On the Initial Transient Problem for Steady-State Simulation

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Outline of Talk

1. The Steady-State Simulation Problem
   - What is it?
   - Why is it relevant?
   - Challenges
2. The Initial Transient Problem
   - Is it a serious problem?
   - When is it a serious problem?
3. The Basic Approaches to the Initial Transient Problem
   - Simulating a stationary version
   - Identifying the initial transient period
   - Low bias estimators

Steady-State Simulation

$Y(t)$ = **rate at which "reward" increases at time** t

Assume there exists a (deterministic) constant α **such that**

$$\frac{1}{t}\int_0^t Y(s)ds \Rightarrow \alpha$$

as $t \longrightarrow \infty$**.**

Goal: Compute α

Examples

$Y(t) =$ **number-in-system (in queue) at time** t

$Y(t) =$ **work-in-process (in manufacturing system) at time** t

$$Y(t) = I(Q(t) \geq b)$$

Why the emphasis on steady-state simulation?

To compute $\alpha(t,x) = \mathrm{E}_x\, f(X(t))$**:**

$$\alpha'(t) = A\alpha(t)$$

$$\alpha(0) = f$$

To compute $\alpha = \sum_x \pi(x) f(x)$**:**

$$\pi = \pi A$$

s/t $\sum_x \pi(x) = 1$

$$\alpha = \pi f$$

Analytical tractability? No!

Modeling Issues

(favoring use of a steady-state formulation)

- **no need to specify time horizon**
- **no need to specify initial distribution**
- **appropriate in many applications**

A Computational Issue

(favoring use of a steady-state formulation)

Goal: Compute $\mathrm{E}_x f(X(t))$ with t large

Method 1: Averaging over independent replications of $f(X(t))$

Error $\approx \frac{t^{1/2}\sigma(\infty)}{\sqrt{c}} N(0,1)$

Method 2: Average one replication of X over $[0, c]$

Error $\approx ae^{-\eta t} + \frac{\sigma}{\sqrt{c}} N(0,1)$

Method 1 is superior when $c >> \frac{t}{a^2} e^{2\eta t}$

(computational budget c needs to be really large!)

Steady-State Simulation: Challenge 1

- **The steady state mean α involves the "infinite time behavior" of $(Y(s) : s \geq 0)$**

- **How do we compute α based on a finite-horizon simulation?**

- **Mathematically:** $\mathrm{E}\,\frac{1}{t}\int_0^t Y(s)ds \neq \alpha$

- **Conceptually:**

  Initial condition is atypical of steady-state

  $\Downarrow$

  "initial transient"

  $\Downarrow$

  "initial bias"

Steady-State Simulation: Challenge 2

In view of Challenge 1, choose time horizon t large

$$\Downarrow$$

One observation of process Y over $[0, t]$

$$\Downarrow$$

How to compute an estimator for the variance of

$$\frac{1}{t}\int_0^t Y(s)ds\,?$$

A Connection between the Two Challenges

$$\mathrm{E}_x\, f(X(t)) = \alpha + a(x)e^{-\eta t}(1+o(1))$$

and

$$\begin{aligned}
&\operatorname{cov}(f(X^*(0)), f(X^*(t))) \\
&\quad = \quad \mathrm{E}_\pi\, f_c(X(0))\, f_c(X(t)) \\
&\quad = \quad \mathrm{E}_\pi\, f_c(X(0)) \cdot \mathrm{E}[f_c(X(t))|X(0)] \\
&\quad = \quad \mathrm{E}_\pi\, f_c(X(0)) \cdot a(X(0))e^{-\eta t}(1+o(1))
\end{aligned}$$

- **used intensively**
- **doesn't work in presence of non-Markov processes**

Today: We focus on Challenge 1

"The Initial Transient Problem"

How serious a problem is the Initial Transient?

