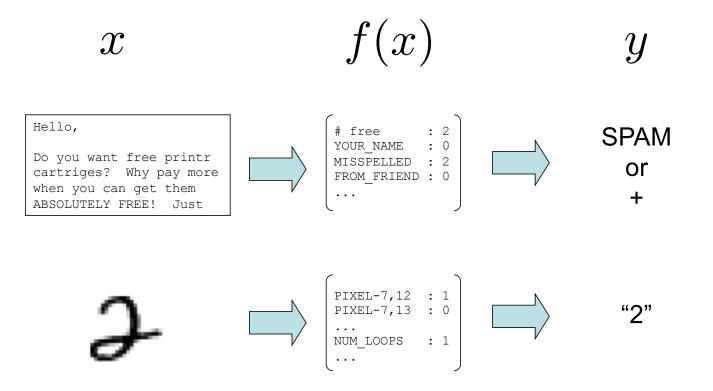
## CS 188: Artificial Intelligence Linear and Logistic Regression

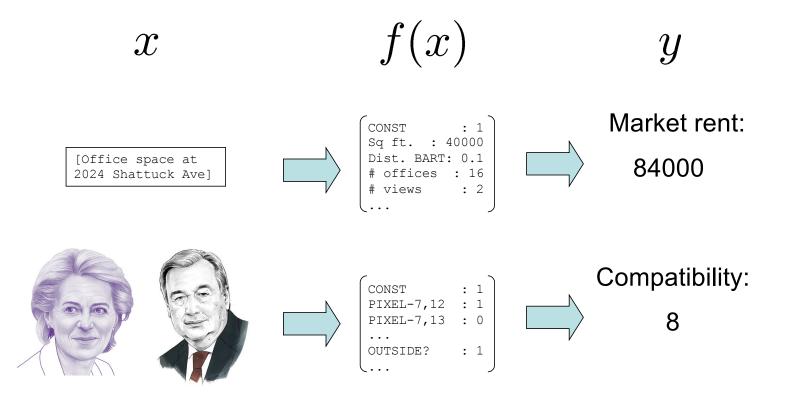
Spring 2024

University of California, Berkeley

## **Classification with Feature Vectors**



## **Regression with Feature Vectors**

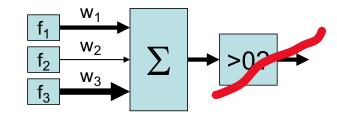


## Linear Classifiers Regression

- Inputs are feature values
- Each feature has a weight
- Sum is the activation prediction

activation 
$$w(x) = \sum_{i} w_i \cdot f_i(x) = w \cdot f(x)$$

If the activation Is:
 Positive, output +1
 Negative, output -1
 Output h<sub>w</sub>



# Weights

Dot product  $w \cdot f$  gives the prediction

w .	$f(x_1)$
CONST : 5000	CONST : 1
Sq ft. : 0.8	Sq ft. : 40000
Dist. BART: 100	Dist. BART: 0.1
# offices : 300	# offices : 16
# views : 1000	# views : 2
w .	$f(x_2)$
CONST : 5000	CONST : 1
Sq ft. : 0.8	Sq ft. : 50000
Dist. BART: 100	Dist. BART: 0.2
# offices : 300	# offices : 4
# views : 1000	# views : 0

Which weight makes the least sense for predicting office rent?

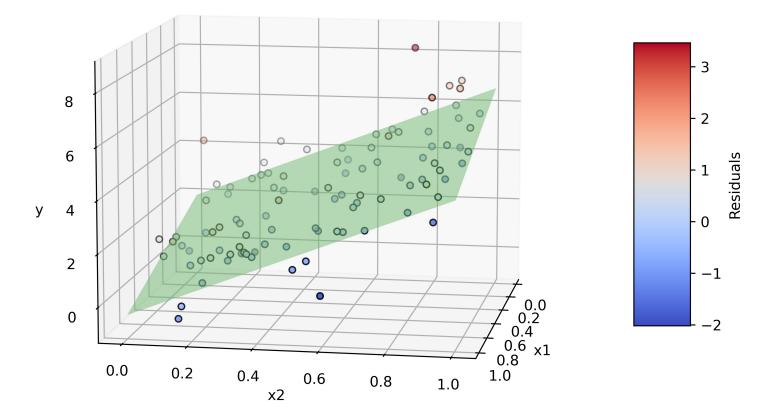
## **Linear Regression**

- Inputs are feature values
- Each feature has a weight
- Sum is the prediction

*Either* make sure one of the features is a constant *or* add this  $w_0$  to the equation (equivalent)

$$h_w(x) = \sum_i w_i \cdot f_i(x) = w \cdot f(x) + W_0$$

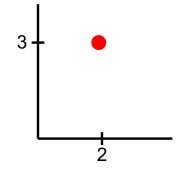
#### Linear Regression with 2d Feature Vector



Code credit: Claude3

#### **Review: Vectors**

• A tuple like (2,3) can be interpreted two different ways:



