Regression & Regularization

Danna Gurari
University of Texas at Austin
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Review

- Last week:
  - Machine learning today
  - History of machine learning
  - How does a machine learn?

- Assignments (Canvas)
  - Problem Set 1 due yesterday
  - Problem Set 2 due next week
  - Lab Assignment 1 due in two weeks

- Questions?

Today’s Topics

- Regression applications
- Evaluating regression models
- Background: notation
- Linear regression
- Polynomial regression
- Regularization (Ridge regression and Lasso regression)
- Lab

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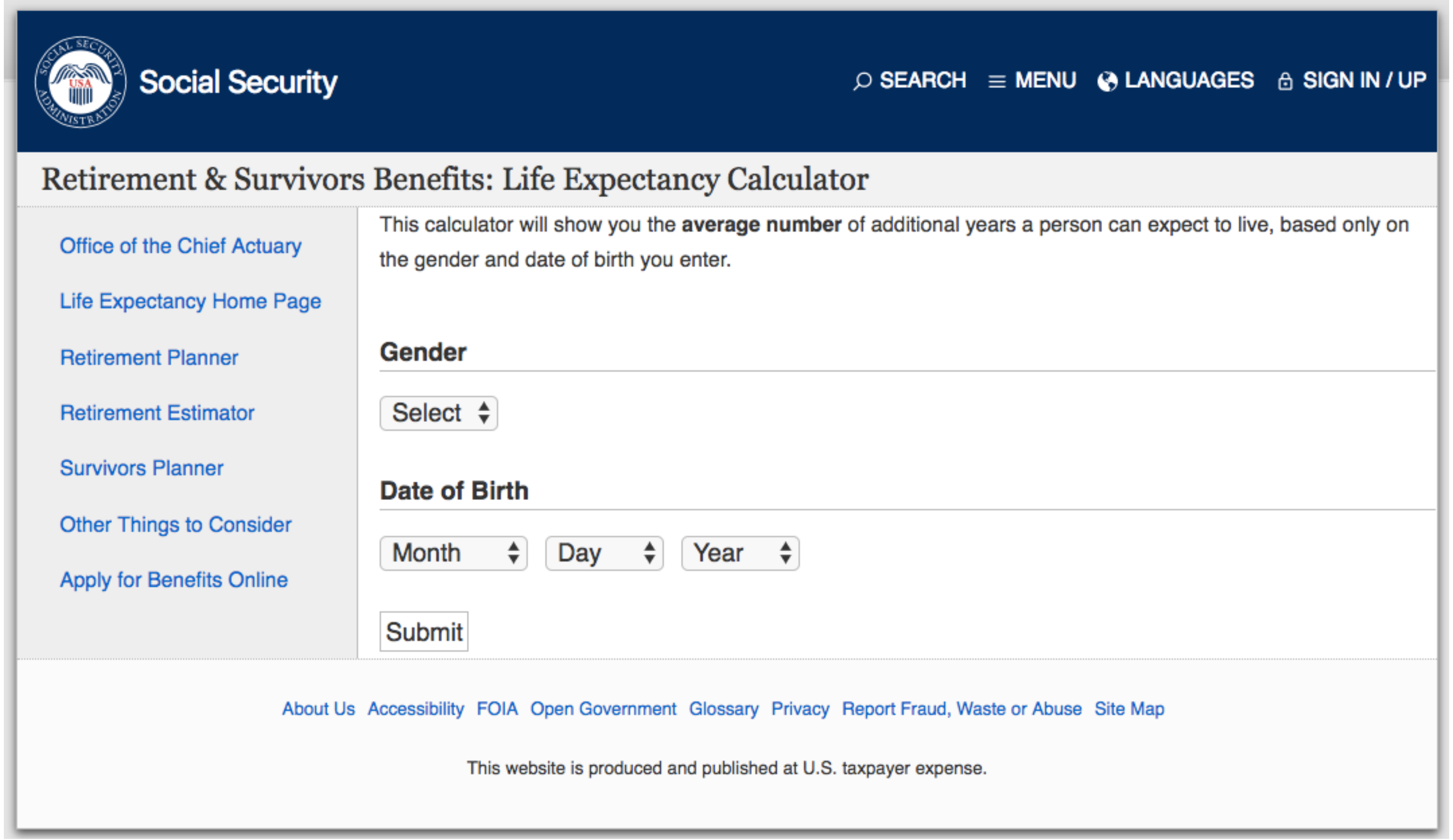
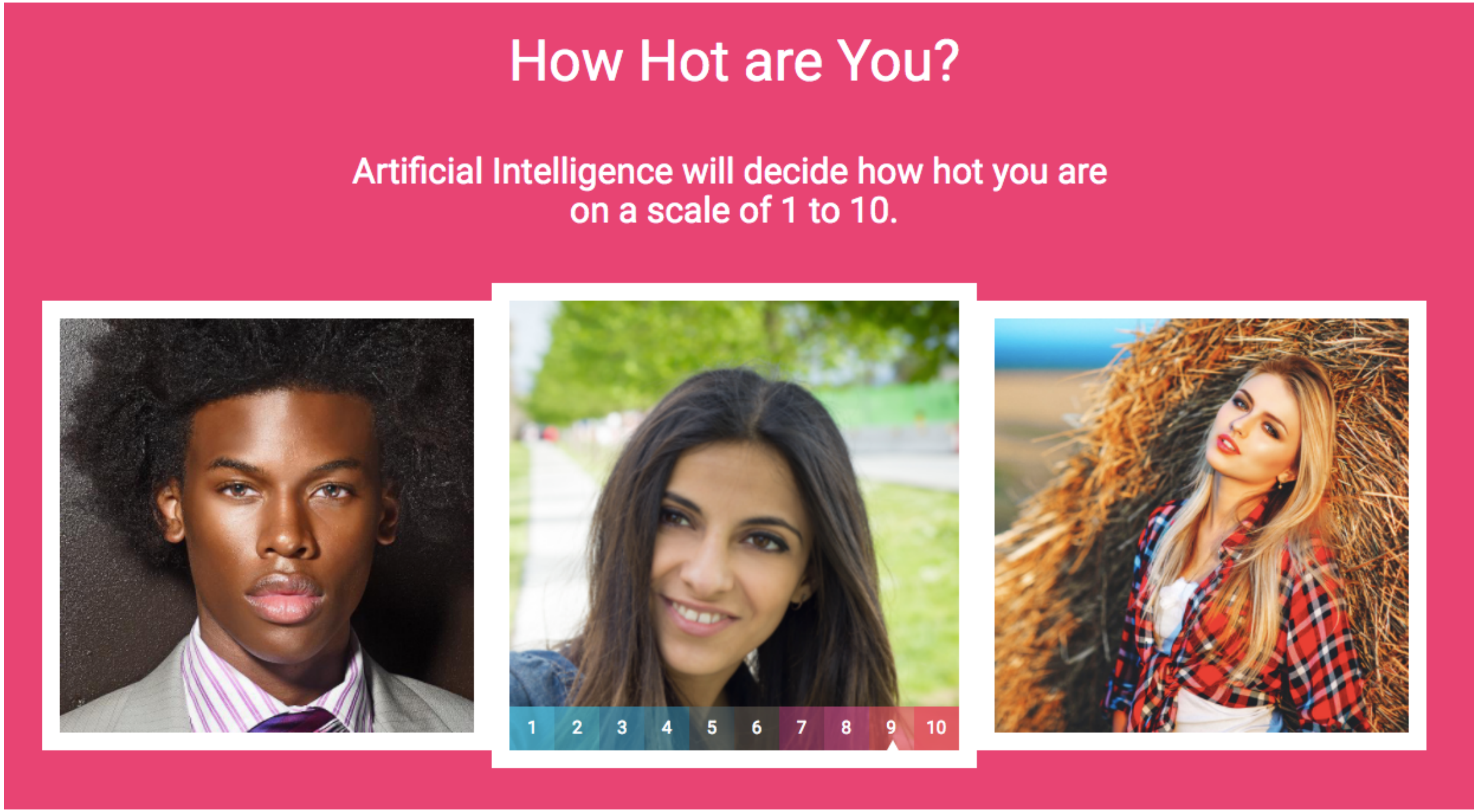
Today’s Focus: Regression