For geometrically ergodic (Markov) processes,

$$Y(t) \Rightarrow Y(\infty) \text{ as } t \to \infty \text{ and}$$

$$\mathrm{E}\,Y(t) = \mathrm{E}\,Y(\infty) + O(e^{-\eta t})$$

so

$$\begin{aligned}
&\mathrm{E}\,\frac{1}{t}\int_0^t Y(s)ds - \alpha \\
&\quad = \quad \frac{1}{t}\int_0^\infty \{\mathrm{E}\,Y(s) - \mathrm{E}\,Y(\infty)\}ds - \frac{1}{t}\int_t^\infty \{\mathrm{E}\,Y(s) - \mathrm{E}\,Y(\infty)\}ds \\
&\quad = \quad b/t + O(e^{-\eta t})
\end{aligned}$$

Also, $t^{1/2}\left(\frac{1}{t}\int_0^t Y(s)ds - \alpha\right) \Rightarrow \sigma N(0,\,1)$

$$\mathrm{var}\left(\frac{1}{t}\int_0^t Y(s)ds\right) \sim \sigma^2/t$$

Conclusion

- **Initial bias effect is small relative to sampling variability**

- **For most OR-related steady-state simulations, initial transient is not serious and can be ignored**

  Why: Any time-horizon large enough to make the sampling variability small effectively eliminates the effect of the initial transient.

There are exceptions

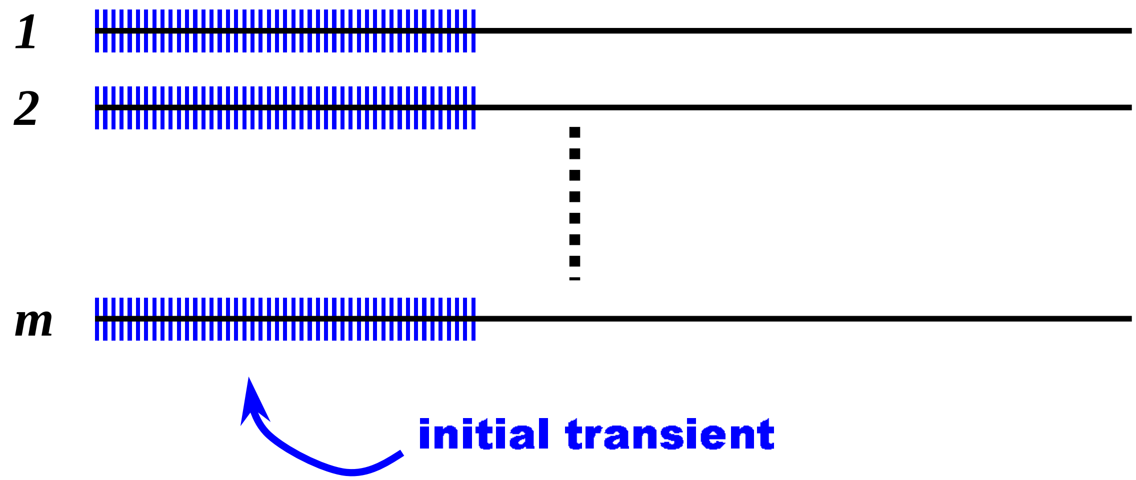
- **parallel simulation**

- **long-range dependent processes**

- **multi-modal behavior / nearly decomposable systems**

- **high dimensional systems**

Parallel Simulation



- **MSE analysis:**

$$\textbf{variance}\left(\frac{1}{m}\sum_{i=1}^{m}\frac{1}{t}\int_0^t Y_i(s)ds\right) \sim \frac{\sigma^2}{mt}$$

$$\textbf{bias}\left(\frac{1}{m}\sum_{i=1}^{m}\frac{1}{t}\int_0^t Y_i(s)ds\right) \sim \frac{b}{t}$$

- **If $m \gg t$, initial transient becomes dominant effect.**

GH 90's

Long-range dependence

- **In the presence of long-range dependence,**

$$\mathrm{var}\left(\frac{1}{t}\int_0^t Y(s)ds\right) \sim \frac{\sigma^2}{t^{2-2H}} \qquad (1/2 < H < 1)$$

- **How to allocate c units of computer time in single processor setting?**

m **independent replications of length** c/m

$$\mathrm{var}\left(\frac{1}{m}\sum_{i=1}^{m}\frac{1}{c/m}\int_0^{c/m} Y_i(s)ds\right) \approx \frac{\sigma^2 m^{1-2H}}{c^{2-2H}}$$

- **Choose m large ...**

- **Same initial bias problem as in parallel simulation setting**

Nearly Decomposable Systems

$$P = \begin{pmatrix} P_{11} & & & & \\ & P_{22} & & \varepsilon & \\ & & \ddots & & \\ & \varepsilon & & \ddots & \\ & & & & P_{dd} \end{pmatrix}$$

- Particularly challenging context . . .
- Any statistically based "detection rule" can be fooled
- Arises in Markov chain Monte Carlo context
- Random re-start

High-Dimensional Systems

$$\overrightarrow{Y}(t) = (Y_1(t), \ldots, Y_d(t))$$

independent

$$\|P(Y_i(t) \in \cdot) - P(Y_i(\infty) \in \cdot)\|y \sim ce^{-\lambda t}$$

$$\|P(\overrightarrow{Y}(t) \in \cdot) - P(\overrightarrow{Y}(\infty) \in \cdot)\| \sim dce^{-\lambda t} \qquad \text{G05}$$

Slows down convergence rate...

