# Monte Carlo Methods for Assessing Solution Quality in Stochastic Optimization

David Morton

Graduate Program in Operations Research

The University of Texas at Austin

Joint work with: Güzin Bayraksan, Anukal Chiralaksanakul, Amit Partani and Kevin Wood.

## Stochastic Programming Models

$$z^* = \min_{x \in X} E\, f(x, \tilde{\xi})$$

Such problems arise in stochastic dynamic programming, statistics, simulation, and mathematical programming.

Choice of $f$ determines problem class

Motivating Applications

- Hedge Fund of Funds Construction. Deutsche Asset Management

  Elmira Popova, Ivilina Popova, Ken Yip and Ming Zhong

- Interdicting Nuclear Material Smuggling. Los Alamos National Laboratory

  Bill Charlton, Feng Pan, and Kevin Saeger

- Hydroelectric Scheduling. Pacific Gas & Electric Company

  Jonathan Jacobs, Gary Freeman, Jan Grygier, Gary Schultz,
  Konstantin Staschus, Jery Stedinger, Zhiming Wang and Bin Zhang

Time dynamics: static to two stage to multi stage

# Hedge Fund of Funds Construction

Funds w/ returns $\tilde{\xi} = (\tilde{\xi}_1, \ldots, \tilde{\xi}_m)$; decision, % of fund $i$: $x = (x_1, \ldots, x_m)$

$$z^* = \max_x \; Ef\left(\sum_{i=1}^m \tilde{\xi}_i x_i\right)$$
$$\text{s.t.} \;\; x \in X \equiv \left\{ x \, : \, \sum_{i=1}^m x_i = 1, x \geq 0 \right\}$$

where

$$f(\xi x) = I(\xi x \geq r_o) - \lambda (r_1 - \xi x)^+, \;\; \lambda \geq 0$$

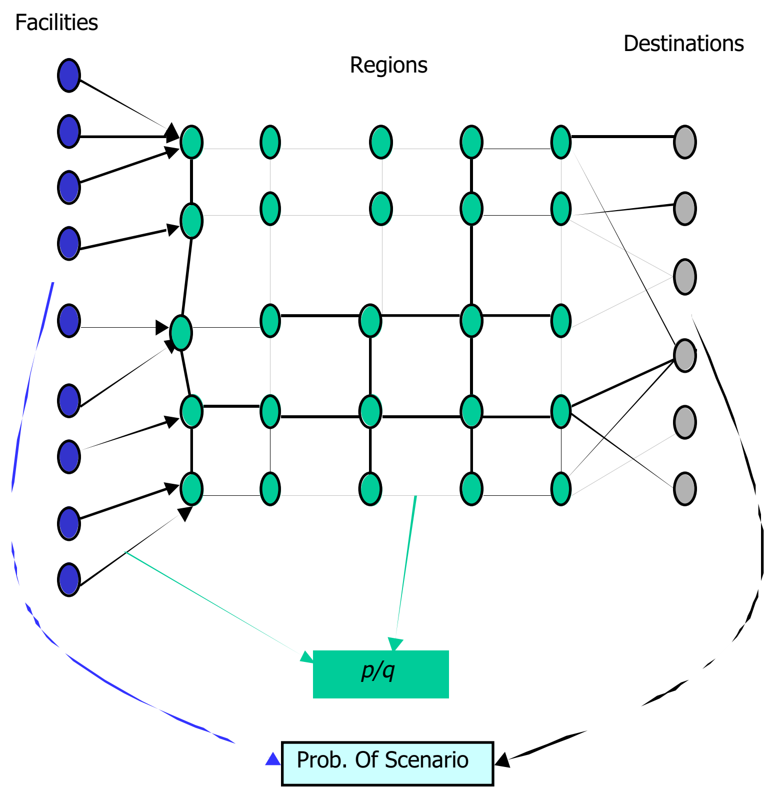
Monte Carlo sampling approximation:

$$z_n^* = \max_{x \in X} \frac{1}{n} \sum_{i=1}^n f\left(\tilde{\xi}^i x\right) \quad \text{with optimal solution} \quad x_n^*$$

Here, $\tilde{\xi}^1, \ldots, \tilde{\xi}^n$ i.i.d. as $\tilde{\xi}$ or from another sampling scheme

