## CS 188: Artificial Intelligence

 Perceptrons, Linear/Logistic Regression

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(Slides adapted from Pieter Abbeel, Dan Klein, Anca Dragan, Stuart Russell and Dawn Song)

## Supervised Learning



Regression
learning a function with real-valued output value


Classification
learning a function with discrete output value

## Linear Regression



Model: Linear functions

## Linear Regression

$(x, y), x$ : house size, $y$ : house price


Berkeley house prices, 2009

## Linear regression $=$ fitting a straight line $/$ hyperplane



Prediction: $h_{w}(x)=w_{0}+w_{1} x$


House size in square feet
Berkeley house prices, 2009

## Prediction error

Error on one instance: $\mathrm{y}-\mathrm{h}_{\mathrm{w}}(\mathrm{x})$


## Find w

- Define loss function
- Find $\mathrm{w}^{*}$ to minimize loss function


## Least squares: Minimizing squared error

- L2 loss function: sum of squared errors over all examples
- Loss = $\qquad$
- We want the weights $\mathrm{w}^{*}$ that minimize loss
- At $\mathrm{w}^{*}$ the derivatives of loss w.r.t. each weight are zero:
- $\partial$ Loss $/ \partial \mathrm{w}_{0}=$ $\qquad$
- $\partial$ Loss $/ \partial w_{1}=$ $\qquad$
- Exact solutions for N examples:
- $w_{1}=\left[N \sum_{j} x_{j} y_{j}-\left(\sum_{j} x_{j}\right)\left(\sum_{j} y_{j}\right)\right] /\left[N \sum_{j} x_{j}^{2}-\left(\sum_{j} x_{j}\right)^{2}\right]$ and $w_{0}=\frac{1}{N}\left[\sum_{j} y_{j}-w_{1} \sum_{j} x_{j}\right]$
- For the general case where $x$ is an $n$-dimensional vector
- X is the data matrix (all the data, one example per row); y is the column of labels
- $\mathbf{w}^{*}=\left(\mathbf{X}^{\mathrm{T}} \mathbf{X}\right)^{-1} \mathbf{X}^{\mathrm{T}} \mathbf{y}$


## Least squares: Minimizing squared error

- L2 loss function: sum of squared errors over all examples
- Loss $=\Sigma_{\mathrm{j}}\left(\mathrm{y}_{\mathrm{j}}-\mathrm{h}_{\mathrm{w}}\left(\mathrm{x}_{\mathrm{j}}\right)\right)^{2}=\Sigma_{\mathrm{j}}\left(\mathrm{y}_{\mathrm{j}}-\left(\mathrm{w}_{0}+\mathrm{w}_{1} \mathrm{x}_{\mathrm{j}}\right)\right)^{2}$
- We want the weights $\mathrm{w}^{*}$ that minimize loss
- At $w^{*}$ the derivatives of loss w.r.t. each weight are zero:
- $\partial$ Loss $/ \partial \mathrm{w}_{0}=-2 \Sigma_{\mathrm{j}}\left(\mathrm{y}_{\mathrm{j}}-\left(\mathrm{w}_{0}+\mathrm{w}_{1} \mathrm{x}_{\mathrm{j}}\right)\right)=0$
- $\partial$ Loss $/ \partial \mathrm{w}_{1}=-2 \Sigma_{\mathrm{j}}\left(\mathrm{y}_{\mathrm{j}}-\left(\mathrm{w}_{0}+\mathrm{w}_{1} \mathrm{x}_{\mathrm{j}}\right)\right) \mathrm{x}_{\mathrm{j}}=0$
- Exact solutions for N examples:
- $w_{1}=\left[N \sum_{j} x_{j} y_{j}-\left(\sum_{j} x_{j}\right)\left(\sum_{j} y_{j}\right)\right] /\left[N \sum_{j} x_{j}^{2}-\left(\sum_{j} x_{j}\right)^{2}\right]$ and $w_{0}=\frac{1}{N}\left[\sum_{j} y_{j}-w_{1} \sum_{j} x_{j}\right]$
- For the general case where $x$ is an $n$-dimensional vector
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## Regression vs Classification

