

# Scenario Generation and Sampling Methods

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Let's Start with a Recap

# Sample Average Approximation

We want to solve the “true” problem

$$\min_{x \in X} \{g(x) := \mathbb{E}[G(x, \xi)]\}, \quad (\text{SP})$$

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but it is typically very difficult or impossible to solve.

Generate a sample  $\{\xi^1, \xi^2, \dots, \xi^N\}$  and solve the Sample Average Approximation (SAA):

$$\min_{x \in X} \left\{ \hat{g}_N(x) := \frac{1}{N} \sum_{j=1}^N G(x, \xi^j) \right\}. \quad (\text{SP}_N)$$

# Sample Average Approximation

Recall

$x^*$  := an optimal solution of (SP)

$S^*$  := the set of optimal solutions of (SP)

$\nu^*$  := the optimal value of (SP)

and

$\hat{x}_N$  := an optimal solution of  $(SP_N)$

$S_N$  := the set of optimal solutions of  $(SP_N)$

$\nu_N$  := the optimal value of  $(SP_N)$

View  $(x^*, S^*, \nu^*)$  as “statistical estimators” of  $(\hat{x}_N, S_N, \nu_N)$

# Sample Average Approximation

So far... **Standard Monte Carlo**:  $\{\xi^1, \xi^2, \dots, \xi^N\}$  generated independent and identically distributed (iid) as  $\xi$

And... Looked at the properties of statistical estimators

- Negative Bias:  $\mathbb{E}[\nu_N] \leq \nu^*$
- Strong Consistency: e.g.,  $\nu_N \rightarrow \nu^*$ , w.p.1.
- Rates of Convergence: e.g.,  
 $\sqrt{N}(\nu_N - \nu^*) \xrightarrow{d} \text{Normal}(0, \sigma(x^*))$
- Large Deviations; Exponential Rates of Convergence; ...

## Why Variance Reduction?

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- Consider  $g(x) = \mathbb{E}[G(x, \xi)]$  for a fixed  $x \in \mathcal{X}$ .
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- For illustration purposes, suppose we provide a Confidence Interval (CI) on the value of  $g(x)$  as

$$\left[ \hat{g}_N(x) - 2\sqrt{\text{Var}[\hat{g}_N(x)]}, \hat{g}_N(x) + 2\sqrt{\text{Var}[\hat{g}_N(x)]} \right]$$

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Suppose we have 2 estimators:

<b>Estimator</b>	<b><math>\hat{g}_N(x)</math></b>	<b><math>\text{Var}[\hat{g}_N(x)]</math></b>	<b>CI</b>
1	10	25	[0, 20]
2	10	0.25	[9, 11]

Which one is preferable? Clearly...

# Why Variance Reduction?

Suppose we use standard Monte Carlo with iid  $\{\xi^1, \xi^2, \dots, \xi^N\}$ . In this case:

$$\text{Var}[\hat{g}_N(x)] = \text{Var} \left[ \frac{1}{N} \sum_{j=1}^N G(x, \xi^j) \right] = \frac{\text{Var}[G(x, \xi)]}{N}.$$

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So... to decrease variance we can increase the sample size  $N$

**NOTE:** Although  $\text{Var}[G(x, \xi)]$  is typically unknown, it can be estimated by a sample variance as follows:

$$S_N^2(x) := \frac{\sum_{j=1}^N [G(x, \xi^j) - \hat{g}_N(x)]^2}{N - 1}.$$

The above estimator is unbiased, i.e.,  $\mathbb{E}[S_N^2(x)] = \text{Var}[G(x, \xi)]$ .

