CSCI567 Machine Learning (Fall 2021)

Prof. Haipeng Luo

U of Southern California

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Administration

- HW 1 is due on Tue, 9/14.
- recall the late day policy: 3 in total, at most 1 for each homework

Outline

Outline

Regression

Predicting a continuous outcome variable using past observations

- temperature, amount of rainfall, house price, etc.

Key difference from classification

- continuous vs discrete
- measure *prediction errors* differently.
- lead to quite different learning algorithms.

Linear Regression: regression with linear models: $f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$

Least square solution

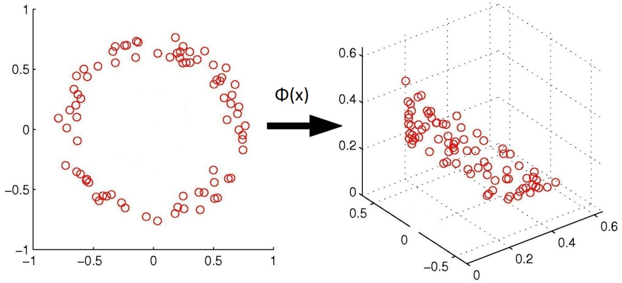
$$
\begin{aligned}
\boldsymbol{w}^* &= \underset{\boldsymbol{w}}{\operatorname{argmin}}\, \mathrm{RSS}(\boldsymbol{w}) \\
&= \underset{\boldsymbol{w}}{\operatorname{argmin}}\, \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|_2^2 \\
&= \left(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}\right)^{-1}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{y}
\end{aligned}
$$

$$
\boldsymbol{X} = \begin{pmatrix} \boldsymbol{x}_1^{\mathrm{T}} \\ \boldsymbol{x}_2^{\mathrm{T}} \\ \vdots \\ \boldsymbol{x}_{\mathsf{N}}^{\mathrm{T}} \end{pmatrix}, \quad \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{\mathsf{N}} \end{pmatrix}
$$

Two approaches to find the minimum:

- find **stationary points** by setting gradient $= \mathbf{0}$
- "**complete the square**"

Regression with nonlinear basis



Model: $f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x})$ where $\boldsymbol{w} \in \mathbb{R}^M$

Similar least square solution: $\boldsymbol{w}^* = \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y}$

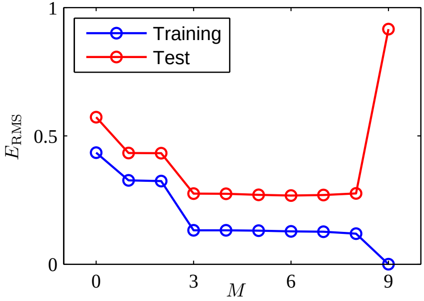
Underfitting and Overfitting

$M \leq 2$ is *underfitting* the data

- large training error
- large test error

$M \geq 9$ is *overfitting* the data

- small training error
- **large test error**



How to prevent overfitting? more data + regularization

$$\boldsymbol{w}^* = \operatorname*{argmin}_{\boldsymbol{w}} \left(\mathrm{RSS}(\boldsymbol{w}) + \lambda \|\boldsymbol{w}\|_2^2\right) = \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi} + \lambda \boldsymbol{I}\right)^{-1} \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y}$$

General idea to derive ML algorithms

Step 1. Pick a set of **models** $\mathcal{F}$

- e.g. $\mathcal{F} = \{f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{D}}\}$
- e.g. $\mathcal{F} = \{f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{\Phi}(\boldsymbol{x}) \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{M}}\}$

Step 2. Define **error/loss** $L(y', y)$

Step 3. Find **(regularized) empirical risk minimizer (ERM)**:

$$\boldsymbol{f}^* = \operatorname*{argmin}_{f \in \mathcal{F}} \sum_{n=1}^{N} L(f(x_n), y_n) + \lambda R(f)$$

ML becomes optimization

Today: another exercise of this recipe + a closer look at Step 3

Outline

Classification

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, fraud or not, price up or down...)

We have discussed **nearest neighbor classifier**:

- require carrying the training set
- more like a heuristic

Deriving classification algorithms

Let's follow the recipe:

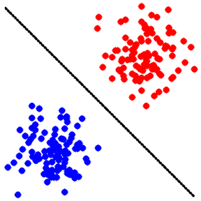
Step 1. Pick a set of models $\mathcal{F}$.