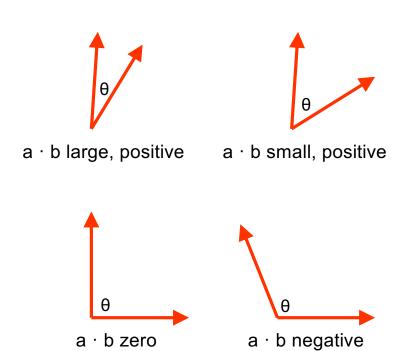
A point on a coordinate grid

2 A **vector** in space. Notice we are not on a coordinate grid.

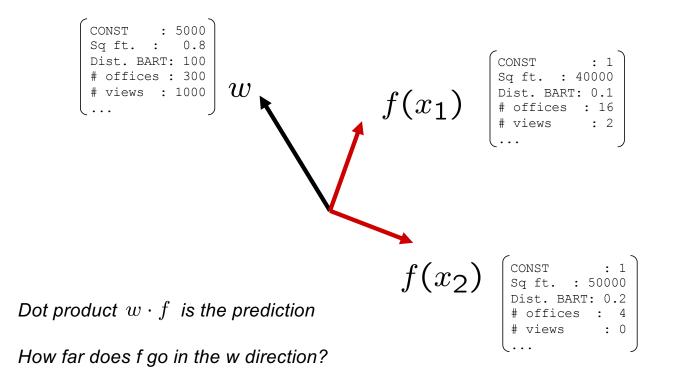
 A tuple with more elements like (2, 7, -3, 6) is a point or vector in higherdimensional space (hard to visualize)

## **Review: Vectors**

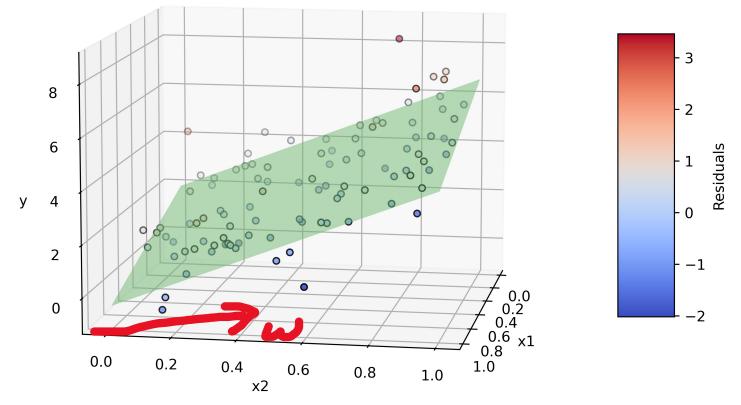
- Definition of dot product:
  - $\mathbf{a} \cdot \mathbf{b} = \Sigma_i \mathbf{a}_i \mathbf{b}_i = |\mathbf{a}| |\mathbf{b}| \cos(\theta)$
  - θ is the angle between the vectors a and b
- Consequences of this definition:
  - Vectors closer together
    - = "similar" vectors
    - = smaller angle  $\theta$  between vectors
    - = larger (more positive) dot product
  - If  $\theta < 90^\circ$ , then dot product is positive
  - If  $\theta = 90^\circ$ , then dot product is zero
  - If θ > 90°, then dot product is negative



## Weights



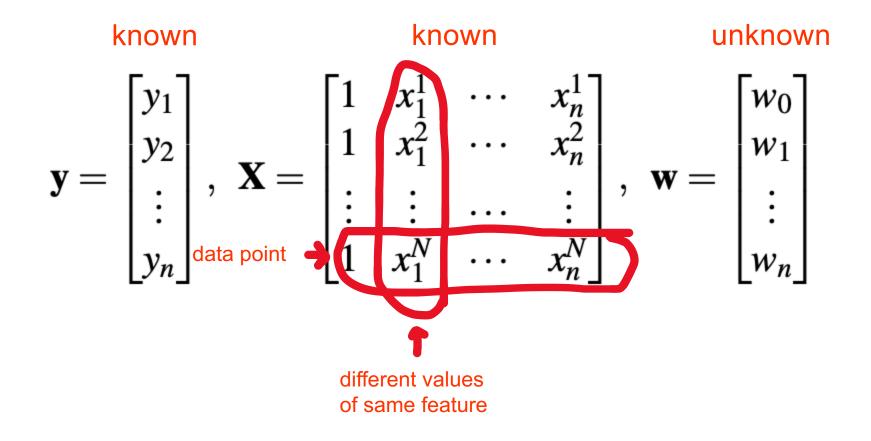
#### Linear Regression with 2d Feature Vector



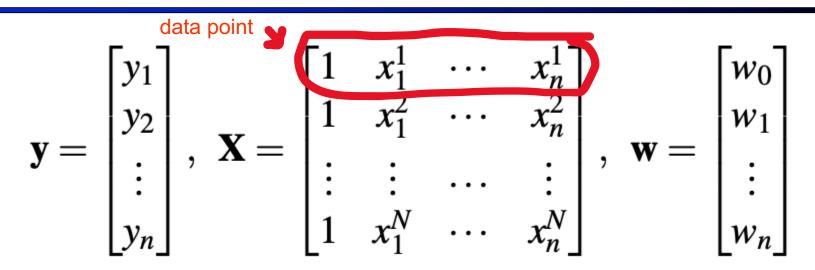
w points in direction where best-fit plane is steepest

Code credit: Claude3

## How to find the weights?



## How to find the weights?



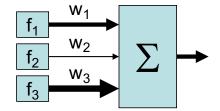
What does matrix product Xw look like?Vector like w and yWhat is the entry in the first row and<br/>first (and only) column of Xw? $w_0 + w_1x_1^1 + ... + w_nx_n^1$ 

