10-315
Introduction to ML

Feature Engineering

Instructor: Pat Virtue

Today

Student support

Feature engineering

- Just touch on polynomial feature engineering
- — stop —
- We'll get back to more feature engineering and feature learning later in the semester

Logistic Regression

Poll 1

How many appointment slots does Pat have available this Friday?

See pinned OH post on Piazza

Poll 2

Linear regression. What is linear about it?

Select all that apply.

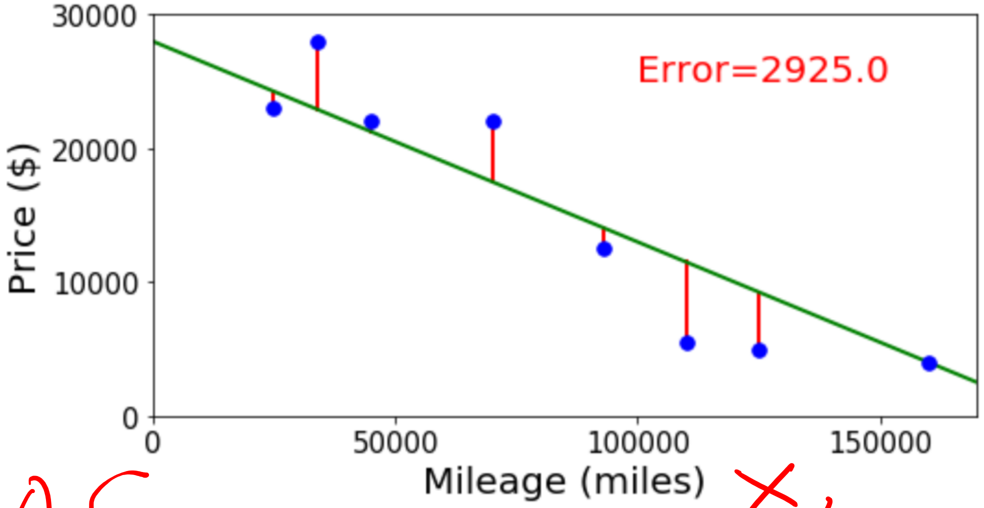
%

43 A. Always fits a linear (or affine) shape to the data

22 B. Linear objective function with respect to the input

82 C. Linear objective function with respect to the parameters

7 D. None of the above



A

$\hat{y} = w^T x + b$

$= w_1 x_1 + w_2 x_2 + b$

x_1

$x_2 = x_1^2$

