Appendix A:
Basics of Monte Carlo

Mathematical Foundations of Deep Neural Networks

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Monte Carlo

We quickly cover some basic notions of Monte Carlo simulations.

These concepts will be used with VAEs.

These ideas are also extensively used in reinforcement learning (although not a topic of this course).

Monte Carlo estimation

Consider IID data $X_1, \ldots, X_N \sim f$. Let $\phi(X) \geq 0$ be some function*. Consider the problem of estimating

$$I = \mathbb{E}_{X\sim f}[\phi(X)] = \int \phi(x) f(x)\, dx$$

One commonly uses

$$\hat{I}_N = \frac{1}{N} \sum_{i=1}^{N} \phi(X_i)$$

to estimate I. After all, $\mathbb{E}\left[\hat{I}_N\right] = I$ and $\hat{I}_N \to I$ by the law of large numbers.#

*The assumption $\phi(X) \geq 0$ can be relaxed.

#Convergence in probability by weak law of large numbers and almost sure convergence by strong law of large numbers.

Monte Carlo estimation

We can quantify convergence with variance:

$$\mathrm{Var}_{X\sim f}\left(\hat{I}_N\right) = \sum_{i=1}^{N} \mathrm{Var}_{X_i\sim f}\left(\frac{\phi(X_i)}{N}\right) = \frac{1}{N}\mathrm{Var}_{X\sim f}\left(\phi(X)\right)$$

In other words

$$\mathbb{E}\left[\left(\hat{I}_N - I\right)^2\right] = \frac{1}{N}\mathrm{Var}_{X\sim f}\left(\phi(X)\right)$$

and

$$\mathbb{E}\left[\left(\hat{I}_N - I\right)^2\right] \to 0$$

as $N \to \infty$.[#]

[#] So $\hat{I}_n \to I$ in L^2 provided that $\mathrm{Var}_{X\sim f}\left(\phi(X)\right) < \infty$.

Empirical risk minimization

In machine learning and statistics, we often wish to solve

$$\underset{\theta \in \Theta}{\text{minimize}} \quad \mathcal{L}(\theta)$$

where the objective function

$$\mathcal{L}(\theta) = \mathbb{E}_{X \sim p_X}[\ell(f_\theta(X), f_\star(X))]$$

Is the (true) *risk*. However, the evaluation of $\mathbb{E}_{X \sim p_X}$ is impossible (if p_X is unknown) or intractable (if p_X is known but the expectation has no closed-form solution). Therefore, we define the proxy loss function

$$\mathcal{L}_N(\theta) = \frac{1}{N} \sum_{i=1}^{N} \ell(f_\theta(X_i), f_\star(X_i))$$

which we call the *empirical risk,* and solve

$$\underset{\theta \in \Theta}{\text{minimize}} \quad \mathcal{L}_N(\theta)$$

Empirical risk minimization

This is called *empirical risk minimization* (ERM). The idea is that

$$\mathcal{L}_N(\theta) \approx \mathcal{L}(\theta)$$

with high probability, so minimizing $\mathcal{L}_N(\theta)$ should be similar to minimizing $\mathcal{L}(\theta)$.

Technical note) The law of large numbers tells us that

$$\mathbb{P}(|\mathcal{L}_N(\theta) - \mathcal{L}(\theta)| > \varepsilon) = \mathrm{small}$$

for any given θ, but we need

$$\mathbb{P}\left(\sup_{\theta \in \Theta} |\mathcal{L}_N(\theta) - \mathcal{L}(\theta)| > \varepsilon\right) = \mathrm{small}$$

for all compact Θ in order to conclude that the argmins of the two losses to be similar. These types of results are established by a *uniform law of large numbers*.

Importance sampling

Importance sampling (IS) is a technique for reducing the variance of a Monte Carlo estimator.