We want Xw to look like y

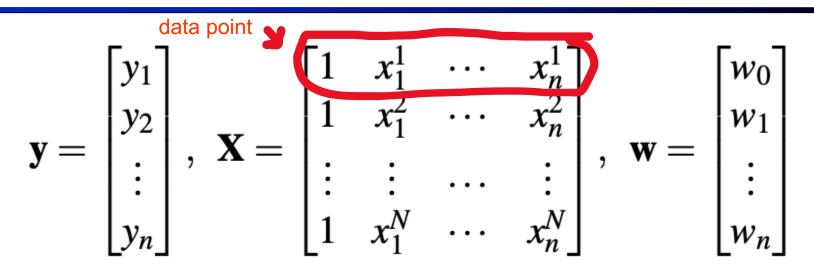
#### **Linear Regression**

- Inputs are feature values
- Each feature has a weight
- Sum is the prediction

$$h_w(x) = \sum_i w_i \cdot f_i(x) = w \cdot f(x)$$



## Premise of linear regression

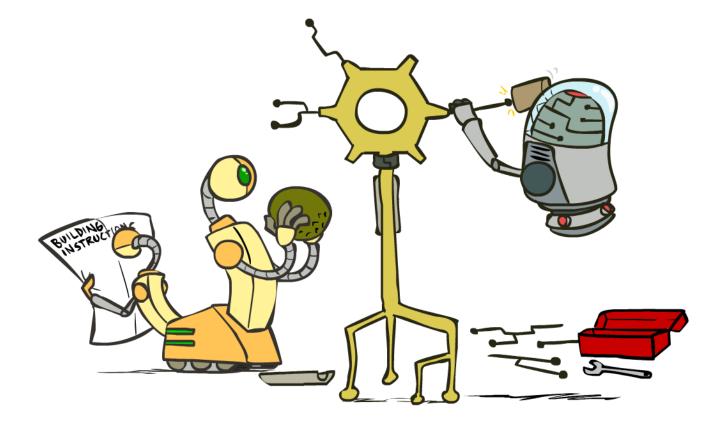


For a proposed weight vector w, its badness is  $|Xw - y|^2 / 2$ |v| is the length of the vector;  $|v|^2 = \Sigma_i v_i^2 = v^T v_i^2$ Loss So badness(w) =  $\Sigma_i (h_w(x^i)w - y_i)^2 / 2$ 

# Solving for w

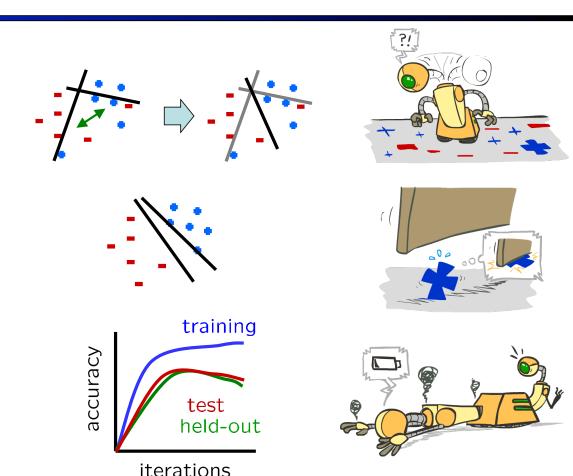
$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \ \mathbf{X} = \begin{bmatrix} \mathbf{1} & \mathbf{x}_1^T & \cdots & \mathbf{x}_n^T \\ 1 & \mathbf{x}_1^T & \cdots & \mathbf{x}_n^T \\ \vdots & \vdots & \cdots & \vdots \\ 1 & \mathbf{x}_1^N & \cdots & \mathbf{x}_n^N \end{bmatrix}, \ \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_n \end{bmatrix} \qquad \text{Find } \operatorname{argmin}_{\mathbf{w}} |\mathbf{X}\mathbf{w} - \mathbf{y}|^2 / 2$$
$$\nabla_{\mathbf{w}} \frac{1}{2} (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w}) = \mathbf{0}$$
$$= \nabla_{\mathbf{w}} \frac{1}{2} (\mathbf{y}^T \mathbf{y} - \mathbf{y}^T \mathbf{X}\mathbf{w} - \mathbf{w}^T \mathbf{X}^T \mathbf{y} + \mathbf{w}^T \mathbf{X}^T \mathbf{X}\mathbf{w})$$
$$= \nabla_{\mathbf{w}} \frac{1}{2} (\mathbf{y}^T \mathbf{y} - 2\mathbf{w}^T \mathbf{X}^T \mathbf{y} + \mathbf{w}^T \mathbf{X}^T \mathbf{x}\mathbf{w}) = -\mathbf{X}^T \mathbf{y} + \mathbf{X}^T \mathbf{X}\mathbf{w}$$
$$\begin{bmatrix} \mathbf{\hat{w}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} \end{bmatrix} \qquad \text{If you ever actually need to do this sort of stuff:}$$
$$\begin{array}{c} \text{https://cs.nyu.edu/~roweis/} \\ \text{notes/matrixid.pdf} \end{array}$$

