CSCI 567: Machine Learning

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Fall 2022

Lecture 2, Sep 1

USC University of Southern California

Administrivia

- HW1 is out
- Due in about 2 weeks (9/14 at 2pm). **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?

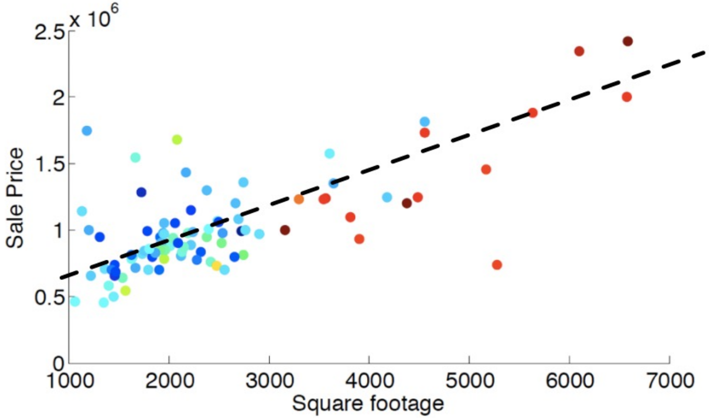
Optimization: How can we efficiently solve the empirical risk minimization problem?

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** × square footage + **fixed_expense**

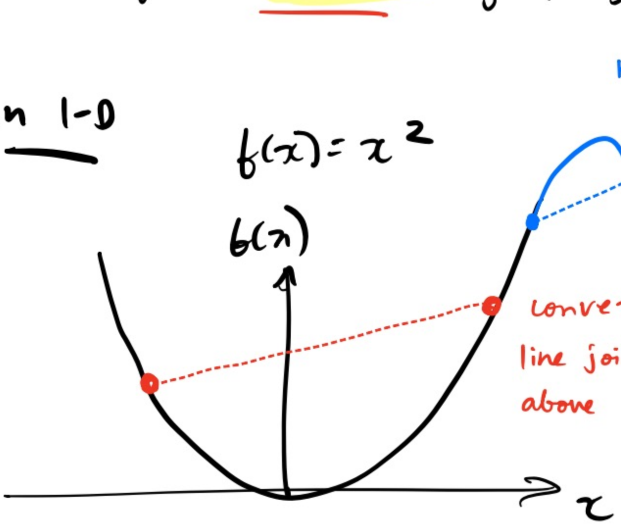


How to solve this? Find **stationary points**

Are stationary points minimizers?

Yes, for convex objectives!

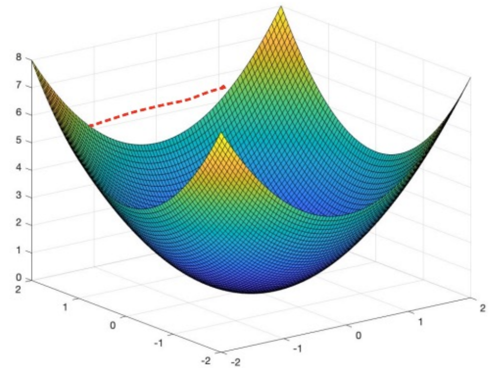
In 1-D



convex $\iff$ line joining 2 points above function

$f''(x) \geq 0 \;\; \forall x$ $\longrightarrow$ $\nabla^2(F(x))$ is positive semi-definite (psd)

In high dimensions:



General least square solution

Objective

$$\mathrm{RSS}(\tilde{\boldsymbol{w}}) = \sum_i (\tilde{\boldsymbol{x}}_i^{\mathrm{T}} \tilde{\boldsymbol{w}} - y_i)^2$$

Find stationary points:

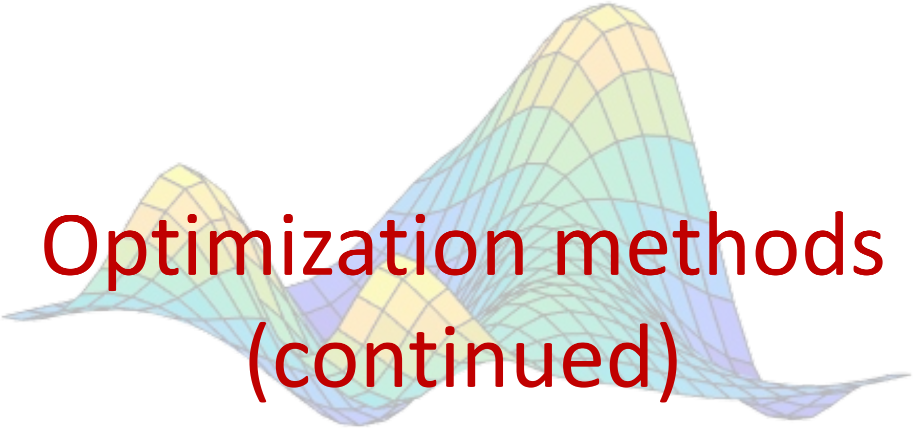
$$\begin{aligned}\nabla \mathrm{RSS}(\tilde{\boldsymbol{w}}) &= 2 \sum_i \tilde{\boldsymbol{x}}_i (\tilde{\boldsymbol{x}}_i^{\mathrm{T}} \tilde{\boldsymbol{w}} - y_i) \propto \left(\sum_i \tilde{\boldsymbol{x}}_i \tilde{\boldsymbol{x}}_i^{\mathrm{T}} \right) \tilde{\boldsymbol{w}} - \sum_i \tilde{\boldsymbol{x}}_i y_i \\ &= (\tilde{\boldsymbol{X}}^{\mathrm{T}} \tilde{\boldsymbol{X}}) \tilde{\boldsymbol{w}} - \tilde{\boldsymbol{X}}^{\mathrm{T}} \boldsymbol{y}\end{aligned}$$

