

Regression

Spring 2018

Review

- Last week:
 - Why machine learning?
 - What does a machine learn?
 - Designing a “supervised” machine learning algorithm
- Assignments (Canvas)
 - Problem Set 1 due yesterday
 - Lab Assignment 1 out
- Questions?

Today's Topics

- Regression Applications
- Discussion: Building Regression Datasets
- Linear Regression
- Polynomial Regression
- Regularization (Ridge Regression and Lasso Regression)
- Evaluating Regression Models
- Lab

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Today's Focus: Regression

Predict **continuous** value

Predict Road Trip Fuel Cost

www.fueleconomy.gov

the official U.S. government source for fuel economy information

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Trip Calculator

Trip Vehicles



2004 Nissan Sentra

1.8 L, 4 cyl, Automatic 4-spd, Regular



Comb. MPG: **27.0**

Trip fuel cost: **\$110.19**

Predict Price to Charge for Your Home

Airbnb

Book unique homes and
experiences all over the world.

🔍 Try "Orlando"

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Predict Future Value of a House You Buy



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Estimate your Home Value Appreciation and the Profits from its Future Sale

Today's Mortgage Rate

3.04%
APR 15 Year Fixed

Select Loan Amount

lendingtree

[Calculate Payment >](#)

Terms & Conditions apply. NMLS#1138


Predict Perceived “Hot”-ness

How Hot are You?

Artificial Intelligence will decide how hot you are
on a scale of 1 to 10.



Predict Life Expectancy

**Social Security**

SEARCH MENU LANGUAGES SIGN IN / UP

Retirement & Survivors Benefits: Life Expectancy Calculator

[Office of the Chief Actuary](#)
[Life Expectancy Home Page](#)
[Retirement Planner](#)
[Retirement Estimator](#)
[Survivors Planner](#)
[Other Things to Consider](#)
[Apply for Benefits Online](#)

This calculator will show you the **average number** of additional years a person can expect to live, based only on the gender and date of birth you enter.

Gender

Select ▾

Date of Birth

Month ▾ Day ▾ Year ▾

Submit

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Machine Learning For Trading – How To Predict Stock Prices Using Regression?

What Else to Predict?

Insurance Cost

Popularity of Social Media Posts

Public Opinion

Factory Analysis

Political Party Preference

Call Center Complaints

Weather

Class Ratings

Animal Behavior

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Class Task: Predict Your Salary if You Become a Machine Learning Engineer

Machine Learning Engineer Salaries in Austin, TX

60 Salaries

All Industries



All Company Sizes



All Years of Experience



Average Base Pay

\$103,313 /yr

15% below national average

Not enough reports to show salary distribution



https://www.glassdoor.com/Salaries/machine-learning-engineer-salary-SRCH_KO0,25.htm

Class Task: Predict Your Salary if You Become a Machine Learning Engineer

- What cues would be predictive of your salary?
- Where can you find the data (predictive cues + true labels)?
- What would introduce noise to your data?

Class Task: Predict Your Salary if You Become a Machine Learning Engineer

Each person enter 4 data samples into the following spreadsheet:

https://docs.google.com/spreadsheets/d/1M_-qPmvWmA_uCAOWCuRKi18upaZILUmD2zsa6yTb5H8/edit?usp=sharing

Today's Topics

- Regression Applications
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- **Linear Regression**
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Linear Models for Regression

- General formula:

$$\hat{y} = w[0] * x[0] + w[1] * x[1] + \dots + w[p] * x[p] + b$$

Feature vector: $\mathbf{x} = x[0], x[1], \dots, x[p]$

- How many features are there?
 - $p+1$

Parameter vector to learn: $\mathbf{w} = w[0], w[1], \dots, w[p]$

- How many parameters are there?
 - $p+2$

Predicted value

“Simple” Linear Regression Model

- Formula:

$$\hat{y} = w[0] * x[0] + b$$

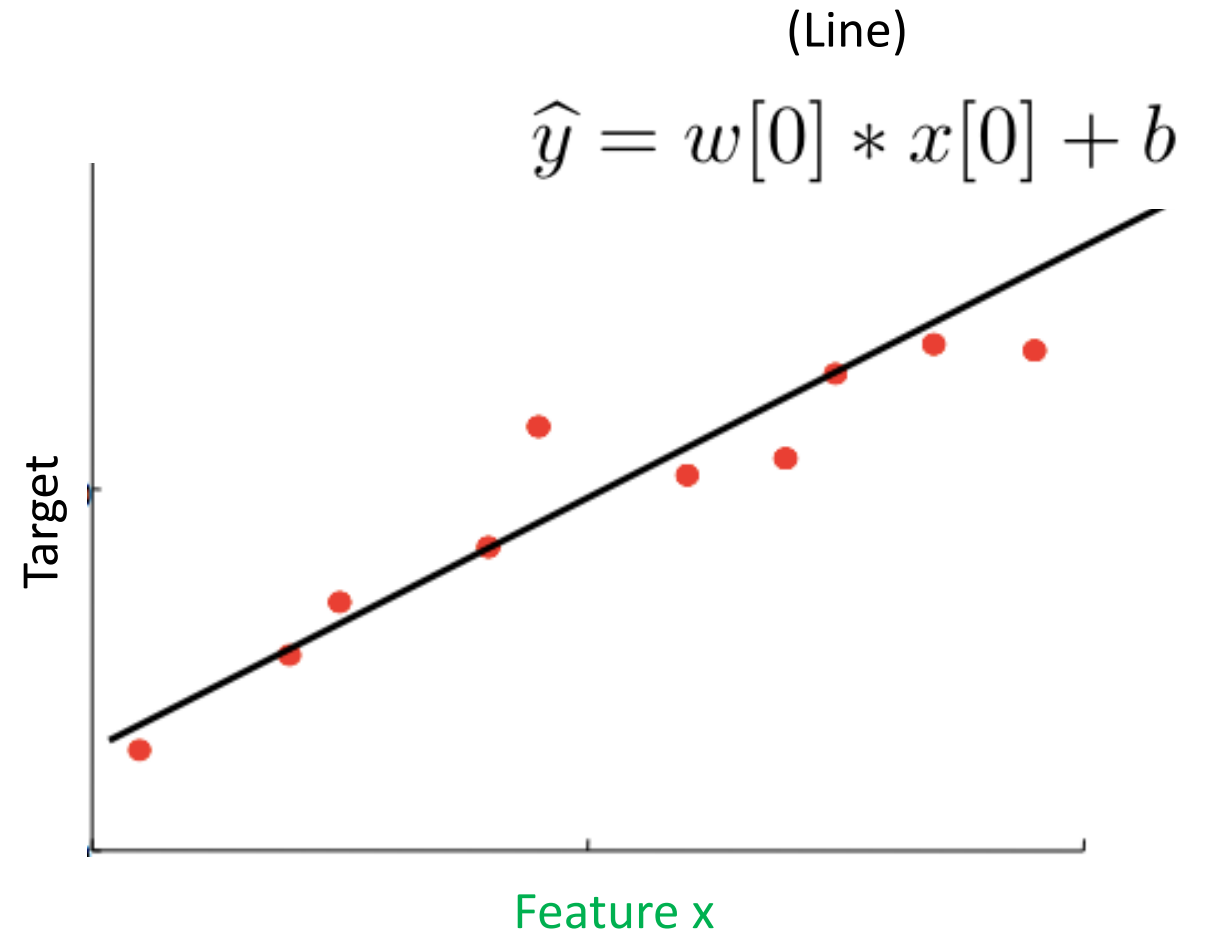
Feature vector

- How many features are there?
 - 1

Parameter vector to learn

- How many parameters are there?
 - 2

Predicted value



“Multiple” Linear Regression Model

- Formula:

$$\hat{y} = w[0] * x[0] + w[1] * x[1] + b$$

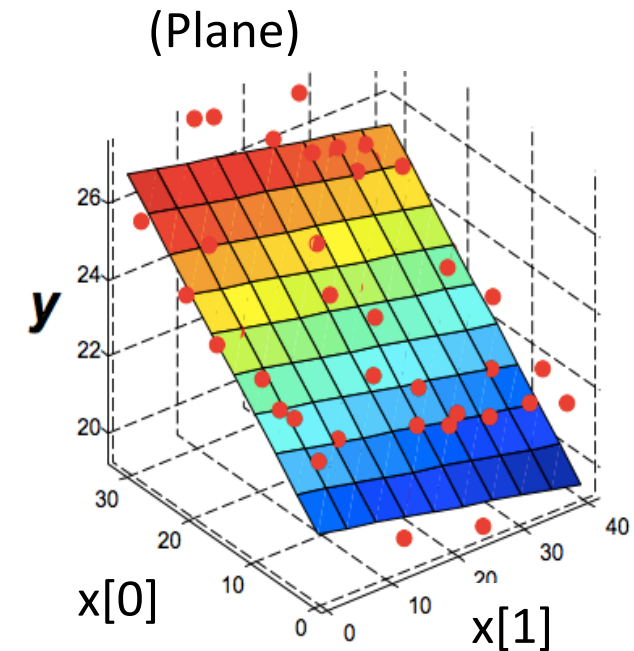
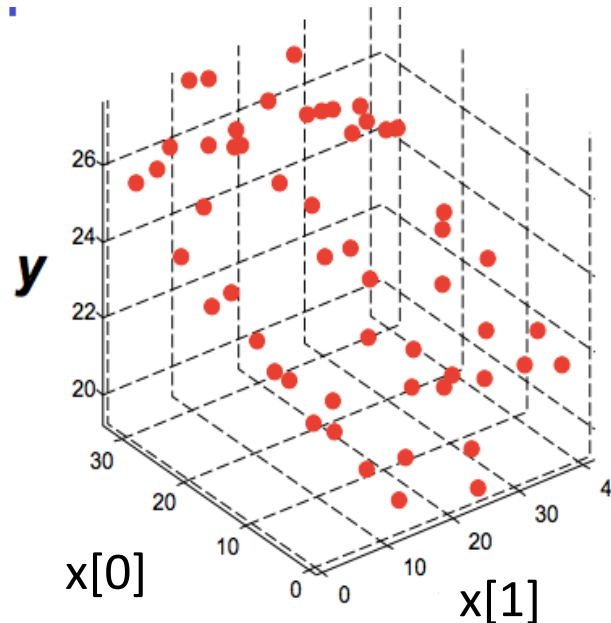
Feature vector

- How many features are there?
 - 2

Parameter vector to learn

- How many parameters are there?
 - 3

Predicted value



Linear Model: Predict Salary as a ML Engineer

(Solution is a hyperplane)

$$\hat{y} = w[0] * x[0] + w[1] * x[1] + \dots + w[p] * x[p] + b$$

- How would you write the linear model equation?
- How would you weight the different predictive cues?

How to Learn Model Parameters?

- Given: dataset (split into train and test partitions!)

Convention: X is $n \times d$ design matrix of sample pts
 y is n -vector of scalars [constants]

$$\begin{bmatrix} X_{11} & X_{12} & \dots & X_{1j} & \dots & X_{1d} \\ X_{21} & X_{22} & & X_{2j} & & X_{2d} \\ \vdots & & & & & \\ X_{i1} & X_{i2} & & X_{ij} & & X_{id} \\ \vdots & & & & & \\ X_{n1} & X_{n2} & & X_{nj} & & X_{nd} \end{bmatrix} \leftarrow \text{point } X_i^\top$$