- Linear regression when output is binary, $y \in\{-1,1\}$
- $h_{w}(x)=w_{0}+w_{1} x$
- Linear classification

- Used with discrete output values
- Threshold a linear function
- $h_{w}(x)=1$, if $w_{0}+w_{1} x \geq 0$
- $h_{w}(x)=-1$, if $w_{0}+w_{1} x<0$



## Linear Classifiers



## Feature Vectors

$$
x
$$

$$
f(x)
$$

$y$

| Hello, |
| :--- |
| Do you want free printr |
| cartriges? Why pay more |
| when you can get them |
| ABSOLUTELY FREE! Just |



SPAM
or
$+$

 "2"

## Linear Classifiers

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


$$
\operatorname{activation}_{w}(x)=\sum_{i} w_{i} \cdot f_{i}(x)=w \cdot f(x)
$$

- If the activation is:
- Positive, output +1
- Negative, output-1



## Weights

- Binary case: compare features to a weight vector
- Learning: figure out the weight vector from examples




## Binary Decision Rule

- In the space of feature vectors
- Examples are points
- Any weight vector is a hyperplane
- One side corresponds to $Y=+1$

- Other corresponds to $\mathrm{Y}=-1$
$w$

| BIAS | $:$ | -3 |
| :--- | :--- | ---: |
| free | $:$ | 4 |
| money | $:$ | 2 |
| $\cdots$ |  |  |



## Binary Decision Rule

- In the space of feature vectors
- Examples are points
- Any weight vector is a hyperplane
- One side corresponds to $Y=+1$

- Other corresponds to $Y=-1$
$w$

| BIAS | $:$ | -3 |
| :--- | :--- | ---: |
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| $\cdots$ |  |  |



Weight Updates


## Learning: Binary Perceptron

- Start with weights $=0$
- For each training instance:
- Classify with current weights

- If correct (i.e., $\mathrm{y}=\mathrm{y}^{*}$ ), no change!

- If wrong: adjust the weight vector



## Learning: Binary Perceptron

- Start with weights $=0$
- For each training instance:
- Classify with current weights

$$
y= \begin{cases}+1 & \text { if } w \cdot f(x) \geq 0 \\ -1 & \text { if } w \cdot f(x)<0\end{cases}
$$

- If correct (i.e., $\mathrm{y}=\mathrm{y}^{*}$ ), no change!
- If wrong: adjust the weight vector by adding or subtracting the feature vector. Subtract if $\mathrm{y}^{*}$ is -1 .

$$
w=w+y^{*} \cdot f
$$



$$
\begin{aligned}
& \text { Before: } w f \\
& \text { After: } w f+y^{\star} f f \\
& f f>=0
\end{aligned}
$$

## Examples: Perceptron

- Separable Case



## Multiclass Decision Rule

- If we have multiple classes:
- A weight vector for each class:

$$
w_{y}
$$



- Score (activation) of a class y:

$$
w_{y} \cdot f(x)
$$

- Prediction highest score wins

$$
y=\arg \max _{y} w_{y} \cdot f(x)
$$



## Learning: Multiclass Perceptron

- Start with all weights $=0$
- Pick up training examples one by one
- Predict with current weights

$$
y=\arg \max _{y} w_{y} \cdot f(x)
$$

- If correct, no change!
- If wrong: lower score of wrong answer, raise score of right answer

$$
\begin{aligned}
& w_{y}=w_{y}-f(x) \\
& w_{y^{*}}=w_{y^{*}}+f(x)
\end{aligned}
$$

## Example: Multiclass Perceptron

"win the vote"
[1 100111$]$
"win the election" [11001]
"win the game" [11101]


