SEQUENTIAL MONTE CARLO TECHNIQUES FOR THE SOLUTION OF LINEAR SYSTEMS

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ABSTRACT

Given a *linear system*

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b},$$

where $\boldsymbol{x}$ is an m-vector, *direct numerical methods*, such as Gaussian elimination, take time $O(m^3)$ to find $\boldsymbol{x}$.

Iterative numerical methods, such as the Gauss-Seidel method or SOR, reduce the system to the form

$$\boldsymbol{x} = \boldsymbol{a} + \boldsymbol{H}\boldsymbol{x},$$

whence $$\boldsymbol{x} = \sum_{r=0}^{\infty} \boldsymbol{H}^r \boldsymbol{a};$$

and then apply the iterations

$$\boldsymbol{x}_0 = \boldsymbol{a}, \boldsymbol{x}_{s+1} = \boldsymbol{a} + \boldsymbol{H}\boldsymbol{x}_s,$$

until sufficient accuracy is achieved; this takes time $O(m^2)$ per iteration. They generate the truncated sums

$$\boldsymbol{x}_s = \sum_{r=0}^{s} \boldsymbol{H}^r \boldsymbol{a}.$$

The usual *plain Monte Carlo* approach uses independent "random walks," to give an approximation to the truncated sum $\boldsymbol{x}_s$, taking time $O(m)$ per random step.

Unfortunately, millions of random steps are typically needed to achieve reasonable accuracy (say, 1% r.m.s. error). Nevertheless, this is what has had to be done, if m is itself of the order of a million or more.

The alternative presented here, is to apply a sequential Monte Carlo method, in which the sampling scheme is iteratively improved. Simply put, if

$$\boldsymbol{x} = \boldsymbol{y} + \boldsymbol{z},$$

where $\boldsymbol{y}$ is a current estimate of $\boldsymbol{x}$, then its correction, $\boldsymbol{z}$, satisfies

$$\boldsymbol{z} = \boldsymbol{d} + \boldsymbol{H}\boldsymbol{z},$$

where $$\boldsymbol{d} = \boldsymbol{a} + \boldsymbol{H}\boldsymbol{y} - \boldsymbol{y}.$$

At each stage, one uses plain Monte Carlo to estimate $\boldsymbol{z}$, and so, the new estimate $\boldsymbol{y}$. If the sequential computation of $\boldsymbol{d}$ is itself approximated, numerically or stochastically, then the expected time for this process to reach a given accuracy is again $O(m)$ per random step; but the number of steps is dramatically reduced [improvement factors of about 5,000, 26,000, and 700 have been obtained in preliminary tests].

A. THE MONTE CARLO METHOD

The Monte Carlo method, which uses statistical sampling and estimation techniques, applied to synthetically constructed random populations with appropriate parameters, to evaluate the solutions to mathematical problems (whether they have a probabilistic background or not), is very ancient in its origins; but its systematic use dates back essentially to the 1940s.[1] The author's survey paper[2] gives definitions, explanations, history, and references. The method is used as a last resort for solving many very large and computationally intractable problems, in such areas as the design of nuclear reactors, radiation shielding, nuclear fission and fusion bombs; studies of percolation and diffusion; quantum chemistry of atoms, molecules, polymer chains, and ferromagnets; complex illumination, reflectance, and shadowing problems in high-quality computer graphics; the design of VLSI chips and PC boards (routing and placement problems); economic models, cell population and epidemiological studies; and a variety of problems in optimization, operations research, and systems analysis.

The underlying mathematical concept is simple. We consider the problem of numerically evaluating a finite *Lebesgue-Stieltjes integral,*

$$\theta = \int_S f(s)\,\mathrm{d}\omega(s), \tag{A1}$$

where f is an integrable function in a measure-space $(S, \boldsymbol{S}, \omega)$. If we can derive a random variable (r.v.) g in a probability space $(M, \boldsymbol{M}, \mu)$, such that the expected value of g is

$$E[g] = \int_M g(t)\,\mathrm{d}\mu(t) = \theta, \tag{A2}$$

also, then repeated independent sampling of $\tau_1, \tau_2, \ldots, \tau_w$ from M yields independent values $g(\tau_u)$ of the "unbiased primary estimator" g of θ, and hence "secondary estimators"

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1 See, e.g., BUSLENKO et al. **(1)**, ERMAKOV **(10)**, HAMMERSLEY and HANDSCOMB **(47)**, KALOS and WHITLOCK **(50)**, KLEIJNEN, **(51)** and **(52)**, RUBINSTEIN **(65)**, SOBOL' **(66)**, SPANIER and GELBARD **(67)**, and YAKOWITZ **(78)**—such numbers refer to the Bibliography.

2 HALTON **(29)**.

$$G_w(\tau_1, \tau_2, \ldots, \tau_w) = \frac{1}{w}\sum_{u=1}^{w} g(\tau_u); \tag{A3}$$

for which

$$E[G_w] = E[g] = \theta \quad \text{and} \quad Var[G_w] = \frac{1}{w}Var[g] = \frac{\sigma^2}{w}. \tag{A4}$$

Furthermore, the Kolmogorov Strong Law of Large Numbers, indicates that[3]

$$G_w \to \theta \left\{ \begin{matrix} \text{(q.m.)} \\ \text{(p.)} \\ \text{(a.s.)} \end{matrix} \right\} \text{ as } w \to \infty. \tag{A5}$$

More generally,[4] if $\left[K_w\right]_{w=1}^{\infty}$ is any sequence of random variables and we are given that the r.v. K_w converge *stochastically*, in some way, to θ, then we call the sequence $\left[K_w\right]_{w=1}^{\infty}$ a **Monte Carlo process**[5] for θ. Thus, we see that it is possible to estimate the solution θ to our problem by random sampling.

For our purposes, it suffices to consider the problem of evaluating a *finite sum*

$$\theta = \sum_{t=1}^{N} f(t). \tag{A6}$$

We can arbitrarily select a probability function $p(t) \geq 0$ in the *index set*[6]

$$N_N = \{1, 2, \ldots, N\}, \tag{A7}$$

such that

$$\sum_{t=1}^{N} p(t) = 1, \tag{A8}$$

with the further proviso:[7]

$$\text{if} \quad f(t) \neq 0, \quad \text{then} \quad p(t) > 0; \tag{A9}$$

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[3] The abbreviation "a.s." denotes "almost sure" convergence (also termed convergence "with probability one"); "p." denotes convergence "in probability"; "q.m." denotes convergence "in quadratic mean."

[4] See HALTON **(17)**, **(21)**, **(22)**, **(24)**, **(26)**, and **(29)**.

[5] These K_w, also, are then referred to as *secondary estimators* for θ.

[6] Here, $M = N_{N'}$, $\boldsymbol{M} = 2^{N_N}$, the power set of $N_{N'}$, and μ is defined by $\mu(\{t\}) = p(t)$.

[7] This is **very important**, but is usually omitted in discussions elsewhere.

and randomly sample index-values τ from N_N with probability $p(\tau)$, yielding a primary estimator of the form

$$g(\tau) = \left\{ \begin{array}{ccc} \dfrac{f(\tau)}{p(\tau)} & \text{if} & p(t)>0 \\ 0 & \text{if} & p(t)=0 \end{array} \right\}. \tag{A10}$$

By (A6)–(A10), $$E[g] = \sum_{t=1}^{N} g(t)p(t) = \sum_{t:f(t)\neq 0} f(t) = \theta, \tag{A11}$$

as required for (A2); so (A3)–(A5) follow. Note that the choice of the probability p, and, indeed, of any preliminary transformation of the function f that preserves the sum—more generally, the Lebesgue-Stieltjes integral—θ, has yet to be made.

Apart from the search for ever broader and subtler applications, Monte Carlo research has two main branches. The first is the development of *Monte Carlo algorithms* in general, and of *variance-reduction techniques* in particular, to yield estimators of ever-increasing efficiency and breadth of application; the second is the design and analysis of *random generators* to use in applying these techniques. The author has had extensive experience, with considerable success, in both of these main areas of research, over the last thirty-six years.

By (A4), the r.m.s. error of the secondary estimator G_w behaves like $w^{-1/2}$, as $w \to \infty$. While this rate of convergence is adequate, it is hardly satisfactory—to get one additional decimal place of accuracy in our estimate, we are compelled to sample a hundred times as many values of the primary estimator g! If we use this straightforward approach, it is therefore important—in order to maximize efficiency—to make the s.d., σ, of g as small as possible. The problem of **variance reduction** is a central one in the theory of the Monte Carlo method.[8] The author has contributed results on *correlated* and *importance sampling*,[9] including the problem of *negative*

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[8] See, e.g., BUSLENKO et al. **(1)** §II.2 [the techniques are given non-standard names, but most of them are mentioned], HALTON **(29)** §2.2, HAMMERSLEY and HANDSCOMB **(47)** §5.3–5.9 and 6.1–6.4, KALOS and WHITLOCK **(50)** §§4.1–4.5, KLEIJNEN **(51)** Chap. III, and SPANIER and GELBARD **(67)** Chap. 3.

[9] These two very widely used techniques depend on the use of an "easy function" $\varphi(t)$ to approximate the summand $f(t)$ in (A1): in *correlated sampling*, a difference estimator of the form $A + f(\tau) - \varphi(\tau)$ is used, usually with uniform sampling; in *importance sampling*, a probability $p(t)$ proportional to $\varphi(t)$ is adopted, thus yielding a quotient estimator of the form $B\, f(\tau)/\varphi(\tau)$. In both cases, the variance is diminished. See HALTON, **(23)** and **(25)**, and HALTON, MAYNARD, and RAGHEB **(32)**.

probabilities in importance sampling, and on *smoothing transformations*,[10] including general *antithetic variates* and *stratified sampling*.

In order to sample index-values τ randomly from $\mathbb{N}_N$ with probability $p(\tau)$, we must use some *physical device* (usually, but not always, a program installed in computer) called a **random generator,** which yields successive sample values of the r.v. τ. Almost always, what we are provided with is a **canonical random generator**, a specialized device or algorithm, which yields successive sample values ξ of independent random variables, *uniformly distributed in the interval*[11] [0,1). In practice, these random generators are *pseudo-random* and *quasi-random* generators, which are, in fact, deterministic in nature, unlike truly random generators (such as dice, roulette wheels, radioactive phenomena, and the like). From this, it can be demonstrated[12] that suitable independent samples of τ can be generated by taking τ such that[13]

$$\sum_{t=1}^{\tau-1} p(t) \le \xi < \sum_{t=1}^{\tau} p(t). \tag{A12}$$

In the case of "crude Monte Carlo," when τ is uniformly distributed in $\mathbb{N}_N$, we take $p(t) = 1/N$, and it is clear that, given a canonical random variable (c.r.v.) ξ, we may put[14]

$$\tau = \lfloor N\xi \rfloor + 1. \tag{A13}$$

The author has done some work on the generation of *arbitrarily distributed* random variables,[15] but has mainly concentrated on the generation of *canonical r.v.*, both *pseudo-random* [deterministic sequences exhibiting

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[10] Here, the summand $f(t)$ is suitably folded upon itself to reduce the variance. This work originates in the papers of HAMMERSLEY and MAULDON **(45)**, HAMMERSLEY and MORTON **(46)**, and is generalized and extended in HALTON and HANDSCOMB **(15)**, HANDSCOMB **(48)**, LAURENT **(53)**, and HALTON **(33)**. Other kinds of smoothing transformations are discussed by FROLOV and CHENTSOV **(14)**, and by HALTON and ZEIDMAN, **(28)** and **(30)**.

[11] This is the set of real x such that $0 \le x < 1$. In practice, it is restricted, in a computer, to the set of binary fractions of the form $p \times 2^{-q}$, where p and q are integers, with $q > 0$ and $0 \le p \le 2^q - 1$.

[12] See LÉVY **(55)** and HALTON **(40)**.

[13] The probability that ξ lies in the interval (A12) is just the difference of the extreme values in the inequality—namely, $p(\tau)$—as required.

[14] $\lfloor x \rfloor$ will denote the *floor function* of x, i.e., the integer infimum of x—the greatest integer not greater than x—this is also sometimes called the *integer part* of x and is often denoted by $[x]$ or by $\lfloor x \rfloor$. Similarly, $\lceil x \rceil$ will denote the *roof* (or *ceiling*) *function* of x, i.e., the integer supremum of x—the least integer not smaller than x—this is also often denoted by $\lceil x \rceil$.

[15] See HALTON, **(18)**, **(29)**, **(36)**, and **(41)**.

many of the statistical properties of truly random sequences], in parallel and tree-structured series,[16] and *quasi-random* [deterministic sequences having near-optimal uniformity properties].[17]

B. LINEAR SYSTEMS

A very prominent problem in numerical computation is that of solving *linear systems of equations*, of the general form

$$\boldsymbol{A}\boldsymbol{X} = \boldsymbol{B}; \tag{B1}$$

where the $(m \times m)$ matrix $\boldsymbol{A}$ and the $(m \times n)$ matrix $\boldsymbol{B}$ are known, while the $(m \times n)$ matrix $\boldsymbol{X}$ is the unknown quantity to be determined. We limit our consideration to situations in which the columns of $\boldsymbol{A}$ are linearly independent and a solution of (B1) exists for *all* choices of the matrix $\boldsymbol{B}$. It is then well-known that the solution is *unique*.

There are many classical numerical methods for solving an $(m \times m \times n)$ system (B1) of linear algebraic equations.[18] The *direct methods*, such as the *Gaussian* and *Gauss-Jordan* elimination, and *LU* and *Cholesky decomposition* techniques, take time

$$\mathbb{T}_{\text{DIRECT}}(m, n) = O(m^3) + O(m^2 n); \tag{B2}$$

while the *iterative methods*, such as the *Jacobi*, *Gauss-Seidel*, and various *relaxation* techniques, take time

$$\mathbb{T}_{\text{ITER}}(m, n, s) = O(m^2 n s), \tag{B3}$$

if there are s iterations. Even if s and n are relatively small (say, e.g., $n = 1$, with $s = 300$, or even $s = 5$), this becomes too laborious if m is large (say, e.g., $m = 1{,}000{,}000$, or even $m = 20{,}000$).