## Back to Classification: Improving the Perceptron

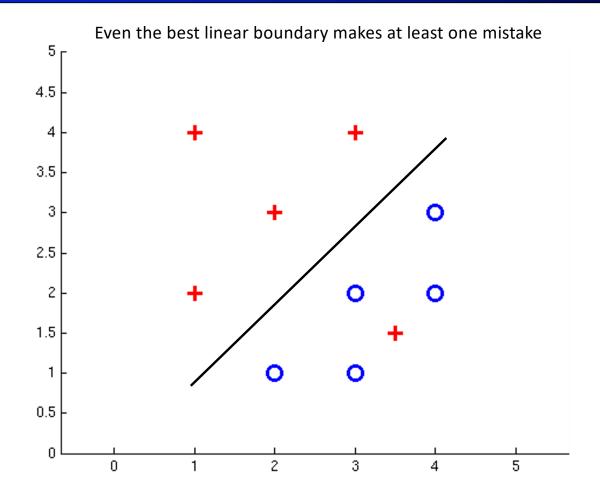


## Problems with the Perceptron

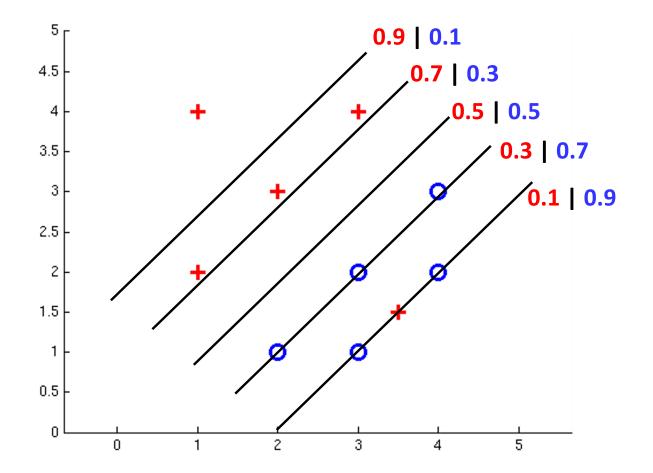
- Noise: if the data isn't separable, weights might thrash
  - Averaging weight vectors over time can help (averaged perceptron)
- Mediocre generalization: finds a "barely" separating solution
- Overtraining: test / held-out accuracy usually rises, then falls
  - Overtraining is a kind of overfitting



## Non-Separable Case: Deterministic Decision



## Non-Separable Case: Probabilistic Decision



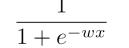
## Perceptrons give deterministic decisions

- Perceptron scoring:  $z = w \cdot f(x)$
- If  $z = w \cdot f(x)$  positive  $\rightarrow$  classifier says: 1.0 probability this is class +1
- If  $z = w \cdot f(x)$  negative  $\rightarrow$  classifier says: 0.0 probability this is class +1
- Step function  $H(z) = \begin{cases} 1 & z > 0 \\ 0 & z \le 0 \end{cases}$   $H(z) = \begin{cases} 1 & z > 0 \\ 0 & z \le 0 \end{cases}$
- z = output of perceptron
   H(z) = probability the class is +1, according to the classifier

## How to get probabilistic decisions?

- Perceptron scoring:  $z = w \cdot f(x)$
- If  $z = w \cdot f(x)$  very positive  $\rightarrow$  probability of class +1 should approach 1.0
- If  $z = w \cdot f(x)$  very negative  $\rightarrow$  probability of class +1 should approach 0.0
- Sigmoid function  $\phi(z) = \frac{1}{1 + e^{-z}}$
- z = output of perceptron
- $\phi(z)$  = probability the class is +1, according to the classifier

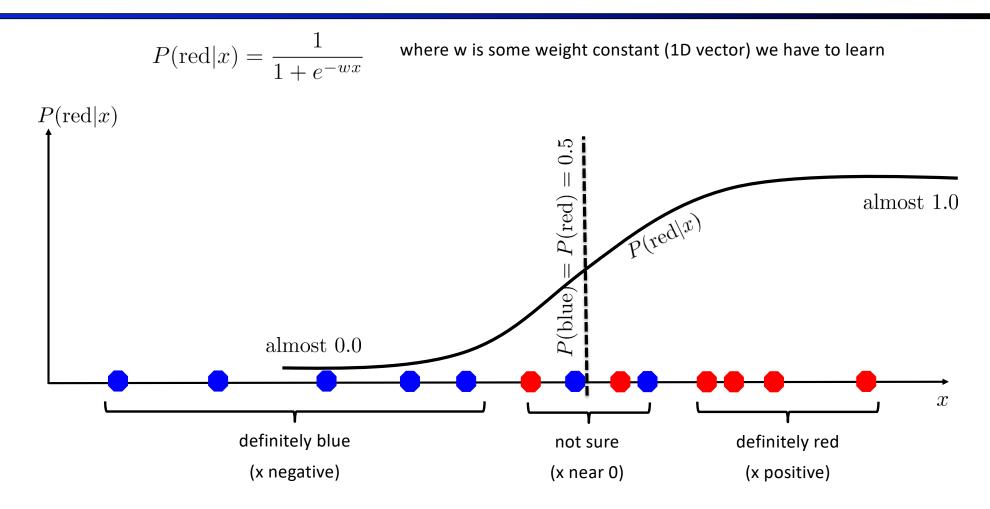
# **Probabilistic Decisions: Example**



 $\frac{1}{1 + e^{-wx}}$  where w is some weight constant (vector) we have to learn, and wx is the dot product of w and x

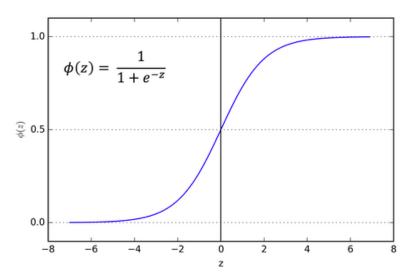
- Suppose w = [-3, 4, 2] and x = [1, 2, 0]
- What label will be selected if we classify deterministically?
  - wx = -3+8+0 = 5
  - 5 is positive, so the classifier guesses the positive label
- What are the probabilities of each label if we classify probabilistically?
  - $1/(1 + e^{-5}) = 0.9933$  probability of positive label
  - 1 0.9933 = 0.0067 probability of negative label

## A 1D Example



# Where does the sigmoid function come from?

- Suppose we have two hypotheses:
  - A: P(heads) = 2/3
  - B: P(heads) = 1/3
- Each heads we see is a "bit" or factor of 2 of evidence for Hypothesis A
- Each tails we see is a "bit" of evidence for B
- If we have n more heads than tails:
  - A is 2<sup>n</sup> times more likely than B
  - $P(A) = 2^n / (1 + 2^n)$
  - = 1 / (1 + 2<sup>-n</sup>)
  - ... but we like e better than 2



Recall maximum likelihood estimation: Choose the w value that maximizes the probability of the observed (training) data

