Introduction to Regression

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Agenda

- Introduction
- Cost Functions & Gradient Descent
  - Minimization
  - Implementation
- Hands-on Example
- Evaluating Regression Models
- Regularization

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Notation

- x^i – The feature vector for the ith data object
  - $x^i = [x_1^i, x_2^i, \dots, x_m^i]$
- X – The set of all x^i
- y^i – The true target value for the ith data object
- Y – The set of all y^i
- n – Number of rows in the dataset
- m – Number of columns in the dataset

Example: Ozone Levels

- Daily measurements of weather data
- Predict ozone level for public awareness

ozone <- read.table('Datasets/Ozone/ozone.data')

head(ozone)

	y	x_1	x_2	x_3
	ozone	radiation	temperature	wind
y^1	41	190	67	7.4
y^2	36	118	72	8.0
y^3	12	149	74	12.6
	18	313	62	11.5
	23	299	65	8.6
	19	99	59	13.8

$x^1 = [190, 67, 7.4]$

$x^2 = [118, 72, 8.0]$

$x^3 = [149, 74, 12.6]$

Example: Ozone Levels

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Y X

Regression vs Classification

- Classification
  - Target is discrete with finite value set
  - Ex: survived/dead, face/non-face, fraud/non-fraud, product categories, ranking
- Regression
  - Target is continuous or ordinal
  - Ex: price, weight, height, temperature, ranking

Non-Parametric Algorithms

- Cannot be represented as a single closed form function
- Many different assumptions about underlying structure of data
- Ex: Decision Trees, Neural Nets

Parametric Algorithms

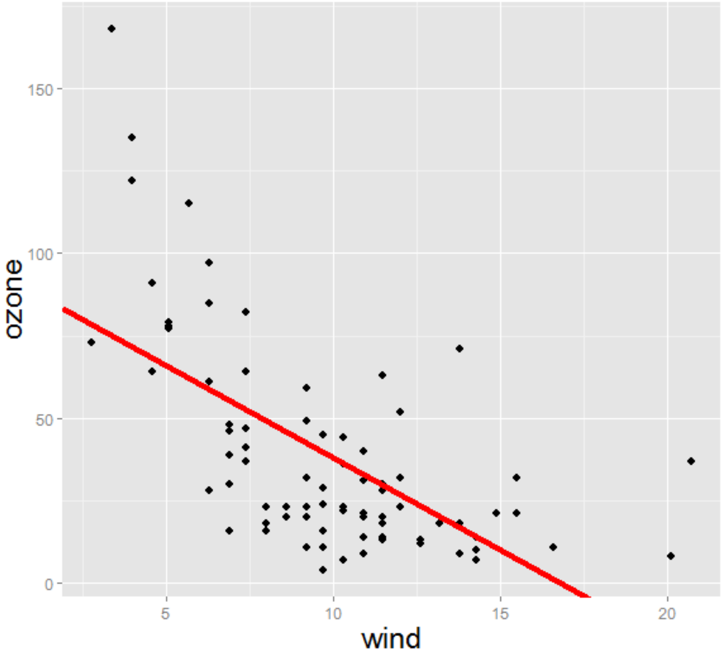
- Assumption: Relationship between features and target can be represented as a closed form function
- This function "maps" $X \rightarrow Y$
- Used in traditional scientific modeling
- Ex: $y = 1 + 2x$
  - Parameters: [1, 2]

Parametric Notation

- h – A specific functional form (line, exponential, Poisson distribution, logit, etc.)
- θ – A vector of function parameters which define a specific hypothesis
- h_θ – A specific hypothesis (estimate) for the mapping $X \rightarrow Y$

Regression Example

- How do we define a line?
  - $y = mx + b$
- What is…
  - θ?
  - h_θ?



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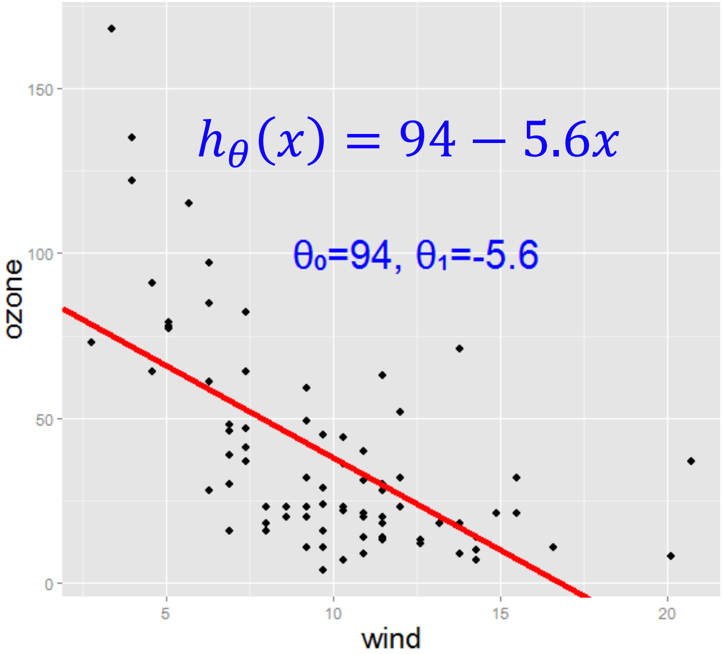

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Regression Example

- What about with three features?
- What is…
  - θ?
  - h_θ?

y	x_1	x_2	x_3
ozone	radiation	temperature	wind
41	190	67	7.4
36	118	72	8.0
12	149	74	12.6
18	313	62	11.5
23	299	65	8.6
19	99	59	13.8

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$$

Regression Example

- What about with more features?
- What is…
  - θ?
  - h_θ?