There are models for which initial transient is significant

3 Approaches to Dealing with the Initial Transient

- **Approach 1** Simulate a stationary version of Y
  exact simulation / perfect simulation

- **Approach 2** Identify the initial transient interval $[0, t]$

- **Approach 3** Modify the estimator so as to reduce the "initial bias" effect

Approach 1: Simulate a stationary version of Y

$$Y(t) = f(X(t))$$

- **Choose** $X(0) \sim \pi$
- **Don't know** π**!**
- **Can we sample from** π **based on the ability to do a dynamic simulation of** X**?**
- **Exact/ perfect simulation**

$$\begin{aligned}
\pi(\cdot) &= \frac{\mathrm{E} \int_0^{\tau} I(X(s) \in \cdot) ds}{\mathrm{E}\, \tau} \\
&= \int_0^{\infty} \mathrm{P}\left(X(s) \in \cdot \mid \tau > s\right) \frac{\mathrm{P}(\tau > s) ds}{\mathrm{E}\, \tau} \\
&= \mathrm{P}(X(Z) \in \cdot)
\end{aligned}$$

AGT 92

$$Z \sim \frac{\mathrm{P}(\tau > \cdot)}{\mathrm{E}\, \tau}$$

- **Are there any interesting problem classes for which**

$$\mathrm{P}(\tau > \cdot)/\,\mathrm{E}\,\tau$$

is known, but simulating from $\pi(\cdot)$ directly is hard?

- **Yes . . .**

$$P^m(x,y) \geq \varepsilon\phi(y)$$

$$P^m(x,y) = \varepsilon\phi(y) + (1-\varepsilon)q(x,y)$$

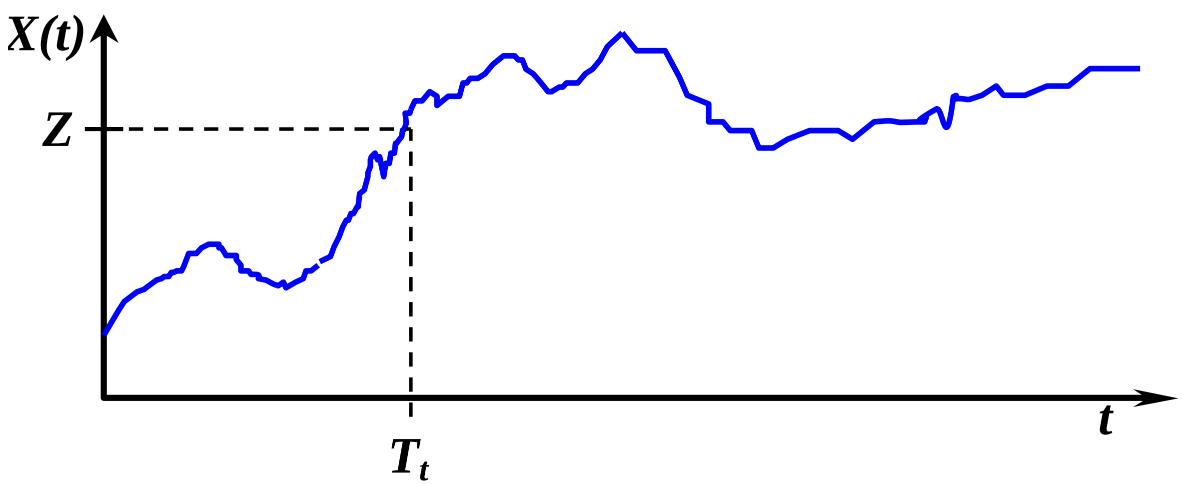
$$P(\tau = mk) = \varepsilon(1-\varepsilon)^{k-1}$$

