Supervised Learning (in 1 Lecture)

Lucas Janson and Sham Kakade

CS/Stat 184: Introduction to Reinforcement Learning
Fall 2023

Today

- Feedback from last lecture
- Recap
- Supervised learning setup
- Linear regression
- Neural networks

Feedback from feedback forms

1. Thank you to everyone who filled out the forms!
2.

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Recap

- Thompson sampling is a good heuristic for bandits
- Couple more slides on it, then we move on (rest of today unrelated to bandits)

Thompson sampling in practice (cont'd)

So Thompson sampling is basically exactly optimal for large T

What could go wrong for smaller T? Suppose $K = 2$ and $T = 3$, and:

- $t = 0$: $a_0 = 1, r_0 = 1$
- $t = 1$: $a_1 = 2, r_1 = 0$
- $t = 2$ (last time step, with $\hat{\mu}_2^{(1)} = 1$ and $\hat{\mu}_2^{(2)} = 0$): $a_2 = ?$

Thompson sampling has a decent probability of choosing $a_2 = 2$, since with just one sample from each arm, Thompson sampling isn't sure which arm is best.

But $a_2 = 1$ is clear right choice here: there is no future value to learning more, i.e., no reason to explore rather than exploit.

Thompson sampling doesn't know this, and neither does UCB (although UCB wouldn't happen to make the same mistake in this case).

Thompson sampling in practice (cont'd)

For small T, Thompson sampling is not greedy enough

Fix: add a tuning parameter to make it more greedy. Some possibilities:

- Update the Beta parameters by $1+\epsilon$ instead of just 1 each time
- Instead of just taking one sample of $\boldsymbol{\mu}$ and computing the greedy action with respect to it, take n samples, compute the greedy action with respect to each, and pick the *mode* of those greedy actions

All of these favor arms that the algorithm has more confidence are good (i.e., arms that have worked well so far), as opposed to arms that *may* be good

Such tuning can improve Thompson sampling's performance even for reasonably large T (the asymptotic optimality of vanilla TS is *very* asymptotic)

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Supervised learning setup

Data: i.i.d. pairs $(y_1, x_1), \ldots, (y_n, x_n)$ drawn from distribution $\mathbb{P}(y, x) = \mathbb{P}(y \mid x)\mathbb{P}(x)$

Goal: learn a good predictor $f(x)$ of y

Note: $\mathbb{E}[y \mid x]$ minimizes mean squared error

$$\begin{aligned}
\text{MSE}(f) &= \mathbb{E}[(y - f(x))^2] \\
&= \mathbb{E}[(y - \mathbb{E}[y \mid x] + \mathbb{E}[y \mid x] - f(x))^2] \\
&= \mathbb{E}[(y - \mathbb{E}[y \mid x])^2] + \mathbb{E}[(\mathbb{E}[y \mid x] - f(x))^2] + 2\mathbb{E}[(y - \mathbb{E}[y \mid x])(\mathbb{E}[y \mid x] - f(x))]
\end{aligned}$$

$$\begin{aligned}
\mathbb{E}\left[\left(y - \mathbb{E}[y \mid x]\right)\left(\mathbb{E}[y \mid x] - f(x)\right)\right] &= \mathbb{E}\left[\mathbb{E}\left[\left(y - \mathbb{E}[y \mid x]\right)\left(\mathbb{E}[y \mid x] - f(x)\right) \,\middle|\, x\right]\right] \\
&= \mathbb{E}\left[\mathbb{E}\left[\left(y - \mathbb{E}[y \mid x]\right) \,\middle|\, x\right]\left(\mathbb{E}[y \mid x] - f(x)\right)\right] = 0
\end{aligned}$$

How do we now know that $f(x) = \mathbb{E}[y \mid x]$ minimizes MSE?

Empirical risk minimization (ERM)

Fact: $\mathbb{E}[y \mid x] = \arg\min_f \mathbb{E}[(y - f(x))^2]$

This fact both motivates $\mathbb{E}[y \mid x]$ as a target for learning, and suggests how to do it

Law of large numbers: $\mathbb{E}[(y - f(x))^2] \approx \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2 \; =:$ training error of f

Empirical risk minimization (ERM): $\hat{f}(x) = \arg\min_f \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2$

Seems great, but if we allow f in the argmin to range over *all* functions, we can get ridiculous solutions. Can anyone think of one?

E.g., $f(x) = \sum_{i=1}^{n} y_i 1_{\{x = x_i\}}$ achieves zero training error (as long as no ties in the x_i's)

But it predicts 0 at every x value not in the training data, regardless of the data!

Function classes

Need to constrain ERM to a function class $\mathcal{F}$: $\hat{f}(x) = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2$

E.g. (if x scalar) quadratic functions: $\mathcal{F} = \{f(x) = ax^2 + bx + c : (a, b, c) \in \mathbb{R}^3\}$

How to choose $\mathcal{F}$? Three main high-level criteria:

1. Approximation: $\mathbb{E}[y \mid x] \approx \arg\min_{f \in \mathcal{F}} \mathbb{E}[(y - f(x))^2]$
2. Complexity: $\mathcal{F}$ doesn't contain "too many" functions/dimensions
3. Optimizable: need to be able to compute the argmin (or something like it)

Statistical learning theory: the ERM optimum (criterion 3) $\hat{f}$ will perform well if $\mathcal{F}$'s approximation error (criterion 1) and complexity (criterion 2) are low

Optimization

Typically our function class $\mathcal{F}$ is parameterized by a parameter vector $\theta \in \mathbb{R}^d$,
i.e., every $f \in \mathcal{F}$ can be written as $f_\theta(x)$ for some $\theta \in \mathbb{R}^d$