Likelihood = P(training data|w)

$$= \prod_{i} P(\text{training datapoint } i \mid w)$$
$$= \prod_{i} P(\text{point } x^{(i)} \text{ has label } y^{(i)} \mid w)$$
$$= \prod_{i} P(y^{(i)} \mid x^{(i)}; w)$$
Log Likelihood = 
$$\sum_{i} \log P(y^{(i)} \mid x^{(i)}; w)$$

Recall maximum likelihood estimation: Choose the w value that maximizes the probability of the observed (training) data

$$P(\text{point } x^{(i)} \text{ has label } y^{(i)} = +1 \mid w)$$
  
=  $P(y^{(i)} = +1 \mid x^{(i)}; w)$   
=  $\frac{1}{1 + e^{-w \cdot x^{(i)}}}$ 

 $P(\text{point } x^{(i)} \text{ has label } y^{(i)} = -1 \mid w)$ =  $P(y^{(i)} = -1 \mid x^{(i)}; w)$ =  $1 - \frac{1}{1 + e^{-w \cdot x^{(i)}}}$ 

Maximum likelihood estimation:

$$\begin{split} \max_{w} & ll(w) = \max_{w} \quad \sum_{i} \log P(y^{(i)} | x^{(i)}; w) \\ \text{with:} & P(y^{(i)} = +1 | x^{(i)}; w) = \frac{1}{1 + e^{-w \cdot f(x^{(i)})}} \\ & P(y^{(i)} = -1 | x^{(i)}; w) = 1 - \frac{1}{1 + e^{-w \cdot f(x^{(i)})}} \\ \text{That's Logistic Regression} & \text{Loss(w) = -log likelihood(w)} \end{split}$$

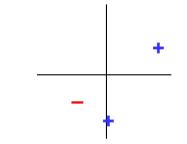
## Logistic Regression Example

- What function are we trying to maximize for this training data?
  - Data point [2, 1] is class +1
  - Data point [0, -2] is class +1
  - Data point [-1, -1] is class -1

$$\max_{w} ll(w) = \max_{w} \sum_{i} \log P(y^{(i)} | x^{(i)}; w)$$
$$P(y^{(i)} = +1 | x^{(i)}; w) = \frac{1}{1 + e^{-w \cdot f(x^{(i)})}}$$
$$P(y^{(i)} = -1 | x^{(i)}; w) = 1 - \frac{1}{1 + e^{-w \cdot f(x^{(i)})}}$$

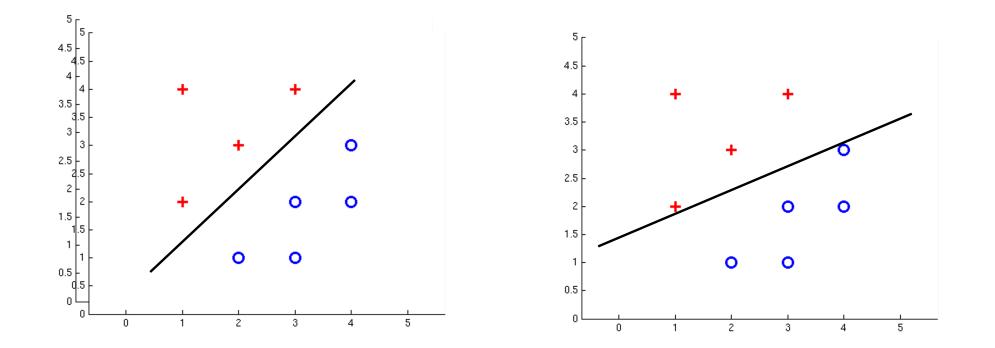
## Logistic Regression Example

- What function are we trying to maximize for this training data?
  - Data point [2, 1] is class +1
  - Data point [0, -2] is class +1
  - Data point [-1, -1] is class -1

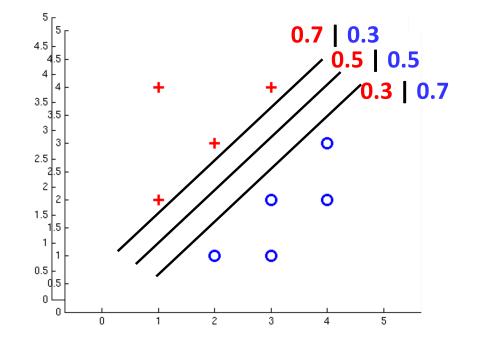


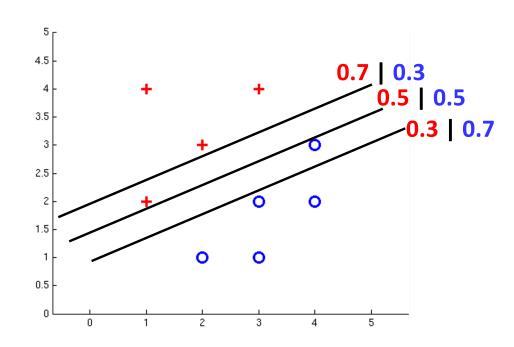
$$\underset{w}{\operatorname{argmax}} \left[ \log \left( \frac{1}{1 + e^{-(2w_1 + w_2)}} \right) + \log \left( \frac{1}{1 + e^{-(-2w_2)}} \right) + \log \left( 1 - \frac{1}{1 + e^{-(-w_1 - w_2)}} \right) \right]$$

