

#### 10-301/601 Introduction to Machine Learning

Machine Learning Department School of Computer Science Carnegie Mellon University

## Logistic Regression + Feature Engineering + Regularization

Matt Gormley & Henry Chai Lecture 10 Oct. 1, 2021

### Reminders

- Homework 4: Logistic Regression
  - Out: Fri, Oct. 1
  - Due: Mon, Oct. 11 at 11:59pm

### MAXIMUM LIKELIHOOD ESTIMATION

### MLE

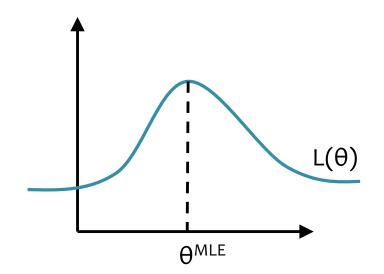
Suppose we have data  $\mathcal{D} = \{x^{(i)}\}_{i=1}^N$ 

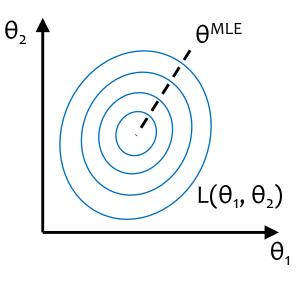
### **Principle of Maximum Likelihood Estimation:**

Choose the parameters that maximize the likelihood of the data.  $\theta^{\text{MLE}} = \operatorname{argmax} \prod p(\mathbf{x}^{(i)} | \theta)$ 



θ





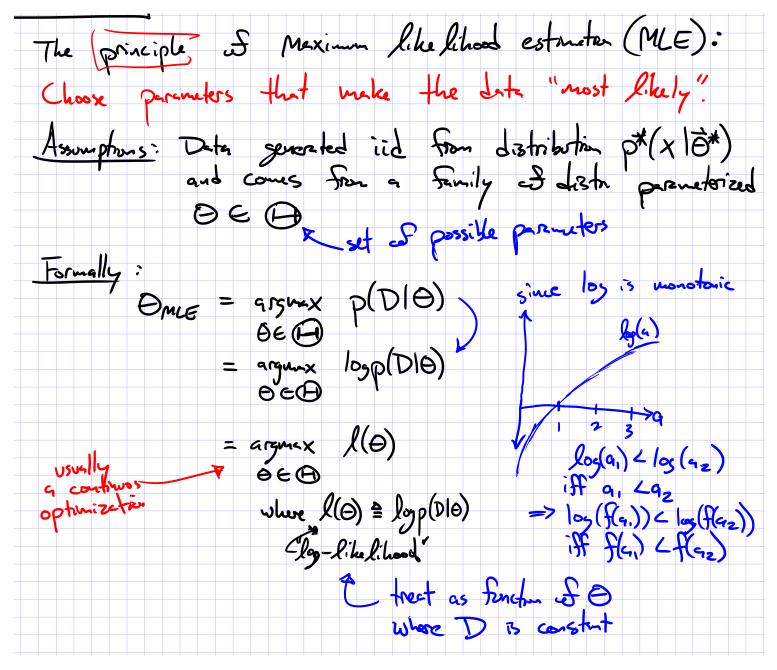
### MLE

What does maximizing likelihood accomplish?

- There is only a finite amount of probability mass (i.e. sum-to-one constraint)
- MLE tries to allocate as much probability mass as possible to the things we have observed...

... at the expense of the things we have not observed

### Maximum Likelihood Estimation



### MOTIVATION: LOGISTIC REGRESSION

### Example: Image Classification

- ImageNet LSVRC-2010 contest:
  - Dataset: 1.2 million labeled images, 1000 classes
  - Task: Given a new image, label it with the correct class
  - **Multiclass** classification problem
- Examples from http://image-net.org/



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### Example: Image Classification

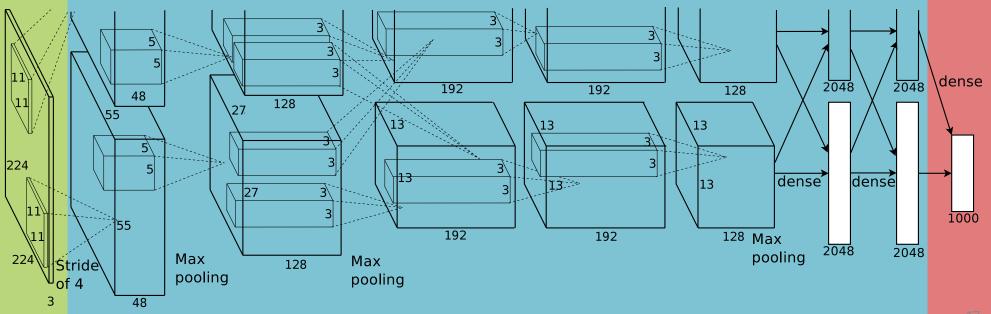
**CNN for Image Classification** (Krizhevsky, Sutskever & Hinton, 2011) 17.5% error on ImageNet LSVRC-2010 contest

Input

image

(pixels)

- Five convolutional layers (w/max-pooling)
- Three fully connected layers

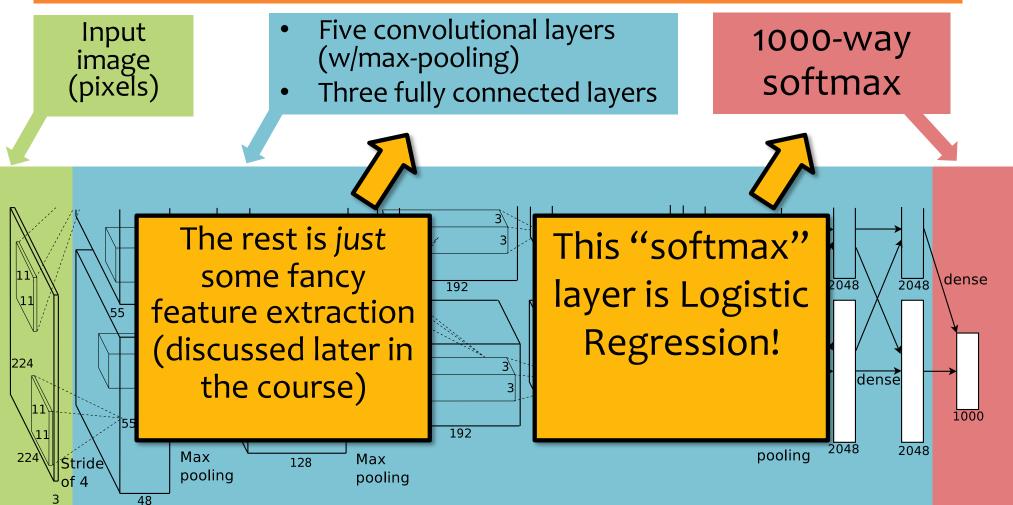


1000-way

softmax

### Example: Image Classification

**CNN for Image Classification** (Krizhevsky, Sutskever & Hinton, 2011) 17.5% error on ImageNet LSVRC-2010 contest



### LOGISTIC REGRESSION

**Data:** Inputs are continuous vectors of length M. Outputs are discrete.

 $\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^N$  where  $\mathbf{x} \in \mathbb{R}^M$  and  $y \in \{0, 1\}$ 

We are back to classification.