$J(\theta) = \frac{1}{N} \| \hat{y} - X\theta \|_2^2$

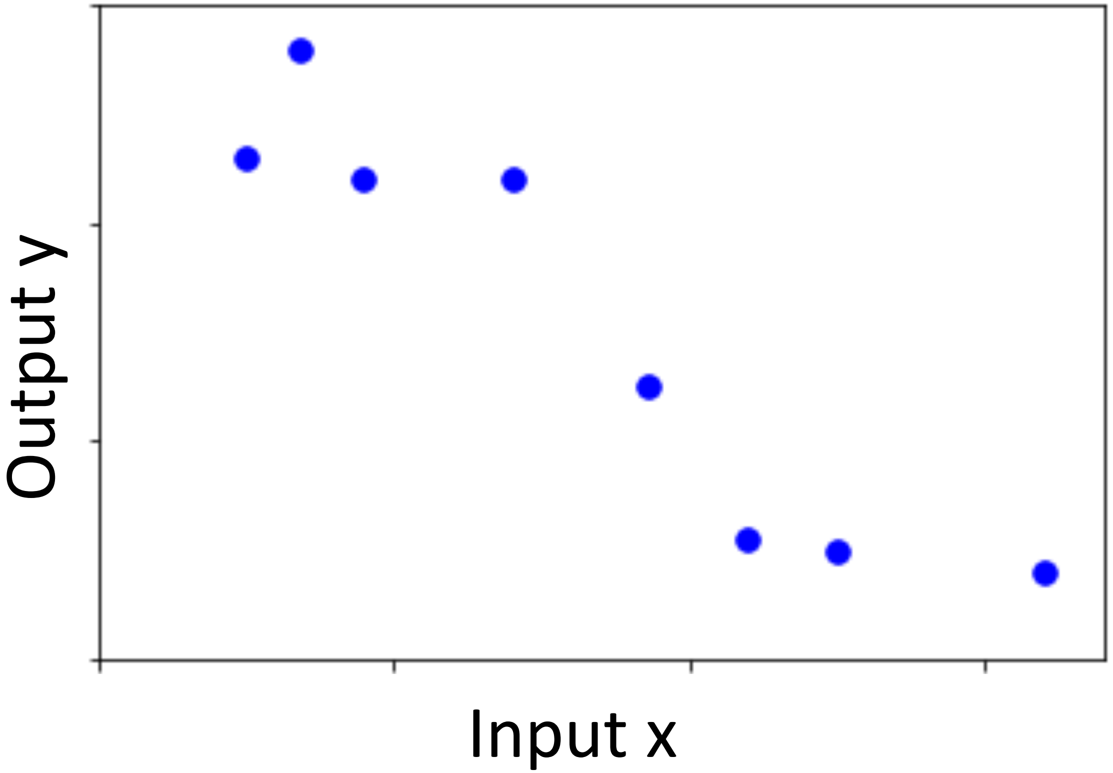
$\|\vec{v}\|_2 \quad \|A\|_F$

Pre-reading

Polynomial Features

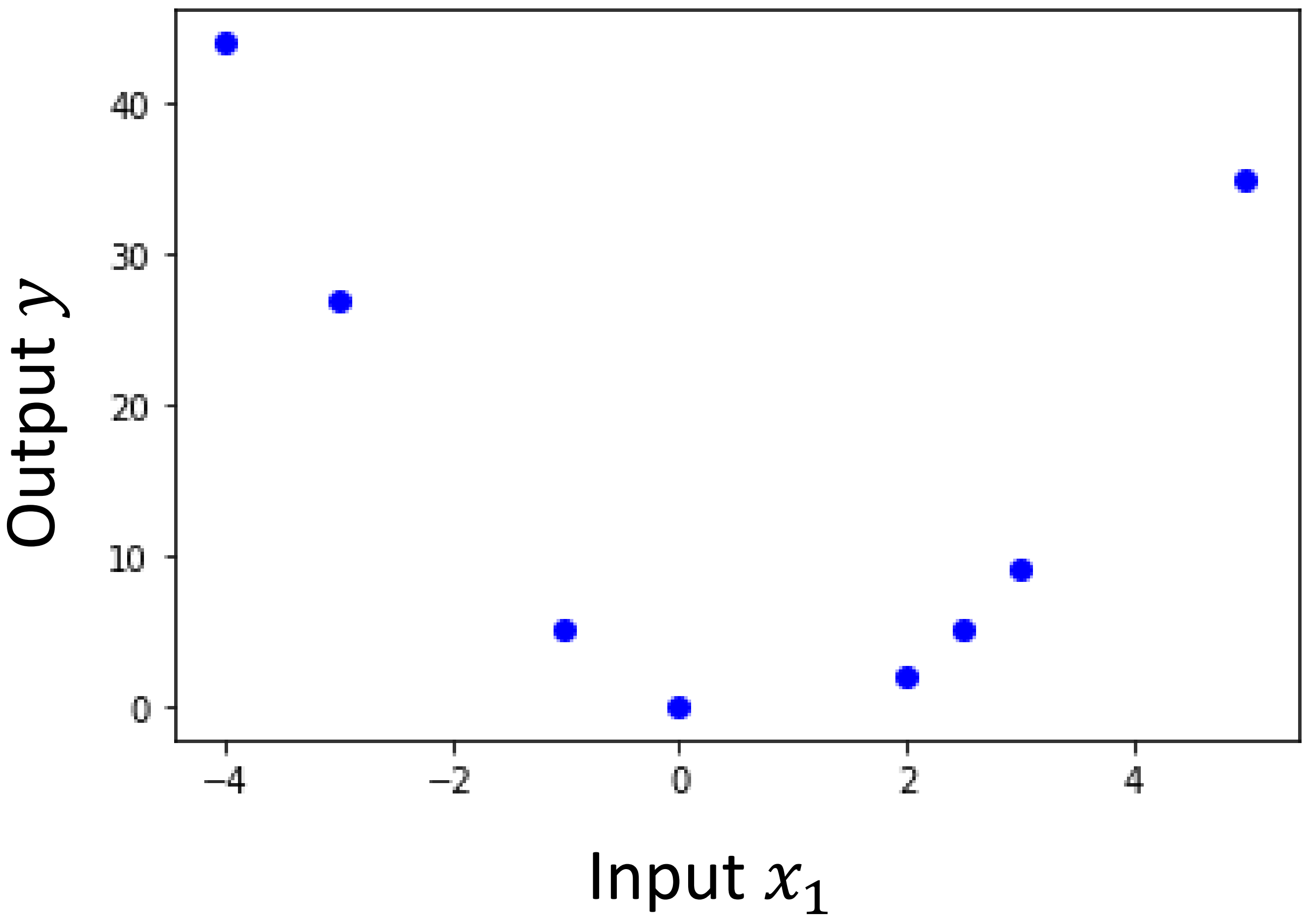
Linear Data

Regression on simple linear dataset



Non-linear Data

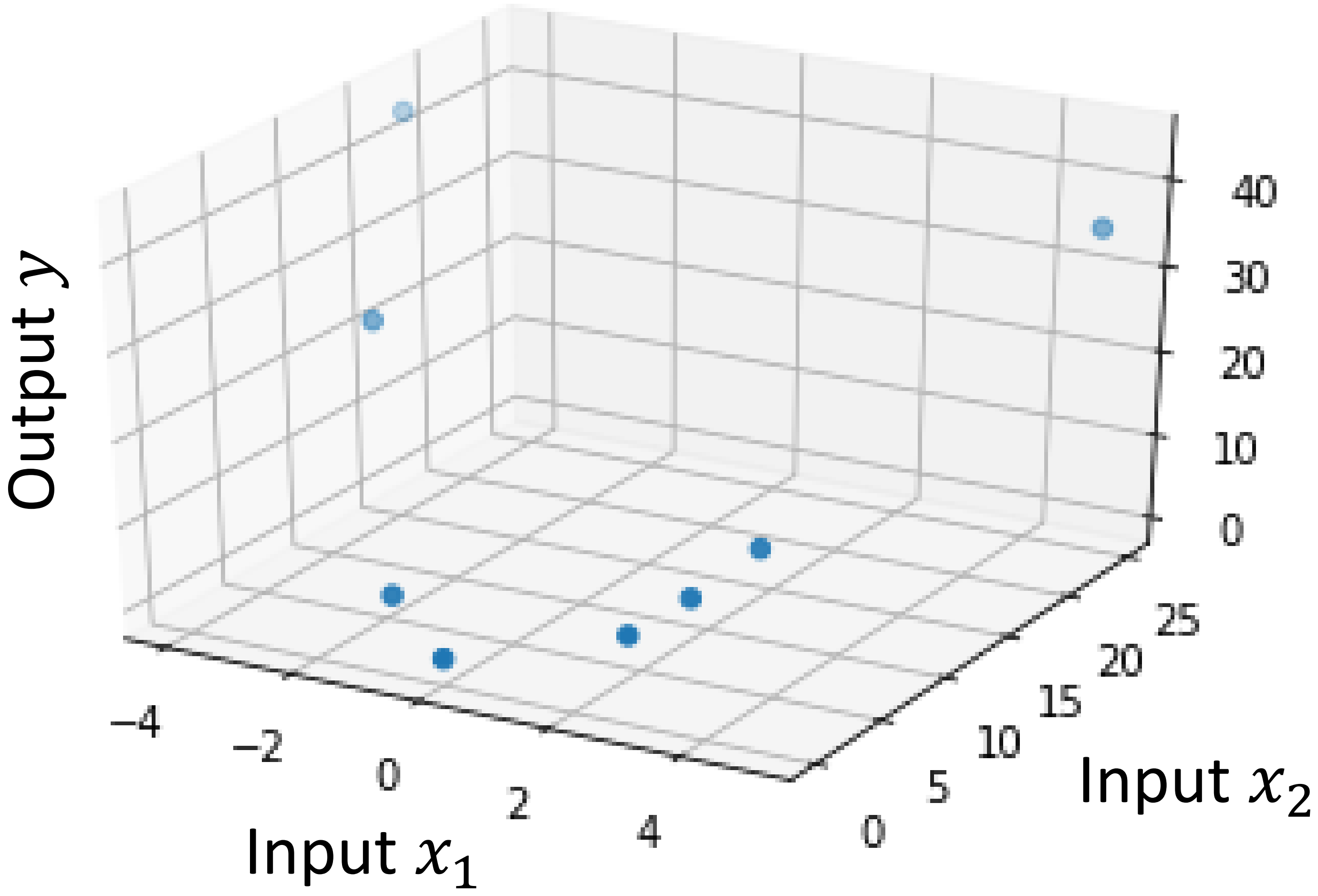
Linear regression on polynomial data?



y	x_1
44	-4
27	-3
5	-1
0	0
2	2
5	2.5
9	3
35	5

Non-linear Data

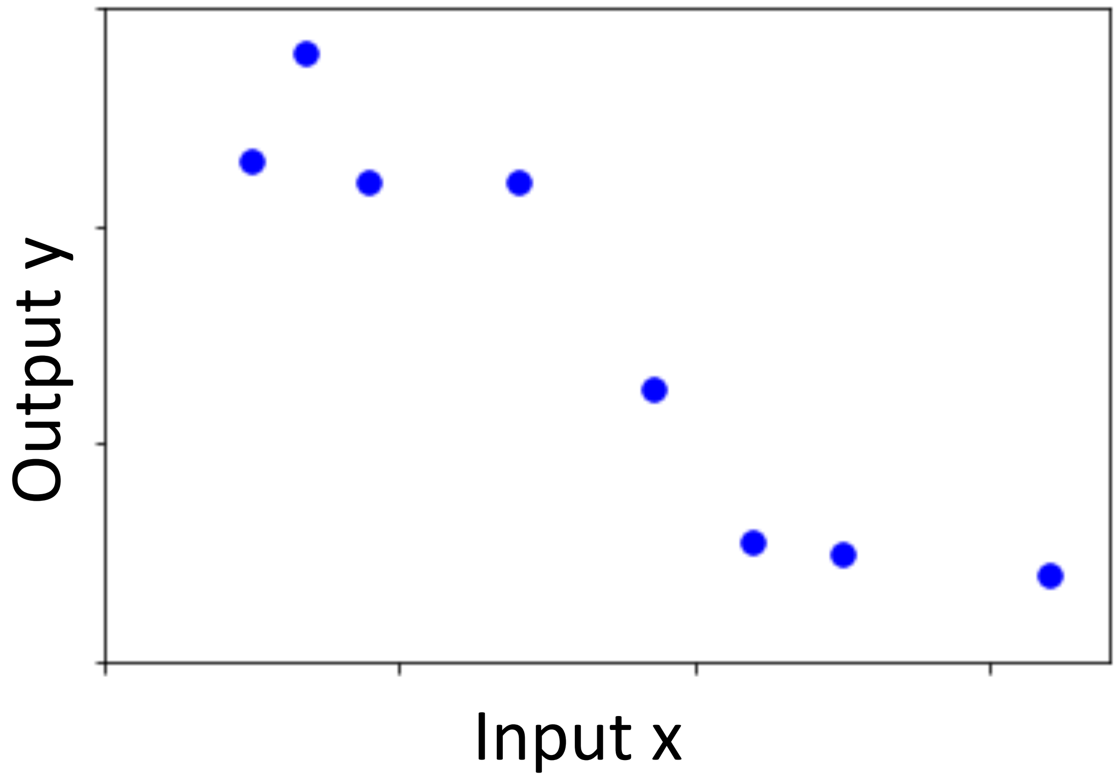
Regression on simple linear dataset



y	x_1	x_2
44	-4	16
27	-3	9
5	-1	1
0	0	0
2	2	4
5	2.5	6.25
9	3	9
35	5	25

Non-linear Data

Polynomial feature map for linear regression

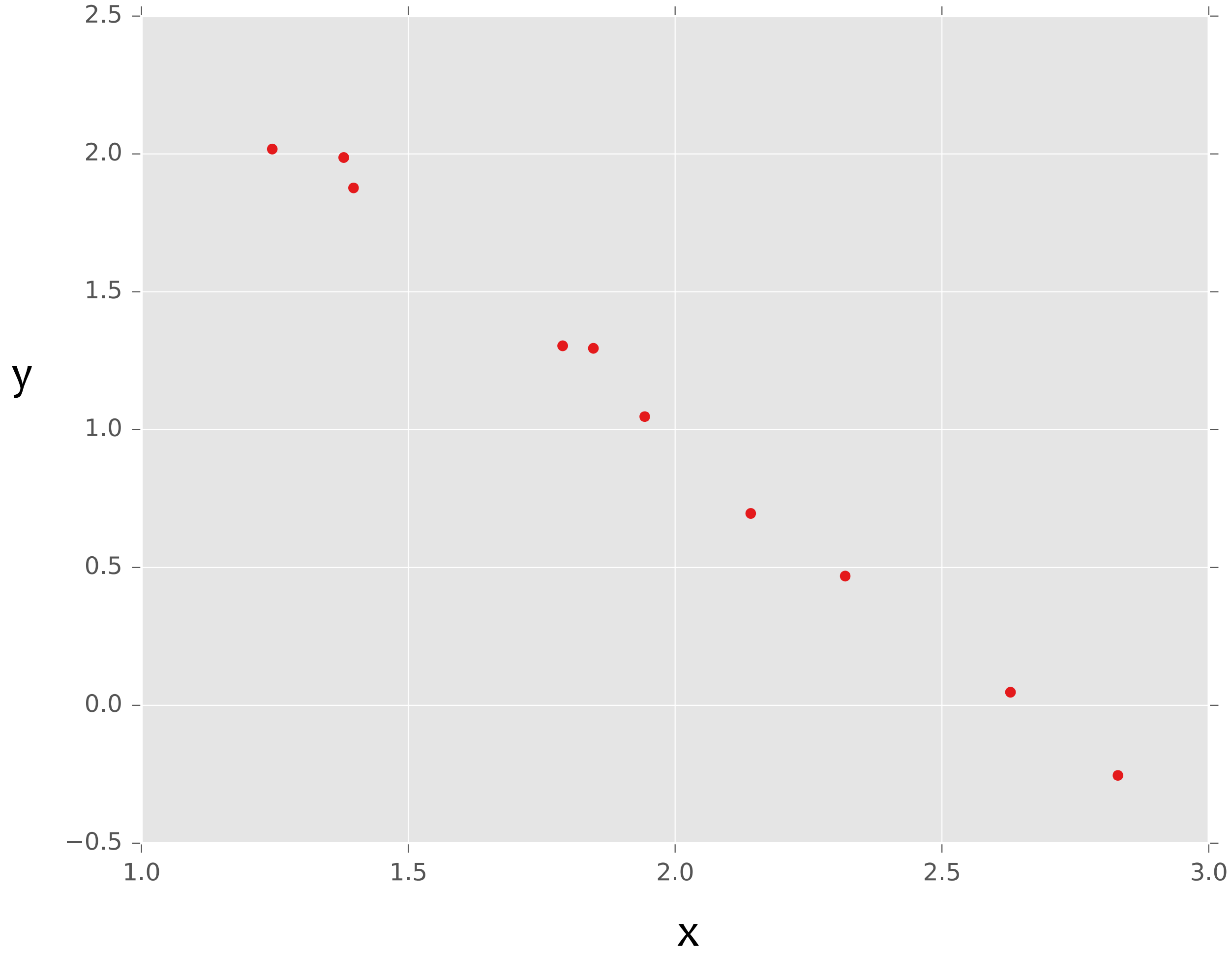


Example: Linear Regression

Goal: Learn y = $\mathbf{w}^T$ f($\mathbf{x}$) + b
where f(.) is a polynomial basis function