where

$$\tilde{\boldsymbol{X}} = \begin{pmatrix} \tilde{\boldsymbol{x}}_1^{\mathrm{T}} \\ \tilde{\boldsymbol{x}}_2^{\mathrm{T}} \\ \vdots \\ \tilde{\boldsymbol{x}}_n^{\mathrm{T}} \end{pmatrix} \in \mathbb{R}^{n \times (d+1)}, \quad \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} \in \mathbb{R}^n$$

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

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 $t = 0, 1, 2, \ldots$

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

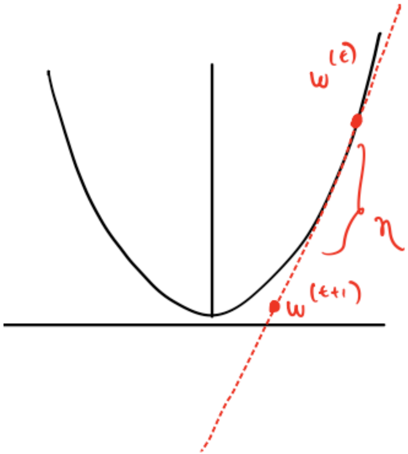
where $\eta > 0$ is called <u>step size</u> or <u>learning rate</u>

- in theory η 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

$$F(w) \approx F(w^{(t)}) + \nabla F(w^{(t)})^T (w - w^{(t)})$$



$$F(w^{(t+1)}) \approx F(w^{(t)}) - \eta \underbrace{\|\nabla F(w^{(t)})\|_2^2}_{\geq 0}$$

$$\Rightarrow F(w^{(t+1)}) \underset{\sim}{\leq} F(w^{(t)})$$

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

Convergence guarantees for GD

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

$$F(\boldsymbol{w}^{(t)}) - F(\boldsymbol{w}^{*}) \le \varepsilon$$

Convergence guarantees for GD

Many results for GD (and many variants) on *convexobjectives*.
They tell you how many iterations t (in terms of ε) are needed to achieve

$$F(\boldsymbol{w}^{(t)}) - F(\boldsymbol{w}^{*}) \le \varepsilon$$

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

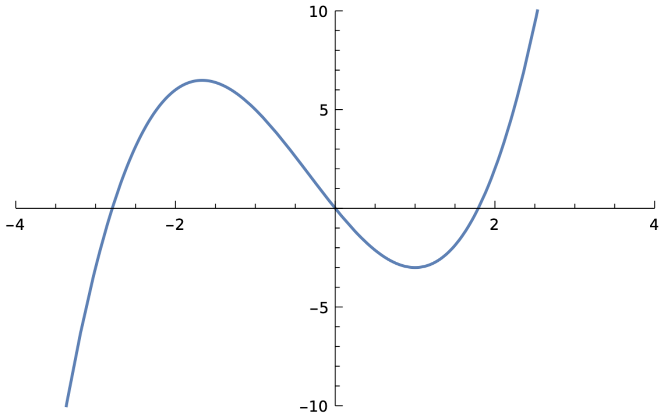
$$\left\|\nabla F(\boldsymbol{w}^{(t)})\right\| \le \varepsilon$$

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).

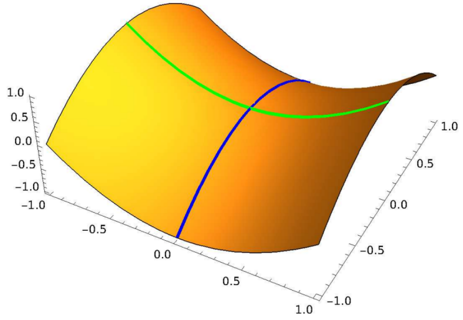


$$f(w) = w^3 + w^2 - 5w$$

Stationary points: non convex objectives

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

- $f(\boldsymbol{w}) = w_1^2 - w_2^2$
- $\nabla f(\boldsymbol{w}) = (2w_1, -2w_2)$
- so $\boldsymbol{w} = (0, 0)$ is stationary
- local max for blue direction $(w_1 = 0)$
- local min for green direction $(w_2 = 0)$