# Why Variance Reduction?

However, increasing the sample size is not desirable:

- 1 Estimation of  $G(x, \xi^j)$  for a fixed  $x \in X$  could be very expensive
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**WANT: decrease variance without increasing sample size**

- A well studied topic in statistics and simulation
- When we optimize  $\min_{x \in X} \hat{g}_N(x)$ , variance reduction can be more important
- Poor estimates of objective and/or gradients can slow down the convergence of Monte Carlo simulation-based methods

# Variance Reduction Techniques

We will discuss:

- Antithetic Variates
- Latin Hypercube Sampling
- Quasi-Monte Carlo (QMC) and Randomized QMC
- Importance Sampling
- Control Variates



We will:

- Introduce these techniques in the context of estimating  $G(x, \xi)$  for a fixed  $x \in X$
- Point to literature that uses them for stochastic optimization
- Discuss the properties of resulting statistical estimators when used in the context of stochastic optimization

Some common themes to reduce variance:

- 1 Exploitation of Correlations
- 2 Sampling more “uniformly” than random sampling (or “filling in the space better”)
- 3 Concentrating the sampling to important regions

## Antithetic Variates (AV)

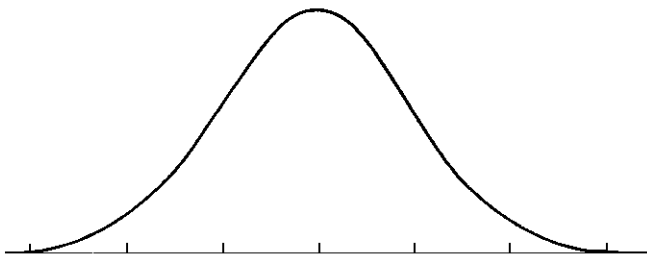
**Idea:** use pairs of negatively correlated random variables to reduce variance

Suppose  $N$  is even and components of  $\xi$  are independent:

- 1 Sample observations  $\{U^1, \dots, U^{\frac{N}{2}}\}$  from a  $U(0, 1)^{d_\xi}$  distribution.
- 2 Calculate the antithetic pairs  $\{U^{1'}, \dots, U^{\frac{N}{2}'}\} = \{1 - U^1, \dots, 1 - U^{\frac{N}{2}}\}$ .
- 3 Apply the inverse cumulative distribution function to obtain  $N$  observations  $\{\xi^1, \xi^{1'}, \xi^2, \xi^{2'} \dots, \xi^{\frac{N}{2}}, \xi^{\frac{N}{2}'}\}$ .

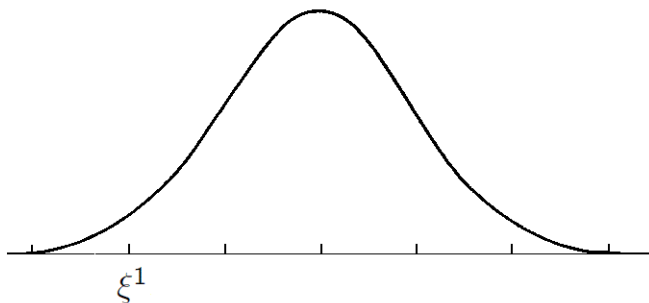
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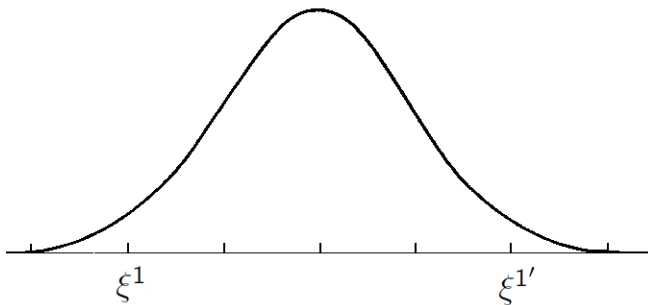
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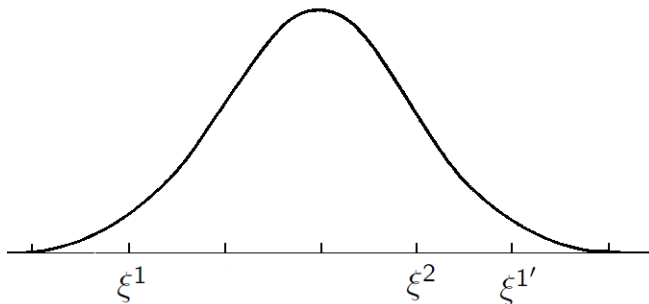
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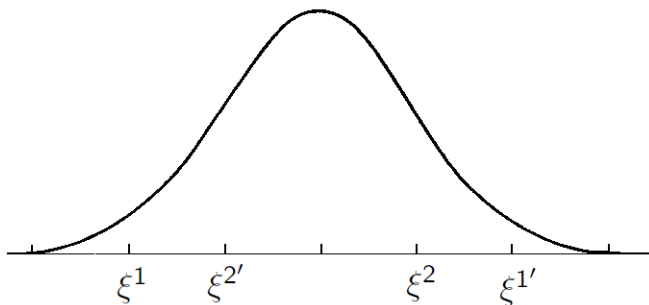
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AV estimator of  $\mathbb{E}[G(x, \xi)]$  is:

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- Unbiased:  $\mathbb{E}[\hat{g}_{N,AV}(x)] = \mathbb{E}[G(x, \xi)]$
- Has variance:

$$\text{Var}[\hat{g}_{N,AV}(x)] = \underbrace{\frac{\text{Var}[G(x, \xi)]}{N}}_{\text{Var of Standard MC!}} + \underbrace{\frac{1}{N} \text{Cov}[G(x, \xi^j), G(x, \xi^{j'})]}_{\text{If Cov} < 0, \text{ AV reduces var!}}$$

The amount of variance reduction depends on how much negative correlation between  $U$  and  $U'$  is preserved when:

- (i) Transforming to  $\xi$  and  $\xi'$
- (ii) Applying  $G(x, \cdot)$

It is well known that  $G(x, \cdot)$  preserves negative correlation when:

- (i)  $G(x, \cdot)$  is bounded and monotone in each component of  $\xi$
- (ii)  $G(x, \cdot)$  is not constant in the interior of  $\Xi$

# AV: Amount of Variance Reduction

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**Example:** Two-stage stochastic linear programs with recourse

$$\begin{aligned} \min_x \quad & \mathbb{E}[G(x, \xi)] = \mathbb{E}[cx + h(x, \xi)] \\ \text{s.t.} \quad & Ax = b, \quad x \geq 0, \end{aligned}$$

where  $h(x, \xi)$  is the optimal value of the linear program

$$\begin{aligned} h(x, \xi) = \min_y \quad & \tilde{q}y \\ \text{s.t.} \quad & Wy \geq \tilde{r} - Tx, \quad y \geq 0. \end{aligned}$$

Here,  $\xi$  is a random vector that is comprised of random elements of  $\tilde{q}$ ,  $\tilde{r}$ .

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**Example Cont'd:** Two-Stage Stochastic Linear Programs are Monotone when:

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**Be careful!** AV can backfire



shows when monotonicity is lost, AV can increase variance

When used for optimization:

-  Analytically show the extent of variance reduction using AV on a newsvendor problem
  - Decreases bias of  $\nu_N$  ( $\mathbb{E}[\nu_N] \leq \nu^*$ )
  - Can increase or decrease variance depending on parameters

# AV: In the Context of Optimization



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# Latin Hypercube Sampling (LHS)



**Idea:** use stratified sampling but in a less computationally intensive way

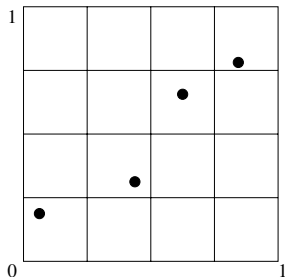
Suppose components of  $\xi$  are independent:

- 1 For each component of  $\tilde{\xi}$ :
  - 1.1 Sample observations  $U^i \sim U(\frac{i-1}{N}, \frac{i}{N})$  for  $i = 1, \dots, N$ .
  - 1.2 Randomly permute these  $N$  observations.
- 2 Apply the inverse cumulative distribution function to obtain  $\{\xi^1, \dots, \xi^N\}$ .