y	x
2.0	1.2
1.3	1.7
0.1	2.7
1.1	1.9

true "unknown" target function is linear with negative slope and gaussian noise



Slide credit: CMU MLD Matt Gormley

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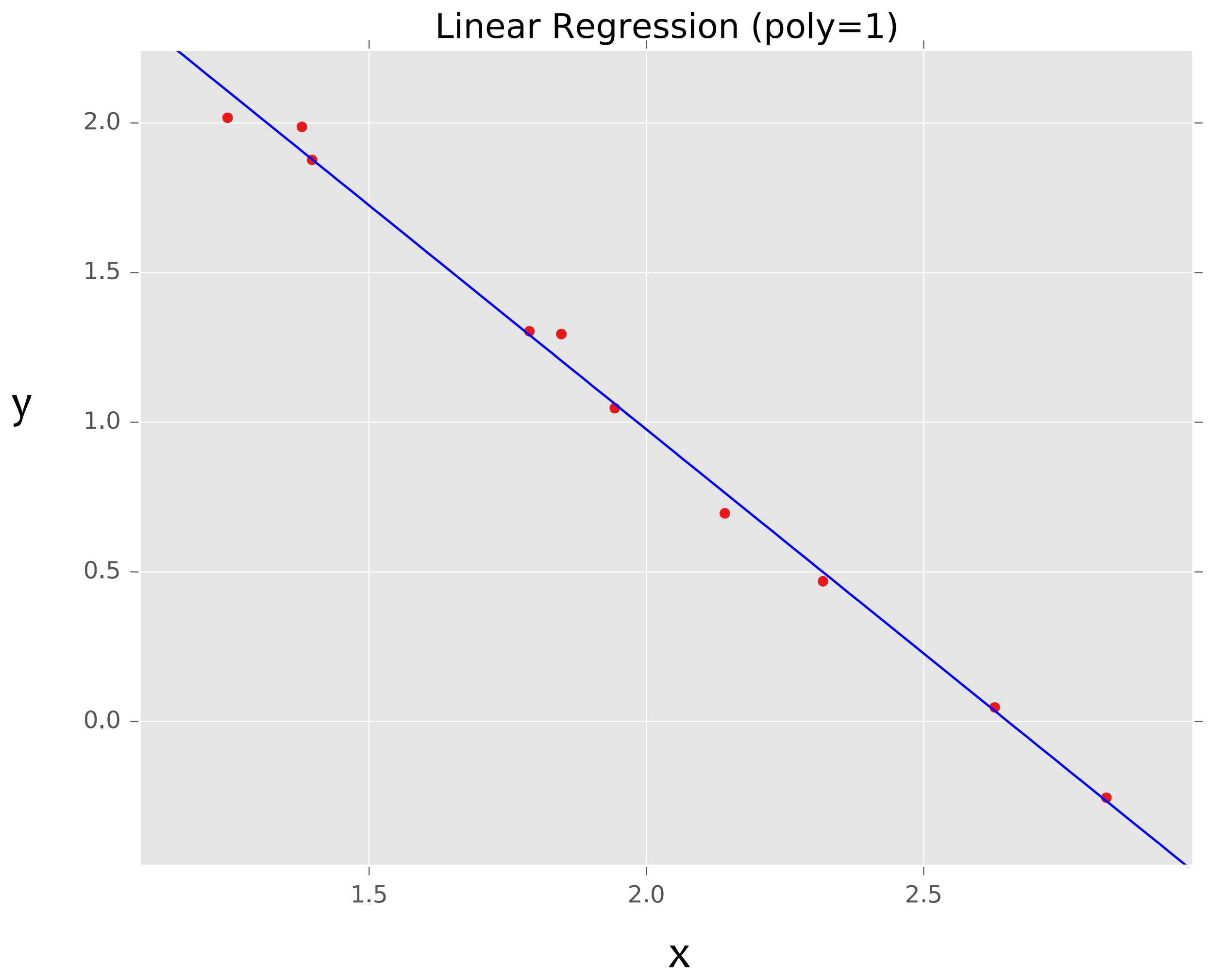

Slide credit: CMU MLD Matt Gormley

Example: Linear Regression

Goal: Learn y = $\mathbf{w}^T f(\mathbf{x}) + b$
where f(.) is a polynomial basis function

y	x	x^2
2.0	1.2	$(1.2)^2$
1.3	1.7	$(1.7)^2$
0.1	2.7	$(2.7)^2$
1.1	1.9	$(1.9)^2$

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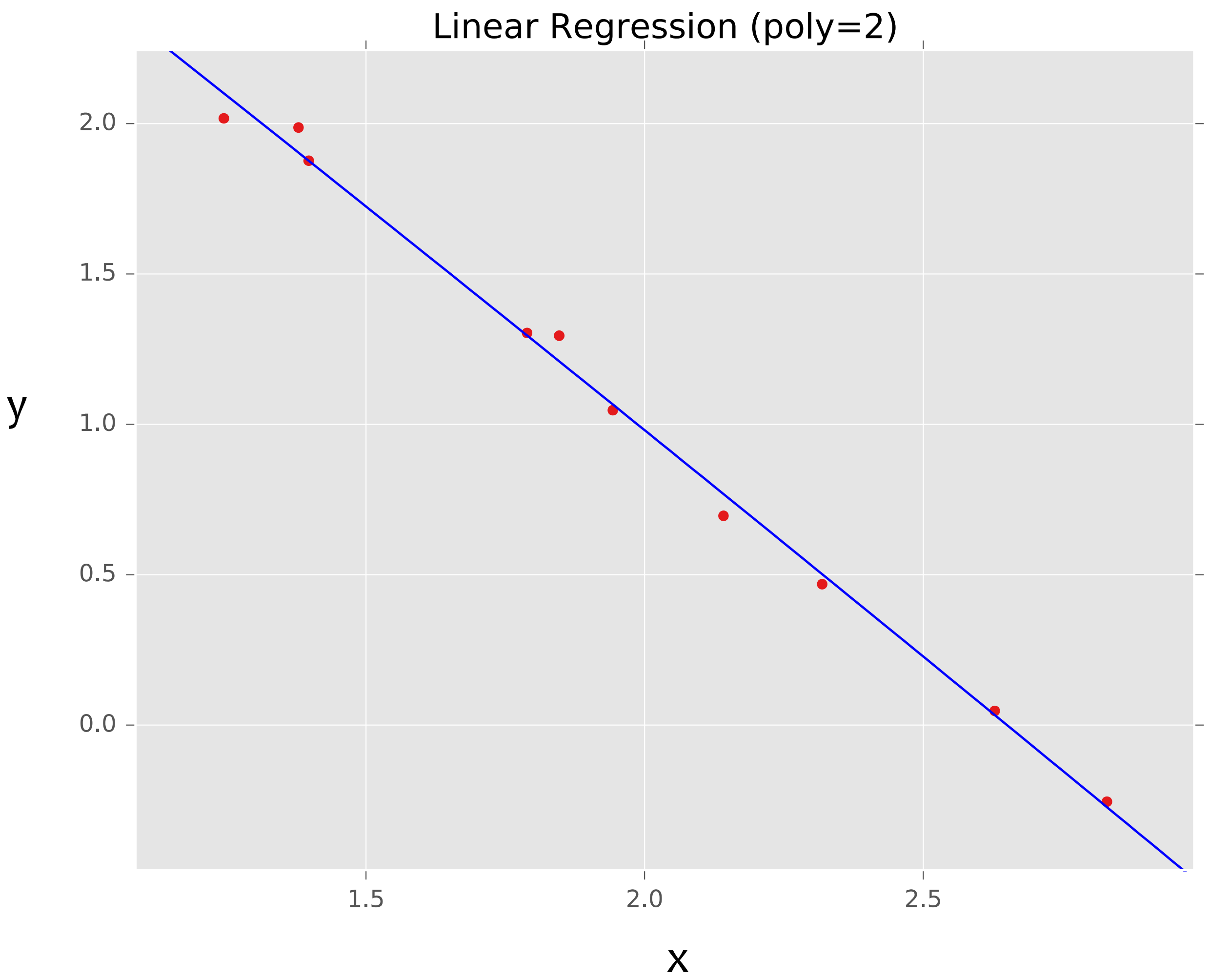