Despite the name logistic **regression**.

## Linear Models for Classification

### Key idea: Try to learn this hyperplane directly

#### Looking ahead:

- We'll see a number of commonly used Linear Classifiers
- These include:
  - Perceptron
  - Logistic Regression
  - Naïve Bayes (under certain conditions)
  - Support Vector Machines

Directly modeling the hyperplane would use a decision function:

 $h(\mathbf{x}) = \operatorname{sign}(\boldsymbol{\theta}^T \mathbf{x})$ 

for:

 $y \in \{-1, +1\}$ 



### **Background:** Hyperplanes

Notation Trick: fold the bias b and the weights w into a single vector  $\boldsymbol{\theta}$  by prepending a constant to **x** and increasing dimensionality by one to get x'!

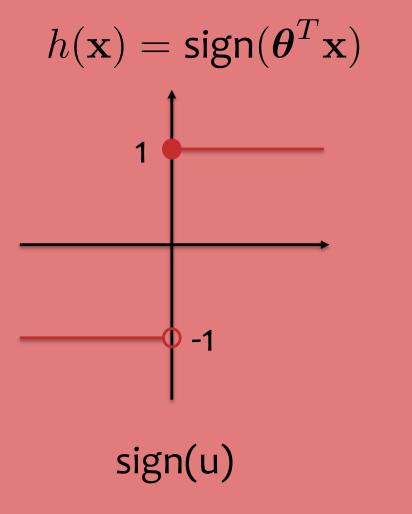
Half-spaces:

Hyperplane (Definition 1):  $\mathcal{H} = \{\mathbf{x} : \mathbf{w}^T \mathbf{x} = b\}$ Hyperplane (Definition 2):  $\mathcal{H} = \{\mathbf{x}': \boldsymbol{\theta}^T \mathbf{x}' = 0\}$ and  $x_{1} = 1$  $\boldsymbol{\theta} = [b, w_1, \dots, w_M]^T$  $\mathbf{x}' = [1, x_1, \dots, x_M]^T$  $\mathcal{H}^+ = \{ \mathbf{x} : \boldsymbol{\theta}^T \mathbf{x} > 0 \text{ and } x_1 = 1 \}$  $\mathcal{H}^- = \{\mathbf{x} : \boldsymbol{\theta}^T \mathbf{x} < 0 \text{ and } x_1 = 1\}$ 

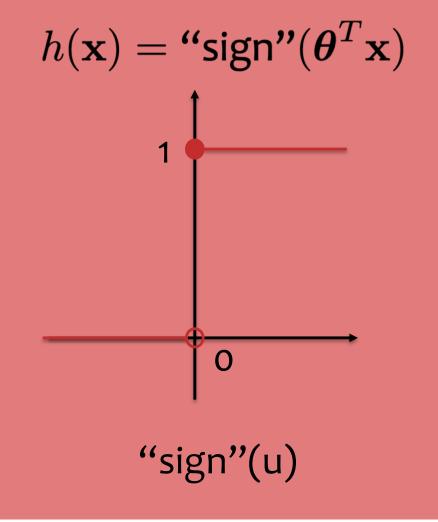
Key idea behind today's lecture:

- 1. Define a linear classifier (logistic regression)
- 2. Define an objective function (likelihood)
- 3. Optimize it with gradient descent to learn parameters
- 4. Predict the class with highest probability under the model

Suppose we wanted to learn a linear classifier, but instead of predicting  $y \in \{-1,+1\}$  we wanted to predict  $y \in \{0,1\}$ 



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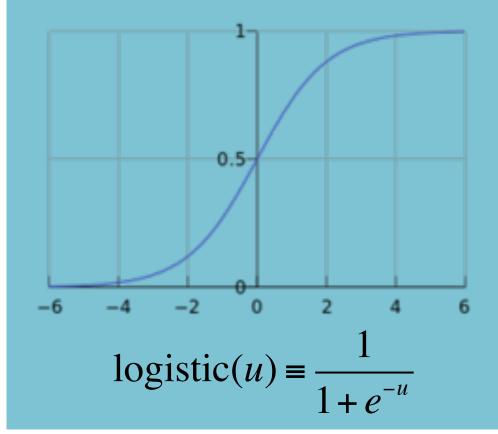


**Goal:** Learn a linear classifier with Gradient Descent

But this decision function isn't differentiable...

$$h(\mathbf{x}) = \text{"sign"}(\boldsymbol{\theta}^T \mathbf{x})$$

Use a differentiable function instead!  $p_{\theta}(y = 1 | \mathbf{x}) = \frac{1}{1 + \exp(-\theta^T \mathbf{x})}$ 



"sign"(u)

0

Whiteboard

- Conceptual Change: 2D classification in 3D
- Why is it called Logistic Regression and not Logistic Classification?

**Data:** Inputs are continuous vectors of length M. Outputs are discrete.

 $\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^N$  where  $\mathbf{x} \in \mathbb{R}^M$  and  $y \in \{0, 1\}$ 

**Model:** Logistic function applied to dot product of parameters with input vector.  $p_{\theta}(y = 1 | \mathbf{x}) = \frac{1}{1 + \exp(-\theta^T \mathbf{x})}$ 

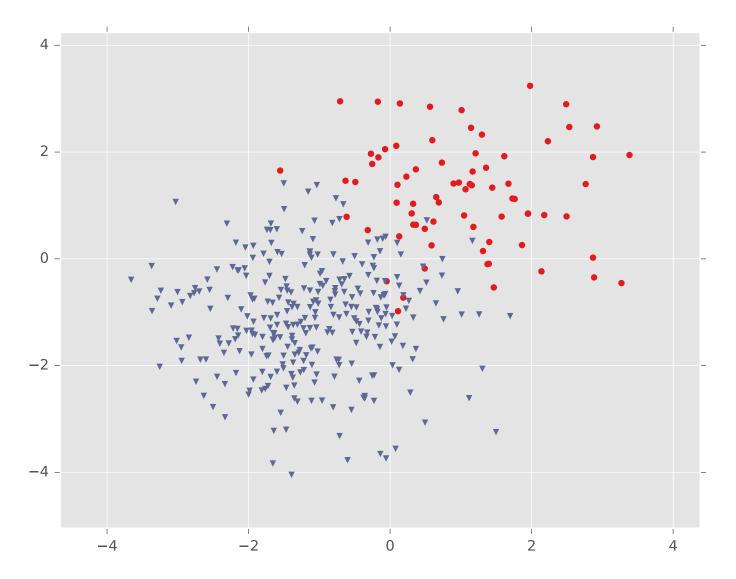
**Learning:** finds the parameters that minimize some objective function.  $\theta^* = \operatorname*{argmin}_{\theta} J(\theta)$ 