## Properties of Perceptrons

- Separability: true if some parameters get the training set perfectly correct
- Convergence: if the training is separable, perceptron will eventually converge (binary case)



## 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

iterations



## Improving the Perceptron



## Non-Separable Case: Deterministic Decision

Even the best linear boundary makes at least one mistake


Non-Separable Case: Probabilistic Decision


## How to get probabilistic decisions?

- Perceptron scoring: $z=w \cdot f(x)$
- If $\quad z=w \cdot f(x) \quad$ very positive $\rightarrow$ want probability going to 1
- If $z=w \cdot f(x) \quad$ very negative $\rightarrow$ want probability going to 0
- Sigmoid function

$$
\phi(z)=\frac{1}{1+e^{-z}}
$$



## A 1D Example



## The Soft Max



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

## Best w?

- Maximum likelihood estimation:

$$
\max _{w} l l(w)=\max _{w} \sum_{i} \log P\left(y^{(i)} \mid x^{(i)} ; w\right)
$$

with:

$$
\begin{aligned}
& P\left(y^{(i)}=+1 \mid x^{(i)} ; w\right)=\frac{1}{1+e^{-w \cdot f\left(x^{(i)}\right)}} \\
& P\left(y^{(i)}=-1 \mid x^{(i)} ; w\right)=1-\frac{1}{1+e^{-w \cdot f\left(x^{(i)}\right)}}
\end{aligned}
$$

= Logistic Regression

## Separable Case: Deterministic Decision - Many Options




## Separable Case: Probabilistic Decision - Clear Preference




## Multiclass Logistic Regression

- Recall Perceptron:
- A weight vector for each class: $w_{y}$
- Score (activation) of a class y: $w_{y} \cdot f(x)$
- Prediction highest score wins $y=\arg \underset{y}{\max } w_{y} \cdot f(x)$

- How to make the scores into probabilities?

original activations
softmax activations


## Best w?

- Maximum likelihood estimation:

$$
\begin{gathered}
\max _{w} l l(w)=\max _{w} \sum_{i} \log P\left(y^{(i)} \mid x^{(i)} ; w\right) \\
P\left(y^{(i)} \mid x^{(i)} ; w\right)=\frac{e^{w_{y}(i) \cdot f\left(x^{(i)}\right)}}{\sum_{y} e^{w_{y} \cdot f\left(x^{(i)}\right)}}
\end{gathered}
$$

## Optimization

## Optimization

i.e., how do we solve:

$$
\max _{w} l l(w)=\max _{w} \sum_{i} \log P\left(y^{(i)} \mid x^{(i)} ; w\right)
$$

## Hill Climbing

Recall from CSPs lecture: 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 $g\left(w_{0}+h\right)$ and $g\left(w_{0}-h\right)$
Then step in best direction
Or, evaluate derivative: $\frac{\partial g\left(w_{0}\right)}{\partial w}=\lim _{h \rightarrow 0} \frac{g\left(w_{0}+h\right)-g\left(w_{0}-h\right)}{2 h}$
Tells which direction to step into

## 2-D Optimization



## 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: $g\left(w_{1}, w_{2}\right)$

Updates:

$$
\begin{aligned}
& w_{1} \leftarrow w_{1}+\alpha * \frac{\partial g}{\partial w_{1}}\left(w_{1}, w_{2}\right) \\
& w_{2} \leftarrow w_{2}+\alpha * \frac{\partial g}{\partial w_{2}}\left(w_{1}, w_{2}\right)
\end{aligned}
$$

- Updates in vector notation:

$$
w \leftarrow w+\alpha * \nabla_{w} g(w)
$$

with: $\nabla_{w} g(w)=\left[\begin{array}{l}\frac{\partial g}{\partial w_{1}}(w) \\ \frac{\partial g}{\partial w_{2}}(w)\end{array}\right] \quad=$ gradient