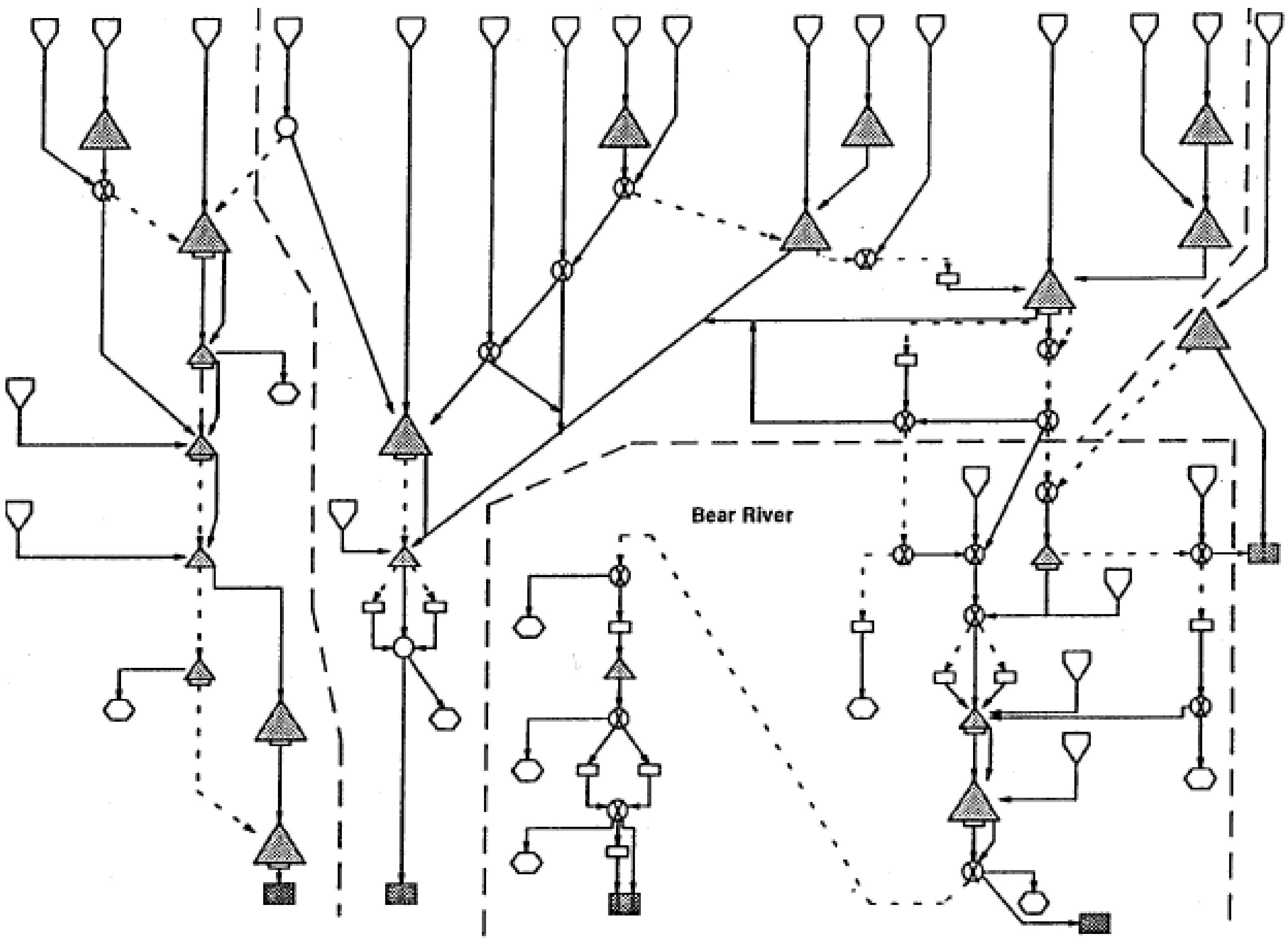
Typical size: $m = 10$ funds, $r_o = 15\%$, $\lambda = 0$ (most computationally demanding), $n = 500$

# Interdicting Nuclear Material Smuggling: Second Line of Defense




- Goal: Minimize probability of successful smuggling of nuclear material
- Approach: Install radiation sensors at key locations, subject to budget constraint
- 85 facilities, 91 geographic regions, 263 customs checkpoints, 9 destinations