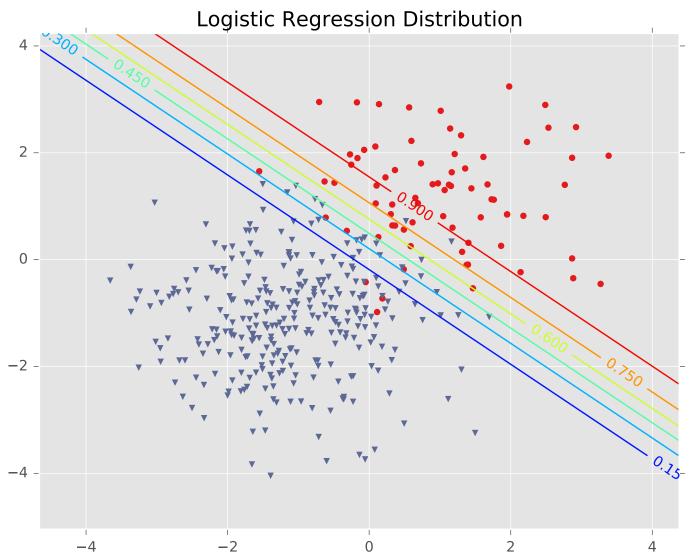
**Prediction:** Output is the most probable class.  $\hat{y} = \operatorname*{argmax}_{y \in \{0,1\}} p_{\theta}(y|\mathbf{x})$ 

Whiteboard

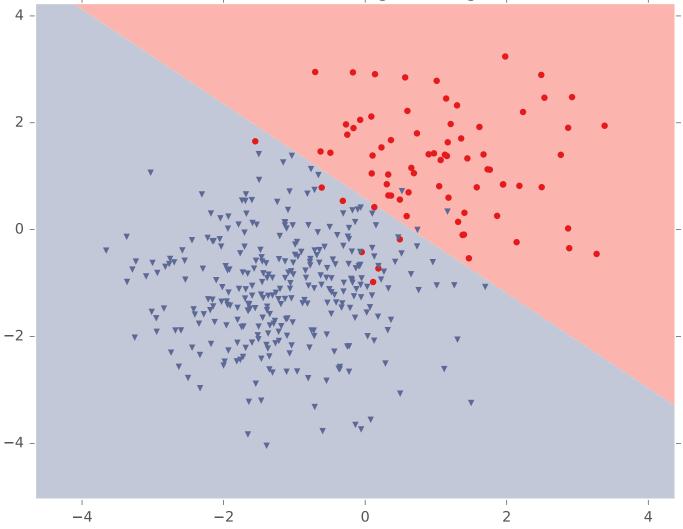
- Logistic Regression Model
- Partial derivative for logistic regression
- Gradient for logistic regression
- Decision boundary

### LOGISTIC REGRESSION ON GAUSSIAN DATA





Classification with Logistic Regression



### LEARNING LOGISTIC REGRESSION

### Maximum **Conditional** Likelihood Estimation

**Learning:** finds the parameters that minimize some objective function.

 $\boldsymbol{\theta}^* = \operatorname*{argmin}_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$ 

We minimize the *negative* log conditional likelihood:

$$J(\boldsymbol{\theta}) = -\log \prod_{i=1}^{N} p_{\boldsymbol{\theta}}(y^{(i)} | \mathbf{x}^{(i)})$$

Why?

- 1. We can't maximize likelihood (as in Naïve Bayes) because we don't have a joint model p(x,y)
- 2. It worked well for Linear Regression (least squares is MCLE)

### Maximum **Conditional** Likelihood Estimation

**Learning:** Four approaches to solving  $\theta^* = \operatorname{argmin}_{\theta} J(\theta)$ 

**Approach 1:** Gradient Descent (take larger – more certain – steps opposite the gradient)

**Approach 2:** Stochastic Gradient Descent (SGD) (take many small steps opposite the gradient)

**Approach 3:** Newton's Method (use second derivatives to better follow curvature)

**Approach 4:** Closed Form??? (set derivatives equal to zero and solve for parameters)

### Maximum **Conditional** Likelihood Estimation

**Learning:** Four approaches to solving  $\theta^* = \operatorname{argmin}_{\theta} J(\theta)$ 

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Approach 4: Closed Form???

(set derivatives equal to zero and solve for parameters)

Logistic Regression does not have a closed form solution for MLE parameters.

### SGD for Logistic Regression

#### **Question:**

Which of the following is a correct description of SGD for Logistic Regression?

#### Answer:

At each step (i.e. iteration) of SGD for Logistic Regression we...

- A. (1) compute the gradient of the log-likelihood for all examples (2) update all the parameters using the gradient
- B. (1) ask Matt for a description of SGD for Logistic Regression, (2) write it down, (3) report that answer
- C. (1) compute the gradient of the log-likelihood for all examples (2) randomly pick an example (3) update only the parameters for that example
- D. (1) randomly pick a parameter, (2) compute the partial derivative of the loglikelihood with respect to that parameter, (3) update that parameter for all examples
- E. (1) randomly pick an example, (2) compute the gradient of the log-likelihood for that example, (3) update all the parameters using that gradient
- F. (1) randomly pick a parameter and an example, (2) compute the gradient of the log-likelihood for that example with respect to that parameter, (3) update that parameter using that gradient



A When survey is active, respond at pollev.com/10301601polls

### Lecture 10: In-Class Poll





the When poll is active, respond at pollew.com/10301601polls



Question 1





### Gradient Descent

Algorithm 1 Gradient Descent

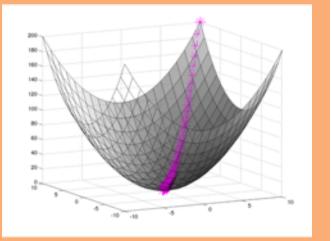
1: procedure 
$$GD(\mathcal{D}, \boldsymbol{\theta}^{(0)})$$

2: 
$$\boldsymbol{ heta} \leftarrow \boldsymbol{ heta}^{(0)}$$

3: while not converged do 4:  $\theta \leftarrow \theta - \gamma \nabla_{\theta} J(\theta)$ 

$$: \quad \mathbf{0} \leftarrow \mathbf{0} - \mathbf{1} \lor \mathbf{\theta}$$





In order to apply GD to Logistic Regression all we need is the **gradient** of the objective  $\nabla_{\theta} J(\theta) =$ function (i.e. vector of partial derivatives).

$$\begin{bmatrix} \frac{d}{d\theta_1} J(\boldsymbol{\theta}) \\ \frac{d}{d\theta_2} J(\boldsymbol{\theta}) \\ \vdots \\ \frac{d}{d\theta_2} J(\boldsymbol{\theta}) \end{bmatrix}$$

 $uv_M$ 

# Stochastic Gradient Descent (SGD)

0.4 0.3 0.2 0.1

-0.1 -0.2 -0.3

-500

1000

500

1500

2000

Algorithm 1 Stochastic Gradient Descent (SGD)

1: procedure SGD(
$$\mathcal{D}, \theta^{(0)}$$
)  
2:  $\theta \leftarrow \theta^{(0)}$   
3: while not converged do  
4: for  $i \in \text{shuffle}(\{1, 2, ..., N\})$  do  
5:  $\theta \leftarrow \theta - \gamma \nabla_{\theta} J^{(i)}(\theta)$   
6: return  $\theta$ 



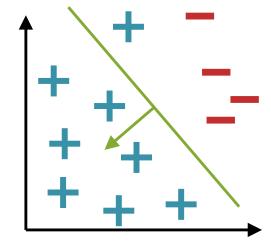
We need a per-example objective:

Let 
$$J(\boldsymbol{\theta}) = \sum_{i=1}^{N} J^{(i)}(\boldsymbol{\theta})$$
  
where  $J^{(i)}(\boldsymbol{\theta}) = -\log p_{\boldsymbol{\theta}}(y^{i}|\mathbf{x}^{i})$ .

