Monte-Carlo Gradient Estimation for Machine Learning
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Presentation Overview

Introduction

How do we compute the gradient of function expectations?

$$\mathcal{F}(\boldsymbol{\theta}) := \int d\boldsymbol{x} P(\boldsymbol{x};\boldsymbol{\theta}) f(\boldsymbol{x};\phi) = \mathbb{E}_{P(\boldsymbol{x};\boldsymbol{\theta})}[f(\boldsymbol{x};\phi)] \quad (1)$$

$$\boldsymbol{\eta} := \nabla_{\boldsymbol{\theta}} \mathcal{F}(\boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}} \mathbb{E}_{P(\boldsymbol{x};\boldsymbol{\theta})}[f(\boldsymbol{x};\phi)] (2)$$

We estimate it!

Key Targets

- **Consistency** ✓
  The estimator, $\boldsymbol{\eta}$, gets better with more samples.
- **Unbiasdness**
  $\nabla \mathbb{E}_{P(\boldsymbol{x};\boldsymbol{\theta})}[\bar{\mathcal{F}}_N] = \nabla \mathbb{E}_{P(\boldsymbol{x};\boldsymbol{\theta})}[f(\boldsymbol{x};\boldsymbol{\phi})]$. This ensures that we have an accurate estimator.
- **Minimum Variance**
  The more precise an estimate given a constant number of samples, N, the better.
- **Computational Efficiency**
  Blazingly Fast!

Score Function Estimators

$$\boldsymbol{\eta} = \nabla_{\boldsymbol{\theta}} \mathbb{E}_{P(\boldsymbol{x};\boldsymbol{\theta})}[f(\boldsymbol{x};\phi)] \tag{3}$$

$$= \int P(\boldsymbol{x};\boldsymbol{\theta}) \frac{\nabla_{\boldsymbol{\theta}} P(\boldsymbol{x};\boldsymbol{\theta})}{P(\boldsymbol{x};\boldsymbol{\theta})} f(\boldsymbol{x};\phi) d\boldsymbol{x} \tag{4}$$

$$= \int P(\boldsymbol{x};\boldsymbol{\theta}) f(\boldsymbol{x};\phi) \nabla_{\boldsymbol{\theta}} \log(P(\boldsymbol{x};\boldsymbol{\theta})) d\boldsymbol{x}, \tag{5}$$

$$\approx \bar{\boldsymbol{\eta}}_N = \frac{1}{N} \sum_{n=1}^{N} f(\hat{\boldsymbol{x}}^{(n)};\boldsymbol{\phi}) \nabla_{\boldsymbol{\theta}} \log(P(\hat{\boldsymbol{x}}^{(n)};\boldsymbol{\theta})). \tag{6}$$

- **Idea**: Swap the order of integration and differentiation, then use the Monte-Carlo estimate.

Consideration of SFE

- **Unbiasedness** ✓: The estimator is unbiased in common ML settings.
- **Minimum Variance** ×: The estimator is the highest variance for a constant number of samples compared with the other two.
- **Computational Efficiency** ✓: Certified Blazingly Fast!
  - $\mathcal{O}(N(D_\theta + L_{f(\boldsymbol{x};\phi)}))$
  - An estimate can be made with a single sample.

Further Considerations:

- Black Box score function allowed.
- Higher order differentials are conceptually simple but can be expensive.

Pathwise Gradient Estimator

$$\hat{x} \sim P(\boldsymbol{x}; \boldsymbol{\theta}) \quad \equiv \quad \hat{x} = g(\hat{\epsilon}, \theta), \ \hat{\epsilon} \sim p(\epsilon) \tag{7}$$

- **Idea**: Reparameterise expectation using knowledge of the sampling path g and the base distribution $P(\epsilon)$ to swap order of derivative and integral