Predict **continuous** value

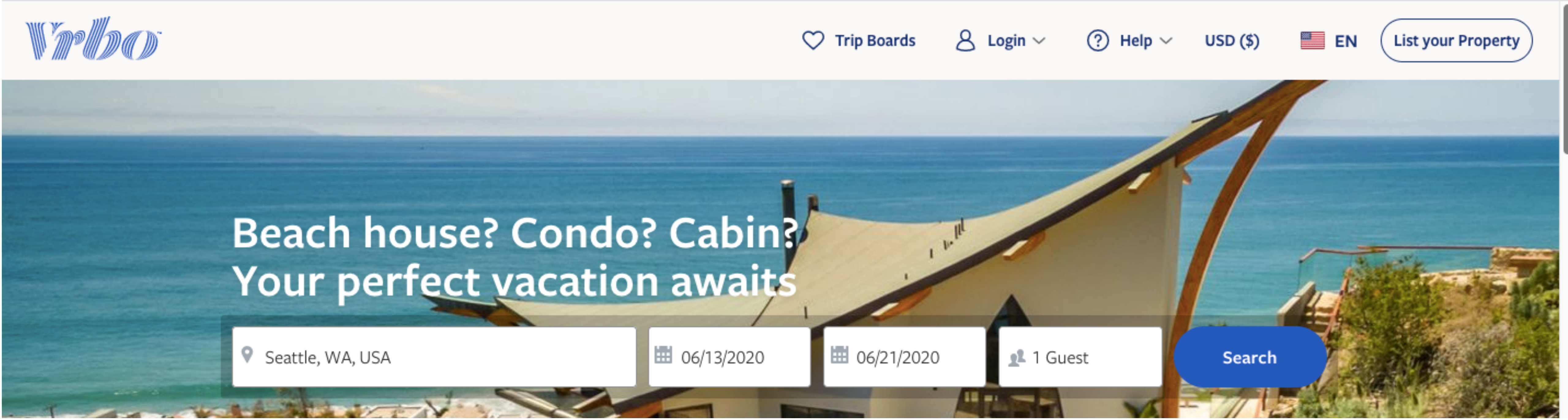
Predict Life Expectancy



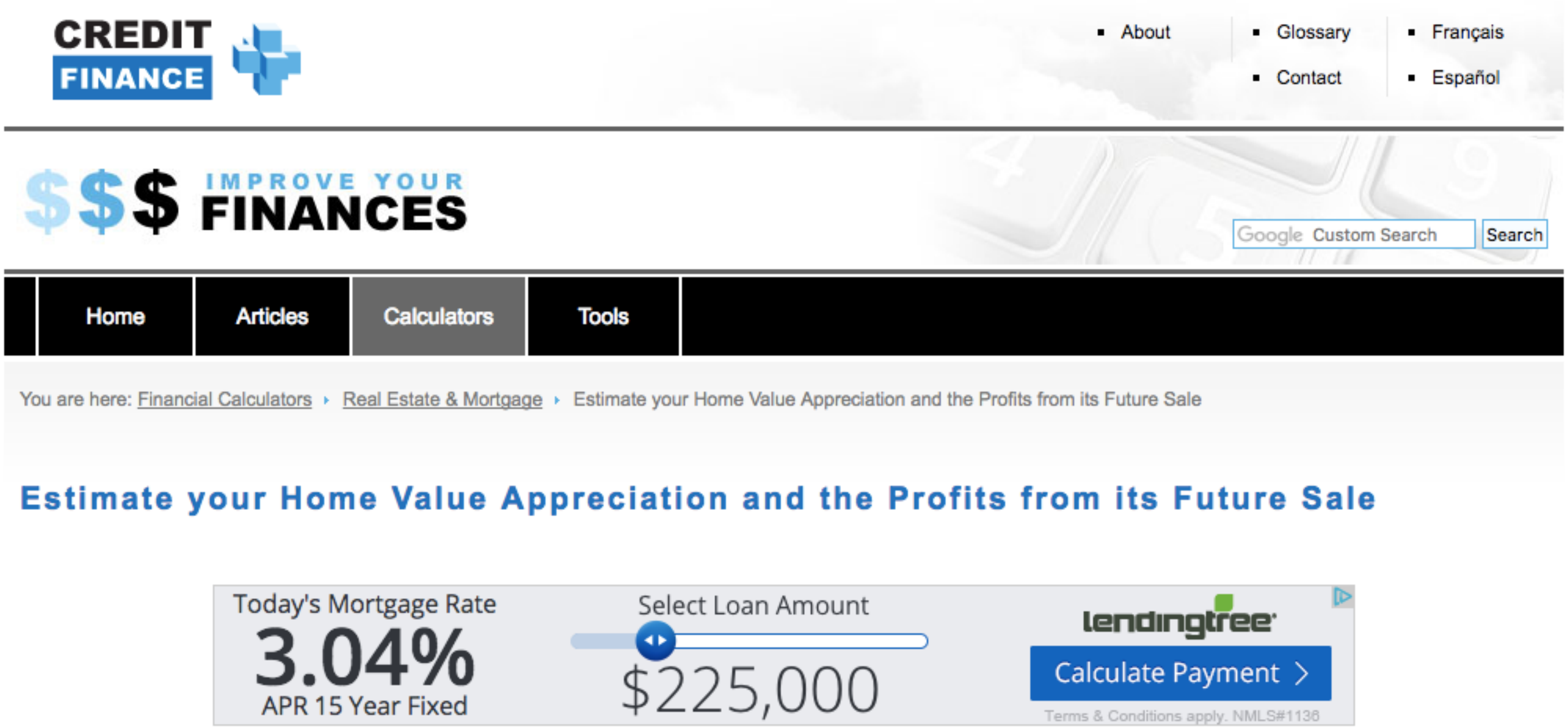
Predict Perceived "Hot"-ness



Predict Price to Charge for Your Home



Predict Future Value of a House You Buy



Predict Future Stock Price

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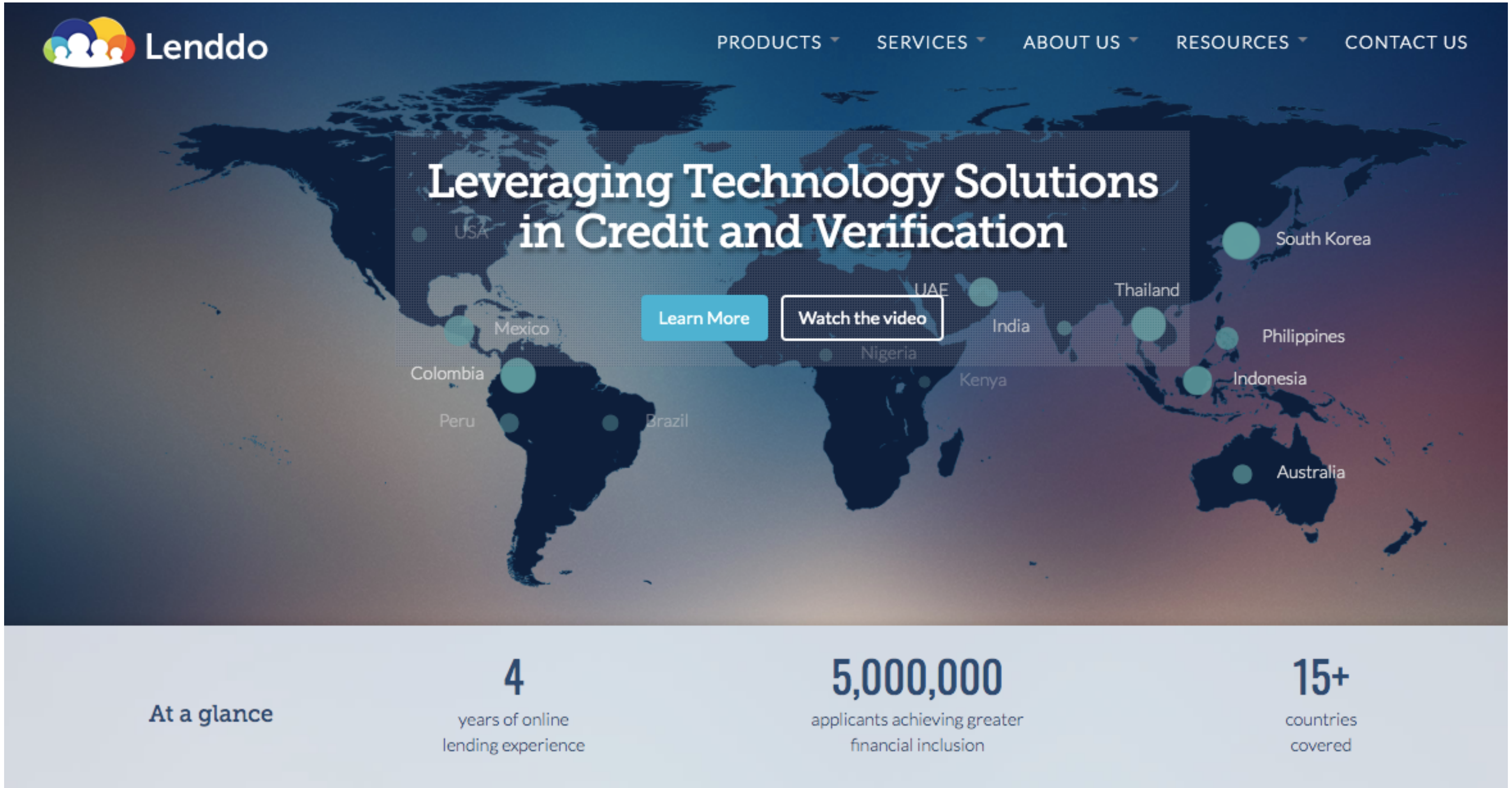
Home > Blog > Trading Strategies

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

Predict Credit Score for Loan Lenders



Demo: https://www.youtube.com/watch?time_continue=6&v=0bEJO4Twgu4&feature=emb_logo

https://emerj.com/ai-sector-overviews/artificial-intelligence-applications-lending-loan-management/

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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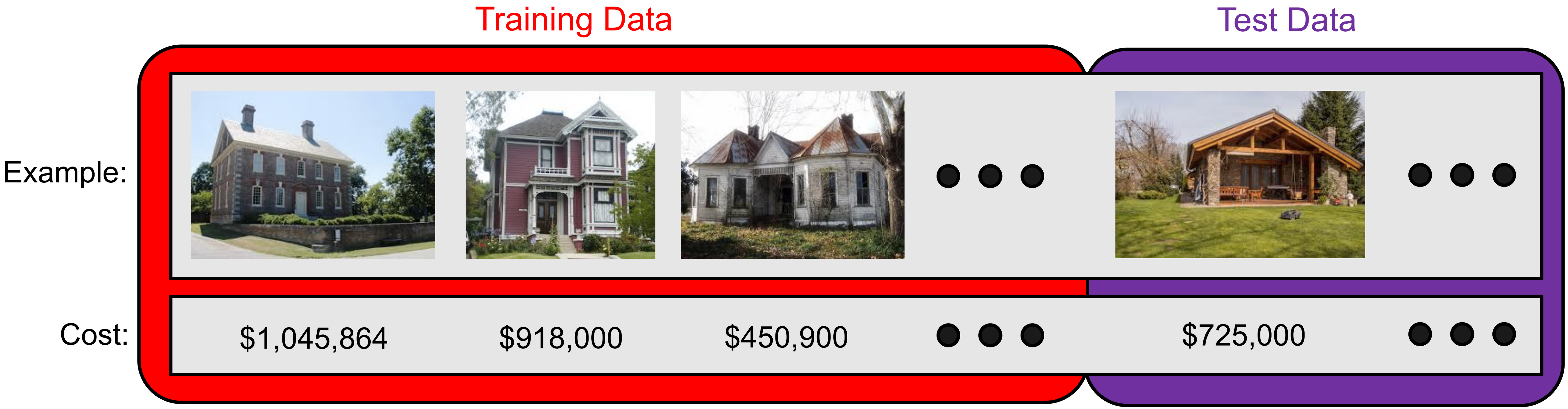
Goal: Design Models that **Generalize** Well to New, Previously Unseen Examples