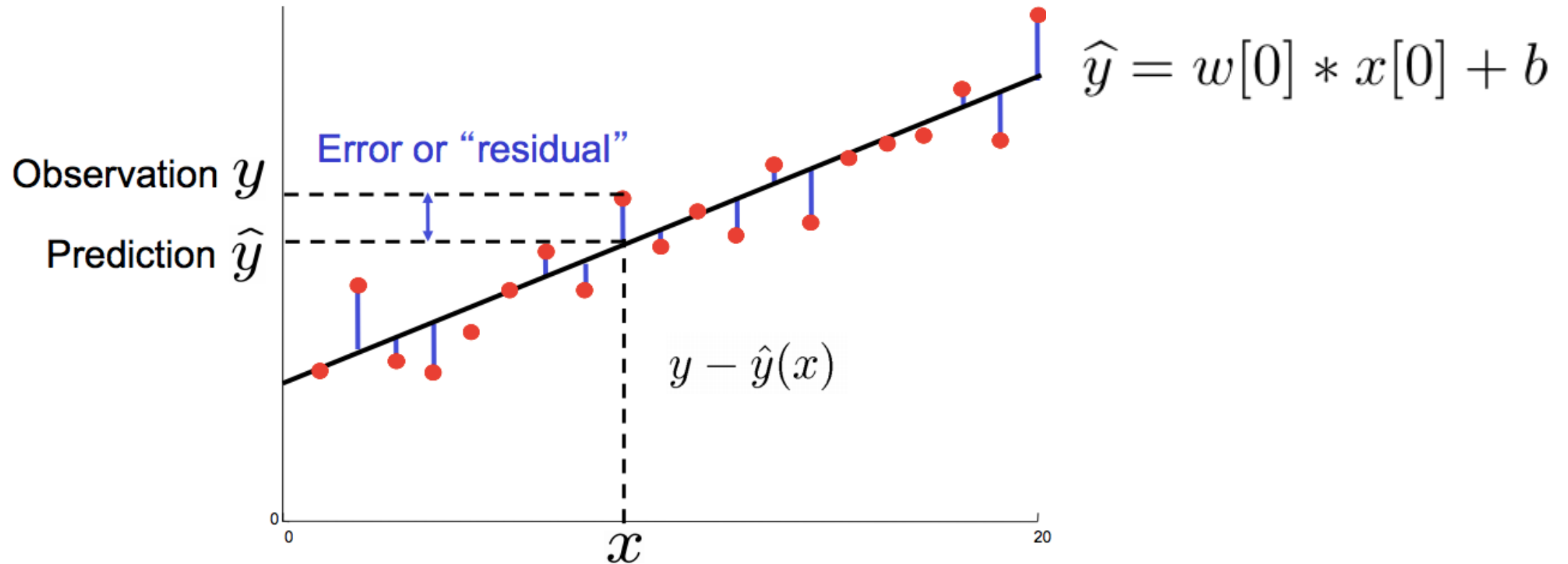
\uparrow
feature column X_{*j}

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

\uparrow
 y

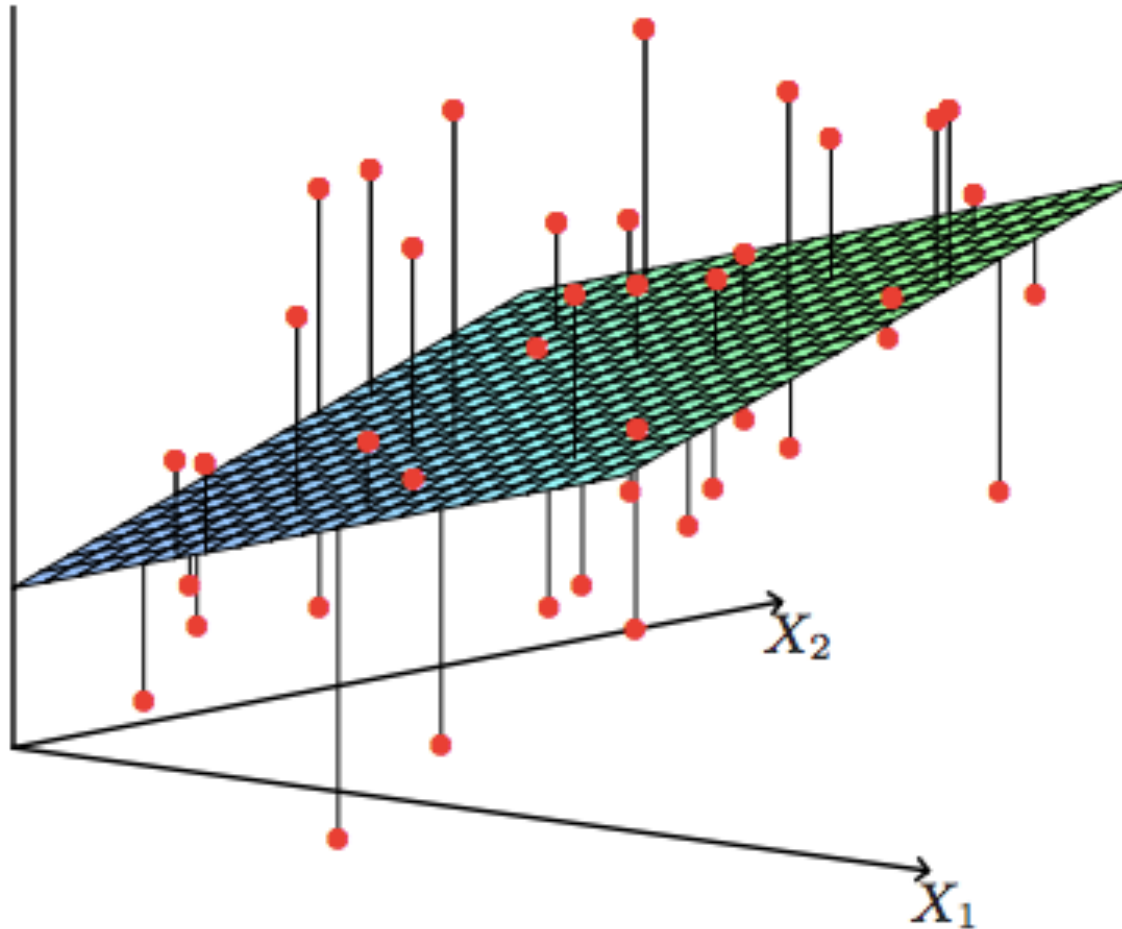
How to Learn Model Parameters?

- (Gauss, 1801) Least squares: *minimize* total squared error (“residual”)
 - Why square the error?



How to Learn Model Parameters?

- (Gauss, 1801) Least squares: *minimize* total squared error (“residual”)



How to Learn Model Parameters?

- (Gauss, 1801) Least squares: *minimize* total squared error (“residual”)
 - Take derivatives, set to zero, and solve for parameters

$$\frac{\partial}{\partial w} \sum_i (y_i - wx_i)^2 = 2 \sum_i -x_i (y_i - wx_i) \Rightarrow$$

$$2 \sum_i x_i (y_i - wx_i) = 0 \Rightarrow$$

$$\sum_i x_i y_i = \sum_i wx_i^2 \Rightarrow$$

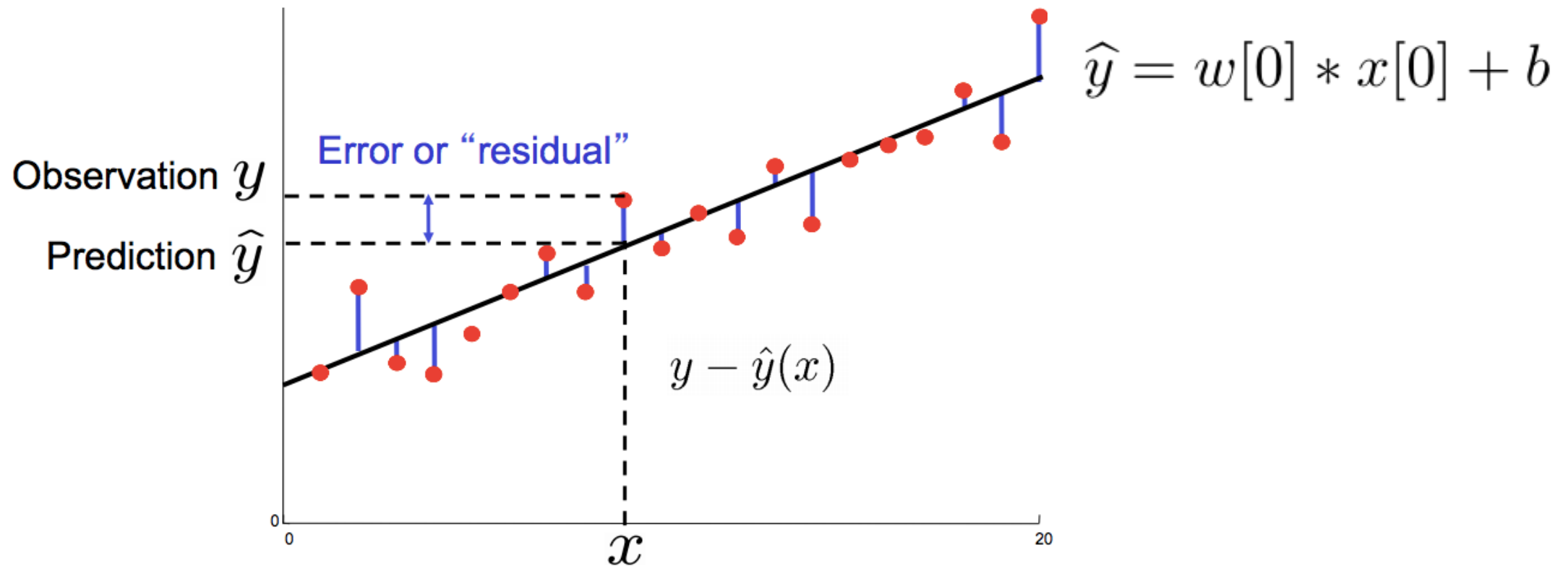
$$w = \frac{\sum_i x_i y_i}{\sum_i x_i^2}$$

How to Learn Model Parameters?

- (Gauss, 1801) Least squares: *minimize* total squared error (“residual”)
 - Gradient Descent: online learning solution
 - Slower
 - Not guaranteed to find optimal solution
 - But works for large datasets!

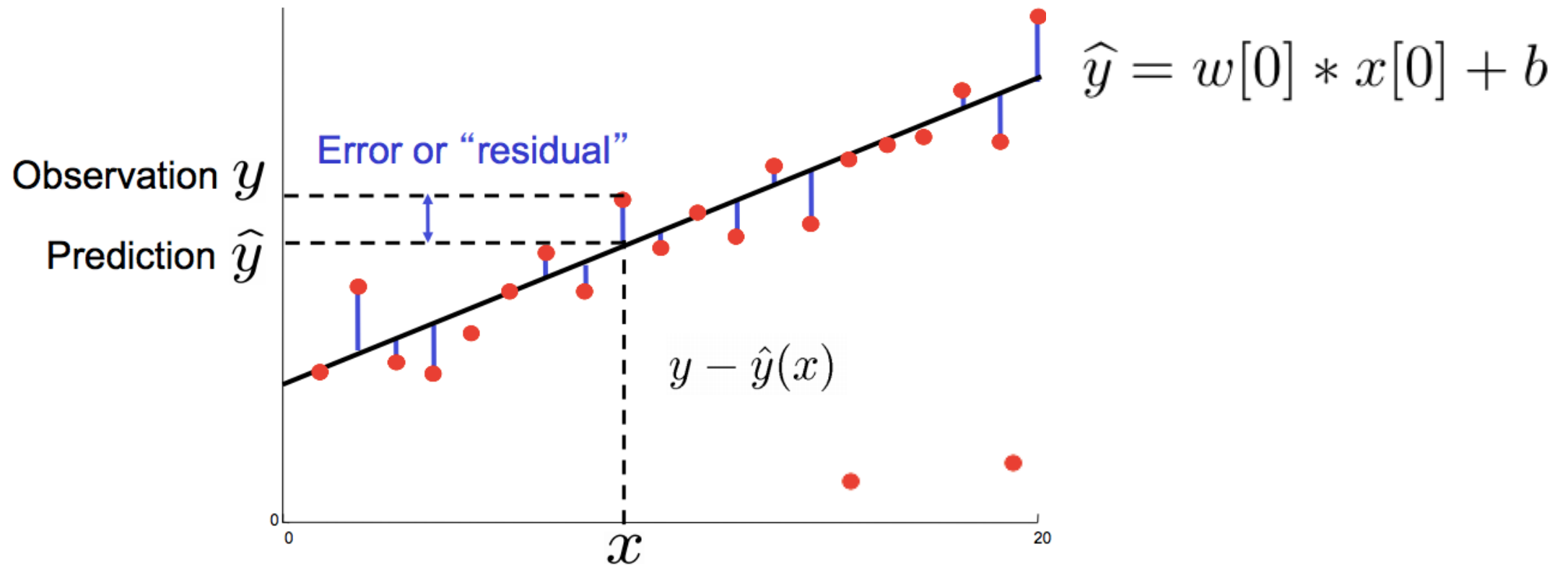
What Does the Error Represent?

