# CSCI 567: Machine Learning 

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## Administrivia

- HW1 is out
- Due in about 3 weeks ( $2 / 7$ midnight). Start early!!!
- Post on Ed Discussion if you're looking for teammates.

Recap

## Supervised learning in one slide

## Loss function: What is the right loss function for the task?

Representation: What class of functions should we use?
Optimization: How can we efficiently solve the empirical risk minimization problem?

Generalization: Will the predictions of our model transfer gracefully to unseen examples?

All related! And the fuel which powers everything is data.

## Linear regression

Predicted sale price = price_per_sqft $\times$ square footage + fixed_expense


How to solve this? Find stationary points

Are stationary points minimizers?
Yes, for convex objectives !
In high dimensions:


$\nabla^{2}(f(x))$ is positive semi- definite (ps)

## General least square solution

Objective

$$
\operatorname{RSS}(\tilde{\boldsymbol{w}})=\sum_{i}\left(\tilde{\boldsymbol{x}}_{i}^{\mathrm{T}} \tilde{\boldsymbol{w}}-y_{i}\right)^{2}
$$

Find stationary points:

$$
\begin{aligned}
\nabla \operatorname{RSS}(\tilde{\boldsymbol{w}}) & =2 \sum_{i} \tilde{\boldsymbol{x}}_{i}\left(\tilde{\boldsymbol{x}}_{i}^{\mathrm{T}} \tilde{\boldsymbol{w}}-y_{i}\right) \propto\left(\sum_{i} \tilde{\boldsymbol{x}}_{i} \tilde{\boldsymbol{x}}_{i}^{\mathrm{T}}\right) \tilde{\boldsymbol{w}}-\sum_{i} \tilde{\boldsymbol{x}}_{i} y_{i} \\
& =\left(\tilde{\boldsymbol{X}}^{\mathrm{T}} \tilde{\boldsymbol{X}}\right) \tilde{\boldsymbol{w}}-\tilde{\boldsymbol{X}}^{\mathrm{T}} \boldsymbol{y}
\end{aligned}
$$

where

$$
\tilde{\boldsymbol{X}}=\left(\begin{array}{c}
\tilde{\boldsymbol{x}}_{1}^{\mathrm{T}} \\
\tilde{\boldsymbol{x}}_{2}^{\mathrm{T}} \\
\vdots \\
\tilde{\boldsymbol{x}}_{n}^{\mathrm{T}}
\end{array}\right) \in \mathbb{R}^{n \times(d+1)}, \quad \boldsymbol{y}=\left(\begin{array}{c}
y_{1} \\
y_{2} \\
\vdots \\
y_{n}
\end{array}\right) \in \mathbb{R}^{n}
$$

$$
\left(\tilde{\boldsymbol{X}}^{\mathrm{T}} \tilde{\boldsymbol{X}}\right) \tilde{\boldsymbol{w}}-\tilde{\boldsymbol{X}}^{\mathrm{T}} \boldsymbol{y}=\mathbf{0} \quad \Rightarrow \quad \tilde{\boldsymbol{w}}^{*}=\left(\tilde{\boldsymbol{X}}^{\mathrm{T}} \tilde{\boldsymbol{X}}\right)^{-1} \tilde{\boldsymbol{X}}^{\mathrm{T}} \boldsymbol{y}
$$

Optimization methods (continued)

## Problem setup

Given: a function $\mathrm{F}(\boldsymbol{w})$
Goal: minimize $\mathrm{F}(\boldsymbol{w})$ (approximately)

Two simple yet extremely popular methods Gradient Descent (GD): simple and fundamental Stochastic Gradient Descent (SGD): faster, effective for large-scale problems

Gradient is the first-order information of a function. Therefore, these methods are called first-order methods.