Example:				● ● ●		● ● ●
Cost:	$1,045,864	$918,000	$450,900	● ● ●	$725,000	● ● ●

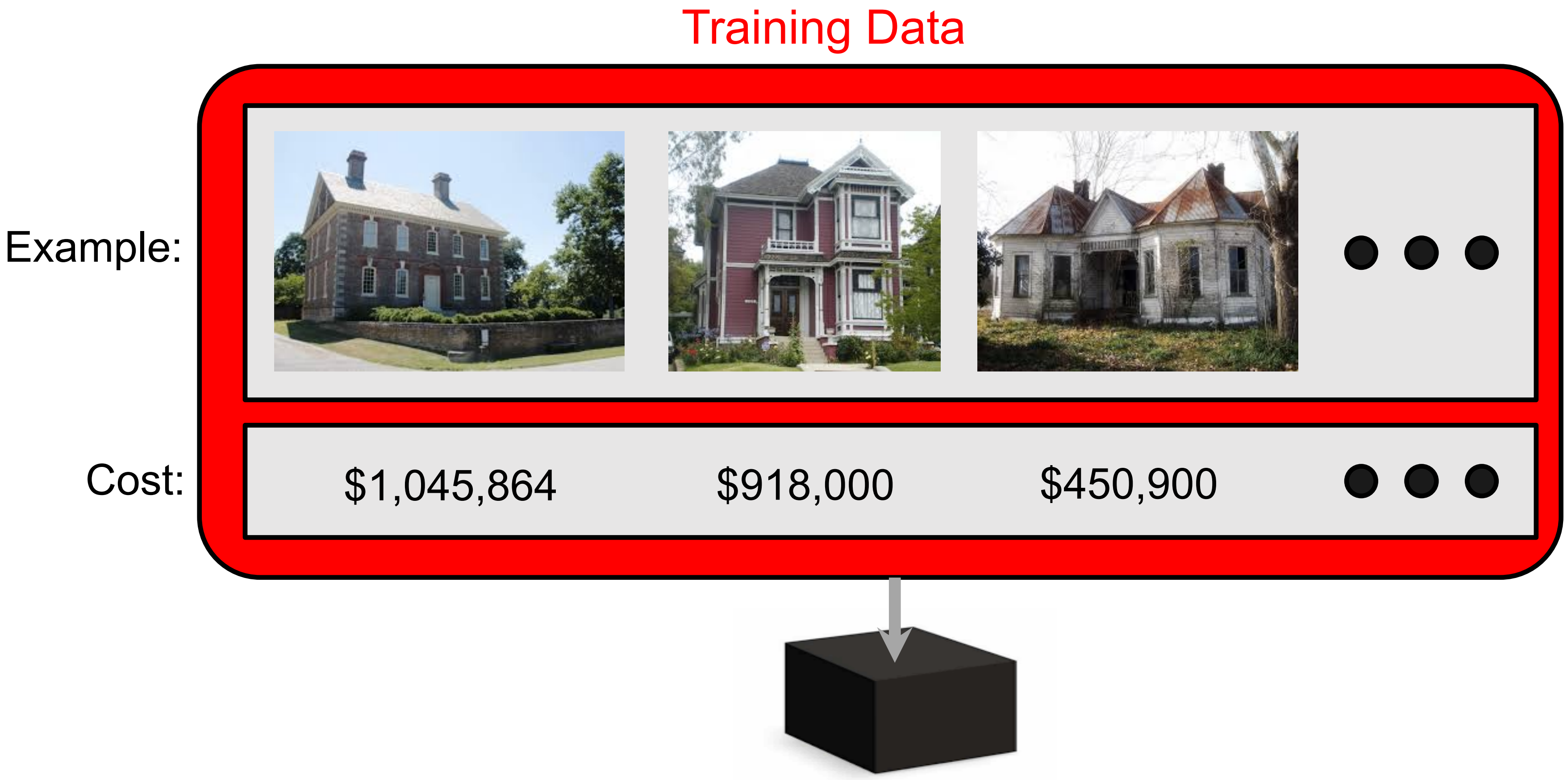
Goal: Design Models that **Generalize** Well to New, Previously Unseen Examples

1. Split data into a "training set" and "test set"



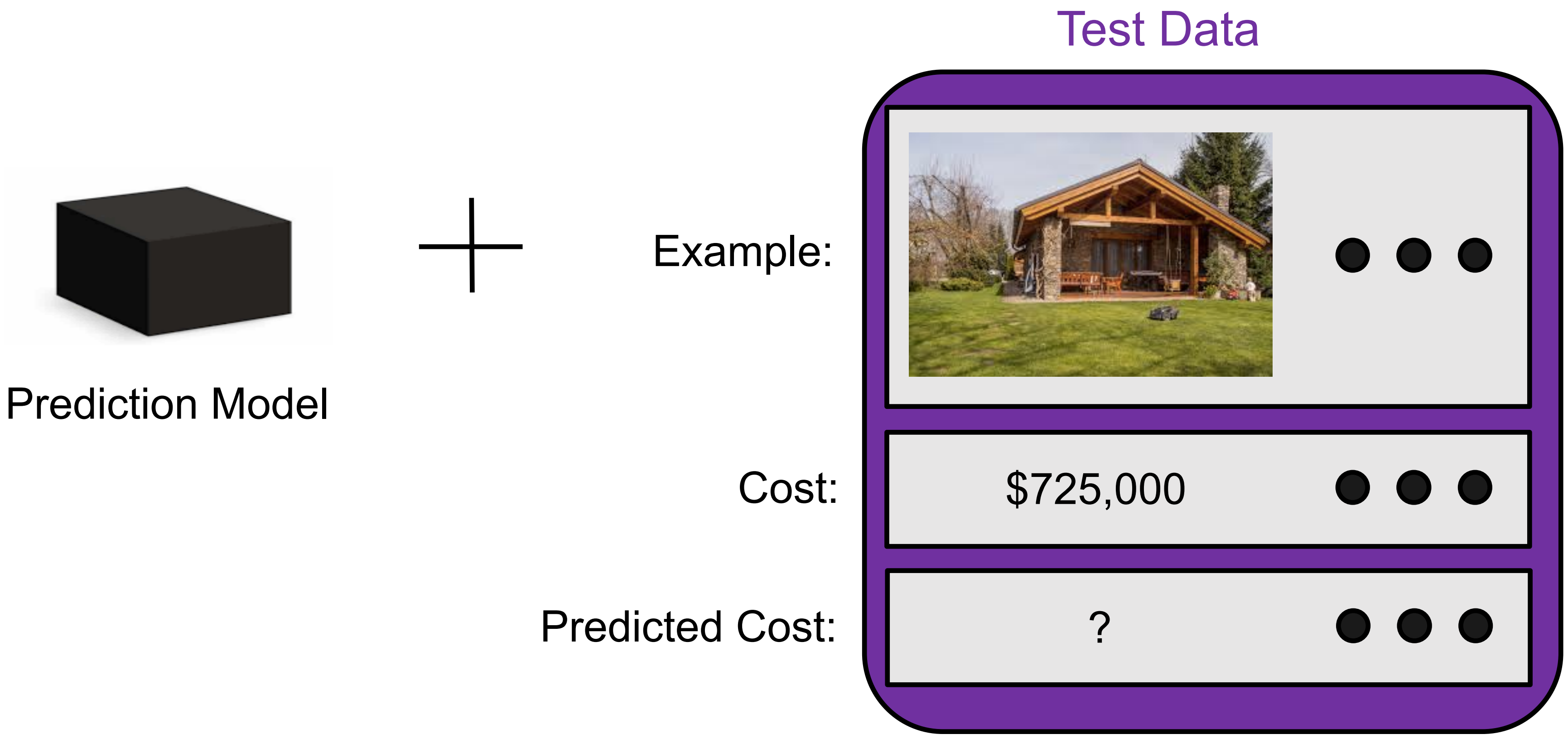
Goal: Design Models that **Generalize** Well to New, Previously Unseen Examples

2. Train model on "training set" to try to minimize prediction error on it



Goal: Design Models that **Generalize** Well to New, Previously Unseen Examples

3. Apply trained model on "test set" to measure generalization error



Goal: Design Models that **Generalize** Well to New, Previously Unseen Examples

3. Apply trained model on "test set" to measure generalization error

Prediction Model

+

Test Data

Example:  ● ● ●

Cost: $725,000 ● ● ●

Predicted Cost: $615,000 ● ● ●

Regression Evaluation Metrics

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	[illegible]	[illegible]	[illegible]
5	0	0.232	0.232
6	[illegible]	[illegible]	[illegible]
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	[illegible]	[illegible]	[illegible]
13	0.505	0.28	-0.225
14	[illegible]	[illegible]	[illegible]
15	0.12	0.178	0.058
16	0.254	0.235	-0.018

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

Regression Evaluation Metrics

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

- Mean absolute error
- Mean squared error
  - Why square the errors?

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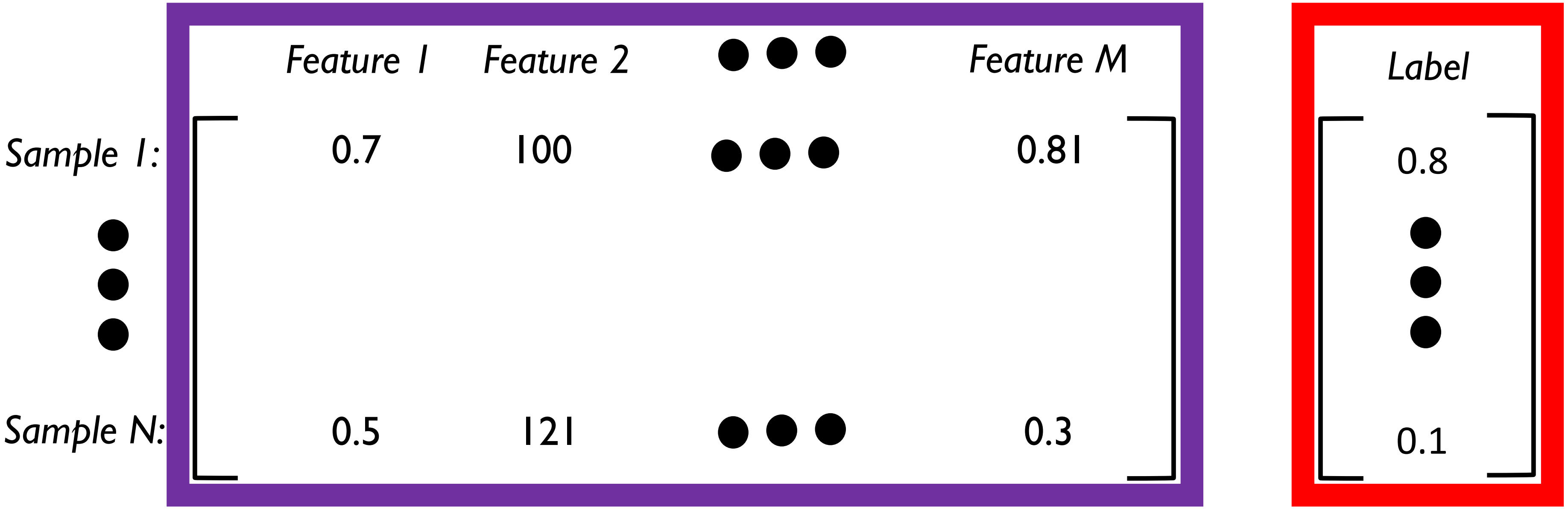
Matrices and Vectors

- **X** : each feature is in its own column and each sample is in its own row
- **y** : each row is the target value for the sample



Matrices and Vectors

- **X** : each feature is in its own column and each sample is in its own row
- **y** : each row is the target value for the sample

$$
\begin{bmatrix}
X_{11} & X_{12} & \cdots & X_{1j} & \cdots & X_{1d} \\
X_{21} & X_{22} & & X_{2j} & & X_{2d} \\
\vdots & & & & & \\
X_{i1} & X_{i2} & & X_{ij} & & X_{id} \\
\vdots & & & & & \\
X_{n1} & X_{n2} & & X_{nj} & & X_{nd}
\end{bmatrix}
\begin{matrix} \\ \\ \\ \leftarrow \text{point } X_i^\top \\ \\ \\ \end{matrix}
\qquad
\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}
$$

$\uparrow$ feature column X_{*j} $\qquad$ $\uparrow$ y

Vector-Vector Product

$$\boldsymbol{w}^T\boldsymbol{x} = \begin{bmatrix} w_1 & w_2 & w_3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = w_1x_1 + \cdots + w_mx_m$$

e.g.,

$$\begin{bmatrix} 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} = (1\text{x}4 + 2\text{x}5 + 3\text{x}6) = 32$$

Excellent Review: http://www.cs.cmu.edu/~zkolter/course/15-884/linalg-review.pdf

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

indeed | Find Jobs | Company Reviews | **Find Salaries** | Find Resumes | Employers / Post Job

Machine Learning Engineer Salaries in Austin, TX

Salary estimated from 44 employees, users, and past and present job advertisements on Indeed in the past 36 months. Last updated: August 18, 2018

Location

Austin

Average in Austin, TX

$142,418 per year

•Meets national average

How much does a Machine Learning Engineer make in Austin, TX?

