Math of Data Science: Lecture 5

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Course progress

Last lecture:

- Basics of probability: Probabilistic inequalities
- Jointly distributed random variables: independence and covariance
- This lecture:
 - Finish probability review: LLNs, Gaussian RVs and CLT
 - Presentation based on reference [1] and [3]
 - Optimization review
 - Presentation based on references [2], [4] and [5]

Motivation for expectation/LLN

- As with the sample mean, we can think of E[X] as indicating where the values taken by X 'typically' lie (even though E[X] may not actually equal any of the possible values of X)
- There are plenty of other quantities that can be used this way (such as 'median' and 'mode' in statistics).
- But the expectation has a better theory and more computational tools available, making it more useful to solve problems.
- For example, if the loss function depends on random inputs, its expectation is is a natural choice of the thing to minimize in machine learning problems
- The LLN connects expectations with long-run averages when we perform an experiment many independent times

One of our basic intuitions about probability is this: If we perform an experiment independently many times, and *E* is an event that can happen for each performance of the experiment, then in the long-run average

frequency of occurrence of $E \approx P(E)$.

- For instance, if 37% (not a real statistic) of US citizens have visible dandruff, and we randomly select a few thousand citizens (a large number, but much less than US population), then we expect about 37% of those sampled to have visible dandruff.
- So this is saying that, under these long-run average conditions, this 'frequency random variable' settles down, in some approximate sense, to the fixed value P(E).

- Instead of an event E, assume our basic experiment has a random variable X, e.g., 1_E indicator function of the event E
- Independent repeats of the experiment give independent copies of this random variable, say X₁, X₂,
- In general, a sequence of RVs X₁, X₂,... are independent and identically distributed ('i.i.d.') if (i) they are independent, and (ii) they all have the same distribution. Let

$$\mu_n = \frac{1}{n} \sum_i X_i$$

► (Weak Law of Large Numbers, 'WLLN'). For any ε > 0, we have

$$P(|\mu_n - E[X]| \ge \epsilon) o 0$$
 as $n o \infty$

where μ_n is the sample mean defined previously

- (Weak) Law of Large Numbers:
- For any $\epsilon > 0$, we have

$$P(|\mu_n - E[X]| \geq \epsilon)
ightarrow 0$$
 as $n
ightarrow \infty$

- We will justify this result subject to the extra assumption that every X has a well-defined and finite variance (some RVs don't). This must be the same for every X_i - call it σ².
- (LLN is actually true without this assumption.)

LLN justification

- ▶ By linearity of expectation, we have $E[\mu_n] = E[X]$
- We've previously shown that

$$Var(aX) = Cov(aX, aX) = a^2 Cov(X, X) = a^2 Var(X)$$

Also since X_is are independent,

$$Var(\sum_{i=1}^{n} X_i) = \sum_{i=1}^{n} Var(X_i) = \sum_{i=1}^{n} \sigma_i^2$$

• Using these results and that X_i 's have the same variance,

$$Var(\mu_n) = Var(\frac{1}{n}\sum_{i=1}^n X_i) = \frac{\sigma^2}{n}$$

Then, since $E|\mu_n - E[X]|^2 = Var(\mu_n)$, by Chebychev

$$P(|\mu_n - E[X]| \ge \epsilon) = P(|\mu_n - E[X]|^2 \ge \epsilon^2) \le \frac{\sigma^2}{n\epsilon^2}$$

Let X_i 's be i.i.d. with expectation E[X], the sample mean is

$$\mu_n = \frac{1}{n} \sum_i X_i$$

• (Weak) Law of Large Numbers: Then for any $\epsilon > 0$,

$$P(|\mu_n - E[X]| \ge \epsilon) o 0$$
 as $n o \infty$

- How large n has to be depends on how good an approximation you want
- Our proof gave an explicit estimate for how long we have to wait, given *ε*.
- Another way of visualizing the n Bernoulli-trials case: once n is large, then ¹/_n binom(p, n), PMF puts almost all of its mass into a narrow window around the mean p.