Key insight of important sampling:

$$I = \int \phi(x) f(x)\, dx = \int \frac{\phi(x) f(x)}{g(x)} g(x)\, dx = \mathbb{E}_{X\sim g}\left[\frac{\phi(X) f(X)}{g(X)}\right]$$

(We do have to be mindful of division by 0.) Then

$$\hat{I}_N = \frac{1}{N}\sum_{i=1}^{N} \phi(X_i) \frac{f(X_i)}{g(X_i)}$$

with $X_1, \dots, X_N \sim g$ is also an estimator of I. Indeed, $\mathbb{E}[\hat{I}_N] = I$ and $\hat{I}_N \to I$. The weight $\frac{f(x)}{g(x)}$ is called the *likelihood ratio* or the Radon–Nikodym derivative.

So we can use samples from g to compute expectation with respect to f.

IS example: Low probability events

Consider the setup of estimating the probability

$$\mathbb{P}(X > 3) = 0.00135$$

where $X \sim \mathcal{N}(0,1)$. If we use the regular Monte Carlo estimator

$$\hat{I}_N = \frac{1}{N}\sum_{i=1}^{N} \mathbf{1}_{\{X_i > 3\}}$$

where $X_i \sim \mathcal{N}(0,1)$, if N is not sufficiently large, we can have $\hat{I}_N = 0$. Inaccurate estimate.

If we use the IS estimator

$$\hat{I}_N = \frac{1}{N}\sum_{i=1}^{N} \mathbf{1}_{\{Y_i > 3\}} \exp\left(\frac{(Y_i - 3)^2 - Y_i^2}{2}\right)$$

where $Y_i \sim \mathcal{N}(3,1)$, having $\hat{I}_N = 0$ is much less likely. Estimate is much more accurate.

Importance sampling

Benefit of IS quantified by with variance:

$$\mathrm{Var}_{X\sim g}\left(\hat{I}_N\right) = \sum_{i=1}^{N} \mathrm{Var}_{X\sim g}\left(\frac{\phi(X_i)f(X_i)}{ng(X_i)}\right) = \frac{1}{N}\mathrm{Var}_{X\sim g}\left(\frac{\phi(X)f(X)}{g(X)}\right)$$

If $\mathrm{Var}_{X\sim g}\left(\frac{\phi(X)f(X)}{g(X)}\right) < \mathrm{Var}_{X\sim f}\left(\phi(X)\right)$, then IS provides variance reduction.

We call g the *importance* or *sampling distribution*. Choosing g poorly can increase the variance. What is the best choice of g?

Optimal sampling distribution

The sampling distribution

$$g(x) = \frac{\phi(x)f(x)}{I}$$

makes $\mathrm{Var}_{X\sim g}\left(\frac{\phi(X)f(X)}{g(X)}\right) = \mathrm{Var}_{X\sim g}(I) = 0$ and therefore is optimal. (I serves as the normalizing factor that ensures the density g integrates to 1.)

Problem: Since we do not know the normalizing factor I, the answer we wish to estimate, sampling from g is usually difficult.

Optimized/trained sampling distribution

Instead, we consider the optimization problem

$$\underset{g\in\mathcal{G}}{\text{minimize}} \quad D_{\text{KL}}\left(g \| \frac{\phi f}{I}\right)$$

and compute a suboptimal, but good, sampling distribution within a class of sampling distributions $\mathcal{G}$. (In ML, $\mathcal{G} = \{g_\theta | \theta \in \Theta\}$ is parameterized by neural networks.)

Importantly, this optimization problem does not require knowledge of I.

$$\begin{aligned} D_{\text{KL}}(g_\theta \| \phi f / I) &= \mathbb{E}_{X\sim g_\theta}\left[\log\left(\frac{I g_\theta(X)}{\phi(X) f(X)}\right)\right] \\ &= \mathbb{E}_{X\sim g_\theta}\left[\log\left(\frac{g_\theta(X)}{\phi(X) f(X)}\right)\right] + \log I \\ &= \mathbb{E}_{X\sim g_\theta}\left[\log\left(\frac{g_\theta(X)}{\phi(X) f(X)}\right)\right] + \text{constant independent of } \theta \end{aligned}$$

How do we compute stochastic gradients?