$$\theta = [\theta_0, \theta_1, \theta_2, \dots, \theta_m]$$

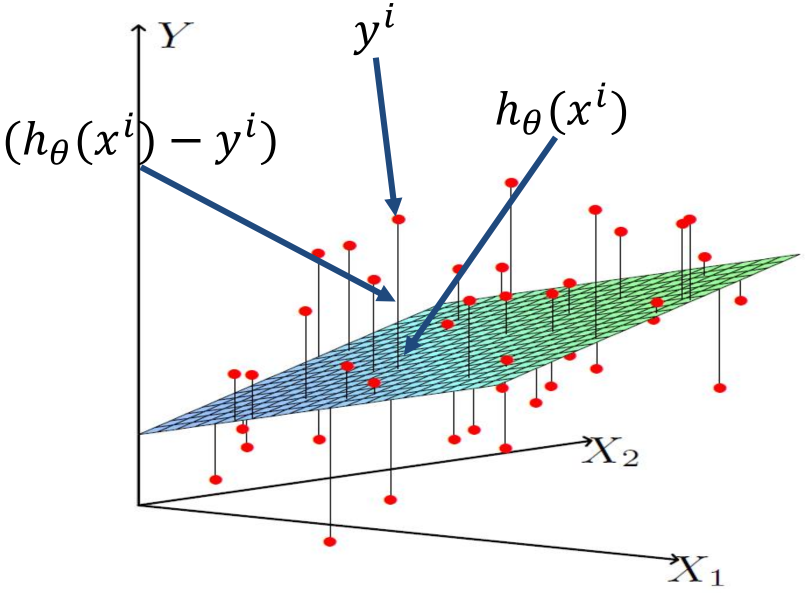
$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_m x_m$$

Regression Algorithms

- $\theta = [\theta_0, \theta_1, \theta_2, \ldots, \theta_m]$, $x = [x_1, x_2, \ldots, x_m]$
- Linear Regression
  - h – a line function
  - $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_m x_m = \theta^T x$
- Logistic Regression
  - h – a logit function
  - $h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$

Note: Logistic Regression is a classification algorithm

Regression Errors



- How do we assess the error of a model?
- "Residual" – difference between predicted and actual target value
  - $res = (h_\theta(x^i) - y^i)$

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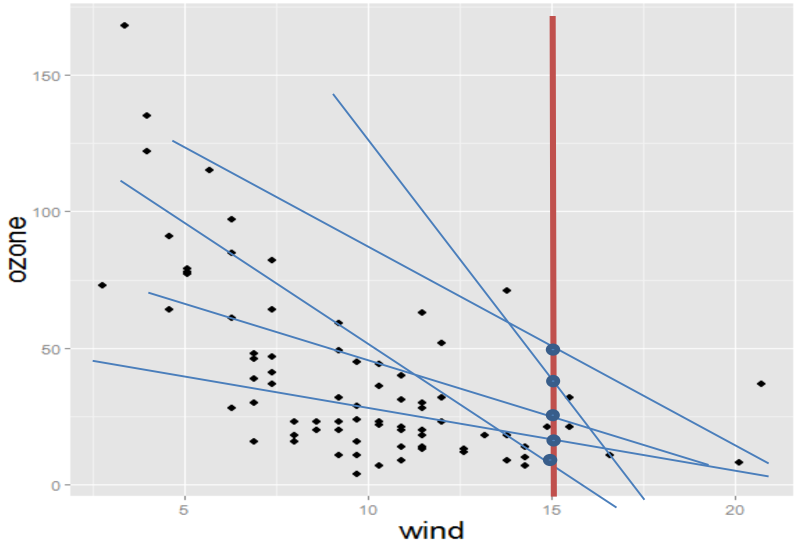
Regression Training

- Wind Speed=15 mph
- Ozone = ?
- Use the line that is somewhere in the middle
- How do we define "middle"?



$$h_\theta(x) = \theta_0 + \theta_1 x$$

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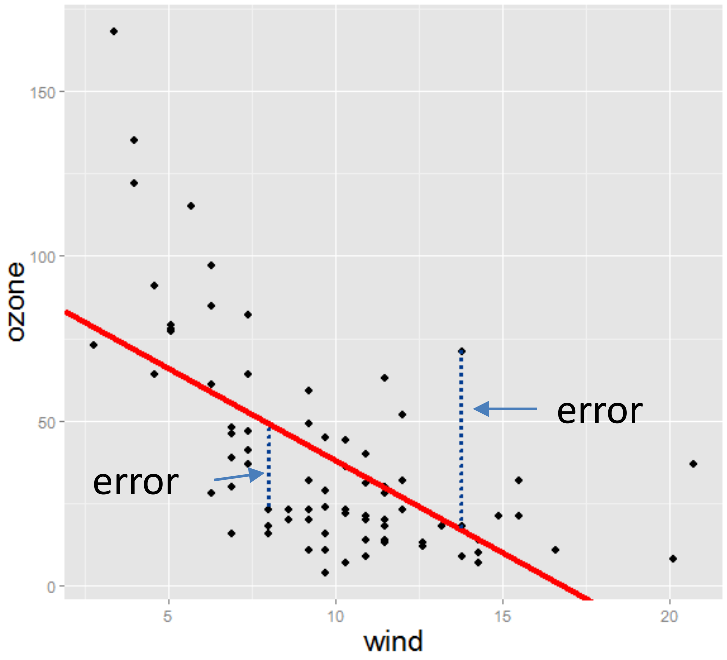
Cost Function

- Want: a "cost" or "loss" function – $J(\theta)$
  - Smaller for lower error
  - Larger for higher error
- Residuals – a measure of error
  - Simple sum doesn't work – why?
- Solution: Square them!
  - "Mean Square Error"