- The WLLN does not say that X_n is guaranteed to be close to p, only that this is very likely.
- Of course, if we're very unlucky, we might toss a fair coin but still get the outcome

НННННННННН or maybe ННТНТТННТННН

For these very unlikely outcomes, the sample mean takes the values 1 and 2/3 respectively, far away from the true mean, which is 1/2.

- If we consider our running sequence of sample means μ_n, then WLLN says that, for each individual large value of n, μ_n is unlikely be far away from E[X].
- But that's an infinite sequence of unlikely events.
- Even though their individual probabilities are small, we can still imagine that one of them occurs very occasionally.
- That is, it could be that μ_n mostly stays close to E[X], but as n increases μ_n very occasionally makes a large deviation away from μ.
- Strong LLN says this doesn't happen.

$$\mathsf{P}(\lim_{n\to\infty}\mu_n=\mathsf{E}[X])=1$$

▶ Proof is more difficult that WLLN (e.g., can use estimates of the 4th moments $E[\mu_n^4]/n^4$)

Back to our dandruff example:

- If 37% of US citizens have visible dandruff, and we randomly select a thousand citizens (a large number, but much less than the US population), then we expect about 37% of those sampled to have visible dandruff.
- Taking $X_i = \mathbb{1}_{i-\text{th person has dandruff}}$
- Now SLLN ensures that

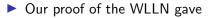
$$P(\lim_{n\to\infty}\mu_n=E[X]=P(\text{person has dandruff}))=1$$

But how confident can we be of this approximation? Is a sample of a thousand large enough for the effect to be reliable?

In the LLN context our question was: Pick two error tolerances, ε > 0 and α > 0. How large does n have to be so that

$$P(|\mu_n - E[X]| \ge \epsilon) < \alpha$$

(There were really two kinds of error tolerance involved all along: ε is how close you want μ_n to be to E[X] = p, and α is the small probability of error that you allow.



$$P(|\mu_n - E[X]| \ge \epsilon) \le \frac{\sigma^2}{n\epsilon^2}$$

I.e., bound on the probability of the tails

- Now our question is: effectively how wide are spikes around the mean as $n \rightarrow \infty$.
- E.g., for a Bernoulli $X_1, ..., X_n$ with p = 1/2, let

$$S_n = \sum_{i=1}^n X_i$$

We want to approximate the 'shape' of the PMF

$$P(S_n=k)$$

when k/n is close to 1/2, i.e. in a range

$$n/2 - n\epsilon < k < n/2 + n\epsilon$$

Gaussian

The normal distribution with mean m and variance σ², or N(m, σ²) is given by the Gaussian density

$$p(x) = \frac{1}{\sigma\sqrt{2\pi}}e^{-(x-m)^2/(2\sigma^2)}$$

• The the CDF of standard normal N(0,1) is

$$\Phi(a) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{a} e^{-x^2/2}$$

• Let $X_1, ..., X_n$ be i.i.d with mean E[X] and $Var(X) = \sigma^2$ and

$$\mu_n = \frac{1}{n}(X_1 + \dots + X_n)$$

► The Central Limit Theorem: The limiting distribution of √n(µ_n − E[X]) is N(0, 1), in the following sense.

$$P(a < rac{\sqrt{n}}{\sigma}(\mu_n - E[X]) < b)
ightarrow \Phi(b) - \Phi(a)$$

as $n \to \infty$.

