COMPSCI 589
Lecture 8: Linear Regression, Ridge, and Lasso

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Outline

Views on Machine Learning

Mitchell (1997): "A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E."

Substitute "training data D" for "experience E."

The Regression Task

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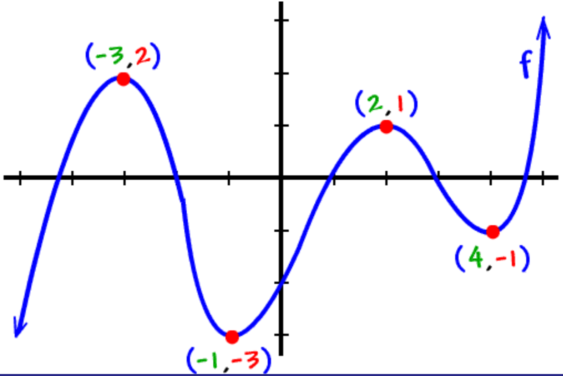
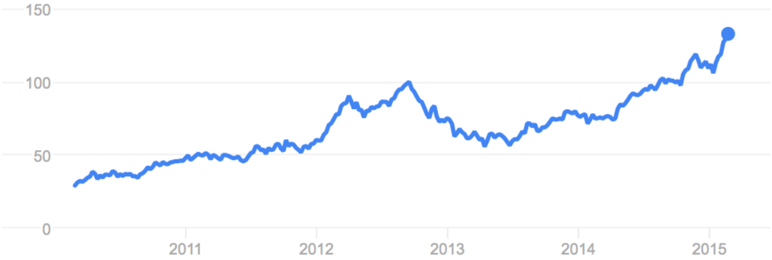
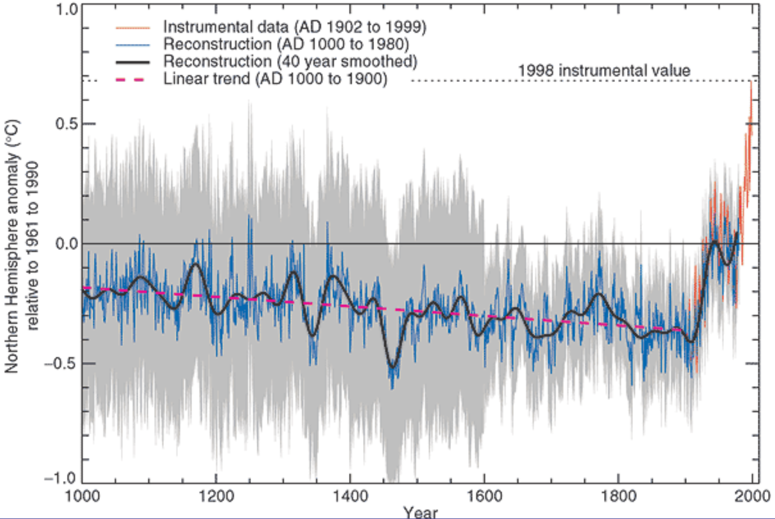


Example: Stock Prices

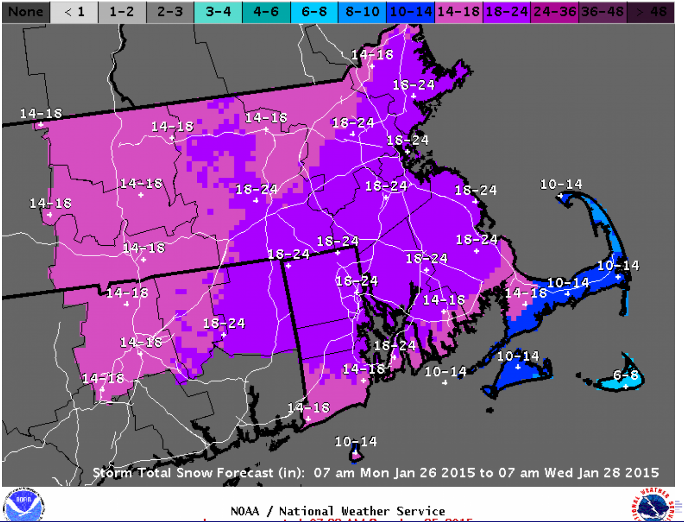


Open	130.02	Market cap	755.53B
High	133.00	P/E ratio (ttm)	17.92
Low	129.66	Dividend yield	1.41%