Again try 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:

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

(Sometimes use sgn for sign too.)



The models

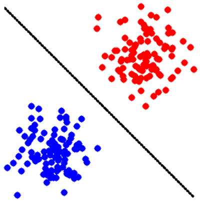
The set of **(separating) hyperplanes**:

$$\mathcal{F} = \{f(\boldsymbol{x}) = \mathsf{sgn}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}) \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{D}}\}$$

Good choice for *linearly separable* data, i.e., $\exists \boldsymbol{w}$ s.t.

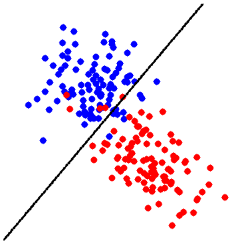
$$\mathsf{sgn}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x_n}) = y_n \quad \text{or} \quad y_n\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x_n} > 0$$

for all $n \in [N]$.



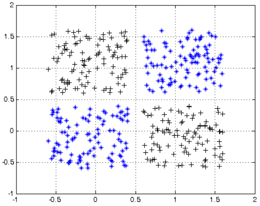
The models

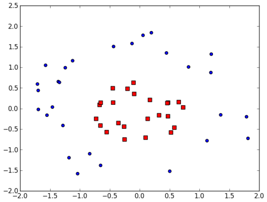
Still makes sense for “almost” linearly separable data



The models

For clearly not linearly separable data,





Again can apply a **nonlinear mapping** $\mathbf{\Phi}$:

$$\mathcal{F} = \{f(\boldsymbol{x}) = \text{sgn}(\boldsymbol{w}^{\mathrm{T}}\mathbf{\Phi}(\boldsymbol{x})) \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{M}}\}$$

More discussions in the next two lectures.

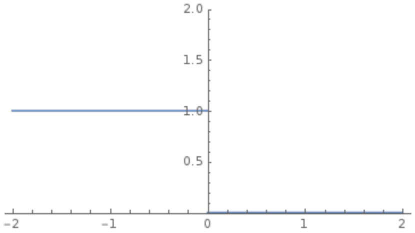
0-1 Loss

Step 2. Define error/loss $L(y', y)$.

Most natural one for classification: **0-1 loss** $L(y', y) = \mathbb{I}[y' \neq y]$

For classification, more convenient to look at the loss **as a function of** $y\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$. That is, with

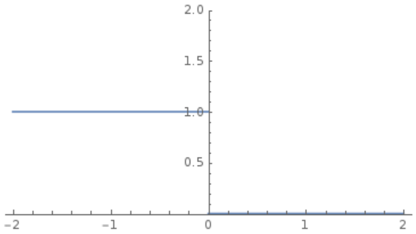
$$\ell_{\text{0-1}}(z) = \mathbb{I}[z \leq 0]$$



the loss for hyperplane $\boldsymbol{w}$ on example $(\boldsymbol{x}, y)$ is $\ell_{\text{0-1}}(y\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x})$

Minimizing 0-1 loss is hard

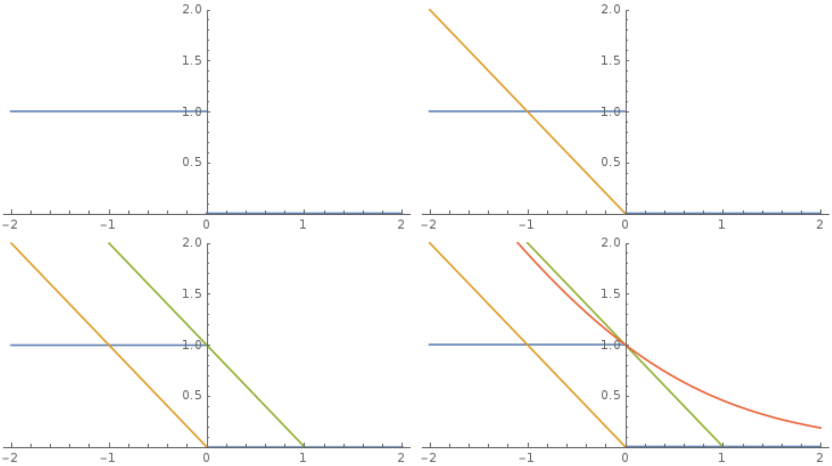
However, 0-1 loss is *not convex*.