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**Example:** Dimension  $d_{\xi} = 2$  and sample size  $N = 4$



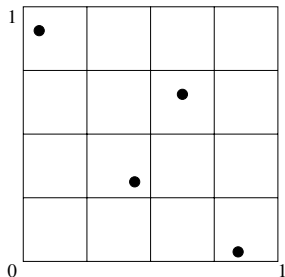
(a) Stratified

(Images: )

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(b) LHS

(Images: )

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- More generally

$$\text{Var} [\hat{g}_{N,\text{LHS}}(x)] \leq \frac{N}{N-1} \text{Var} [\hat{g}_N(x)]$$

When used for optimization:

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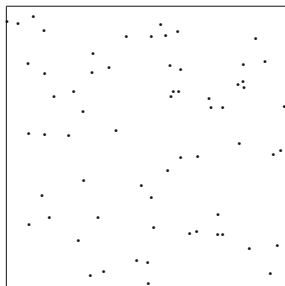
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  - Completely removes bias of  $\nu_N$  ( $\mathbb{E}[\nu_N] = \nu^*$ ) –A really nice side effect!
  - Decreases variance considerably
- Many studies show LHS effectively reduces variance and bias for several classes of stochastic programs; e.g., (???)

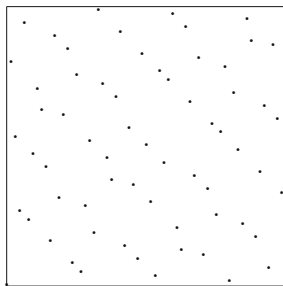


# Quasi-Monte Carlo (QMC) and Randomized Quasi-Monte Carlo (RQMC)

**Idea:** use a low-discrepancy sequence to sample more uniformly. The sequence doesn't have to be independent or random.



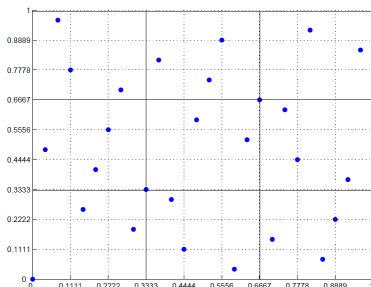
(a) Random Sequence



(b) Sobol' Sequence

(Images: Lemieux (2009))

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(c) (0,3,2)-net in base b=3

(Image: Homem-de-Mello and Bayraksan (2014))

Many different ways to generate these sequences:

- Sobol'
- Niederreiter
- Lattice rules
- Digital nets and sequences
- ...

For simplicity, we will assume  $\xi$  is a random vector with independent components, each with uniform distribution over  $[0, 1]$



How to measure the quality (or “uniformity”) of these sequences?

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## Star Discrepancy

- Consider a  $d_\xi$  dimensional unit cube  $[0, 1)^{d_\xi}$
- A point set  $P = \{\xi^j\}_{j=1}^\infty$  inside  $[0, 1)^{d_\xi}$
- $P_N$  denotes the first  $N$  points from the point set  $P$
- Consider hyper-rectangles with a corner at the origin

$$B(\mathbf{v}) = \prod_{i=1}^{d_\xi} [0, v_i]$$

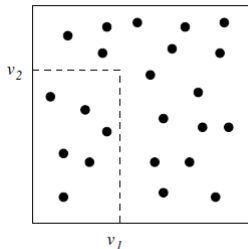
where  $\mathbf{v}$  is a vector  $(v_1 \ v_2 \ \dots \ v_{d_\xi})$

# Star Discrepancy

Star Discrepancy is the Kolmogorov-Smirnov distance between the point set and the uniform distribution over the unit cube:

$$D^*(P_N) := \sup_{\mathbf{v} \in [0,1]^{d_\xi}} \left| \frac{\text{Number of } \xi^j \in B(\mathbf{v})}{N} - \prod_{i=1}^{d_\xi} v_i \right|$$