# Logistic Regression vs. Perceptron

### **Question:**

True or False: Just like Perceptron, one step (i.e. iteration) of SGD for Logistic Regression will result in a change to the parameters only if the current example is incorrectly classified.



### Answer:



th When poll is active, respond at pollev.com/10301601polls



**Question 2** 

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В		
C		

### **OPTIMIZATION METHOD #4: MINI-BATCH SGD**

## Mini-Batch SGD

### • Gradient Descent:

Compute true gradient exactly from all N examples

• Stochastic Gradient Descent (SGD): Approximate true gradient by the gradient of one randomly chosen example

### • Mini-Batch SGD:

Approximate true gradient by the average gradient of K randomly chosen examples

### Mini-Batch SGD

while not converged: 
$$oldsymbol{ heta} \leftarrow oldsymbol{ heta} - \lambda \mathbf{g}$$

### Three variants of first-order optimization:

Gradient Descent:  $\mathbf{g} = \nabla J(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} \nabla J^{(i)}(\boldsymbol{\theta})$ SGD:  $\mathbf{g} = \nabla J^{(i)}(\boldsymbol{\theta})$  where i sampled uniformly Mini-batch SGD:  $\mathbf{g} = \frac{1}{S} \sum_{s=1}^{S} \nabla J^{(i_s)}(\boldsymbol{\theta})$  where  $i_s$  sampled uniformly  $\forall s$ 

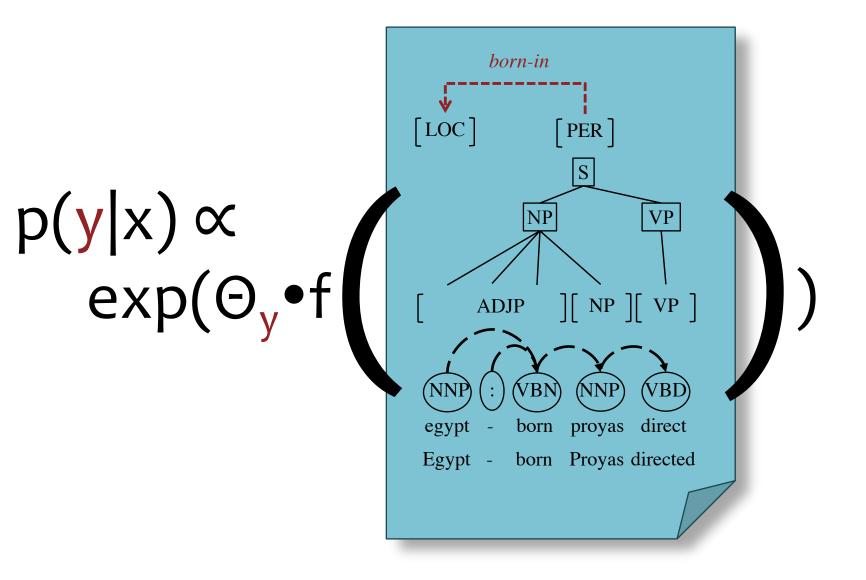
# Logistic Regression Objectives

You should be able to...

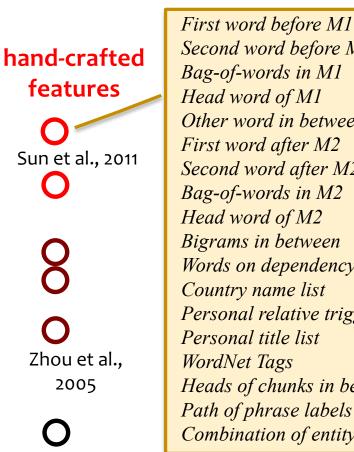
- Apply the principle of maximum likelihood estimation (MLE) to learn the parameters of a probabilistic model
- Given a discriminative probabilistic model, derive the conditional log-likelihood, its gradient, and the corresponding Bayes Classifier
- Explain the practical reasons why we work with the log of the likelihood
- Implement logistic regression for binary or multiclass classification
- Prove that the decision boundary of binary logistic regression is linear
- For linear regression, show that the parameters which minimize squared error are equivalent to those that maximize conditional likelihood