This implies

$$P(|\mu_n - E[X]| < \frac{c}{\sqrt{n}}) \rightarrow \Phi\left(\frac{c}{\sigma}\right) - \Phi\left(-\frac{c}{\sigma}\right)$$

• and taking $\epsilon = \frac{c}{\sqrt{n}}$

$$P(|\mu_n - E[X]| < \epsilon) \rightarrow \Phi\left(\frac{\epsilon\sqrt{n}}{\sigma}\right) - \Phi\left(-\frac{\epsilon\sqrt{n}}{\sigma}\right)$$

Note that CLT gives

$$P(|\mu_n - E[X]| < \epsilon) \rightarrow \Phi\left(\frac{\epsilon\sqrt{n}}{\sigma}\right) - \Phi\left(-\frac{\epsilon\sqrt{n}}{\sigma}\right)$$

On the other hand, if we wanted to bound the probability mass around the mean rather than the tails, the WLLN is not informative as n → ∞

$$P(|\mu_n - E[X]| < \epsilon) \ge 1 - \frac{\sigma^2}{n\epsilon^2}$$

This follows from

$$1 - P(|\mu_n - E[X]| < \epsilon) = P(|\mu_n - E[X]| \ge \epsilon) \le \frac{\sigma^2}{n\epsilon^2}$$

Optimization review - convexity

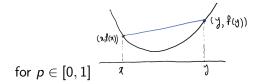
K is a convex set: if x, y ∈ K, then so is the line segment from x to y, i.e.

$$px + (1 - p)y \in K$$

for $p \in [0, 1]$.

f is a convex fcn if the set of points on and above the graph of F is convex, i.e.

$$f(px+(1-p)y) \leq pf(x)+(1-p)f(y)$$



Convex optimization

Convex optimization

 $\min_{x\in K}f(x)$

where K is a convex set and f(x) is a convex function

- Thm: Any local minimum is global, and there will be no isolated local min
- Justification: if that wasn't true, then the line between two local min would intersect with the graph of f

Gradient descent

Let's start with an unconstrained problem

 $\min_{x} f(x)$

Gradient descent algorithm is an iterative method given by

$$x_{k+1} = x_k - s_k \nabla f(x_k)$$

- x₀ is an initial (often random) guess
- We'll discuss the step size (also called learning rate s_k > 0) shortly.

GD and learning

 Let's look at our linear regression objective (typically scale the loss by the number of data points in ML, but that shouldn't affect the minimization)

$$R(x) = \frac{1}{n} ||Ax - b||^2 = \frac{1}{n} \sum_{i=1}^n (x^T a_i - b_i)^2$$

To learn x, we can follow the GD descent algorithm

$$x_{k+1} = x_k - s_k \nabla R(x)$$

where

$$\nabla R(x) = \frac{1}{n} (2x^{\top} A^{\top} A - 2b^{\top} A) = \frac{1}{n} \sum_{i=1}^{n} 2(x^{\top} a_i - b_i) a_i$$

GD and learning

Our linear regression objective uses a square loss to measures the difference between the prediction of a linear model x^Ta_i and the actual data b_i

$$\ell_i(x) = (x^T a_i - b_i)^2$$

You can generalize this to other loss functions and learning algorithms

$$\ell_i(x) = \ell(F(x,a_i) - b_i)^2$$

- E.g., F can represent a neural network, which outputs a label F(x, a) given features a and parameters x.
- The training, i.e., learning x given the data, can be done by minimizing

$$L(x) = \frac{1}{n} \sum_{i=1}^{n} \ell_i(x)$$

Sometimes the above term is called is called empirical risk, and the training process is called empirical risk minimization

Learning rate

- Several ways to determine sk depending on the algorithm
- ► For GD, a convergence guarantee is available for a fixed step size s ≤ 1/M where M is the Lipschitz constant of the gradient

$$\|\nabla f(x) - \nabla f(y)\| \le M \|x - y\|$$

uniformly over the domain

If f is C², then M would be the bound of the eigenvalues λ_i of the Hessian

$$|\lambda_i| \leq M$$

for all i uniformly in x.