#### Separable Case: Deterministic Decision – Many Options

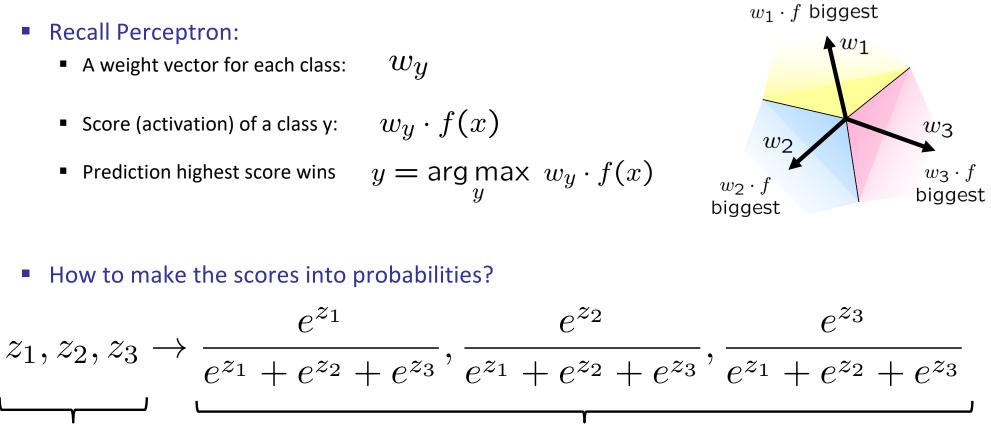


## Separable Case: Probabilistic Decision – Clear Preference





## **Multiclass Logistic Regression**



original activations

softmax activations

## Multi-Class Probabilistic Decisions: Example

$$z_1, z_2, z_3 \to \frac{e^{z_1}}{e^{z_1} + e^{z_2} + e^{z_3}}, \frac{e^{z_2}}{e^{z_1} + e^{z_2} + e^{z_3}}, \frac{e^{z_3}}{e^{z_1} + e^{z_2} + e^{z_3}}, \frac{e^{z_3}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

- Suppose w<sub>1</sub> = [-3, 4, 2], w<sub>2</sub> = [2, 2, 7], w<sub>3</sub> = [0, -1, 0], and x = [1, 2, 0]
- What label will be selected if we classify deterministically?
  - $w_1 \cdot x = 5$ , and  $w_2 \cdot x = 6$ , and  $w_3 \cdot x = -2$
  - w<sub>2</sub>·x has the highest score, so the classifier guesses class 2
- What are the probabilities of each label if we classify probabilistically?
  - Probability of class 1: e<sup>5</sup> / (e<sup>5</sup> + e<sup>6</sup> + e<sup>-2</sup>) = 0.2689
  - Probability of class 2: e<sup>6</sup> / (e<sup>5</sup> + e<sup>6</sup> + e<sup>-2</sup>) = 0.7310
  - Probability of class 3: e<sup>-2</sup> / (e<sup>5</sup> + e<sup>6</sup> + e<sup>-2</sup>) = 0.0002

Recall maximum likelihood estimation: Choose the w value that maximizes the probability of the observed (training) data

Likelihood = P(training data|w)

$$= \prod_{i} P(\text{training datapoint } i \mid w)$$
$$= \prod_{i} P(\text{point } x^{(i)} \text{ has label } y^{(i)} \mid w)$$
$$= \prod_{i} P(y^{(i)} \mid x^{(i)}; w)$$
Log Likelihood = 
$$\sum_{i} \log P(y^{(i)} \mid x^{(i)}; w)$$

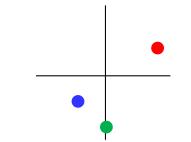
Maximum likelihood estimation:

$$\max_{w} \quad ll(w) = \max_{w} \quad \sum_{i} \log P(y^{(i)} | x^{(i)}; w)$$
with: 
$$P(y^{(i)} | x^{(i)}; w) = \frac{e^{w_{y^{(i)}} \cdot f(x^{(i)})}}{\sum_{y} e^{w_{y} \cdot f(x^{(i)})}}$$

#### = Multi-Class Logistic Regression

## Multi-Class Logistic Regression Example

- What function are we trying to maximize for this training data?
  - Data point [2, 1] is class Red
  - Data point [0, -2] is class Green
  - Data point [-1, -1] is class Blue

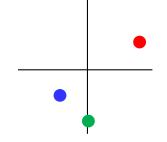


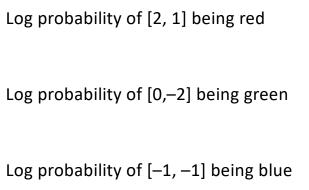
$$\max_{w} ll(w) = \max_{w} \sum_{i} \log P(y^{(i)} | x^{(i)}; w)$$
$$P(y^{(i)} | x^{(i)}; w) = \frac{e^{w_{y^{(i)}} \cdot f(x^{(i)})}}{\sum_{y} e^{w_{y} \cdot f(x^{(i)})}}$$

## Multi-Class Logistic Regression Example

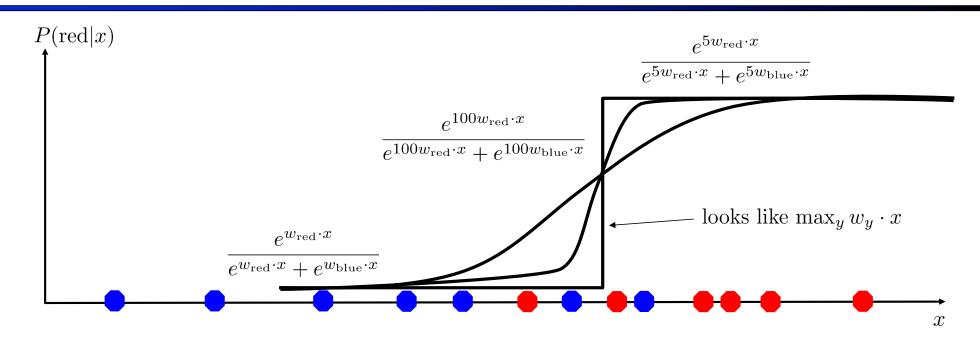
- What function are we trying to maximize for this training data?
  - Data point [2, 1] is class Red
  - Data point [0, -2] is class Green
  - Data point [-1, -1] is class Blue