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16 This work—see HALTON, **(34)**, **(35)**, **(37)**, and **(38)**—is an extension to more complicated structures, of the pioneering pseudo-random sequence work of LEHMER **(54)**, FRANKLIN **(13)**, COVEYOU **(4)**, ROTENBERG **(64)**, and, later, of AHRENS, DIETER, MARSAGLIA, and many others. Prior to **(34)**, the new concept of random trees has only been investigated empirically, to a slight extent. Further theoretical research on this is both badly needed and ripe for development. One promising area in which research should certainly be done is that of the development and analysis of corresponding *quasi-random trees.*

17 See FAURE **(11)**, HALTON, **(16)**, **(20)**, and **(31)**, HALTON and SMITH **(19)**, HALTON and ZAREMBA **(27)**, NIEDERREITER, **(59)–(61)**, PEART **(63)**.

18 See any standard text on linear numerical analysis, e.g., DAHLQUIST and BJÖRCK **(8)**, ISAACSON and KELLER **(49)**, STEWART **(68)**, VARGA **(69)**, or WILKINSON **(75)**.

In addition, algebraic equations of the form (B1) often arise from *discretizations* of differential and/or integral equations, such as

$$\left\{\lambda(\xi,\eta)\ \frac{\partial^2}{\partial\xi^2}+\mu(\xi,\eta)\qquad \frac{\partial^2}{\partial\eta^2}\right\}X(\xi,\,\eta,\,\omega)\ =\ B(\xi,\,\eta,\,\omega) \tag{B4a}$$

or

$$\int_a^b A(\xi,\eta)X(\eta,\omega)\mathrm{d}\eta\ =\ B(\xi,\,\omega), \tag{B4b}$$

and the corresponding algebraic solutions ($\boldsymbol{X}$, i.e., X_{jk}) are, essentially, only useful as approximations to the continuous solutions—e.g., $X(\xi,\,\eta,\,\omega)$ or $X(\eta,\,\omega)$—of the original differential and/or integral equations. Thus, while a relatively coarse discretization of the continuous *solution* may be completely adequate, a similarly coarse discretization of the differential and/or integral *equations* may well lead to gross differences between the algebraic approximation and the continuous solution. However, a fine-grained discretization of the problem, requiring large values of m, usually becomes prohibitively laborious, and effectively entails the computation of the entire, fine-grained algebraic solution with m components, even when most of these components are of no appreciable interest.

We shall see that, by contrast, the *Monte Carlo* techniques presented here take time

$$\mathbb{T}_{\mathrm{MC}}(m,\,c,\,n,\,s,\,w)\ =\ O\Big((m+cn)sw\ \Big) \tag{B5}$$

(or less), if there are, on average, w samples, involving random walks of average length s, to determine the nc components in a subset of c rows of $\boldsymbol{X}$.[19] In comparison with iterative methods, we have w replacing mn; and cw replacing m^2. Thus, since $c < m$; so long as $w < m$, this is far more efficient than the classical methods. In addition, it will be seen that, unlike the traditional sampling methods, in which the expected errors are of order $w^{-1/2}$, requiring large numbers, w, of samples for acceptable accuracy; the **sequential methods**, which form the main thrust of this paper, converge much more rapidly, with errors of order κ^w, for some constant κ such that $|\kappa| < 1$.

To solve the $(m \times m \times n)$ system (B1) for $\boldsymbol{X}$, we select a non-singular $(m \times m)$ matrix $\boldsymbol{G}$ (so that the reciprocal matrix $\boldsymbol{G}^{-1}$ exists) and put

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[19] Since the n columns of $\boldsymbol{B}$ and of $\boldsymbol{X}$ are entirely unrelated, there is no point in mentioning any columns whose components are not needed for the solution.

$$\boldsymbol{L} = \boldsymbol{GB} \quad \text{and} \quad \boldsymbol{H} = \mathbf{I} - \boldsymbol{GA}, \tag{B6}$$

where $\mathbf{I}$ is the $(m \times m)$ unit matrix. This yields

$$\boldsymbol{X} = \boldsymbol{L} + \boldsymbol{HX}. \tag{B7}$$

Now $\boldsymbol{X}$ is a solution of (B1) if and only if it is a solution of (B7). Furthermore,

$$\boldsymbol{X} = \sum_{r=0}^{\infty} \boldsymbol{H}^r \boldsymbol{L} = \boldsymbol{L} + \boldsymbol{HL} + \boldsymbol{H}^2\boldsymbol{L} + \ldots + \boldsymbol{H}^r\boldsymbol{L} + \ldots, \tag{B8}$$

whenever the Neumann series (B8) converges. This is the case if the spectral radius $\rho(\boldsymbol{H})$[20] of the matrix $\boldsymbol{H}$satisfies

$$\rho(\boldsymbol{H}) < 1. \tag{B9}$$

The theory of *iterative processes* for solving equations of the form (B1) now tells us that, if $\rho(\boldsymbol{H}) < 1$, the sequence of matrices $\boldsymbol{X}_0, \boldsymbol{X}_1, \boldsymbol{X}_2, \ldots$, satisfying

$$\boldsymbol{X}_{s+1} = \boldsymbol{L} + \boldsymbol{HX}_s, \tag{B10}$$

converges to the solution matrix $\boldsymbol{X}$.

Furthermore, if $\boldsymbol{Y}$ is an *estimate* of $\boldsymbol{X}$, and

$$\boldsymbol{X} = \boldsymbol{Y} + \boldsymbol{Z}, \tag{B11}$$

then

$$\boldsymbol{Z} = \boldsymbol{D} + \boldsymbol{HZ}, \tag{B12}$$

where

$$\boldsymbol{D} = \boldsymbol{L} + \boldsymbol{HY} - \boldsymbol{Y}. \tag{B13}$$

Comparison of the equations (B7) and (B12) shows that $\boldsymbol{Z}$ satisfies the same form of equation as $\boldsymbol{X}$ does, with the same factor-matrix $\boldsymbol{H}$, but with $\boldsymbol{L}$ replaced by the *error*, $\boldsymbol{D}$, made when (B7) is applied to $\boldsymbol{Y}$.

It should also be noted that, in many cases, what is required is not the complete solution $\boldsymbol{X}$, but a (possibly vector) **functional** of the form

$$U(\phi, \omega) = \int_a^b \mathrm{d}\xi \int_a^b \mathrm{d}\eta \; F(\phi, \xi, \eta)\, X(\xi, \eta, \omega) \tag{B14a}$$

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[20] $\rho(\boldsymbol{H}) = \max\{|\lambda| : (\exists \boldsymbol{v} \neq \mathbf{0})\ \boldsymbol{Hv} = \lambda \boldsymbol{v}\}$ is the maximum absolute value of the eigenvalues of $\boldsymbol{H}$. For any vector $\boldsymbol{x}$, if $\rho(\boldsymbol{H}) < 1$, then $\boldsymbol{H}^r\boldsymbol{x} \to \mathbf{0}$ as $s \to \infty$.

or
$$U(\phi, \omega) = \int_a^b \mathrm{d}\eta \; F(\phi, \eta)\, X(\eta, \omega), \tag{B14b}$$

which reduces to the algebraic form

$$\boldsymbol{U} = \boldsymbol{FX}, \tag{B15}$$

with $\boldsymbol{F}$ a $(d \times m)$ matrix [often, $d = 1$]. This is tantamount to taking $c = d$ above. The case in which we require only *one* row, $\boldsymbol{X}_{j\bullet}$, of $\boldsymbol{X}$ corresponds to $d = 1$ and

$$(\boldsymbol{F})_{1h} = \delta_{jh} = \left\{ \begin{matrix} 1 \text{if} h = j \\ 0 \text{if} h \neq j \end{matrix} \right\}. \tag{B16}$$

Now, by (B8),

$$\boldsymbol{U} = \boldsymbol{FX} = \sum_{r=0}^{\infty} \boldsymbol{FH}^r\boldsymbol{L} = \boldsymbol{FL} + \boldsymbol{FHL} + \boldsymbol{FH}^2\boldsymbol{L} + \ldots + \boldsymbol{FH}^r\boldsymbol{L} + \ldots . \tag{B17}$$

The simplicity of the form (B17) and its close similarity to (B8) allows us to omit explicit mention of the functional forms in much of what follows.

C. MONTE CARLO FOR LINEAR SYSTEMS

An area of intense, long-standing activity by Monte Carlo researchers and practitioners has been the application of statistical sampling methods for solving linear systems of equations.

If we expand (B8) for a specific component, we see that

$$X_{ik} = \sum_{r=0}^{\infty} \sum_{j_1=1}^{m} \sum_{j_2=1}^{m} \cdots \sum_{j_{r-1}=1}^{m} \sum_{j_r=1}^{m} H_{ij_1} H_{j_1 j_2} \ldots H_{j_{r-1} j_r} L_{j_r k}, \tag{C1}$$

so that the result is an infinite sum of finite sums. If we apply the ideas of §A to these sums, we can develop a variety of Monte Carlo estimators for the X_{ik}, and this has been widely exploited for many years.[21]

[21] See CARTER and CASHWELL **(2)**, COURANT, FRIEDRICHS and LEWY **(3)**, CURTISS, **(5)** and **(6)**, CUTKOSKY **(7)**, EDMUNDSON **(9)**, FORSYTHE and LEIBLER **(12)**, HALTON, **(22)**, **(29)**, **(39)**, **(42)**, and **(43)**, MULLER, **(57)** and **(58)**, PAGE **(62)**, SPANIER and GELBARD **(67)**, and WASOW, **(71)–(74)**.

In particular, we shall note what are called **direct**, and **adjoint**, **homogeneous random walk estimators** using the **augmented index set**.

First, define a **stochastic** $(m \times m)$ **matrix** $\boldsymbol{P}$, such that

$$(\forall j, j') \quad P_{jj'} \geq 0, \quad \text{and,} \quad \text{if} \quad H_{jj'} \neq 0, \quad \text{then} \quad P_{jj'} > 0, \tag{C2}$$

and

$$(\forall j) \quad \sum_{j'=1}^{m} P_{jj'} = 1, \tag{C3}$$

and a stochastic m-vector $\boldsymbol{R}$, such that

$$(\forall j') \quad R_{j'} \geq 0, \quad \text{and,} \quad \text{if} \quad (\exists i) \quad H_{ij'} \neq 0, \quad \text{then} \quad R_{j'} > 0, \tag{C4}$$

and

$$\sum_{j'=1}^{m} R_{j'} = 1. \tag{C5}$$

We can now define a **Markov process**, or **random walk**,

$$\Gamma = [\gamma_1, \gamma_2, \gamma_3, \ldots, \gamma_r, \ldots], \tag{C6}$$

in which, first, $\gamma_1 \in \mathbb{N}_m$ is sampled with probability R_{γ_1}, and then, for $r = 1, 2, \ldots$, when $\gamma_1, \gamma_2, \ldots, \gamma_r$ have already been sampled, $\gamma_{r+1} \in \mathbb{N}_m$ is sampled with probability $P_{\gamma_r \gamma_{r+1}}$. This process yields an index-sequence $[\gamma_1, \gamma_2, \gamma_3, \ldots, \gamma_r]$ with probability

$$\mathit{Prob}\,[\gamma_1, \gamma_2, \gamma_3, \ldots, \gamma_r] = R_{\gamma_1} P_{\gamma_1 \gamma_2} P_{\gamma_2 \gamma_3} \ldots P_{\gamma_{r-1} \gamma_r}; \tag{C7}$$

and hence, in the spirit of (A10), we can, for $r = 0, 1, 2, \ldots$, generate a **direct** unbiased primary estimator of the r-term of the infinite series in (C1), of the form[22]

$$g^{\mathrm{DIR}}_{rik}(\Gamma) = \frac{H_{i\gamma_1} H_{\gamma_1 \gamma_2} H_{\gamma_2 \gamma_3} \ldots H_{\gamma_{r-1} \gamma_r} L_{\gamma_r k}}{R_{\gamma_1} P_{\gamma_1 \gamma_2} P_{\gamma_2 \gamma_3} \ldots P_{\gamma_{r-1} \gamma_r}}. \tag{C8}$$

If we replace (C2) and (C4) by

$$(\forall j, j') \quad P_{jj'} \geq 0, \quad \text{and,} \quad \text{if} \quad H_{j'j} \neq 0, \quad \text{then} \quad P_{jj'} > 0, \tag{C9}$$

and

$$(\forall j') \quad R_{j'} \geq 0, \quad \text{and,} \quad \text{if} \quad (\exists k) \quad L_{j'k} \neq 0, \quad \text{then} \quad R_{j'} > 0, \tag{C10}$$

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[22] Of course, $g^{\mathrm{DIR}}_{rik}(\Gamma) = g^{\mathrm{ADJ}}_{rik}(\Gamma) = L_{ik}$, which is a constant.

we effectively run the random walk "in reverse" and obtain the corresponding **adjoint** estimator

$$g_{rik}^{\mathrm{ADJ}}(\Gamma) = \frac{H_{i\gamma_r} H_{\gamma_r\gamma_{r-1}} H_{\gamma_{r-1}\gamma_{r-2}} \ldots H_{\gamma_2\gamma_1} L_{\gamma_1 k}}{R_{\gamma_1} P_{\gamma_1\gamma_2} P_{\gamma_2\gamma_3} \ldots P_{\gamma_{r\ -1}\gamma_r}}. \tag{C11}$$

In the case of *functionals*,[23] we take an initial extra step; the random walk becomes

$$\Gamma = [\gamma_0, \gamma_1, \gamma_2, \ldots, \gamma_r, \ldots], \tag{C12}$$

in which, first, $\gamma_0 \in \mathbb{N}_m$ is sampled with probability R_{γ_0}, and then, when $\gamma_0, \gamma_1, \gamma_2, \ldots, \gamma_r$ have already been sampled, $\gamma_{r+1} \in \mathbb{N}_m$ is sampled with probability $P_{\gamma_r\gamma_{r+1}}$, as before. This process yields an index-sequence $[\gamma_0, \gamma_1, \gamma_2, \ldots, \gamma_r]$ with probability

$$\mathit{Prob}\,[\gamma_0, \gamma_1, \gamma_2, \ldots, \gamma_r] = R_{\gamma_0} P_{\gamma_0\gamma_1} P_{\gamma_1\gamma_2} \ldots P_{\gamma_{r-1}\gamma_r}; \tag{C13}$$

and we can generate both *direct* and *adjoint* estimators, of the form

$$g_{rhk}^{\mathrm{DIR-F}}(\Gamma) = \frac{F_{h\gamma_0} H_{\gamma_0\gamma_1} H_{\gamma_1\gamma_2} \ldots H_{\gamma_{r\ -1}\gamma_r} L_{\gamma_r k}}{R_{\gamma_0} P_{\gamma_0\gamma_1} P_{\gamma_1\gamma_2} \ldots P_{\gamma_{r\ -1}\gamma_r}} \tag{C14}$$

and

$$g_{rhk}^{\mathrm{ADJ-F}}(\Gamma) = \frac{F_{h\gamma_r} H_{\gamma_r\gamma_{r-1}} H_{\gamma_{r-1}\gamma_{r-2}} \ldots H_{\gamma_1\gamma_0} L_{\gamma_0 k}}{R_{\gamma_0} P_{\gamma_0\gamma_1} P_{\gamma_1\gamma_2} \ldots P_{\gamma_{r\ -1}\gamma_r}}. \tag{C15}$$

In theory, we can now estimate X_{ik} or U_{hk} by the infinite sum of such estimators.[24] In practice, what has usually been done, to make the methods workable in finite time, has been to *truncate* the series, such as (C1)—and the underlying series (B8)—at a point where the residual sum can be predicted to be negligible. However, it is possible to proceed otherwise, in an easier and more elegant manner.