### FEATURE ENGINEERING

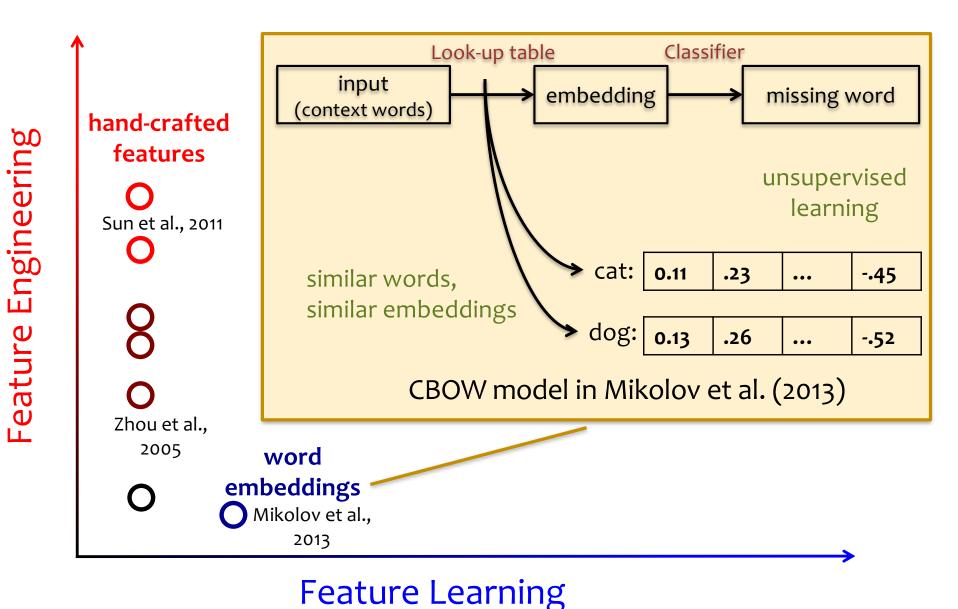
### Handcrafted Features

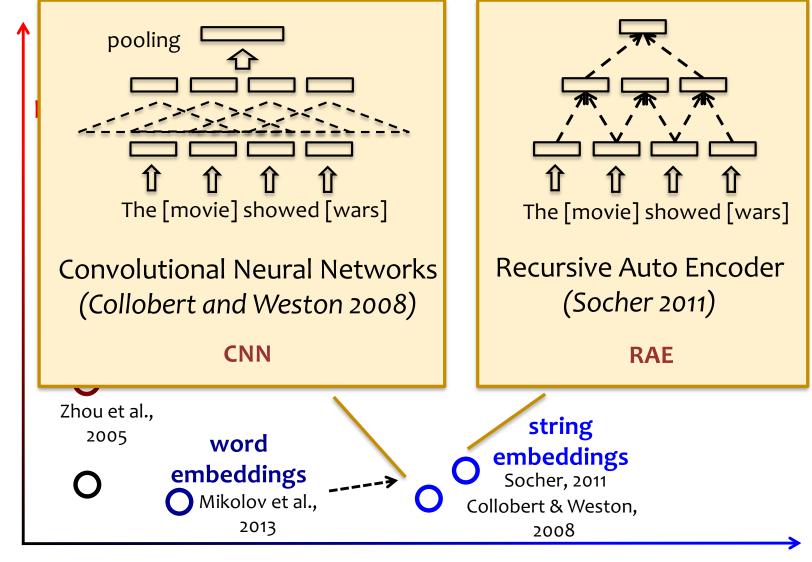


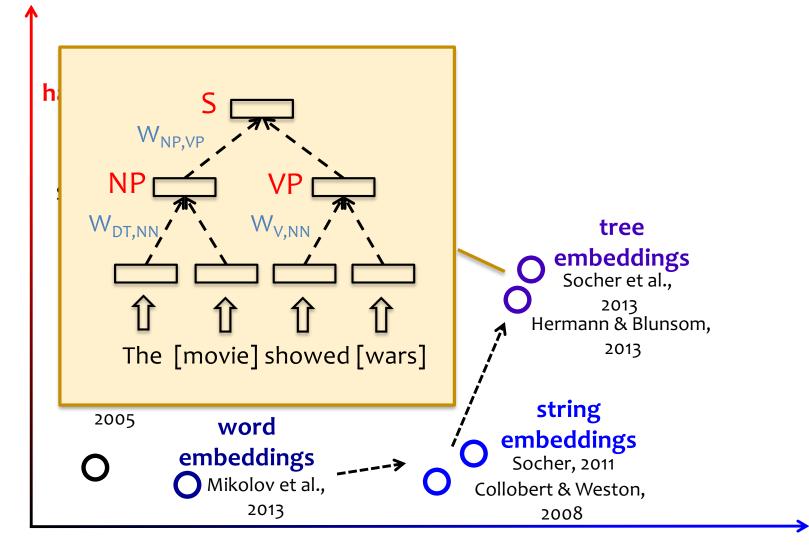
Feature Engineering



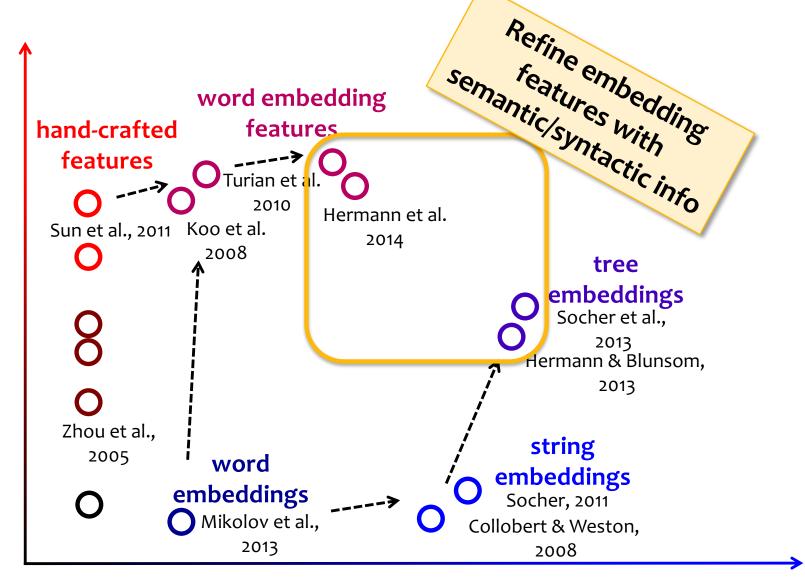
Second word before M1 Bag-of-words in M1 Head word of M1 Other word in between First word after M2 Second word after M2 Bag-of-words in M2 *Head word of M2* Bigrams in between Words on dependency path Country name list Personal relative triggers Personal title list WordNet Tags Heads of chunks in between Path of phrase labels *Combination of entity types* 



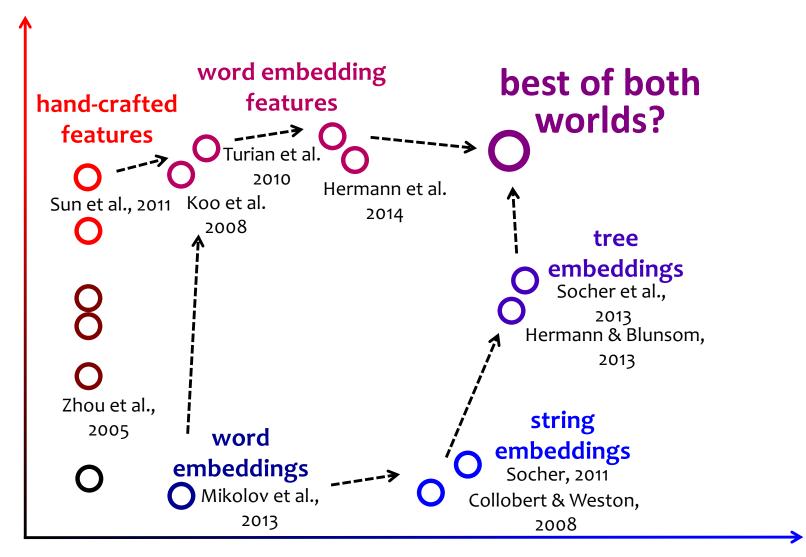




Feature Engineering



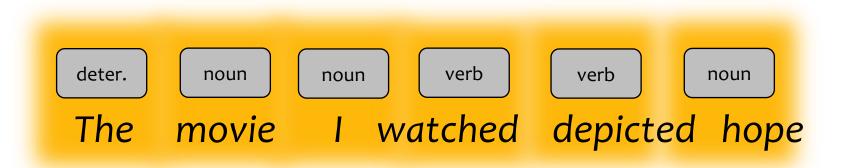
Feature Engineering



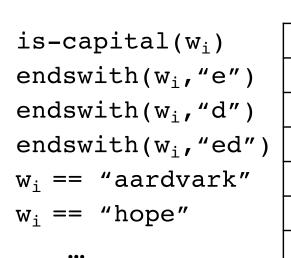
Feature Engineering

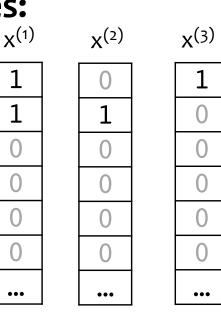
Suppose you build a logistic regression model to predict a part-of-speech (POS) tag for each word in a sentence.

### What features should you use?



#### **Per-word Features:**





1

1

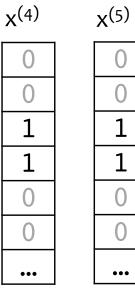
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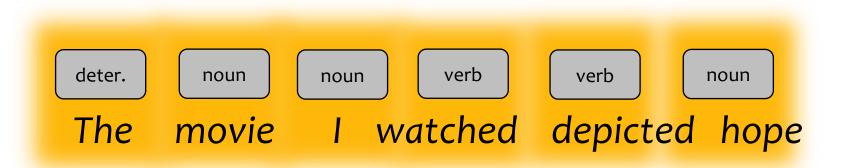
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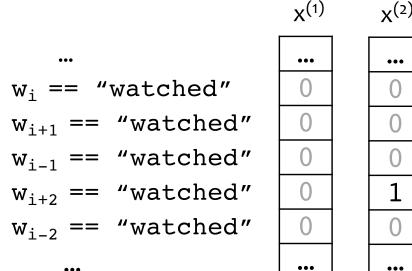
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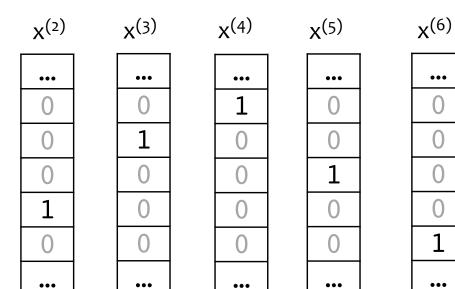
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v(6)



#### **Context Features:**





...