Pathwise Gradient Estimator

$$\boldsymbol{\eta} = \nabla_{\boldsymbol{\theta}} \mathbb{E}_{P(\boldsymbol{x};\boldsymbol{\theta})}[f(\boldsymbol{x};\phi)] \tag{8}$$

$$= \nabla \boldsymbol{\theta} \int P(\boldsymbol{\epsilon}) f(g(\boldsymbol{\epsilon};\boldsymbol{\theta})) d\boldsymbol{\epsilon} \tag{9}$$

$$= \mathbb{E}_{P(\boldsymbol{\epsilon})}[\nabla \boldsymbol{\theta} f(g(\boldsymbol{\epsilon};\boldsymbol{\theta}))] \tag{10}$$

$$\approx \bar{\boldsymbol{\eta}}_N = \frac{1}{N} \sum_{n=1}^{N} \nabla \boldsymbol{\theta} f(g(\hat{\boldsymbol{\epsilon}}^{(n)};\boldsymbol{\theta})); \quad \hat{\boldsymbol{\epsilon}}^{(n)} \sim P(\epsilon) \tag{11}$$

- **Idea**: Reparameterise expectation using knowledge of the sampling path g and the base distribution $P(\epsilon)$ to swap order of derivative and integral

Consideration of Pathwise Estimators

- **Unbiasedness** $\times$
  Function needs to be differentiable
- **Minimum Variance** $\checkmark$
  Variance bounds are independent of parameter dimensionality
- **Computational Efficiency** $\checkmark$
  Same computational cost as SFE
  - $\mathcal{O}(N(D_\theta + L_{f(\boldsymbol{x};\phi)}))$
  - An estimate can be made with a single sample.

Measure-valued Gradient Estimator

For D dimensional parameters θ, we can write the gradient for the ith parameter θ_i as

$$
\begin{aligned}
\eta_i &= \nabla_{\theta_i} \mathbb{E}_{P(\boldsymbol{x};\boldsymbol{\theta})}[f(\boldsymbol{x};\phi)] && (12)\\
&= \int \nabla_{\theta_i} P(\boldsymbol{x};\boldsymbol{\theta}) f(\boldsymbol{x};\phi) d\boldsymbol{x} && (13)\\
&= c_{\theta_i}(\mathbb{E}_{p_i^+(\boldsymbol{x};\boldsymbol{\theta})}[f(\boldsymbol{x};\phi)] - \mathbb{E}_{p_i^-(\boldsymbol{x};\boldsymbol{\theta})}[f(\boldsymbol{x};\phi)]) && (14)\\
&\approx \bar{\eta}_{i,N} = \frac{c_{\theta_i}}{N} \left(\sum_{n=1}^{N} f(\dot{\boldsymbol{x}}^{(n)}) - f(\ddot{\boldsymbol{x}}^{(n)}) \right); && (15)
\end{aligned}
$$

$$\dot{\boldsymbol{x}}^{(n)} \sim p_i^+(\boldsymbol{x};\boldsymbol{\theta}), \ddot{\boldsymbol{x}}^{(n)} \sim p_i^-(\boldsymbol{x};\boldsymbol{\theta})$$

- **Idea**: Use properties of signed measures to compute gradient by decomposing it into a weighted difference of two expectations

Consideration of Measure-valued Estimators

- **Unbiasedness** ✓: The estimator is unbiased in common ML settings
- **Minimum Variance** ✓: Variance depends on choice of decomposition so can be chosen to be low
- **Computational Efficiency** ✗: Expensive
  - $\mathcal{O}(2ND_\theta L_{f(\boldsymbol{x};\phi)})$
  - Typically not preferred in a high-dimensional setting

Variance Reduction

We introduce three common methods of variance reduction:

- Large-samples
- Coupling
- Control variates

Variance Reduction
Method 1: Large-samples

Large-samples is the simplest method, which means increasing the sample size, N, if we can.

- Variance shrinks in the order of $\mathcal{O}(\frac{1}{N})$
- Computational cost increases linearly in N
- It serves as a baseline method for other more complex methods

Variance Reduction
Method 2: Coupling

Coupling is designed for estimators that take the form of the difference between two expectations:

$$\eta = \mathbb{E}_{p_1(x)}[f(x)] - \mathbb{E}_{p_2(x)}[f(x)] \tag{16}$$

$$\begin{aligned} \mathbb{V}_{p_{12}(x_1,x_2)}[\bar{\eta}_{cpl}] &= \mathbb{V}_{p_{12}(x_1,x_2)}[f(x_1) - f(x_2)] \qquad (17) \\ &= \mathbb{V}_{p_1(x)}[f(x_1)] + \mathbb{V}_{p_2(x)}[f(x_2)] - 2\mathrm{Cov}_{p_{12}(x_1,x_2)}[f(x_1), f(x_2)] \qquad (18) \end{aligned}$$

Coupling ensures that the blue term is positive by picking a **Common random number** and using it as a seed when we sample x_1 and x_2.