First, we note that the index set $\mathbb{N}_m = \{1, 2, \ldots, m\}$ of the summations in (C1) can be *augmented* to size

$$m^{\mathrm{j}} = m + 1, \tag{C16}$$

by adding an index 0, yielding

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[23] See (B14)–(B15).

[24] The appropriate rigorous limit theorems have been derived by the proposer; see HALTON, **(17)**, **(26)**, **(39)**, **(42)**, and **(43)**.

$$N^{\mathrm{j}}_{m} = \{0, 1, 2, \ldots, m\}, \tag{C17}$$

and we adopt the convention that, in any *"augmented matrix"*—marked by the superscript $^{\mathrm{j}}$—*any element with the index* 0 *is made to vanish;* i.e., if $1 \le i \le m$ and $1 \le j \le m$, and if $\boldsymbol{M}$ denotes any $(m \times m)$ matrix, such as $\boldsymbol{H}$, $\boldsymbol{A}$, or $\boldsymbol{G}$, then

$$(\boldsymbol{M}^{\mathrm{j}})_{ij} = M_{ij}, \quad (\boldsymbol{M}^{\mathrm{j}})_{i0} = (\boldsymbol{M}^{\mathrm{j}})_{0j} = (\boldsymbol{M}^{\mathrm{j}})_{00} = 0; \tag{C18}$$

while if $1 \le k \le n$, and if $\boldsymbol{N}$ denotes any $(m \times n)$ matrix, such as $\boldsymbol{B}$, $\boldsymbol{X}$, $\boldsymbol{L}$, $\boldsymbol{X}_s$, $\boldsymbol{E}_s$, $\boldsymbol{Y}$, $\boldsymbol{Z}$, or $\boldsymbol{D}$, then[25]

$$(\boldsymbol{N}^{\mathrm{j}})_{jk} = N_{jk}, \quad (\boldsymbol{N}^{\mathrm{j}})_{0k} = 0. \tag{C19}$$

It is then readily apparent that the augmented matrices satisfy relations identical in form to (B1), (B6)–(B13), (B15), and (B17), when every matrix symbol is decorated with the superscript $^{\mathrm{j}}$. We may define a stochastic $(m^{\mathrm{j}} \times m^{\mathrm{j}})$ matrix $\boldsymbol{P}^{<}$ and a stochastic m^{j}-vector $\boldsymbol{R}^{<}$, satisfying conditions analogous to (C2)–(C5),[26] and generate random walks Γ^{j} of the form (C6), but on the augmented index-set N^{j}_{m}, and estimators analogous to (C8), (C11), (C14), or (C15). We now observe that, if[27]

$$\gamma_1 = \gamma_2 = \gamma_3 = \ldots = \gamma_{s-1} > 0, \quad \gamma_s = 0, \tag{C20}$$

in the sampled random walk Γ^{j}, then (C18) ensures that a vanishing factor will occur in the numerator of every estimator (C8), (C11), (C14), or (C15), with $r \ge s$. This ensures that all terms with $r \ge s$. in the infinite-series estimators for all the X_{ik} will vanish; so that the series effectively **terminate** after s terms, making them *computable without truncation*.

We shall henceforth assume that the index set has been augmented in this manner, and **omit the superscripts** $^{\mathrm{j}}$ and $^{<}$, for simplicity, wherever they occur.

The concept of *automatic stopping*, by way of an **augmented index set** $N^{\mathrm{j}}_{m} = \{0, 1, 2, \ldots, m\}$, as outlined in (C16)–(C20), has not been found

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25 For *functionals*, we correspondingly put $(\boldsymbol{F}^{\mathrm{j}})_{hi} = F_{hi}$, $(\boldsymbol{F}^{\mathrm{j}})_{h0} = 0$.

26 This is for the *direct* estimator; for the *adjoint* estimator, we take (C3), (C9), (C5), and (C10). Note that, here, **we do *not* require the conditions (C14)–(C15)**.

27 For *functionals*, we begin with $\gamma_0 > 0$.

in the literature;[28] it is a simple, elegant, and effective technique, and should be utilized much more frequently, and further investigated. It has been found in practice that short random walks (i.e., large stopping probabilities ϖ) can give accurate estimates of series with slow convergence. The relation between the selection of ϖ and the choice of the stochastic matrices $\boldsymbol{R}$ and $\boldsymbol{P}$ in general [see (C2)–(C5)] is unclear; it, too, merits further investigation.

We note that *all* the methods used hitherto to solve linear systems (B1) or (B7), however ingeniously devised, reduce to variations on the above theme, and finally lead to timings of the form (B5);[29] while the r.m.s. errors are firmly pegged at a rate of the form $A w^{-1/2}$, as $w \to \infty$, where w is the number of random walks. This is painfully slow. As with other problems of variance reduction, there is a limited degree of improvement that can be obtained by subtlety of sampling, and the "easy functions" used[30] are constructed in ways based more on hunches and experience than on rigorous analysis.

D. SEQUENTIAL MONTE CARLO FOR LINEAR SYSTEMS

The simple observation, that information obtained during statistical sampling can be used to improve the sampling scheme, is familiar to statisticians in the theory of estimation.[31] The idea of applying this concept in a limited way to the Monte Carlo computation of simple integrals was originally proposed by Marshall;[32] though he did not carry it very far, limiting himself to a single sequential improvement of an importance-sampling scheme. The concept was greatly expanded and analyzed mathematically by the author.[33] His methods were devised

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28 This concept is quite different from the *absorption* probability occurring in particle-transport computations, because the random walk occurring in the Monte Carlo treatment need not have any direct relation to the history of any physical or semi-physical particle.

29 The second term in (B5), $O(cnsw)$, is due to the computation of the needed estimators (C8) or (C11). The first term, $O(msw)$, is due to the determination of sw random indices; the method assumed is the successive computation of the partial sums of probabilities in (A12). The *precomputation* of *all* these sums takes time $O(m^2)$, which is prohibitively laborious, for large m. If only q of the probabilities in any row of $\boldsymbol{P}$ are non-zero, the first term of (B5) becomes $O(qsw)$. If one can, instead, use a simple *formula*, as in the case of *uniform sampling* [see (A13)], then this contributes a time only $O(sw)$, for a total time $O(cnsw)$, but this is not always possible.

30 See Footnote[9].

31 See WALD and WOLFOWITZ **(70)**, and WOLFOWITZ, **(76)** and **(77)**.

32 See MARSHALL **(56)**.

33 See HALTON, **(17)**, **(21)**, **(22)**, **(24)**, **(26)**, **(29)**, **(39)**, and **(42)**–**(44)**.

for solving systems of linear equations like (B1) or (B7). The "First Sequential Method" used ideas analogous to *(unbiased) importance sampling*; the "Second Sequential Method" used ideas analogous to *biased importance sampling* (a new concept); and the "Third Sequential Method" used ideas analogous to *correlated sampling*. We shall limit ourselves here to considering a generalization and modification of what the author termed the Third Sequential Method; the convergence bounds obtained by him for this (and for his First and Second Sequential Methods), as well as a limited amount of computational experience, indicate that this Third Method is the fastest-converging and most easily applied of the three.

The method is based on the results (B11)–(B13). It is iterative in nature and proceeds in *sequential stages*, denoted by the superscript $^{(\nu)}$, taking $\nu = 0, 1, 2, \ldots$. Initially, for simplicity, we can take

$$\boldsymbol{\Upsilon}^{(0)} = \mathbf{O}. \tag{D1}$$

Thereafter, we put $$\boldsymbol{X} = \boldsymbol{\Upsilon}^{(\nu)} + \boldsymbol{Z}^{(\nu)}. \tag{D2}$$

and $$\boldsymbol{D}^{(\nu)} = \boldsymbol{D}^{(\nu)}\big(\boldsymbol{\Upsilon}^{(\nu)}\big) = \boldsymbol{L} + \boldsymbol{H}\boldsymbol{\Upsilon}^{(\nu)} - \boldsymbol{\Upsilon}^{(\nu)} = \boldsymbol{Z}^{(\nu)} - \boldsymbol{H}\boldsymbol{Z}^{(\nu)}. \tag{D3}$$

Note that, initially, $$\boldsymbol{D}^{(0)} = \boldsymbol{L}. \tag{D4}$$

Now, we use the Monte Carlo technique described in §C to obtain a *random walk* $\Gamma^{(\nu)}$ on the augmented index set $\mathbb{N}^{\mathrm{j}}_m = \{0, 1, 2, \ldots, m\}$, and hence *unbiased augmented homogeneous estimators* [see (C8), (C11), (C14), and (C15)][34]

$$g^{\mathrm{DIR},(\nu)}_{i\,k}(\Gamma^{(\nu)}) = \sum_{r=0}^{\infty} \frac{H_{i\gamma_1} H_{\gamma_1\gamma_2} H_{\gamma_2\gamma_3} \ldots H_{\gamma_r\ \ -1\gamma_r} D^{(\nu)}_{\gamma_r k}}{R_{\gamma_1} P_{\gamma_1\gamma_2} P_{\gamma_2\gamma_3} \ldots P_{\gamma_r\ \ -1\gamma_r}} \tag{D5}$$

or $$g^{\mathrm{ADJ},(\nu)}_{i\,k}(\Gamma^{(\nu)}) = \sum_{r=0}^{\infty} \frac{H_{i\gamma_r} H_{\gamma_r\gamma_r\ -1} H_{\gamma_{r-1}\gamma_{r-2}} \ldots H_{\gamma_2\gamma_1} D^{(\nu)}{}_{\gamma_1 k}}{R_{\gamma_1} P_{\gamma_1\gamma_2} P_{\gamma_2\gamma_3} \ldots P_{\gamma_r\ \ -1\gamma_r}} \tag{D6}$$

for the *corrections* $Z^{(\nu)}_{i\,k}$ to our approximations $\Upsilon^{(\nu)}_{i\,k}$. By taking, at stage ν, w_ν independent random walks $\Gamma^{(\nu)}_u$ $(u = 1, 2, \ldots, w_\nu)$, we can generate unbiased secondary estimators, respectively

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[34] Estimators entirely analogous to these can also be constructed, by way of (C14) and (C15), for functionals.

$$\boldsymbol{G}_{w_\nu}^{\mathrm{DIR},(\nu)} = \frac{1}{w_\nu} \sum_{u=1}^{w_\nu} \boldsymbol{g}^{\mathrm{DIR},(\nu)}(\Gamma_u^{(\nu)}) \tag{D7}$$

or
$$\boldsymbol{G}_{w_\nu}^{\mathrm{ADJ},(\nu)} = \frac{1}{w_\nu} \sum_{u=1}^{w_\nu} \boldsymbol{g}^{\mathrm{ADJ},(\nu)}(\Gamma_u^{(\nu)}), \tag{D8}$$

and take $\boldsymbol{\Upsilon}^{(\nu+1)} = \boldsymbol{\Upsilon}^{(\nu)} + \boldsymbol{G}_{w_\nu}^{(\nu)}$, whence $\boldsymbol{\Upsilon}^{(\nu)} = \sum_{\mu=0}^{\nu-1} \boldsymbol{G}_{w_\mu}^{(\mu)}$. (D9)

with the appropriate superscript $^{\mathrm{DIR}}$ or $^{\mathrm{ADJ}}$. Clearly, for each matrix component,

$$Var\,[\,\Upsilon_{ik}^{(\nu+1)} \,|\, \boldsymbol{\Upsilon}^{(\nu)}\,] = Var\,[\,G_{w_\nu ik}^{(\nu)} \,|\, \boldsymbol{\Upsilon}^{(\nu)}\,] = \frac{Var[g_{ik}^{(\nu)} \,|\, \boldsymbol{\Upsilon}^{(\nu)}]}{w_\nu}. \tag{D10}$$

E. THE ESTIMATION OF VARIANCE—DIRECT ESTIMATORS

We prove the following results in the context of *sequential Monte Carlo*; but all the results apply equally to *plain Monte Carlo*, by taking $\nu = 0$, when $\boldsymbol{D}^{(\nu)}$ reverts to $\boldsymbol{L}$. The results derived here apply to any single sequential stage.