## Gradient descent

GD: keep moving in the negative gradient direction
Start from some $\boldsymbol{w}^{(0)}$. For $t=0,1,2, \ldots$

$$
\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)}-\eta \nabla F\left(\boldsymbol{w}^{(t)}\right)
$$

where $\eta>0$ is called step size or learning rate

- in theory $\eta$ should be set in terms of some parameters of $F$
- in practice we just try several small values
- might need to be changing over iterations (think $F(w)=|w|$ )
- adaptive and automatic step size tuning is an active research area


## Why GD?

Intuition: First-order Taylor approximation

$$
F(\boldsymbol{w}) \approx F\left(\boldsymbol{w}^{(t)}\right)+\nabla F\left(\boldsymbol{w}^{(t)}\right)^{T}\left(\boldsymbol{w}_{\left(\boldsymbol{w}-\boldsymbol{w}^{(t)}\right)}\right.
$$



For $\boldsymbol{w}=\boldsymbol{w}^{(t+1)}=\boldsymbol{w}^{(t)}-\eta \nabla F\left(\boldsymbol{w}^{(t)}\right)$, we can write,

$$
\begin{gathered}
F\left(\boldsymbol{w}^{(t+1)}\right) \approx F\left(\boldsymbol{w}^{(t)}\right)-\eta\left\|\nabla F\left(\boldsymbol{w}^{(t)}\right)\right\|_{2}^{2} \\
\Longrightarrow F\left(\boldsymbol{w}^{(t+1)}\right) \lesssim F\left(\boldsymbol{w}^{(t)}\right)
\end{gathered}
$$

(Note that this is only an approximation, and can be invalid if the step size is too large.)

$$
\nabla f\left(w^{(t)}\right)^{\top} \nabla F\left(w^{(t)}\right)=\left\|\nabla F\left(w^{(t)}\right)\right\|_{2}^{2}
$$

## Switch to Colab

## $\triangle$ optimization.ipynb

File Edit View Insert Runtime Tools Help
Code + Text
(1) this_theta[1] $=$ last_theta[1] - eta * grad
theta. append (this_theta)
J.append(cost_func (*this_theta))

* Annotate the objective function plot with coloured points indicating the \# parameters chosen and red arrows indicating the steps down the gradient. ax.annotate( ${ }^{\prime}$ '
arrowprops=\{'arrowstyle' :
va='center', ha='center')
ax.scatter(*zip(*theta), facecolors='none', edgecolors='r', $1 \mathrm{w}=1.5$ )
itles and a legend.
ax.set_xlabel(r'sw_1s')
ax.set_ylabel( $r$ SW_ $2 S$ ' $)$
ax.set_title(' ${ }^{\circ}$ objective function')
plt.show()
[



## Convergence guarantees for GD

Many results for GD (and many variants) on convex objectives. They tell you how many iterations $t$ (in terms of $\varepsilon$ ) are needed to achieve

$$
F\left(\boldsymbol{w}^{(t)}\right)-F\left(\boldsymbol{w}^{*}\right) \leq \varepsilon
$$

## Convergence guarantees for GD

Many results for GD (and many variants) on convex objectives.
They tell you how many iterations $t$ (in terms of $\varepsilon$ ) are needed to achieve

$$
F\left(\boldsymbol{w}^{(t)}\right)-F\left(\boldsymbol{w}^{*}\right) \leq \varepsilon
$$

Even for nonconvex objectives, some guarantees exist:
e.g. how many iterations $t$ (in terms of $\varepsilon$ ) are needed to achieve

$$
\left\|\nabla F\left(\boldsymbol{w}^{(t)}\right)\right\| \leq \varepsilon
$$

that is, how close is $\boldsymbol{w}^{(t)}$ as an approximate stationary point
for convex objectives, stationary point $\Rightarrow$ global minimizer
for nonconvex objectives, what does it mean?

## Stationary points: non-convex objectives

A stationary point can be a local minimizer or even a local/global maximizer (but the latter is not an issue for GD).


$$
f(w)=w^{3}+w^{2}-5 w
$$

## Stationary points: non convex objectives

A stationary point can also be neither a local minimizer nor a local maximizer!

- $f(\boldsymbol{w})=w_{1}^{2}-w_{2}^{2}$
- $\nabla f(\boldsymbol{w})=\left(2 w_{1},-2 w_{2}\right)$
- so $\boldsymbol{w}=(0,0)$ is stationary
- local max for blue direction $\left(w_{1}=0\right)$

- local min for green direction $\left(w_{2}=0\right)$


## Stationary points: non convex objectives

This is known as a saddle point


- but GD gets stuck at $(0,0)$ only if initialized along the green direction
- so not a real issue especially when initialized randomly


## Stationary points: non convex objectives

But not all saddle points look like a "saddle"...