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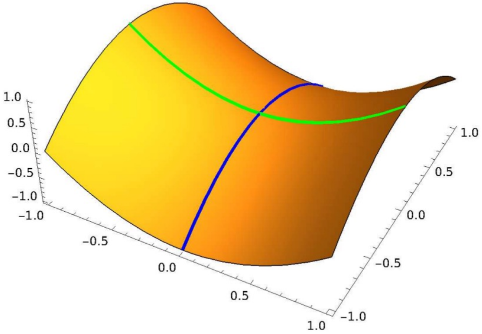
Stationary points: non convex objectives

This is known as a saddle point

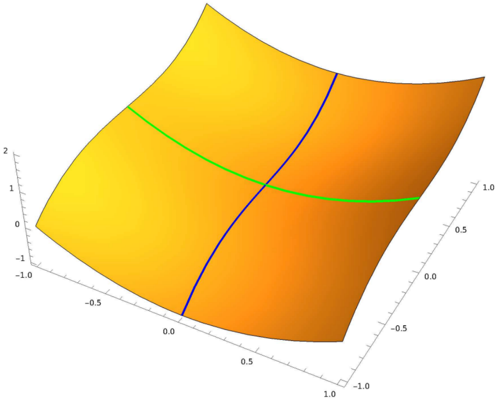


- but GD gets stuck at $(0, 0)$ only if initialized along the green direction
- so not a real issue especially *when initialized randomly*

Stationary points: non convex objectives

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

- $f(\boldsymbol{w}) = w_1^2 + w_2^3$
- $\nabla f(\boldsymbol{w}) = (2w_1, 3w_2^2)$
- so $\boldsymbol{w} = (0, 0)$ is stationary
- not local min/max for blue direction ($w_1 = 0$)



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Stationary points: non convex objectives

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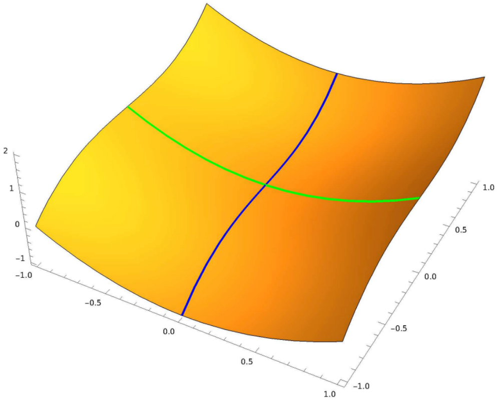
- $\nabla f(\boldsymbol{w}) = (2w_1, 3w_2^2)$
- so $\boldsymbol{w} = (0, 0)$ is stationary
- not local min/max for blue direction ($w_1 = 0$)
- GD gets stuck at $(0, 0)$ for *any initial point with $w_2 \geq 0$ and small η*



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*

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

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

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

Stochastic Gradient descent

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

- 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.

Switch to Colab

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: first-order Taylor approximation

$$F(w) \simeq F(w^{(t)}) + \nabla F(w^{(t)})^T (w - w^{(t)})$$

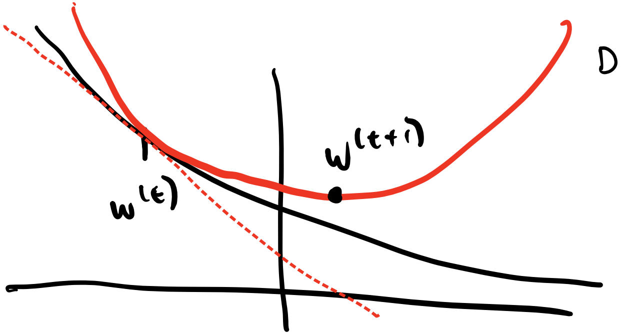
$$f(y) \simeq f(x) + f'(x)(y-x) + \frac{f''(x)}{2} \cdot (y-x)^2$$

What about a second-order Taylor approximation?

$$F(w) \simeq F(w^{(t)}) + \nabla F(w^{(t)})^T (w - w^{(t)}) + \frac{1}{2} (w - w^{(t)})^T H_t (w - w^{(t)})$$

where $H_t = \nabla^2 F(w^{(t)}) \in \mathbb{R}^{d \times d}$ is Hessian of F at $w^{(t)}$

$$H_{t,i,j} = \frac{\partial^2 F(w)}{\partial w_i \partial w_j} \Bigg|_{w = w^{(t)}}$$



Define $\tilde{F}(w) :=$ 2nd order approximation

Set $\nabla \tilde{F}(w) = 0$ to find minima.