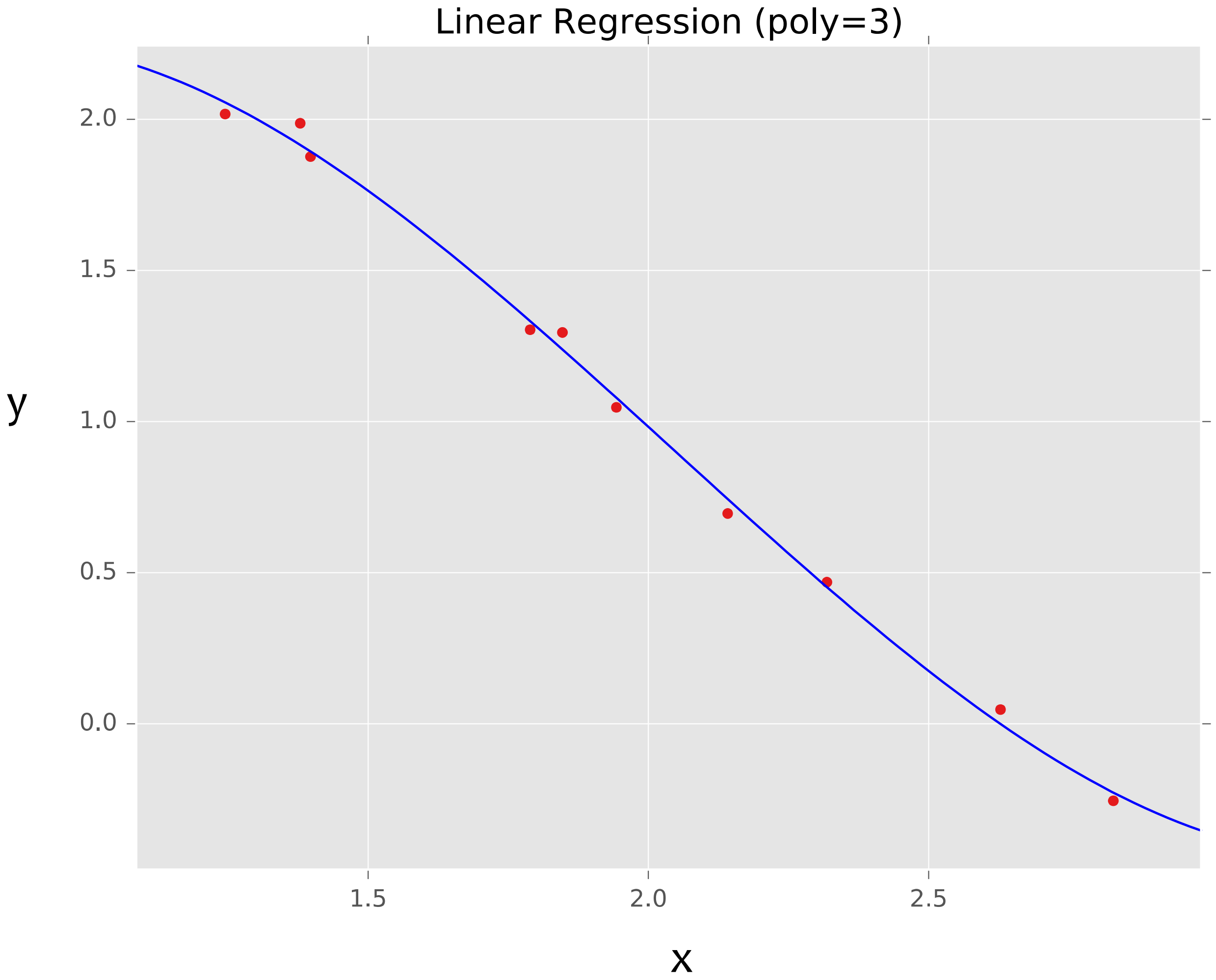
Slide credit: CMU MLD Matt Gormley

Example: Linear Regression

Goal: Learn y = $\mathbf{w}^T f(\mathbf{x}) + b$
where f(.) is a polynomial basis function

y	x	x^2	x^3
2.0	1.2	$(1.2)^2$	$(1.2)^3$
1.3	1.7	$(1.7)^2$	$(1.7)^3$
0.1	2.7	$(2.7)^2$	$(2.7)^3$
1.1	1.9	$(1.9)^2$	$(1.9)^3$

true "unknown" target function is linear with negative slope and gaussian noise



Slide credit: CMU MLD Matt Gormley

Example: Linear Regression

Goal: Learn y = $\mathbf{w}^T$ f($\mathbf{x}$) + b
where f(.) is a polynomial basis function

y	x	x^2	…	x^5
2.0	1.2	$(1.2)^2$	…	$(1.2)^5$
1.3	1.7	$(1.7)^2$	…	$(1.7)^5$
0.1	2.7	$(2.7)^2$	…	$(2.7)^5$
1.1	1.9	$(1.9)^2$	…	$(1.9)^5$

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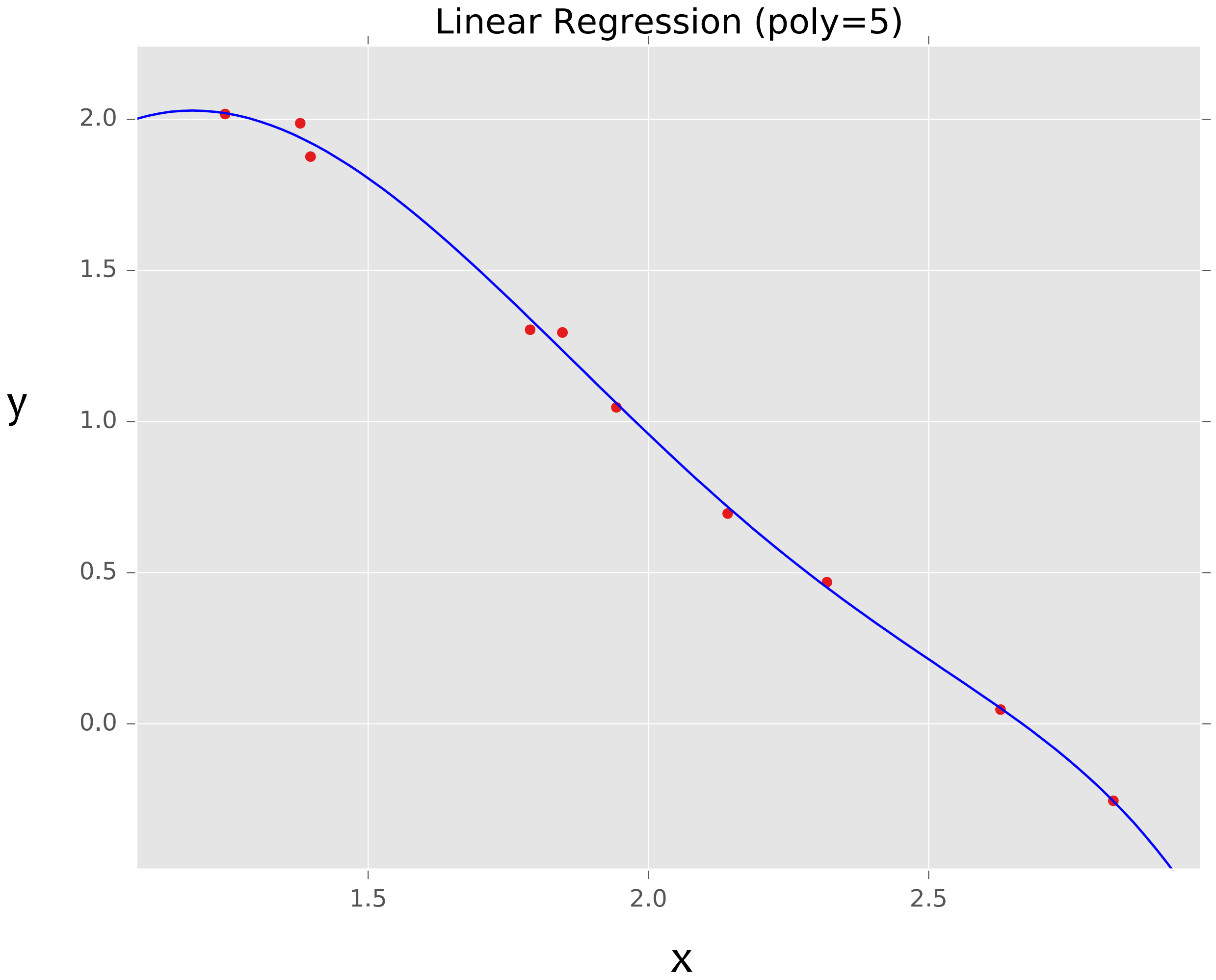


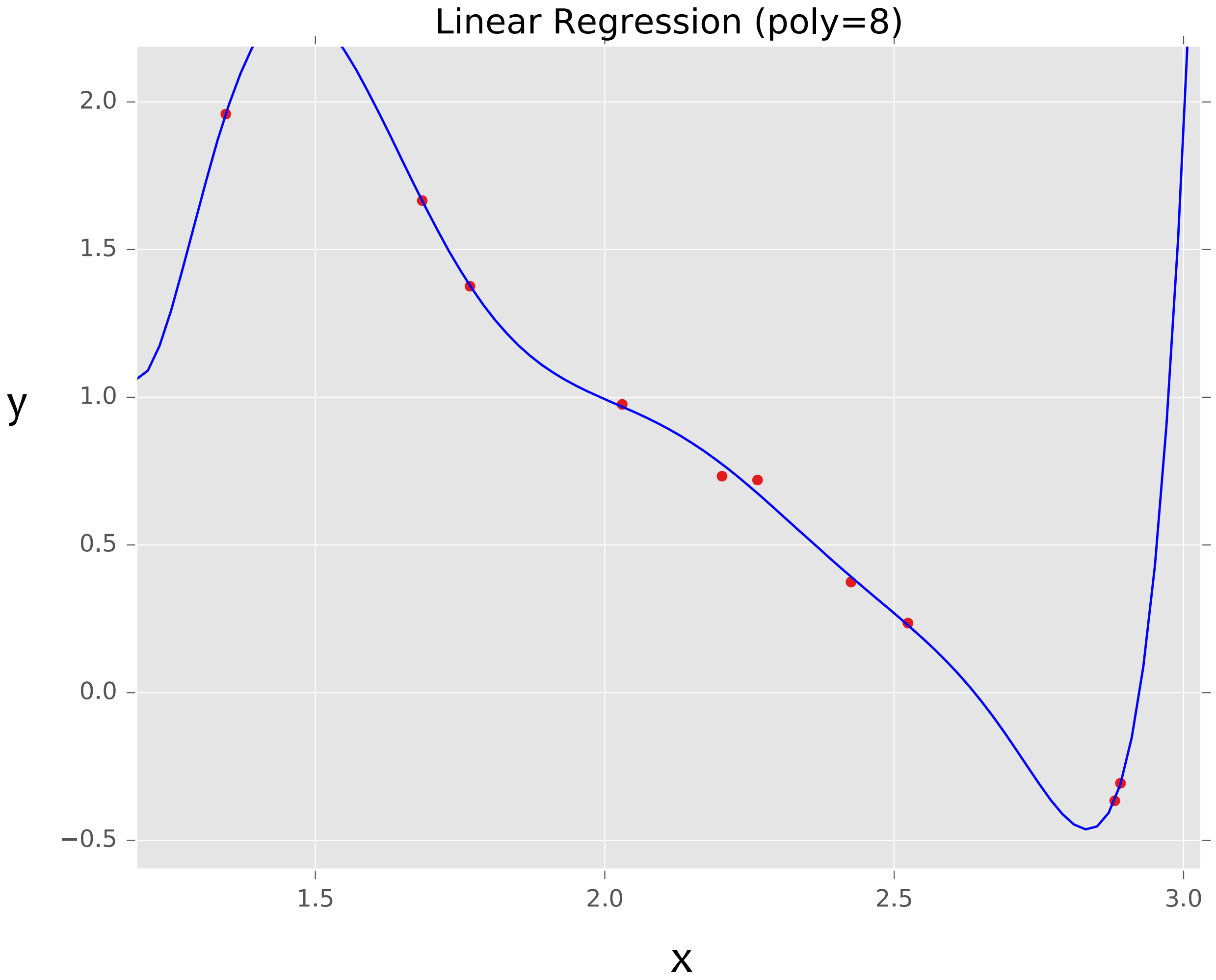
Slide credit: CMU MLD Matt Gormley

Example: Linear Regression

Goal: Learn $y = \mathbf{w}^T f(\mathbf{x}) + b$
where f(.) is a polynomial
basis function