- (Gauss, 1801) Least squares: *minimize* total squared error (“residual”)
 - Noise



What Happens to the Learned Model in the Presence of Outliers?

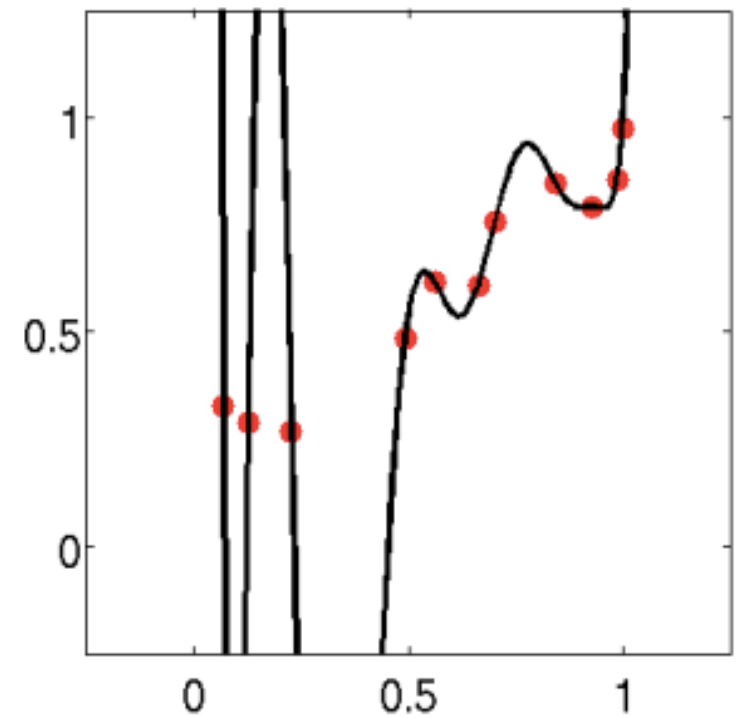
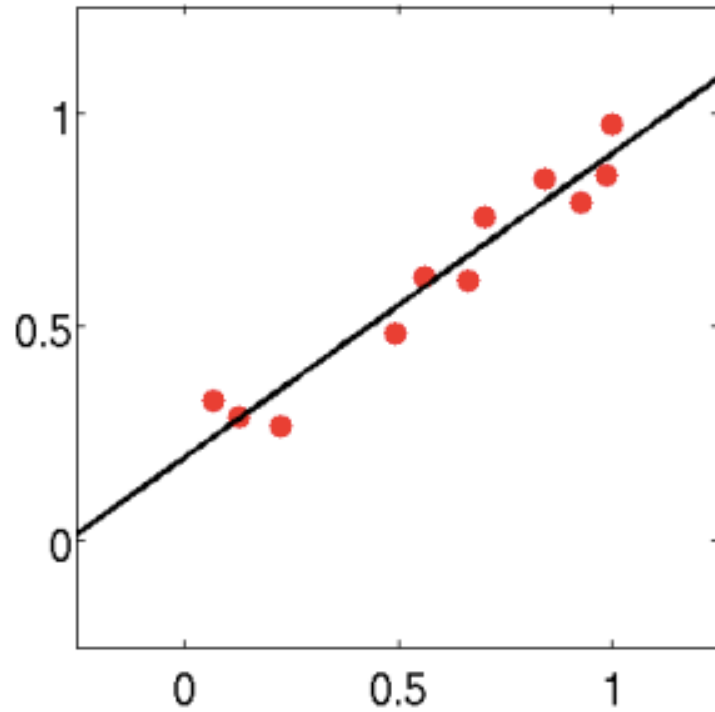
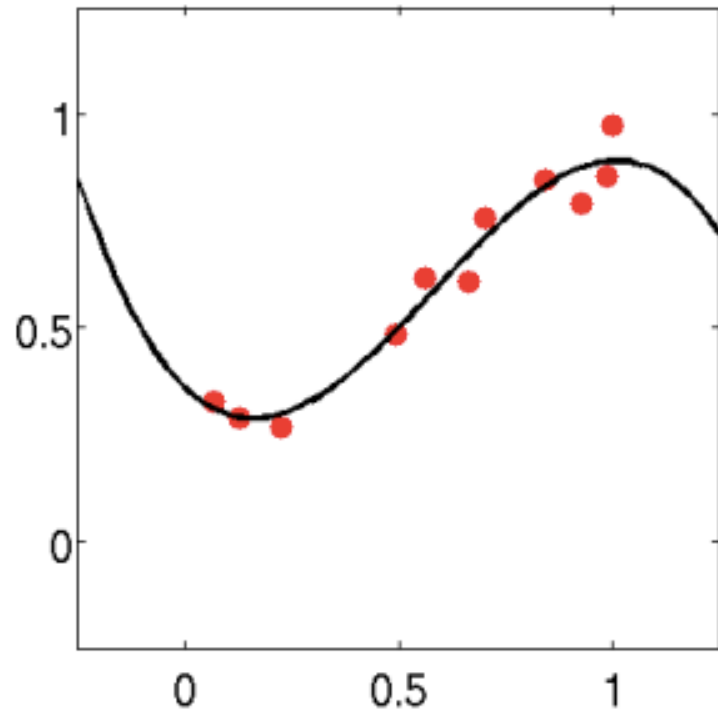
- (Gauss, 1801) Least squares: *minimize* total squared error (“residual”)



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What if Linear Models Are Not Good Enough?



Model Non-Linear Relationships by Transforming Features

- e.g., (Recall) Formula:

$$\hat{y} = w[0] * x[0] + w[1] * x[1] + b$$

Predicted value

- e.g., New Formula:

$$\hat{y} = w[0] * x[0] + w[1] * x[0]^2 + b$$

Parameter vector

Feature vector

- Same model parameters...
- Still a linear model!
- But can now model more complex relationships!!

Model Non-Linear Relationships by Transforming Features

- e.g., feature conversion for polynomial degree 3

$$D = \{(x^{(j)}, y^{(j)})\} \longrightarrow D = \{([x^{(j)}, (x^{(j)})^2, (x^{(j)})^3], y^{(j)})\}$$

- e.g., What is the new feature vector with polynomial degree up to 3?

$$\begin{array}{l} \text{Example 1:} \\ \text{Example 2:} \\ \text{Example 3:} \end{array} \begin{bmatrix} 2 \\ 3 \\ 4 \end{bmatrix} \longrightarrow \begin{array}{l} \text{Example 1:} \\ \text{Example 2:} \\ \text{Example 3:} \end{array} \begin{bmatrix} 2 & 4 & 8 \\ 3 & 9 & 27 \\ 4 & 16 & 64 \end{bmatrix}$$

Basis Functions to Transform Features: Polynomial and Beyond...