$$\nabla F(w^{(t)}) + \frac{H_t w}{2} - \frac{H_t w^{(t)}}{2} - \frac{1}{2} H_t w^{(t)} = 0$$

$$H_t w = H_t w^{(t)} - \nabla F(w^{(t)})$$

$$\Rightarrow \quad w = w^{(t)} - H_t^{-1} \nabla F(w^{(t)})$$

Newton's method: $w^{(t+1)} \leftarrow w^{(t)} - H_t^{-1} \nabla F(w^{(t)})$

GD: $w^{(t+1)} \leftarrow w^{(t)} - \eta \nabla F(w^{(t)})$

Newton's method	GD
* no learning rate	* need to tune η
* super fast convergence	* slower convergence
* Know & invert Hessian (inversion takes $O(d^3)$ time naively)	* fast! $O(d)$ time

Linear classifiers

The Setup

Recall the setup:

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

This lecture: **binary classification**

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

Representation: Choosing the **function class**

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

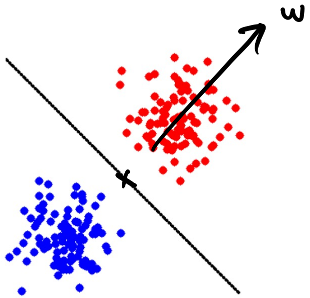
We continue with linear models, but how to predict a label using $\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$?

Sign of $\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$ predicts the label:

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

(Sometimes use sgn for sign too.)

Representation: Choosing the **function class**

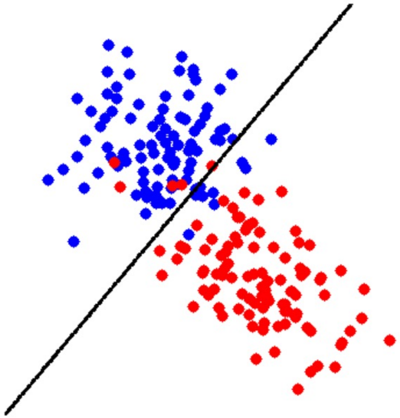


Good choice if data is linearly separated.

Definition: The function class of separating hyperplanes is defined as:

$$\mathcal{F} = \{ f(x) = \mathrm{sgn}(w^T x) : w \in \mathbb{R}^d \}.$$

Still makes sense for “almost” linearly separable data

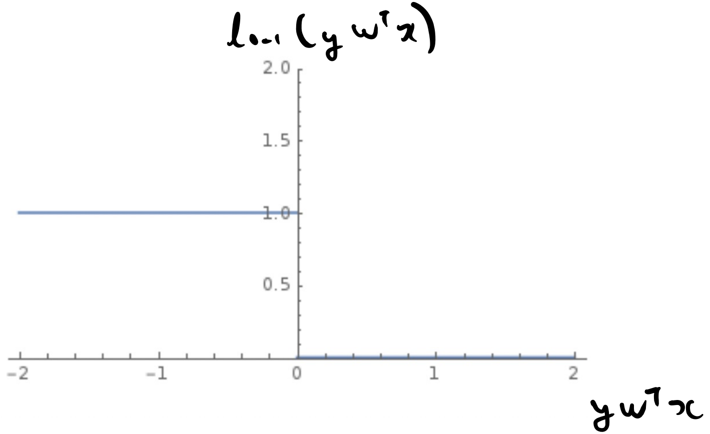


Choosing the **loss function**

Most common loss $\ell(f(x), y) = \mathbb{1}(f(x) \neq y)$

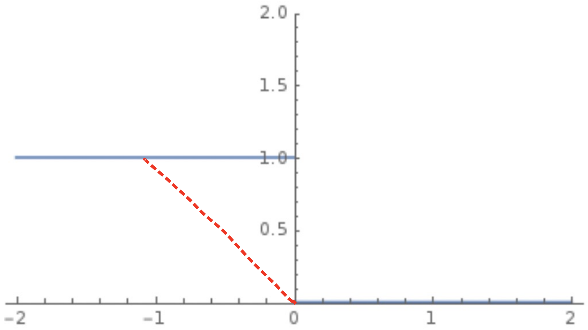
Loss as a function of yw^Tx

$$\ell_{0-1}(yw^Tx) = \mathbb{1}(yw^Tx \leq 0)$$



Choosing the loss function: **minimizing 0/1 loss is hard**

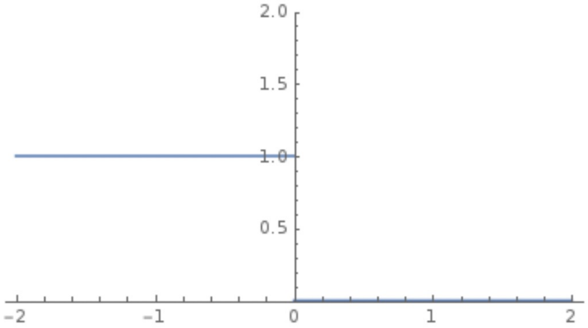
However, 0-1 loss is not convex.