Often *M* is not known, but we can extend the convergence guarantees to *exact line search*

$$s_k = \arg\min_{s\geq 0} f(x_k - s\nabla f(x_k))$$

And backtracking line search, which iteratively reduces sk until

$$f(x_{k+1}) \leq f(x_k) - \frac{1}{2} s_k \| \nabla f(x_k) \|_2^2$$

► Let
$$G = \|\nabla f(x_k)\|_2^2$$
: the 2nd order Taylor expansion is
 $f(x_{k+1})$
 $= f(x_k) + \langle \nabla f(x_k), x_{k+1} - x_k \rangle + \frac{1}{2}(x_{k+1} - x_k)^T H(\xi)(x_{k+1} - x_k)$
 $= f(x_k) - sG + \frac{1}{2}(x_{k+1} - x_k)^T H(\xi)(x_{k+1} - x_k)$

for some ξ on the segment between x_{k+1} and x_k (mean value form of the remainder)

▶ If the eigenvalues λ_i of H are $|\lambda_i| \leq M$ for all i uniformly in x

$$f(x_{k+1}) \leq f(x_k) - sG + \frac{s^2M}{2}G = f(x_k) - \frac{1}{2M}G$$

The RHS is minimized taking the step size s = 1/M.
 But any s < 2/M will reduce f

From the previous slide

$$f(x_{k+1}) \leq f(x_k) - \frac{1}{2M}G$$

taking the step size $s = \frac{1}{M}$ where $G = \|\nabla f(x_k)\|_2^2$.

- Assume that f is bounded below by f* (reasonable in ML since the loss function is typically nonnegative)
- Idea of a convergence argument
 - Start at some $f(x_0)$ and at each step decrease f by at least $\frac{1}{2M}G$
 - We can't decrease f(xk) below f*
 - So G must be going to zero "fast enough"

From the previous slide

$$f(x_{k+1}) \leq f(x_k) - \frac{1}{2M}G$$

taking the step size $s = \frac{1}{M}$ where $G = \|\nabla f(x_k)\|_2^2$.

rearrange

$$G \leq 2M(f(x_k) - f(x_{k+1}))$$

sum over time periods

$$\sum_{k=0}^{t} \|\nabla f(x_k)\|_2^2 \leq 2M \sum_{k=0}^{t} [f(x_k) - f(x_{k+1})]$$

From the previous slide

$$\sum_{k=0}^{t-1} \|\nabla f(x_k)\|_2^2 \leq 2M \sum_{k=0}^{t-1} [f(x_k) - f(x_{k+1})]$$

Replacing ∇f(x_k) with min_k ∇f(x_k) on the LHS, using the telescoping sum on the RHS and then the fact that f(x_t) ≥ f*

$$t \min_{0 \le k \le t-1} \|\nabla f(x_k)\|_2^2 \le 2M[f(x_0) - f(x_t)] \le 2M[f(x_0) - f^*]$$

Therefore

$$\min_{0 \le k \le t-1} \|\nabla f(x_k)\|_2^2 \le \frac{2M[f(x_0) - f^*]}{t} = O(1/t)$$

From the previous slide

$$\min_{0 \le k \le t-1} \|\nabla f(x_k)\|_2^2 \le \frac{2M[f(x_0) - f^*]}{t} = O(1/t)$$

• So the norm is below ϵ if

$$\frac{2M[f(x_0)-f^*]}{t} \le \epsilon$$

This is guaranteed for

$$\frac{2M[f(x_0)-f^*]}{\epsilon} \leq t$$

So GD requires $t = O(1/\epsilon)$ iterations to achieve $\|\nabla f(x_k)\|_2^2 \le \epsilon$

- The previous argument didn't assume that f is convex, so the GD was converging to a local minimum (theoretically could also converge to a saddle point).
- Guaranteeing convergence to a global minimum of a nonconvex function requires multiple random initializations or grid search
- This requires t = O(1/e^d) iterations to achieve ||∇f(x_k)||₂² ≤ e for functions with Lipschitz continuous gradients and x ∈ ℝ^d
- In practice gradient-based methods work well for non-convex functions used in ML/NN even though there are not theoretical convergence guarantees
- ▶ If f is convex, then $\nabla f(x^*) = 0$ at a global minimizer x^*
- Therefore the above argument guarantees convergence to the global min at the above rate