# Hydro-Electric Scheduling: YBSF Hydrological Basin



## Hydro-Thermal Scheduling: Verbal Description

Minimize    Expected system operation cost

subject to

- Satisfying load
- Bounds on thermal generation
- Bounds on hydro releases, reservoir volumes, and spills
- Hydro network-flow constraints
- Side constraints, e.g., decrees

with

- Stochastic natural inflows
- Nonlinear cost function ($/MWh)
- Subperiod modeling for weekday & weekend peak & offpeak
- Planning horizon $\approx$ two years
- End effects: target reservoir levels or future value function
- $\approx$ Four stochastic stages
- $\approx$ 10 hydrological basins
- $\leq$ 12 reservoirs per basin

45 scenario YBSF model: 70,000 constraints and 250,000 decision variables

# Monte Carlo Methods in Stochastic Programming

- True/population problem:

$$(SP) \qquad z^* = \min_{x \in X} E\, f(x, \tilde{\xi})$$

Denote optimal solution $x^*$

- Sample problem:

$$(SP_n) \qquad z_n^* = \min_{x \in X} \left[ \frac{1}{n} \sum_{i=1}^{n} f(x, \tilde{\xi}^i) \right]$$

Here, $\tilde{\xi}^1, \ldots, \tilde{\xi}^n$ i.i.d. as $\tilde{\xi}$. Denote optimal solution $x_n^*$

- View $z_n^*$ as an estimator of $z^*$ and $x_n^*$ as an estimator of $x^*$

- What can we say about $z_n^*$ and $x_n^*$ as $n \to \infty$?

Note: Variety of names . . . external sampling method, sample-path optimization, sample average approximation, stochastic counterpart, non-recursive method, and retrospective optimization

# Monte Carlo Methods in SP: Example

$$(SP) \qquad z^* = \min_{-1 \le x \le 1} \left[ E\, f(x, \tilde{\xi}) = E\tilde{\xi} x \right], \text{ where } \tilde{\xi} \sim N(0,1)$$

Every feasible solution, $x \in [-1, 1]$ is optimal and $z^* = 0$

$$(SP_n) \qquad z_n^* = \min_{-1 \le x \le 1} \left( \frac{1}{n} \sum_{i=1}^{n} \tilde{\xi}^i \right) x$$

$x_n^* = \pm 1$, $z_n^* = -\left| N(0, 1/n) \right|$

## Observations

1. $E z_n^* \le z^* \, \forall n$ (negative bias)
2. $E z_n^* \le E z_{n+1}^* \, \forall n$ (monotonically shrinking bias)
3. $z_n^* \to z^*$, wp1 (strongly consistent)
4. $\sqrt{n}(z_n^* - z^*) = -\left| N(0,1) \right|$ (non-normal errors)
5. $B_z(n) = E z_n^* - z^* = a_1 / \sqrt{n}$ ($O(n^{-1/2})$ bias)

So, *optimization* changes the nature of sample-mean estimators

Note: What if $x \in [-1, 1]$ is replaced with $x \in \Re$?

# Monte Carlo Methods in SP: Bias

$$\min_{x \in X} E\left[\frac{1}{n}\sum_{i=1}^{n} f(x, \tilde{\xi}^i)\right] = \min_{x \in X} E\, f(x, \tilde{\xi}) = z^*$$

and so we obtain

$$E z_n^* = E\left[\min_{x \in X} \frac{1}{n}\sum_{i=1}^{n} f(x, \tilde{\xi}^i)\right] \leq \min_{x \in X} E\, f(x, \tilde{\xi}) = z^*, \text{ i.e., } \boxed{E z_n^* \leq z^*}$$

Simple example when $n = 1$

$$E \min_{x \in X} f(x, \tilde{\xi}) \leq \min_{x \in X} E f(x, \tilde{\xi})$$

Interpretation: We'll do better if we get to "wait and see" $\tilde{\xi}$ before choosing $x$

Also, can show bias decreases monotonically

$$\boxed{E z_n^* \leq E z_{n+1}^* \leq z^*}$$

# Assessing Solution Quality

$$(SP) \qquad z^* = \min_{x \in X} E\, f(x, \tilde{\xi})$$

Our goal: Given $\hat{x} \in X$ and $\alpha$ we want to find a (random) confidence interval width $\tilde{\epsilon}$ with:

$$\boxed{P(E\, f(\hat{x}, \tilde{\xi}) \leq z^* + \tilde{\epsilon}) \approx 1 - \alpha}$$