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

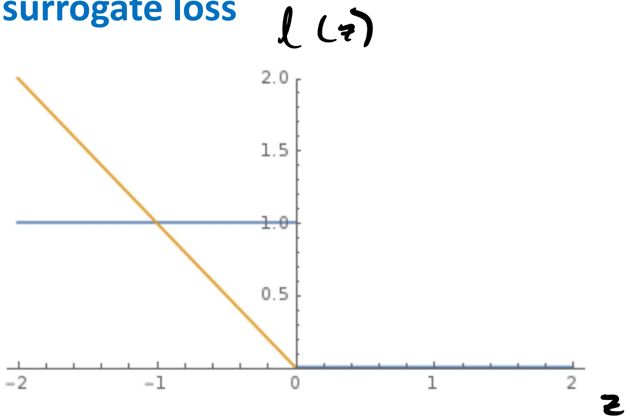
Choosing the loss function: **surrogate losses**

Solution: use a **convex surrogate loss**



Choosing the loss function: surrogate losses

Solution: use a **convex surrogate loss**



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

Choosing the loss function: **surrogate losses**

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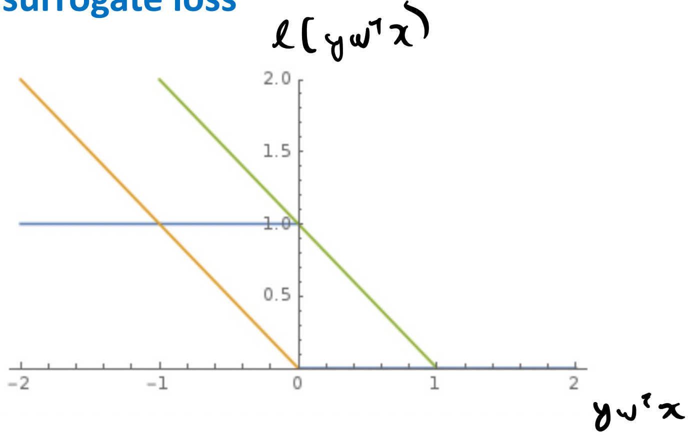

- perceptron loss $\ell_{\text{perceptron}}(z) = \max\{0, -z\}$ (used in Perceptron)
- hinge loss $\ell_{\text{hinge}}(z) = \max\{0, 1 - z\}$(used in SVM and many others)

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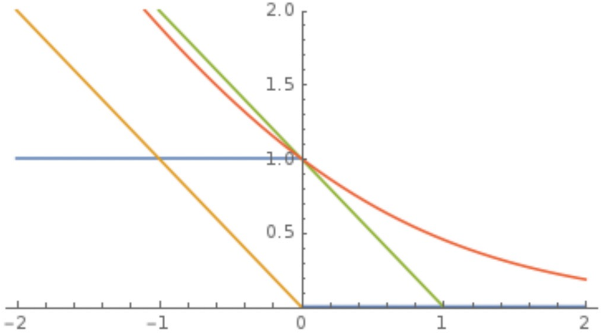


yw^Tx

- 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**!

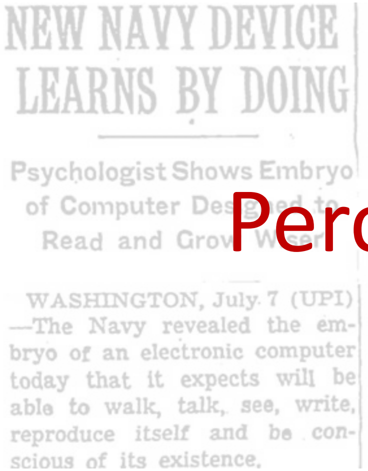
Find ERM :

$$w^* = \underset{w \in \mathbb{R}^d}{\operatorname{argmin}} \; \frac{1}{n} \left(\sum_{i=1}^{n} \ell(y_i w^T x_i) \right)$$

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

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

New York Times, 1958



NEW NAVY DEVICE LEARNS BY DOING

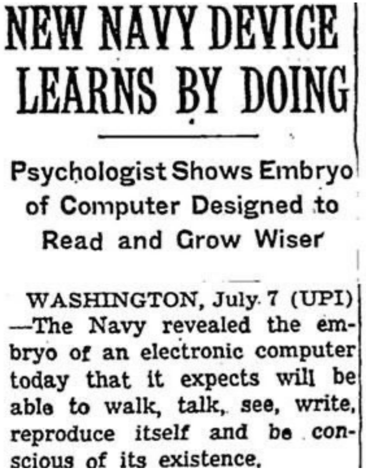
Psychologist Shows Embryo of Computer Designed to Read and Grow Wiser

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.