- General idea: **project data into a higher dimension** to fit more complicated relationships to a linear fit
- How to **project data into a higher dimension**?

e.g., Polynomial: $\phi_j(x) = x^j$ for $j=0 \dots n$

Gaussian: $\phi_j(x) = \frac{(x - \mu_j)}{2\sigma_j^2}$

Sigmoid: $\phi_j(x) = \frac{1}{1 + \exp(-s_j x)}$

Polynomial Function to Transform Features

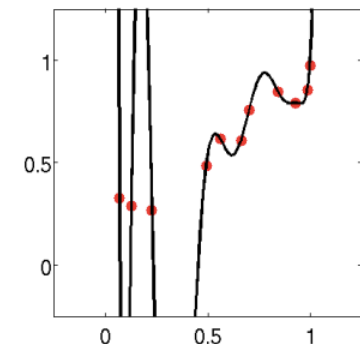
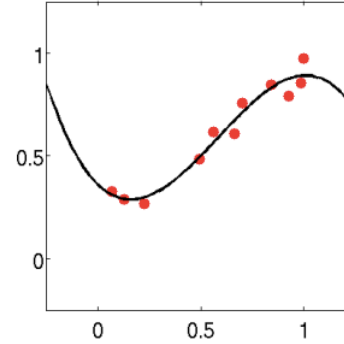
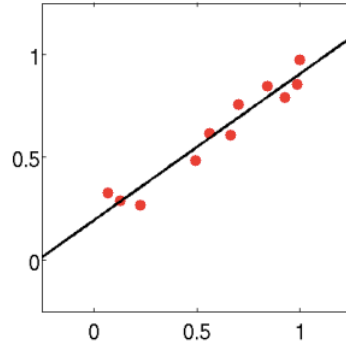
- M-th order polynomial function:

$$\mu(x, \mathbf{w}) = w_0 + \sum_{j=1}^M w_j x^j$$

- Linear model... so still learn model parameters by solving same analytical/gradient descent methods as discussed in previous section

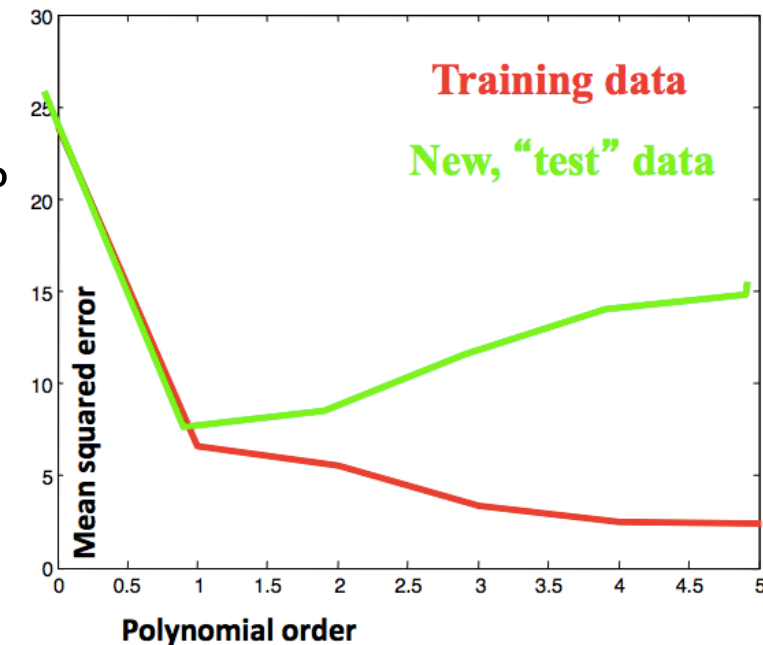
Choosing a Feature Transformation

- Are more features better?



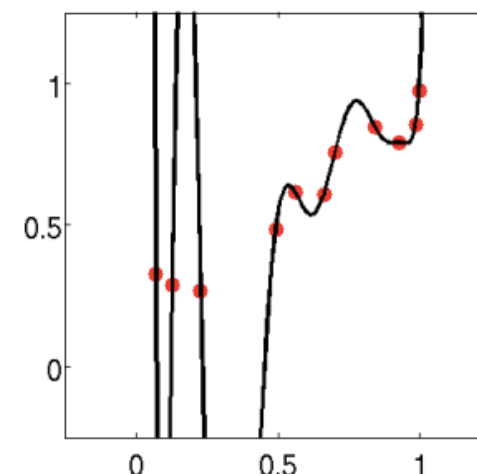
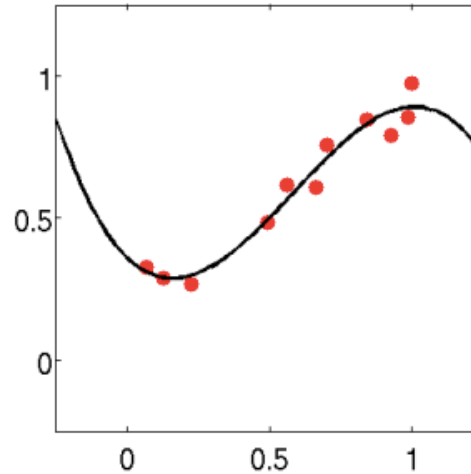
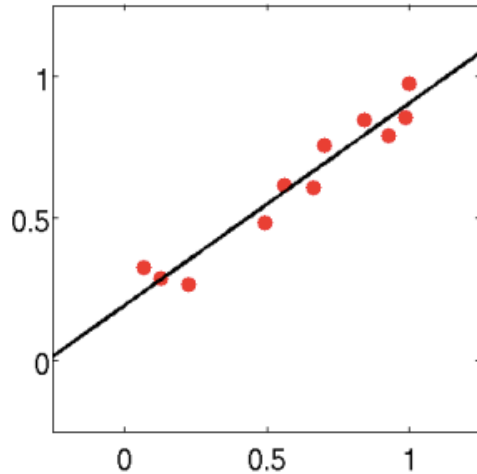
- Example plot of error on training dataset and testing dataset:

- What happens to training data error with larger polynomial order?
- What happens to testing data error with larger polynomial order?
 - Recall data has noise
 - Higher order is more able to model this noise!
 - Higher order is more likely therefore to **“overfit”** to training data and so not generalize to new unobserved test data



How to Avoid Overfitting?