$$\operatorname{argmax}_{w} \left[ \begin{array}{c} \log\left(\frac{e^{2w_{1}+w_{2}}}{e^{2w_{1}+w_{2}}+e^{2w_{1}+w_{2}}+e^{2w_{1}+w_{2}}}\right) \\ +\log\left(\frac{e^{-2w_{2}}}{e^{-2w_{2}}+e^{-2w_{2}}+e^{-2w_{2}}}\right) \\ +\log\left(\frac{e^{-w_{1}-w_{2}}}{e^{-w_{1}-w_{2}}+e^{-w_{1}-w_{2}}+e^{-w_{1}-w_{2}}}\right) \end{array} \right]$$





## Softmax with Different Bases



$$P(\operatorname{red}|x) = \frac{e^{w_{\operatorname{red}} \cdot x}}{e^{w_{\operatorname{red}} \cdot x} + e^{w_{\operatorname{blue}} \cdot x}}$$

## Softmax and Sigmoid

- Binary perceptron is a special case of multi-class perceptron
  - Multi-class: Compute  $w_y \cdot f(x)$  for each class y, pick class with the highest activation
  - Binary case:
     Let the weight vector of +1 be w (which we learn).
     Let the weight vector of -1 always be 0 (constant).
  - Binary classification as a multi-class problem: Activation of negative class is always 0.
     If w · f is positive, then activation of +1 (w · f) is higher than -1 (0).
     If w · f is negative, then activation of -1 (0) is higher than +1 (w · f).

$$\begin{array}{ll} \text{Softmax} & \text{Sigmoid} \\ P(\operatorname{red}|x) = \frac{e^{w_{\operatorname{red}} \cdot x}}{e^{w_{\operatorname{red}} \cdot x} + e^{w_{\operatorname{blue}} \cdot x}} & \text{with } \mathsf{w}_{\operatorname{red}} = \mathsf{0} \text{ becomes:} & P(\operatorname{red}|x) = \frac{1}{1 + e^{-wx}} \end{array}$$

## Next Up

#### Optimization

• i.e., how do we solve:

$$\max_{w} \ ll(w) = \max_{w} \ \sum_{i} \log P(y^{(i)} | x^{(i)}; w)$$

# CS 188: Artificial Intelligence Optimization

Spring 2024 --- University of California, Berkeley

[These slides were created by Dan Klein and Pieter Abbeel for CS188 Intro to AI at UC Berkeley. All CS188 materials are available at http://ai.berkeley.edu.]

## **Review: Derivatives and Gradients**

• What is the derivative of the function  $g(x) = x^2 + 3$ ?

$$\frac{dg}{dx} = 2x$$

What is the derivative of g(x) at x=5?

$$\frac{dg}{dx}\Big|_{x=5} = 10$$

## **Review:** Derivatives and Gradients

- What is the gradient of the function  $g(x, y) = x^2 y$  ?
  - Recall: Gradient is a vector of partial derivatives with respect to each variable

$$\nabla g = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \\ \frac{\partial f}{\partial y} \end{bmatrix} = \begin{bmatrix} 2xy \\ \\ x^2 \end{bmatrix}$$

What is the derivative of g(x, y) at x=0.5, y=0.5?

$$\nabla g|_{x=0.5,y=0.5} = \begin{bmatrix} 2(0.5)(0.5)\\ (0.5^2) \end{bmatrix} = \begin{bmatrix} 0.5\\ 0.25 \end{bmatrix}$$

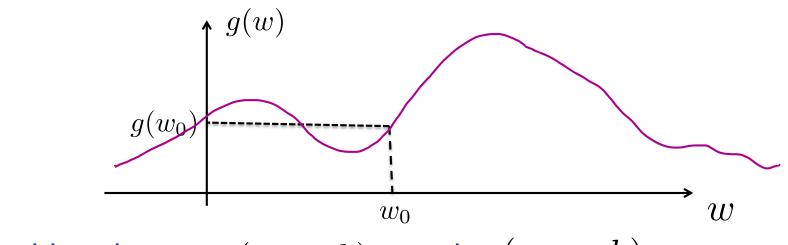
# Hill Climbing

- Recall from local search: simple, general idea
  - Start wherever
  - Repeat: move to the best neighboring state
  - If no neighbors better than current, quit



- What's particularly tricky when hill-climbing for multiclass logistic regression?
  - Optimization over a continuous space
    - Infinitely many neighbors!
    - How to do this efficiently?

## **1-D Optimization**



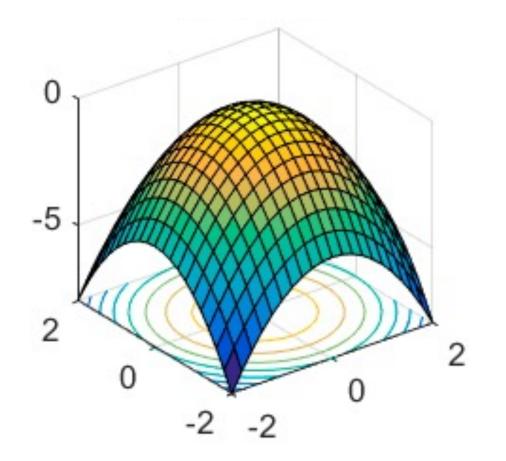
• Could evaluate  $g(w_0 + h)$  and  $g(w_0 - h)$ 