Perceptron

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 non-living mechanism able to "perceive, recognize and identify its surroundings without human training or control."*

New York Times, 1958



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Recall perceptron loss

$$F(w) = \frac{1}{n} \sum_{i=1}^{n} l_{percep}(y_i w^T x_i)$$

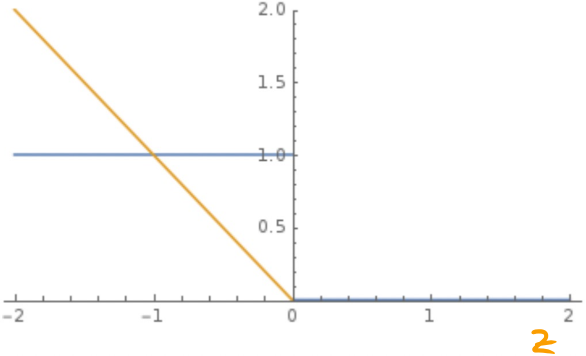
$$= \frac{1}{n} \sum_{i=1}^{n} \max\{0, -y_i w^T x_i\}$$

Let's try GD / SGD.

What's the gradient:

$$\begin{cases} 0, & z > 0 \\ -1, & z \le 0 \end{cases}$$

$l_{percep}(z)$



Applying GD to perceptron loss

Gradient is

$$\nabla F(w) = (1/n) \sum_{i=1}^{n} - \mathbb{1}[y_i w^T x_i \leq 0]\, y_i x_i$$

(only misclassified examples count)

GD : $w \leftarrow w + \frac{\eta}{n} \underbrace{\sum_{i=1}^{n}} \mathbb{1}[y_i w^T x_i \leq 0]\, y_i x_i$

need the entire training set for every GD update.

Applying SGD to perceptron loss

How to get a stochastic gradient?

Objective function of most ML tasks is a finite sum, trick applies generally

→ pick one example $i \in [n]$ uniformly at random, let

$$\tilde{\nabla} F(w^{(t)}) = -\mathbb{1}[y_i w^T x_i \leq 0] y_i x_i$$

Unbiased. why?

$$\mathbb{E}[\tilde{\nabla} F(w^{(t)})] = \frac{1}{n} \sum_{i=1}^{n} -\mathbb{1}[y_i w^T x_i \leq 0] y_i x_i$$

$$= \nabla F(w^{(t)})$$

SGD update: $w \leftarrow w + \eta \mathbb{1}(y_i w^T x_i \leq 0) y_i x_i$

fast! one datapoint per update

Perceptron algorithm

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

Initialize $w = 0$

Repeat

- Pick $x_i \sim \text{Unif}(x_1, \dots, x_n)$
- If $\text{sgn}(w^T x_i) \neq y_i$

$$w \leftarrow w + y_i x_i$$

Perceptron algorithm: Intuition

Say that w makes mistake on (x_i, y_i)

$$y_i w^T x_i < 0$$

Consider $w' = w + y_i x_i$

$$y_i (w')^T x_i = y_i w^T x_i + y_i^2 x_i^T x_i$$

if $x_i \neq 0$

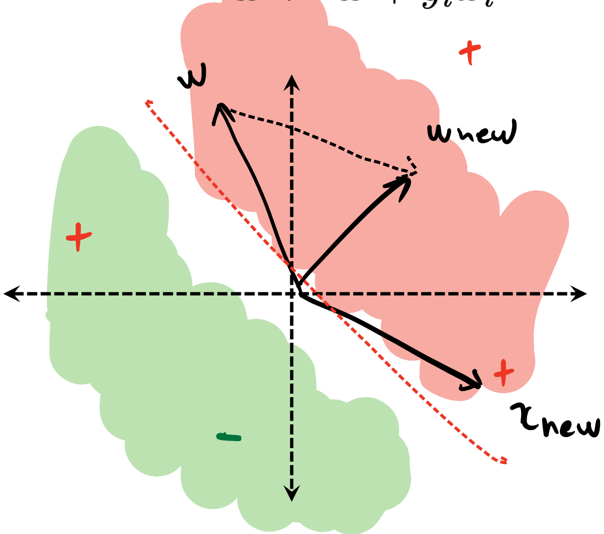
$$y_i (w')^T x_i > y_i w^T x_i$$

Perceptron algorithm: visually

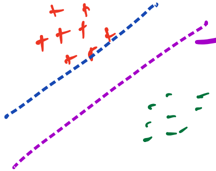
Repeat:

- Pick a data point $\boldsymbol{x}_i$ uniformly at random
- If $\operatorname{sgn}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_i) \neq y_i$

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + y_i \boldsymbol{x}_i$$



Related to question in class: if there are multiple ways to classify data:



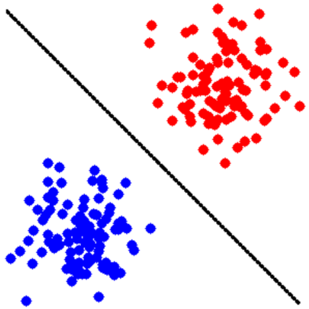
→ This might be better

Perceptron itself could find any of these hyperpl

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 regression

Logistic loss

$$F(w) = \frac{1}{n} \sum_{i=1}^{n} \ell_{\log}(y_i w^T x_i)$$

$$= \frac{1}{n} \sum_{i=1}^{n} \ln(1 + e^{-y_i w^T x_i})$$

Predicting probabilities

Instead of $\{\pm 1\}$, predict the probability.

