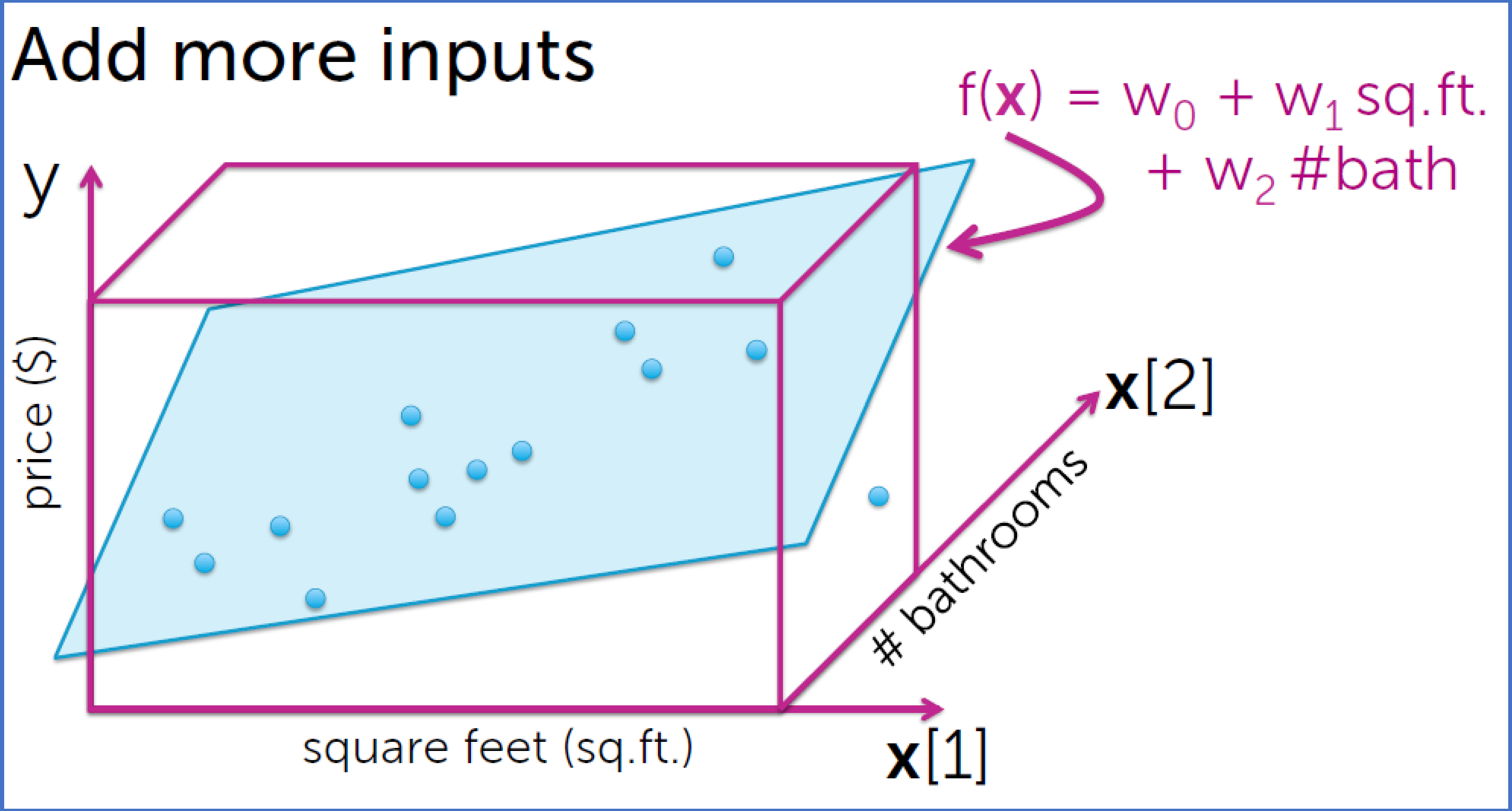


Figure Credit: Emily Fox & Carlos Guestrin, University of Washington

Polynomial Regression

Model:

$$y_i = w_0 + w_1 x_i + w_2 x_i^2 + \ldots + w_p x_i^p + \varepsilon_i$$

treat as different **features**

feature 1 = 1 (constant)	*parameter* 1 = w_0
feature 2 = x	*parameter* 2 = w_1
feature 3 = x^2	*parameter* 3 = w_2
…	…
feature p+1 = x^p	*parameter* p+1 = w_p

Figure Credit: Emily Fox & Carlos Guestrin, University of Washington

Error Sum of Squares

$$SSE = \sum_{i=1}^{n} \left(y_i - \sum_{j=1}^{p} x_{ij} w_j \right)^2$$

LASSO and Ridge Regression

A tuning parameter is added which lets you change the complexity or smoothness of the model.