Let us first consider the direct augmented homogeneous estimator,[35] which, for $r \geq 1$, takes the form

$$g_{rik}^{\mathrm{DIR},(\nu)}(\Gamma) = \frac{H_{i\gamma_1} H_{\gamma_1\gamma_2} H_{\gamma_2\gamma_3} \ldots H_{\gamma_r\ \ -1\gamma_r} D_{\gamma_r k}^{(\nu)}}{R_{\gamma_1} P_{\gamma_1\gamma_2} P_{\gamma_2\gamma_3} \ldots P_{\gamma_r\ \ -1\gamma_r}}. \tag{E1}$$

Write
$$G_0^{(\nu)}(\Gamma) = G_{0\gamma_1}^{(\nu)} = 0 \tag{E2}$$

and, for $r \geq 1$,
$$G_r^{(\nu)}(\Gamma) = G_{r\gamma_1}^{(\nu)} = \frac{H_{\gamma_1\gamma_2} H_{\gamma_2\gamma_3} \ldots H_{\gamma_r\ \ -1\gamma_r} D_{\gamma_r k}^{(\nu)}}{P_{\gamma_1\gamma_2} P_{\gamma_2\gamma_3} \ldots P_{\gamma_r\ \ -1\gamma_r}}; \tag{E3}$$

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[35] See (C8) and (D5). We shall return to the three other types of estimators—adjoint and functional and both—in §F.

so that, for all $r \ge 0$, $$g^{\mathrm{DIR},(v)}_{rik}(\Gamma) \;=\; \delta_{r0} D^{(v)}_{ik} + \frac{H_{i\gamma_1}}{R_{\gamma_1}} G^{(v)}_{r\gamma_1}. \tag{E4}$$

Given a random walk

$$\Gamma \;=\; \Gamma(\gamma_1) \;=\; [\gamma_1, \gamma_2, \gamma_3, \gamma_4, \dots] \tag{E5}$$

starting at index γ_1 and using the Markov probabilities $P_{jj'}$,[36] write

$$\Gamma^{*} \;=\; \Gamma^{*}(\gamma_2) \;=\; [\gamma_2, \gamma_3, \gamma_4, \dots] \tag{E6}$$

for the "continuation walk," starting at the second index, γ_2, of Γ. Then we have that

$$\Gamma(\gamma_1) \;=\; [\gamma_1, \Gamma^{*}(\gamma_2)], \tag{E7}$$

and we see that Γ^{*} is exactly the same *kind* of random walk as Γ, but starting at index γ_2 instead of index γ_1.[37]

Returning to (E3), we easily observe, for all $r \ge 2$, the *recurrence relation*

$$G^{(v)}_{r}(\Gamma(\gamma_1)) \;=\; \frac{H_{\gamma_1\gamma_2}}{P_{\gamma_1\gamma_2}} G^{(v)}_{r-1}(\Gamma^{*}(\gamma_2)), \tag{E8}$$

and, since the statistical properties of Γ and Γ^{*} are the same, we can safely abbreviate this to the form

$$G^{(v)}_{r\gamma_1} \;=\; \frac{H_{\gamma_1\gamma_2}}{P_{\gamma_1\gamma_2}} G^{(v)}_{(r-1)\gamma_2}\,. \tag{E9}$$

Now, let us define the series

$$M^{(v)}_{\gamma_1 k} \;=\; \sum_{r=1}^{\infty} G^{(v)}_{r\gamma_1}, \tag{E10}$$

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36 Note that, here, in the walk Γ, the starting index γ_1 is arbitrarily given; earlier, we took the first index itself to be random, with probability R_{γ_1}.

37 That is, both Γ and Γ^{*} are samples of random walks from the space of all Markov processes starting and moving in $\{1, 2, \dots, m\}$ and controlled by the stochastic matrix $\boldsymbol{P}$.

which clearly converges, since we assume that the estimator series (D5) converges in a stochastic sense[38]. Then, by (E9),

$$M^{(\nu)}_{\gamma_1 k} \;=\; D^{(\nu)}_{\gamma_1 k} + \frac{H_{\gamma_1\gamma_2}}{P_{\gamma_1\gamma_2}} \sum_{r=2}^{\infty} G^{(\nu)}_{(r-1)\gamma_2} \;=\; D^{(\nu)}_{\gamma_1 k} + \frac{H_{\gamma_1\gamma_2}}{P_{\gamma_1\gamma_2}} \sum_{r=1}^{\infty} G^{(\nu)}_{r\gamma_2}\,;$$

i.e.,
$$M^{(\nu)}_{\gamma_1 k} \;=\; D^{(\nu)}_{\gamma_1 k} + \frac{H_{\gamma_1\gamma_2}}{P_{\gamma_1\gamma_2}}\, M^{(\nu)}_{\gamma_2 k}\,. \tag{E11}$$

By (D5) and (E4), we correspondingly get that

$$g^{\mathrm{DIR},(\nu)}_{i\,k}(\Gamma) \;=\; D^{(\nu)}_{i\,k} + \frac{H_{i\gamma_1}}{R_{\gamma_1}}\, M^{(\nu)}_{\gamma_1 k}\,. \tag{E12}$$

We now adopt a usefully concise notation. For any square matrix $\boldsymbol{M}$, if $\mathbf{I} - \boldsymbol{M}$ is *invertible*[39], we can write

$$(\mathbf{I} - \boldsymbol{M})^{-1} \;=\; \boldsymbol{M}^{\mathbf{t}}, \tag{E13}$$

and if furthermore $\rho(\boldsymbol{M}) < 1$, then

$$\boldsymbol{M}^{\mathbf{t}} \;=\; \sum_{s=0}^{\infty} \boldsymbol{M}^s \tag{E14}$$

(see (B7)–(B9)). We observe that, since $(\mathbf{I} - \boldsymbol{M})(\mathbf{I} - \boldsymbol{M})^{-1} = \mathbf{I} = (\mathbf{I} - \boldsymbol{M})^{-1}(\mathbf{I} - \boldsymbol{M})$, it follows that

$$(\mathbf{I} - \boldsymbol{M})\boldsymbol{M}^{\mathbf{t}} \;=\; \mathbf{I} \;=\; \boldsymbol{M}^{\mathbf{t}}(\mathbf{I} - \boldsymbol{M}), \tag{E15}$$

whence
$$\boldsymbol{M}\,\boldsymbol{M}^{\mathbf{t}} \;=\; \boldsymbol{M}^{\mathbf{t}} - \mathbf{I} \;=\; \boldsymbol{M}^{\mathbf{t}}\boldsymbol{M}\,. \tag{E16}$$

Also, by the usual rule about transposing products of matrices, namely,

$$(\boldsymbol{M}_1\boldsymbol{M}_2)^{\mathsf{T}} \;=\; \boldsymbol{M}_2{}^{\mathsf{T}}\boldsymbol{M}_1{}^{\mathsf{T}}; \tag{E17}$$

and with (E14) (applied both to $\boldsymbol{M}$ and to $\boldsymbol{M}^{\mathsf{T}}$), we get that

$$\begin{aligned}(\boldsymbol{M}^{\mathbf{t}})^{\mathsf{T}} \;&=\; (\boldsymbol{M}^{\mathbf{t}})^{\mathsf{T}}(\mathbf{I} - \boldsymbol{M}^{\mathsf{T}})(\boldsymbol{M}^{\mathsf{T}})^{\mathbf{t}} \;=\; (\boldsymbol{M}^{\mathbf{t}})^{\mathsf{T}}(\mathbf{I} - \boldsymbol{M})^{\mathsf{T}}(\boldsymbol{M}^{\mathsf{T}})^{\mathbf{t}} \\ &=\; \big((\mathbf{I} - \boldsymbol{M})\boldsymbol{M}^{\mathbf{t}}\big)^{\mathsf{T}}(\boldsymbol{M}^{\mathsf{T}})^{\mathbf{t}} \;=\; \mathbf{I}^{\mathsf{T}}(\boldsymbol{M}^{\mathsf{T}})^{\mathbf{t}} \;=\; \mathbf{I}\,(\boldsymbol{M}^{\mathsf{T}})^{\mathbf{t}} \;=\; (\boldsymbol{M}^{\mathsf{T}})^{\mathbf{t}};\end{aligned}$$

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[38] See HALTON, **(39)**, and **(42)**–**(44)**. In **(42)** §12, it is shown that the convergence is very strong (almost sure, in probability, in mean, and in distribution), provided only that $\rho(\boldsymbol{H}^{+}) < 1$, where $\boldsymbol{H}^{+}$ is the matrix of absolute values of the corresponding components of $\boldsymbol{H}$.

[39] This holds, for instance, if $\rho(\boldsymbol{M}) < 1$.

i.e., $$(\boldsymbol{M}^{\mathbf{t}})^{\mathsf{T}} \;=\; (\boldsymbol{M}^{\mathsf{T}})^{\mathbf{t}}. \tag{E18}$$

Now, by (E3), (E10), and (E14),

$$E\,[\,M^{(\nu)}_{\gamma_1 k}\,|\,\boldsymbol{\Upsilon}^{(\nu)}\,]\;=\;(\boldsymbol{H}^{\mathbf{t}}\boldsymbol{D}^{(\nu)})_{\gamma_1 k}. \tag{E19}$$

From (E12), we now deduce that

$$E\,[\,\mathcal{g}^{\mathrm{DIR},(\nu)}_{i\,k}\,|\,\boldsymbol{\Upsilon}^{(\nu)}\,]\;=\;D^{(\nu)}_{i\,k}+(\boldsymbol{H}\boldsymbol{H}^{\mathbf{t}}\boldsymbol{D}^{(\nu)})_{ik}\,;$$

i.e., by (E16), $$E\,[\,\mathcal{g}^{\mathrm{DIR},(\nu)}_{i\,k}\,|\,\boldsymbol{\Upsilon}^{(\nu)}\,]\;=\;(\boldsymbol{H}^{\mathbf{t}}\boldsymbol{D}^{(\nu)})_{ik}\,. \tag{E20}$$

and this leads, by the analog of (B8) applied to (B11)–(B13) with (E14), to the well-known fact that

$$E\,[\,\mathcal{g}^{\mathrm{DIR},(\nu)}_{i\,k}\,|\,\boldsymbol{\Upsilon}^{(\nu)}\,]\;=\;(\boldsymbol{H}^{\mathbf{t}}\boldsymbol{D}^{(\nu)})_{ik}\;=\;Z^{(\nu)}_{i\,k}. \tag{E21}$$

When we take the mathematical expectation of the *squares* of the two sides of (E11), and apply (E16) and (E21), we obtain something much less well-known:

$$E\,[\,(M^{(\nu)}_{\gamma_1 k})^2\,|\,\boldsymbol{\Upsilon}^{(\nu)}\,]\;=\;E\left[\;\left(D^{(\nu)}_{\gamma_1 k}+\frac{H_{\gamma_1\gamma_2}}{P_{\gamma_1\gamma_2}}M^{(\nu)}_{\gamma_2 k}\right)^2\,\middle|\,\boldsymbol{\Upsilon}^{(\nu)}\;\right]$$

$$=\;E\left[\;(D^{(\nu)}_{\gamma_1 k})^2+2D^{(\nu)}_{\gamma_1 k}\frac{H_{\gamma_1\gamma_2}}{P_{\gamma_1\gamma_2}}M^{(\nu)}_{\gamma_2 k}+\frac{H^{\,2}_{\gamma_1\gamma_2}}{P^{\,2}_{\gamma_1\gamma_2}}(M^{(\nu)}_{\gamma_2 k})^2\,\middle|\,\boldsymbol{\Upsilon}^{(\nu)}\;\right]$$

$$=\;(D^{(\nu)}_{\gamma_1 k})^2+2D^{(\nu)}_{\gamma_1 k}\sum_{\beta=1}^{m}H_{\gamma_1\beta}\,E\,[\,M^{(\nu)}_{\beta k}\,|\,\boldsymbol{\Upsilon}^{(\nu)}\,]+\sum_{\beta=1}^{m}\frac{H^{\,2}_{\gamma_1\beta}}{P_{\gamma_1\beta}}E[(M^{(\nu)}_{\beta k})^2\,|\,\boldsymbol{\Upsilon}^{(\nu)}$$

]

$$=\;(D^{(\nu)}_{\gamma_1 k})^2+2D^{(\nu)}_{\gamma_1 k}\,(\boldsymbol{H}\boldsymbol{H}^{\mathbf{t}}\boldsymbol{D}^{(\nu)})_{\gamma_1 k}+\sum_{\beta=1}^{m}K_{\gamma_1\beta}\,E\,[\,(M^{(\nu)}_{\beta k})^2\,|\,\boldsymbol{\Upsilon}^{(\nu)}\,]$$

$$=\;2D^{(\nu)}_{\gamma_1 k}\,Z^{(\nu)}_{\gamma_1 k}\;-(D^{(\nu)}_{\gamma_1 k})^2+\;\sum_{\beta=1}^{m}K_{\gamma_1\beta}E[(M^{(\nu)}{}_{\beta k})^2\,|\,\boldsymbol{\Upsilon}^{(\nu)}]\,, \tag{E22}$$

where we define $$(\boldsymbol{K})_{\alpha\beta} \;=\; K_{\alpha\beta} \;=\; \frac{H_{\alpha\beta}^{\;2}}{P_{\alpha\beta}}. \tag{E23}$$

Hence, if we define new matrices $\boldsymbol{N}^{(\nu)}$ and $\boldsymbol{J}^{(\nu)}$ by

$$(\boldsymbol{N}^{(\nu)})_{\alpha k} \;=\; N_{\alpha k}^{(\nu)} \;=\; E\,[\,(M_{\alpha k}^{(\nu)})^2\,] \tag{E24}$$

and $$(\boldsymbol{J}^{(\nu)})_{\alpha k} \;=\; J_{\alpha k}^{(\nu)} \;=\; 2D_{\alpha k}^{(\nu)}\,Z_{\alpha k}^{(\nu)} \;-\; (D_{\alpha k}^{(\nu)})^2, \tag{E25}$$

then (E22) gives the matrix equation [compare (B7) and (B12)]

$$\boldsymbol{N}^{(\nu)} \;=\; \boldsymbol{J}^{(\nu)} + \boldsymbol{K}\boldsymbol{N}^{(\nu)}, \tag{E26}$$

whence, if $$\rho(\boldsymbol{K}) < 1, \tag{E27}$$

we can put $$\boldsymbol{N}^{(\nu)} \;=\; \boldsymbol{K}^{\mathrm{t}}\boldsymbol{J}^{(\nu)}. \tag{E28}$$