y	x	x^2	…	x^8
2.0	1.2	$(1.2)^2$	…	$(1.2)^8$
1.3	1.7	$(1.7)^2$	…	$(1.7)^8$
0.1	2.7	$(2.7)^2$	…	$(2.7)^8$
1.1	1.9	$(1.9)^2$	…	$(1.9)^8$

true "unknown" target function is linear with negative slope and gaussian noise



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Example: Linear Regression

Goal: Learn y = $\mathbf{w}^T f(\mathbf{x}) + b$
where f(.) is a polynomial basis function

y	x	x^2	…	x^9
2.0	1.2	$(1.2)^2$	…	$(1.2)^9$
1.3	1.7	$(1.7)^2$	…	$(1.7)^9$
0.1	2.7	$(2.7)^2$	…	$(2.7)^9$
1.1	1.9	$(1.9)^2$	…	$(1.9)^9$

true "unknown" target function is linear with negative slope and gaussian noise

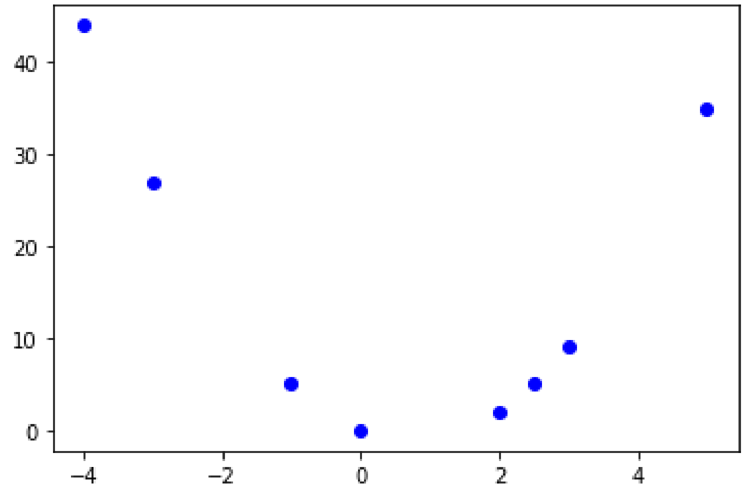
Slide credit: CMU MLD Matt Gormley

Polynomial Features

Design Matrix

$\phi(\vec{x}) : \mathbb{R}^M \to \mathbb{R}^{M'}$

N datapoints



y	x_1
44	-4
27	-3
5	-1
0	0
2	2
5	2.5
9	3
35	5

$N \times M$

$$X = \begin{bmatrix} — \mathbf{x}^{(1)\top} — \\ — \mathbf{x}^{(2)\top} — \\ — \mathbf{x}^{(3)\top} — \\ \cdots \\ — \mathbf{x}^{(N)\top} — \end{bmatrix}$$

$N \times M'$

$$\phi(X) = \begin{bmatrix} — \phi\left(\mathbf{x}^{(1)}\right)^\top — \\ — \phi\left(\mathbf{x}^{(2)}\right)^\top — \\ — \phi\left(\mathbf{x}^{(3)}\right)^\top — \\ \cdots \\ — \phi\left(\mathbf{x}^{(N)}\right)^\top — \end{bmatrix}$$

$\Phi(X) =$

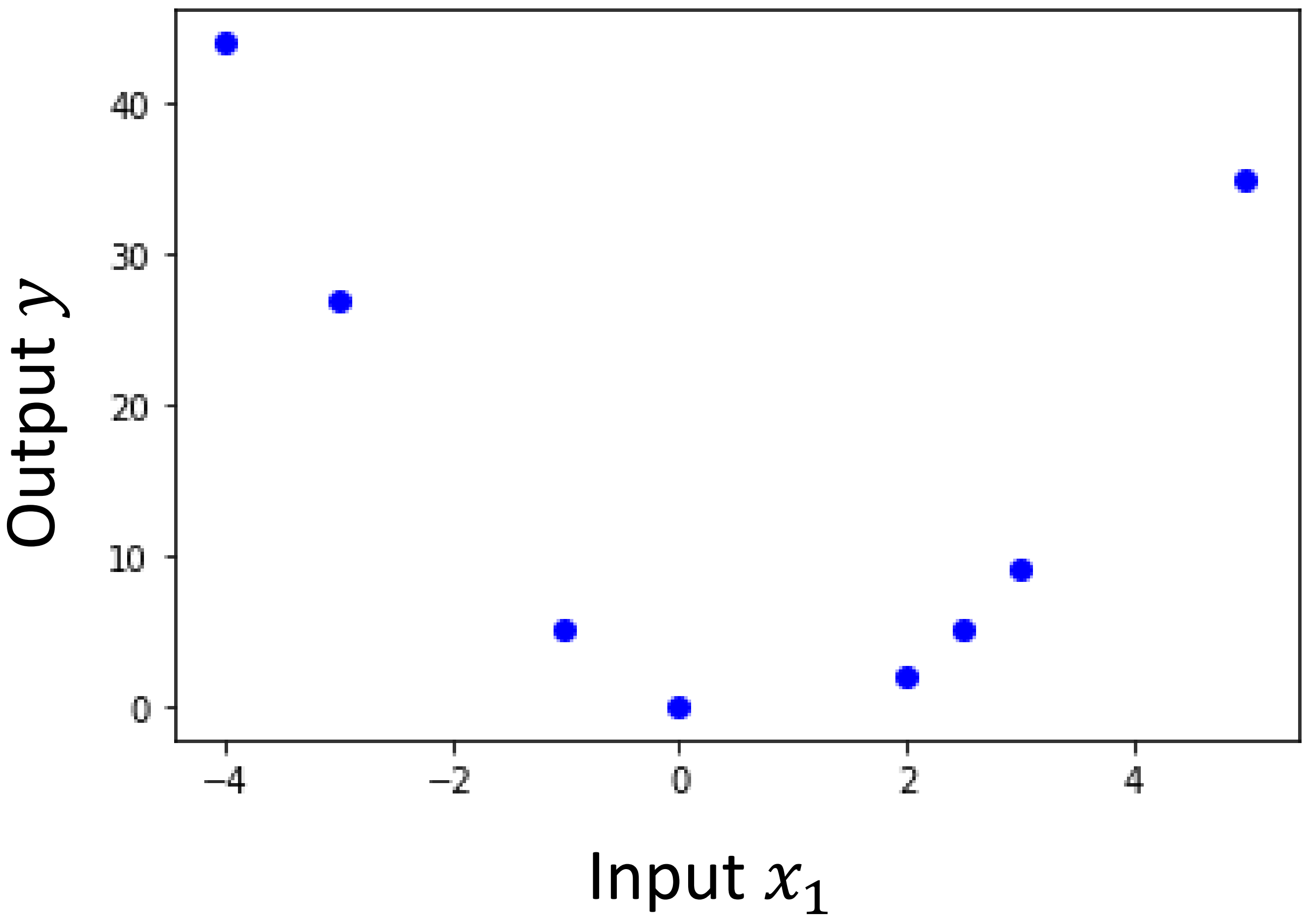
$\underline{\Phi}$

X

Polynomial Features

Non-linear Data

Linear regression on polynomial data?



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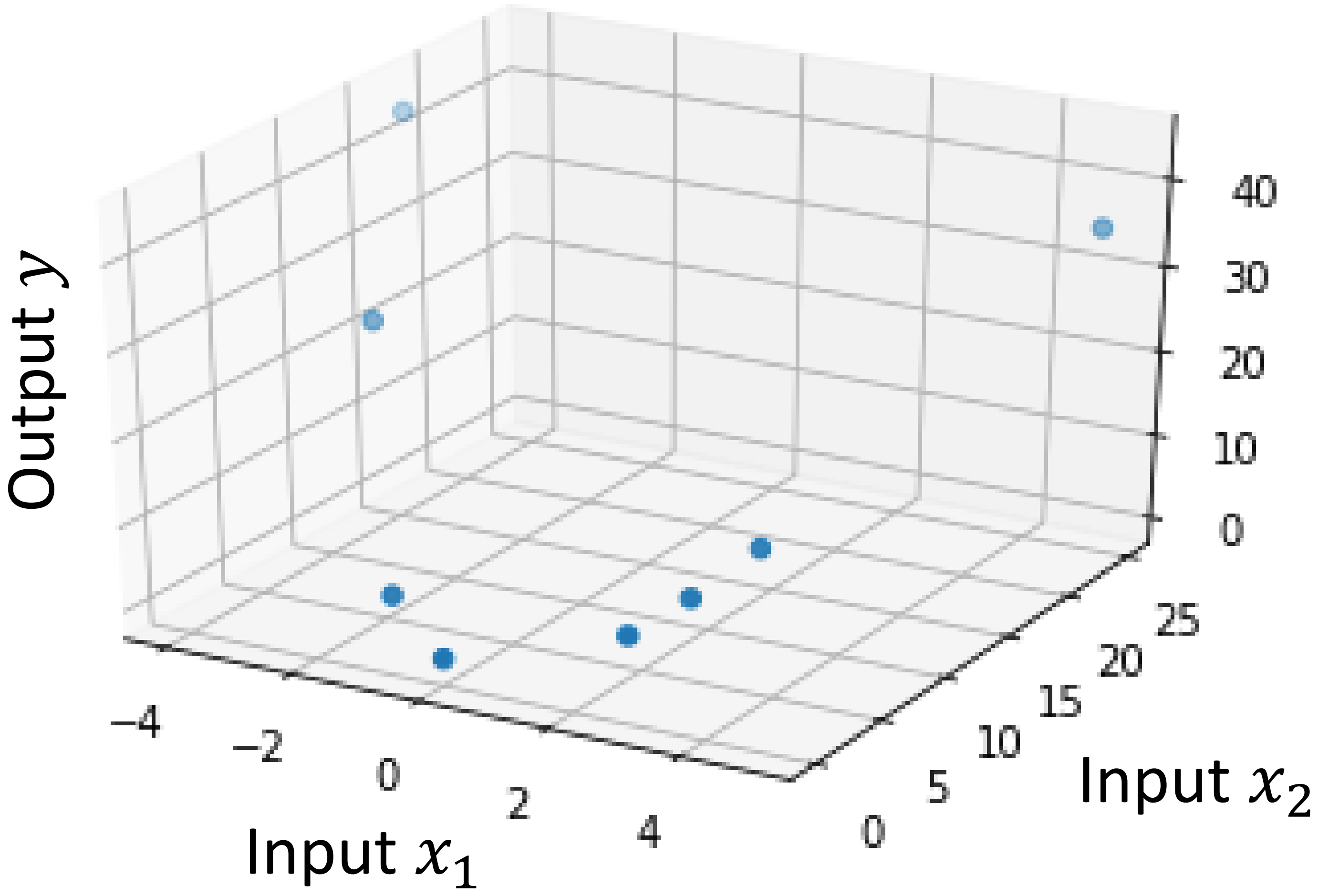
Non-linear Data