## Example (Lemieux, 2009):



$v_1 = 0.4$ ,  $v_2 = 0.7$  and  $6/23$  points inside the box, gives a discrepancy of  $|6/23 - 0.4 \times 0.7| = 0.019$

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- Conjecture that for deterministic sequences, the best that can be achieved is  $D^*(P_N) \in O\left(\frac{(\log N)^{d\xi}}{N}\right)$

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- *Koksma-Hlawka inequality* gives a bound on the error

$$|\hat{g}_{N,\text{QMC}}(x) - g(x)| \leq D^*(P_N)V(G(x, \cdot))$$

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- For large  $d_\xi$ , QMC can backfire! (esp. with low  $N$ )
- One way to deal with this is to find the “effective” dimension of the problem and use LHS or Standard MC on the other dimensions; e.g., (Drew and Homem-de-Mello, 2006; Drew, 2007)

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→ So that we do better than standard MC!

Many different ways to do randomization

- Random shift
- Digital shift (for digital nets)
- Scrambling and Permutations, ...

# RQMC: Cranley Patterson Random Shift

Generate a random vector  $\mathbf{u} \sim U([0.1]^{d_\xi})$

Let

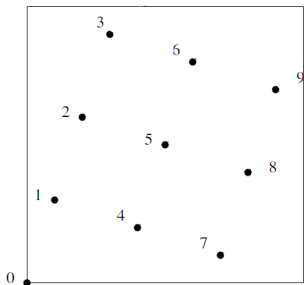
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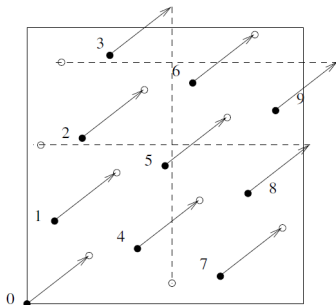


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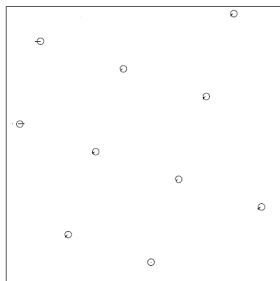


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# RQMC: Estimation of Error

Generate  $m$  iid RQMC sequences  $\tilde{P}_N$

$$\hat{g}_{N,\text{RQMC}}^l(x) = \frac{1}{N} \sum_{j=1}^N G(x, \tilde{\xi}^j), \quad l = 1, 2, \dots, m$$

and use the estimator

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- This estimator is unbiased:  $\mathbb{E}[\hat{g}_{N,\text{RQMC}}(x)] = g(x)$
- And the error can be estimated through the variance

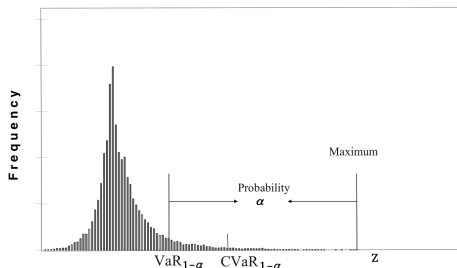
$$\frac{1}{m-1} \sum_{l=1}^m \left( \hat{g}_{N,\text{RQMC}}^l(x) - \hat{g}_{N,\text{RQMC}}(x) \right)^2$$

# Importance Sampling (IS)



# Importance Sampling: Motivation

**Idea:** Concentrate samples to most important areas. Especially can be useful for “rare” events.



$$\text{CVaR}_{1-\alpha}[G(x, \xi)] = \min_{\eta} \left\{ \eta + \frac{1}{\alpha} \mathbb{E} [(G(x, \xi) - \eta)_+] \right\}$$

If  $\alpha = 0.05$ , 95% of the standard Monte Carlo samples do not contribute to positive values in this expectation!

