Chapter 15

SIMULATION-BASED OPTIMIZATION II: STOCHASTIC GRADIENT AND SAMPLE PATH METHODS

• Organization of chapter in ISSO
  – Introduction to gradient estimation
  – Interchange of derivative and integral
  – Gradient estimation techniques
    • Likelihood ratio/score function (LR/SF)
    • Infinitesimal perturbation analysis (IPA)
  – Optimization with gradient estimates
  – Sample path method
Issues in Gradient Estimation

• Estimate the gradient of the loss function with respect to parameters for optimization from simulation outputs

\[ g(\theta) = \frac{\partial L(\theta)}{\partial \theta} \]

where \( L(\theta) \) is a scalar-valued loss function to minimize and \( \theta \) is a \( p \)-dimensional vector of parameters

• Essential properties of gradient estimates
  — Unbiased:
    \[ E[\hat{g}(\theta)] = g(\theta) \]
  — Small variance
Two Types of Parameters

\[ L(\theta) = E\left[ Q(\theta, V) \right] = \int Q(\theta^S, \nu) \rho_V(\nu | \theta^D) d\nu \]

where \( V \) is the random effect in the system, \( \rho_V(\nu | \theta) \) is the probability density function of \( V \)

- **Distributional parameters** \( \theta^D \): Elements of \( \theta \) that enter via their effect on probability distribution of \( V \). For example, if scalar \( V \) has distribution \( N(\mu, \sigma^2) \), then \( \mu \) and \( \sigma^2 \) are distributional parameters

- **Structural parameters** \( \theta^S \): Elements of \( \theta \) that have effects directly on the loss function (via \( Q \))

- Distinction not always obvious
Interchange of Derivative and Integral

• Unbiased gradient estimations using only one simulation require the interchange of derivative and integral:

\[
\frac{\partial L}{\partial \theta} = \frac{\partial}{\partial \theta} \int Q(\theta, \nu) p_{\nu} (\nu | \theta) d\nu = \int \frac{\partial \left[ Q(\theta, \nu) p_{\nu} (\nu | \theta) \right]}{\partial \theta} d\nu
\]

• Above generally not true. Technical conditions needed for validity:
  — \( Q \cdot p_{\nu} \) and \( \frac{\partial (Q \cdot p_{\nu})}{\partial \theta} \) are continuous
  — \( \left| Q(\theta, \nu) p_{\nu} (\nu | \theta) \right| \leq q_0 (\nu), \int q_0 (\nu) d\nu < \infty \)
  — \( \left\| \frac{\partial \left[ Q(\theta, \nu) p_{\nu} (\nu | \theta) \right]}{\partial \theta} \right\| \leq q_1 (\nu), \int q_1 (\nu) d\nu < \infty \)

• Above has implications in practical applications
A General Form of Gradient Estimate

• Assume that all the conditions required for the exchange of derivative and integral are satisfied,

\[
g(\theta) = \int \left[ Q(\theta, \nu) \frac{\partial p_v(\nu | \theta)}{\partial \theta} + \frac{\partial Q(\theta, \nu)}{\partial \theta} p_v(\nu | \theta) \right] d\nu
\]

\[
= \int \left[ Q(\theta, \nu) p_v(\nu | \theta)^{-1} \frac{\partial p_v(\nu | \theta)}{\partial \theta} + \frac{\partial Q(\theta, \nu)}{\partial \theta} \right] p_v(\nu | \theta) d\nu
\]

\[
= E \left[ Q(\theta, \nu) \frac{\partial \log p_v(\nu | \theta)}{\partial \theta} + \frac{\partial Q(\theta, \nu)}{\partial \theta} \right]
\]

• Hence, an unbiased gradient estimate can be obtained as

\[
\hat{g}(\theta) = Q(\theta, \nu) \frac{\partial \log p_v(\nu | \theta)}{\partial \theta} + \frac{\partial Q(\theta, \nu)}{\partial \theta}
\]

Output from one simulation!
Two Gradient Estimates: LR/SF and IPA

\[
\hat{g}(\theta) = Q(\theta, V) \frac{\partial \log p_V(V | \theta)}{\partial \theta} + \frac{\partial Q(\theta, V)}{\partial \theta}
\]

- Likelihood Ratio/ Score Function (LR/SF): only distributional parameters

\[
\hat{g}_{LR/SF}(\theta) = Q(\theta, V) \frac{\partial \log p_V(V | \theta)}{\partial \theta}
\]

- Infinitesimal Perturbation Analysis (IPA): only structural parameters

\[
\hat{g}_{IPA}(\theta) = \frac{\partial Q(\theta, V)}{\partial \theta}
\]