Regression on simple linear dataset



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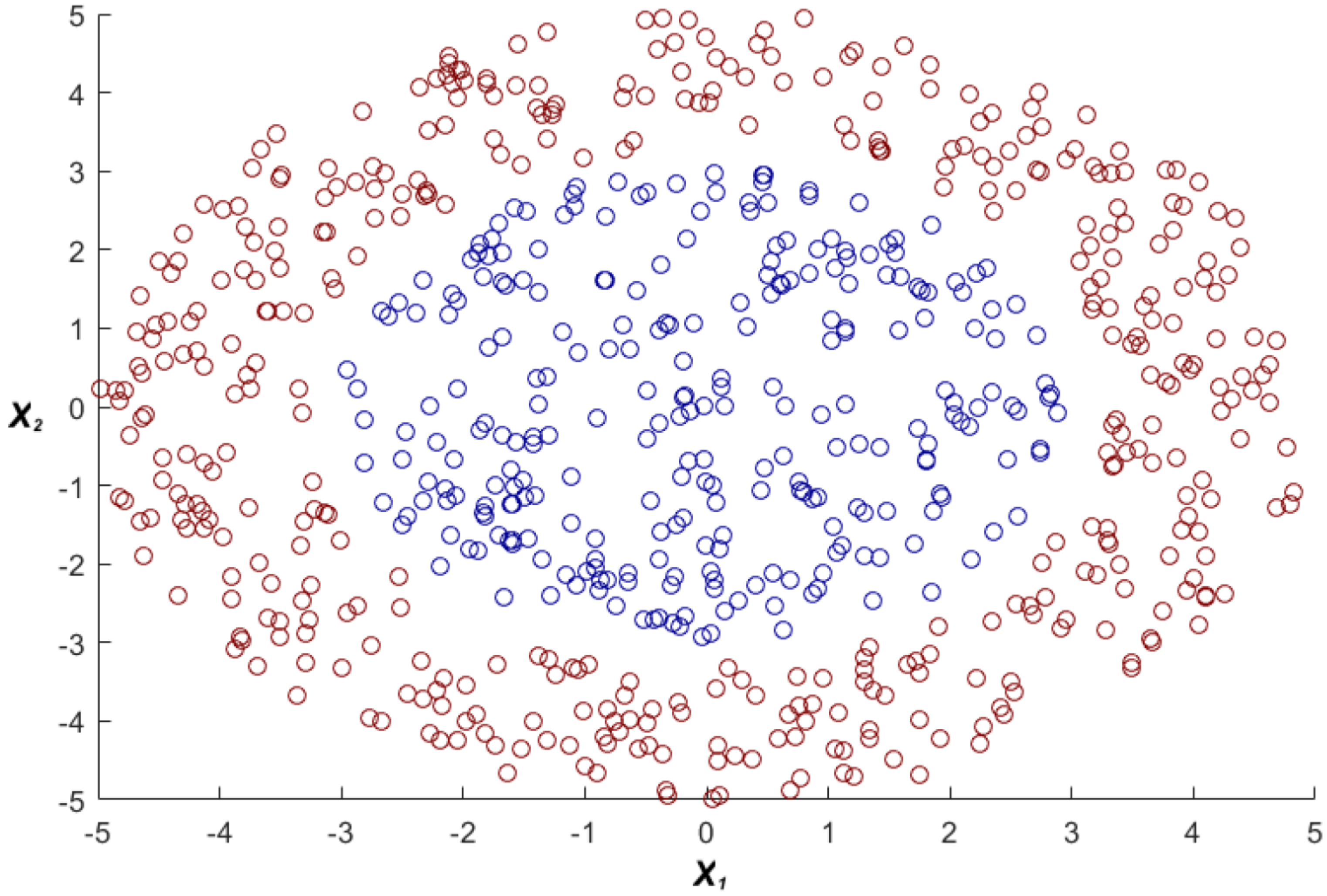
5	-1	1
0	0	0
2	2	4
5	2.5	6.25
9	3	9
35	5	25

Non-linear Data

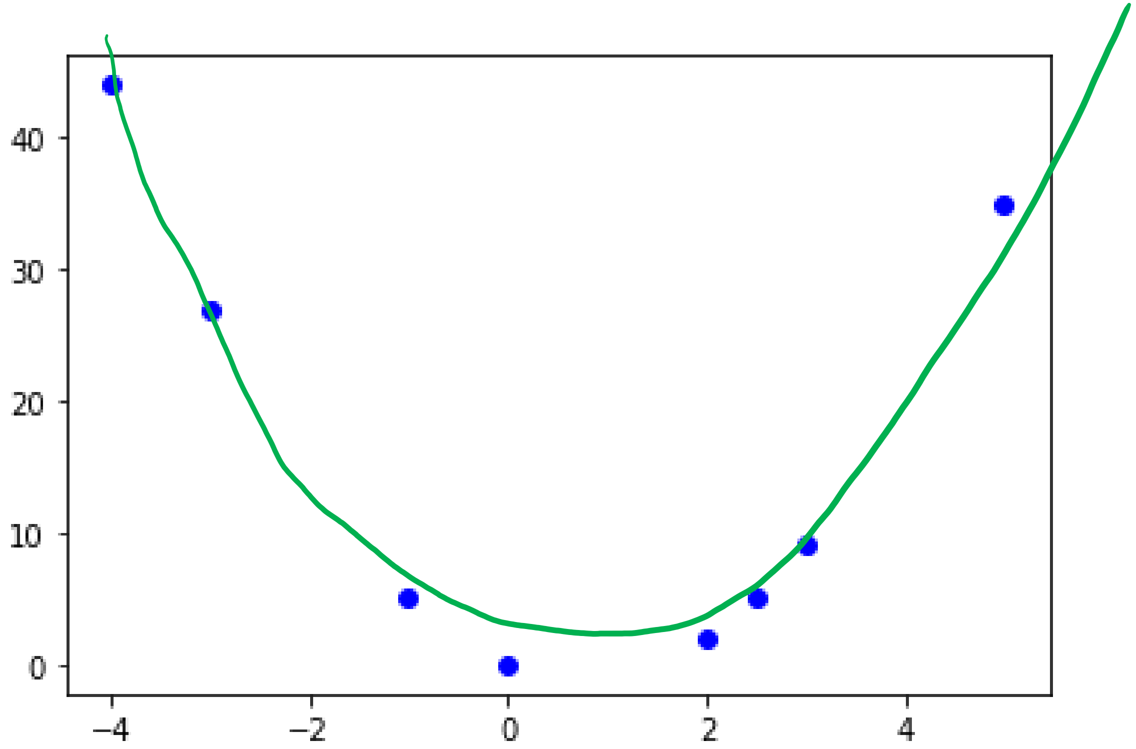
Polynomial feature map for linear classification