Parameterized ERM optimization: $\hat{\theta} = \arg\min_{\theta \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} (y_i - f_\theta(x_i))^2$; $\hat{f} = f_{\hat{\theta}}$

Notation: $L_i(\theta) = (y_i - f_\theta(x_i))^2$, $L(\theta) = \frac{1}{n} \sum_{i=1}^{n} L_i(\theta)$, gradient operator ∇_θ

Gradient descent: initialize at θ_0, update via $\theta^{(i+1)} = \theta^{(i)} - \eta \nabla_\theta L(\theta^{(i)})$

Downside: computing $\nabla_\theta L(\theta^{(i)})$ at each step expensive for big data

Stochastic gradient descent: initialize at θ_0, update via $\theta^{(i+1)} = \theta^{(i)} - \eta \nabla_\theta L_i(\theta^{(i)})$

Can do multiple passes of data, or uses batch size $b > 1$ at each step

Main takeaway: this works (for good choices of b and η, which may vary with i)

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Linear model

Linear model (if $d = \dim(x)$, let $\theta \in \mathbb{R}^d$): $f_\theta(x) = x^\top \theta$

ERM optimization: $\hat{\theta} = \arg\min_{\theta \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} (y_i - x_i^\top \theta)^2$

Let $Y := (y_1, \ldots, y_n) \in \mathbb{R}^n$ and $X := (x_1^\top; \ldots; x_n^\top) \in \mathbb{R}^{n \times d}$, can rewrite ERM as:

$$\hat{\theta} = \arg\min_{\theta \in \mathbb{R}^d} \frac{1}{2} \|Y - X\theta\|^2$$

Let $L(\theta) = \frac{1}{2}\|Y - X\theta\|^2$: $\quad \nabla_\theta L(\theta) = X^\top (Y - X\theta), \quad \nabla_\theta L_i(\theta) = x_i (y_i - x_i^\top \theta)$

Instead of (S)GD, $\nabla_\theta L(\theta) = 0$ leads to closed-form solution $\hat{\theta} = (X^\top X)^{-1} X^\top Y$

If $n < d$, $X^\top X$ non-invertible; many solutions exists (think: fitting line through 1 point)

Surprising fact: GD initialized at 0 finds solution with smallest norm!

Notes on linear models

1. Can work surprisingly well in practice, especially in high dimensions
   a) Linear functions approximate smooth functions pretty well, if very smooth
2. Need good features
   a) Can use domain knowledge to construct transformation $\phi(x)$ which can be higher- or lower-dimensional than x, and then just use linear model in $\phi(x)$
3. Adding penalty to ERM objective can help a lot, especially in high dimensions
   a) Ridge penalty: add $\lambda \sum_{j=1}^{d} \theta_j^2$ to training loss to discourage huge $\hat{\theta}$ entries
   b) Lasso penalty: add $\lambda \sum_{j=1}^{d} |\theta_j|$ to training loss to encourage sparse $\hat{\theta}$

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Neural network model

Building blocks:

1. Linear transformation (multiplication by matrix W, then addition by vector b)
2. Nonlinear transformation σ, e.g., ReLU $\sigma(a) = \max(a,0)$, applied element-wise

Simplest nontrivial NN is $f(x) = W_2\sigma(W_1x+b_1)+b_2$. Can think of as:

1. Start with input $x \in \mathbb{R}^d$,
2. Linearly transform with $W_1 \in \mathbb{R}^{m\times d}$ and $b_1 \in \mathbb{R}^m$ to get $W_1x+b_1 \in \mathbb{R}^m$
3. Apply (element-wise) the nonlinearity σ to get $\sigma(W_1x+b_1) \in \mathbb{R}^m$
4. Linearly transform with $W_2 \in \mathbb{R}^{m\times 1}$ and $b_2 \in \mathbb{R}$ to get $W_2\sigma(W_1x+b_1)+b_2 \in \mathbb{R}$

With p layers: $f(x) = W_p\sigma(W_{p-1}\sigma(\cdots\ \sigma(W_1x+b_1)\ \cdots)+b_{p-1})+b_p$

Parameter vector θ concatenates all W's and b's; $\dim(\theta)$ scales as width $\times$ depth

Optimizing the neural network

Computing gradients, even stochastic gradients $\nabla_\theta L_i(\theta)$, is daunting

A trick called backpropagation allows such gradients to be computed efficiently

Too notationally cumbersome to cover here, but basically the hierarchical structure of neural networks plays very nicely with the chain rule (see Wikipedia or many other sources on internet for more)

Unfortunately, $L(\theta)$ is non-convex, i.e., it will in general have many local optima

We hope that SGD finds a good one… in practice there are optimization tricks that are like SGD but perform better, e.g., one very popular one is called Adam

Notes on NNs

1. Work well for all problems, breaking criterion 1 (approximation)
    a) Actually, NNs need a lot of data, and are often worse than classical methods on smaller data sets
    b) Many of the most famous / impressive NNs, such as CNNs for vision or AlphaFold for protein structure, heavily incorporate problem-specific structure into their models
2. Work better when larger / more complex, breaking criterion 2 (complexity)
    a) This is true, though larger / more complex NNs also need more data to train
    b) The number of NN parameters is not a good measure of its “complexity”
3. Are highly non-convex, breaking criterion 3 (optimization)
    a) The optimizers used for NNs don’t find arbitrary solutions, they actually find “low-complexity” solutions!

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Summary:

- Given data comprised of a bunch of (y, x) pairs, there exists a huge toolbox (a whole field's worth) to approximate the function $\mathbb{E}[y \mid x]$
- Generally, we write down a squared-error loss function for a parameterized function class and optimize it via (possibly stochastic) gradient descent

Attendance:

bit.ly/3RcTC9T

Feedback:

bit.ly/3RHtlxy