The regularization value imposes a special penalty on complex models.

L2 Regularization – Ridge Regression

- The L2 penalty is the sum of the square of the weights.
- Adds “squared magnitude” of coefficient as penalty term to the loss function.
- Penalizes large coefficients, which are associated with overfitting in linear regression.

$$\sum_{i=1}^{n}\left(y_i - \sum_{j=1}^{p} x_{ij} w_j\right)^2 + \lambda \sum_{j=1}^{p} w_j^2$$

Figure Credit: Adapted from Gene Olafsen, Regularization, 3/14/18

L1 Regularization – LASSO Regression

- The L1 penalty is the sum of the weight magnitudes.
- Lasso shrinks the less important feature's coefficient to zero removing some feature altogether. This works well for feature selection in cases having a huge number of features.
- As lambda increases, the number of non-zero weights decreases.

$$\sum_{i=1}^{n}\left(y_i - \sum_{j=1}^{p} x_{ij} w_j\right)^2 + \boldsymbol{\lambda} \sum_{j=1}^{p} \left|w_j\right|$$

Figure Credit: Adapted from Gene Olafsen, Regularization, 3/14/18

Change in Weights as Lambda Increase (L2)

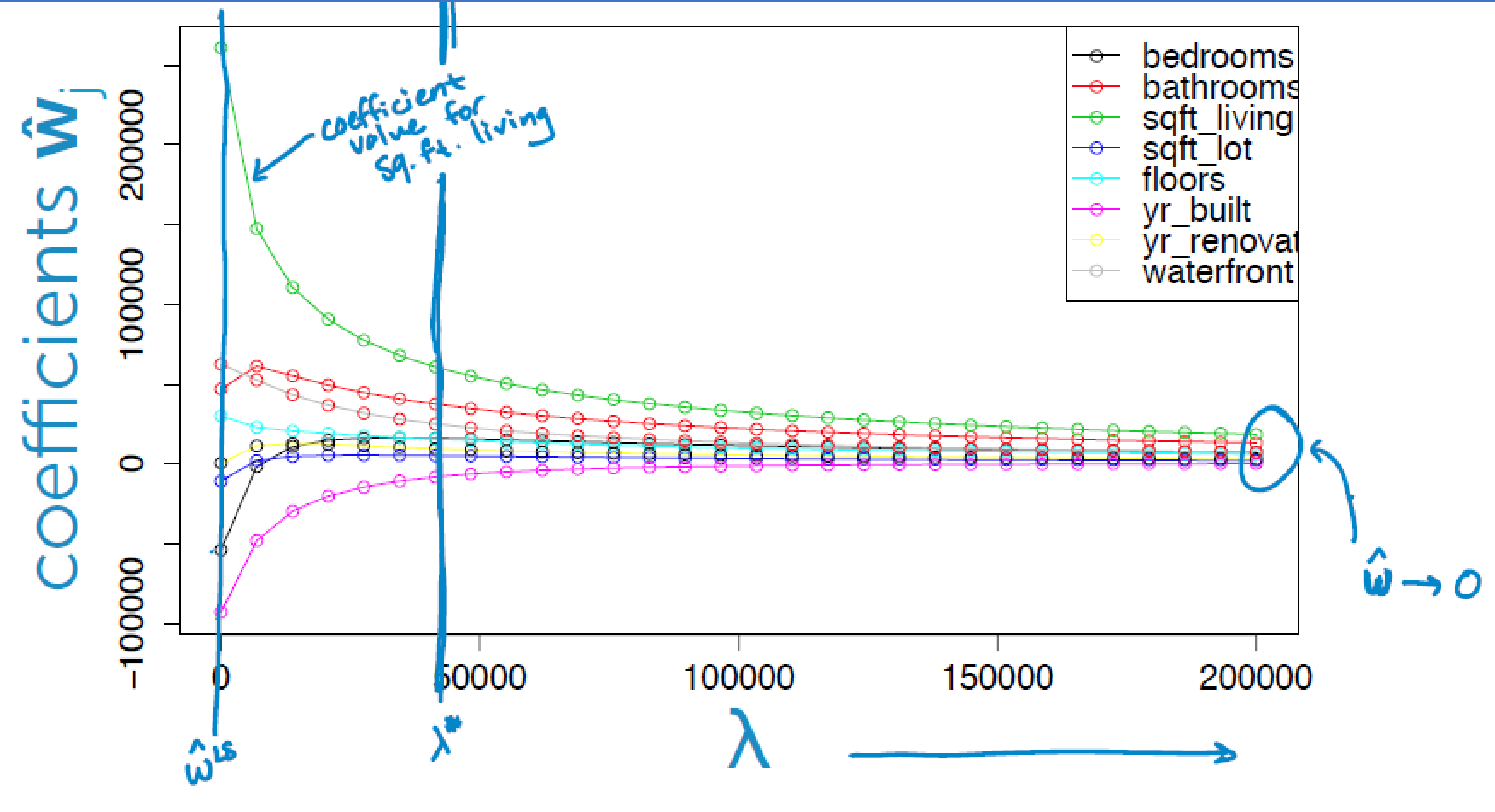


Figure Credit: Emily Fox & Carlos Guestrin, University of Washington

Change in Weights as Lambda Increase (L1)