The average salary for a Machine Learning Engineer is $142,418 per year in Austin, TX, which meets the national average. Salary estimates are based on 44 salaries submitted anonymously to Indeed by Machine Learning Engineer employees, users, and collected from past and present job advertisements on Indeed in the past 36 months. The typical tenure for a Machine Learning Engineer is less than 1 year.

Machine Learning Engineer job openings

Machine Learning Scientist
Amazon.com
Austin, TX
30+ days ago

Machine Learning Developer - Reinforcement Learning | INZONE.AI
Inzone
Austin, TX
30+ days ago

Junior Software Development Engineer in Test (SDET)
CACI
Austin, TX
13 days ago

Machine Learning Inference Engineer (67954)
Advanced Micro Devices, Inc.
Austin, TX

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

- What features would be predictive of your salary?
- Where can you find data for model training and evaluation (features + true values)?
- What would introduce noise to your data?
- Create a matrix/vector representation of three examples.

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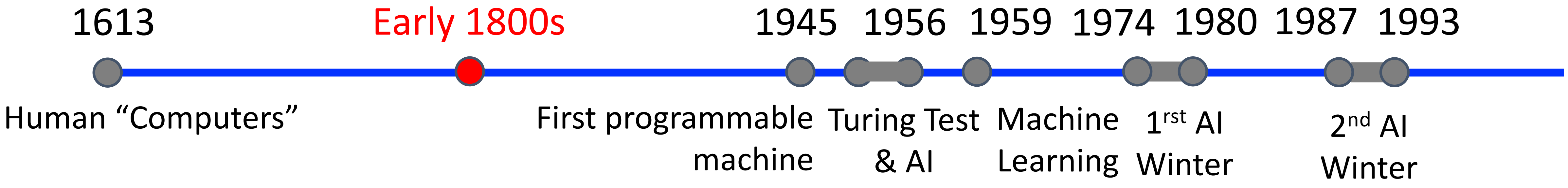
Linear Regression: Historical Context

Learning Linear Regression Models with Least Squares



Legendre (1805) and Gauss (1809): https://en.wikipedia.org/wiki/Linear_regression

Linear Regression Model

- General formula:

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

Feature vector: **x** = x[0], x[1], …, x[p]

- How many features are there?
  - p+1

Parameter vector to learn: **w** = w[0], w[1], …, w[p]

- How many parameters are there?
  - p+2

Predicted value

“Simple” Linear Regression Model

- Formula:

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

Feature vector
- How many features are there?
  - 1

Parameter vector to learn
- How many parameters are there?
  - 2

Predicted value

(Line)

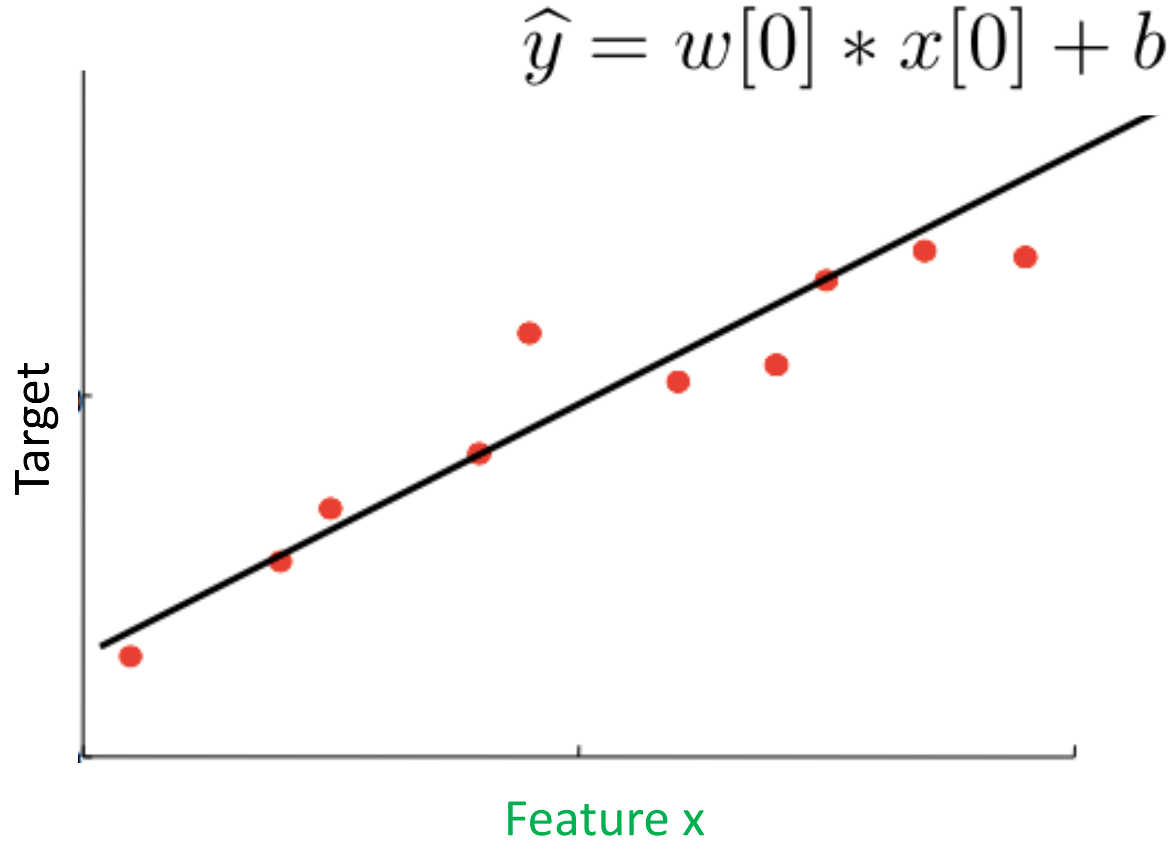


Figure Credit: http://sli.ics.uci.edu/Classes/2015W-273a?action=download&upname=04-linRegress.pdf

“Multiple” Linear Regression Model

- Formula:

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

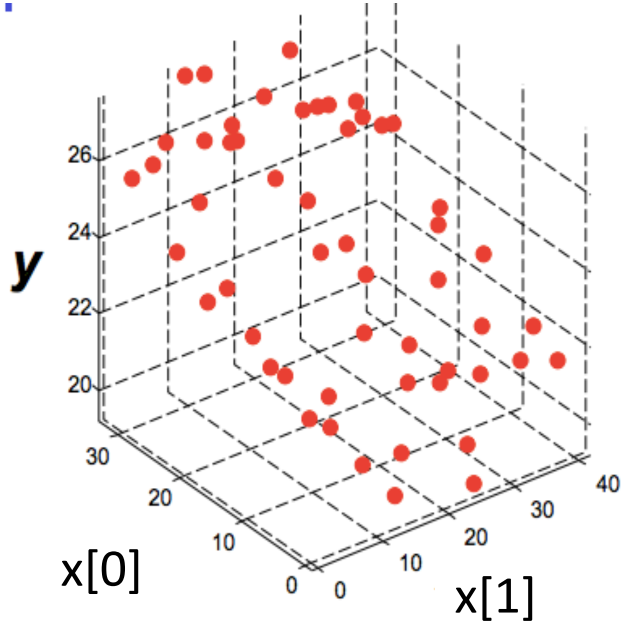
Feature vector

- How many features are there?
  - 2

Parameter vector to learn

- How many parameters are there?
  - 3

Predicted value



(Plane)

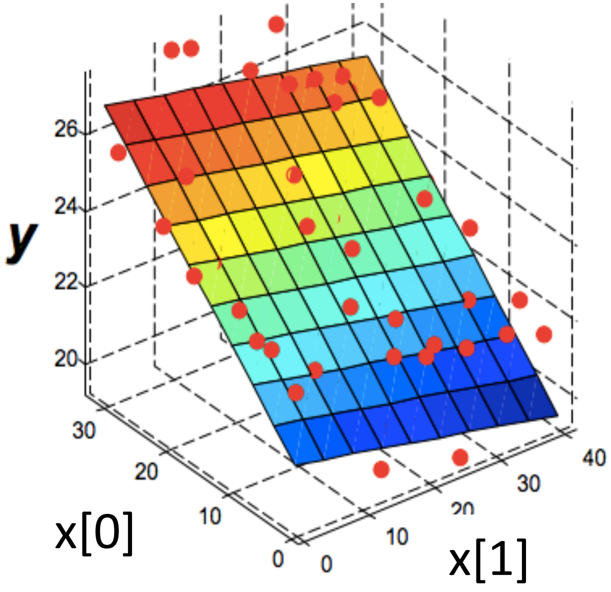


Figure Credit: http://sli.ics.uci.edu/Classes/2015W-273a?action=download&upname=04-linRegress.pdf

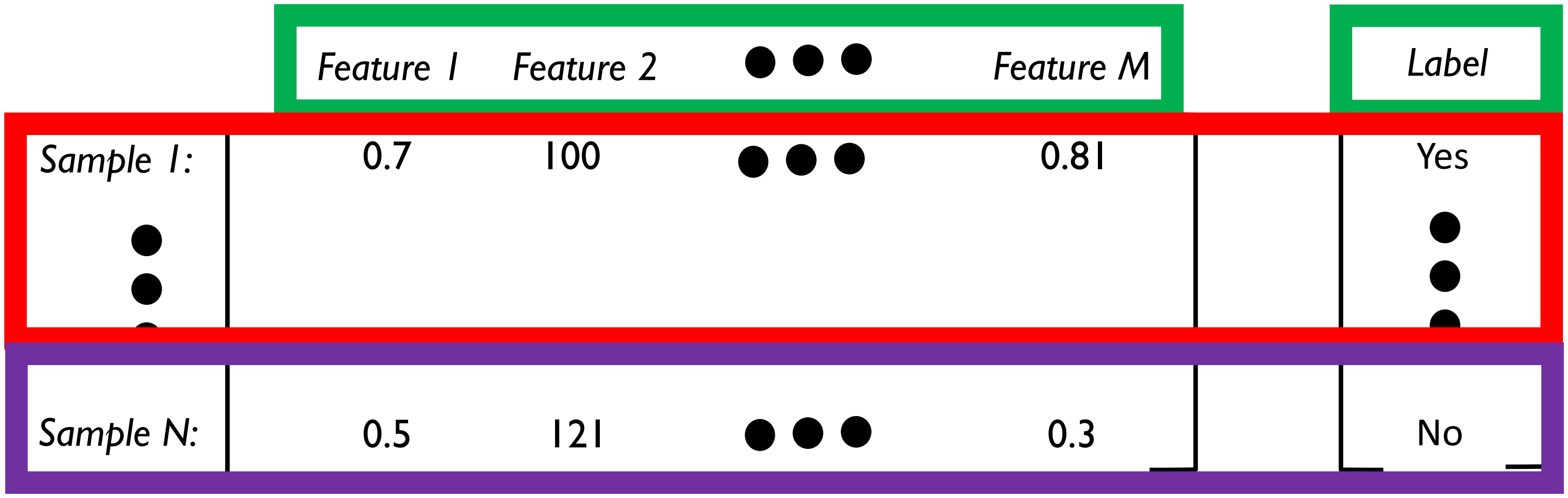
Linear Regression Model: How to Learn?