Recall bias result $E z_n^* \leq z^*$ where

$$(SP_n) \qquad z_n^* = \min_{x \in X} \left[ \frac{1}{n} \sum_{i=1}^{n} f(x, \tilde{\xi}^i) \right]$$

So,

$$\underbrace{E \left[ \frac{1}{n} \sum_{i=1}^{n} f(\hat{x}, \tilde{\xi}^i) - \min_{x \in X} \frac{1}{n} \sum_{i=1}^{n} f(x, \tilde{\xi}^i) \right]}_{G_n} \geq E f(\hat{x}, \tilde{\xi}) - z^*$$

Remarks

- Anticipate var $G_n \leq$ var $U_n +$ var $L_n$
- $G_n \geq 0$
- $G_n$ is not asymptotically normal (what to do?)

## Assessing Solution Quality: Multiple Replication Procedure (MRP)

1. Find $\hat{x} \in X$, candidate solution
2. Generate $n_g$ batches of size $n$:

$$\tilde{\xi}^{11}, \tilde{\xi}^{12}, \ldots, \tilde{\xi}^{1n}$$

$$\tilde{\xi}^{21}, \tilde{\xi}^{22}, \ldots, \tilde{\xi}^{2n}$$

$$\vdots$$

$$\tilde{\xi}^{n_g 1}, \tilde{\xi}^{n_g 2}, \ldots, \tilde{\xi}^{n_g n}$$

3. Calculate point estimate: $\bar{G}(n_g) = \dfrac{1}{n_g} \displaystyle\sum_{i=1}^{n_g} G_n^i = \dfrac{1}{n_g} \sum_{i=1}^{n_g} \left[ \dfrac{1}{n} \sum_{j=1}^{n} f(\hat{x}, \tilde{\xi}^{ij}) - \min_{x \in X} \dfrac{1}{n} \sum_{i=1}^{n} f(x, \tilde{\xi}^{ij}) \right]$

Based on the central limit theorem for i.i.d.r.v.'s:

$$\sqrt{n_g} \left[ \bar{G}(n_g) - EG_n \right] \Rightarrow N(0, \sigma_g^2) \text{ as } n_g \to \infty$$

Construct $(1-\alpha)$-level confidence interval for optimality gap $= Ef(\hat{x}, \tilde{\xi}) - z^*$

$$\left[ 0, \bar{G}(n_g) + \frac{t_{n_g-1,\alpha} s_g(n_g)}{\sqrt{n_g}} \right]$$

## Related Work and Connections

- Stochastic Programming

  Wait-and-see generalized to all-pairs and all-tuples problems: Birge

  Within sampling-based cutting-plane algorithms: Higle & Sen and Dantzig, Glynn & Infanger

  Estimating bounds w/in branch-and-bound: Norkin, Pflug & Ruszczynski

  Estimating bounds via duality: Higle & Sen

  Statistical verification of KKT conditions: Higle & Sen and Shapiro & Homem-de-Mello

- Stochastic dynamic programming and Markov decision processes

  Reinforcement learning in MDPs

  Confidence intervals for American-style option prices: Broadie and Glasserman

  Bias and variance for value functions in MDPs: Mannor, Simester, Sun & Tsitsiklis

- Statistics and Simulation

  Constrained MLE estimation: Huber

  Confidence regions in stochastic approximation: Pflug

  Indifference (or not) zones in ranking and selection: Goldsman & Nelson

  Mesh-based optimization: Ensor & Glynn

  IPA gradient-estimators with common random numbers: Atlason, Epelman & Henderson

## Shortcomings of the MRP

1. We solve one SP to obtain $\hat{x}$/policy and then thirty more just to assess $\hat{x}$/policy's quality
2. The bias of $z_n^*$ can be large
3. The error due to sampling can be large
4. $\hat{x}$/policy may be a poor solution

Recall the confidence interval is:

$$\left[0, \bar{G}(n_g) \; + \; \frac{t_{n_g-1,\alpha} s_g(n_g)}{\sqrt{n_g}}\right]$$

where

$$\bar{G}(n_g) = \frac{1}{n_g} \sum_{i=1}^{n_g} \left[ \frac{1}{n} \sum_{j=1}^{n} f(\hat{x}, \tilde{\xi}^{ij}) - \min_{x \in X} \frac{1}{n} \sum_{i=1}^{n} f(x, \tilde{\xi}^{ij}) \right]$$

We'll discuss ideas to circumvent 1-3, but not 4.