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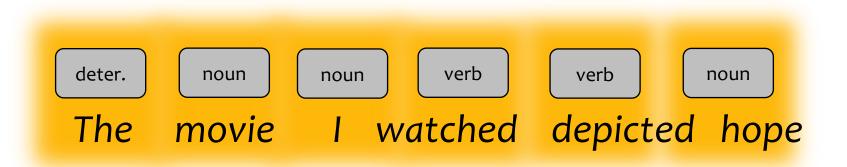
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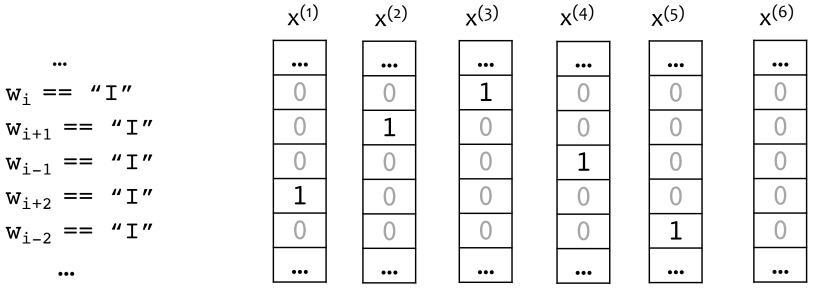
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**Context Features:** 



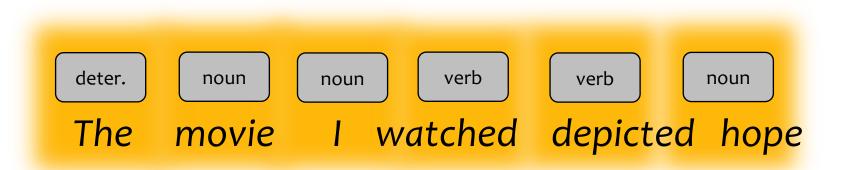
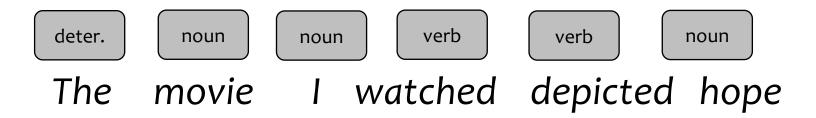
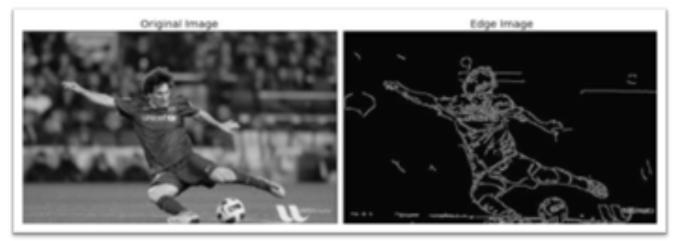


Table 3. Tagging accuracies with different feature templates and other changes on the WSJ 19-21 development set.

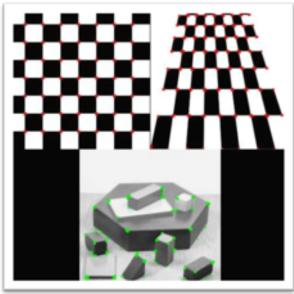
Model	Feature Templates	#	Sent.	Token	Unk.
		Feats	Acc.	Acc.	Acc.
3gramMemm	See text	248,798	52.07%	96.92%	88.99%
NAACL 2003	See text and [1]	460,552	55.31%	97.15%	88.61%
Replication	See text and [1]	460,551	55.62%	97.18%	88.92%
Replication'	+rareFeatureThresh = 5	482,364	55.67%	97.19%	88.96%
5w	$+(t_0, w_{-2}), (t_0, w_2)$	730,178	56.23%	97.20%	89.03%
5wShapes	$+\langle t_0, s_{-1} \rangle, \langle t_0, s_0 \rangle, \langle t_0, s_{+1} \rangle$	731,661	56.52%	97.25%	89.81%
5wShapesDS	+ distributional similarity	737,955	56.79%	97.28%	90.46%



Edge detection (Canny)



#### Corner Detection (Harris)



### Scale Invariant Feature Transform (SIFT)



Figure 3: Model images of planar objects are shown in the oprow. Recognition results below show model outlines and mage keys used for matching.

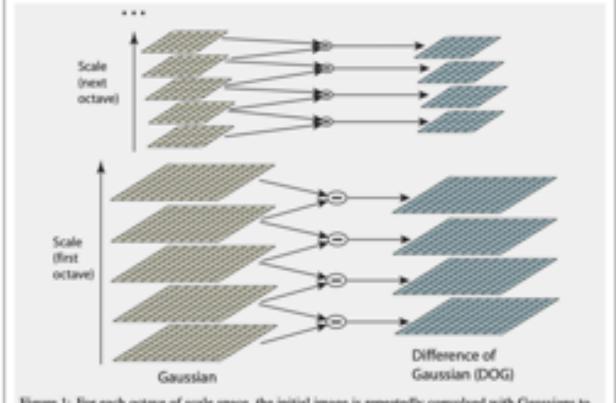


Figure 1: For each octave of scale space, the initial image is repeatedly convolved with Gaussians to produce the set of scale space images shown on the left. Adjacent Gaussian images are subtracted to produce the difference-of-Gaussian images on the right. After each octave, the Gaussian image is down-sampled by a factor of 2, and the process repeated.

### **NON-LINEAR FEATURES**

### Nonlinear Features

- aka. "nonlinear basis functions"
- So far, input was always  $\mathbf{x} = [x_1, \dots, x_M]$ ullet
- **Key Idea:** let input be some function of **x** ullet
  - original input:  $\mathbf{x} \in \mathbb{R}^M$ where M' > M (usually)

– new input: 
$$\mathbf{x}' \in \mathbb{R}^{M'}$$

- define  $\mathbf{x}' = b(\mathbf{x}) = [b_1(\mathbf{x}), b_2(\mathbf{x}), \dots, b_{M'}(\mathbf{x})]$ 

where  $b_i : \mathbb{R}^M \to \mathbb{R}$  is any function

**Examples:** (M = 1)• polynomial

radial basis function

$$b_j(x) = x^j \quad \forall j \in \{1, \dots, J\}$$
$$b_j(x) = \exp\left(\frac{-(x - \mu_j)^2}{2\sigma_j^2}\right)$$
$$b_j(x) = \frac{1}{1 + \exp(-\omega_j x)}$$
$$b_j(x) = \log(x)$$

For a linear model: still a linear function of b(x) even though a nonlinear function of X