$$\widehat{y} = \boxed{w[0]} * x[0] + \boxed{w[1]} * x[1] + \ldots + \boxed{w[p]} * x[p] + \boxed{b}$$

- Weight coefficients:
  - Indicates how much the predicted value will vary when that feature varies while holding all the other features constant

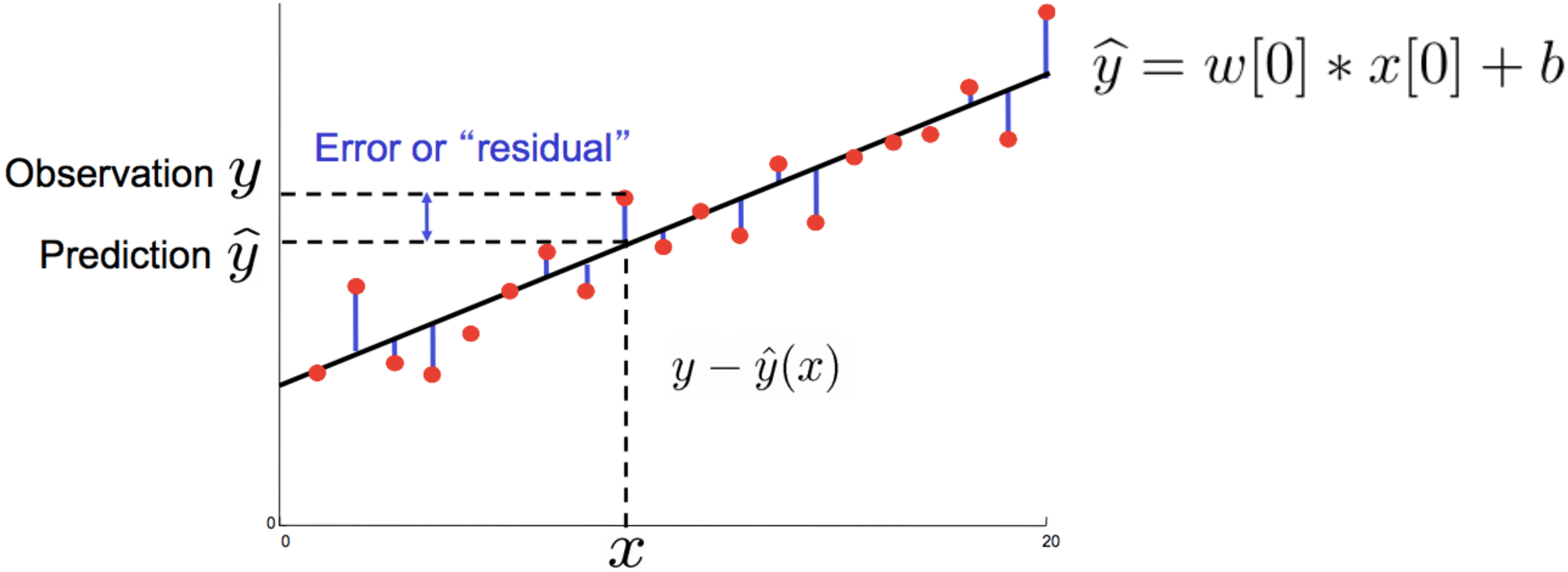
Linear Regression Model: Learning Parameters

- Split data into a "training set" and "testing set"



Linear Regression Model: Learning Parameters

- Least squares: *minimize* total squared error ("residual") on "training set"
  - Why square the error?



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Linear Regression Model: Learning Parameters

- Least squares: *minimize* total squared error ("residual") on "training set"

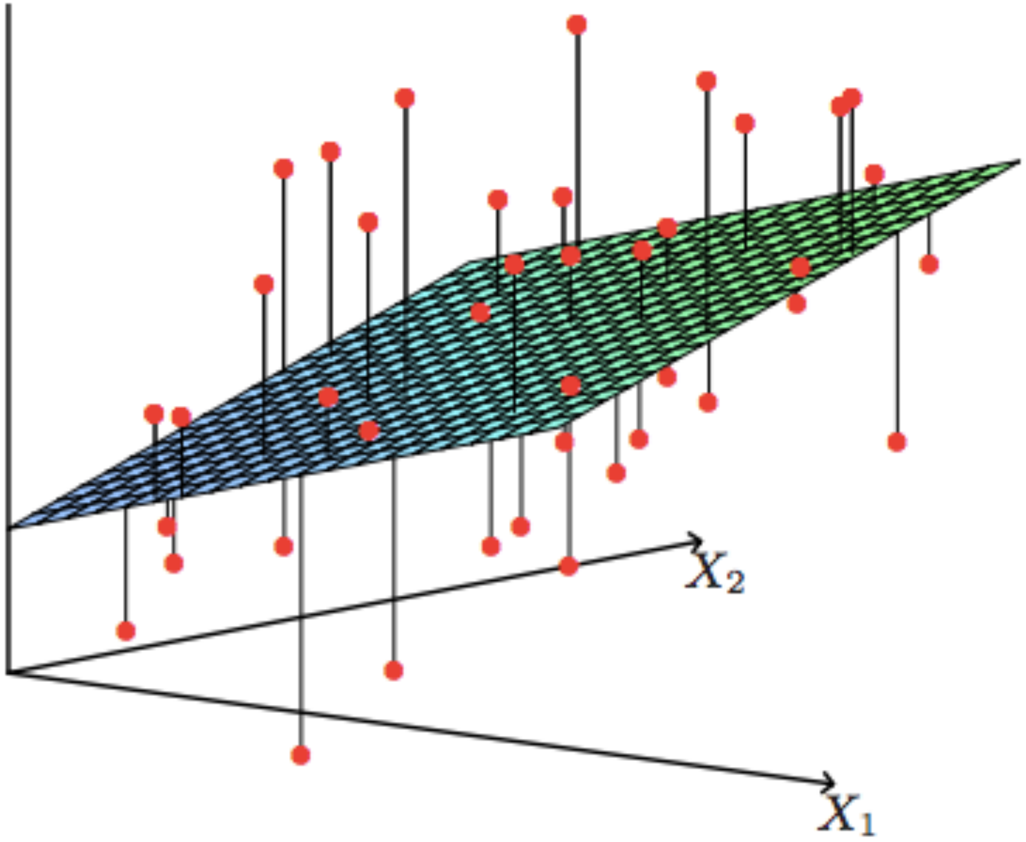

Figure Source: https://web.stanford.edu/~hastie/Papers/ESLII.pdf

Linear Regression Model: Learning Parameters

- Least squares: *minimize* total squared error ("residual") on "training set"
  - Take derivatives, set to zero, and solve for parameters

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

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

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

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

Great tutorial: http://www.cns.nyu.edu/~eero/NOTES/leastSquares.pdf

Linear Regression Model: Learning Parameters

- Least squares: *minimize* total squared error ("residual") on "training set"
  - What would be the impact of outliers in the training data?

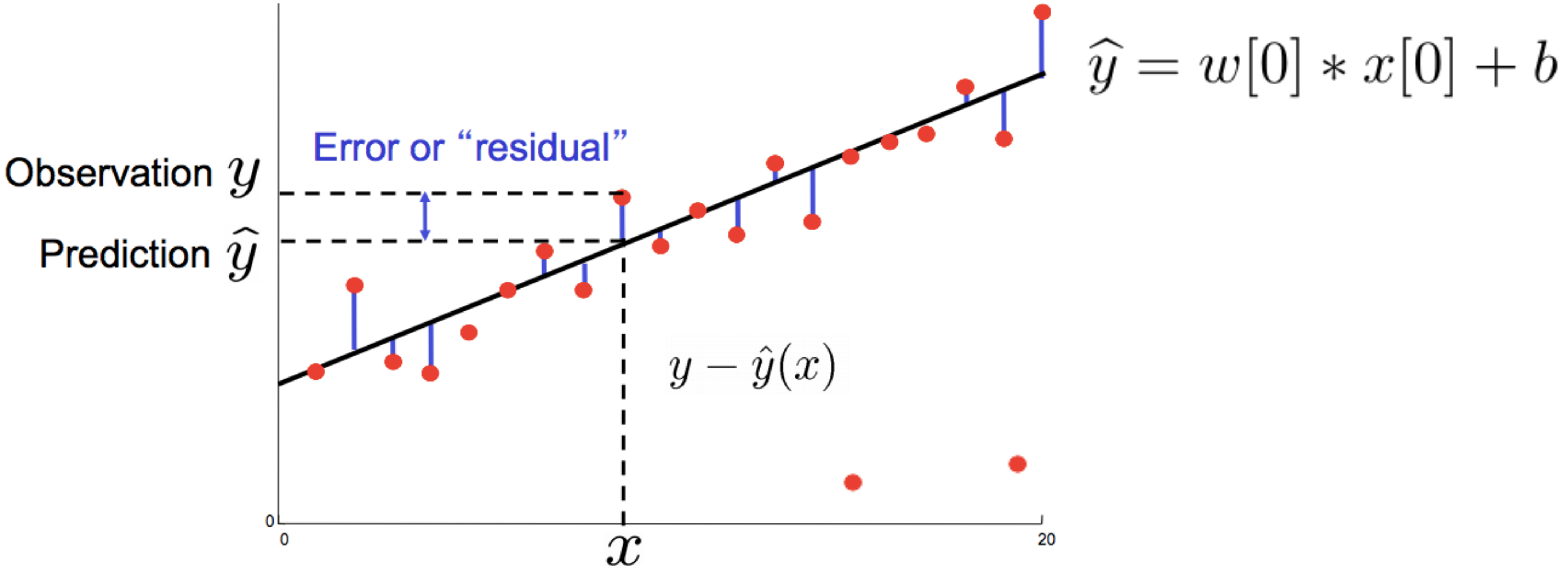

Figure Credit: http://sli.ics.uci.edu/Classes/2015W-273a?action=download&upname=04-linRegress.pdf

Linear Regression: Predict Salary of ML Engineer

(Solution is a hyperplane)

$$\widehat{y} = \boxed{w[0]} * x[0] + \boxed{w[1]} * x[1] + \ldots + \boxed{w[p]} * x[p] + \boxed{b}$$