# IS: How does it work?

For simplicity, suppose  $\xi$  has density  $f$ . Then,

$$g(x) = \mathbb{E}[G(x, \xi)] = \int_{\Xi} G(x, \xi) f(\xi) d\xi$$

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Here,  $\mathcal{L}(\xi) = \frac{f(\xi)}{q(\xi)}$  is the **likelihood ratio**, which we assume is well defined  
(for this, we may set  $\mathcal{L}$  to zero whenever both  $f$  and  $q$  are zero).

# IS: How does it work?

Standard MC: iid sample  $\{\xi^1, \xi^2, \dots, \xi^N\}$  from density  $f$

Importance Sampling: iid sample  $\{\tilde{\xi}_q^1, \tilde{\xi}_q^2, \dots, \tilde{\xi}_q^N\}$  from density  $q$

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The importance sampling estimator:

$$\hat{g}_{N,IS}(x) = \frac{1}{N} \sum_{j=1}^N G(x, \tilde{\xi}_q^j) \mathcal{L}(\tilde{\xi}_q^j)$$

- Unbiased:  $\mathbb{E}[\hat{g}_{N,IS}(x)] = g(x)$



**How to obtain  $q$ ?**

## How to obtain $q$ ?

→ To reduce variance! To understand this better, let's take a look at the variance of the IS estimator.

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Consider the following facts:

- $\mathbb{E}[G(x, \tilde{\xi}_q)\mathcal{L}(\tilde{\xi}_q)] = \mathbb{E}[G(x, \xi)]$
- $\mathbb{E}[G^2(x, \tilde{\xi}_q)\mathcal{L}^2(\tilde{\xi}_q)] = \mathbb{E}[G^2(x, \xi)\mathcal{L}(\xi)]$
- Therefore, the variance of the IS estimator is

$$\text{Var}[\hat{g}_{N,\text{IS}}(x)] = \frac{1}{N} [\mathbb{E}[G^2(x, \xi)\mathcal{L}(\xi)] - (\mathbb{E}[G(x, \xi)])^2],$$

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→ Reduce Variance when  $\mathbb{E}[G^2(x, \xi)\mathcal{L}(\xi)] < \mathbb{E}[G^2(x, \xi)]$

# How to obtain IS distribution?

When  $G(x, \cdot) \geq 0$ , setting  $\text{Var} [\hat{g}_{N, \text{IS}}(x)] = 0$  results in the **optimal zero-variance density**

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Too good to be true? **YES!** Requires knowledge of unknown quantity!

Nevertheless, select  $q$

$$q(\xi) \propto f(\xi)G(x, \xi)$$

to achieve variance reduction even though the proportionality constant may not be known

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Many different ways to obtain the IS distribution

- Exponential Tilting
- Using Large Deviations
- Nonparametric methods, . . .
- Exploit the problem structure
- Still an open area of research

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The nominal probability mass function (pmf) is:  $f(\xi) = \frac{1}{|\Xi|}$
- Instead of the expensive evaluations  $G(x, \xi)$ , suppose there is a good *approximation function*  $H(x, \xi)$  that:
  - estimates the value of  $G(x, \xi)$  cheaply and
  - orders the values  $G(x, \xi)$  in the same way

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$$g(\xi) = \begin{cases} \frac{1}{2} \frac{1}{\lfloor \alpha |\Xi| \rfloor}, & \xi : H(x, \xi) \geq V_H \\ \frac{1}{2} \frac{1}{|\Xi| - \lfloor \alpha |\Xi| \rfloor}, & \xi : H(x, \xi) < V_H \end{cases}$$

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- Barrera et al. (2016) apply IS to a chance constrained problem with rare probabilities.
- They show consistency of the SAA problem formed using IS (optimal values converge, etc.)
- They make two important improvements:
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Think of  $\mathcal{L}_x(\xi)$  instead of  $\mathcal{L}(\xi)$
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## Control Variates (CV)