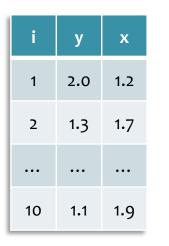
#### **Examples:**

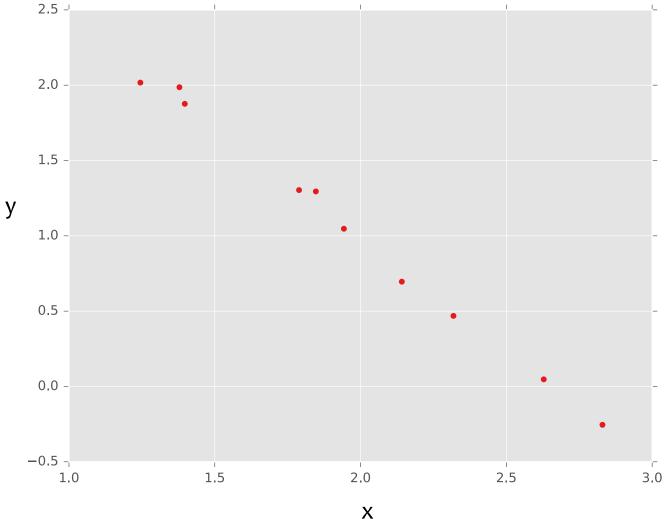
- Perceptron
- Linear regression
- Logistic regression

sigmoid

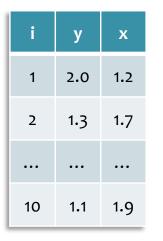
log

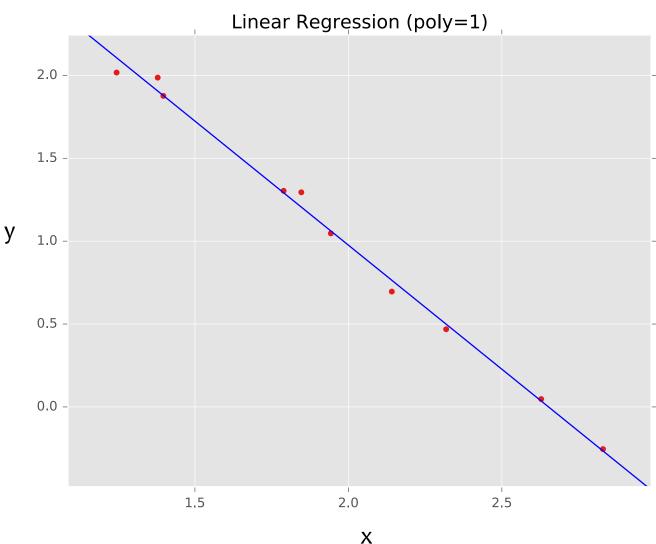
**Goal:** Learn  $y = w^T f(x) + b$ where f(.) is a polynomial basis function





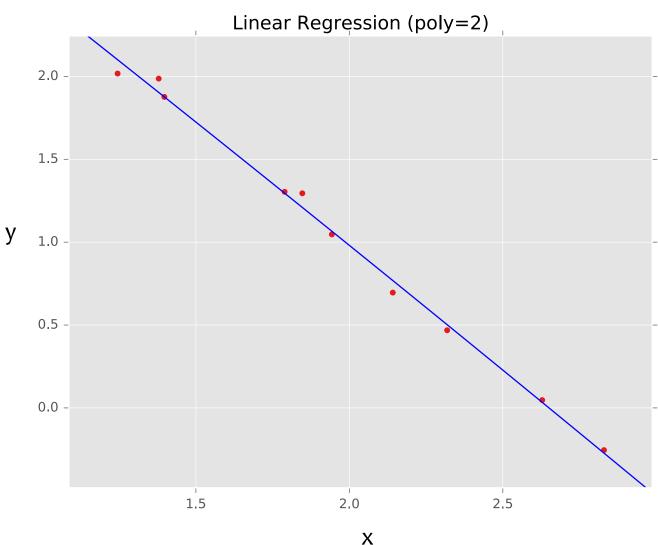
**Goal:** Learn  $y = w^T f(x) + b$  where f(.) is a polynomial basis function





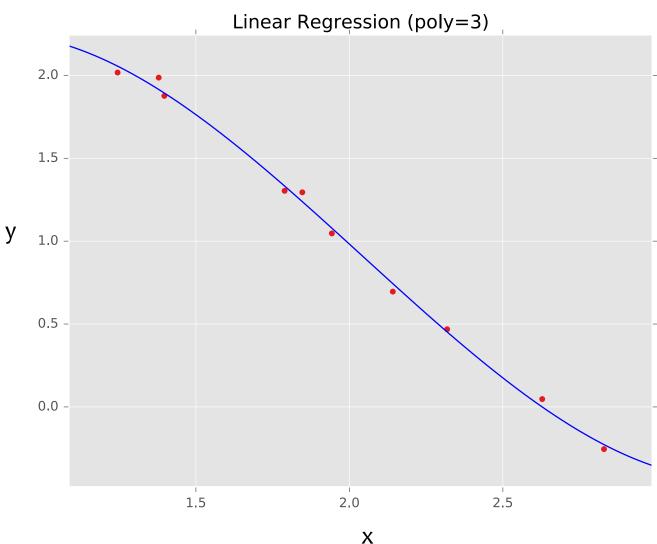
**Goal:** Learn  $y = w^T f(x) + b$  where f(.) is a polynomial basis function

i	у	x	<b>X</b> <sup>2</sup>
1	2.0	1.2	(1.2)2
2	1.3	1.7	(1.7)2
10	1.1	1.9	(1.9)2



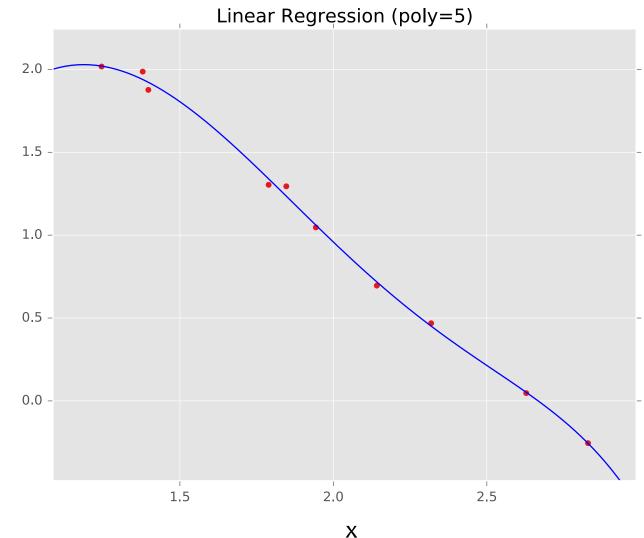
**Goal:** Learn  $y = w^T f(x) + b$  where f(.) is a polynomial basis function

i	у	x	X <sup>2</sup>	Х <sup>3</sup>
1	2.0	1.2	(1.2)2	(1.2)3
2	1.3	1.7	(1.7)2	(1.7) <sup>3</sup>
10	1.1	1.9	(1.9) <sup>2</sup>	(1 <b>.9)</b> <sup>3</sup>