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

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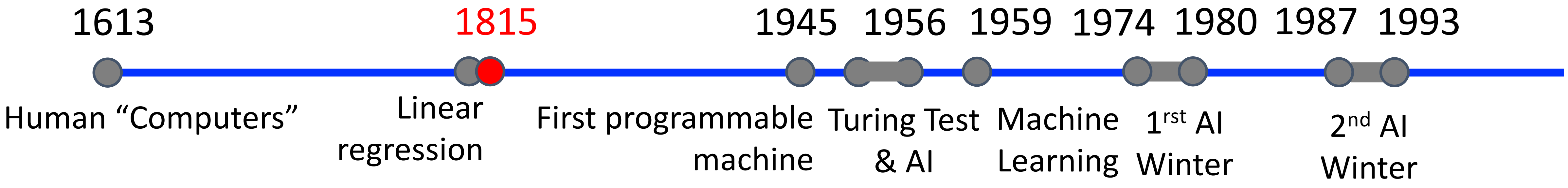
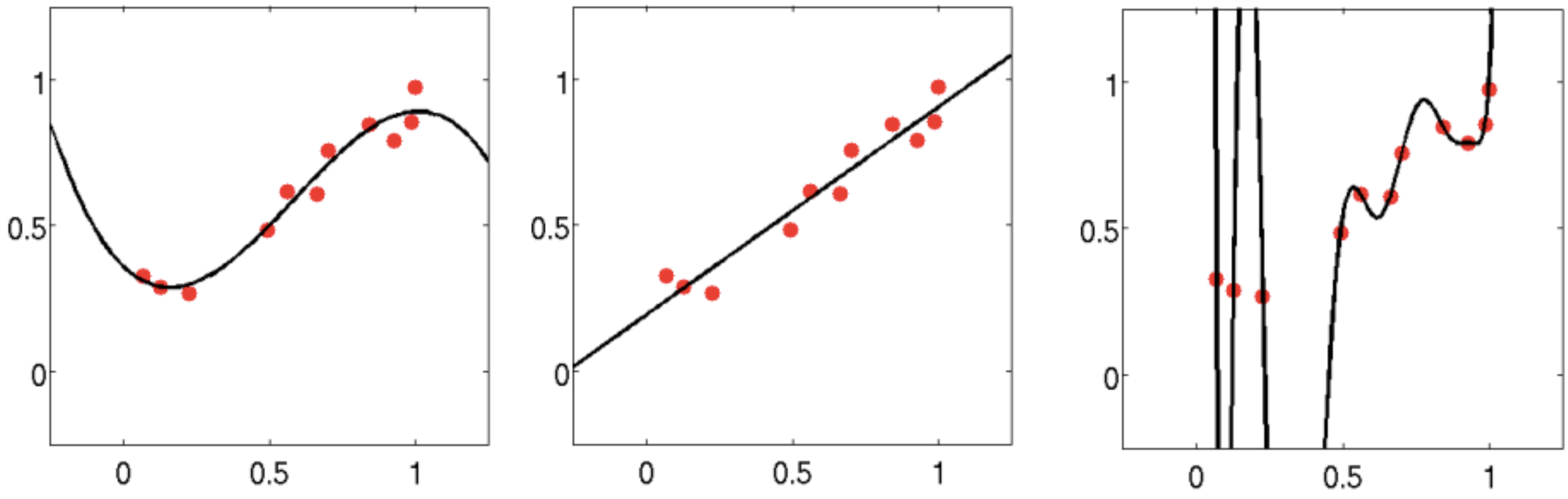
Linear Regression: Historical Context

Learning Polynomial Regression Models with Least Squares



Gergonne, J. D. (November 1974) [1815]. "The application of the method of least squares to the interpolation of sequences". *Historia Mathematica* (Translated by Ralph St. John and S. M. Stigler from the 1815 French ed.). **1** (4): 439–447.

Linear Models: When They Are Not Good Enough, Increase Representational Capacity



polynomial equations (higher capacity)

linear equations (lowest capacity)

polynomial equations (highest capacity)

Polynomial Regression: Transform Features to Model Non-Linear Relationships

- e.g., (Recall) Formula:

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

- e.g., New Formula:

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

Predicted value

Parameter vector

Feature vector

- **Still a linear model!**
- **But can now model more complex relationships!!**

Polynomial Regression: Transform Features to Model Non-Linear Relationships

- 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?

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

Polynomial Regression: Transform Features to Model Non-Linear Relationships

- 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 … 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 Regression Model: Learning Parameters

- M-th order polynomial function: $y(x, \mathbf{w}) = w_0 + \sum_{j=1}^{M} w_j x^j$
- Still linear model, so can learn with same approach as for linear regression

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

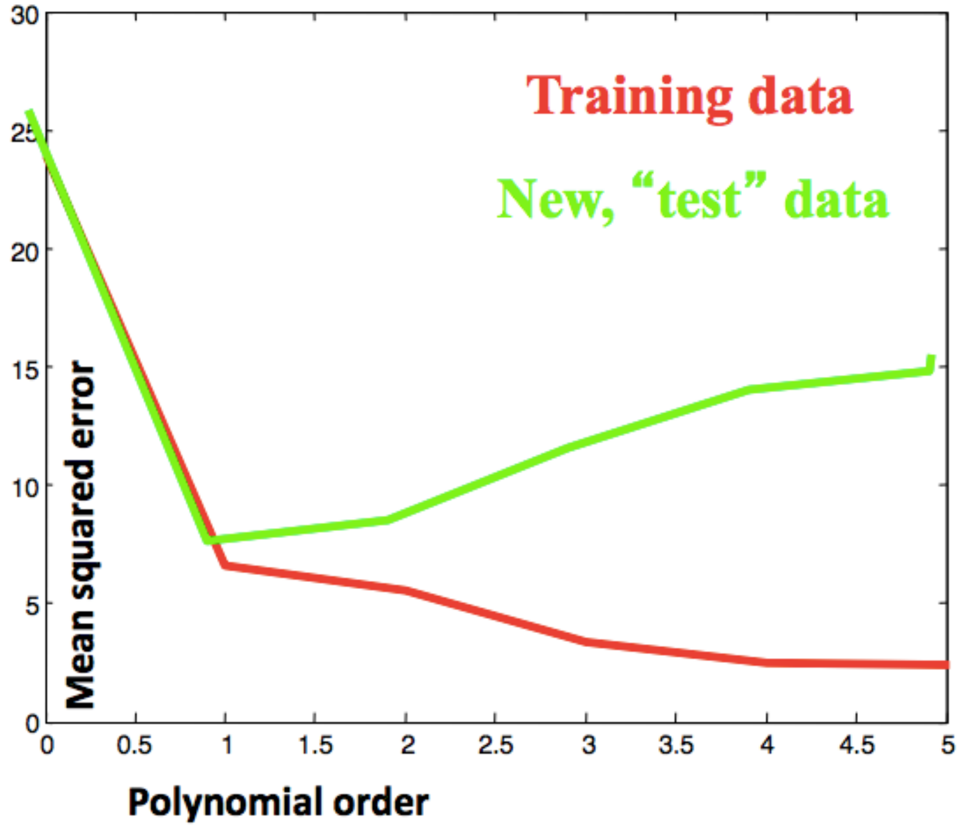
$$2\sum_i x_i(y_i - wx_i) = 0 \Rightarrow$$

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

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

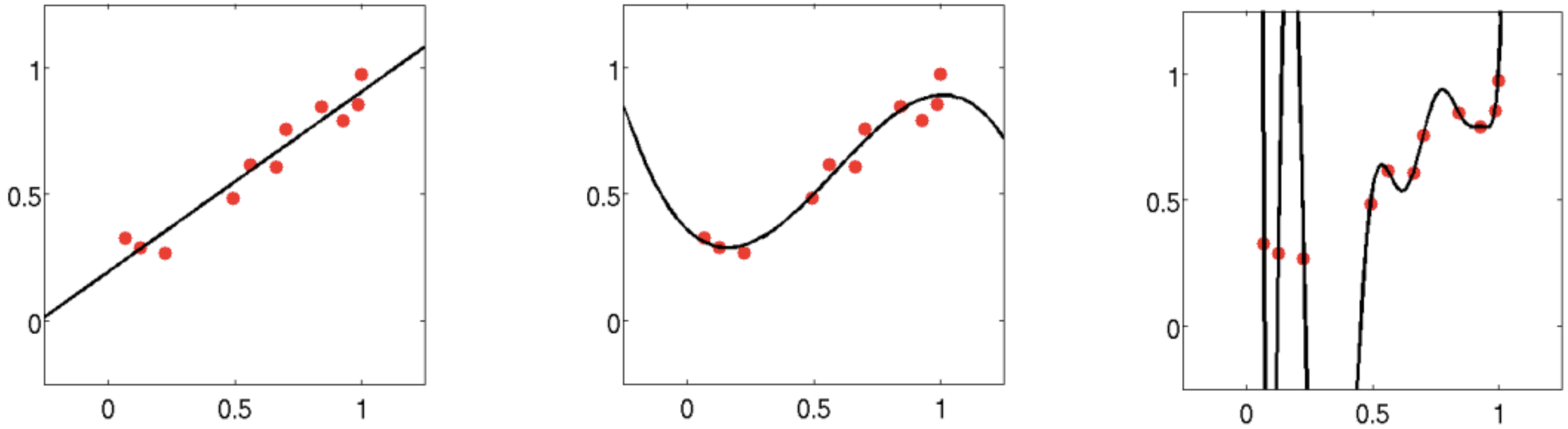
Polynomial Regression Model: What Feature Transformation to Use?

- Example plot of error on training and test sets:
  - What happens to training data error with larger polynomial order?
    - Shrinks
  - What happens to test data error with larger polynomial order?
    - Error shrinks and then grows
    - Higher order can model 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?

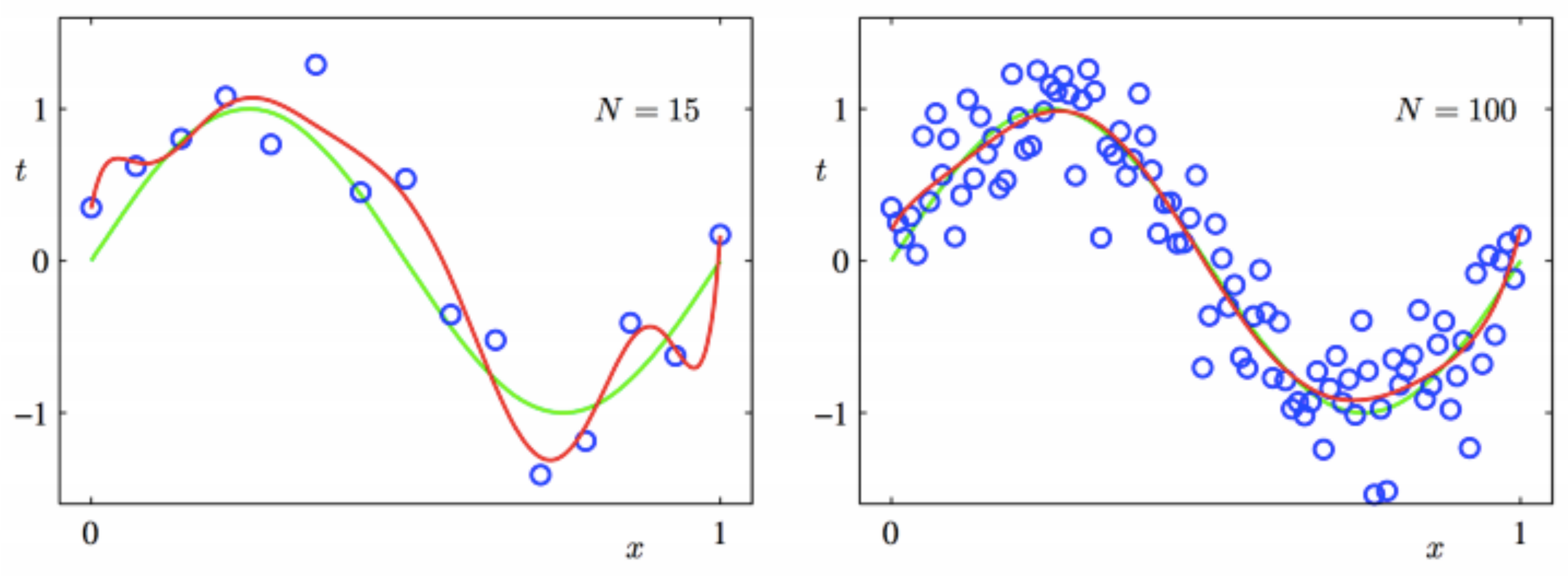
- Use lower degree polynomial:



- Risk: may be underfitting again

How to Avoid Overfitting?