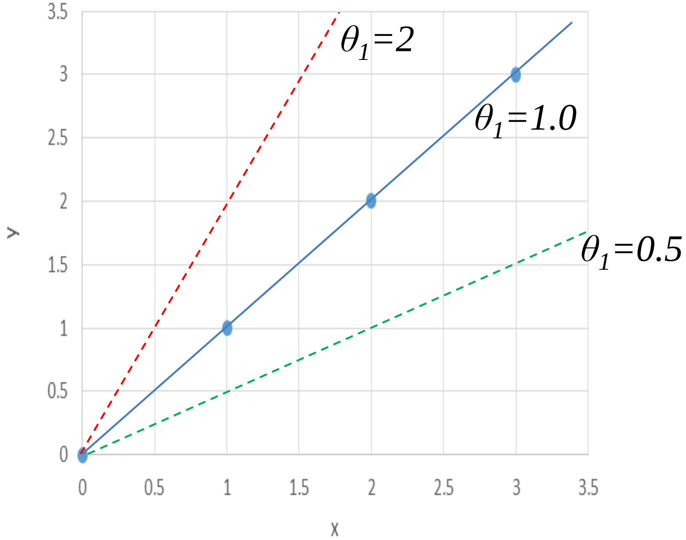


$$J(\theta) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_\theta(x^i) - y^i\right)^2$$

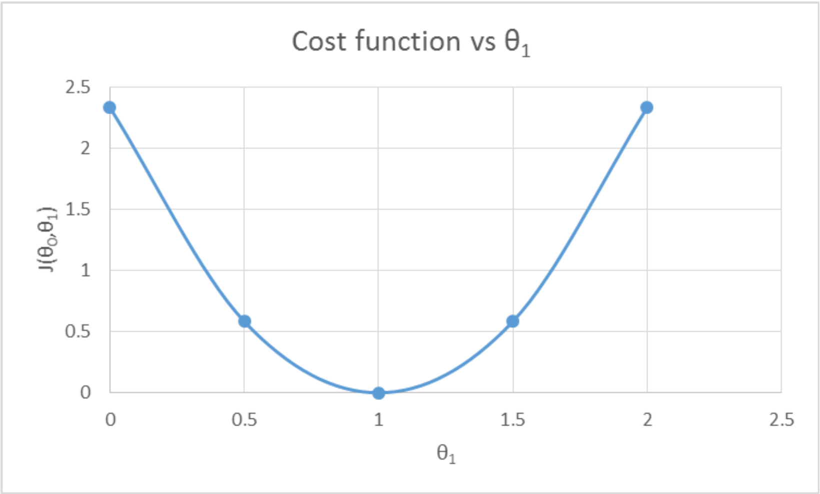
Mean Square Error – 1D

$$h_\theta(x) = \theta_0 + \theta_1 x$$

$$J(\theta) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_\theta(x^i) - y^i\right)^2$$



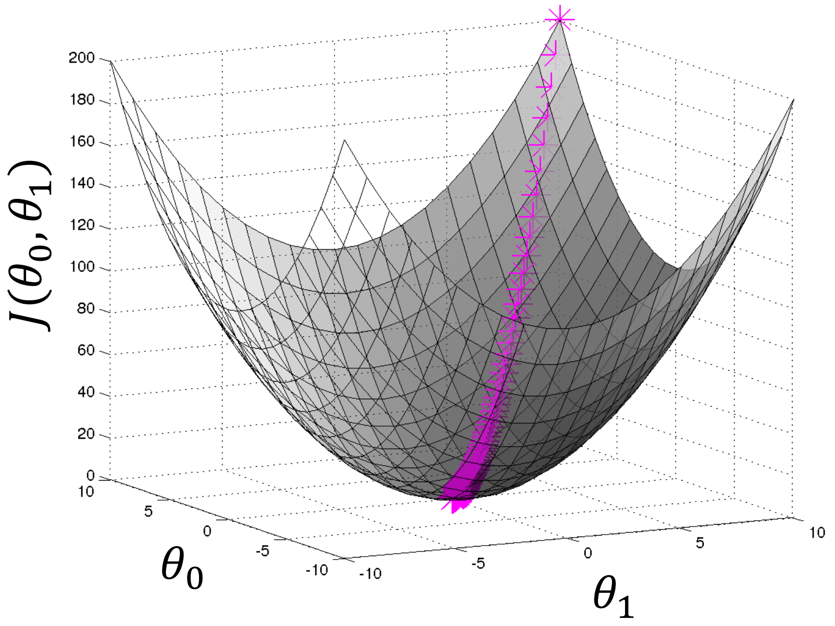
θ_0=0



Mean Square Error – 2D

$$h_\theta(x) = \theta_0 + \theta_1 x$$

$$J(\theta) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_\theta(x^i) - y^i\right)^2$$



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Maximum/Minimum Problem

Find two nonnegative numbers whose sum is 9 and so that the product of one number and the square of the other number is a maximum.