Log-derivative trick

Generally, consider the setup where we wish to solve

$$\underset{\theta \in \mathbb{R}^p}{\text{minimize}} \quad \mathbb{E}_{X \sim f_\theta}[\phi(X)]$$

with SGD.

(Previous slide had θ-dependence both on and inside the expectation. For now, let's simplify the problem so that ϕ does not depend on θ.)

Incorrect gradient computation:

$$\nabla_\theta \mathbb{E}_{X \sim f_\theta}[\phi(X)] \stackrel{?}{=} \mathbb{E}_{X \sim f_\theta}[\nabla_\theta \phi(X)] = \mathbb{E}_{X \sim f_\theta}[0] = 0$$

Log-derivative trick

Correct gradient computation:

$$\nabla_\theta \mathbb{E}_{X\sim f_\theta}[\phi(X)] = \nabla_\theta \int \phi(x) f_\theta(x)\, dx = \int \phi(x) \nabla_\theta f_\theta(x)\, dx$$

$$= \int \phi(x) \frac{\nabla_\theta f_\theta(x)}{f_\theta(x)} f_\theta(x)\, dx = \mathbb{E}_{X\sim f_\theta}\left[\phi(X)\frac{\nabla_\theta f_\theta(X)}{f_\theta(X)}\right]$$

$$= \mathbb{E}_{X\sim f_\theta}\left[\phi(X)\nabla_\theta \log(f_\theta(X))\right]$$

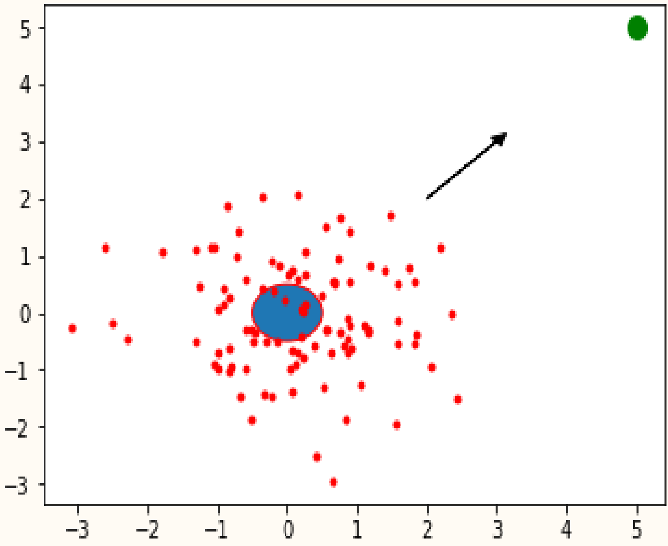
Therefore, $\phi(X)\nabla_\theta \log(f_\theta(X))$ with $X \sim f_\theta$ is a stochastic gradient of the loss function. This technique is called the *log-derivative trick*, the *likelihood ratio gradient*[#], or *REINFORCE*[*].

Formula with the log-derivative ($\nabla_\theta \log(\cdot)$) is convenient when dealing with Gaussians, or more generally exponential families, since the densities are of the form

$$f_\theta(x) = h(x)\exp(\text{function of } \theta)$$

[#]P. W. Glynn, Likelihood ratio gradient estimation for stochastic systems, *Communications of the ACM*, 1990.
[*]R. J. Williams, Simple statistical gradient-following algorithms for connectionist reinforcement learning. *Machine Learning*, 1992.