- Add more training data



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

How to Avoid Overfitting?

- Or regularize the model…

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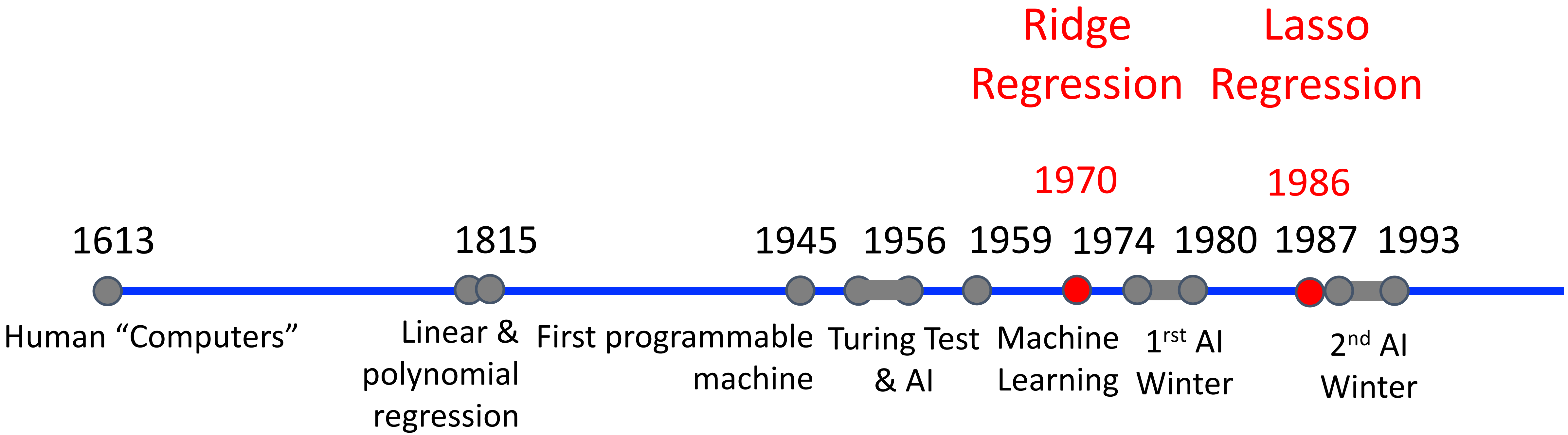
Linear Regression: Historical Context



Santosa, Fadil; Symes, William W. (1986). "Linear inversion of band-limited reflection seismograms". *SIAM Journal on Scientific and Statistical Computing*. SIAM. **7** (4): 1307–1330.

Tibshirani, Robert (1996). "Regression Shrinkage and Selection via the lasso". *Journal of the Royal Statistical Society*. Series B (methodological). Wiley. **58** (1): 267–88.

Arthur E. Hoerl and Robert W. Kennard, "Ridge regression: Biased estimation for nonorthogonal problems", Technometrics. 1970.

Problem: Overfitting

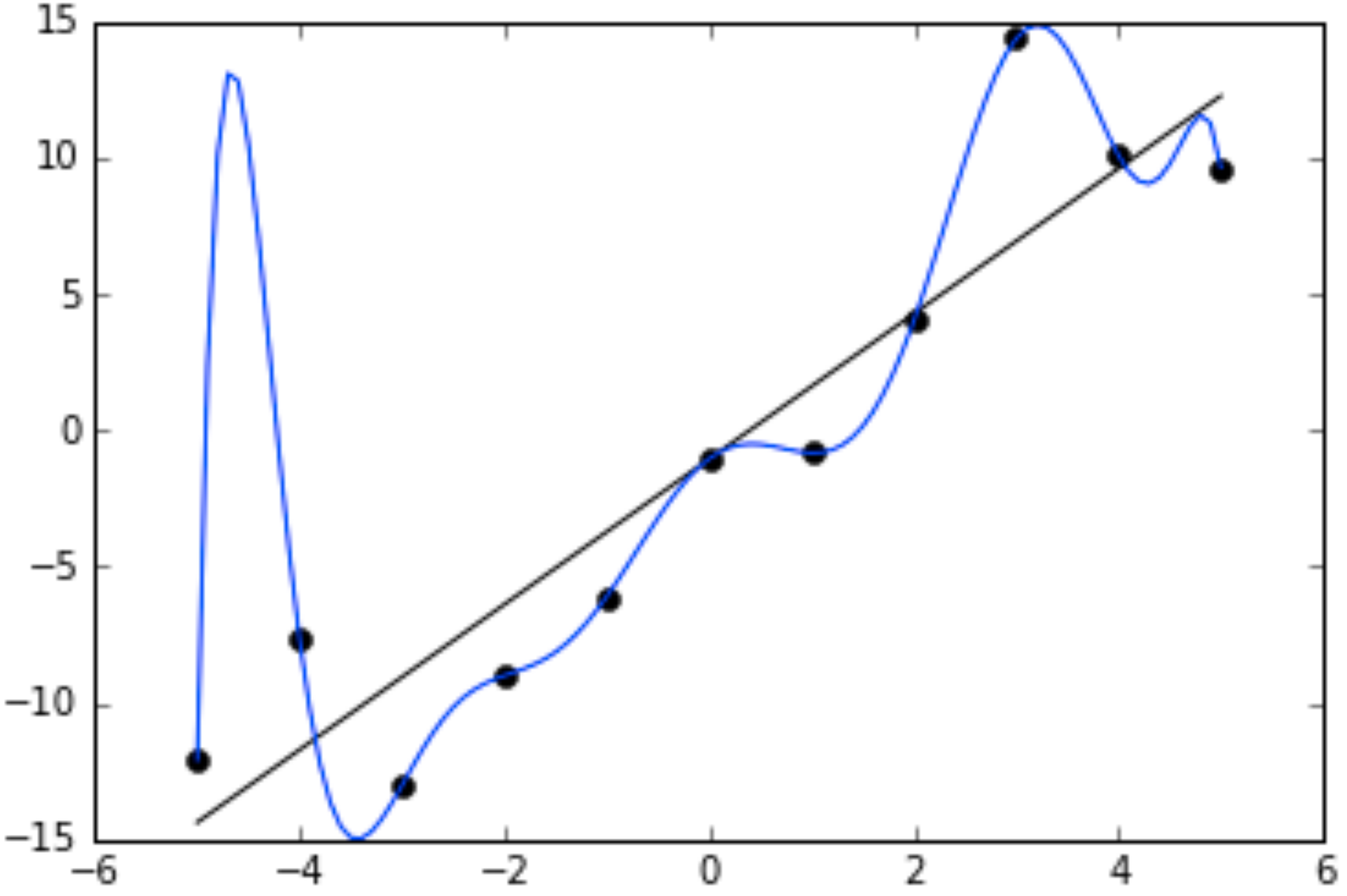


Figure Source: https://en.wikipedia.org/wiki/Overfitting

Problem: Overfitting

- e.g., weights learned for fitting a model to a sine wave function (polynomial degrees 0, 1, …, 9)

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

- Sign of overfitting: weights blow up and cancel each other out to fit the training data

Solution: Regularization

- Regularize model (add constraints)

	$M = 0$	$M = 1$	$M = 6$	$M = 9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
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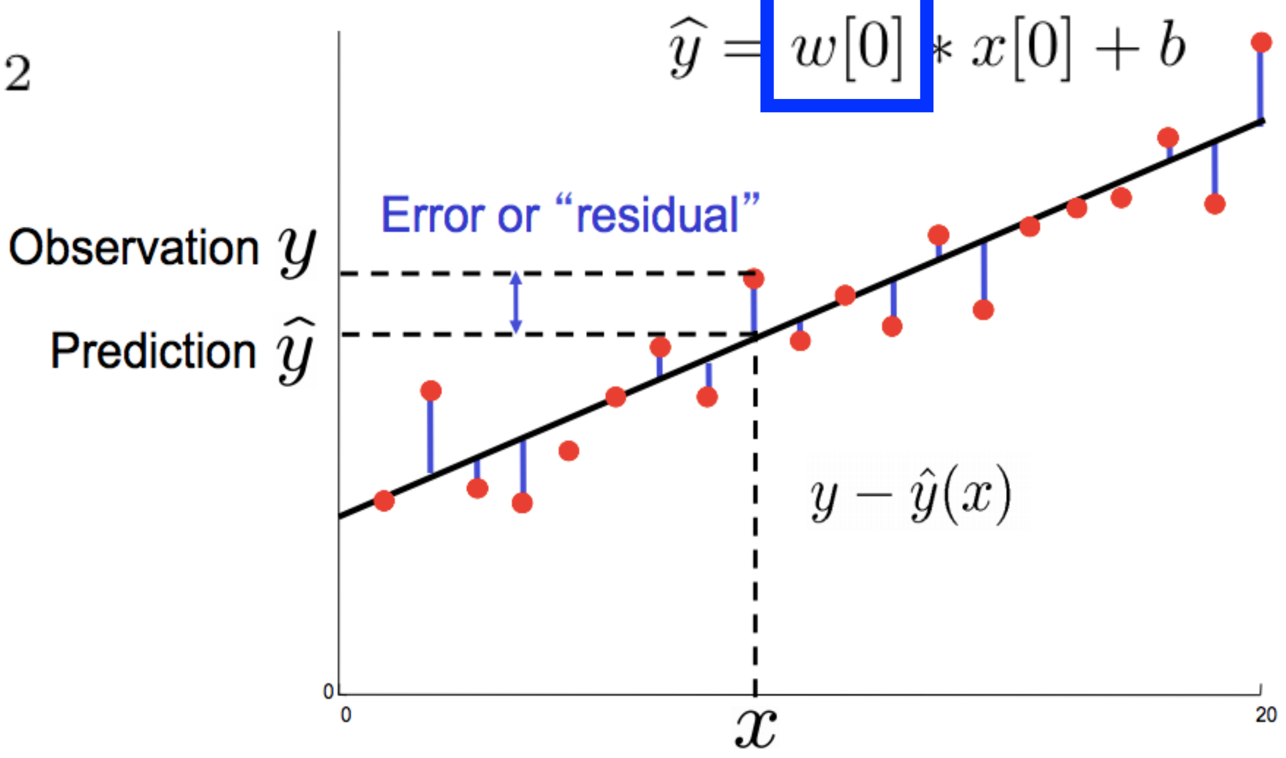
$w_8^\star$				-557682.99
$w_9^\star$				125201.43

- Idea: add constraint to minimize presence of large weights in models!