Now, take the expectation of the squares of both sides of (E12); then, by very similar manipulations, with (E19), (E21), and (E24), we get that

$$E\,[\,(\mathcal{E}_{i\,k}^{\mathrm{DIR},(\nu)})^2 \,|\, \boldsymbol{\Upsilon}^{(\nu)}\,] \;=\; E\left[\;\left(D_{i\,k}^{(\nu)} + \frac{H_{i\gamma_1}}{R_{\gamma_1}} M_{\gamma_1 k}^{(\nu)}\right)^2 \,\middle|\, \boldsymbol{\Upsilon}^{(\nu)}\;\right]$$

$$= E\left[\;(D_{i\,k}^{(\nu)})^2 + 2D_{i\,k}^{(\nu)}\,\frac{H_{i\gamma_1}}{R_{\gamma_1}} M_{\gamma_1 k}^{(\nu)} + \frac{H_{i\gamma_1}^{\;2}}{R_{\gamma_1}^{\;2}} (M_{\gamma_1 k}^{(\nu)})^2 \,\middle|\, \boldsymbol{\Upsilon}^{(\nu)}\;\right];$$

$$= (D_{i\,k}^{(\nu)})^2 + 2D_{i\,k}^{(\nu)} \sum_{\alpha=1}^{m} H_{i\alpha}\, E\,[\,M_{\alpha k}^{(\nu)} \,|\, \boldsymbol{\Upsilon}^{(\nu)}\,] + \sum_{\alpha=1}^{m} \frac{H_{i\alpha}^{\;2}}{R_\alpha}\, E\,[\,(M_{\alpha k}^{(\nu)})^2 \,|\, \boldsymbol{\Upsilon}^{(\nu)}$$

];

$$= (D_{i\,k}^{(\nu)})^2 + 2D_{i\,k}^{(\nu)} \sum_{\alpha=1}^{m} H_{i\alpha}\,(\boldsymbol{H}^{\mathrm{t}}\;\boldsymbol{D}^{(\nu)})_{\alpha k} + \sum_{\alpha=1}^{m} K^{\dagger}_{\;i\alpha}\, N_{\alpha k}^{(\nu)}$$

$$= 2D_{i\,k}^{(\nu)}\,Z_{i\,k}^{(\nu)} - (D_{i\,k}^{(\nu)})^2 + (\boldsymbol{K}^{\dagger}\boldsymbol{N}^{(\nu)})_{ik}, \tag{E29}$$

where we have defined [compare (E23)]

$$(\boldsymbol{K}^{\dagger})_{i\alpha} \;=\; K_{i\alpha}^{\dagger} \;=\; \frac{H_{i\alpha}^{\;2}}{R_\alpha}. \tag{E30}$$

Therefore, by (E29), with (E16) and (E20),

$$\begin{aligned} Var\,[\,g_{ik}^{\mathrm{DIR},(\nu)} \,|\, \Upsilon^{(\nu)}\,] &= E\,[\,(g_{ik}^{\mathrm{DIR},(\nu)})^2 \,|\, \Upsilon^{(\nu)}\,] - \left\{E[g_{ik}^{\mathrm{DIR},(\nu)} \;\; |\, \Upsilon^{(\nu)}]\right\}^2 \\ &= 2D_{ik}^{(\nu)}\, Z_{ik}^{(\nu)} - (D_{ik}^{(\nu)})^2 + (\boldsymbol{K}^{\dagger}\boldsymbol{N}^{(\nu)})_{ik} - (Z_{ik}^{(\nu)})^2 \\ &= (\boldsymbol{K}^{\dagger}\boldsymbol{N}^{(\nu)})_{ik} - \left(Z_{ik}^{(\nu)} - D_{ik}^{(\nu)}\right)^2, \end{aligned} \tag{E31}$$

or, in matrix form,
$$\boldsymbol{V}^{(\nu)} = \boldsymbol{K}^{\dagger}\boldsymbol{N}^{(\nu)} - \boldsymbol{W}^{(\nu)}, \tag{E32}$$

when we define
$$(\boldsymbol{V}^{(\nu)})_{ik} = V_{ik}^{(\nu)} = Var\,[\,g_{ik}^{\mathrm{DIR},(\nu)} \,|\, \Upsilon^{(\nu)}\,] \tag{E33}$$

and
$$(\boldsymbol{W}^{(\nu)})_{ik} = W_{ik}^{(\nu)} = \left(Z_{ik}^{(\nu)} - D_{ik}^{(\nu)}\right)^2. \tag{E34}$$

With the definitions given in (E1)–(E3), (E10), (E14), (E23)–(E25), (E30), (E33), and (E34); and the conditions (B9), (E27), and[40]

$$\rho(\boldsymbol{H}^{+}) < 1; \tag{E35}$$

it now follows from (E28) and (E32), that

$$\boldsymbol{V}^{(\nu)} = \boldsymbol{K}^{\dagger}\boldsymbol{K}^{\mathrm{t}}\boldsymbol{J}^{(\nu)} - \boldsymbol{W}^{(\nu)}. \tag{E36}$$

We have thus verified the following theorem.

THEOREM 1. *Given the "infinite-series" estimator* $g_{ik}^{\mathrm{DIR},(\nu)}(\boldsymbol{\Gamma})$ *of the "direct augmented homogeneous" type, as defined in (D5), satisfying the convergence conditions (B9), (E27), and (E35); the variances of these estimators are given by the formula (E36); or, in detail,*

$$\begin{aligned} Var\,[\,g_{ik}^{\mathrm{DIR},(\nu)} \,|\, \Upsilon^{(\nu)}\,] = \sum_{\alpha=1}^{m}\sum_{\beta=1}^{m} \frac{H_{i\alpha}^{\;2}}{R_{\alpha}} (\boldsymbol{K}^{\mathrm{t}})_{\alpha\beta} \left[2D_{\beta k}^{(\nu)}\, Z_{\beta k}^{(\nu)} - (D_{\beta k}^{(\nu)})^2\right] \\ - \left(Z_{ik}^{(\nu)} - D_{ik}^{(\nu)}\right)^2. \end{aligned} \tag{E37}$$

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[40] See Footnote[38]. Note that it can be proved [see **(42)** and **(43)**] that (E39) implies (B9).

Now, consider the following mathematical expectations, obtained from (B7), (D2), (D3), and (D9),

$$\left.\begin{aligned} &\boldsymbol{\Upsilon}^{(\nu)}=\boldsymbol{\Upsilon}^{(\nu-1)}+\boldsymbol{G}\,w_{\nu-1}^{(\nu-1)}, \\ &E[\boldsymbol{\Upsilon}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}]=\boldsymbol{\Upsilon}^{(\nu-1)}+\boldsymbol{Z}^{(\nu)}=\boldsymbol{X}, \end{aligned}\right\} \tag{E38}$$

$$\left.\begin{aligned} &\boldsymbol{Z}^{(\nu)}=\boldsymbol{X}-\boldsymbol{\Upsilon}^{(\nu)}, \\ &E[\boldsymbol{Z}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}]=\mathbf{O}, \end{aligned}\right\} \tag{E39}$$

$$\left.\begin{aligned} &\boldsymbol{D}^{(\nu)}=\boldsymbol{L}+\boldsymbol{H}\boldsymbol{\Upsilon}^{(\nu)}-\boldsymbol{\Upsilon}^{(\nu)}, \\ &E[\boldsymbol{D}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}]=\boldsymbol{L}+\boldsymbol{H}\boldsymbol{X}-\boldsymbol{X}=\mathbf{O}, \end{aligned}\right\} \tag{E40}$$

and
$$\boldsymbol{L}+\boldsymbol{H}\boldsymbol{X}-\boldsymbol{X}\;=\;\mathbf{O}; \tag{E41}$$

so
$$\begin{aligned} &E\left[\;2D_{\beta k}^{(\nu)}\,Z_{\beta k}^{(\nu)}-(D_{\beta k}^{(\nu)})^2\;\middle|\;\boldsymbol{\Upsilon}^{(\nu-1)}\;\right] \\ &\quad=E\left[2\left(L_{\beta k}+\sum_{\gamma=1}^{m}H_{\beta\gamma}\Upsilon_{\gamma k}^{(\nu)}-\Upsilon_{\beta k}^{(\nu)}\right)\left(X_{\beta k}-\Upsilon_{\beta k}^{(\nu)}\right)\right. \\ &\qquad\qquad\left.-\left(L_{\beta k}+\sum_{\gamma=1}^{m}H_{\beta\gamma}\Upsilon_{\gamma k}^{(\nu)}-\Upsilon_{\beta k}^{(\nu)}\right)^2\;\middle|\;\boldsymbol{\Upsilon}^{(\nu-1)}\right] \\ &\quad=E\left[\left(X_{\beta k}-\Upsilon_{\beta k}^{(\nu)}\right)^2\right. \\ &\qquad\left.-\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m}H_{\beta\gamma}H_{\beta\delta}\left(X_{\gamma k}-\Upsilon_{\gamma k}^{(\nu)}\right)\left(X_{\delta k}-\Upsilon_{\delta k}^{(\nu)}\right)\;\middle|\;\boldsymbol{\Upsilon}^{(\nu-1)}\right] \\ &\quad=Var\,[\,\Upsilon_{\beta k}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}\,] \\ &\qquad-\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m}H_{\beta\gamma}H_{\beta\delta}\,Cov\,[\,\Upsilon_{\gamma k}^{(\nu)},\,\Upsilon_{\delta k}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}\,]. \end{aligned} \tag{E42}$$

and, by (E38),

$$E\left[\left(Z_{i\,k}^{(\nu)} - D_{i\,k}^{(\nu)}\right)^2 \,\middle|\, \boldsymbol{\Upsilon}^{(\nu-1)} \right] = E\left[\left(\sum_{\gamma=1}^{m} H_{i\gamma} Z_{\gamma k}^{(\nu)} \right)^2 \,\middle|\, \boldsymbol{\Upsilon}^{(\nu-1)} \right]$$

$$= E\left[\left\{ \sum_{\gamma=1}^{m} H_{i\gamma} \left(X_{\gamma k} - \Upsilon_{\gamma k}^{(\nu)}\right) \right\}^2 \,\middle|\, \boldsymbol{\Upsilon}^{(\nu-1)} \right]$$

$$= E\left[\sum_{\gamma=1}^{m} H_{i\gamma} \left(X_{\gamma k} - \Upsilon_{\gamma k}^{(\nu)}\right) \sum_{\delta=1}^{m} H_{i\delta} \left(X_{\delta k} - \Upsilon_{\delta k}^{(\nu)}\right) \,\middle|\, \boldsymbol{\Upsilon}^{(\nu-1)} \right]$$

$$= \sum_{\gamma=1}^{m} \sum_{\delta=1}^{m} H_{i\gamma} H_{i\delta} \, Cov\left[\Upsilon_{\gamma k}^{(\nu)}, \Upsilon_{\delta k}^{(\nu)} \,\middle|\, \boldsymbol{\Upsilon}^{(\nu-1)} \right]. \qquad \text{(E43)}$$

Therefore, by (E37), (E42), and (E43),

$$Var\left[g_{i\,k}^{\mathrm{DIR},(\nu)} \,\middle|\, \boldsymbol{\Upsilon}^{(\nu-1)} \right]$$

$$= \sum_{\alpha=1}^{m} \sum_{\beta=1}^{m} \frac{H_{i\alpha}^{\,2}}{R_\alpha} \left(\boldsymbol{K}^{\mathbf{t}}\right)_{\alpha\beta} E\left[2 D_{\beta k}^{(\nu)} Z_{\beta k}^{(\nu)} - \left(D_{\beta k}^{(\nu)}\right)^2 \,\middle|\, \boldsymbol{\Upsilon}^{(\nu-1)} \right]$$

$$- E\left[\left(Z_{i\,k}^{(\nu)} - D_{i\,k}^{(\nu)}\right)^2 \,\middle|\, \boldsymbol{\Upsilon}^{(\nu-1)} \right]$$

$$= \sum_{\alpha=1}^{m} \sum_{\beta=1}^{m} \frac{H_{i\alpha}^{\,2}}{R_\alpha} \left(\boldsymbol{K}^{\mathbf{t}}\right)_{\alpha\beta} \left\{ Var\left[\Upsilon_{\beta k}^{(\nu)} \,\middle|\, \boldsymbol{\Upsilon}^{(\nu-1)} \right] \right.$$

$$\left. - \sum_{\gamma=1}^{m} \sum_{\delta=1}^{m} H_{\beta\gamma} H_{\beta\delta} \, Cov\left[\Upsilon_{\gamma k}^{(\nu)}, \Upsilon_{\delta k}^{(\nu)} \,\middle|\, \boldsymbol{\Upsilon}^{(\nu-1)} \right] \right\}$$

$$- \sum_{\gamma=1}^{m} \sum_{\delta=1}^{m} H_{i\gamma} H_{i\delta} \, Cov\left[\Upsilon_{\gamma k}^{(\nu)}, \Upsilon_{\delta k}^{(\nu)} \,\middle|\, \boldsymbol{\Upsilon}^{(\nu-1)} \right]. \qquad \text{(E44)}$$

Now, by the well-known statistical form of Cauchy's inequality,

$$Cov\,[\,Y^{(\nu)}_{\gamma k}, Y^{(\nu)}_{\delta k} \,|\, \boldsymbol{\Upsilon}^{(\nu-1)}\,] \le \Big(Var[\,Y^{(\nu)}_{\gamma k} \,|\, \boldsymbol{\Upsilon}^{(\nu-1)}] Var[\,Y^{(\nu)}_{\delta k} \,|\, \boldsymbol{\Upsilon}^{(\nu-1)}] \,\Big)^{1/2}, \qquad \text{(E45)}$$

whence

$$Cov\,[\,Y^{(\nu)}_{\gamma k}, Y^{(\nu)}_{\delta k} \,|\, \boldsymbol{\Upsilon}^{(\nu-1)}\,] \le \max_{1\le j\le m} \Big\{ Var[\,Y^{(\nu)}_{jk} \,|\, \boldsymbol{\Upsilon}^{(\nu-1)}] \,\Big\}. \qquad \text{(E46)}$$

