CSCI 567: Machine Learning

Vatsal Sharan Spring 2024

Lecture 2, Jan 19



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?

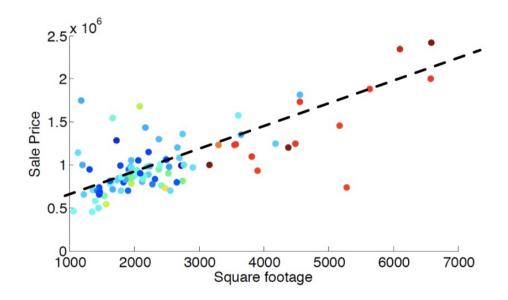
Generalization: Will the predictions of our model transfer

gracefully to unseen examples?

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

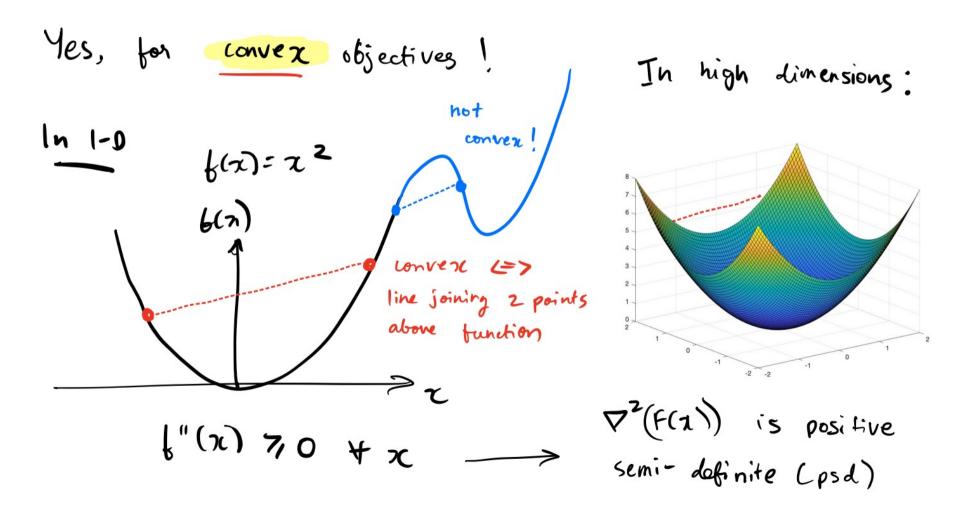
Linear regression

Predicted sale price = price_per_sqft × square footage + fixed_expense



How to solve this? Find stationary points

Are stationary points minimizers?



General least square solution

Objective

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

Find stationary points:

$$egin{aligned}
abla ext{RSS}(ilde{m{w}}) &= 2 \sum_i ilde{m{x}}_i (ilde{m{x}}_i^{ ext{T}} ilde{m{w}} - y_i) \propto \left(\sum_i ilde{m{x}}_i ilde{m{x}}_i^{ ext{T}}
ight) ilde{m{w}} - \sum_i ilde{m{x}}_i y_i \ &= (ilde{m{X}}^{ ext{T}} ilde{m{X}}) ilde{m{w}} - ilde{m{X}}^{ ext{T}} m{y} \end{aligned}$$

where

$$oldsymbol{ ilde{X}} = \left(egin{array}{c} ilde{oldsymbol{x}}_1^{\mathrm{T}} \ ilde{oldsymbol{x}}_2^{\mathrm{T}} \ dots \ ilde{oldsymbol{x}}_n^{\mathrm{T}} \end{array}
ight) \in \mathbb{R}^{n imes (d+1)}, \quad oldsymbol{y} = \left(egin{array}{c} y_1 \ y_2 \ dots \ y_n \end{array}
ight) \in \mathbb{R}^n$$

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

Optimization methods (continued)

Problem setup

Given: a function F(w)

Goal: minimize F(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 $t=0,1,2,\ldots$

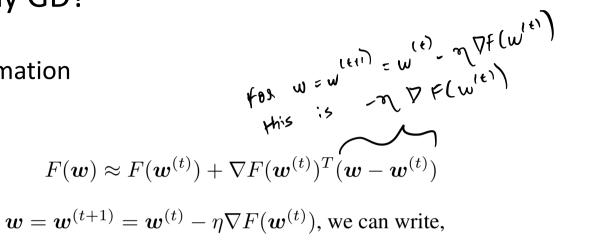
$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \eta \nabla F(\boldsymbol{w}^{(t)})$$