Solution

Sum of number is 9

$$9 = x + y$$

Product of two numbers is

$$P = x\,y^2$$

$$= x\,(\,9 - x)^2$$

Solution

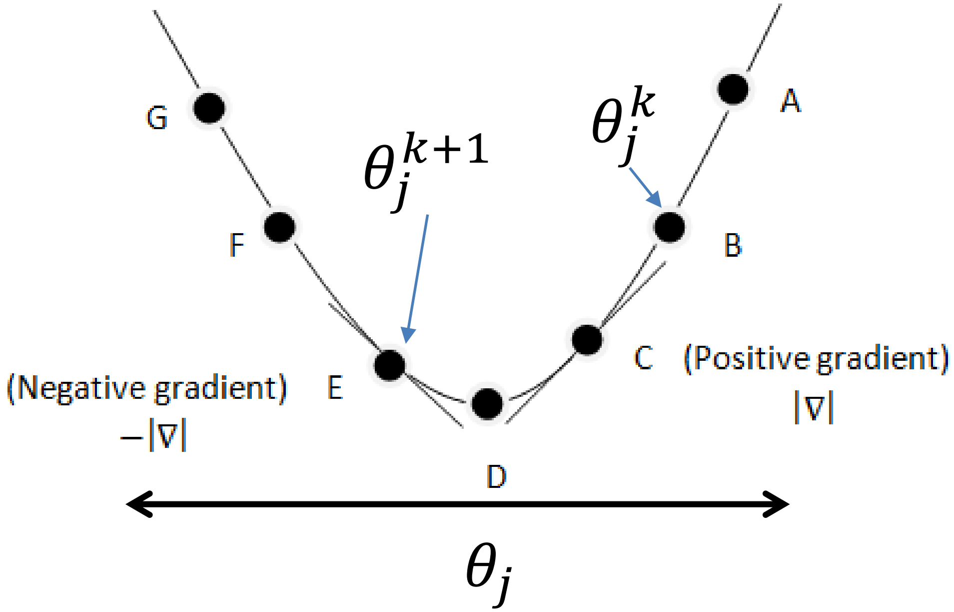
$$P' = x\,(2)\,(9-x)(-1) + (1)\,(9-x)^2$$
$$= (9-x)\,[\,-2x + (9-x)\,]$$
$$= (9-x)\,[\,9-3x\,]$$
$$= (9-x)\,(3)[\,3-x\,]$$
$$= 0$$

$x=9$ or $x=3$

Gradients

- Derivatives: slope in one direction
- What about more features?
- Gradient: a multi-dimensional derivative
    - $\nabla J(\theta) = [\frac{\partial J}{\partial \theta_0}, \frac{\partial J}{\partial \theta_1}, \ldots, \frac{\partial J}{\partial \theta_m}]$
    - Treat each dimension independently

Intuition



$$\theta_j^{k+1} := \theta_j^k - \alpha \frac{\partial}{\partial \theta_j} J(\theta^k)$$

Gradient Descent

- Goal : minimize $J(\theta)$
- Start with some initial θ and then perform an update on each θ_j in turn:

$$\theta_j^{k+1} := \theta_j^k - \alpha \frac{\partial}{\partial \theta_j} J(\theta^k)$$

- Repeat until θ converges

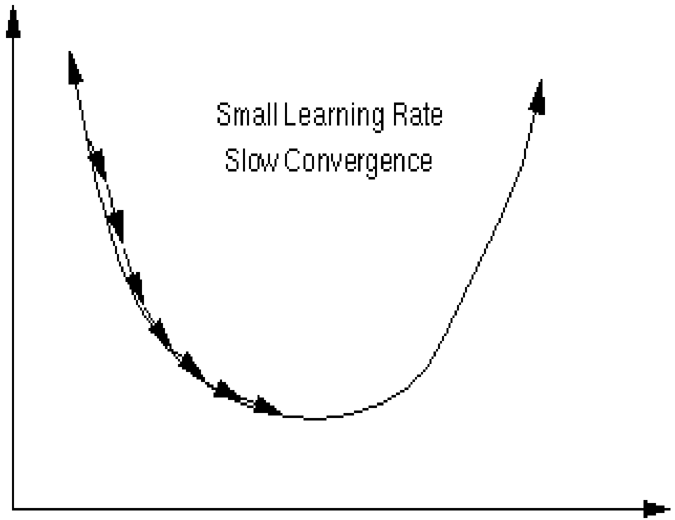
Gradient Descent

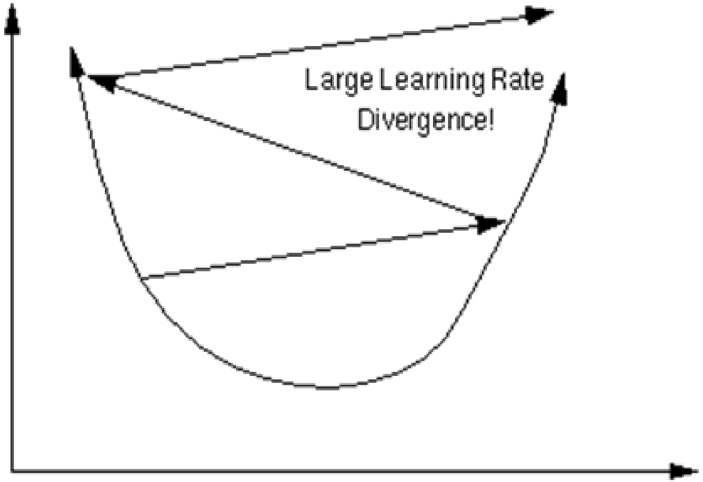
$$\theta_j^{k+1} := \theta_j^k - \alpha \frac{\partial}{\partial \theta_j} J(\theta^k)$$

- α is known as the learning rate; set by user
- Each time the algorithm takes a step in the direction of the steepest descent and $J(\theta)$ decreases.
- α determines how quickly or slowly the algorithm will converge to a solution

Learning Rate Effects

$$\theta_j^{k+1} := \theta_j^k - \alpha \frac{\partial}{\partial \theta_j} J(\theta^k)$$





Gradient Descent Animations

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Gradient Descent Implementation

- Ordinary least squares, linear regression
$$\theta_j^{k+1} := \theta_j^k - \alpha\big(y - h_\theta(x)\big)x_j$$
- When do we stop updating ("converge")?
  - When θ stops changing
    - i.e. θ^{k+1} very close to θ^k
  - When error stops dropping
    - i.e. $J\left(\theta^{k+1}\right)$ very close to $\mathrm{J}\left(\theta^k\right)$
  - "close" can be absolute or relative

Batch Gradient Descent

- How do we incorporate all our data?
- Loop!