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

Surrogate Losses

Solution: find a **convex surrogate loss**



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

ML becomes convex optimization

Step 3. Find ERM:

$$\boldsymbol{w}^* = \operatorname*{argmin}_{\boldsymbol{w}\in\mathbb{R}^{\mathsf{D}}} \sum_{n=1}^{N} \ell(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) = \operatorname*{argmin}_{\boldsymbol{w}\in\mathbb{R}^{\mathsf{D}}} \frac{1}{N} \sum_{n=1}^{N} \ell(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)$$

where $\ell(\cdot)$ can be perceptron/hinge/logistic loss

- *no closed-form* in general (unlike linear regression)
- can apply general convex optimization methods

Note: minimizing perceptron loss *does not really make sense* (try $\boldsymbol{w} = \mathbf{0}$), but the algorithm derived from this perspective does.

Outline

Numerical optimization

Problem setup

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

First-order optimization methods

Two simple yet extremely popular methods

- **Gradient Descent (GD)**: simple and fundamental
- **Stochastic Gradient Descent (SGD)**: faster, effective for large-scale problems

Gradient is sometimes referred to as *first-order* information of a function. Therefore, these methods are called *first-order methods*.

Gradient Descent (GD)

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

An example

Example: $F(\boldsymbol{w}) = 0.5(w_1^2 - w_2)^2 + 0.5(w_1 - 1)^2$. Gradient is

$$\frac{\partial F}{\partial w_1} = 2(w_1^2 - w_2)w_1 + w_1 - 1 \qquad \frac{\partial F}{\partial w_2} = -(w_1^2 - w_2)$$

GD:

- Initialize $w_1^{(0)}$ and $w_2^{(0)}$ (to be 0 or *randomly*), $t = 0$
- do

$$\begin{aligned} w_1^{(t+1)} &\leftarrow w_1^{(t)} - \eta \left[2({w_1^{(t)}}^2 - w_2^{(t)}) w_1^{(t)} + w_1^{(t)} - 1 \right] \\ w_2^{(t+1)} &\leftarrow w_2^{(t)} - \eta \left[-({w_1^{(t)}}^2 - w_2^{(t)}) \right] \\ t &\leftarrow t + 1 \end{aligned}$$

- until $F(w^{(t)})$ **does not change much** or t **reaches a fixed number**

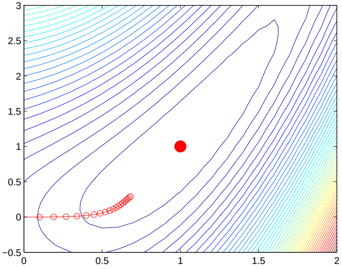
Why GD?

Intuition: by first-order **Taylor approximation**

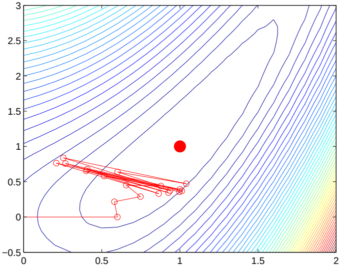
$$F(\boldsymbol{w}) \approx F(\boldsymbol{w}^{(t)}) + \nabla F(\boldsymbol{w}^{(t)})^{\mathrm{T}}(\boldsymbol{w} - \boldsymbol{w}^{(t)})$$

GD ensures

$$F(\boldsymbol{w}^{(t+1)}) \approx F(\boldsymbol{w}^{(t)}) - \eta \|\nabla F(\boldsymbol{w}^{(t)})\|_2^2 \leq F(\boldsymbol{w}^{(t)})$$



reasonable η decreases function value



but large η is unstable

Stochastic Gradient Descent (SGD)

GD: keep moving in the negative gradient direction

SGD: keep moving in some *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.

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

Key point: it could be *much faster to obtain a stochastic gradient!* (examples coming soon)

Convergence guarantees — convex objectives

Many for both GD and SGD on **convex objectives**.