Log-derivative trick example



Learn $\mu \in \mathbb{R}^2$ to minimize the objective below.

$$\underset{\mu \in \mathbb{R}^2}{\text{minimize}} \quad \mathbb{E}_{X \sim \mathcal{N}(\mu, I)} \left\| X - \begin{pmatrix} 5 \\ 5 \end{pmatrix} \right\|^2$$

Then the loss function is

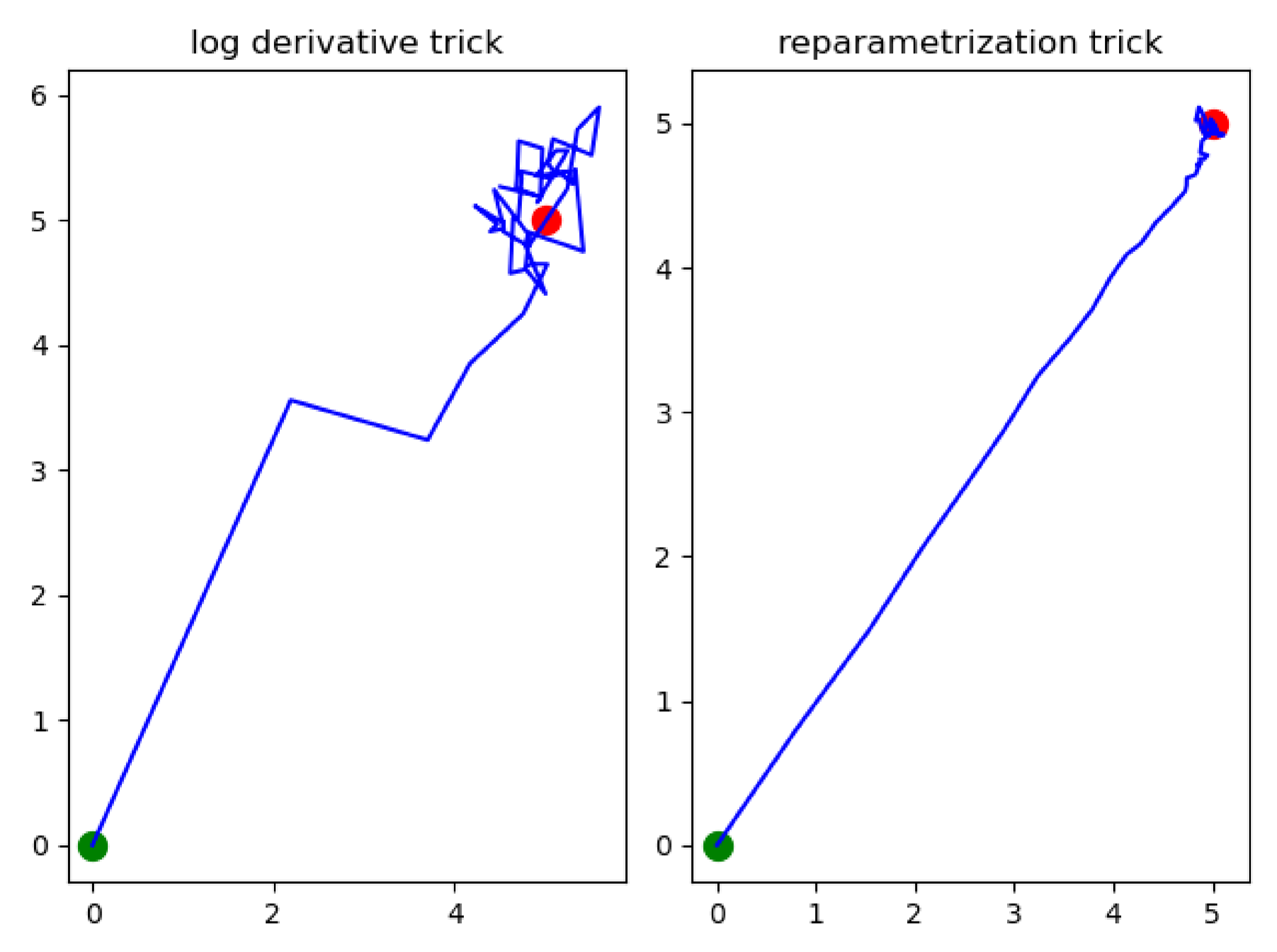
$$\mathcal{L}(\mu) = \mathbb{E}_{X \sim \mathcal{N}(\mu, I)} \left\| X - \begin{pmatrix} 5 \\ 5 \end{pmatrix} \right\|^2 = \int \left\| x - \begin{pmatrix} 5 \\ 5 \end{pmatrix} \right\|^2 \frac{1}{2\pi} \exp\left(-\frac{1}{2} \|x - \mu\|^2 \right) \, dx$$