For j from 0 to m:

$$\theta_j^{k+1} := \theta_j^k + \alpha \sum_{i=1}^{n} \left(y^i - h_\theta\left(x^i\right)\right) x_j^i$$

- h_θ is updated only once the loop has completed
- Weaknesses?

Stochastic Gradient Descent

- Consider an alternative approach:

for i from 1 to n:

for j from 0 to m:

$$\theta_j^{k+1} := \theta_j^k + \alpha \left(y^i - h_\theta\left(x^i\right) \right) x_j^i$$

- h_θ is updated when inner loop is complete
- If the training set is big, converges quicker than batch
- May oscillate around a minimum of $J(\theta)$ and never converge

Batch vs. Stochastic

Batch Gradient Descent

Repeat until convergence {

For j from 0 to m:

$$\theta_j^{k+1} := \theta_j^k + \alpha \sum_{i=1}^{n} \left(y^i - h_\theta\left(x^i\right)\right) x_j^i$$

}

- To update each parameter value, scan through the whole training data
- Converges to the minimum value slowly
- Preferred for small datasets

Stochastic Gradient Descent

Repeat until convergence {

for i from 1 to n:

for j from 0 to m:

$$\theta_j^{k+1} := \theta_j^k + \alpha \left(y^i - h_\theta\left(x^i\right)\right) x_j^i$$

}

- Update the parameter values with one training example at a time
- Converges to the 'proximity' of minimum value fast but may keep oscillating near the minimum
- Preferred for large datasets

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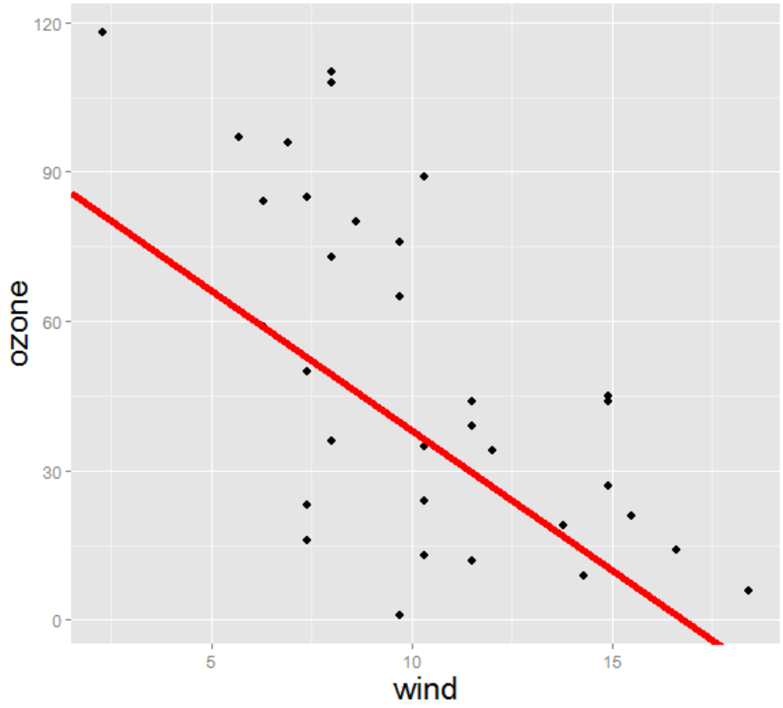
Regression Example

- From earlier:
  - $h_\theta(x) = 94 - 5.6 * x$
  - How do we evaluate?
    - Train/Test Split
- What metrics to use?
  - $J(\theta)$?



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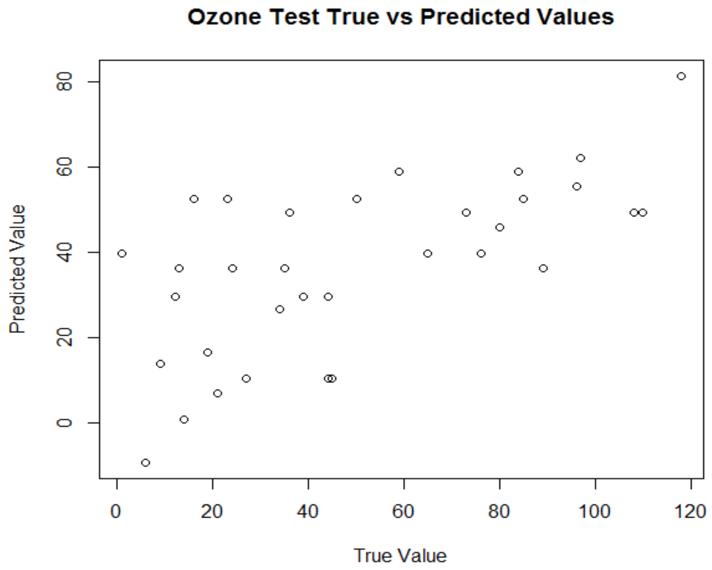
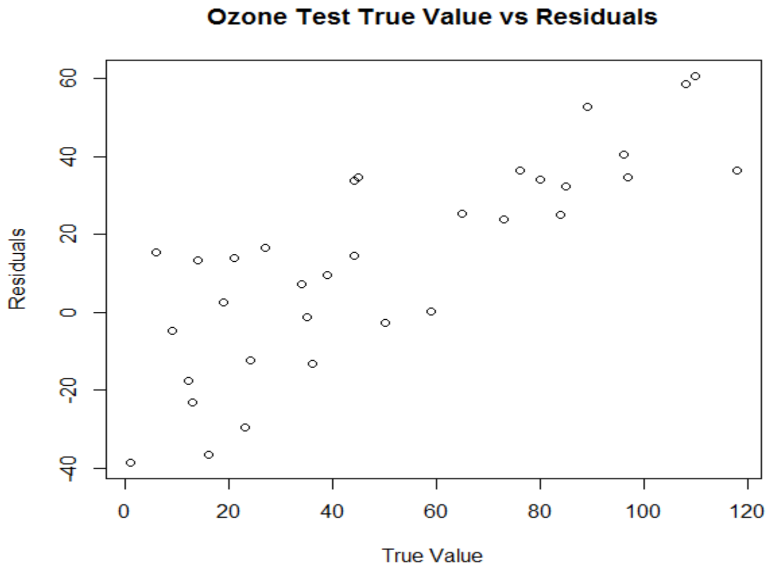
Graphical Evaluation Methods