- $f(\boldsymbol{w})=w_{1}^{2}+w_{2}^{3}$
- $\nabla f(\boldsymbol{w})=\left(2 w_{1}, 3 w_{2}^{2}\right)$
- so $\boldsymbol{w}=(0,0)$ is stationary
- not local min/max for blue direction $\left(w_{1}=0\right)$



## Stationary points: non convex objectives

But not all saddle points look like a "saddle"...

- $f(\boldsymbol{w})=w_{1}^{2}+w_{2}^{3}$
- $\nabla f(\boldsymbol{w})=\left(2 w_{1}, 3 w_{2}^{2}\right)$
- so $\boldsymbol{w}=(0,0)$ is stationary
- not local min/max for blue direction $\left(w_{1}=0\right)$
- GD gets stuck at $(0,0)$ for any initial point with $w_{2} \geq 0$ and small $\eta$


Even worse, distinguishing local min and saddle point is generally NP-hard.

## Stochastic Gradient descent

GD: keep moving in the negative gradient direction
SGD: keep moving in the noisy negative gradient direction

$$
\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)}-\eta \tilde{\nabla} F\left(\boldsymbol{w}^{(t)}\right)
$$

where $\tilde{\nabla} F\left(\boldsymbol{w}^{(t)}\right)$ is a random variable (called stochastic gradient) s.t.

$$
\mathbb{E}\left[\tilde{\nabla} F\left(\boldsymbol{w}^{(t)}\right)\right]=\nabla F\left(\boldsymbol{w}^{(t)}\right) \quad \text { (unbiasedness) }
$$

## Stochastic Gradient descent

GD: keep moving in the negative gradient direction
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\mathbb{E}\left[\tilde{\nabla} F\left(\boldsymbol{w}^{(t)}\right)\right]=\nabla F\left(\boldsymbol{w}^{(t)}\right) \quad \text { (unbiasedness) }
$$

- Key point: it could be much faster to obtain a stochastic gradient!
- Similar convergence guarantees, usually needs more iterations but each iteration takes less time.


## Summary: Gradient descent \& Stochastic Gradient descent

- GD/SGD coverages to a stationary point
- for convex objectives, this is all we need


## Summary: Gradient descent \& Stochastic Gradient descent

- GD/SGD coverages to a stationary point
- for convex objectives, this is all we need
- for nonconvex objectives, can get stuck at local minimizers or "bad" saddle points (random initialization escapes "good" saddle points)
- recent research shows that many problems have no "bad" saddle points or even "bad" local minimizers
- justify the practical effectiveness of GD/SGD (default method to try)

Second-order methods
GD: Est order Taylor

$$
\begin{gathered}
F(w) \approx F\left(w^{(t)}\right)+\nabla F\left(w^{(t)}\right)^{\top}\left(w-w^{(t)}\right) \\
f(y)=f(x)+f^{\prime}(x)(y-x)+\frac{f^{\prime \prime}(x)}{2}(y-x)^{2} \\
F(w) \approx F\left(w^{(t)}\right)+\nabla F\left(w^{(t)}\right)^{\top}\left(w-w^{(t)}\right)+\frac{1}{2}\left(w-w^{(t)}\right)^{\top} H_{t}\left(w \cdot w^{(t)}\right)
\end{gathered}
$$

where $H_{t}=\nabla^{2} F\left(\omega^{(t)}\right) \in \mathbb{R}^{d+d}$ is Hessian of $F$ at $\omega^{(t)}$

$$
\left(H_{t}\right)_{i, j}=\left.\frac{\partial^{2} F(w)}{\partial w_{i} w_{j}}\right|_{w=w^{(t)}}
$$