## A Single Replication Procedure

*Input:* Desired CI level $1-\alpha$, sample size $n$ and a candidate solution $\hat{x} \in X$

*Output:* $(1-\alpha)$-level confidence interval on $Ef(\hat{x},\tilde{\xi}) - z^*$

1. Sample i.i.d. observations $\tilde{\xi}^1, \ldots, \tilde{\xi}^n$ from the distribution of $\tilde{\xi}$
2. Solve (SP$_n$) to obtain $x_n^*$
3. Calculate $G_n(\hat{x})$ and $s_n^2(x_n^*)$

$$G_n(\hat{x}) = \bar{f}_n(\hat{x}) - \bar{f}_n(x_n^*)$$

$$s_n^2(x_n^*) = \frac{1}{n-1}\sum_{i=1}^{n}\left[(f(\hat{x},\tilde{\xi}^i) - f(x_n^*,\tilde{\xi}^i)) - (\bar{f}_n(\hat{x}) - \bar{f}_n(x_n^*))\right]^2$$

4. Output one-sided CI on $Ef(\hat{x},\tilde{\xi}) - z^*$,

$$\left[0,\ G_n(\hat{x}) + \frac{t_{n-1,\alpha}s_n(x_n^*)}{\sqrt{n}}\right]$$

## Justifying a Single Replication Procedure

**Theorem 1** *Let* $0 < \alpha < 1$, $\hat{x} \in X$, *and* $\tilde{\xi}^1, \ldots, \tilde{\xi}^n$ *be i.i.d. as* $\tilde{\xi}$. *Then, under mild conditions*

$$\liminf_{n \to \infty} P\left( \frac{\left[\bar{f}_n(\hat{x}) - \bar{f}_n(x_n^*)\right] - \left[Ef(\hat{x}, \tilde{\xi}) - z^*\right]}{s_n(x_n^*)/\sqrt{n}} \geq -z_\alpha \right) \geq 1 - \alpha$$

From this we infer that for sufficiently large values of $n$

$$P\left( Ef(\hat{x}, \tilde{\xi}) - z^* \leq \left[\bar{f}_n(\hat{x}) - \bar{f}_n(x_n^*)\right] + z_\alpha s_n(x_n^*)/\sqrt{n} \right) \approx 1 - \alpha$$

Here,

$$s_n^2(x_n^*) = \widehat{\text{var}} \left[ f(\hat{x}, \tilde{\xi}) - f(x_n^*, \tilde{\xi}) \right]$$

So, we can employ common random number in the single-replication procedure

Aside: Just because we *can* run a single-replication procedure doesn't mean it's the most computationally efficient approach

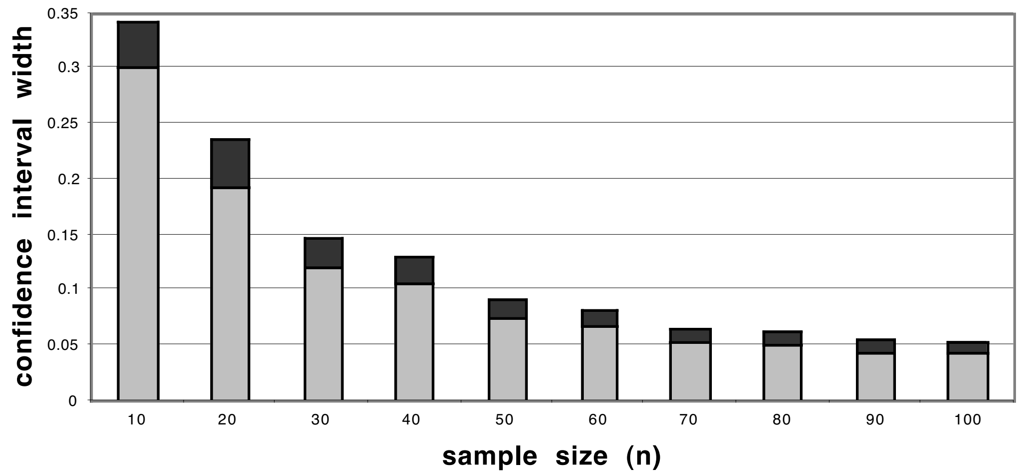
If sampling error dominates lower-bound bias then we may prefer to solve 10 small instances of $(SP_n)$ instead of one large $(SP_n)$

## Lower-Bound Bias Reduction: Motivation

A two-stage stochastic LP TELE (Higle and Sen). Based on larger SSN model.