Ideal: Straight line with slope 1



Ideal: Randomly distributed about 0



Common Metrics

- Mean Absolute Error (MAE)
- Root-Mean-Square Error (RMSE)
  - Root-Mean-Square Deviation
- Coefficient of Determination (R^2)

Mean Absolute Error

$$MAE(\theta) = \frac{\sum_{i=1}^{n} \left| h_\theta\left(x^i\right) - y^i \right|}{n}$$

- Mean of residual values
- "Pure" measure of error

Mean Absolute Error - Example

$$y = \{36, 19, 34, 6, 1, 45 \ldots\}$$

$$h_\theta(x) = \{27, -2.6, 13, -7.3, -2.6, 48 \ldots\}$$

$$|h_\theta(x) - y| = \{9, 21.6, 21, 13.3, 3.6, 3 \ldots\}$$

$$MAE(\theta) = \frac{71.5}{6} = 11.9$$

Root-Mean-Square Error

$$RMSE(\theta) = \sqrt{\frac{\sum_{i=1}^{n}(h_\theta(x^i) - y^i)^2}{n}}$$

- Square root of mean of squared residuals
- Penalizes large errors more than small
- Good when large errors particularly bad

RMSE - Example

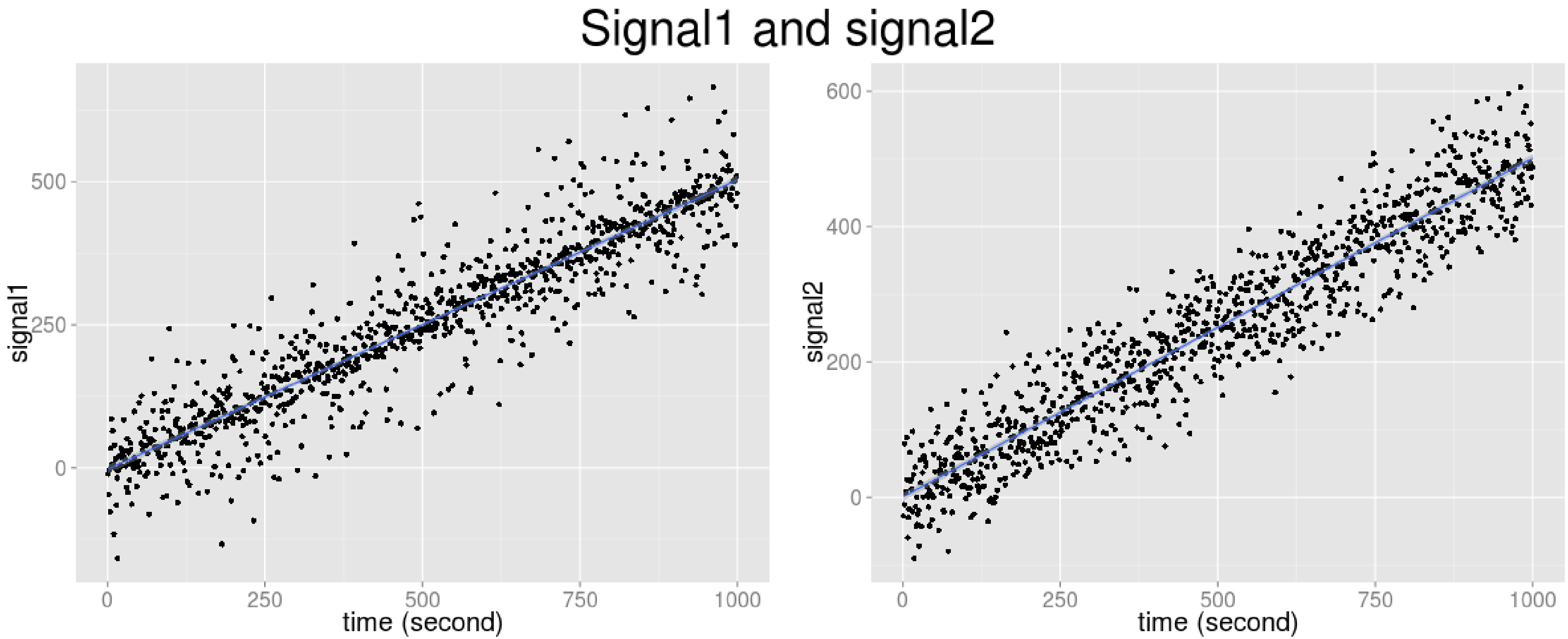
$$y = \{36, 19, 34, 6, 1, 45, \dots\}$$

$$h_\theta(x) = \{27, -2.6, 13, -7.3, -2.6, 48, \dots\}$$