And, using $X_1, \ldots, X_B \sim \mathcal{N}(\mu, I)$, we have stochastic gradients

$$\nabla_\mu \mathcal{L}(\mu) = \mathbb{E}_{X \sim q_\mu} \left[\left\| x - \begin{pmatrix} 5 \\ 5 \end{pmatrix} \right\|^2 \nabla_\mu \left(-\frac{1}{2} \|x - \mu\|^2 \right) \right] \approx \frac{1}{B} \sum_{i=1}^{B} \left\| X_i - \begin{pmatrix} 5 \\ 5 \end{pmatrix} \right\|^2 (X_i - \mu)$$

These stochastic gradients have large variance and thus SGD is slow.

Log-derivative trick example



Reparameterization trick

The *reparameterization trick* (RT) or the *pathwise derivative* (PD) relies on the key insight.

$$\mathbb{E}_{X\sim\mathcal{N}(\mu,\sigma^2)}\left[\phi(X)\right] = \mathbb{E}_{Y\sim\mathcal{N}(0,1)}\left[\phi\left(\mu+\sigma Y\right)\right]$$

Gradient computation:

$$\begin{aligned}\nabla_{\mu,\sigma}\mathbb{E}_{X\sim\mathcal{N}(\mu,\sigma^2)}\left[\phi(X)\right] = \mathbb{E}_{Y\sim\mathcal{N}(0,1)}\left[\nabla_{\mu,\sigma}\phi(\mu+\sigma Y)\right] &= \mathbb{E}_{Y\sim\mathcal{N}(0,1)}\left[\phi'(\mu+\sigma Y)\begin{bmatrix}1\\ Y\end{bmatrix}\right]\\ &\approx \frac{1}{B}\sum_{i=1}^{B}\phi'(\mu+\sigma Y_i)\begin{bmatrix}1\\ Y_i\end{bmatrix}, \qquad Y_1,\dots,Y_B\sim\mathcal{N}(0,I)\end{aligned}$$

RT is less general than log-derivative trick, but it usually produces stochastic gradients with lower variance.

Reparameterization trick example

Consider the same example as before

$$\mathcal{L}(\mu) = \mathbb{E}_{X\sim\mathcal{N}(\mu,I)} \left\| X - \begin{pmatrix} 5 \\ 5 \end{pmatrix} \right\|^2 = \mathbb{E}_{Y\sim\mathcal{N}(0,I)} \left\| Y + \mu - \begin{pmatrix} 5 \\ 5 \end{pmatrix} \right\|^2$$

Gradient computation:

$$\nabla_\mu \mathcal{L}(\mu) = \mathbb{E}_{Y\sim\mathcal{N}(0,I)} \nabla_\mu \left\| Y + \mu - \begin{pmatrix} 5 \\ 5 \end{pmatrix} \right\|^2 = 2\mathbb{E}_{Y\sim\mathcal{N}(0,I)} \left(Y + \mu - \begin{pmatrix} 5 \\ 5 \end{pmatrix} \right)$$

$$\approx \frac{2}{B} \sum_{i=1}^{B} \left(Y_i + \mu - \begin{pmatrix} 5 \\ 5 \end{pmatrix} \right), \qquad Y_1, \ldots, Y_B \sim \mathcal{N}(0, I)$$

These stochastic gradients have smaller variance and thus SGD is faster.

Reparameterization trick example