Variance Reduction
Method 3: Control Variates

Control Variates is a general method. It reduces variance by constructing a **substitute function**, $\tilde{f}(x)$ with properties:

- $\mathbb{E}(\tilde{f}(x)) = \mathbb{E}(f(x))$
- $\mathbb{V}(\tilde{f}(x)) < \mathbb{V}(f(x))$

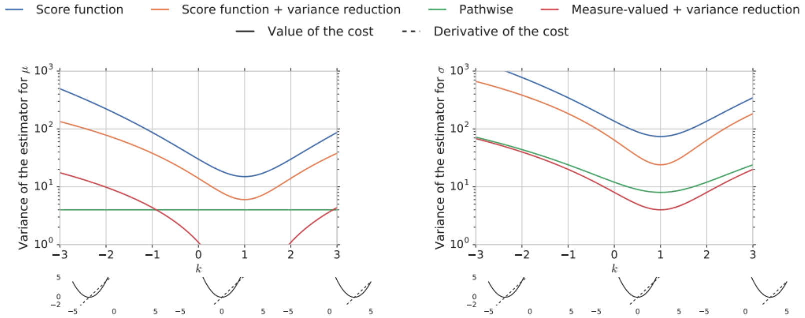
Design a function $h(x)$ with known $\mathbb{E}_{p(x;\theta)}(h(x))$, then we have:

$$\tilde{f}(x) = f(x) - \beta\Big[\underbrace{h(x)}_{\text{control variate}} - \mathbb{E}_{p(x;\theta)}[h(x)]\Big] \tag{19}$$

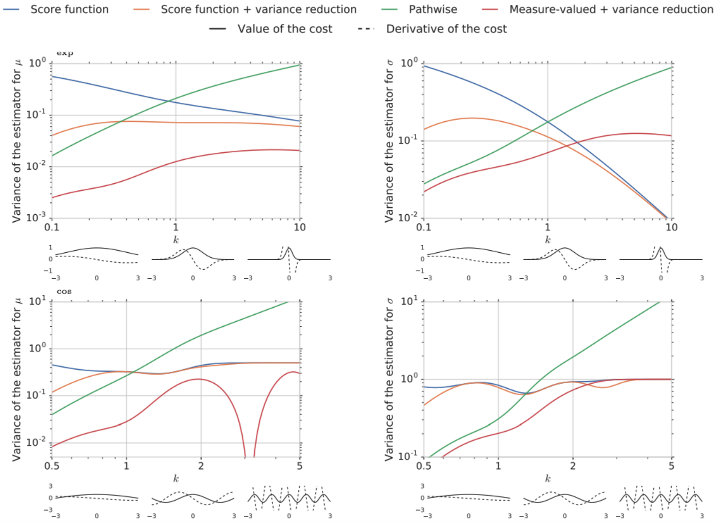
$$\frac{\mathbb{V}[\tilde{f}(x)]}{\mathbb{V}[f(x)]} = \frac{\mathbb{V}\left[f(x) - \beta\left(h(x) - \mathbb{E}_{p(x;\theta)}[h(x)]\right)\right]}{\mathbb{V}[f(x)]} = 1 - \frac{\mathrm{Cov}^2(f,h)}{\mathbb{V}[f]\mathbb{V}[h]} \tag{20}$$

Intuitive Case Study
Quadratic Cost function

$$\eta = \nabla_\theta \int \underbrace{\mathcal{N}(x \,|\, \mu, \sigma^2)}_{\text{Gaussian}} f(x;k)dx; \qquad f \in \left\{(x-k)^2,\ \exp\{-kx^2\},\ \cos(kx)\right\}$$



Intuitive Case Study
Exponential and Cosine cost functions



Conclusion

The big takeaway here is that the lack of universal ranking is a general property of gradient estimators.

This table may be helpful in terms of which method to choose:

-	Score Function	Pathwise	Measure-valued
Consistency	✓	✓	✓
Unbiasedness	✓	×	✓
min. Var.	×	✓	✓
cmpt. eff.	✓	✓	×

Variance reduction is always recommended since it indeed reduces variance for any method we choose.