## Gradient Ascent

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


## Gradient in n dimensions

$$
\nabla g=\left[\begin{array}{c}
\frac{\partial g}{\partial w_{1}} \\
\frac{\partial g}{\partial w_{2}} \\
\cdots \\
\frac{\partial g}{\partial w_{n}}
\end{array}\right]
$$

## Optimization Procedure: Gradient Ascent

$$
\begin{aligned}
& \text { init } u \text { f } \\
& \text { for iter }=1,2 \text {, ... } \\
& \qquad w \leftarrow w+\alpha * \nabla g(w)
\end{aligned}
$$

- $\alpha$ : learning rate --- tweaking parameter that needs to be chosen carefully


## Batch Gradient Ascent on the Log Likelihood Objective

$$
\max _{w} l l(w)=\max _{w} \underbrace{\sum_{i} \log P\left(y^{(i)} \mid x^{(i)} ; w\right)}_{g(w)}
$$

$$
\begin{aligned}
& \text { init } u \\
& \text { for iter }=1,2, \ldots \\
& w \leftarrow w+\alpha * \sum_{i} \nabla \log P\left(y^{(i)} \mid x^{(i)} ; w\right)
\end{aligned}
$$

## Stochastic Gradient Ascent on the Log Likelihood Objective

$$
\max _{w} l l(w)=\max _{w} \sum_{i} \log P\left(y^{(i)} \mid x^{(i)} ; w\right)
$$

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

$$
\begin{aligned}
& \text { init } w \\
& \text { for iter }=1,2, \ldots \\
& \quad \text { pick random j } \\
& \quad w \leftarrow w+\alpha * \nabla \log P\left(y^{(j)} \mid x^{(j)} ; w\right)
\end{aligned}
$$

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

$$
\max _{w} l l(w)=\max _{w} \sum_{i} \log P\left(y^{(i)} \mid x^{(i)} ; w\right)
$$

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

$$
\begin{aligned}
& \text { init } u \\
& \text { for iter }=1,2, \ldots \\
& \text { pick random subset of training examples J } \\
& \qquad w \leftarrow w+\alpha * \sum_{j \in J} \nabla \log P\left(y^{(j)} \mid x^{(j)} ; w\right)
\end{aligned}
$$

## What will gradient ascent do in multi-class logistic regression?

$$
\begin{aligned}
& w \leftarrow w+\alpha * \sum_{i} \nabla \log P\left(y^{(i)} \mid x^{(i)} ; w\right) \\
& P\left(y^{(i)} \mid x^{(i)} ; w\right)=\frac{e^{w_{y}(i) \cdot f\left(x^{(i)}\right)}}{\sum_{y} e^{w_{y} \cdot f\left(x^{(i)}\right)}} \\
& \begin{array}{l}
\nabla w_{y^{(i)}} f\left(x^{(i)}\right)-\nabla \log \sum_{y} e^{w_{y} f\left(x^{(i)}\right)} \\
\text { adds } \mathrm{f} \text { to the correct }
\end{array} \\
& \text { adds } \mathrm{f} \text { to the correct } \\
& \text { class weights } \\
& \frac{1}{\sum_{y} e^{w_{y} f\left(x^{(i)}\right)}} \sum_{y}\left(e^{w_{y} f\left(x^{(i)}\right)}\left[0^{T} f\left(x^{(i)}\right)^{T} 0^{T}\right]^{T}\right) \\
& \text { for } y^{\prime} \text { weights: } \frac{1}{\sum_{y} e^{w_{y} f\left(x^{(i)}\right)}} e^{w_{y^{\prime}} f\left(x^{(i)}\right)} f\left(x^{(i)}\right) \\
& P\left(y^{\prime} \mid x^{(i)} ; w\right) f\left(x^{(i)}\right) \quad \begin{array}{c}
\text { subtracts } \mathrm{f} \text { from } \mathrm{y}^{\prime} \text { weights in proportion to } \\
\text { the probability current weights give to } \mathrm{y}^{\prime}
\end{array}
\end{aligned}
$$