$$(h_\theta(x) - y)^2 = \{81, 467, 441, 177, 13, 9, \dots\}$$

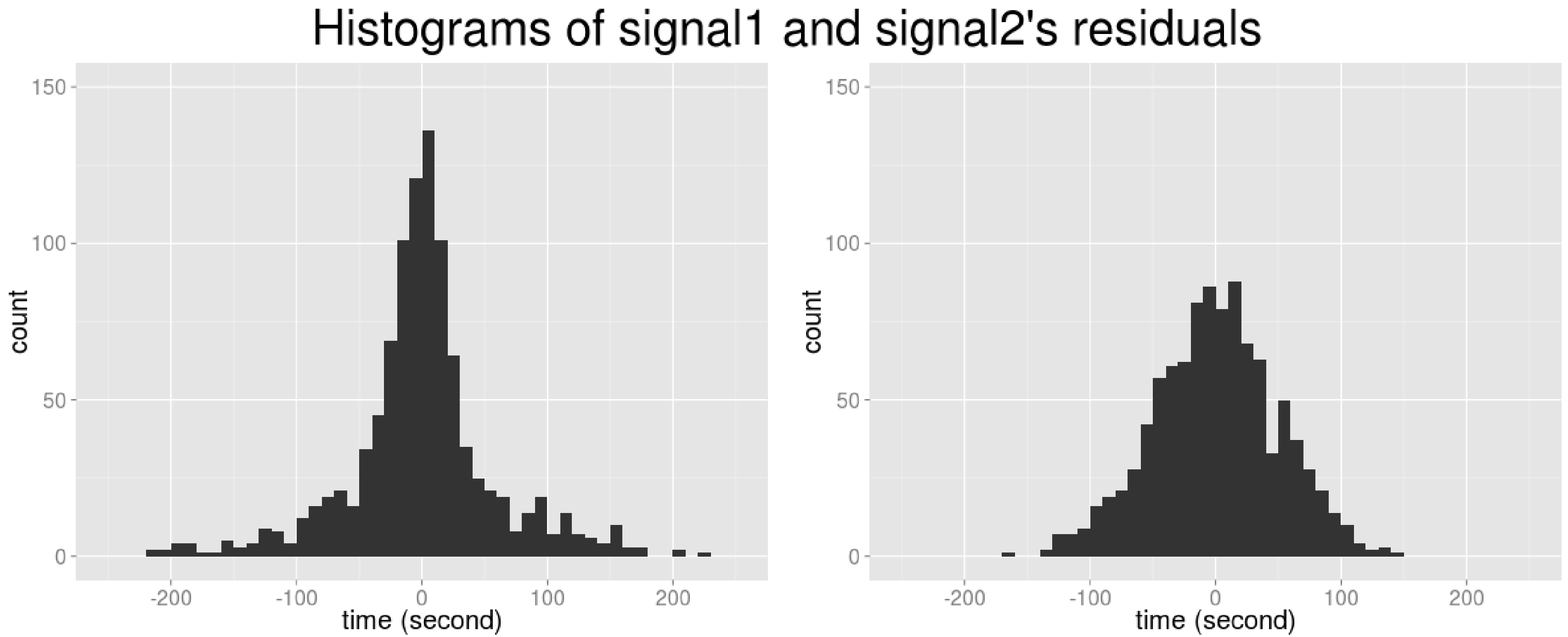
$$MAE(\theta) = \sqrt{\frac{1218}{6}} = 14.2$$

MAE vs RMSE



Signal1 and signal2
signal1
500
250
0
0
250
500
750
1000
time (second)
signal2
600
400
200
0
0
250
500
750
1000
time (second)

MAE vs RMSE



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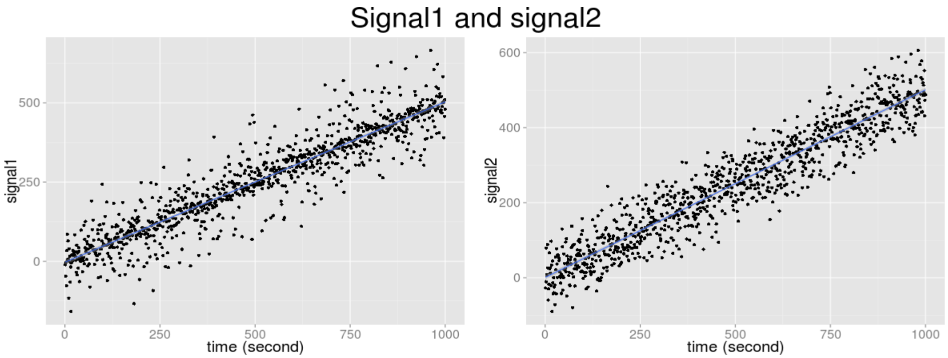
MAE vs RMSE



- MAE: **41.926** < 43.199
- RMSE: 64.458 > **54.516**
- Large deviation is penalized more by RMSE

Coefficient of Determination (R^2)

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

where

$$SS_{res} = \sum_{i=1}^{n} \left(h_\theta\left(x^i\right) - y^i\right)^2 \qquad SS_{tot} = \sum_{i=1}^{n} \left(y^i - \bar{y}\right)^2$$

- SS_{res} – Sum of squared residuals (i.e. total squared error)
- SS_{tot} – Sum of squared differences from mean (i.e. total variation in dataset)
- Result: Measure of how well the model explains the data
    - "Fraction of variation in data explained by model"