- ▶ If f is strongly convex, i.e, the eigenvalues λ_i of the Hessian H are also $0 < m \le \lambda_i$ uniformly in x, the convergence $O((1 \frac{m}{M})^k)$ for 0 < c < 1.
- This means that a bound of

$$f(x_k) - f(x^*) \le \epsilon$$

can be achieved using only $O(\log(1/\epsilon))$ iterations.

- This rate is called "linear convergence" for historic reasons (the error lies below a line on a log-linear plot of the error vs iteration number)
- Many loss functions in ML are not strongly convex, e.g., Relu and softmax are convex but not strongly convex
- \blacktriangleright Adding an ℓ^2 regularization term will make them such and can improve convergence

Gradient descent convergence

► Let $G = \|\nabla f(x_k)\|_2^2$: the 2nd order Taylor expansion is $f(x_{k+1})$ $= f(x_k) + \langle \nabla f(x_k), x_{k+1} - x_k \rangle + \frac{1}{2}(x_{k+1} - x_k)^T H(\xi)(x_{k+1} - x_k)$ $= f(x_k) - sG + \frac{1}{2}(x_{k+1} - x_k)^T H(\xi)(x_{k+1} - x_k)$

for some ξ on the segment between x_{k+1} and x_k (mean value form of the remainder)

• If the eigenvalues λ_i of H are $m \leq \lambda_i \leq M$ for all i

$$f(x_{k+1}) \leq f(x_k) - sG + \frac{s^2M}{2}G = f(x_k) - \frac{1}{2M}G$$

taking $s = \frac{1}{M}$ (exact line search) For the optimal x^* ,

$$f(x_{k+1}) - f(x^*) \le f(x_k) - f(x^*) - \frac{1}{2M}G$$

Gradient descent convergence

By a similar argument

$$f(x^{*}) = f(x_{k}) + \langle \nabla f(x_{k}), x^{*} - x_{k} \rangle + \frac{1}{2} (x^{*} - x_{k})^{T} H(\xi) (x^{*} - x_{k})$$

$$\geq f(x_{k}) + \langle \nabla f(x_{k}), \tilde{x} - x_{k} \rangle + \frac{m}{2} \|\tilde{x} - x_{k}\|^{2}$$

$$= f(x_{k}) - \frac{1}{2m} G$$

where $\tilde{x} = x_k - \frac{1}{m} \nabla f(x_k)$ is determined by minimizing the above expression with respect to \tilde{x}

we get

$$f(x_{k+1}) - f(x^*) \le (1 - \frac{m}{M})(f(x_k) - f(x^*))$$

Learning rate-GD line search

- The previous discussion suggested a fixed step size of 1/M
- In practice, the Lipschitz of constant of the gradient is not known
- so "try a big step-size, and decrease it if isn't satisfying a progress bound."
- Another alternative is *exact line search*:

$$s_k = \arg\min_s f(x_k - s \nabla f(x_k))$$

The previous bounds relied on

$$f(x_{k+1}) \leq f(x_k) - \frac{1}{2M}G$$

where x_{k+1} is determined using a fixed step size $s = \frac{1}{M}$. For x_{k+1}^* determined by an exact line search

$$f(x_{k+1}^*) \leq f(x_{k+1})$$

so all the convergence guarantees still hold

Exact line search can be also computationally expensive since we need to optimize f in 1D

 $t = \beta t$

For α ∈ (0, 0.5), β ∈ (0, 1), initial t = 1, backtracking line search entails iteratively reducing s = αt via

until
$$f(x_{k+1}) \leq f(x_k) - \alpha t \|\nabla f(x_k)\|_2^2$$

Figure: The backtracking condition is that f lies below the upper dashed line Fig 9.1 from [5]

- Since −∇f(x_k) is a descent direction, the backtracking condition is satisfied for a sufficiently small t ∈ (0, t₀].
- Therefore, the line search stops with t = 1 or $t \in (\beta t_0, t_0]$.