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

- 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

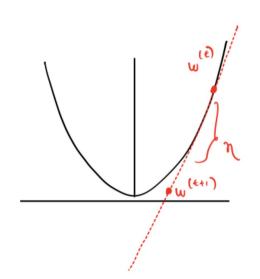


For $\boldsymbol{w} = \boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \eta \nabla F(\boldsymbol{w}^{(t)})$, we can write,

$$F(\boldsymbol{w}^{(t+1)}) \approx F(\boldsymbol{w}^{(t)}) - \eta \|\nabla F(\boldsymbol{w}^{(t)})\|_{2}^{2}$$

$$\implies F(\boldsymbol{w}^{(t+1)}) \lessapprox F(\boldsymbol{w}^{(t)})$$

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



Switch to Colab

```
🛆 optimization.jpvnb 🕱
 File Edit View Insert Runtime Tools Help
+ Code + Text
         this theta[1] = last theta[1] - eta * grad1
         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.
     for j in range(1,N):
        ax.annotate('', xy=theta[j], xytext=theta[j-1],
                        arrowprops={'arrowstyle': '->', 'color': 'orange', 'lw': 1},
                        va='center', ha='center')
     ax.scatter(*zip(*theta), facecolors='none', edgecolors='r', lw=1.5)
     # Labels, titles and a legend.
     ax.set xlabel(r'$w 1$')
     ax.set_ylabel(r'$w_2$')
     ax.set_title('objective function')
     plt.show()
 ₽
                                     objective function
```

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

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

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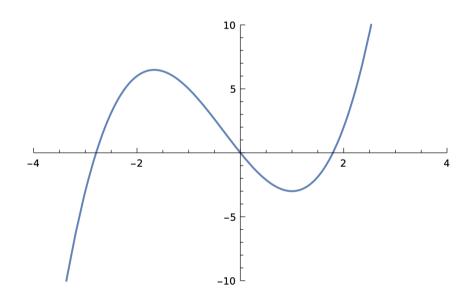
Even for *nonconvex objectives*, some guarantees exist: e.g. how many iterations t (in terms of ε) are needed to achieve

$$\|\nabla F(\mathbf{w}^{(t)})\| \leq \varepsilon$$

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?

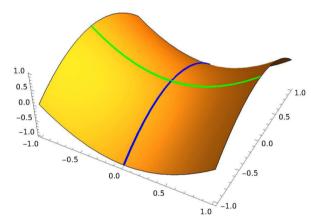
A stationary point can be a local minimizer or even a local/global maximizer (but the latter is not an issue for GD).



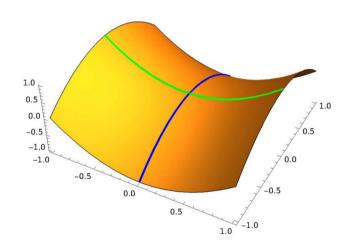
 $f(w) = w^3 + w^2 - 5w$

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

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



This is known as a saddle point

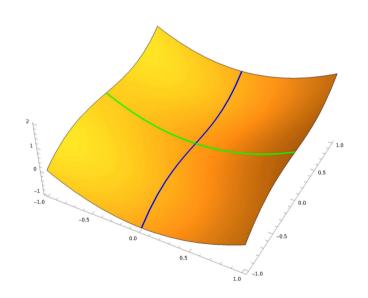




- but GD gets stuck at (0,0) only if initialized along the green direction
- so not a real issue especially when initialized randomly

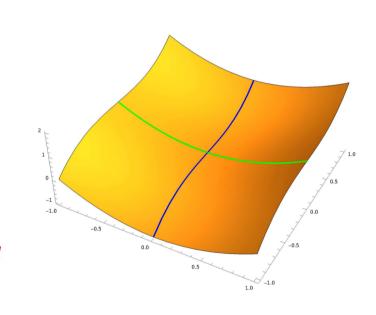
But not all saddle points look like a "saddle" ...