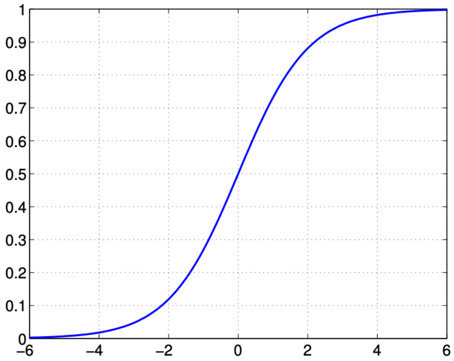
(i.e. regression on probability)

Sigmoid + linear model:

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

where $\sigma(z) = \dfrac{1}{1+e^{-z}}$

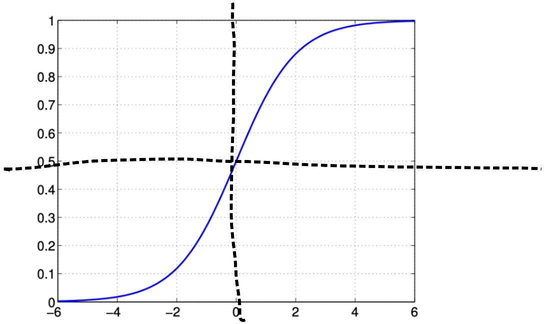
(sigmoid)



The sigmoid function

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

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



$$\mathbb{P}(y = -1 \mid \boldsymbol{x}; \boldsymbol{w}) = 1 - \mathbb{P}(y = +1 \mid \boldsymbol{x}; \boldsymbol{w})$$
$$= 1 - \sigma(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}) = \sigma(-\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x})$$

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

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 $\boldsymbol{x_1}, \cdots, \boldsymbol{x_n}$, as a function of some $\boldsymbol{w}$?

$$P(\boldsymbol{w}) = \prod_{i=1}^{N} \mathbb{P}(y_i \mid \boldsymbol{x_i}; \boldsymbol{w})$$

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

Maximum likelihood solution

$$\begin{aligned}
\boldsymbol{w}^* &= \operatorname*{argmax}_{\boldsymbol{w}} P(\boldsymbol{w}) = \operatorname*{argmax}_{\boldsymbol{w}} \prod_{i=1}^{n} \mathbb{P}(y_i \mid \boldsymbol{x_i}; \boldsymbol{w}) \\
&= \operatorname*{argmax}_{\boldsymbol{w}} \sum_{i=1}^{n} \ln \mathbb{P}(y_i \mid \boldsymbol{x_i}; \boldsymbol{w}) \\
&= \operatorname*{argmin}_{\boldsymbol{w}} \sum_{i=1}^{n} - \ln \mathbb{P}(y_i \mid \boldsymbol{x_i}; \boldsymbol{w}) \\
&= \operatorname*{argmin}_{\boldsymbol{w}} \sum_{i=1}^{n} \ln(1 + e^{-y_i \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x_i}}) \\
&= \operatorname*{argmin}_{\boldsymbol{w}} \sum_{i=1}^{n} \ell_{\text{logistic}}(y_i \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_i) \\
&= \operatorname*{argmin}_{\boldsymbol{w}} F(\boldsymbol{w})
\end{aligned}$$

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

SGD to logistic loss

$$
\begin{aligned}
\boldsymbol{w} &\leftarrow \boldsymbol{w} - \eta \tilde{\nabla} F(\boldsymbol{w}) \\
&= \boldsymbol{w} - \eta \nabla_{\boldsymbol{w}} \ell_{\text{logistic}}(y_i \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_i) \\
&= \boldsymbol{w} - \eta \left(\left. \frac{\partial \ell_{\text{logistic}}(z)}{\partial z} \right|_{z = y_i \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_i} \right) y_i \boldsymbol{x}_i \\
&= \boldsymbol{w} - \eta \left(\left. \frac{-e^{-z}}{1 + e^{-z}} \right|_{z = y_i \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_i} \right) y_i \boldsymbol{x}_i \\
&= \boldsymbol{w} + \eta \sigma(-y_i \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_i) y_i \boldsymbol{x}_i \\
&= \boldsymbol{w} + \eta \mathbb{P}(-y_i \mid \boldsymbol{x}_i; \boldsymbol{w}) y_i \boldsymbol{x}_i
\end{aligned}
$$

