CSCI 567: Machine Learning

Vatsal Sharan

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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

$f(x) = x^2$

convex $\Leftrightarrow$ line joining 2 points above function

$f''(x) \geq 0 \ \forall x \longrightarrow$

In high dimensions:

$\nabla^2(F(x))$ is positive semi-definite (psd)

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

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

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

$$\Rightarrow F(w^{(t+1)}) \overset{\approx}{\leq} F(w^{(t)})$$

(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

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

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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

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

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

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

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).

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

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 $(w_2 = 0)$

Switch to Colab

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"...

- $f(\boldsymbol{w}) = w_1^2 + w_2^3$
- $\nabla f(\boldsymbol{w}) = (2w_1, 3w_2^2)$
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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 $w_2 \geq 0$ 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.

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

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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.

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

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:

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

(Sometimes use sgn for sign too.)

Representation: Choosing the **function class**

Still makes sense for “almost” linearly separable data

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.

Choosing the loss function: **surrogate losses**

Solution: use a **convex surrogate loss**

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Onto **Optimization**!

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

Perceptron

New York Times, 1958

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Recall perceptron loss

Applying **GD to perceptron loss**

Applying **SGD to perceptron loss**

Perceptron algorithm

Perceptron algorithm: Intuition

Perceptron algorithm: visually

Repeat:

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

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

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

Predicting probabilities

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 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

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

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 <u>Maximum Likelihood Estimation (MLE)</u>

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

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

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

SGD to logistic loss

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

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)
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Representation

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

Optimization

Empirical risk minimization (ERM) problem:

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

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: $f(\boldsymbol{x}) : \mathcal{X} \to \mathcal{Y}$
- 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, $\ell(f(\boldsymbol{x}, y)) = \mathbb{1}(f(\boldsymbol{x}) \neq y)$.

Intuition: When does ERM generalize?

Relaxing our assumptions

- We assumed that the function class is finite-sized. Results can be extended to **infinite function classes** (such as separating hyperplanes).
- We considered 0-1 loss. Can extend to **real-valued loss** (such as for regression).
- We assumed realizability. Can prove similar theorem which guarantees small generalization gap **without realizability** (but with an ϵ^2 instead of ϵ in the denominator). This is called agnostic learning.

Rule of thumb for generalization

Suppose the functions f in our function class $\mathcal{F}$ have d parameters which can be set. Assume we discretize these parameters so they can take W possible values each. How much data do we need to have small generalization gap?

A useful rule of thumb: to guarantee generalization, make sure that your training data set size n is at least linear in the number d of free parameters in the function that you're trying to learn.