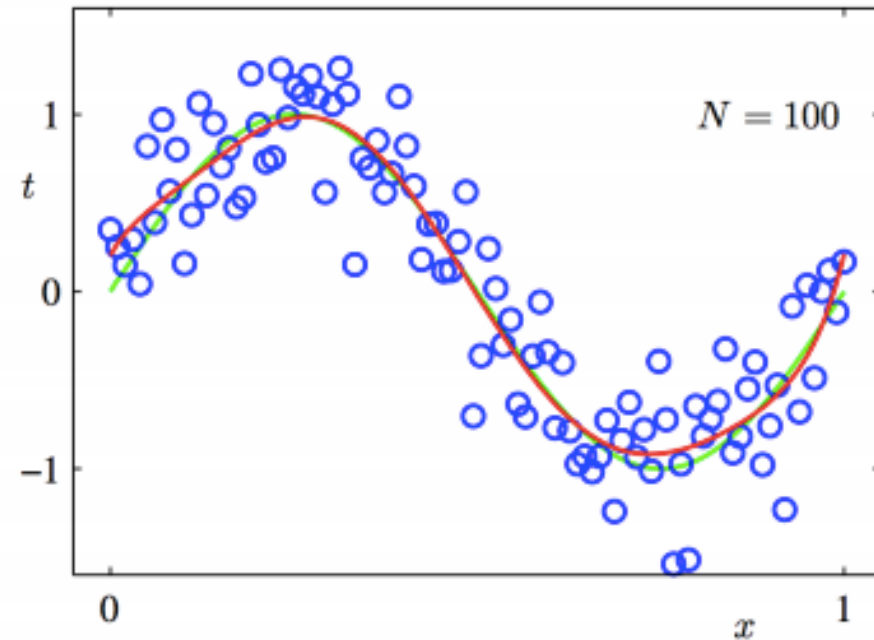
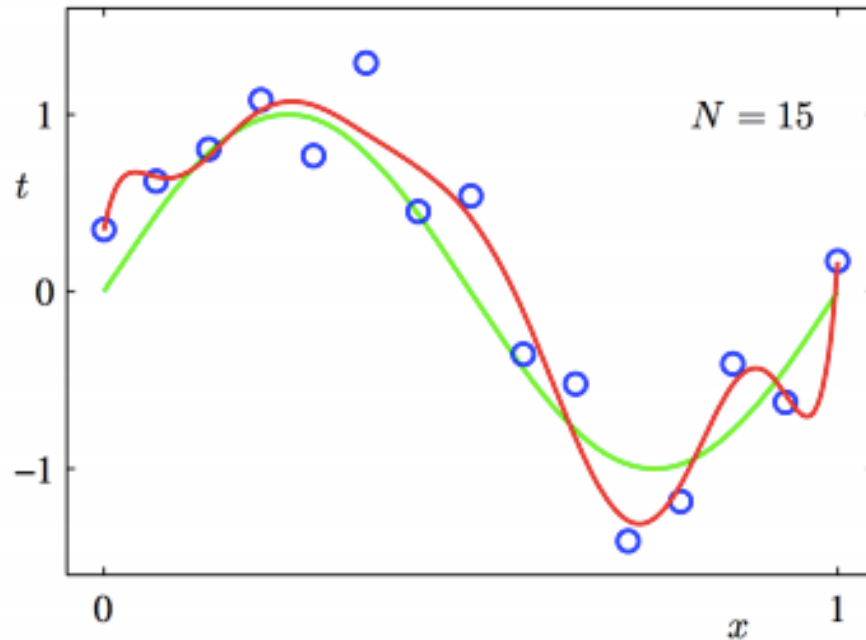
- Use lower degree polynomial:



- Risk: may be underfitting again

How to Avoid Overfitting?

- Add more training data



- What are the challenges/costs with collecting more training data?

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How to Avoid Overfitting?

- **Regularize** model (add constraints)... but how?
 - e.g., weights learned for fitting a model to a sine wave function (polynomial degrees 0, 1, ..., 9)

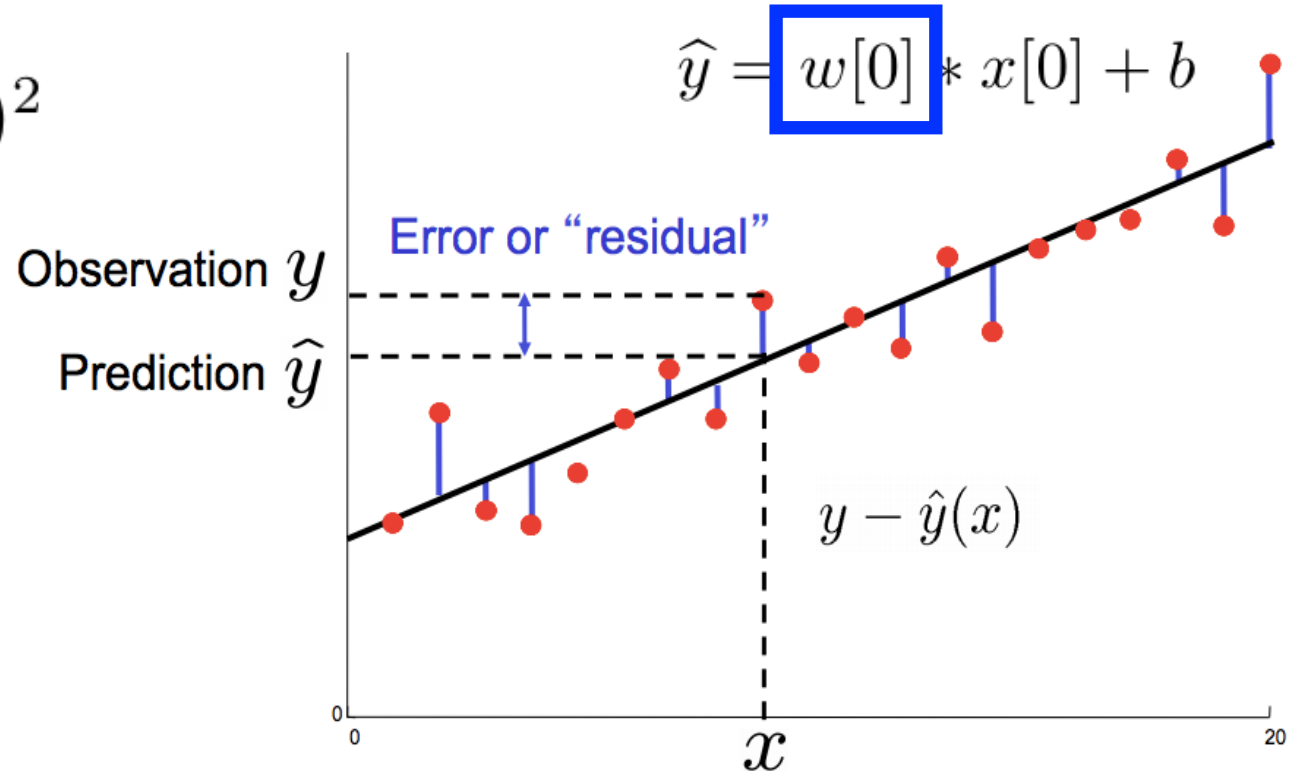
| | $M = 0$ | $M = 1$ | $M = 6$ | $M = 9$ |
|---------|---------|---------|---------|-------------|
| w_0^* | 0.19 | 0.82 | 0.31 | 0.35 |
| w_1^* | | -1.27 | 7.99 | 232.37 |
| w_2^* | | | -25.43 | -5321.83 |
| w_3^* | | | 17.37 | 48568.31 |
| w_4^* | | | | -231639.30 |
| w_5^* | | | | 640042.26 |
| w_6^* | | | | -1061800.52 |
| w_7^* | | | | 1042400.18 |
| w_8^* | | | | -557682.99 |
| w_9^* | | | | 125201.43 |

- Sign of overfitting: weights blow up and cancel each other out to fit the training data
- **Idea**: add constraint to minimize presence of large weights in models!

How to Avoid Overfitting?

- **Idea:** add constraint to minimize presence of large weights in models
- **Recall:** we previously learned models by *minimizing* sum of squared errors (SSE) for all n training examples:

$$SSE = \sum_{i=1}^n (y^{(i)} - \hat{y}^{(i)})^2$$



How to Avoid Overfitting?

- **Idea:** add constraint to minimize presence of large weights in models
- **Recall:** we previously learned models by *minimizing* sum of squared errors (SSE) for all n training examples:

$$SSE = \sum_{i=1}^n (y^{(i)} - \hat{y}^{(i)})^2$$

- **Ridge Regression:** add constraint to penalize squared weight values

$$Error = \sum_{i=1}^n (y^{(i)} - \hat{y}^{(i)})^2 + \alpha \sum_{j=1}^m w_j^2$$

- **Lasso Regression:** add constraint to penalize absolute weight values

$$Error = \sum_{i=1}^n (y^{(i)} - \hat{y}^{(i)})^2 + \alpha \sum_{j=1}^m |w_j|$$

How to Set Alpha?

Recall: $\hat{y} = \sum_{j=1}^m w_j x_j + w_0$

What happens when you set alpha to 0?

What happens when you set alpha to 1?