TELE has 7 first-stage decision variables, 14 stochastic parameters and $4.1 \times 10^7$ scenarios.

Number of replications is $n_g = 20$, $\alpha = 0.05$ and $\hat{x}$ was found by solving $(SP_n)$ with $n = 1000$.




Plot of $\bar{G}_{n_g} + \epsilon_g$ versus $n$

Contribution CI width by $\bar{G}_{n_g}$ (gray) is significantly larger than the sampling error, $\epsilon_g$ (black)

Separate estimation shows $Ef(\hat{x}, \tilde{\xi}) \approx 8.298 \pm 0.005\,(95\%)$

## Lower-Bound Bias Reduction
## Generalized Jackknife and Adaptive Jackknife

Generalized jackknife estimator is used to eliminate $O(n^{-p})$ bias (Gray and Schucany)

Let $g_n$ be an estimator of $g_\mu$ that is based on $n$ i.i.d. observations and assume

$$B_g(n) = Eg_n - g_\mu = a_1/n^p + a_2/n^{p+1} + \cdots .$$

Now,

$$n^p Eg_n = n^p g_\mu + a_1 + a_2/n + \cdots$$

and

$$(n-1)^p Eg_{n-1} = (n-1)^p g_\mu + a_1 + a_2/(n-1) + \cdots$$

So,

$$E \underbrace{\left[ \frac{n^p g_n - (n-1)^p g_{n-1}}{n^p - (n-1)^p} \right]}_{J^{(n)}(p)} = g_\mu + O(n^{-2})$$

This assumes $p$ is known, but it's unknown ...

$\longrightarrow$ Adaptive jackknife includes a *third* equation to eliminate both $a_1$ and $p$

## Multistage Lower-Bound Bias Reduction

In multistage problems, allocate samples in nonuniform empirical scenario tree to reduce bias

Applied to stochastic lot-sizing and American-style option pricing

Derive analytical bias estimator: $\hat{b}_t(I_t^i, n(t,i))$

Allocate sample size for stage $t$ by solving

$$\begin{aligned} \min_{n(t,1),\ldots,n(t,m_t)} \quad & \sum_{i=1}^{m_t} \hat{p}_t^i \, \hat{b}_t(I_t^i, n(t,i)) \\ \text{s.t.} \quad & \sum_{i=1}^{m_t} n(t,i) = n_{t+1} \\ & n(t,i) \geq \underline{n}(t,i), \; i = 1, \ldots, m_t. \end{aligned}$$

Here, $p_t^i = P(\tilde{I}_t = I_t^i)$

## Towards Variance Reduction: Quasi-Monte Carlo

Recall methods for computing

$$\int_{a_1}^{b_1} \cdots \int_{a_d}^{b_d} g(u_1, \ldots, u_d) du_d \ldots du_1$$

1. **Analytical Integration**
2. **Numerical Quadrature** (e.g., Simpson's rule in $\Re^d$)

   Quality: deterministic error bounds

   Viability: limited by dimension $d$, say, $d \leq 2, 3$
3. **Monte Carlo Integration**

   Quality: statistical error bounds

   Viability: converges slowly ($\propto 1/\sqrt{n}$) but rate independent of $d$

**QMC methods** lie between 2 and 3, trying to avoid dimensional effect of 2 and trying to improve on convergence rate of 3

*Low-discrepancy* sequences of points achieve $O(n^{-1} \log^d n)$ rate of convergence

For sufficiently large $n$, $n^{-1} \log^d n \leq n^{-1/2}$.