Define $\tilde{F}(\omega)=$ and order approximation
Set $\nabla^{\nu} \tilde{F}^{(w)}=0$

$$
\begin{aligned}
& \frac{d F\left(w^{(t)}\right)}{d w}=0 \quad \frac{d}{d w}\left(\nabla F\left(w^{(t)}\right)^{\top}\left(w-w^{(t)}\right)\right)=\nabla F\left(w^{(t)}\right) \\
& \frac{d}{d w}\left(\frac{1}{2} w^{\top} H_{t} w\right)=H t w \quad \frac{d}{d w}\left(\frac{-1}{2} w H_{t} w^{(t)}\right)=\frac{-1}{2} H_{t w}^{(t)} \\
& \frac{d}{d w}\left(-\frac{1}{2} w^{(t)} H_{t} w\right)=\frac{-1}{2} H_{t w^{(t)}} \quad \frac{d}{d w}\left(\frac{1}{2} w^{(t)} H_{t} w^{(t)}\right)=0
\end{aligned}
$$

$$
\begin{aligned}
& \nabla \tilde{F}(w)=\nabla F\left(w^{(t)}+H \in w-\frac{1}{2} H_{t} w^{(t)}+z\right. \\
& \text { Set } \nabla \tilde{F}(w)=0 \\
& H_{t} w=H_{t} w^{(t)}-\nabla F\left(w^{(t)}\right) \\
& \Rightarrow w=w^{(t)}-H_{t}^{-1} \nabla F\left(w^{(t)}\right)
\end{aligned}
$$

Newton's method: $w^{(t+1)}=w^{(t)}-H_{t}^{-1} \nabla F\left(w^{(+1)}\right)$
GD: $w^{(t+1)}=w^{(t)}-\eta \nabla F\left(w^{(t)}\right)$

| Newton's Method | Gradient Descent |
| :---: | :---: |
| No learning rate | Need to tune learning rate |
| Super fast convergence | Slower convergence |
| Know and invert Hessian <br> (inversion takes $O\left(d^{3}\right)$ time <br> naively) | Fast! |



## Linear classifiers

## The Setup

Recall the setup:

- input (feature vector): $\boldsymbol{x} \in \mathbb{R}^{\mathrm{d}}$
- output (label): $y \in[\mathrm{C}]=\{1,2, \cdots, \mathrm{C}\}$
- goal: learn a mapping $f: \mathbb{R}^{\mathrm{d}} \rightarrow[\mathrm{C}]$

This lecture: binary classification

- Number of classes: $\mathrm{C}=2$
- Labels: $\{-1,+1\}$ (cat or dog)


## Representation: Choosing the function class

Let's follow the recipe, and pick a function class $\mathcal{F}$.

We continue with linear models, but how to predict a label using $\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}$ ?
Sign of $\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}$ predicts the label:

$$
\operatorname{sign}\left(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}\right)= \begin{cases}+1 & \text { if } \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}>0 \\ -1 & \text { if } \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x} \leq 0\end{cases}
$$

(Sometimes use sgn for sign too.)

Representation: Choosing the function class


Definition: The function class of separating hyperplanes (or linear classifiers) is:

$$
f=\left\{f(x)=\operatorname{sign}\left(w^{\top} x\right): w \in \mathbb{R}^{d}\right\}
$$

Still makes sense for "almost" linearly separable data


## Iris dataset

iris setosa

iris versicolor

iris virginica


## Features:

1. Sepal length
2. Sepal width



Choosing the loss function
Most common loss $\quad \ell(f(x), y)=11(f(x) \neq y)$
Loss as a function of $y w^{\top} x$

$$
\begin{aligned}
& \operatorname{lor-1}^{\operatorname{lo-1}_{2.0}\left(y \omega^{\top} x\right)}(y)=\mathbb{1}\left(y \omega^{\top} x \leq 0\right) \\
& \hline 0.5
\end{aligned}
$$

## Choosing the loss function: minimizing $0 / 1$ loss is hard

However, 0-1 loss is not convex.


Even worse, minimizing 0-1 loss is NP-hard in general.

## Choosing the loss function: surrogate losses

Solution: use a convex surrogate loss


## Choosing the loss function: surrogate losses

Solution: use a convex surrogate loss $\ell(z)$


- perceptron loss $\ell_{\text {perceptron }}(z)=\max \{0,-z\}$ (used in Perceptron)


## Choosing the loss function: surrogate losses

Solution: use a convex surrogate loss


- perceptron loss $\ell_{\text {perceptron }}(z)=\max \{0,-z\}$ (used in Perceptron)
- hinge loss $\ell_{\text {hinge }}(z)=\max \{0,1-z\}$ (used in SVM and many others)