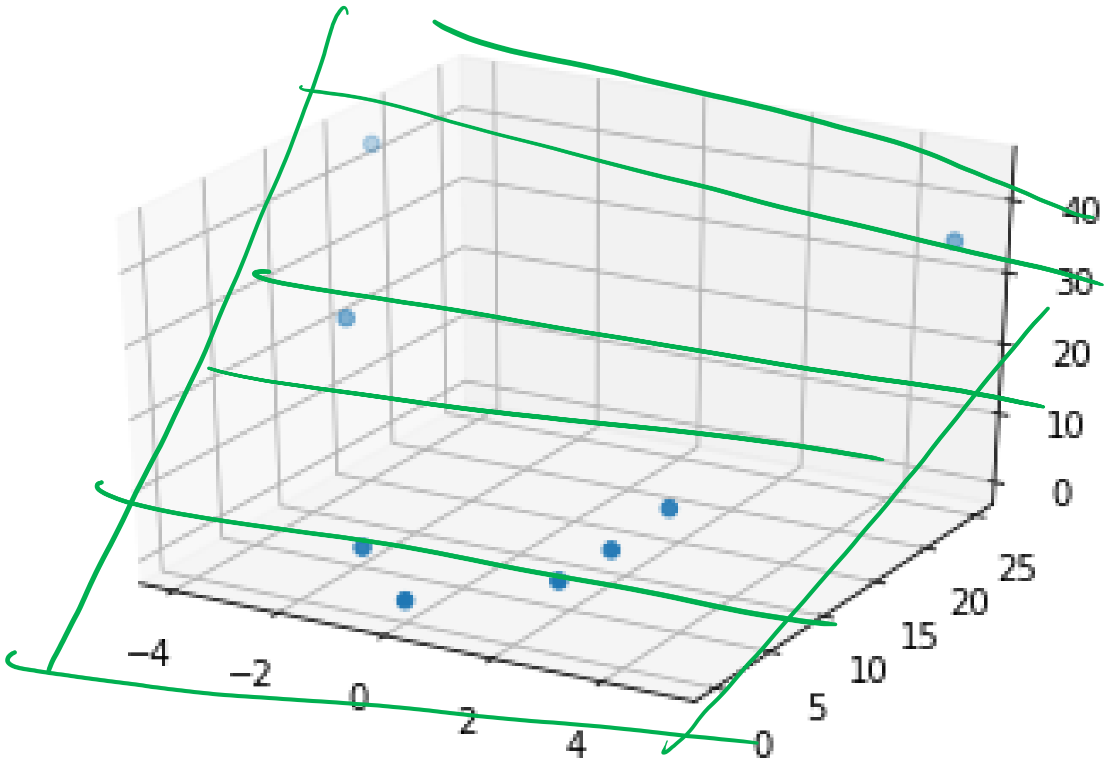


https://www.youtube.com/watch?v=3liCbRZPrZA

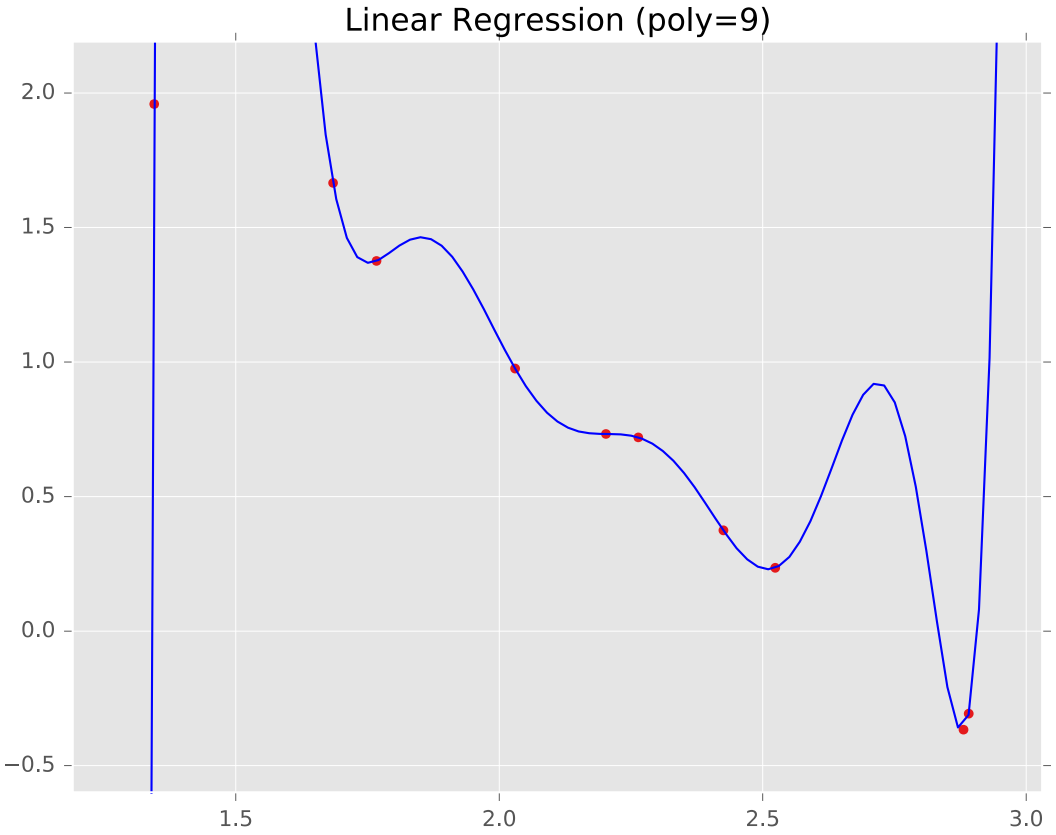
Feature Maps

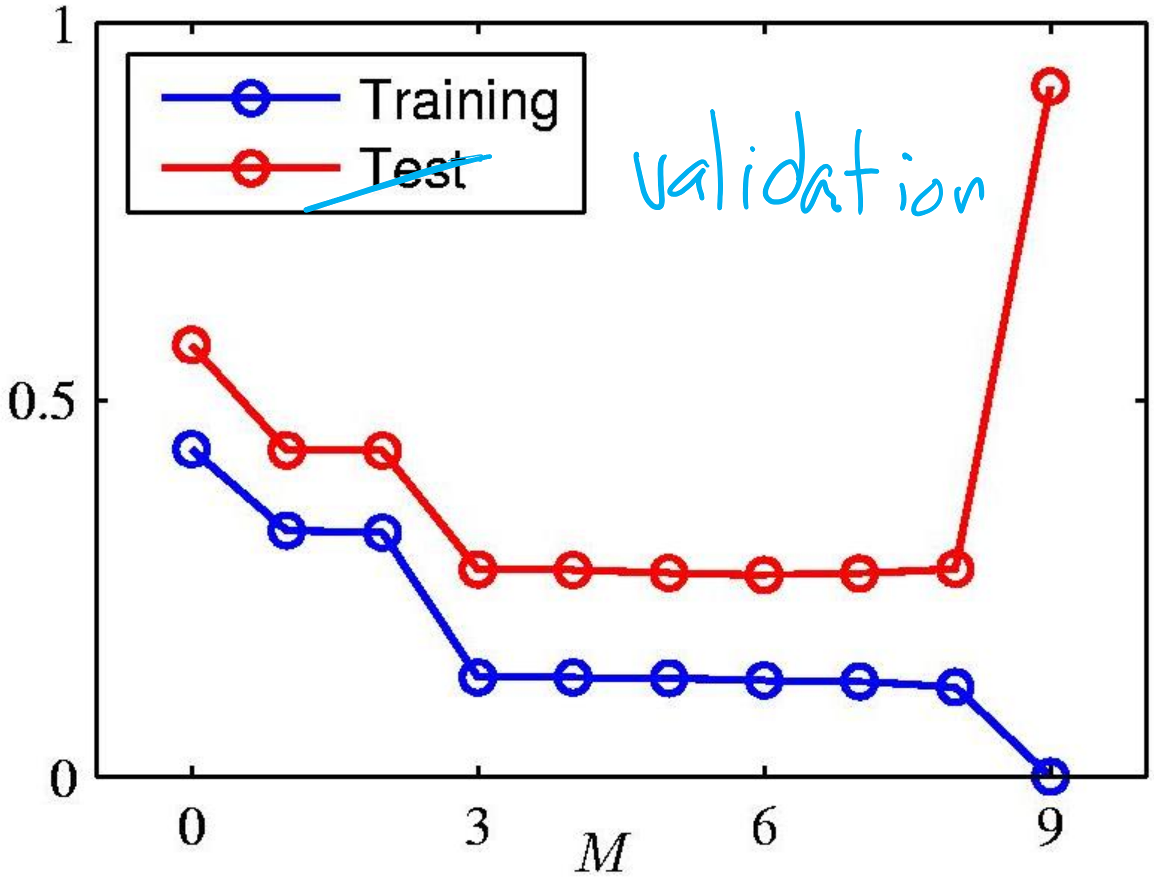
Two ways to think about it





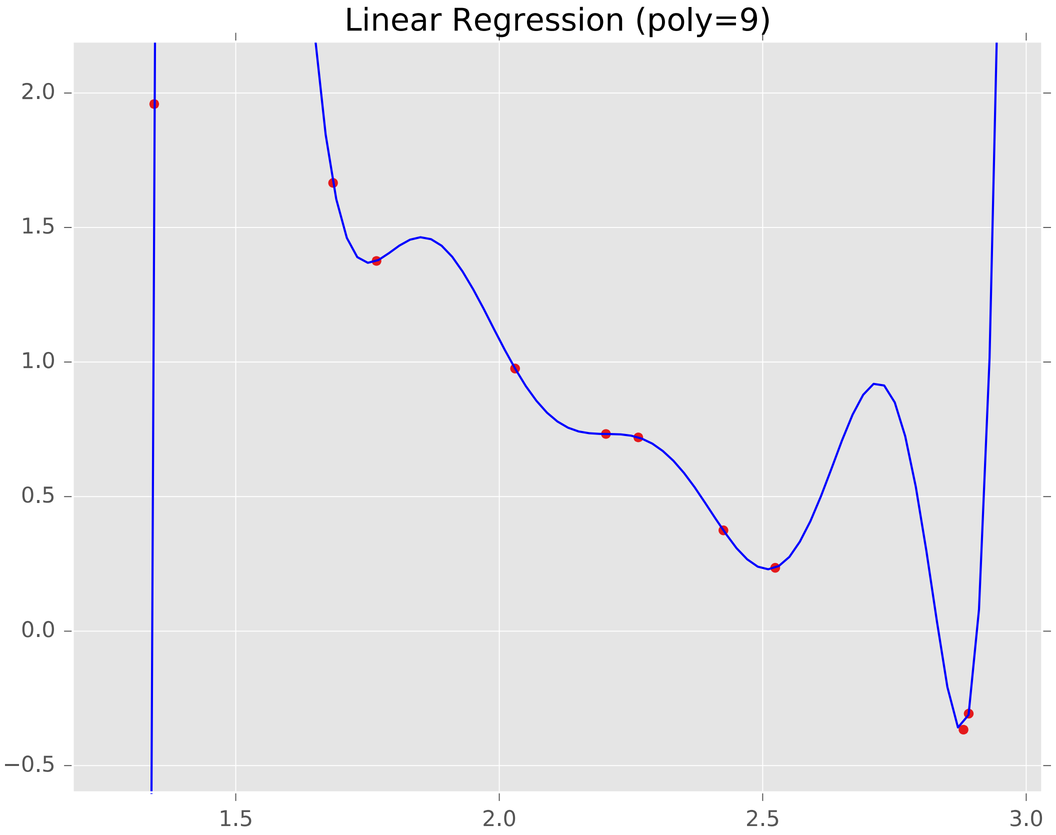
Overfitting: Symptoms





Slide credit: CMU MLD William Cohen

Overfitting: Symptoms



	$M=0$	$M=1$	$M=3$	$M=9$
θ_0	0.19	0.82	0.31	0.35
θ_1		-1.27	7.99	232.37
θ_2			-25.43	-5321.83
θ_3			17.37	48568.31
θ_4				-231639.30
θ_5				640042.26
θ_6				-1061800.52
θ_7				1042400.18
θ_8				-557682.99
θ_9				125201.43

9

Overfitting: Fix?