$\frac{\tau}{m}$ **geometric**

AGT (1992)
Propp/Wilson (1996)
⋮

A Statistically-based alternative

- **Simulate Markov process** X **over** $[0, t]$
- **Compute** $\widehat{\pi}_t(x) = \frac{1}{t}\int_0^t I(X(s) = x)ds$
- **Generate** $Z_t \sim \widehat{\pi}_t$
- **Put** $T_t = \inf\{s \geq 0 : X(s) = Z_t\}$
- **Then,** $\|(X(s) : T_t \leq s \leq T_t{+}t) - (X^*(s) : 0 \leq s \leq t)\| \longrightarrow 0$



G 93

Approach 2: Identify initial transient interval $[0, t_0]$

- **Use analytic bounds to compute t_0 for which**

$$||\mathrm{P}(Y(t_0) \in \cdot) - \mathrm{P}(Y(\infty) \in \cdot)|| < \varepsilon$$

For many geometrically ergodic processes,

$$\mathrm{E}_x f(X(t)) = \alpha + a(x)e^{-\gamma t + i\theta t}(1 + o(1))$$

where $\gamma > 0$. Here, $z = -\gamma + i\theta$ is second largest (in modulus) eigenvalue of A.

  - **For highly structured models, one can sometimes compute asymptotics for z (Diaconis)**
  - **For reversible systems, one can compute analytic bounds on z (Cheeger)**
  - **For regenerative systems, one can obtain bounds on $||\mathrm{P}(Y(t) \in \cdot) - \mathrm{P}(Y(\infty) \in \cdot)||$ (Roberts, Rosenthal)**

- **Use an approximating analytic model to identify t_0:**

$$Y(t) \stackrel{\mathscr{D}}{\approx} \widetilde{Y}(t)$$

Single-server FIFO queue in "heavy-traffic":

$$Y(t) \stackrel{\mathscr{D}}{\approx} \mathrm{RBM}(t)$$

$$t_0 = c(1-\rho)^{-2}$$

For infinite-server queue in "heavy-traffic":

$$Y(t) \stackrel{\mathscr{D}}{\approx} \text{Gaussian process}$$

$$t_0 \approx F^{-1}(1-\varepsilon)$$

Problems

- good approximations hard to compute for most models (networks)

  Possible remedy:

  - simulate simplified model first; determine t_0 based on simulation
  - then simulate real model

- note that time to stationarity t_0 depends on functional being computed

t_0 for "number-in-system"
$\neq t_0$ for "buffer loss"

γ for "number-in-system"
$\neq \widetilde{\gamma}$ for exponential moments of "number-in-system"

Statistically Based Methods

- Many proposals have been made

  e.g. discard initial observations until the first one left is neither the maximum nor the minimum of the remaining observations (Conway 1963)

- Problematic both in theory and in practice

A Basic Difficulty

- In general, one has only one realization of the initial transient on which to base one's statistical analysis.

- Any rigorous rule needs to "model" the initial transient

  e.g., autoregressive process

$$X_{n+1} = \rho X_n + \varepsilon_{n+1}$$

Regenerative Processes

$$a(t) = \mathrm{E}\,Y(t)$$

$$a = b + F * a \qquad \textbf{(renewal eqn)}$$

Solution is

$$a = U * b$$

If b, F are known, choose t_0 such that $|a(t_0) - a(\infty)| < \varepsilon$

If b, F are unknown, estimate these from cycles simulated:

$$\widehat{F}_n(t) = \tfrac{1}{n}\sum_{i=1}^{n} I(\tau_i \le t)$$

$$\widehat{b}_n(t) = \tfrac{1}{n}\sum_{i=1}^{n} b_i(t)$$

Choose $\widehat{t}$ so that

$$|(\widehat{U}_n * \widehat{b}_n)(\widehat{t}) - (\widehat{U}_n * \widehat{b}_n)(\infty)| < \varepsilon \qquad \text{BG06, KG06}$$

Approach 3: Low Bias Estimators

Attempt 1

$$\mathrm{E}\,\frac{1}{t}\int_0^t Y(s)ds = \alpha + \frac{b}{t} + O(e^{-\lambda t})$$