$\mathbb{E}[\tilde{\nabla} F(w)] = \nabla F(w)$

(i is drawn uniformly from $[n]$)

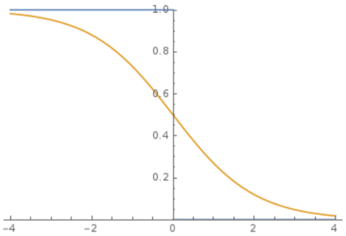
(chain rule)

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

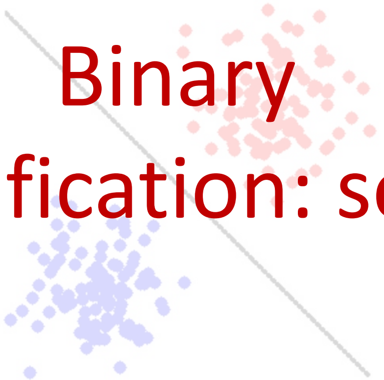
$$\sigma(-z) = 1 - \sigma(z) = 1 - \frac{1}{1+e^{-z}} = \frac{e^{-z}}{1+e^{-z}}$$

This is a *soft version of Perceptron!*

$\mathbb{P}(-y_i | \boldsymbol{x}_i; \boldsymbol{w})$ versus $\mathbb{I}[y_i \neq \text{sgn}(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_i)]$



Binary classification: so far



Supervised learning in one slide

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

Representation: What class of functions should we use?

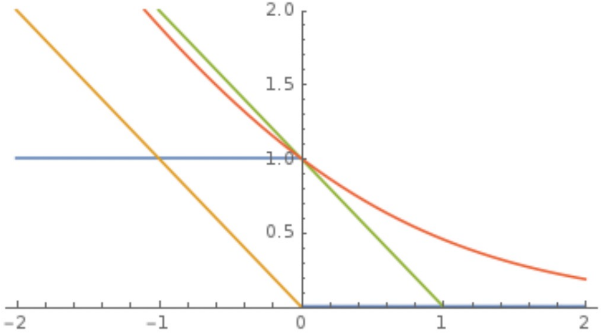
Optimization: How can we efficiently solve the empirical risk minimization problem?

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

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

Loss function

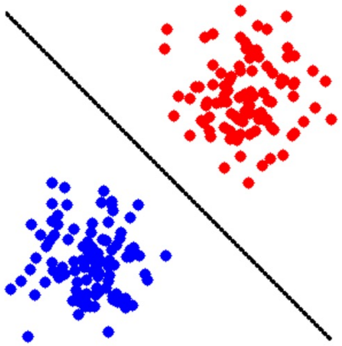
Use a **convex surrogate loss**



- 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)
- logistic loss $\ell_{\text{logistic}}(z) = \log(1 + \exp(-z))$ (used in logistic regression; the base of $\log$ doesn't matter)

Representation

Definition: The **function class of separating hyperplanes** is defined as
$\mathcal{F} = \{f(\boldsymbol{x}) = sign(\boldsymbol{w}^T\boldsymbol{x}) \colon \boldsymbol{w} \in \mathbb{R}^d\}$.



Optimization

Empirical risk minimization (ERM) problem:

$$\boldsymbol{w}^* = \operatorname*{argmin}_{\boldsymbol{w}\in\mathbb{R}^{\mathsf{d}}} \frac{1}{n}\sum_{i=1}^{n} \ell(y_i \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_i)$$

Solve using a suitable optimization algorithm:

- **GD:** $\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta \nabla F(\boldsymbol{w})$
- **SGD:** $\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta \tilde{\nabla} F(\boldsymbol{w})$ $\quad (\mathbb{E}[\tilde{\nabla} F(\boldsymbol{w})] = \nabla F(\boldsymbol{w}))$
- **Newton:** $\boldsymbol{w} \leftarrow \boldsymbol{w} - \left(\nabla^2 F(\boldsymbol{w})\right)^{-1} \nabla F(\boldsymbol{w})$

Generalization

Rich theory! Let's see a glimpse ☺

Generalization

Reviewing definitions

- Input space: $\mathcal{X}$
- Output space: $\mathcal{Y}$
- Predictor: $f(\boldsymbol{x}) : \mathcal{X} \rightarrow \mathcal{Y}$
- Distribution D over $(\boldsymbol{x}, y)$.
- Let D^n denote the distribution of n samples $\{(\boldsymbol{x}_i, y_i), i \in [n]\}$ drawn i.i.d. from D.
- Risk of a predictor $f(\boldsymbol{x})$ is $R(f) = \mathbb{E}_{(\boldsymbol{x},y)\sim D}\Big[\ell(f(\boldsymbol{x}), y)\Big]$
- Consider the 0-1 loss, $\ell(f(\boldsymbol{x}, y)) = \mathbb{1}(f(\boldsymbol{x}) \neq y)$.

Next time, we'll see some generalization theory!