- $f(\mathbf{w}) = w_1^2 + w_2^3$
- $\nabla f(\mathbf{w}) = (2w_1, 3w_2^2)$
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- 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 $w_2 > 0$ 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[ilde{
abla}F(oldsymbol{w}^{(t)})
ight] =
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 (unbiasedness)

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- 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

(iD: 1st oxder Taylor

$$f(w) \times f(w^{(t)}) + \nabla f(w^{(t)})^{7}(w-w^{(t)})$$

 $f(y) = f(x) + f'(x) |y-x| + f''(x) (y-x)^{2}$

$$f(w) = f(x) + f'(x) | y - x \rangle + f''(x) | (w - w^{(t)}) \rangle$$

$$f(w) = f(x) + f'(x) | y - x \rangle + f''(x) | (y - x)^{2} \rangle$$

$$f(w) = f(w^{(t)}) + \nabla f(w^{(t)}) | T(w - w^{(t)}) \rangle + \frac{1}{2} (w - w^{(t)}) | T(w - w^{(t)}) \rangle$$
where $H_{t} = \nabla^{2} F(w^{(t)}) \in \mathbb{R}^{d+d}$ is $Hessian$ of F at $w^{(t)}$

$$F(w^{(t)}) \in \mathbb{R}^{n \times n} \text{ is Hessian}$$

$$(H_t)_{i,j} = \frac{\int_{-\infty}^{2} F(w)}{\partial w_i w_j} \Big|_{W=w^{(t)}}$$

Define
$$F(w) = 2nd$$
 order approximation

Set $\nabla F(w) = 0$

$$\frac{dF(w^{(t)})}{dw} = 0$$

$$\frac{d}{dw} \left(\frac{1}{2} w^T H_{E} w \right) = H_{E} w$$

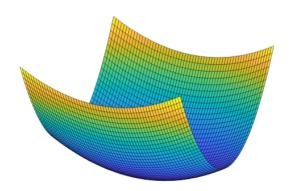
$$\frac{d}{dw} \left(-\frac{1}{2} w H_{E} w \right) = -\frac{1}{2} H_{E} w^{(t)}$$

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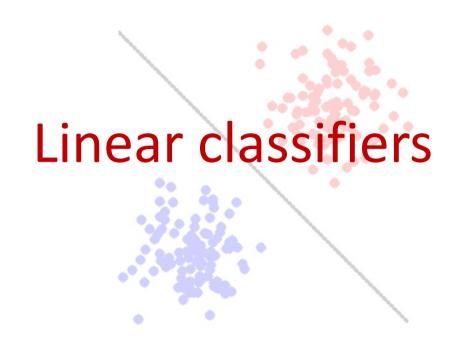
He
$$w = He w^{(f)} - \nabla F(w^{(f)})$$

Hewton's method:
$$w^{(t+1)} = w^{(t)} - H_{\varepsilon}^{-1} \nabla F(w^{(t)})$$
 $\omega^{(t+1)} = w^{(t)} - H_{\varepsilon}^{-1} \nabla F(w^{(t)})$
 $\omega^{(t+1)} = w^{(t)} - \eta \nabla F(w^{(t)})$

Newton's Method	Gradient Descent
No learning rate	Need to tune learning rate
Super fast convergence	Slower convergence
Know and invert Hessian	Fast!
(inversion takes $O(d^3)$ time	(only takes $O(d)$ time)
naively)	



If optimization objective is very flat along a certain direction, 2nd order methods maybe better



The Setup

Recall the setup:

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

This lecture: binary classification

- Number of classes: 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} .

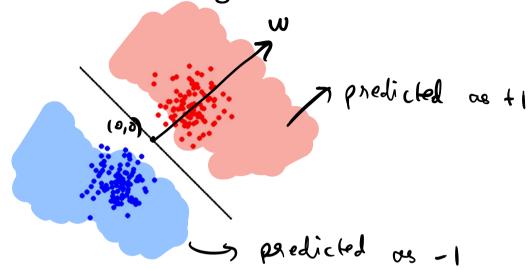
We continue with linear models, but how to predict a label using $w^{\mathrm{T}}x$?