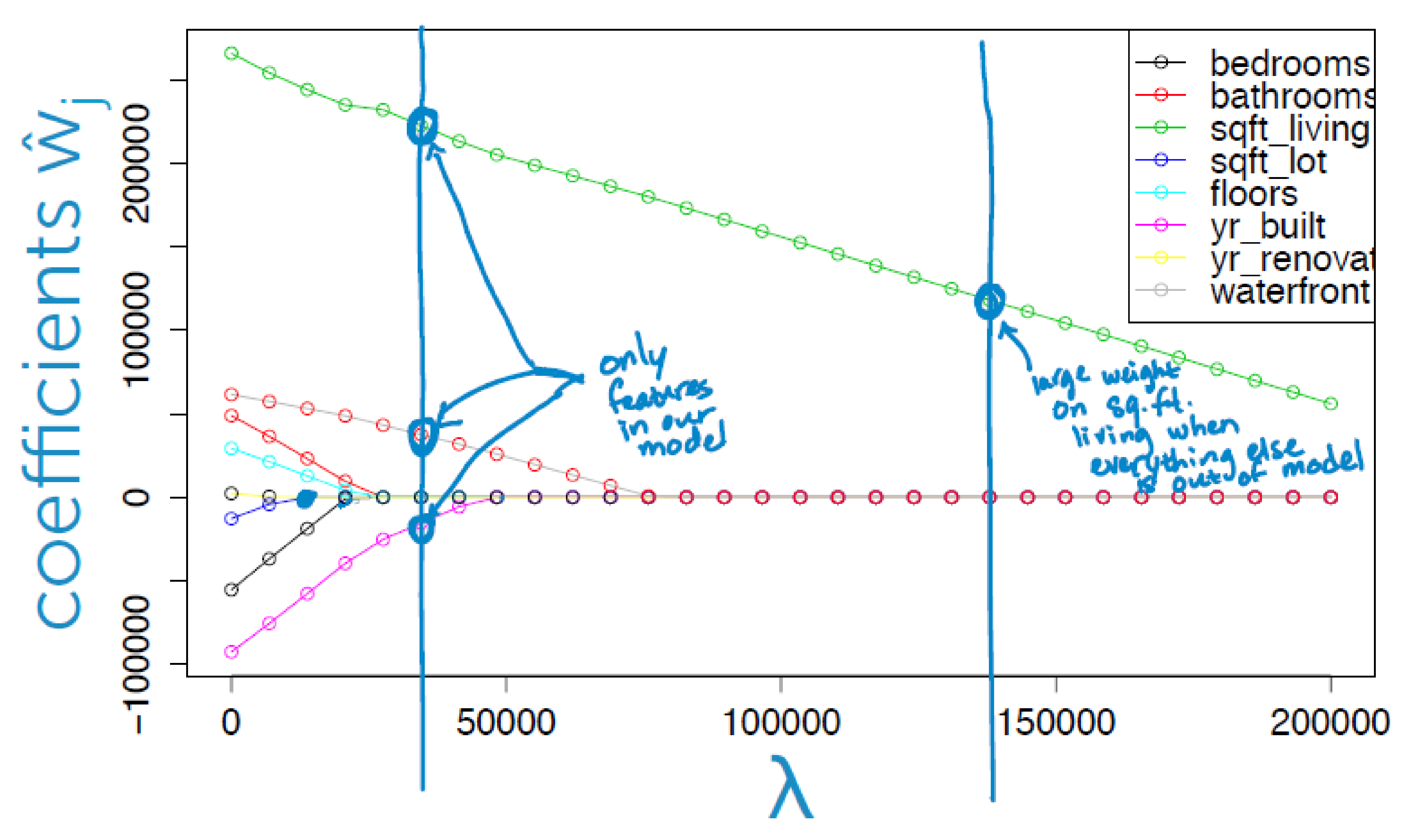


Figure Credit: Emily Fox & Carlos Guestrin, University of Washington

L1 and L2 Summary

L2 regularization	L1 regularization
Computational efficient due to having analytical solutions	Computational inefficient on non-sparse cases
Non-sparse outputs	Sparse outputs
No feature selection	Built-in feature selection

Figure Credit: Gene Olafson, Regularization 3/14/18