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Let  $C$  be a *control variable* with

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With  $\lambda$  a scalar, the control variate estimator of  $\mathbb{E}[G(x, \xi)]$  is given by

$$\hat{g}_{N, CV}(x) = \frac{1}{N} \sum_{j=1}^N (G(x, \xi^j) + \lambda C^j)$$

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- We can **minimize this variance by setting  $\lambda$  to**

$$\lambda^* = \frac{-\text{Cov}[G(x, \xi), C]}{\text{Var}[C]}.$$

Plug  $\lambda^*$  back in:

$$\text{Var}[\hat{g}_{N,\text{CV}}^*(x)] = \frac{1}{N} \left( \sigma^2(x) - \frac{\text{Cov}^2[G(x, \xi), C]}{\text{Var}[C]} \right)$$

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Can be estimated, but when an estimator of  $\lambda^*$  is used:

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- Can still yield significant variance reduction
- Obeys a Central Limit Theorem (CLT) of the form (Nelson, 1990)

$$\sqrt{N}(\hat{g}_{N, CV}(x) - \mathbb{E}[G(x, \xi)]) \xrightarrow{d} \text{Normal}(0, \text{Var}[\hat{g}_{N, CV}^*(x)])$$

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**Example (Pierre-Louis et al., 2011):** Consider two-stage stochastic programs of the form:

$$\min_{x \in X} \{g(x) := c(x) + \mathbb{E}[Q(x, \xi)]\},$$

where

$$\begin{aligned} Q(x, \xi) = \min_{y \geq 0} \quad & q(y) \\ \text{s.t.} \quad & g(y) \leq h(\xi) - T(x, \xi). \end{aligned}$$

Assume:

- (A1)**  $Q(x, \cdot)$  is convex on  $\text{co}(\Xi)$  for all  $x \in X$ ;
- (A2)**  $\xi$  has independent components, and  $h(\cdot)$  and  $T(x, \cdot)$  are affine on  $\mathbb{R}^{d_\xi}$  for all  $x \in X$ .

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This class of problems could be:

- Two-Stage Stochastic Linear Program
- Two-Stage Stochastic Convex Program
- $X$  can have integrality restrictions, leading to a Stochastic Integer Program

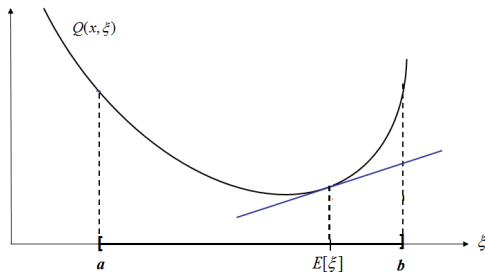


# CV: Example Use in Optimization

Use the first-order Taylor approximation of  $Q(x, \cdot)$  as the control random variable

$$C(x, \xi) = Q(x, \bar{\xi}) + \nabla_{\xi} Q(x, \bar{\xi})(\xi - \bar{\xi})$$

where  $\bar{\xi} = \mathbb{E}[\xi]$



To Sum Up...

# Recap of Variance Reduction Techniques We Discussed

Some change the way we Sample:

- Antithetic Variates
- Latin Hypercube Sampling
- Quasi-Monte Carlo (deterministic!)
- Randomized Quasi-Monte Carlo
- Importance Sampling

Some applied typically for a fixed  $x$  and exploits problem structure:

- Importance Sampling
- Control Variates

Some can backfire if not used properly:

- Antithetic Variates (if cannot induce negative correlation)
- Randomized Quasi-Monte Carlo (for high dimensions)
- Importance Sampling (if IS distribution not selected properly)

Can significantly improve the performance of SAA if used well (and sometimes with minimal effort)

How about properties of SAA with variance reduction?