Example: Climate Change



Example: Weather Forecasting

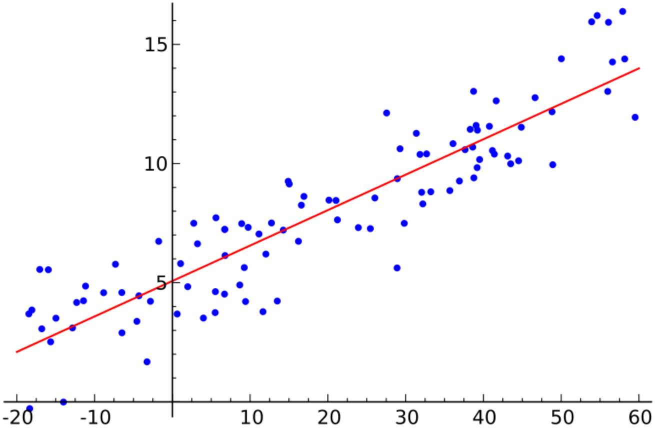


The Regression Learning Problem

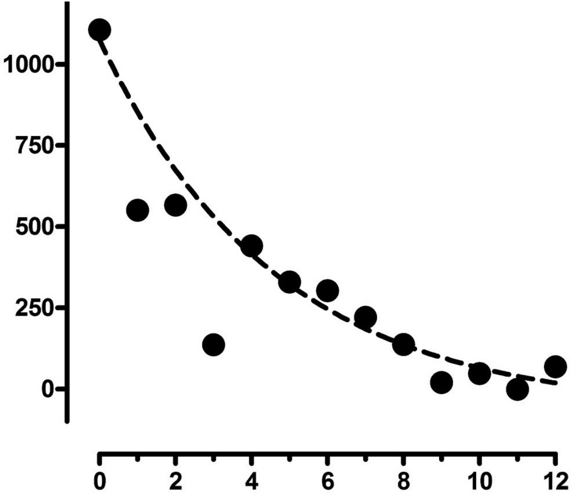
Definition: Regression Learning Problem

Given a data set of example pairs $\mathcal{D} = \{(\mathbf{x}_i, y_i), i = 1 : N\}$ where $\mathbf{x}_i \in \mathbb{R}^D$ is a feature vector and $y_i \in \mathbb{R}$ is the output, learn a function $f : \mathbb{R}^D \to \mathbb{R}$ that accurately predicts y for any feature vector $\mathbf{x}$.

Example: Linear Regression Learning



Example: Non-Linear Regression Learning



Error Measures: MSE

Definition: Mean Squared Error

Given a data set of example pairs $\mathcal{D} = \{(\mathbf{x}_i, y_i), i = 1 : N\}$ and a function $f : \mathbb{R}^D \to \mathcal{Y}$, the mean squared error of f on $\mathcal{D}$ is:

$$MSE(f, \mathcal{D}) = \frac{1}{N} \sum_{i=1}^{N} (y_i - f(\mathbf{x}_i))^2$$

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Related measures include:

Sum of Squared Errors: $SSE(f, \mathcal{D}) = N \cdot MSE(f, \mathcal{D})$

Risidual Sum of Squares: $RSS(f, \mathcal{D}) = N \cdot MSE(f, \mathcal{D})$

Root Mean Squared Error: $RMSE(f, \mathcal{D}) = \sqrt{MSE(f, \mathcal{D})}$

Error Measures: MAE

Definition: Mean Absolute Error

Given a data set of example pairs $\mathcal{D} = \{(\mathbf{x}_i, y_i), i = 1 : N\}$ and a function $f : \mathbb{R}^D \to \mathcal{Y}$, the mean absolute error of f on $\mathcal{D}$ is:

$$MAE(f, \mathcal{D}) = \frac{1}{N} \sum_{i=1}^{N} |y_i - f(\mathbf{x}_i)|$$

Outline

Linear Regression

Linear regression is a parametric regression method that assumes the relationship between y and $\mathbf{x}$ is a linear function with parameters $\mathbf{w} = [w_1, ..., w_D]^T$ and b.