It now follows from (D10), (E44), and (E46) that, if we write

$$V_k^{(\nu+1,\nu-1)} = \max_{1\le i\le m} \Big\{ Var[\,Y^{(\nu+1)}_{ik} \,|\, \boldsymbol{\Upsilon}^{(\nu-1)}] \,\Big\}, \qquad \text{(E47)}$$

then

$$\begin{aligned}
V_k^{(\nu+1,\nu-1)} &= \max_{1\le i\le m} \Big\{ Var[\,Y^{(\nu+1)}_{ik} \,|\, \boldsymbol{\Upsilon}^{(\nu-1)}] \,\Big\} = \frac{\max_{1\le i\le m} \Big\{ Var[\,g^{(\nu)}_{ik} \,|\, \boldsymbol{\Upsilon}^{(\nu-1)}] \,\Big\}}{w_\nu} \\
&= \frac{1}{w_\nu} \max_{1\le i\le m} \Bigg\{ \sum_{\alpha=1}^{m} \sum_{\beta=1}^{m} \frac{H_{i\alpha}{}^2}{R_\alpha} (\boldsymbol{K}^{\mathbf{t}})_{\alpha\beta} \Bigg(Var[\,Y^{(\nu)}_{\beta k} \,|\, \boldsymbol{\Upsilon}^{(\nu-1)}] \\
&\qquad - \sum_{\gamma=1}^{m} \sum_{\delta=1}^{m} H_{\beta\gamma} H_{\beta\delta} Cov[\,Y^{(\nu)}_{\gamma k}, Y^{(\nu)}_{\delta k} \,|\, \boldsymbol{\Upsilon}^{(\nu-1)}] \Bigg) \\
&\qquad - \sum_{\gamma=1}^{m} \sum_{\delta=1}^{m} H_{i\gamma} H_{i\delta} Cov[\,Y^{(\nu)}_{\gamma k}, Y^{(\nu)}_{\delta k} \,|\, \boldsymbol{\Upsilon}^{(\nu-1)}] \Bigg\} \\
&\le \frac{1}{w_\nu} \Bigg[\sum_{\alpha=1}^{m} \sum_{\beta=1}^{m} \frac{\max_{1\le i\le m}\{H_{i\alpha}{}^2\}}{R_\alpha} (\boldsymbol{K}^{\mathbf{t}})_{\alpha\beta} \Bigg(1 + \sum_{\gamma=1}^{m} \sum_{\delta=1}^{m} |H_{\beta\gamma} H_{\beta\delta}| \Bigg) V_k^{(\nu,\nu-1)} \\
&\qquad + \sum_{\gamma=1}^{m} \sum_{\delta=1}^{m} \max_{1\le i\le m}\{|H_{i\gamma} H_{i\delta}|\} V_k^{(\nu,\nu-1)} \Bigg] \\
&= \frac{1}{w_\nu} \Bigg[\sum_{\alpha=1}^{m} \sum_{\beta=1}^{m} \frac{\max_{1\le i\le m}\{H_{i\alpha}{}^2\}}{R_\alpha} (\boldsymbol{K}^{\mathbf{t}})_{\alpha\beta} \Bigg(1 + \sum_{\gamma=1}^{m} \sum_{\delta=1}^{m} |H_{\beta\gamma} H_{\beta\delta}| \Bigg) \\
&\qquad + \sum_{\gamma=1}^{m} \sum_{\delta=1}^{m} \max_{1\le i\le m}\{|H_{i\gamma} H_{i\delta}|\} \Bigg] V_k^{(\nu,\nu-1)}. \qquad \text{(E48)}
\end{aligned}$$

It is clear that the upper bound in (E48) is probably often a gross over-estimate; but it is *finite*, and this suffices. If we put

$$C = \sum_{\alpha=1}^{m}\sum_{\beta=1}^{m} \frac{\max_{1\le i\le m}\{H_{i\alpha}{}^2\}}{R_\alpha} (\boldsymbol{K}^{\mathbf{t}})_{\alpha\beta}\left(1+\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m} |H_{\beta\gamma}H_{\beta\delta}|\right)$$

$$+\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m}\max_{1\le i\le m}\{\,|H_{i\gamma}H_{i\delta}|\,\}, \tag{E49}$$

where we note that the constant C is not dependent on the parameters k and ν, we see that (E47) can be written as

$$V_k^{(\nu+1,\nu-1)} \le \frac{C}{w_\nu} V_k^{(\nu,\nu-1)}. \tag{E50}$$

Now take the expectations of both sides of (E48) or (E50) over all $\boldsymbol{\Upsilon}^{(\nu-1)}$. Then the corresponding *unconditional variances* satisfy the inequality

$$V_k^{(\nu+1,0)} \le \frac{C}{w_\nu} V_k^{(\nu,0)}. \tag{E51}$$

Finally, we observe, therefore, that, if we take constant w_ν—

$$(\forall\,\nu)\quad w_\nu = w \tag{E52}$$

and write $$\lambda = \frac{C}{w} \quad \text{and} \quad V_k^{(\nu)} = V_k^{(\nu,0)}; \tag{E53}$$

then (E51) yields $$V_k^{(\nu)} \le \lambda^\nu V_k^{(0)}. \tag{E54}$$

F. THE ESTIMATION OF VARIANCE—OTHER ESTIMATORS

As well as the basic direct estimator, we now also consider the other three cases of augmented homogeneous estimators—the basic adjoint estimator and the direct and adjoint functional estimators—which take the respective forms[41]

[41] Compare (E1); see (C11), (C14), and (C15), and (D6)—also Footnote[35].

$$g_{rik}^{\mathrm{DIR},(\nu)}(\Gamma) = \frac{H_{i\gamma_1}H_{\gamma_1\gamma_2}H_{\gamma_2\gamma_3}\ldots H_{\gamma_r\ \ -1\gamma_r}D^{(\nu)}_{\gamma_r k}}{R_{\gamma_1}P_{\gamma_1\gamma_2}P_{\gamma_2\gamma_3}\ldots P_{\gamma_r\ \ -1\gamma_r}}, \qquad \text{(E1)} \equiv \text{(F1a)}$$

$$g_{rik}^{\mathrm{ADJ},(\nu)}(\Gamma) = \frac{H_{i\gamma_r}H_{\gamma_r\gamma_{r-1}}H_{\gamma_{r-1}\gamma_{r-2}}\ldots H_{\gamma_2\gamma_1}D^{(\nu)}_{\ \ \gamma_1 k}}{R_{\gamma_1}P_{\gamma_1\gamma_2}P_{\gamma_2\gamma_3}\ldots P_{\gamma_r\ \ -1\gamma_r}}, \qquad \text{(F1b)}$$

$$g_{rhk}^{\mathrm{DIR-F}}(\Gamma) = \frac{F_{h\gamma_0}H_{\gamma_0\gamma_1}H_{\gamma_1\gamma_2}\ldots H_{\gamma_r\ \ -1\gamma_r}D^{(\nu)}_{\gamma_r k}}{R_{\gamma_0}P_{\gamma_0\gamma_1}P_{\gamma_1\gamma_2}\ldots P_{\gamma_r\ \ -1\gamma_r}}, \qquad \text{(F1c)}$$

and

$$g_{rhk}^{\mathrm{ADJ-F}}(\Gamma) = \frac{F_{h\gamma_r}H_{\gamma_r\gamma_{r-1}}H_{\gamma_{r-1}\gamma_{r-2}}\ldots H_{\gamma_1\gamma_0}D^{(\nu)}_{\ \ \gamma_0 k}}{R_{\gamma_0}P_{\gamma_0\gamma_1}P_{\gamma_1\gamma_2}\ldots P_{\gamma_r\ \ -1\gamma_r}}. \qquad \text{(F1d)}$$

We proceed in a manner exactly parallel and analogous to that used for the derivations for direct estimators. By analogy with (E2) and (E3), we take away the initial factors in the numerator and denominator, and respectively put:

for DIR and ADJ and $r = 0$, $\quad G_0^{(\nu)}(\Gamma) = G_{0\gamma_1}^{(\nu)} = 0;$ $\qquad$ (E2) ≡ (F2a/b)

for DIR and $r \geq 1$,

$$G_r^{(\nu)}(\Gamma) = G_{r\gamma_1}^{(\nu)} = \frac{H_{\gamma_1\gamma_2}H_{\gamma_2\gamma_3}\ldots H_{\gamma_r\ \ -1\gamma_r}D^{(\nu)}_{\gamma_r k}}{P_{\gamma_1\gamma_2}P_{\gamma_2\gamma_3}\ldots P_{\gamma_r\ \ -1\gamma_r}}; \qquad \text{(E3)} \equiv \text{(F3a)}$$

for ADJ and $r \geq 1$,

$$G_r^{(\nu)}(\Gamma) = G_{r\gamma_1}^{(\nu)} = \frac{H_{i\gamma_r}H_{\gamma_r\gamma_{r-1}}H_{\gamma_{r-1}\gamma_{r-2}}\ldots H_{\gamma_2\gamma_1}}{P_{\gamma_1\gamma_2}P_{\gamma_2\gamma_3}\ldots P_{\gamma_r\ \ -1\gamma_r}}; \qquad \text{(F3b)}$$

for DIR–F and $r \geq 0$,

$$G_r^{(\nu)}(\Gamma) = G_{r\gamma_0}^{(\nu)} = \frac{H_{\gamma_0\gamma_1}H_{\gamma_1\gamma_2}\ldots H_{\gamma_r\ \ -1\gamma_r}D^{(\nu)}_{\gamma_r k}}{P_{\gamma_0\gamma_1}P_{\gamma_1\gamma_2}\ldots P_{\gamma_r\ \ -1\gamma_r}}; \qquad \text{(F3c)}$$

and,for ADJ–F and $r \geq 0$,

$$G_r^{(\nu)}(\Gamma) = G_{r\gamma_0}^{(\nu)} = \frac{F_{h\gamma_r}H_{\gamma_r\gamma_{r-1}}H_{\gamma_{r-1}\gamma_{r-2}}\ldots H_{\gamma_1\gamma_0}}{P_{\gamma_0\gamma_1}P_{\gamma_1\gamma_2}\ldots P_{\gamma_r\ \ -1\gamma_r}}. \qquad \text{(F3d)}$$

Thus, as in (E4),[42]

$$g^{\mathrm{DIR},(\nu)}_{rik}(\Gamma) = \delta_{r0} D^{(\nu)}_{ik} + \frac{H_{i\gamma_1}}{R_{\gamma_1}} G^{(\nu)}_{r\gamma_1}, \qquad \text{(E4)} \equiv \text{(F4a)}$$

$$g^{\mathrm{ADJ},(\nu)}_{rik}(\Gamma) = \delta_{r0} D^{(\nu)}_{ik} + \frac{D^{(\nu)}_{\gamma_1 k}}{R_{\gamma_1}} G^{(\nu)}_{r\gamma_1}, \qquad \text{(F4b)}$$

$$g^{\mathrm{DIR-F},(\nu)}_{rhk}(\Gamma) = \frac{F_{h\gamma_0}}{R_{\gamma_0}} G^{(\nu)}_{r\gamma_0}, \qquad \text{(F4c)}$$

$$g^{\mathrm{ADJ-F},(\nu)}_{rhk}(\Gamma) = \frac{D^{(\nu)}_{\gamma_0 k}}{R_{\gamma_0}} G^{(\nu)}_{r\gamma_0}. \qquad \text{(F4d)}$$

The recurrence (E9) applies to both direct estimators:[43]

$$G^{(\nu)}_{r\gamma_1} = \frac{H_{\gamma_1\gamma_2}}{P_{\gamma_1\gamma_2}} G^{(\nu)}_{(r-1)\gamma_2}. \qquad \text{(E9)} \equiv \text{(F9a/c)}$$

For the adjoint estimators, we similarly get

$$G^{(\nu)}_{r\gamma_1} = \frac{H_{\gamma_2\gamma_1}}{P_{\gamma_1\gamma_2}} G^{(\nu)}_{(r-1)\gamma_2}. \qquad \text{(F9b/d)}$$

By analogy with (E10), define:

for DIR,
$$M^{(\nu)}_{\gamma_1 k} = \sum_{r=1}^{\infty} G^{(\nu)}_{r\gamma_1}; \qquad \text{(E10)} \equiv \text{(F10a)}$$

for ADJ,
$$M^{(\nu)}_{i\gamma_1} = \sum_{r=1}^{\infty} G^{(\nu)}_{r\gamma_1}; \qquad \text{(F10b)}$$

for DIR–F,
$$M^{(\nu)}_{\gamma_0 k} = \sum_{r=0}^{\infty} G^{(\nu)}_{r\gamma_0}; \qquad \text{(F10c)}$$

for ADJ–F,
$$M^{(\nu)}_{h\gamma_0} = \sum_{r=0}^{\infty} G^{(\nu)}_{r\gamma_0}; \qquad \text{(F10d)}$$

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42 With the corresponding forms of G, as defined in (F3a)–(F3d).

43 In this section, the numbering of equations is *not consecutive*; instead, it parallels the numbering of corresponding equations in §E.

Thus the corresponding recurrences are easily verified to be

$$M^{(\nu)}_{\gamma_1 k} \;=\; D^{(\nu)}_{\gamma_1 k} + \frac{H_{\gamma_1\gamma_2}}{P_{\gamma_1\gamma_2}}\, M^{(\nu)}_{\gamma_2 k}\,. \qquad \text{(E11)} \equiv \text{(F11a)}$$

$$M^{(\nu)}_{i\gamma_1} \;=\; H_{i\gamma_1} + \frac{H_{\gamma_2\gamma_1}}{P_{\gamma_1\gamma_2}}\, M^{(\nu)}_{i\gamma_2}\,. \qquad \text{(F11b)}$$

$$M^{(\nu)}_{\gamma_0 k} \;=\; D^{(\nu)}_{\gamma_0 k} + \frac{H_{\gamma_0\gamma_1}}{P_{\gamma_0\gamma_1}}\, M^{(\nu)}_{\gamma_1 k}\,. \qquad \text{(F11c)}$$

$$M^{(\nu)}_{h\gamma_0} \;=\; F_{h\gamma_0} + \frac{H_{\gamma_1\gamma_0}}{P_{\gamma_0\gamma_1}}\, M^{(\nu)}_{h\gamma_1}\,. \qquad \text{(F11d)}$$

Hence, corresponding to (E12), using (F4a)–(F4d), we get

$$g^{\text{DIR},(\nu)}_{i\,k}(\Gamma) \;=\! D^{(\nu)}_{i\,k} + \frac{H_{i\gamma_1}}{R_{\gamma_1}}\, M^{(\nu)}_{\gamma_1 k}\,, \qquad \text{(E12)} \equiv \text{(F12a)}$$

$$g^{\text{ADJ},(\nu)}_{i\,k}(\Gamma) \;=\! D^{(\nu)}_{i\,k} + \frac{D^{(\nu)}_{\gamma_1 k}}{R_{\gamma_1}}\, M^{(\nu)}_{i\gamma_1}\,, \qquad \text{(F12b)}$$

$$g^{\text{DIR–F},(\nu)}_{h\,k}(\Gamma) \;=\; \frac{F_{h\gamma_0}}{R_{\gamma_0}}\, M^{(\nu)}_{\gamma_0 k}\,, \qquad \text{(F12c)}$$

$$g^{\text{ADJ–F},(\nu)}_{h\,k}(\Gamma) \;=\; \frac{D^{(\nu)}_{\gamma_0 k}}{R_{\gamma_0}}\, M^{(\nu)}_{h\gamma_0}\,. \qquad \text{(F12d)}$$