Regularization

- Idea: add constraint to minimize presence of large weights in models
- Recall: we previously learned models by *minimizing* **s**um of **s**quared **e**rrors (SSE) for all n training examples:

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



Regularization

- Idea: add constraint to minimize presence of large weights in models
- Recall: we previously learned models by *minimizing* **s**um of **s**quared **e**rrors (SSE) for all n training examples:

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

- Ridge Regression: add constraint to penalize squared weight values

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

- Lasso Regression: add constraint to penalize absolute weight values

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

Regularization: How to Set Alpha?

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

What happens when you set alpha to a small value?

What happens when you set alpha to a large value?

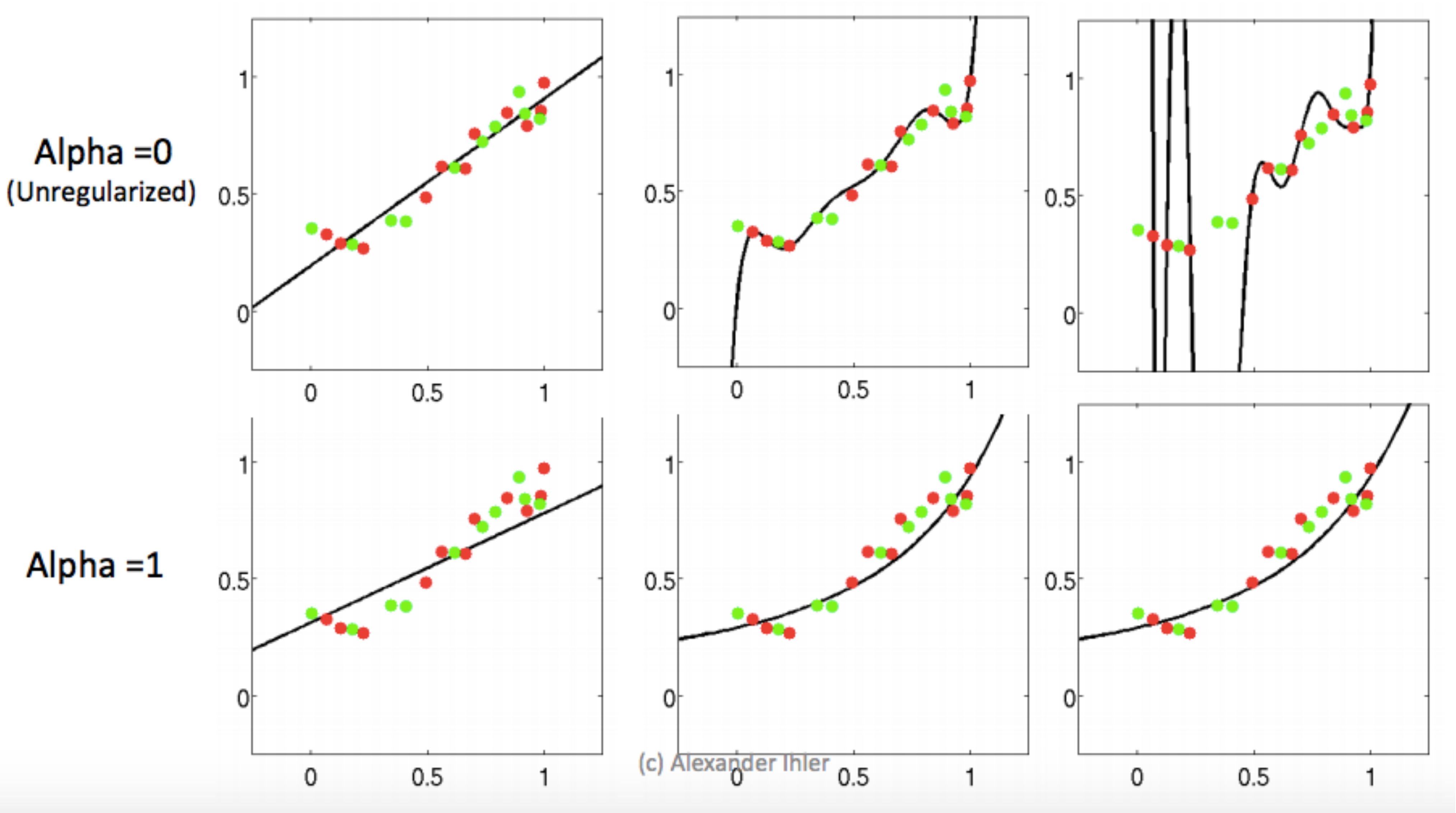
- Ridge Regression: add constraint to penalize squared weight values

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

- Lasso Regression: add constraint to penalize absolute weight values

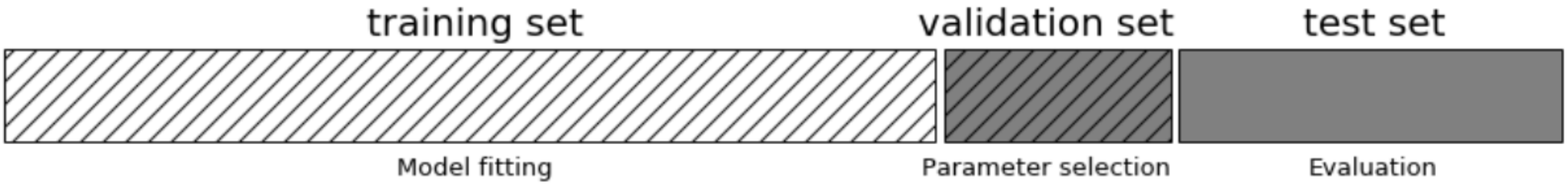
$$Error = \sum_{i=1}^{n} (y^{(i)} - \widehat{y}^{(i)})^2 + \alpha \sum_{j=1}^{m} |w_j|$$

Regularization: How to Set Alpha?



Regularization: How to Set Alpha?

- Split training data into “train” and “validation” datasets



- Algorithm: brute-force, exhaustive approach by evaluating every alpha value to find optimal hyperparameter

Why Choose Lasso Instead of 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

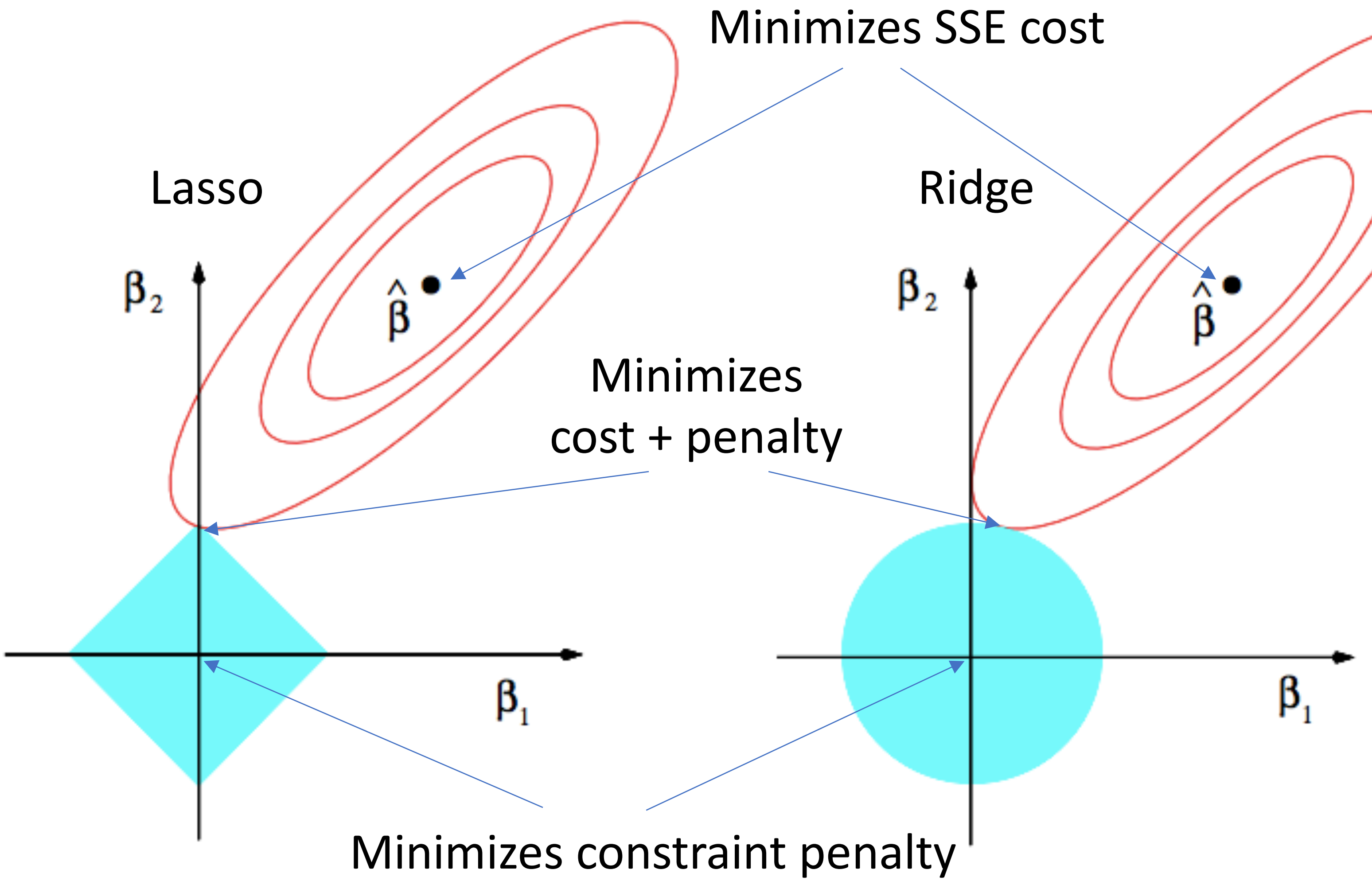
- Ridge Regression: add constraint to penalize squared weight values

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

- Lasso Regression: add constraint to penalize absolute weight values

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

Why Choose Lasso Instead of Ridge Regression? (2D feature example)



Contour of least square error function

Contour of regularization constraint functions:

$$|\beta_1| + |\beta_2| \leq t$$

$$\beta_1^2 + \beta_2^2 \leq t^2$$

https://web.stanford.edu/~hastie/Papers/ESLII.pdf

Today's Topics

- Regression applications
- Evaluating regression models
- Background: notation
- Linear regression
- Polynomial regression
- Regularization (Ridge regression and Lasso regression)
- Lab

Resources Used for Today's Slides

- Deep Learning by Goodfellow et. al
  - pgs. 29-38 for background on linear algebra (e.g., matrices, norms)
- 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