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Question: How can we learn the parameter values $\mathbf{w}$ and b?

Ordinary Least Squares Linear Regression

Ordinary least squares selects the linear regression parameters to minimize the mean squared error (MSE) on the training data set:

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$$\mathbf{w}^*, b^* = \arg\min_{\mathbf{w},b} \frac{1}{N} \sum_{i=1}^{N} (y_i - \mathbf{x}_i \mathbf{w} + b)^2$$

Solving OLS For One Feature

$$\arg\min_{w,b} \frac{1}{N}\sum_{i=1}^{N}(y_i - wx_i - b)^2$$

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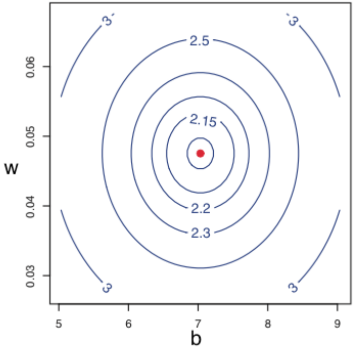

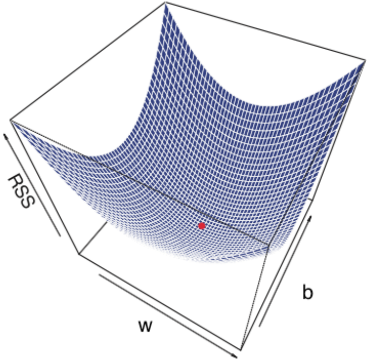

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$$w\left(\sum_{i=1}^{N}x_i^2\right) + b\left(\sum_{i=1}^{N}x_i\right) = \sum_{i=1}^{N}(y_i x_i)$$

$$w\left(\sum_{i=1}^{N}x_i\right) + b(N) = \sum_{i=1}^{N}(y_i)$$

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$$\begin{bmatrix} \sum_{i=1}^N x_i^2 & \sum_{i=1}^N x_i \\ \sum_{i=1}^N x_i & N \end{bmatrix} \begin{bmatrix} w \\ b \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^N y_i x_i \\ \sum_{i=1}^N y_i \end{bmatrix}$$

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$$\begin{bmatrix} w \\ b \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^N x_i^2 & \sum_{i=1}^N x_i \\ \sum_{i=1}^N x_i & N \end{bmatrix}^{-1} \begin{bmatrix} \sum_{i=1}^N y_i x_i \\ \sum_{i=1}^N y_i \end{bmatrix}$$

General OLS Solution

Assume that $\mathbf{X}$ is a data matrix with one data case $\mathbf{x}_i \in \mathbb{R}^D$ per row, and $\mathbf{Y}$ is a column vector containing the corresponding outputs. The general OLS solution is:

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$$
\begin{aligned}
\mathbf{w}^* &= \arg\min_{\mathbf{w}} \frac{1}{N}\sum_{i=1}^{N}(y_i - \mathbf{x}_i\mathbf{w})^2 \\
&= \arg\min_{\mathbf{w}} \frac{1}{N}(\mathbf{Y} - \mathbf{X}\mathbf{w})^T(\mathbf{Y} - \mathbf{X}\mathbf{w}) \\
0 &= \frac{\partial}{\partial \mathbf{w}}\frac{1}{N}(\mathbf{Y} - \mathbf{X}\mathbf{w})^T(\mathbf{Y} - \mathbf{X}\mathbf{w}) \\
0 &= \mathbf{X}^T(\mathbf{Y} - \mathbf{X}\mathbf{w}) \\
\mathbf{X}^T\mathbf{X}\mathbf{w} &= \mathbf{X}^T\mathbf{Y} \\
\mathbf{w}^* &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}
\end{aligned}
$$

Connection to Probabilistic Models

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$$P(y|\mathbf{x}) = \mathcal{N}(y; \mathbf{xw}, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(y - \mathbf{xw})^2\right)$$

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This view shows that OLS assumes the residuals are Normally distributed. This assumption is violated in many real world processes that have significant outliers or heavy-tailed noise.