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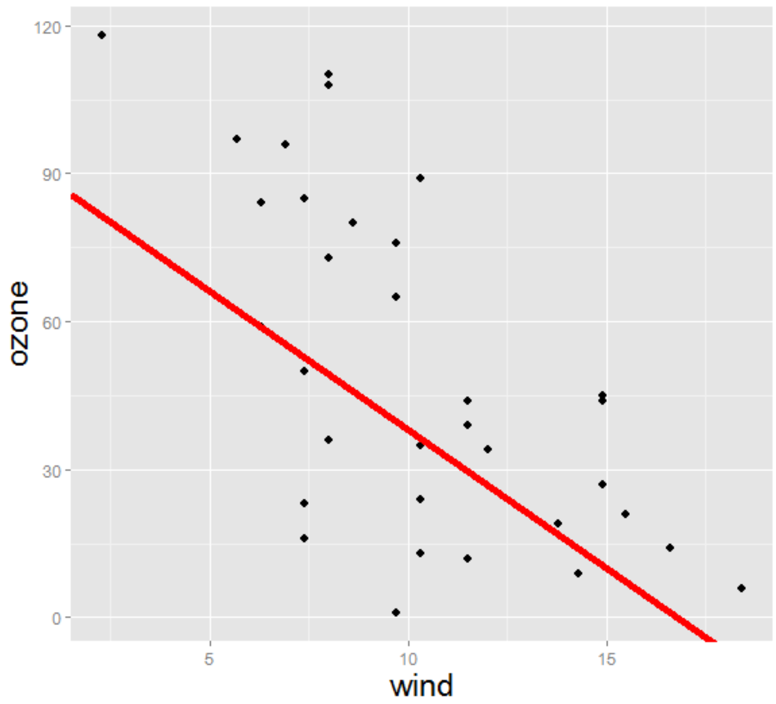
R^2 Example

- $R^2 = 0.277$
- Want a much better model for real application
- $R^2 = 0.6$ can be a good model



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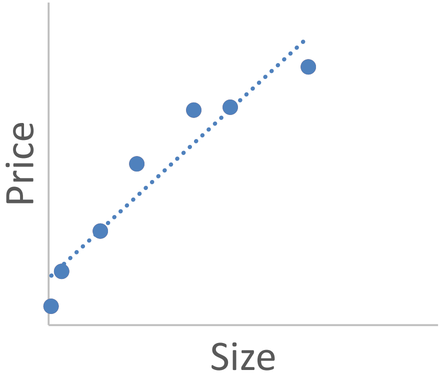
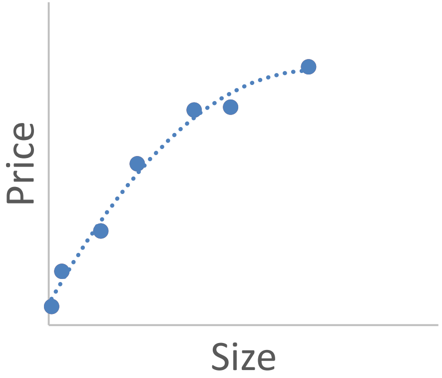
Overfitting

- Want to extract general trends
- Danger: "memorizing" the training set
- A model is **overfit** when model performance on test set is much worse than on training set.

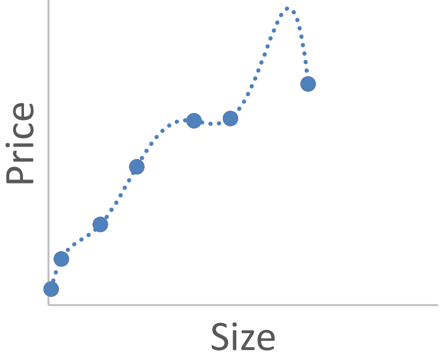
Overfitting



$\theta_0 + \theta_1 x$



$\theta_0 + \theta_1 x + \theta_2 x^2$

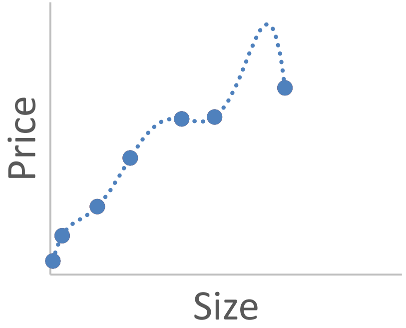


$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

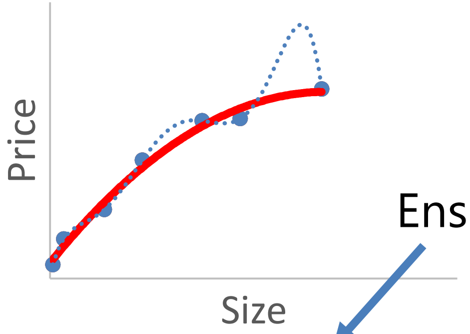
Complexity

- What makes a good model overfit?
  - Nature of training data
  - **Complexity of model**
- How do we handle these?
  - Cross validation
  - Manual model constraint
  - Regularization

Intuition



$$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$



Ensure Small

$$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

- Want to discourage complex models automatically – How?
- Adjust the cost function!
    - Penalize models with large high-order θ terms

$$J'(\theta) = J(\theta) + Penalty$$

Definitions

- Two most common
  - L1 regularization
    - lasso regression
  - L2 regularization
    - ridge regression
    - weight decay

$$J_{L1}(\theta) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_\theta\left(x^i\right) - y^i\right)^2 + \lambda\sum_{j=1}^{m}\left|\theta_j\right|$$

$$J_{L2}(\theta) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_\theta\left(x^i\right) - y^i\right)^2 + \lambda\sum_{j=1}^{m}\theta_j^2$$

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Regularized Regression

$$J_{L1}(\theta) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_\theta\left(x^i\right) - y^i\right)^2 + \lambda\sum_{j=1}^{m}|\theta_j| \qquad J_{L2}(\theta) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_\theta\left(x^i\right) - y^i\right)^2 + \lambda\sum_{j=1}^{m}\theta_j^2$$

- Find the best fit
- Keep the θ_j terms as small as possible.
- λ is a user-set parameter which controls the trade off

Regularized Regression

$$J_{L1}(\theta) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_\theta\left(x^i\right) - y^i\right)^2 + \lambda\sum_{j=1}^{m}\left|\theta_j\right| \qquad J_{L2}(\theta) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_\theta\left(x^i\right) - y^i\right)^2 + \lambda\sum_{j=1}^{m}\theta_j^2$$

- Size of λ important
  - λ too high => no fitting
  - λ too low => no regularization

QUESTIONS

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