When $d = 14$ (TELE) this requires $n \geq 8.3 \times 10^{59}$. Notion of an *effective dimension*

## Variance Reduction: Randomized Quasi-Monte Carlo (RQMC)

### Shortcomings of trying to directly plug QMC into our setting

1. $z_n^*$ isn't biased low, it's not even a random variable
2. Lack of useful error statements

### RQMC circumvents both these difficulties

Denote QMC points $\mathcal{U}_n = \{u^1, \ldots, u^n\}$

Random shift: Redefine each element of $\mathcal{U}_n$ as $\tilde{u}^i = [u^i + v]$ where $v \sim U[0,1]^d$

Perform $n_g$ i.i.d. replications of such a shift. Then, as an immediate consequence (Fox 99, L'Ecuyer and Lemieux 00, Sloan and Joe 92), we obtain

**Proposition 2** *Revise solution-quality procedure to use RQMC to generate the i.i.d. batches. Then,*

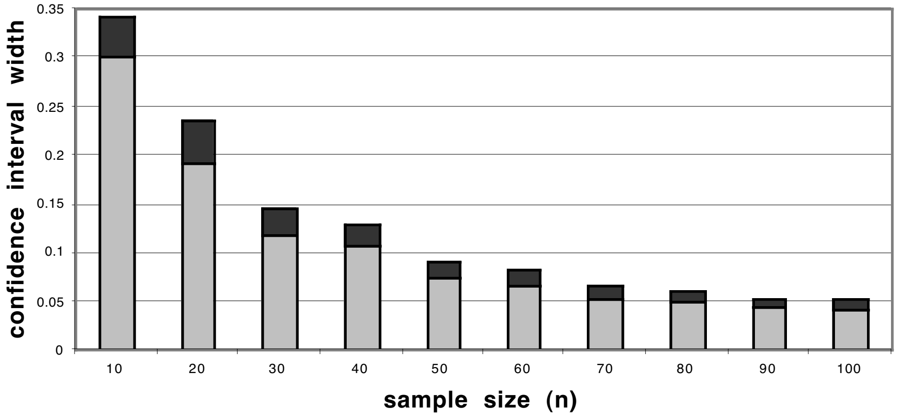
*(i)* $EG_n^1 \geq Ef(\hat{x}, \tilde{\xi}) - z^*$,

*(ii)* $\sqrt{n_g}\left[\bar{G}_{n_g} - EG_n^1\right] \Rightarrow N(0, \sigma_g^2)$ *as* $n_g \rightarrow \infty$ *where* $\sigma_g^2 = \textit{var}\, G_n^1$, *and*

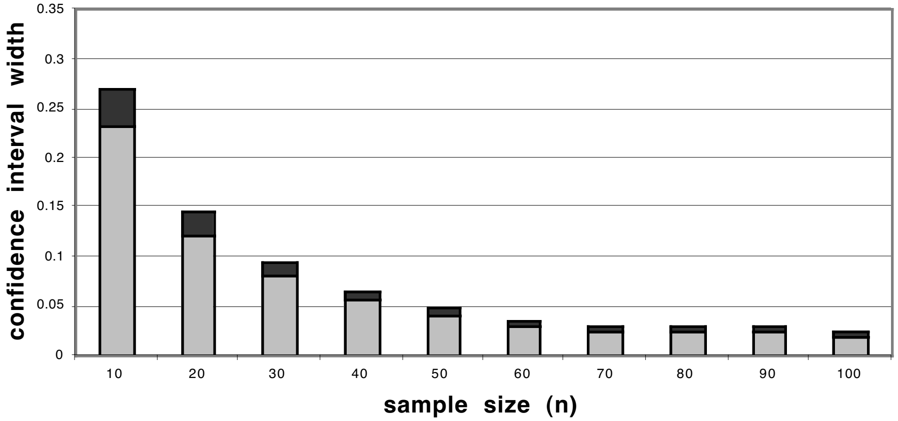
*(iii)* $Es_g^2 = \sigma_g^2$ *and* $s_g^2 = s_g^2(n_g) \rightarrow \sigma_g^2$, *wp1.*

# Variance Reduction: Randomized Quasi-Monte Carlo (RQMC)

## Monte Carlo




## Randomized Quasi-Monte Carlo




Note: Both sampling error and bias appear to shrink

## Assessing Solution Quality in Stochastic Programs: Summary

- Stochastic Programming Models
  - Static asset allocation
  - Two-stage stochastic network interdiction
  - Multi-stage hydro-electric scheduling

- Monte Carlo Integration & Optimization
  - Results for MC
  - Influence of optimization on results

- A MC Procedure for Assessing Solution Quality

- Efficiency Considerations
  - To replicate or not?
  - Reducing bias: generalized jackknife and nonuniform trees
  - Reducing variance: RQMC