They tell you how many iterations t (in terms of ϵ) needed to achieve

$$F(\boldsymbol{w}^{(t)}) - F(\boldsymbol{w}^*) \leq \epsilon$$

- usually SGD needs more iterations
- but then again each iteration takes less time

Convergence guarantees — nonconvex objectives

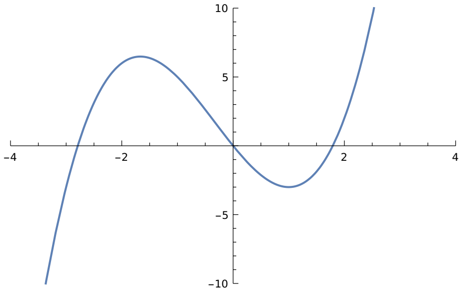
Even for *nonconvex objectives*, some guarantees exist: e.g. how many iterations t (in terms of ϵ) needed to achieve

$$\|\nabla F(\boldsymbol{w}^{(t)})\| \leq \epsilon$$

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

Convergence guarantees — nonconvex objectives

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

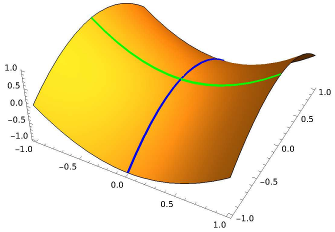


$$f(w) = w^3 + w^2 - 5w$$

Convergence guarantees — nonconvex objectives

A stationary point can also be *neither a local minimizer nor a local maximizer!* This is called a **saddle point**.

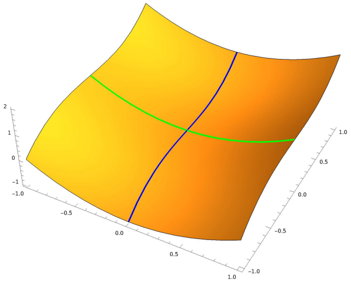
- $f(\boldsymbol{w}) = w_1^2 - w_2^2$
- $\nabla f(\boldsymbol{w}) = (2w_1, -2w_2)$
- so $\boldsymbol{w} = (0, 0)$ is stationary
- local max for blue direction $(w_1 = 0)$
- local min for green direction $(w_2 = 0)$
- but GD gets stuck at $(0, 0)$ only if initialized along the green direction
- so not a real issue especially *when initialized randomly*



Convergence guarantees — nonconvex 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 ($w_1 = 0$)
- 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*.

Convergence guarantees

Summary:

- 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

Recall the intuition of GD: we look at first-order **Taylor approximation**

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

What if we look at *second-order* Taylor approximation?

$$F(\boldsymbol{w}) \approx F(\boldsymbol{w}^{(t)}) + \nabla F(\boldsymbol{w}^{(t)})^{\mathrm{T}}(\boldsymbol{w} - \boldsymbol{w}^{(t)}) + \frac{1}{2}(\boldsymbol{w} - \boldsymbol{w}^{(t)})^{\mathrm{T}}\boldsymbol{H}_t(\boldsymbol{w} - \boldsymbol{w}^{(t)})$$

where $\boldsymbol{H}_t = \nabla^2 F(\boldsymbol{w}^{(t)}) \in \mathbb{R}^{\mathsf{D}\times\mathsf{D}}$ is the *Hessian* of F at $\boldsymbol{w}^{(t)}$, i.e.,

$$H_{t,ij} = \frac{\partial^2 F(\boldsymbol{w})}{\partial w_i \partial w_j}\Big|_{\boldsymbol{w}=\boldsymbol{w}^{(t)}}$$

(think "second derivative" when $D = 1$)

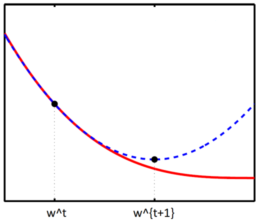
Newton method

If we minimize the second-order approximation (via "complete the square")

$$F(\boldsymbol{w})$$
$$\approx F(\boldsymbol{w}^{(t)}) + \nabla F(\boldsymbol{w}^{(t)})^{\mathrm{T}}(\boldsymbol{w} - \boldsymbol{w}^{(t)}) + \frac{1}{2}(\boldsymbol{w} - \boldsymbol{w}^{(t)})^{\mathrm{T}}\boldsymbol{H}_t(\boldsymbol{w} - \boldsymbol{w}^{(t)})$$
$$= \frac{1}{2}\left(\boldsymbol{w} - \boldsymbol{w}^{(t)} + \boldsymbol{H}_t^{-1}\nabla F(\boldsymbol{w}^{(t)})\right)^{\mathrm{T}} \boldsymbol{H}_t \left(\boldsymbol{w} - \boldsymbol{w}^{(t)} + \boldsymbol{H}_t^{-1}\nabla F(\boldsymbol{w}^{(t)})\right) + \text{cnt}$$

for convex F (so H_t is *positive semidefinite*)
we obtain **Newton method**:

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



Comparing GD and Newton

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

$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \boldsymbol{H}_t^{-1} \nabla F(\boldsymbol{w}^{(t)}) \tag{Newton}$$

Both are iterative optimization procedures, but Newton method

- has no learning rate η (so **no tuning needed!**)
- converges **super fast** in terms of #iterations (for convex objectives)
  - e.g. how many iterations needed when applied to a quadratic?
- computing Hessian in each iteration is *very slow* though
- does not really make sense for *nonconvex objectives* (but generally Hessian can be useful for escaping saddle points)

Outline

Recall the perceptron loss

$$
\begin{aligned}
F(\boldsymbol{w}) &= \frac{1}{N}\sum_{n=1}^{N} \ell_{\textsf{perceptron}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) \\
&= \frac{1}{N}\sum_{n=1}^{N} \max\{0, -y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n\}
\end{aligned}
$$

Let's approximately minimize it with GD/SGD.

Applying GD to perceptron loss

Objective

$$F(\boldsymbol{w}) = \frac{1}{N}\sum_{n=1}^{N} \max\{0, -y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n\}$$

Gradient (or really *sub-gradient*) is

$$\nabla F(\boldsymbol{w}) = \frac{1}{N}\sum_{n=1}^{N} -\mathbb{I}[y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n \leq 0] y_n \boldsymbol{x}_n$$

(only misclassified examples contribute to the gradient)

GD update

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \frac{\eta}{N}\sum_{n=1}^{N} \mathbb{I}[y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n \leq 0] y_n \boldsymbol{x}_n$$

Slow: each update makes one pass of the entire training set!

Applying SGD to perceptron loss

How to construct a stochastic gradient?

One common trick: pick one example $n \in [N]$ uniformly at random, let

$$\tilde{\nabla} F(\boldsymbol{w}^{(t)}) = -\mathbb{I}[y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n \leq 0] y_n \boldsymbol{x}_n$$

clearly unbiased (convince yourself).

SGD update:

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \eta \mathbb{I}[y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n \leq 0] y_n \boldsymbol{x}_n$$

Fast: each update touches only one data point!

Conveniently, objective of most ML tasks is a *finite sum* (over each training point) and the above trick applies!

The Perceptron Algorithm

Perceptron algorithm is SGD with $\eta = 1$ applied to perceptron loss:

Repeat:

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

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + y_n\boldsymbol{x}_n$$

Note:

- $\boldsymbol{w}$ is always a *linear combination* of the training examples
- why $\eta = 1$? Does not really matter in terms of prediction of $\boldsymbol{w}$

Why does it make sense?

If the current weight $\boldsymbol{w}$ makes a mistake

$$y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n < 0$$

then after the update $\boldsymbol{w}' = \boldsymbol{w} + y_n \boldsymbol{x}_n$ we have

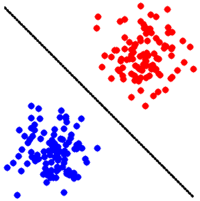
$$y_n {\boldsymbol{w}'}^{\mathrm{T}} \boldsymbol{x}_n = y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n + y_n^2 \boldsymbol{x}_n^{\mathrm{T}} \boldsymbol{x}_n \geq y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n$$

Thus it is more likely to get it right after the update.

Any theory?

(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.

Outline

A simple view

In one sentence: find the minimizer of

$$F(\boldsymbol{w}) = \frac{1}{N}\sum_{n=1}^{N} \ell_{\textsf{logistic}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)$$
$$= \frac{1}{N}\sum_{n=1}^{N} \ln(1 + e^{-y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n})$$

Before optimizing it: *why logistic loss? and why "regression"?*

Predicting probability

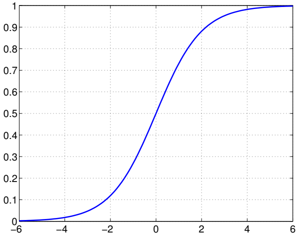
Instead of predicting a discrete label, can we *predict the probability of each label?* i.e. regress the probabilities

One way: **sigmoid function + linear model**

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

where σ is the sigmoid function:

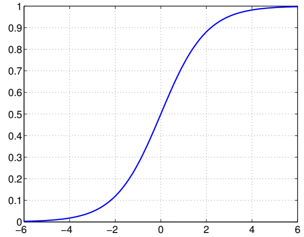
$$\sigma(z) = \frac{1}{1 + e^{-z}}$$



Properties

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 $\operatorname{sgn}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x})$
- 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



The probability of label -1 is naturally

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

and thus

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

How to regress with discrete labels?