- Then step in best direction
- Or, evaluate derivative:

$$\frac{\partial g(w_0)}{\partial w} = \lim_{h \to 0} \frac{g(w_0 + h) - g(w_0 - h)}{2h}$$

Tells which direction to step into

# 2-D Optimization



Source: offconvex.org

## **Gradient Ascent**

- Perform update in uphill direction for each coordinate
- The steeper the slope (i.e. the higher the derivative) the bigger the step for that coordinate
- E.g., consider:  $g(w_1, w_2)$ 
  - Updates:

$$w_1 \leftarrow w_1 + \alpha * \frac{\partial g}{\partial w_1}(w_1, w_2)$$
$$w_2 \leftarrow w_2 + \alpha * \frac{\partial g}{\partial w_2}(w_1, w_2)$$

Updates in vector notation:

$$w \leftarrow w + \alpha * \nabla_w g(w)$$

with: 
$$\nabla_w g(w) = \begin{bmatrix} \frac{\partial g}{\partial w_1}(w) \\ \frac{\partial g}{\partial w_2}(w) \end{bmatrix}$$
 = gradient

## **Gradient Ascent**

- Idea:
  - Start somewhere
  - Repeat: Take a step in the gradient direction

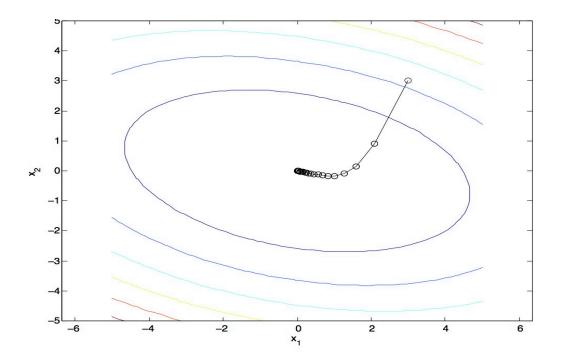


Figure source: Mathworks

## What is the Steepest Direction?\*

$$\max_{\Delta:\Delta_1^2 + \Delta_2^2 \le \varepsilon} g(w + \Delta)$$



• First-Order Taylor Expansion:

$$g(w + \Delta) \approx g(w) + \frac{\partial g}{\partial w_1} \Delta_1 + \frac{\partial g}{\partial w_2} \Delta_2$$

Steepest Descent Direction:

$$\max_{\Delta:\Delta_1^2 + \Delta_2^2 \le \varepsilon} g(w) + \frac{\partial g}{\partial w_1} \Delta_1 + \frac{\partial g}{\partial w_2} \Delta_2$$

• Note:  $\max_{\Delta: \|\Delta\| \le \varepsilon} \Delta^{\top} a \rightarrow \Delta =$ 

$$\Delta = \varepsilon \frac{a}{\|a\|}$$

• Hence, solution:  $\Delta = \varepsilon \frac{\nabla g}{\|\nabla g\|}$ 

**Gradient direction = steepest direction** 

 $\nabla g = \begin{bmatrix} \frac{\partial g}{\partial w_1} \\ \frac{\partial g}{\partial w_2} \end{bmatrix}$ 

## Gradient in n dimensions

$$\nabla g = \begin{bmatrix} \frac{\partial g}{\partial w_1} \\ \frac{\partial g}{\partial w_2} \\ \dots \\ \frac{\partial g}{\partial w_n} \end{bmatrix}$$

## **Optimization Procedure: Gradient Ascent**

```
• init w
• for iter = 1, 2, ...
w \leftarrow w + \alpha * \nabla g(w)
```

- *α*: learning rate --- tweaking parameter that needs to be chosen carefully
- How? Try multiple choices
  - Crude rule of thumb: update changes *W* about 0.1 1 %

## What was the point again?

We want to set w to maximize the log likelihood that logistic regression assigns to the data

$$\max_{w} ll(w) = \max_{w} \sum_{i} \log P(y^{(i)} | x^{(i)}; w)$$
$$P(y^{(i)} = +1 | x^{(i)}; w) = \frac{1}{1 + e^{-w \cdot f(x^{(i)})}}$$
$$P(y^{(i)} = -1 | x^{(i)}; w) = 1 - \frac{1}{1 + e^{-w \cdot f(x^{(i)})}}$$

with:

So we (repeatedly) calculate  $\nabla_w II(w)$  and then use that do gradient ascent

## Batch Gradient Ascent on the Log Likelihood Objective

$$\max_{w} ll(w) = \max_{w} \sum_{i} \log P(y^{(i)} | x^{(i)}; w)$$

• init 
$$w$$
  
• for iter = 1, 2, ...  
 $w \leftarrow w + \alpha * \sum_{i} \nabla \log P(y^{(i)} | x^{(i)}; w)$ 

### Stochastic Gradient Ascent on the Log Likelihood Objective

$$\max_{w} ll(w) = \max_{w} \sum_{i} \log P(y^{(i)}|x^{(i)};w)$$

**Observation:** once gradient on one training example has been computed, might as well incorporate before computing next one

• init w• for iter = 1, 2, ... • pick random j  $w \leftarrow w + \alpha * \nabla \log P(y^{(j)} | x^{(j)}; w)$ 

#### Mini-Batch Gradient Ascent on the Log Likelihood Objective

$$\max_{w} ll(w) = \max_{w} \sum_{i} \log P(y^{(i)}|x^{(i)};w)$$

**Observation:** gradient over small set of training examples (=mini-batch) can be computed in parallel, might as well do that instead of a single one

• init w• for iter = 1, 2, ... • pick random subset of training examples J  $w \leftarrow w + \alpha * \sum_{j \in J} \nabla \log P(y^{(j)} | x^{(j)}; w)$