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

$$\mathsf{sign}(oldsymbol{w}^{\mathrm{T}}oldsymbol{x}) = \left\{ egin{array}{ll} +1 & \mathsf{if} \ oldsymbol{w}^{\mathrm{T}}oldsymbol{x} > 0 \ -1 & \mathsf{if} \ oldsymbol{w}^{\mathrm{T}}oldsymbol{x} \leq 0 \end{array}
ight.$$

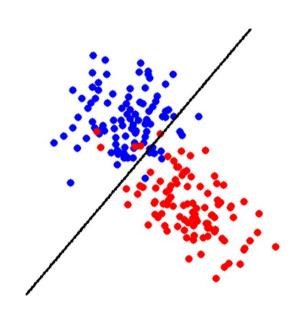
(Sometimes use sgn for sign too.)

Representation: Choosing the function class

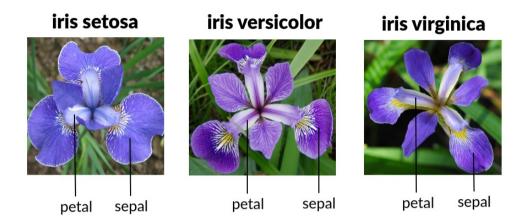


Definition: The function class of separating hyperplanes (on linear classifiens) is: $f(x) = sign(w^{T}x) : w \in \mathbb{R}^{d}$

Still makes sense for "almost" linearly separable data

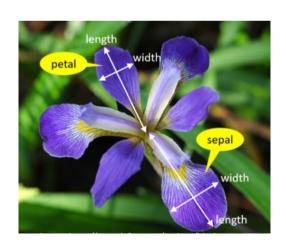


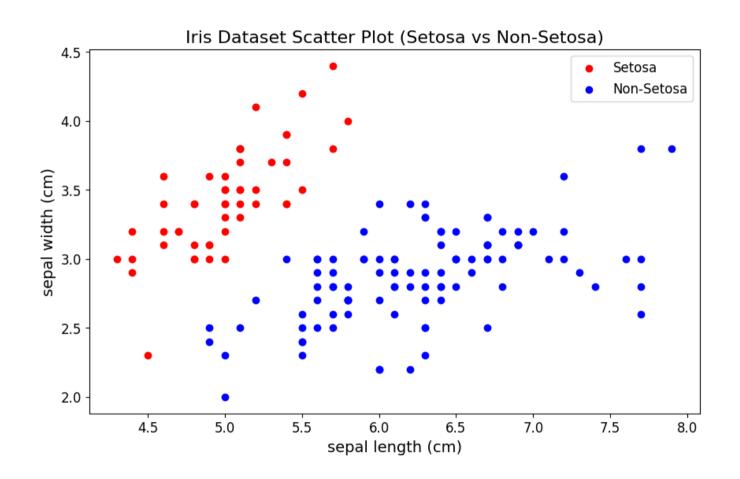
Iris dataset



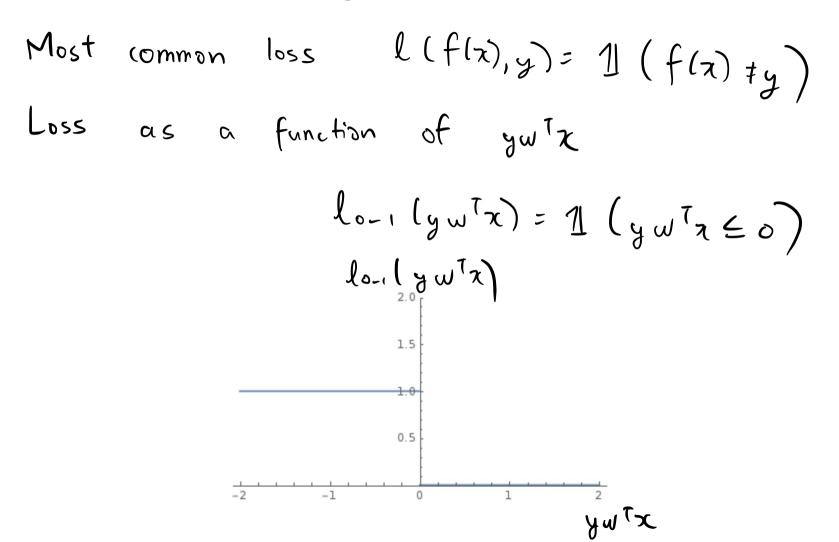
Features:

- 1. Sepal length
- 2. Sepal width



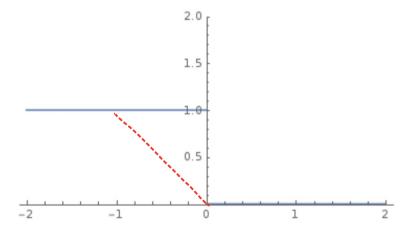


Choosing the loss function



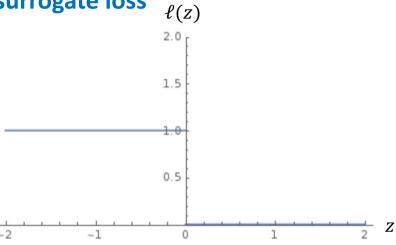
Choosing the loss function: minimizing 0/1 loss is hard

However, 0-1 loss is not convex.

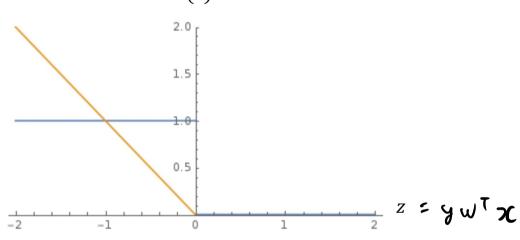


Even worse, minimizing 0-1 loss is NP-hard in general.

Solution: use a **convex surrogate loss**

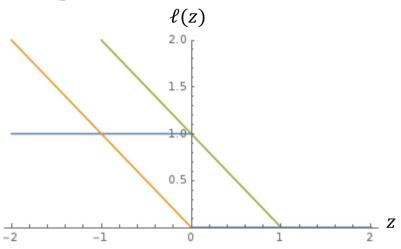


Solution: use a **convex surrogate loss** _{ℓ}



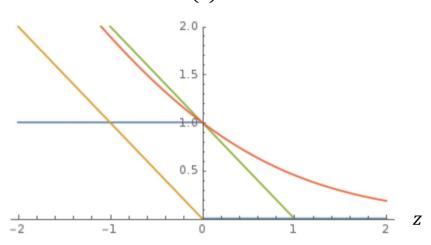
• perceptron loss $\ell_{\mathsf{perceptron}}(z) = \max\{0, -z\}$ (used in Perceptron)

Solution: use a convex surrogate loss



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

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



- perceptron loss $\ell_{perceptron}(z) = \max\{0, -z\}$ (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:

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

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!

Psychologist Shows Embryo

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 embryo of an electronic computer named the **Perceptron** of Computer Despective Cepting of Completed in about a Read and Grow Werrcepting of Cepting of Completed in about a Read and Grow Werrcepting of Cepting o living mechanism able to "perceive, identify recognize and surroundings without human training or control."

NEW NAVY DEVICE LEARNS BY DOING

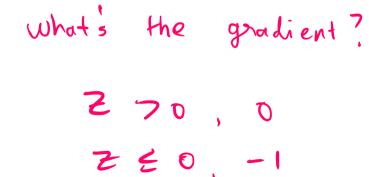
of Computer Designed to
Read and Grow Wiser

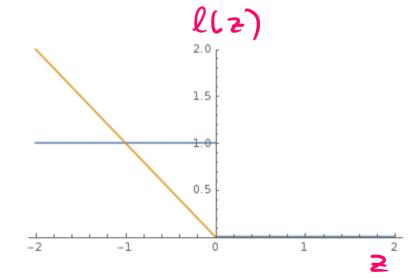
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Recall perceptron loss





Applying GD to perceptron loss

Applying SGD to perceptron loss

How to get stochastic gradient?

$$\nabla F(w^{(t)}) = -1 [y_i w^7 x_i \leq 0] y_i x_i$$

$$IE[\nabla F(w^{(t)}] = \frac{1}{n} \frac{2}{x_i} - 1 [y_i w^7 x_i \leq 0] y_i x_i$$

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

ShD update: w = w + of 1 [yiwtzi = o]yizi

Perceptron algorithm

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

- 1. Initialize w = 0
- 2. Repeat
 - Pick $x_i \sim \text{Unif}(x_1, \dots, x_n)$
 - If $\operatorname{sgn}(\boldsymbol{w}^T\boldsymbol{x_i}) \neq y_i$