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- Variance is generally low unless there are outliers.

Outline

Regularized Linear Regression

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$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \frac{1}{N}\sum_{i=1}^{N}(y_i - \mathbf{x}_i\mathbf{w})^2 + \lambda||\mathbf{w}||$$

$$= \arg\min_{\mathbf{w}} \frac{1}{N}\sum_{i=1}^{N}(y_i - \mathbf{x}_i\mathbf{w})^2 \text{ ... st } ||\mathbf{w}|| \leq c$$

Ridge Regression

Ridge regression is the name given to regularized least squares when the weights are penalized using the square of the ℓ_2 norm $||\mathbf{w}||_2^2 = \mathbf{w}^T\mathbf{w} = \sum_{d=1}^{D} w_d^2$:

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In this case, it is easy to show that the optimal regularized weights are:

$$\mathbf{w}^* = (\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{Y}$$

The Lasso

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The Lasso problem is a quadratic programming problem. However, it can be solved efficiently for all values of λ using an algorithm called *least angle regression* (LARS). The advantage of the Lasso is that it simultaneously performs regularization and feature selection.

Lasso vs Ridge

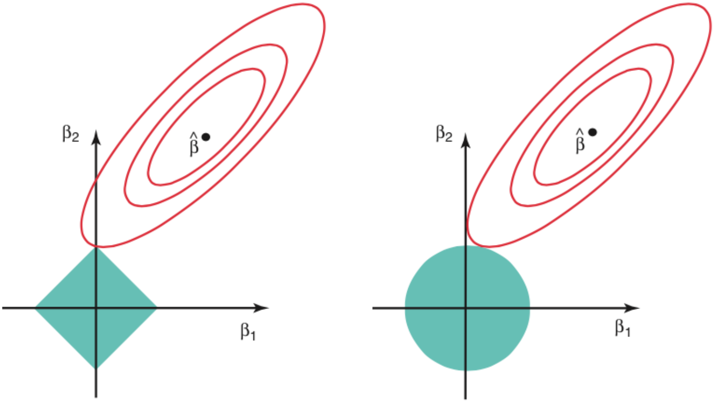

FIGURE 6.7. *Contours of the error and constraint functions for the lasso* (left) *and ridge regression* (right). *The solid blue areas are the constraint regions,* $|\beta_1| + |\beta_2| \leq s$ *and* $\beta_1^2 + \beta_2^2 \leq s$, *while the red ellipses are the contours of the RSS.*

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- Does not solve bias problem
- Computation for ridge is still cubic in data dimension D, but now need to determine regularization parameters. Computation for LARS is similar.

Outline

Basis Expansion

Just as with linear classification models, linear regression models can be extended to capture non-linear relationships using basis function expansions. The polynomial basis is often used for this purpose, although it is not sensible for forecasting.

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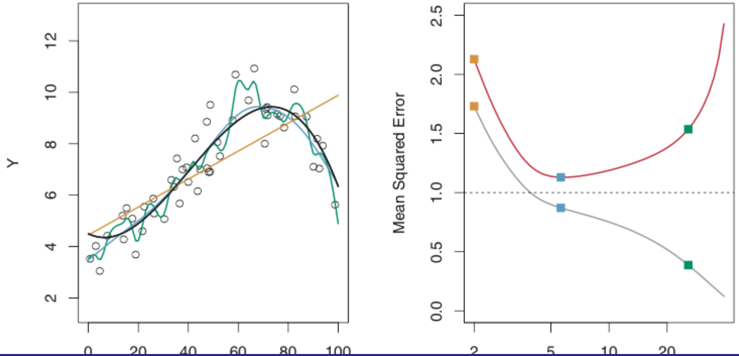

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- Computation is cubic in the dimensionality of the basis function expansion. Can be costly.