As for (E19), by (F3a)–(F3d) and (F10a)–(F10d), we now get:

for DIR, $$E\,[\, M^{(\nu)}_{\gamma_1 k} \,|\, \boldsymbol{\Upsilon}^{(\nu)}\,] \;=\; (\boldsymbol{H}^{\mathbf{t}}\boldsymbol{D}^{(\nu)})_{\gamma_1 k}\,; \qquad \text{(E19)} \equiv \text{(F19a)}$$

for ADJ,[44] $$E\,[\, M^{(\nu)}_{i\gamma_1} \,|\, \boldsymbol{\Upsilon}^{(\nu)}\,] \;=\; (\boldsymbol{H}^{\mathbf{t}})_{i\gamma_1} - \delta_{i\gamma_1}\,; \qquad \text{(F19b)}$$

for DIR–F, $$E\,[\, M^{(\nu)}_{\gamma_0 k} \,|\, \boldsymbol{\Upsilon}^{(\nu)}\,] \;=\; (\boldsymbol{H}^{\mathbf{t}}\boldsymbol{D}^{(\nu)})_{\gamma_0 k}\,; \qquad \text{(F19c)}$$

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[44] We get $\big((\boldsymbol{H}^{\mathsf{T}})^{\mathbf{t}}\boldsymbol{H}^{\mathsf{T}}\big)_{\gamma_1 i} = (\boldsymbol{H}\boldsymbol{H}^{\mathbf{t}})_{i\gamma_1} = (\boldsymbol{H}^{\mathbf{t}} - \mathbf{I})_{i\gamma_1}$, by (E14), (E16), and (E17).

for ADJ–F,[45] $$E\,[\,M_{h\gamma_0}^{(\nu)}\,|\,\boldsymbol{Y}^{(\nu)}\,]\;=\;(\boldsymbol{F}\boldsymbol{H}^{\mathsf{t}})_{h\gamma_0}\,. \tag{F19d}$$

Of course, the equation (E21) will become

$$E\,[\,g_{i\,k}^{\mathrm{DIR},(\nu)}\,|\,\boldsymbol{Y}^{(\nu)}\,]\;=\;(\boldsymbol{H}^{\mathsf{t}}\boldsymbol{D}^{(\nu)})_{ik}\;=\;Z_{i\,k}^{(\nu)}, \tag{E21} \equiv \text{(F21a)}$$

$$E\,[\,g_{i\,k}^{\mathrm{ADJ},(\nu)}\,|\,\boldsymbol{Y}^{(\nu)}\,]\;=\;(\boldsymbol{H}^{\mathsf{t}}\boldsymbol{D}^{(\nu)})_{ik}\;=\;Z_{i\,k}^{(\nu)}, \tag{F21b}$$

$$E\,[\,g_{h\,k}^{\mathrm{DIR–F},(\nu)}\,|\,\boldsymbol{Y}^{(\nu)}\,]\;=\;(\boldsymbol{F}\boldsymbol{H}^{\mathsf{t}}\boldsymbol{D}^{(\nu)})_{hk}\;=\;(\boldsymbol{F}\boldsymbol{Z}^{(\nu)})_{hk}\;, \tag{F21c}$$

$$E\,[\,g_{h\,k}^{\mathrm{ADJ–F},(\nu)}\,|\,\boldsymbol{Y}^{(\nu)}\,]\;=\;(\boldsymbol{F}\boldsymbol{H}^{\mathsf{t}}\boldsymbol{D}^{(\nu)})_{hk}\;=\;(\boldsymbol{F}\boldsymbol{Z}^{(\nu)})_{hk}\;. \tag{F21d}$$

When we take the mathematical expectations of the squares of both sides of (F11a)–(F11d), we can clearly proceed as in (E22), *mutatis mutandis*, and get, in each case, an equation of the form (E26). The definitions corresponding to (E23)–(E25) are respectively:

for DIR and DIR–F,[46] $$(\boldsymbol{K})_{\alpha\beta}\;=\;K_{\alpha\beta}\;=\;\frac{H_{\alpha\beta}^{\,2}}{P_{\alpha\beta}}\,, \tag{E23} \equiv \text{(F23a/c)}$$

$$(\boldsymbol{N}^{(\nu)})_{\alpha k}\;=\;N_{\alpha k}^{(\nu)}\;=\;E\,[\,(M_{\alpha k}^{(\nu)})^2\,], \tag{E24} \equiv \text{(F24a/c)}$$

$$(\boldsymbol{J}^{(\nu)})_{\alpha k}\;=\;J_{\alpha k}^{(\nu)}\;=\;D_{\alpha k}^{(\nu)}\left[2Z_{\alpha k}^{(\nu)}-D^{(\nu)}_{\alpha k}\right]; \tag{E25} \equiv \text{(F25a/c)}$$

for ADJ and ADJ–F, $$(\boldsymbol{K})_{\alpha\beta}\;=\;K_{\alpha\beta}\;=\;\frac{H_{\beta\alpha}^{\,2}}{P_{\alpha\beta}}\,; \tag{F23b/d}$$

for ADJ,[47] $$(\boldsymbol{N}^{(\nu)})_{i\alpha}\;=\;N_{i\alpha}^{(\nu)}\;=\;E\,[\,(M_{i\alpha}^{(\nu)})^2\,], \tag{F24b}$$

$$(\boldsymbol{J}^{(\nu)})_{i\alpha}\;=\;J_{i\alpha}^{(\nu)}\;=\;H_{i\alpha}\left[2(\boldsymbol{H}^{\mathsf{t}})_{i\alpha}-H_{i\alpha}-2\delta_{i\alpha}\quad\right]; \tag{F25b}$$

for ADJ–F, $$(\boldsymbol{N}^{(\nu)})_{h\alpha}\;=\;N_{h\alpha}^{(\nu)}\;=\;E\,[\,(M_{h\alpha}^{(\nu)})^2\,], \tag{F24d}$$

$$(\boldsymbol{J}^{(\nu)})_{h\alpha}\;=\;J_{h\alpha}^{(\nu)}\;=\;F_{h\alpha}\left[2(\boldsymbol{F}\boldsymbol{H}^{\mathsf{t}})_{h\alpha}-F_{h\alpha}\;\right]. \tag{F25d}$$

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45 We get $\left((\boldsymbol{H}^{\mathsf{T}})^{\mathsf{t}}\boldsymbol{F}^{\mathsf{T}}\right)_{\gamma_0 h}=(\boldsymbol{F}\boldsymbol{H}^{\mathsf{t}})_{h\gamma_0}$.

46 (E25) ≡ (F25a/c) comes from (E16) and (E21) ≡ (F21): $(\boldsymbol{H}\boldsymbol{H}^{\mathsf{t}}\boldsymbol{D}^{(\nu)})_{\alpha k}=(\boldsymbol{H}^{\mathsf{t}}\boldsymbol{D}^{(\nu)})_{\alpha k}-D_{\alpha k}^{(\nu)}=Z_{\alpha k}^{(\nu)}-D_{\alpha k}^{(\nu)}$.

47 (F25b) comes from two applications of (E16): $(\boldsymbol{H}\boldsymbol{H}^{\mathsf{t}}\boldsymbol{H})_{h\alpha}=(\boldsymbol{H}^{\mathsf{t}}\boldsymbol{H})_{h\alpha}-H_{h\alpha}=(\boldsymbol{H}^{\mathsf{t}})_{h\alpha}-\delta_{h\alpha}-H_{h\alpha}$.

Now, when we take expectations of the squares of both sides of (F12a)–(F12d), proceeding as in (E29) and (E31), we get an equation of the form (E32). The definitions corresponding to (E30) are respectively:

for DIR, $$(\boldsymbol{K}^{\dagger})_{i\alpha} = K^{\dagger}_{i\alpha} = \frac{H_{i\alpha}{}^2}{R_\alpha}; \qquad \text{(E30)} \equiv \text{(F30a)}$$

for DIR–F, $$(\boldsymbol{K}^{\dagger})_{h\alpha} = K^{\dagger}_{h\alpha} = \frac{F_{h\alpha}{}^2}{R_\alpha}; \qquad \text{(F30c)}$$

for ADJ and ADJ–F, $$(\boldsymbol{K}^{\dagger})_{\alpha k} = K^{\dagger}_{\alpha k} = \frac{(D^{(\nu)}_{\alpha k})^2}{R_\alpha}. \qquad \text{(F30b/d)}$$

The equation (E33) applies to all the estimators:

$$(\boldsymbol{V}^{(\nu)})_{ik} = V^{(\nu)}_{i\,k} = Var\,[\, g^{(\nu)}_{i\,k} \,|\, \boldsymbol{Y}^{(\nu)} \,]. \qquad \text{(F33)}$$

Finally, the equations corresponding to (E34) are:

for DIR and ADJ, $$(\boldsymbol{W}^{(\nu)})_{ik} = W^{(\nu)}_{i\,k} = \left(Z^{(\nu)}_{i\,k} - D^{(\nu)}_{i\,k}\right)^2, \qquad \text{(E34)} \equiv \text{(F34a/b)}$$

for DIR–F and ADJ–F, $$(\boldsymbol{W}^{(\nu)})_{hk} = W^{(\nu)}_{h\,k} = \left((\boldsymbol{F}\boldsymbol{Z}^{(\nu)})_{hk}\right)^2. \qquad \text{(F34c/d)}$$

From all this, it follows that, if the conditions (E27) and (E35) apply, then the equation (E36) will apply in all four cases. Consequently, we can expand Theorem 1 to include all four cases. This is done below.

THEOREM 2. *Given the four "infinite-series"estimators* $g^{\mathrm{DIR},(\nu)}_{i\,k}(\Gamma)$, $g^{\mathrm{ADJ},(\nu)}_{i\,k}(\Gamma)$, $g^{\mathrm{DIR-F},(\nu)}_{h\,k}(\Gamma)$, *and* $g^{\mathrm{ADJ-F},(\nu)}_{h\,k}(\Gamma)$, *of the "augmented homogeneous" type,*[48] *satisfying the convergence conditions (E27) and (E35); the variances of these estimators are given by the formula (E36); or, in detail,*

$$Var\,[\, g^{\mathrm{DIR},(\nu)}_{i\,k} \,|\, \boldsymbol{Y}^{(\nu)} \,] = \sum_{\alpha=1}^{m}\sum_{\beta=1}^{m} \frac{H_{i\alpha}{}^2}{R_\alpha}\,((\boldsymbol{K}^{\mathbf{DIR}})^{\mathbf{t}})_{\alpha\beta}\, D^{(\nu)}_{\beta k}\left[2Z^{(\nu)}_{\beta k} - D^{(\nu)}_{\beta k}\right] - \left(Z^{(\nu)}_{i\,k} - D^{(\nu)}_{i\,k}\right)^2,$$

..... (E37) ≡ (F37a)

$$Var\,[\, g^{\mathrm{ADJ},(\nu)}_{i\,k} \,|\, \boldsymbol{Y}^{(\nu)} \,] = \sum_{\alpha=1}^{m}\sum_{\beta=1}^{m} \frac{(D^{(\nu)}_{\alpha k})^2}{R_\alpha}\,((\boldsymbol{K}^{\mathbf{ADJ}})^{\mathbf{t}})_{\alpha\beta}\, H_{i\beta}\left[2(\boldsymbol{H}^{\mathbf{t}})_{i\beta} - H_{i\beta} - 2\delta_{i\beta}\right] - \left(Z^{(\nu)}_{i\,k} - D^{(\nu)}_{i\,k}\right)^2,$$

..... (F37b)

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[48] These are defined in terms of (F1a)–(F1d), by analogy with (D5) and (D6).

$$Var\,[\,g_{h\,k}^{\mathrm{DIR\text{–}F},(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu)}\,]\;=\;\sum_{\alpha=1}^{m}\sum_{\beta=1}^{m}\frac{F_{h\alpha}^{\,2}}{R_\alpha}\,((\boldsymbol{K}^{\mathbf{DIR}})^{\mathbf{t}})_{\alpha\beta}\,D_{\beta k}^{(\nu)}\left[2Z_{\beta k}^{(\nu)}-D_{\beta k}^{(\nu)}\right]-\left((\boldsymbol{F}\boldsymbol{Z}^{(\nu)})_{hk}\right)^2,$$

.....(F37c)

$$Var\,[\,g_{h\,k}^{\mathrm{ADJ\text{–}F},(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu)}\,]\;=\;\sum_{\alpha=1}^{m}\sum_{\beta=1}^{m}\frac{(D_{\alpha k}^{(\nu)})^2}{R_\alpha}\,((\boldsymbol{K}^{\mathbf{ADJ}})^{\mathbf{t}})_{\alpha\beta}\,F_{h\beta}\left[2(\boldsymbol{F}\boldsymbol{H}^{\mathbf{t}})_{h\beta}-F_{h\beta}\right]-\left((\boldsymbol{F}\boldsymbol{Z}^{(\nu)})_{hk}\right)^2.$$

.....(F37d)