**Bias of  $\nu_N$ :** Let  $\xi^1, \xi^2, \dots, \xi^N$  satisfy

$$\mathbb{E} \left[ \frac{1}{N} \sum_{j=1}^N G(x, \xi^j) \right] = \mathbb{E} [G(x, \xi)], \quad \forall x \in X$$

Then,  $\mathbb{E} [\nu_N] \leq z^*$ .

Unbiasedness condition above is satisfied by many variance reduction techniques we discussed: AV (with adjustments to estimator), LHS, RQMC, IS, CV (under certain conditions)

For AV, LHS, and RQMC Bias reduction have been observed.

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# Strong Consistency of $\nu_N$ and $\hat{\chi}_N$

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- **AV:** Because AV pairs  $(\xi^j, \xi^{j'})$  are iid, results typically follow from iid case with modifications to notation
- **LHS:** Might require additional conditions. For instance, pointwise Strong Law of Large Numbers (SLLN) requires:

$$\mathbb{E} [(G(x, \xi))^2] < \infty$$

Conditions under which consistency results hold are discussed in, e.g., (Drew, 2007; Stockbridge, 2013).

- **RQMC:** One condition that is needed is that the star discrepancy of QMC sequence shrinks to zero

$$D^*(P_N) \searrow 0$$

as  $N \nearrow \infty$ . Then, through *epi-convergence* and under additional assumptions, consistency results are shown (Koivu, 2005)

- **QMC:** Similar results through epi-convergence have been shown for QMC discretization, e.g, (Pennanen and Koivu, 2005)

**Rates of Convergence of Optimal Values:** can be obtained for a class of problems that satisfy (Homem-de-Mello, 2008):

## Assumption PLF

Suppose either

- (i)  $X$  is convex and compact polyhedron
  - (ii)  $G(\cdot, \xi)$  is convex and piecewise linear
  - (iii)  $\xi$  has finite support
- or  $X$  is finite.

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$$\frac{\hat{g}_N(x^*) - g(x^*)}{\sigma_N(x^*)} \xrightarrow{d} \text{Normal}(0, 1)$$

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Then, optimal values also obey a CLT:

$$\frac{\nu_N - \nu^*}{\sigma_N(x^*)} \xrightarrow{d} \text{Normal}(0, 1)$$



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- **AV:** Also by iid case above,  $O(N^{-1/2})$
- **LHS:** Pointwise CLT for LHS holds when  $G$  is bounded

$$\sup_{x \in X, \xi \in \Xi} |G(x, \xi)| < M \quad \text{for some } 0 < M < \infty$$

and  $G(x^*, \cdot)$  is not additive.

Then, rate of convergence is same as standard MC:  $O(N^{-1/2})$

- **RQMC:** For a RQMC where pointwise CLT holds, rate of convergence is

$$O\left(\left[\frac{(\log N)^{d_\xi-1}}{N^3}\right]^{\frac{1}{2}}\right)$$

This rate is asymptotically better than standard MC.

**Rates of Convergence of Optimal Solutions:** have similar properties (Homem-de-Mello, 2008).

For simplicity, let's assume assumption PLF holds.

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If exponential rate of convergence holds pointwise

$$P(|\hat{g}_N(x) - g(x)| \geq \delta) \leq C_x e^{-N\gamma_x(\delta)}, \quad \forall x \in X$$

for all  $N \geq 1$  and  $\delta > 0$  with some constant  $C_x > 0$  and function  $\gamma_x(\cdot)$  such that  $\gamma_x(0) = 0$  and  $\gamma_x(z) > 0$  if  $z > 0$

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**LHS:** Pointwise large deviations results (i.e., exponential rates of convergence) holds, for instance, when  $G(x, \cdot)$  is monotone in each component of  $\xi$

## Some Final Remarks

- Variance Reduction can be very important for optimization because it can significantly improve the statistical estimators
- Many asymptotic (and other) properties of SAA can be recovered when variance reduction techniques are used (sometimes, though, under more stringent conditions)
- If not used properly, some techniques may backfire
- Still more to do with respect to algorithmic (optimization wise) and application-based advances

Thank you

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