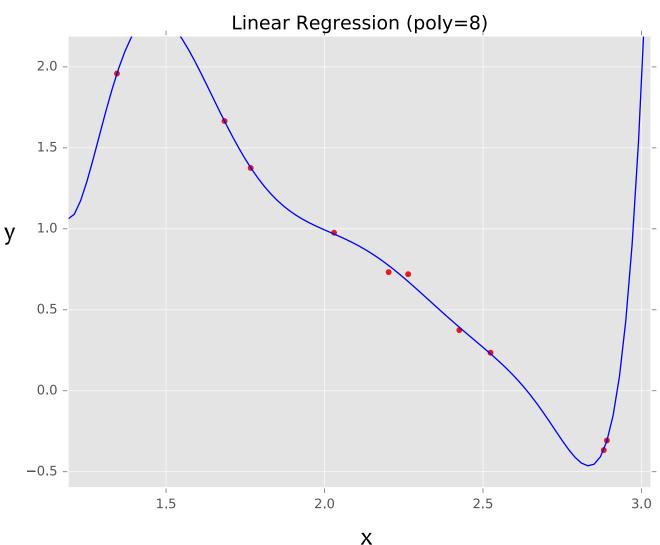
**Goal:** Learn  $y = w^T f(x) + b$  where f(.) is a polynomial basis function

i	у	х	 <b>x</b> <sup>5</sup>	
1	2.0	1.2	 (1.2)5	
2	1.3	1.7	 (1 <b>.</b> 7) <sup>5</sup>	
			 	у
10	1.1	1.9	 (1.9)5	-



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

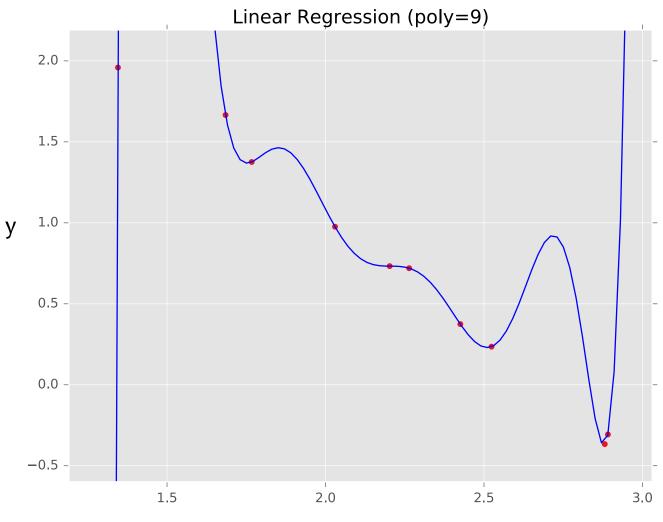
i	у	x	•••	<b>x</b> <sup>8</sup>
1	2.0	1.2		(1.2)8
2	1.3	1.7		(1.7) <sup>8</sup>
10	1.1	1.9		(1.9) <sup>8</sup>



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

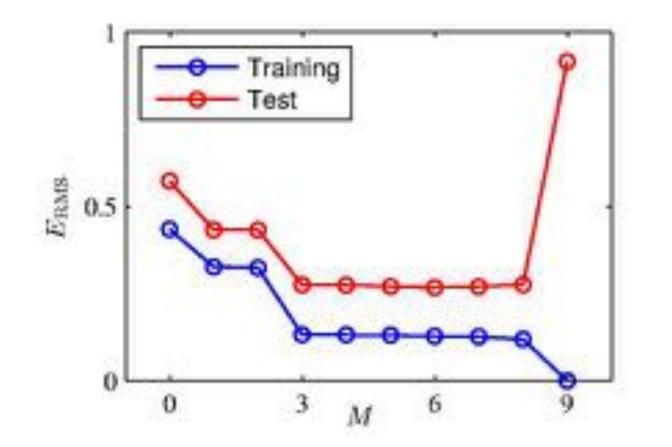
i	у	x	 х <sup>9</sup>
1	2.0	1.2	 (1.2) <sup>9</sup>
2	1.3	1.7	 (1.7) <sup>9</sup>
10	1.1	1.9	 (1.9) <sup>9</sup>

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



Х

# **Over-fitting**



Root-Mean-Square (RMS) Error:  $E_{\text{RMS}} = \sqrt{2E(\mathbf{w}^{\star})/N}$ 

### **Polynomial Coefficients**

	M = 0	M = 1	M=3	M = 9
$ heta_0$	0.19	0.82	0.31	0.35
$ heta_1$		-1.27	7.99	232.37
$ heta_2$			-25.43	-5321.83
$ heta_3$			17.37	48568.31
$ heta_4$				-231639.30
$ heta_5$				640042.26
$ heta_6$				-1061800.52
$ heta_7$				1042400.18
$ heta_8$				-557682.99
$ heta_9$				125201.43

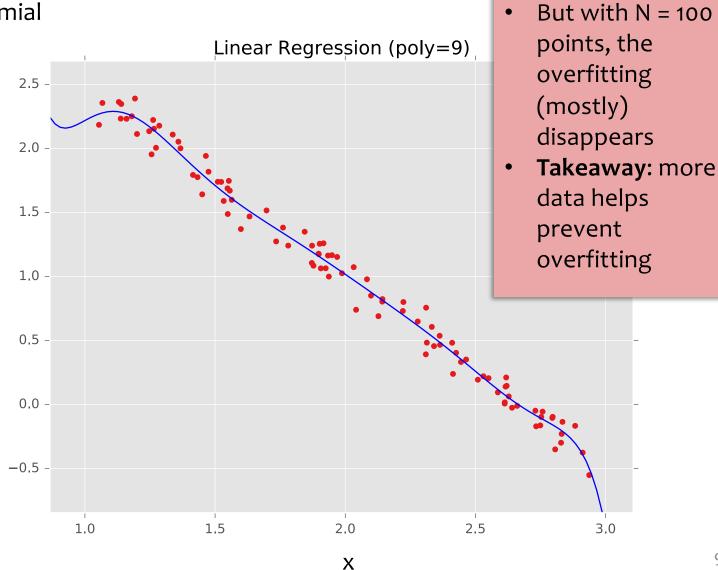
**Goal:** Learn  $y = w^T f(x) + b$ points we overfit! where f(.) is a polynomial But with N = 100• basis function points, the Linear Regression (poly=9) overfitting 2.0 (mostly) **X**<sup>9</sup> X disappears (1.2)<sup>9</sup> 1.2 2.0 ••• Takeaway: more 1 • 1.5 data helps (1.7)<sup>9</sup> 1.7 1.3 ••• 2 prevent 1.0 ••• • • • • • • • • • • • • overfitting V ... (1.9)<sup>9</sup> 1.9 10 1.1 0.5 -0.0 -0.5 1.5 2.0 2.5 3.0

Х

With just N = 10

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

i	у	х	•••	<b>x</b> <sup>9</sup>	
1	2.0	1.2	•••	(1.2) <sup>9</sup>	
2	1.3	1.7	•••	(1.7) <sup>9</sup>	
3	0.1	2.7		(2.7)9	y
4	1.1	1.9	•••	(1.9) <sup>9</sup>	
•••	•••	•••	•••	•••	
			•••		
98	•••	•••			
99					
100	0.9	1.5		(1.5) <sup>9</sup>	



With just N = 10

•

points we overfit!