- **Ridge Regression:** add constraint to penalize squared weight values

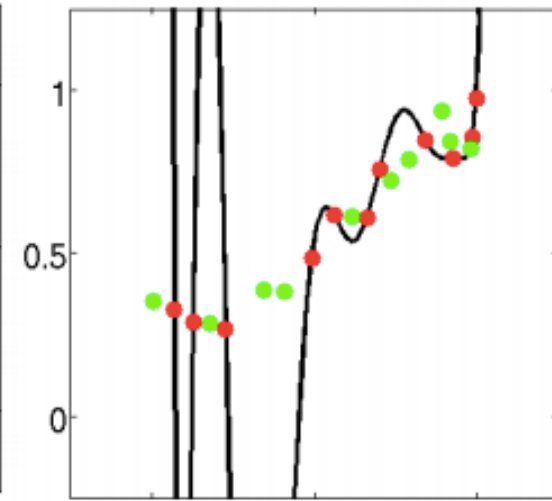
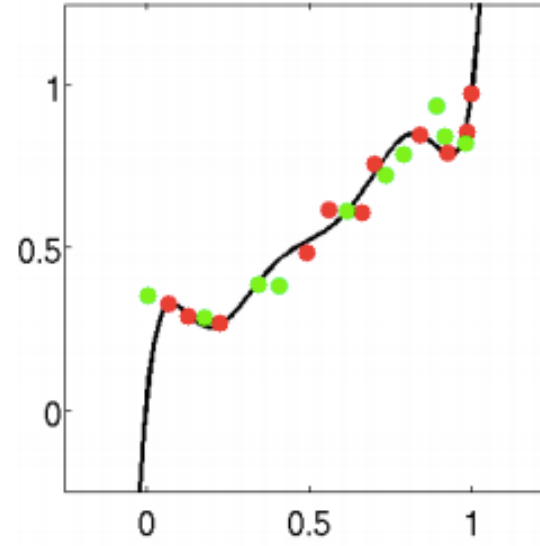
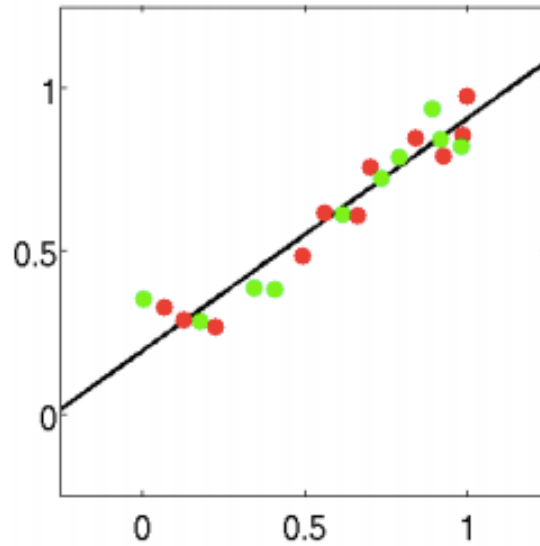
$$Error = \sum_{i=1}^n (y^{(i)} - \hat{y}^{(i)})^2 + \alpha \sum_{j=1}^m w_j^2$$

- **Lasso Regression:** add constraint to penalize absolute weight values

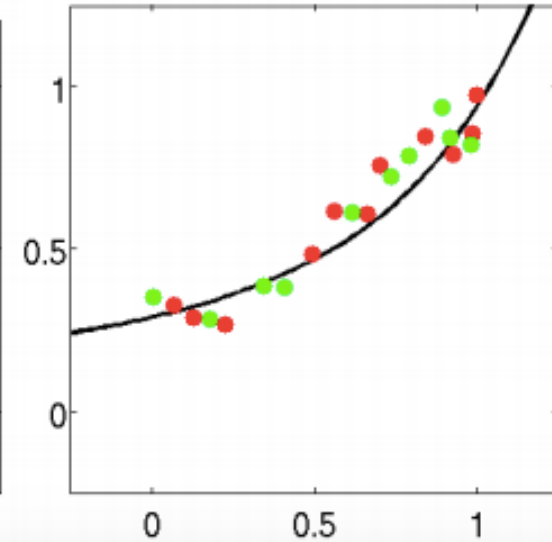
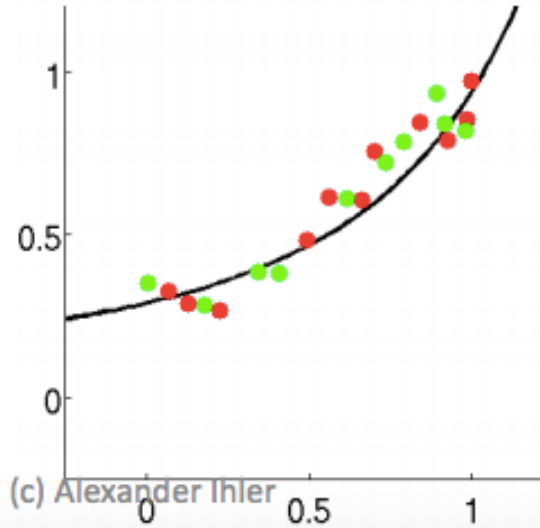
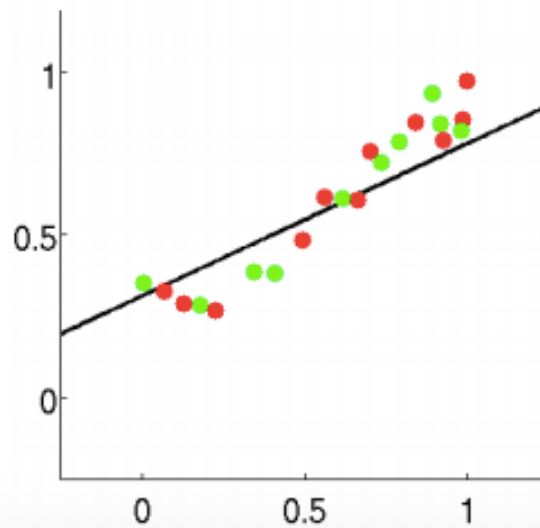
$$Error = \sum_{i=1}^n (y^{(i)} - \hat{y}^{(i)})^2 + \alpha \sum_{j=1}^m |w_j|$$

How to Set Alpha?

Alpha = 0
(Unregularized)



Alpha = 1



Why Choose Lasso Instead vs Ridge Regression

- Lasso: typically creates sparse weight vectors (sets weights to 0)
 - Good to use when there are MANY features and few believed to be relevant
 - Increases interpretability

Today's Topics

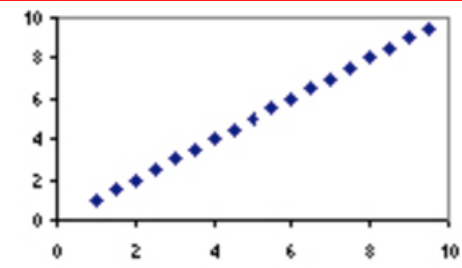
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Evaluating regressors: descriptive statistics

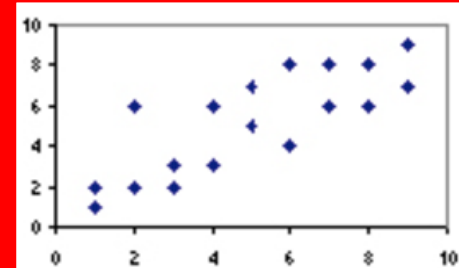
Results: e.g.,

| inst# | actual | predicted | error |
|-------|--------|-----------|--------|
| 1 | 0.18 | 0.272 | 0.092 |
| 2 | 0.122 | 0.434 | 0.312 |
| 3 | 0.088 | 0.344 | 0.256 |
| 4 | 0.125 | 0.238 | 0.112 |
| 5 | 0 | 0.232 | 0.232 |
| 6 | 0 | 0.092 | 0.092 |
| 7 | 0.907 | 0.367 | -0.54 |
| 8 | 0.216 | 0.227 | 0.011 |
| 9 | 0 | 0.367 | 0.367 |
| 10 | 0.048 | 0.108 | 0.061 |
| 11 | 0.198 | 0.145 | -0.053 |
| 12 | 0 | 0.159 | 0.159 |
| 13 | 0.505 | 0.28 | -0.225 |
| 14 | 0.273 | 0.097 | -0.175 |
| 15 | 0.12 | 0.178 | 0.058 |
| 16 | 0.254 | 0.235 | -0.018 |