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + y_i \boldsymbol{x_i}$$

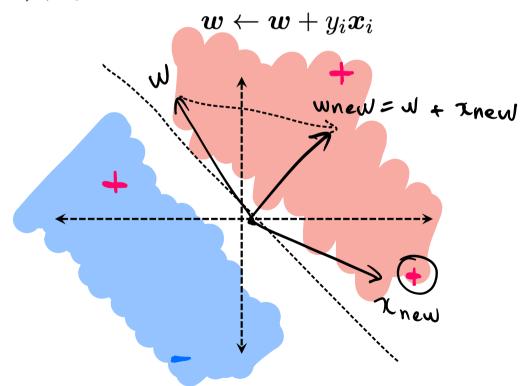
Perceptron algorithm: Intuition

that w makes mistake on (zi, yi) yiwiti Lo Consider w'= w+ yixi y; (w') Tz; = y; w Tx; + y; z z; Tz; ·. if i = a y ξ (w') 'τ' > y; w'τ;

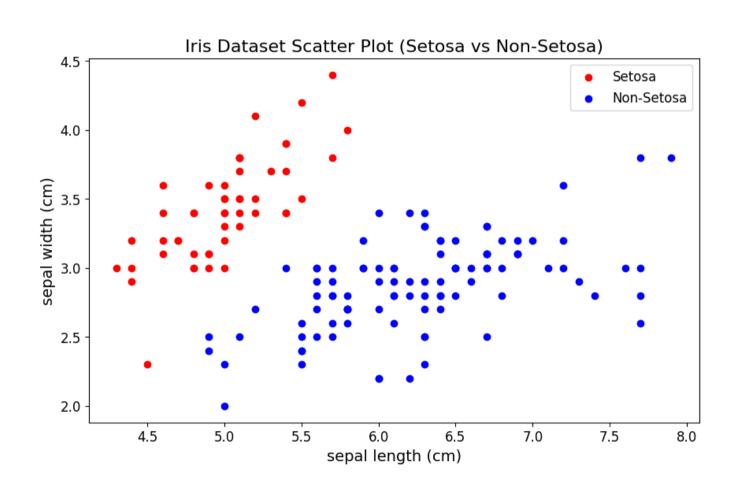
Perceptron algorithm: visually

Repeat:

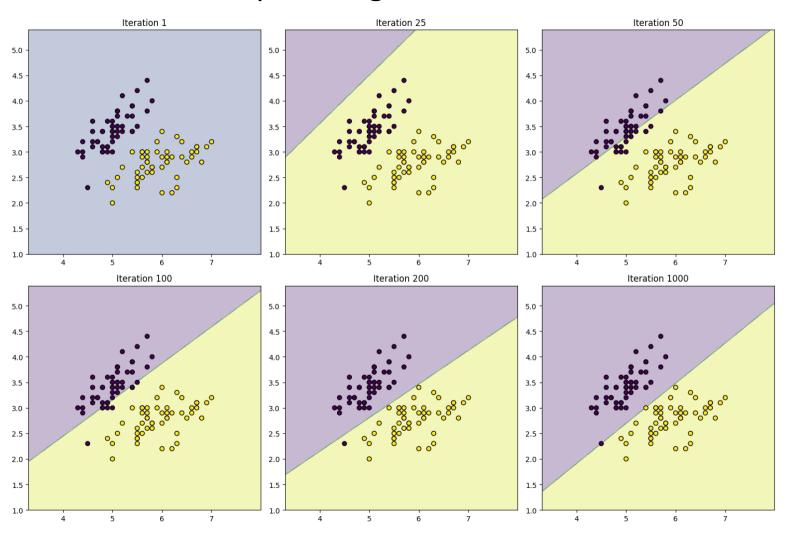
- ullet Pick a data point $oldsymbol{x}_i$ uniformly at random
- If $\operatorname{sgn}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_i) \neq y_i$