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 label $y_1, \cdots, y_n$ given $x_1, \cdots, x_n$, as a function of some $\boldsymbol{w}$?

$$P(\boldsymbol{w}) = \prod_{n=1}^{N} \mathbb{P}(y_n \mid \boldsymbol{x_n}; \boldsymbol{w})$$

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

The MLE solution

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

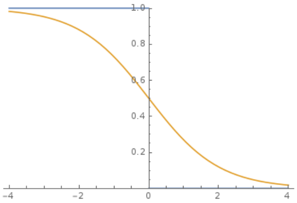
i.e. *minimizing logistic loss is exactly doing MLE for the sigmoid model!*

Let's apply SGD again

$$
\begin{aligned}
\boldsymbol{w} &\leftarrow \boldsymbol{w} - \eta \tilde{\nabla} F(\boldsymbol{w}) \\
&= \boldsymbol{w} - \eta \nabla_{\boldsymbol{w}} \ell_{\text{logistic}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) \qquad (n \in [N] \text{ is drawn u.a.r.}) \\
&= \boldsymbol{w} - \eta \left(\left. \frac{\partial \ell_{\text{logistic}}(z)}{\partial z} \right|_{z = y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n} \right) y_n \boldsymbol{x}_n \\
&= \boldsymbol{w} - \eta \left(\left. \frac{-e^{-z}}{1 + e^{-z}} \right|_{z = y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n} \right) y_n \boldsymbol{x}_n \\
&= \boldsymbol{w} + \eta \sigma(-y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) y_n \boldsymbol{x}_n \\
&= \boldsymbol{w} + \eta \mathbb{P}(-y_n \mid \boldsymbol{x}_n; \boldsymbol{w}) y_n \boldsymbol{x}_n
\end{aligned}
$$

This is a *soft version of Perceptron!*

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



Applying Newton to logistic loss

$$\nabla_{\boldsymbol{w}} \ell_{\text{logistic}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) = -\sigma(-y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) y_n \boldsymbol{x}_n$$

$$\begin{aligned}
\nabla^2_{\boldsymbol{w}} \ell_{\text{logistic}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) &= \left(\left.\frac{\partial \sigma(z)}{\partial z}\right|_{z=-y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n} \right) y_n^2 \boldsymbol{x}_n \boldsymbol{x}_n^{\mathrm{T}} \\
&= \left(\left.\frac{e^{-z}}{(1+e^{-z})^2}\right|_{z=-y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n} \right) \boldsymbol{x}_n \boldsymbol{x}_n^{\mathrm{T}} \\
&= \sigma(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) \left(1 - \sigma(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)\right) \boldsymbol{x}_n \boldsymbol{x}_n^{\mathrm{T}}
\end{aligned}$$

Exercises:

- why is the Hessian of logistic loss positive semidefinite?
- can we apply Newton method to perceptron/hinge loss?

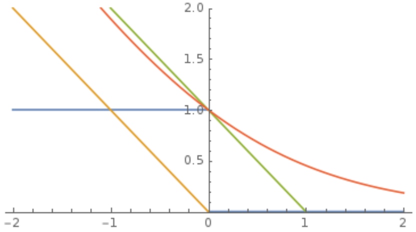
Summary

Linear models for classification:

Step 1. Model is the set of **separating hyperplanes**

$$\mathcal{F} = \{f(\boldsymbol{x}) = \mathsf{sgn}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}) \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{D}}\}$$

Step 2. Pick the **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)

Step 3. Find empirical risk minimizer (ERM):

$$\boldsymbol{w}^* = \operatorname*{argmin}_{\boldsymbol{w} \in \mathbb{R}^{\mathsf{D}}} \frac{1}{N} \sum_{n=1}^{N} \ell(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)$$

using

- **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:** $\boldsymbol{w} \leftarrow \boldsymbol{w} - \left(\nabla^2 F(\boldsymbol{w})\right)^{-1} \nabla F(\boldsymbol{w})$