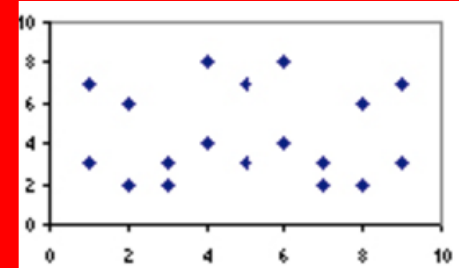
- Correlation coefficient



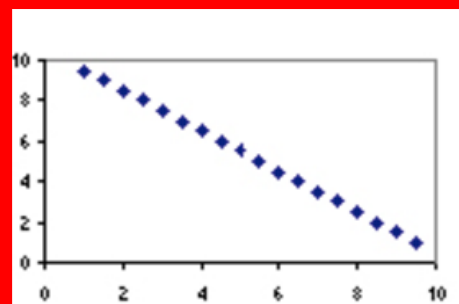
Maximum positive correlation
($r = 1.0$)



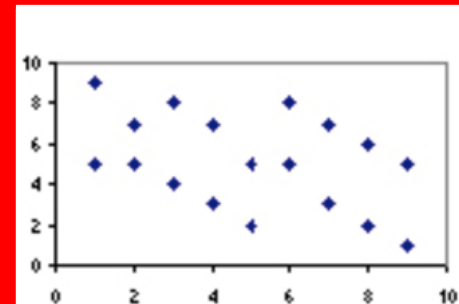
Strong positive correlation
($r = 0.80$)



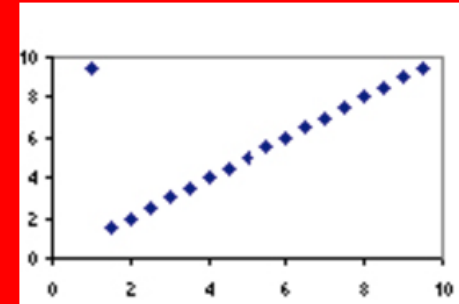
Zero correlation
($r = 0$)



Maximum negative correlation
($r = -1.0$)



Moderate negative correlation
($r = -0.43$)



Strong correlation & outlier
($r = 0.71$)

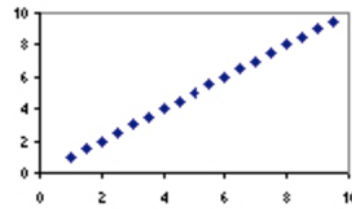
Evaluating regressors: descriptive statistics

Results: e.g.,

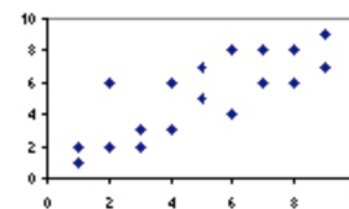
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- Correlation coefficient

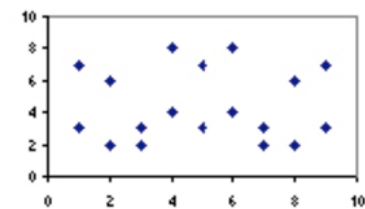
- What is the range of possible values?
- Are larger values better or worse?



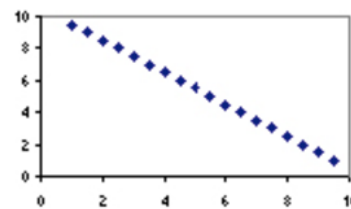
Maximum positive correlation
($r = 1.0$)



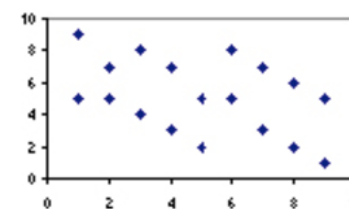
Strong positive correlation
($r = 0.80$)



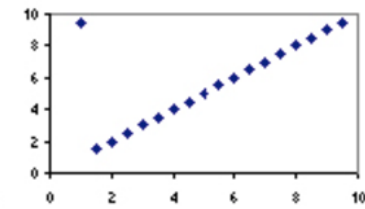
Zero correlation
($r = 0$)



Maximum negative correlation
($r = -1.0$)



Moderate negative correlation
($r = -0.43$)



Strong correlation & outlier
($r = 0.71$)

Evaluating regressors: descriptive statistics

Results: e.g.,

| inst# | actual | predicted | error |
|-------|--------|-----------|--------|
| 1 | 0.18 | 0.272 | 0.092 |
| 2 | 0.122 | 0.434 | 0.312 |
| 3 | 0.088 | 0.344 | 0.256 |
| 4 | 0.125 | 0.338 | 0.213 |
| 5 | 0 | 0.232 | 0.232 |
| 6 | 0 | 0.182 | 0.182 |
| 7 | 0.907 | 0.367 | -0.54 |
| 8 | 0.216 | 0.227 | 0.011 |
| 9 | 0 | 0.367 | 0.367 |
| 10 | 0.048 | 0.108 | 0.061 |
| 11 | 0.198 | 0.145 | -0.053 |
| 12 | 0 | 0.158 | 0.158 |
| 13 | 0.505 | 0.28 | -0.225 |
| 14 | 0.173 | 0.187 | 0.013 |
| 15 | 0.12 | 0.178 | 0.058 |
| 16 | 0.254 | 0.235 | -0.018 |

- Correlation coefficient (Pearson's)
- Mean absolute error
 - What is the range of possible values?
 - Are larger values better or worse?

Today's Topics

- Regression Applications
- Discussion: Building Regression Datasets
- Linear Regression
- Polynomial Regression
- Regularization (Ridge Regression and Lasso Regression)
- Evaluating Regression Models
- Lab

Lab Assignment 1 Out

- “Unofficial TA” – Brandon Dang
- Piazza for class questions/discussion
- Office hours from Microsoft Azure representative this Friday Jan. 26:
 - Choose time slot here: <http://slottd.com/events/izg73js2o8/slots>

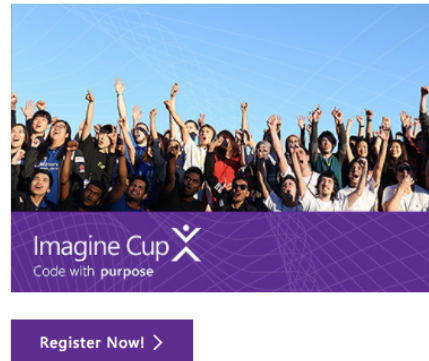
More Resources I Used for Today's Slides

- <http://www.cs.utoronto.ca/~fidler/teaching/2015/slides/CSC411/>
- - <http://www.cs.cmu.edu/~epxing/Class/10701/lecture.html>
- - <http://web.cs.ucla.edu/~sriram/courses/cs188.winter-2017/html/index.html>
- - <https://people.eecs.berkeley.edu/~jrs/189/>
- - <http://alex.smola.org/teaching/cmu2013-10-701/>
- - <http://sli.ics.uci.edu/Classes/2015W-273a>

Imagine Cup Competition

- Microsoft is hosting the annual Imagine Cup competition – both in the US and internationally.
 - The top prize is \$100,000.
 - Learn more at <https://imagine.microsoft.com/en-us/Category/11>

2018 Imagine Cup



- What to do? Build a project using Microsoft technologies