## Choosing the loss function: surrogate losses

Solution: use a convex surrogate loss $\ell(z)$


- perceptron loss $\ell_{\text {perceptron }}(z)=\max \{0,-z\}$ (used in Perceptron)
- hinge loss $\ell_{\text {hinge }}(z)=\max \{0,1-z\}$ (used in SVM and many others)
- logistic loss $\ell_{\text {logistic }}(z)=\log (1+\exp (-z))$ (used in logistic regression; the base of $\log$ doesn't matter)


## Onto Optimization!

Find ERM:

$$
\boldsymbol{w}^{*}=\underset{\boldsymbol{w} \in \mathbb{R}^{d}}{\operatorname{argmin}} \frac{1}{n}\left(\sum_{i=1}^{n} \ell\left(y_{i} \boldsymbol{w}^{\top} \boldsymbol{x}_{\boldsymbol{i}}\right)\right)
$$

where $\ell(\cdot)$ is a convex surrogate loss function.

- No closed-form solution in general (in contrast to linear regression)
- We can use our optimization toolbox!

New York Times, 1958

## Imw way dyice LERRNS BY DOING

The Navy last week demonstrated the embryo of an electronic computer named the Perceptron
Psychologist Shows Embryo of Computer DesP CPOM Ren completed in about a Read and Grov C.C CPC Dected to be the first non-

WASHINGTON, July. 7 (UPI) -The Navy revealed the embryo of an etectronic computer today that it expects will be able to walk, talk, see, write, reproduce itself and bo conscious of its existence.
living mechanism able to "perceive, recognize and identify its surroundings without human
training or control.

New York Times, 1958

## NEW NAVY DEVICE LEARNS BY DOING

Psychologist Shows Embryo of Computer Designed to Read and Grow Wiser

WASHINGTON, July. 7 (UPI) -The Navy revealed the embryo of an electronic computer today that it expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence.

The Navy last week demonstrated the embryo of an electronic computer named the Perceptron which, when completed in about a year, is expected to be the first nonliving mechanism able to "perceive, recognize and identify its surroundings without human training or control."

Recall perceptron loss

$$
\begin{aligned}
f(w) & =\frac{1}{n} \sum_{i=1}^{n} l_{\text {percep }}\left(y_{i} \omega^{\top} x_{i}\right) \\
& =\frac{1}{n} \sum_{i=1}^{n} \operatorname{mat}\left\{0,-y_{i} \omega^{\top} x_{i}\right\}
\end{aligned}
$$

What's the gradient?

$$
\begin{aligned}
& z>0,0 \\
& z \leq 0,-1
\end{aligned}
$$



Applying GD to perceptron loss
Gradient is

$$
\begin{aligned}
& \nabla F(\omega)=\frac{1}{n} \sum_{i=1}^{n}-\mathbb{1}\left[y_{i} \omega^{\top} x_{i} \leq 0\right] y_{i} x_{i} \\
& G_{D}: \omega \leftarrow \omega+\frac{\eta}{n} \sum_{i=1}^{n} \mathbb{1}\left[y_{i} \omega^{\top} x_{i} \leq 0\right]_{y_{i} x_{i}}
\end{aligned}
$$

Applying SGD to perceptron loss
How to get stochastic gradient?
$\rightarrow$ pick one example $i \in[n]$ uniformly at random

$$
\begin{aligned}
\tilde{\nabla} F\left(\omega^{(t)}\right) & =-\mathbb{1}\left[y_{i} \omega^{\top} x_{i} \leq 0\right] y_{i} x_{i} \\
\mathbb{E}\left[\tilde{\nabla} F\left(w^{(t)}\right]\right. & =\frac{1}{n} \sum_{i=1}^{n}-\mathbb{1}\left[y_{i} \omega^{\top} x_{i} \leq 0\right] y_{i} x_{i} \\
& =\nabla F\left(w^{(t)}\right)
\end{aligned}
$$

SGD update : $\omega \in \omega+\eta \mathbb{1}\left[y_{i} w^{\top} x_{i} \leq 0\right]_{y_{i} x_{i}}$

## Perceptron algorithm

SGD with $\eta=1$ on perceptron loss.