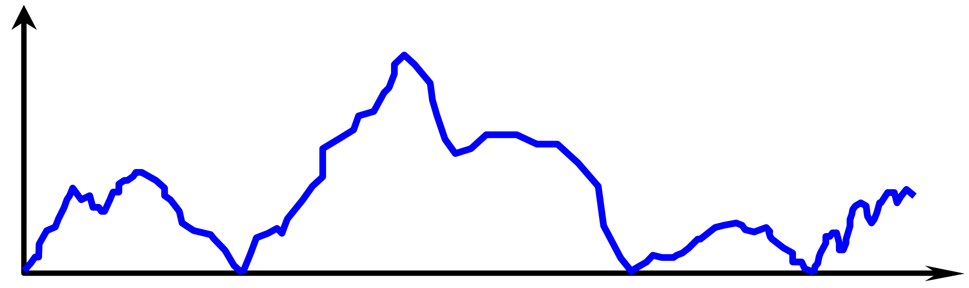
Estimate α, b via a linear regression

Use $\widehat{\alpha}$ from linear regression

Doesn't work ...

As for Approach 2, must “model” initial transient

Regenerative Processes



$$Y = (Y(s) : 0 \leq s \leq T_n)$$

$$(\int_{T_{i-1}}^{T_i} Y(s)ds, T_i - T_{i-1} : 1 \leq i \leq n)$$

$$iid$$

- **No initial transient on time scale of regenerative cycles**
- **Structure of initial transient highly dependent on time scale used**

How does initial bias manifest itself on time scale of regenerative cycles?

$$\alpha = \frac{\mathrm{E}\int_0^{T_1} Y(s)ds}{\mathrm{E}\,T_1} \triangleq \frac{\mathrm{E}\,W}{\mathrm{E}\,T}$$

$$\alpha_n = \frac{\overline{W}_n}{\overline{T}_n} = g(\overline{W}_n, \overline{T}_n)$$

$$\mathrm{E}\alpha_n \neq g(\mathrm{E}\overline{W}_n, \mathrm{E}\overline{T}_n)$$

$\nwarrow$ **non-linearity bias**

Solutions:

- **Taylor expand ...**   **estimate** $\downarrow$

$$\mathrm{E}\alpha_n = \alpha - \frac{1}{n}\frac{\mathrm{E}[(W - \alpha T)T]}{(\mathrm{E}\,T)^2} + \frac{c}{n^2} + O\left(\frac{1}{n^3}\right) \qquad \text{CI75}$$

- **Jack-knife**

On time scale of simulated time:

$$\mathrm{E}\,\frac{1}{t}\int_0^t Y(s)ds = \alpha + \frac{b}{t} + O(e^{-\lambda t})$$

where

$$b = \frac{\mathrm{E}\int_0^{T_1} s[Y(s)-\alpha]ds}{\mathrm{E}\,T_1}$$

$\nearrow$

estimate from cycles completed by t

G 90

Typical Theoretical Analysis

$$\mathrm{E}\,\widehat{\alpha}_L(t) = \alpha + o(1/\tau)$$

$$\mathrm{var}\,\widehat{\alpha}_L(t) \sim \mathrm{var}\,\widehat{\alpha}(t) \qquad \textbf{as } t \longrightarrow \infty.$$

Hence, $\widehat{\alpha}_L(t)$ is better...

A More Careful Analysis

$$
\begin{aligned}
\mathrm{E}\,\widehat{\alpha}(t) &= \alpha + \frac{b}{t} + o(1/t) \\
\mathrm{E}\,\widehat{\alpha}_L(t) &= \alpha + o(1/t) \\
\mathrm{var}\,\widehat{\alpha}(t) &= \frac{\sigma^2}{t} + \frac{c_1}{t^2} + o(1/t^2) \\
\mathrm{var}\,\widehat{\alpha}_L(t) &= \frac{\sigma^2}{t} + \frac{c_2}{t^2} + o(1/t^2) \\
\mathrm{MSE}(\widehat{\alpha}(t)) &= \frac{\sigma^2}{t} + \frac{c_1 + b^2}{t^2} + o(1/t^2) \\
\mathrm{MSE}(\widehat{\alpha}_L(t)) &= \frac{\sigma^2}{t} + \frac{c_2}{t^2} + o(1/t^2)
\end{aligned}
$$

Need to check that $c_2 < c_1 + b^2$! A+G 06

Conclusions

- **There are problems in which initial transient can be a serious issue**
- **There are rigorously supported methods for reducing the effect of the initial transient**

  even in single replication setting!
- **Ideas apply even in nonstationary settings, e.g., when to initialize simulations focused on "rush hours"?**