Perceptron algorithm: Iris dataset



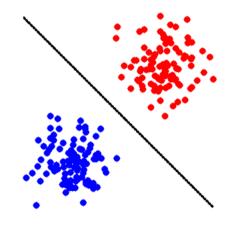
Perceptron algorithm: Iris dataset



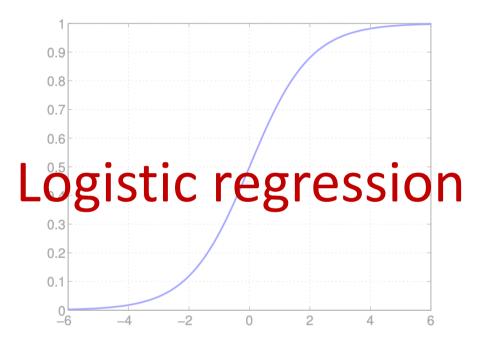
HW1: Theory for perceptron!

(HW 1) If training set is linearly separable

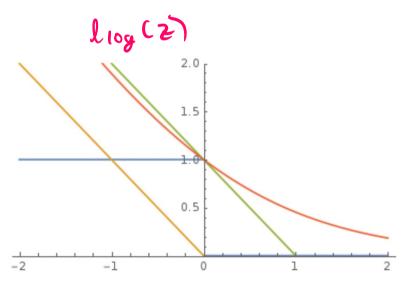
- Perceptron converges in a finite number of steps
- training error is 0



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



Logistic loss



Predicting probabilities

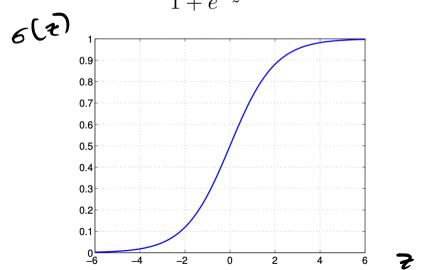
Instead of predicting the $\{\pm 1\}$ label, predict the probability (i.e. regression on probability).

Sigmoid + linear model:

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

where

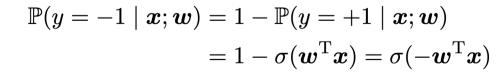
$$\sigma(z) = \frac{1}{1 + e^{-z}}$$
 (Sigmoid function)



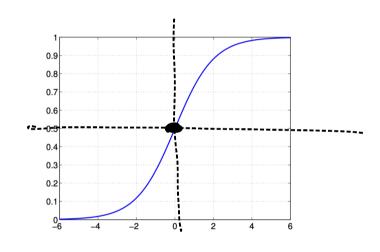
The sigmoid function

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 $w^Tx \Rightarrow$ larger $\sigma(w^Tx) \Rightarrow$ higher confidence in label 1
- $\sigma(z) + \sigma(-z) = 1$ for all z
- ullet Therefore, the probability of label -1 is



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



Maximum likelihood estimation

What we observe are labels, not probabilities.

Take a probabilistic view

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

Specifically, what is the probability of seeing labels y_1, \dots, y_n given x_1, \dots, x_n , as a function of some w?

$$P(w) = \prod_{i=1}^{n} \mathbb{P}(y_i \mid x_i; w)$$
 all datopoints are independent and identically distributed

MLE: find w^* that maximizes the probability P(w)

Maximum likelihood solution

$$w^* = \underset{w}{\operatorname{argmax}} P(w) = \underset{w}{\operatorname{argmax}} \prod_{i=1}^n \mathbb{P}(y_i \mid x_i; w)$$

$$= \underset{w}{\operatorname{argmin}} \sum_{i=1}^n \ln \mathbb{P}(y_i \mid x_i; w)$$

$$= \underset{w}{\operatorname{argmin}} \sum_{i=1}^n -\ln \mathbb{P}(y_i \mid x_i; w)$$

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

$$= \underset{w}{\operatorname{argmin}} \sum_{i=1}^n \ell_{\operatorname{logistic}}(y_i w^T x_i)$$

$$= \underset{w}{\operatorname{argmin}} F(w)$$

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

SGD to logistic loss

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

This is a soft version of Perceptron!

$$\mathbb{P}(-y_i|oldsymbol{x}_i;oldsymbol{w})$$
 versus $\mathbb{I}[y_i
eq \operatorname{sgn}(oldsymbol{w}^{\mathrm{T}}oldsymbol{x}_i)]$