1. Initialize $\boldsymbol{w}=0$
2. Repeat

- Pick $\boldsymbol{x}_{\boldsymbol{i}} \sim \operatorname{Unif}\left(\boldsymbol{x}_{\boldsymbol{1}}, \ldots, \boldsymbol{x}_{\boldsymbol{n}}\right)$
- If $\operatorname{sgn}\left(\boldsymbol{w}^{T} \boldsymbol{x}_{\boldsymbol{i}}\right) \neq y_{i}$

$$
\boldsymbol{w} \leftarrow \boldsymbol{w}+y_{i} \boldsymbol{x}_{\boldsymbol{i}}
$$

Perceptron algorithm: Intuition
Say that $w$ makes mistake on ( $x_{i}, y_{i}$ )

$$
\begin{aligned}
y_{i} w^{\top} x_{i} & <0 \\
\text { Consider } \quad w^{\prime}= & w+y_{i} x_{i} \\
y_{i}\left(w^{\prime}\right)^{\top} x_{i} & =y_{i} w^{\top} x_{i}+y_{i}^{2} x_{i}^{\top} x_{i} \\
\therefore \quad \text { if } x_{i} & =0 \\
& y i\left(w^{1}\right)^{\top} x_{i}>y_{i} w^{\top} x_{i}
\end{aligned}
$$

## Perceptron algorithm: visually

Repeat:

- Pick a data point $\boldsymbol{x}_{i}$ uniformly at random
- If $\operatorname{sgn}\left(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_{i}\right) \neq y_{i}$



## Perceptron algorithm: Iris dataset



## Perceptron algorithm: Iris dataset



## HW1: Theory for perceptron!

(HW 1) If training set is linearly separable

- Perceptron converges in a finite number of steps
- training error is 0


There are also guarantees when the data are not linearly separable.


Logistic loss

$$
\begin{aligned}
F(w) & =\frac{1}{n} \sum_{i=1}^{n} \log \left(y_{i} w^{\top} x_{i}\right) \\
& =\frac{1}{n} \sum_{i=1}^{n} \ln \left(1+e+p\left(-y_{i} w^{\top} x_{i}\right)\right)
\end{aligned}
$$



## Predicting probabilities

Instead of predicting the $\{ \pm 1\}$ label, predict the probability (i.e. regression on probability).

Sigmoid + linear model:

$$
\mathbb{P}(y=+1 \mid \boldsymbol{x}, \boldsymbol{w})=\sigma\left(\boldsymbol{w}^{T} \boldsymbol{x}\right)
$$

where


## The sigmoid function

Properties of sigmoid $\sigma(z)=\frac{1}{1+e^{-z}}$

- between 0 and 1 (good as probability)
- $\sigma\left(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}\right) \geq 0.5 \Leftrightarrow \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x} \geq 0$, consistent with predicting the label with $\operatorname{sgn}\left(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}\right)$
- larger $\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x} \Rightarrow \operatorname{larger} \sigma\left(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}\right) \Rightarrow$ higher confidence in label 1
- $\sigma(z)+\sigma(-z)=1$ for all $z$
- Therefore, the probability of label -1 is


$$
\begin{aligned}
\mathbb{P}(y=-1 \mid \boldsymbol{x} ; \boldsymbol{w}) & =1-\mathbb{P}(y=+1 \mid \boldsymbol{x} ; \boldsymbol{w}) \\
& =1-\sigma\left(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}\right)=\sigma\left(-\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}\right)
\end{aligned}
$$

Therefore, we can model $\mathbb{P}(y \mid \boldsymbol{x} ; \boldsymbol{w})=\sigma\left(y \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}\right)=\frac{1}{1+e^{-y \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}}}$

## Maximum likelihood estimation

What we observe are labels, not probabilities.
Take a probabilistic view

- assume data is independently generated in this way by some $\boldsymbol{w}$
- perform Maximum Likelihood Estimation (MLE)

Specifically, what is the probability of seeing labels $y_{1}, \cdots, y_{n}$ given $x_{1}, \cdots, x_{n}$, as a function of some $\boldsymbol{w}$ ?

$$
P(\boldsymbol{w})=\prod_{i=1}^{n} \mathbb{P}\left(y_{i} \mid \boldsymbol{x}_{\boldsymbol{i}} ; \boldsymbol{w}\right)\left\{\begin{array}{l}
\text { i.i.d. assumption } \\
\text { all datopoints are independent } \\
\text { and identically disTritated }
\end{array}\right.
$$