N = 10 points we overfit!

Goal: Learn $y = \mathbf{w}^T f(\mathbf{x}) + b$ where f(.) is a polynomial basis function

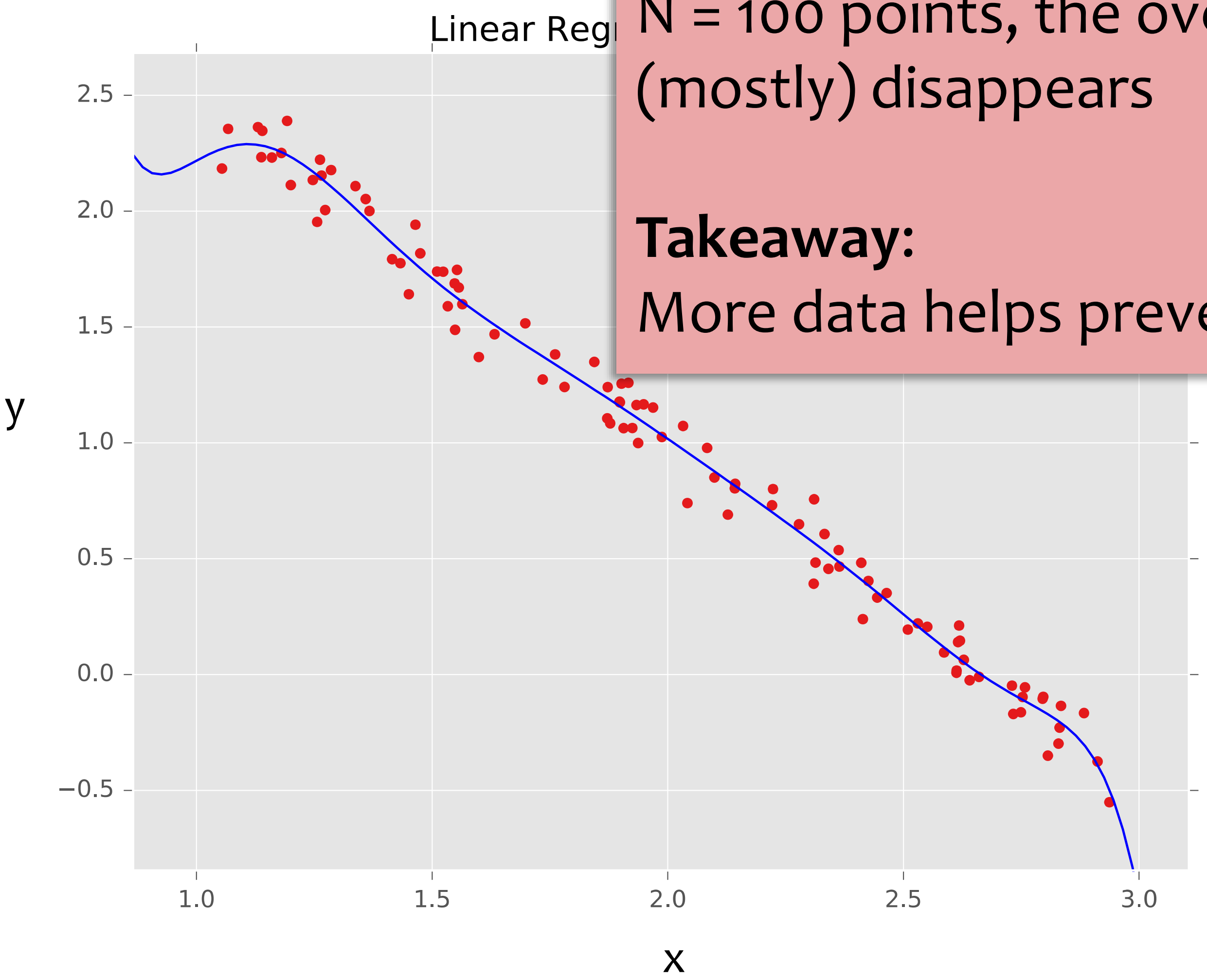
i	y	x	…	x^9
1	2.0	1.2	…	$(1.2)^9$
2	1.3	1.7	…	$(1.7)^9$
…	…	…	…	…
10	1.1	1.9	…	$(1.9)^9$

Slide credit: CMU MLD Matt Gormley

Overfitting: More training data!

Goal: Learn $y = \mathbf{w}^T f(\mathbf{x}) + b$
where f(.) is a polynomial
basis function

i	y	x	…	x^9
1	2.0	1.2	…	$(1.2)^9$
2	1.3	1.7	…	$(1.7)^9$
3	0.1	2.7	…	$(2.7)^9$
4	1.1	1.9	…	$(1.9)^9$
…	…	…	…	…
…	…	…	…	…
…	…	…	…	…
98	…	…	…	…
99	…	…	…	…
100	0.9	1.5	…	$(1.5)^9$



N = 10 points we overfit!

N = 100 points, the overfitting (mostly) disappears

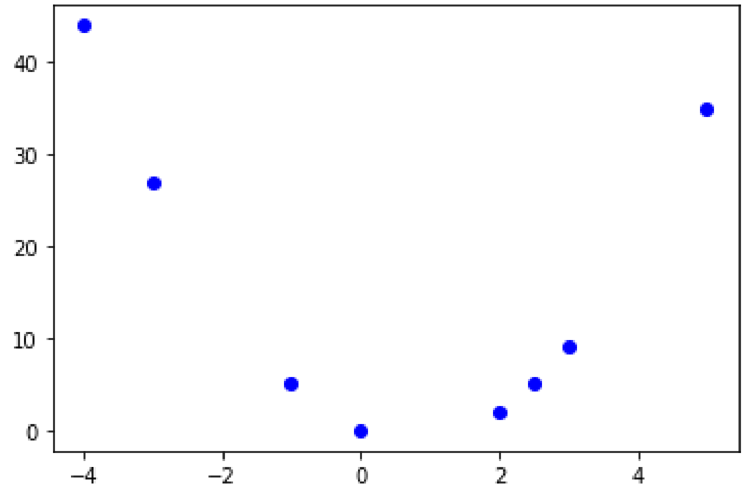
Takeaway:
More data helps prevent overfitting

Polynomial Features

Design Matrix

$\phi(\vec{x}) : R^{M} \rightarrow R^{M'}$

N datapoints



y	x_1
44	-4
27	-3
5	-1
0	0
2	2
5	2.5
9	3
35	5

$N \times M$

$$X = \begin{bmatrix} — & \mathbf{x}^{(1)\top} & — \\ — & \mathbf{x}^{(2)\top} & — \\ — & \mathbf{x}^{(3)\top} & — \\ & \cdots & \\ — & \mathbf{x}^{(N)\top} & — \end{bmatrix}$$

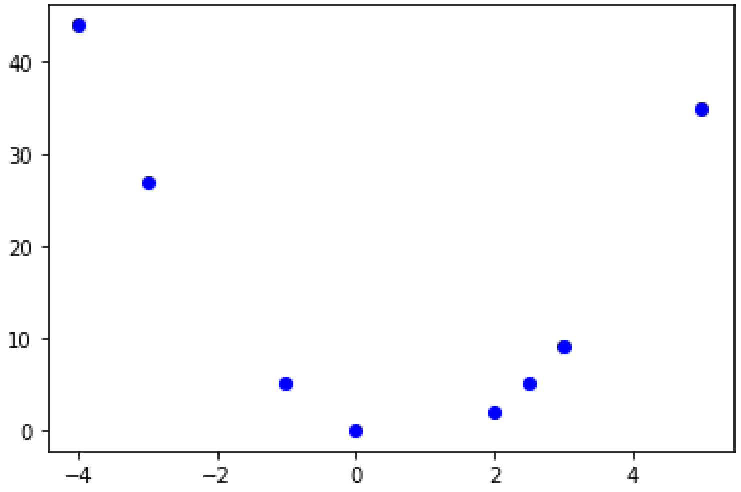
$N \times M'$

$$\phi(X) = \begin{bmatrix} — & \phi\left(\mathbf{x}^{(1)}\right)^\top & — \\ — & \phi\left(\mathbf{x}^{(2)}\right)^\top & — \\ — & \phi\left(\mathbf{x}^{(3)}\right)^\top & — \\ & \cdots & \\ — & \phi\left(\mathbf{x}^{(N)}\right)^\top & — \end{bmatrix}$$

Polynomial Features

Solving linear regression

$$\phi(\vec{x}) = \begin{bmatrix} 1 \\ x_1 \\ x_1^2 \end{bmatrix} \qquad \vec{\theta} = \begin{bmatrix} b \\ w_1 \\ w_2 \end{bmatrix}$$



$\vec{y} \in \mathbb{R}^N \qquad N=8$

	y	x_1
$i=1$	44	-4
	27	-3
	5	-1
	0	0
	2	2
	5	2.5
	9	3
$i=8$	35	5

Feature Engineering vs Feature Learning

Feature engineering

- Humans decide what the features may be useful
- Humans implement feature extraction algorithms

Feature learning

- Humans choose data and performance measure
- Humans decide on structure/algorithm to learn features
  - Features are just intermediate values between input and output
  - Structure defines number of feature values
- Allow machine to map data to feature values as needed

One-hot encoding

Need to convert text for categories into numerical values for input and output

Categorical

color	color	r	g	b
red	1	1	0	0
green	2	0	1	0
blue	3	0	0	1
red	1	1	0	0
red	1	1	0	0

Categorical variables

- Enumeration
- One-hot vector (or one-hot columns)

One-hot vector

- Vector of length M with exactly one 1 and M-1 zeros
- Series of M binary values, exactly one of which is 1

More to come later in the semester

✅ Polynomial feature engineering

✅ Categorical features and one-hot encoding

Images

- Raw data, feature engineering
- Feature learning

Audio

- Raw data, feature engineering
- Feature learning

Text

- Raw data, feature engineering
- Feature learning