- From previous the line search stops with t = 1 or t ∈ (βt₀, t₀]. t ≥ min(t, βt₀)
- By convexity of $g(t) = -t + Mt^2/2$

$$g(x/M + (1-x) \cdot 0)) \le xg(1/M) - (1-x)g(0)$$

This implies

$$-t + Mt^2/2 \le -t/2$$

By the previous slide

$$-t + Mt^2/2 \le -t/2$$

• By an earlier computation, for $G = \|\nabla f(x_k)\|_2^2$

$$f(x_{k+1}) \leq f(x_k) - tG + \frac{t^2M}{2}G$$
$$\leq f(x_k) - \frac{t}{2}G$$
$$\leq f(x_k) - \alpha tG$$

Since the first inequality holds with equality for t = 1/M, the backtracking line search terminates with t = 1 or t ≥ β/M:

$$f(x_{k+1}) \leq f(x_k) - \min\{\alpha, \beta \alpha/M\}G$$

By the previous slide

$$f(x_{k+1}) \leq f(x_k) - \min\{\alpha, \beta \alpha / M\}G$$

We can repeat the earlier argument with a different constant prefactor

$$\min_{0 \le k \le t-1} \|\nabla f(x_k)\|_2^2 \le \frac{[f(x_0) - f^*]}{\min\{\alpha, \beta \alpha/M\}t} = O(1/t)$$

Nesterov accelerated descent

- If f is convex (but not necessarily strongly convex) is the t = O(1/ε) "sublinear convergence" optimal?
- So called Nesterov accelerated descent

$$x_{k+1} = y_k - s \nabla f(y_k) y_{k+1} = x_{k+1} + \beta_k (x_{k+1} - x_k)$$

achieves error of $O(1/t^2)$ after t iterations.

- Can use s = 1/M and $\beta_k = (k-1)/(k+2)$
- ▶ So only needs $t = O(1/\sqrt{\epsilon})$ to get within ϵ of the solution
- It not straightforward to understand why this method works better
- One observation is that this is not a descent method, i.e., the steps may overshoot the minimum and oscillate around it, rather than converging from one direction.
- Used in practice to optimize convex and nonconvex function in ML

Second order methods: Newton's method

• A second order approximation of a convex C^2 function is

$$g(y) = f(x) + \nabla f(y - x) + \frac{1}{2}(y - x)^T \nabla^2 f(x)(y - x)$$

If the Hessian is positive definite,

$$\arg\min_{y} g(y) = x - (\nabla^2 f(x))^{-1} \nabla f(x)$$

This idea leads to Newton's method

$$x_{k+1} = x_k - (\nabla^2 f(x_k))^{-1} \nabla f(x_k)$$

which has quadratic convergence under certain assumptions

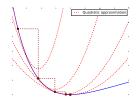


Figure: Quadratic approximation of 1D convex function (Fig14 from [4])

Next steps

- PCA (Sec I.9)
- ► Conjugate gradients (Sec. II.1) and least squares (Sec. II.2)

References I

- [1] Tim Austin, *Theory of Probability unpublished lecture* notes, 2016
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- [3] Ross, A First Course in Probability (9th ed., 2014)
- [4] Carlos Fernandez-Granda, DS-GA 1013 / MATH-GA 2821 Optimization-based Data Analysis, Lecture Notes, 2017 https://math.nyu.edu/~cfgranda/pages/OBDA_ fall17/index.html
- [5] Boyd, Vandenberghe, *Convex Optimization*