MLE: find $\boldsymbol{w}^{*}$ that maximizes the probability $P(\boldsymbol{w})$

Maximum likelihood solution

$$
\begin{aligned}
\boldsymbol{w}^{*} & =\underset{\boldsymbol{w}}{\operatorname{argmax}} P(\boldsymbol{w})=\underset{\boldsymbol{w}}{\operatorname{argmax}} \prod_{i=1}^{n} \mathbb{P}\left(y_{i} \mid \boldsymbol{x}_{\boldsymbol{i}} ; \boldsymbol{w}\right) \\
& =\underset{\boldsymbol{w}}{\operatorname{argmax}} \sum_{i=1}^{n} \ln \mathbb{P}\left(y_{i} \mid \boldsymbol{x}_{\boldsymbol{i}} ; \boldsymbol{w}\right) \\
& =\underset{\boldsymbol{w}}{\operatorname{argmin}} \sum_{i=1}^{n}-\ln \mathbb{P}\left(y_{i} \mid \boldsymbol{x}_{\boldsymbol{i}} ; \boldsymbol{w}\right) \quad \mathbb{P}\left(y_{i} \mid x_{i} ; \boldsymbol{w}\right)=\boldsymbol{\sigma}\left(\boldsymbol{y}_{i} \boldsymbol{w}^{\top} x_{i}\right) \\
& =\underset{\boldsymbol{w}}{\operatorname{argmin}} \sum_{i=1}^{n} \ln \left(1+e^{-y_{i} \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_{\boldsymbol{i}}}\right) \\
& =\underset{\boldsymbol{w}}{\operatorname{argmin}} \sum_{i=1}^{n} \ell_{\text {logistic }}\left(y_{i} \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_{i}\right) \\
& =\underset{\boldsymbol{w}}{\operatorname{argmin}} F(\boldsymbol{w})
\end{aligned}
$$

Minimizing logistic loss is exactly doing MLE for the sigmoid model!

SGD to logistic loss

$$
\boldsymbol{w} \leftarrow \boldsymbol{w}-\eta \tilde{\nabla} F(\boldsymbol{w}) \quad \text { IE }[\tilde{\nabla} F(w)]=\nabla F(w)
$$

$=\boldsymbol{w}-\eta \nabla_{\boldsymbol{w}} \ell_{\text {logistic }}\left(y_{i} \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_{i}\right) \quad$ (xi,yi) drawn uniformly from $\{1, \ldots, n\}$
$=\boldsymbol{w}-\eta\left(\left.\frac{\partial \ell_{\text {logistic }}(z)}{\partial z}\right|_{z=y_{i} \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_{i}}\right) y_{i} \boldsymbol{x}_{i} \quad$ (chain rule)

$$
\begin{aligned}
& =\boldsymbol{w}-\eta\left(\left.\frac{-e^{-z}}{1+e^{-z}}\right|_{z=y_{i} \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_{i}}\right) y_{i} \boldsymbol{x}_{i} \quad \frac{\partial\left(\log \left(1+e^{-z}\right)\right)}{\partial z}=\frac{1}{1+e-z}+\left(-e^{-z}\right) \\
& =\boldsymbol{w}+\eta \sigma\left(-u_{i} \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_{\mathrm{j}}\right) u_{i} \boldsymbol{x}_{i}
\end{aligned}
$$

$$
\begin{array}{lc}
=\boldsymbol{w}+\eta \sigma\left(-y_{i} \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_{i}\right) y_{i} \boldsymbol{x}_{i} & \sigma(-z)=1-\sigma(z)= \\
=\boldsymbol{w}+\eta \mathbb{P}\left(-y_{i} \mid \boldsymbol{x}_{i} ; \boldsymbol{w}\right) y_{i} \boldsymbol{x}_{i}
\end{array} \quad \begin{gathered}
1+e^{-z} \\
1-\frac{1}{1+e^{-z}}=\frac{e^{-z}}{1+e^{-z}}
\end{gathered}
$$

This is a soft version of Perceptron!

$$
=\sigma(-z)
$$

$$
\mathbb{P}\left(-y_{i} \mid \boldsymbol{x}_{i} ; \boldsymbol{w}\right) \quad \text { versus } \quad \square\left[y_{i} \neq \operatorname{sgn}\left(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_{i}\right)\right]
$$