We can now proceed as in (E38)–(E43), evaluating the expectations conditional on $\boldsymbol{\Upsilon}^{(\nu-1)}$ instead of $\boldsymbol{\Upsilon}^{(\nu)}$. Just as we got (E44) for the basic direct estimator, we can obtain

$$\begin{aligned}Var\,[\,g_{i\,k}^{\mathrm{DIR},(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}\,]\;=\;&\sum_{\alpha=1}^{m}\sum_{\beta=1}^{m}\frac{H_{i\alpha}^{\,2}}{R_\alpha}\,((\boldsymbol{K}^{\mathrm{DIR}})^{\mathbf{t}})_{\alpha\beta}\\&\times\left\{Var[\,\Upsilon_{\beta k}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}]-\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m}H_{\beta\gamma}H_{\beta\delta}\,Cov[\,\Upsilon_{\gamma k}^{(\nu)},\Upsilon_{\delta k}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}]\right\}\\&-\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m}H_{i\gamma}H_{i\delta}\,Cov\,[\,\Upsilon_{\gamma k}^{(\nu)},\Upsilon_{\delta k}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}\,],\qquad\text{(E44) ≡ (F44a)}\end{aligned}$$

$$\begin{aligned}Var\,[\,g_{i\,k}^{\mathrm{ADJ},(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}\,]\;=\;&\sum_{\alpha=1}^{m}\sum_{\beta=1}^{m}\frac{1}{R_\alpha}\,((\boldsymbol{K}^{\mathbf{ADJ}})^{\mathbf{t}})_{\alpha\beta}\,H_{i\beta}\left[2(\boldsymbol{H}^{\mathbf{t}})_{i\beta}-H_{i\beta}-2\delta_{i\beta}\right]\\&\times\left\{Var[\,\Upsilon_{\alpha k}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}]-2\sum_{\gamma=1}^{m}H_{\alpha\gamma}\,Cov[\,\Upsilon_{\alpha k}^{(\nu)},\Upsilon_{\gamma k}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}]\right.\\&\qquad\left.+\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m}H_{\alpha\gamma}H_{\alpha\delta}\,Cov[\,\Upsilon_{\gamma k}^{(\nu)},\Upsilon_{\delta k}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}]\right\}\\&-\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m}H_{i\gamma}H_{i\delta}\,Cov\,[\,\Upsilon_{\gamma k}^{(\nu)},\Upsilon_{\delta k}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}\,],\qquad\text{(F44b)}\end{aligned}$$

$$Var\,[\,g_{h\,k}^{\mathrm{DIR\text{–}F},(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}\,]\;=\;\sum_{\alpha=1}^{m}\sum_{\beta=1}^{m}\frac{F_{h\alpha}{}^{2}}{R_\alpha}\,((\boldsymbol{K}^{\mathbf{DIR}})^{\mathbf{t}})_{\alpha\beta}$$

$$\times\left\{Var[\,\Upsilon_{\beta k}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}]-\sum_{\gamma=1}^{n}\sum_{\delta=1}^{m}H_{\beta\gamma}H_{\beta\delta}Cov[\,\Upsilon^{(\nu)}{}_{\gamma k}\,,\Upsilon_{\delta k}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}]\right\}$$

$$-\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m}F_{h\gamma}F_{h\delta}\,Cov\,[\,\Upsilon_{\gamma k}^{(\nu)}\,,\,\Upsilon_{\delta k}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}\,],\qquad\text{(F44c)}$$

$$Var\,[\,g_{h\,k}^{\mathrm{ADJ\text{–}F},(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}\,]\;=\;\sum_{\alpha=1}^{m}\sum_{\beta=1}^{m}\frac{1}{R_\alpha}\,((\boldsymbol{K}^{\mathbf{ADJ}})^{\mathbf{t}})_{\alpha\beta}\,F_{h\beta}\,\big[2(\boldsymbol{F}\boldsymbol{H}^{\mathbf{t}})_{h\beta}-F_{h\beta}\;\big]$$

$$\times\left\{Var[\,\Upsilon_{\alpha k}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}]-2\sum_{\gamma=1}^{n}H_{\alpha\gamma}Cov[\,\Upsilon^{(\nu)}{}_{\alpha k},\Upsilon_{\gamma k}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}]\right.$$

$$\left.+\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m}H_{\alpha\gamma}H_{\alpha\delta}Cov[\,\Upsilon^{(\nu)}{}_{\gamma k}\,,\Upsilon_{\delta k}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}]\;\right\}$$

$$-\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m}F_{h\gamma}F_{h\delta}\,Cov\,[\,\Upsilon_{\gamma k}^{(\nu)}\,,\,\Upsilon_{\delta k}^{(\nu)}\,|\,\boldsymbol{\Upsilon}^{(\nu-1)}\,].\qquad\text{(F44d)}$$

Clearly, we can now apply (E46), with the notation (E47) for each estimator, to get, as in (E48):

for DIR,

$$V_k^{(\nu+1,\nu-1)}\;\le\;\frac{1}{w_\nu}\left[\sum_{\alpha=1}^{m}\sum_{\beta=1}^{m}\frac{\max_i\{H_{i\alpha}{}^{2}\}}{R_\alpha}((\boldsymbol{K}^{\mathrm{DIR}})^{\mathbf{t}}\,)_{\alpha\beta}\left(1+\sum_{\gamma=1}^{n}\sum_{\delta=1}^{m}\,|\,H_{\beta\gamma}H_{\beta\delta}|\;\right)\right.$$

$$\left.+\sum_{\gamma=1}^{n}\sum_{\delta=1}^{m}\max_i\{\,|\,H_{i\gamma}H_{i\delta}|\,\}\;\right]V_k^{(\nu,\nu-1)};\qquad\text{(E48)}\equiv\text{(F48a)}$$

for ADJ,

$$V_k^{(\nu+1,\nu-1)} \le \frac{1}{w_\nu}\left[\sum_{\alpha=1}^{m}\sum_{\beta=1}^{m}\frac{1}{R_\alpha}\left((\boldsymbol{K}^{\mathbf{ADJ}})^{\mathbf{t}}\right)_{\alpha\beta}\max_i\left\{\left|H_{i\beta}\left[\ 2(\boldsymbol{H}^{\mathbf{t}})_{i\beta}-H_{i\beta}-2\delta_{i\beta}\ \right]\right|\right\}\right.$$
$$\left.\times\left(1+\sum_{\gamma=1}^{m}|H_{\alpha\gamma}|\right)^2+\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m}\max_i\{|H_{i\gamma}H_{i\delta}|\}\right]V_k^{(\nu,\nu-1)}; \qquad \text{(F48b)}$$

for DIR–F,

$$V_k^{(\nu+1,\nu-1)} \le \frac{1}{w_\nu}\left[\sum_{\alpha=1}^{m}\sum_{\beta=1}^{m}\frac{{F_{h\alpha}}^2}{R_\alpha}\left((\boldsymbol{K}^{\mathbf{DIR}})^{\mathbf{t}}\right)_{\alpha\beta}\left(1+\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m}|H_{\beta\gamma}H_{\beta\delta}|\right)\right.$$
$$\left.+\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m}\max_h\{|F_{h\gamma}F_{h\delta}|\}\right]V_k^{(\nu,\nu-1)}; \qquad \text{(F48c)}$$

for ADJ–F,

$$V_k^{(\nu+1,\nu-1)} \le \frac{1}{w_\nu}\left[\sum_{\alpha=1}^{m}\sum_{\beta=1}^{m}\frac{1}{R_\alpha}\left((\boldsymbol{K}^{\mathbf{ADJ}})^{\mathbf{t}}\right)_{\alpha\beta}F_{h\beta}\left[2(\boldsymbol{F}\boldsymbol{H}^{\mathbf{t}})_{h\beta}-F_{h\beta}\ \right]\right.$$
$$\left.\times\left(1+\sum_{\gamma=1}^{m}|H_{\alpha\gamma}|\right)^2+\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m}\max_i\{|F_{h\gamma}F_{h\delta}|\}\right]V_k^{(\nu,\nu-1)}. \qquad \text{(F48d)}$$

Now, we can define constants analogous to (E49):

$$C^{\mathrm{DIR}} = \sum_{\alpha=1}^{m}\sum_{\beta=1}^{m}\frac{\max_i\{{H_{i\alpha}}^2\}}{R_\alpha}\left((\boldsymbol{K}^{\mathrm{DIR}})^{\mathbf{t}}\right)_{\alpha\beta}\left(1+\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m}|H_{\beta\gamma}H_{\beta\delta}|\right)$$
$$+\sum_{\gamma=1}^{m}\sum_{\delta=1}^{m}\max_i\{|H_{i\gamma}H_{i\delta}|\}, \qquad \text{(E49)} \equiv \text{(F49a)}$$

$$C^{\mathrm{ADJ}} = \sum_{\alpha=1}^{m}\sum_{\beta=1}^{m} \frac{1}{R_\alpha}\left((\boldsymbol{K}^{\mathbf{ADJ}})^{\mathbf{t}}\right)_{\alpha\beta} \max_i\left\{ \left| H_{i\beta}\left[\; 2(\boldsymbol{H}^{\mathbf{t}})_{i\beta} - H_{i\beta} - 2\delta_{i\beta} \quad \right] \right| \right\}$$

$$\times \left(1 + \sum_{\gamma=1}^{m} |H_{\alpha\gamma}| \right)^2 + \sum_{\gamma=1}^{m}\sum_{\delta=1}^{m} \max_i\{ |H_{i\gamma}H_{i\delta}| \}, \tag{F49b}$$

$$C^{\mathrm{DIR-F}} = \sum_{\alpha=1}^{m}\sum_{\beta=1}^{m} \frac{F_{h\alpha}{}^2}{R_\alpha}\left((\boldsymbol{K}^{\mathbf{DIR}})^{\mathbf{t}}\right)_{\alpha\beta} \left(1 + \sum_{\gamma=1}^{m}\sum_{\delta=1}^{m} |H_{\beta\gamma}H_{\beta\delta}| \right)$$

$$+ \sum_{\gamma=1}^{m}\sum_{\delta=1}^{m} \max_h\{ |F_{h\gamma}F_{h\delta}| \}, \tag{F49c}$$

$$C^{\mathrm{ADJ-F}} = \sum_{\alpha=1}^{m}\sum_{\beta=1}^{m} \frac{1}{R_\alpha}\left((\boldsymbol{K}^{\mathbf{ADJ}})^{\mathbf{t}}\right)_{\alpha\beta} F_{h\beta}\left[2(\boldsymbol{F}\boldsymbol{H}^{\mathbf{t}})_{h\beta} - F_{h\beta} \quad \right]$$

$$\times \left(1 + \sum_{\gamma=1}^{m} |H_{\alpha\gamma}| \right)^2 + \sum_{\gamma=1}^{m}\sum_{\delta=1}^{m} \max_i\{ |F_{h\gamma}F_{h\delta}| \}. \tag{F49d}$$

With these constants, we see that all four cases give rise to the inequalities (E50), (E51), and (E54), if we suitably define the w_ν and λ, as in (E52) and (E53).

We have therefore proved the following powerful theorem.

THEOREM 3. *Given the four "infinite-series"estimators* $g_{i\,k}^{\mathrm{DIR},(\nu)}(\Gamma)$, $g_{i\,k}^{\mathrm{ADJ},(\nu)}(\Gamma)$, $g_{h\,k}^{\mathrm{DIR-F},(\nu)}(\Gamma)$, *and* $g_{h\,k}^{\mathrm{ADJ-F},(\nu)}(\Gamma)$, *of the "augmented homogeneous" type, satisfying the usual convergence conditions (E27) and (E35); and given that the corresponding constants C are defined as in (F49a)–(F49d), with* w_ν *and* λ *defined as in (E52) and (E53); then their variances satisfy in each case the relation (E54).*

This is the very favorable order of convergence κ^w alluded to in §B.[49]

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[49] Choose $\lambda < 1$ such that $\boxed{C/\lambda} = C/\lambda$. The total number of walks after ν sequential stages is then $w = C(\nu+1)/\lambda$, and the r.m.s. error (s.d.) is less than a multiple of $\lambda^{(\nu+1)/2} = \lambda^{(\lambda/2C)w}$. Take $\kappa = \lambda^{\lambda/2C}$; then, clearly, $0 < \kappa < 1$.

G. COMPUTATIONAL RESULTS

Preliminary computations on some simple examples have been very encouraging. Our *first example* is the $(4 \times 4 \times 3)$ linear system (B1), with matrices

$$\boldsymbol{A} = \begin{bmatrix} 1.04 & 0.02 & -0.03 & 0.01 \\ -0.04 & 0.99 & -0.02 & 0.01 \\ -0.02 & 0.03 & 0.97 & -0.05 \\ 0.00 & 0.02 & 0.04 & 1.07 \end{bmatrix}, \boldsymbol{B} = \begin{bmatrix} 1.03 & 8.35 & 0.05 \\ 1.92 & 3.61 & 1.01 \\ 2.75 & 1.85 & -0.94 \\ 4.44 & 1.23 & -0.02 \end{bmatrix}, \boldsymbol{X} = \begin{bmatrix} 1 & 8 & 0 \\ 2 & 4 & 1 \\ 3 & 2 & -1 \\ 4 & 1 & 0 \end{bmatrix}. \quad \text{.....(G1)}$$

We take $\boldsymbol{L} = \boldsymbol{B}$ and $\boldsymbol{H} = \mathbf{I} - \boldsymbol{A}$. The results of three independent runs, to obtain sample estimates, with less than 0.1% relative s.d.,[50] for all components of $\boldsymbol{X}$, both by the standard ("plain") Monte Carlo method described in §C and by the sequential method described above (with all $w_\nu = 4$), with "stopping probability" $\varpi = 0.25$,[51] are tabulated below. w is the total number of random walks in each run, "STEPS" is the overall number of random steps, which is proportional to the Monte Carlo work required (both in finding random indices and in computing the corresponding estimators), and ε is the *greatest actual absolute error*, among all components.

PLAIN MONTE CARLO			SEQUENTIAL MONTE CARLO				WORK RATIO
w	STEPS_1	ε	ν	w	STEPS_2	ε	$\text{STEPS}_1/\text{STEPS}_2$
69,564	276,668	0.004 953	3	16	47	0.003 211	5,886.55
69,739	279,883	0.001 200	3	16	67	0.004 533	4,177.36
69,651	277,938	0.001 605	3	16	59	0.005 969	4,710.81

[50] Since all components of $\boldsymbol{X}$ are either 0 or not less than 1, we take the regular sample s.d., if the sample mean is less than 0.1 in magnitude; otherwise, we divide by the sample mean.

[51] This is the probability R_0 (more properly, $R_0^<$) or P_{j0} (i.e., $P_{j0}^<$) of going to index 0. In the present sampling scheme, these all equal $\varpi = 0.25$, and all other $R_{j'}$ and $P_{jj'} = (1 - \varpi)/m$.

Our *second example* is the $(6 \times 6 \times 4)$ linear-system (B1) with matrices

$$\boldsymbol{A} = \begin{bmatrix} 10.04 & -0.06 & 0.03 & -0.05 & 0.06 & -0.04 \\ -0.06 & 9.96 & -0.02 & 0.11 & -0.08 & 0.15 \\ 0.03 & -0.02 & 10.10 & 0.15 & 0.12 & 0.07 \\ -0.05 & 0.11 & 0.15 & 10.12 & 0.03 & 0.02 \\ 0.06 & -0.08 & 0.12 & 0.03 & 9.90 & -0.03 \\ -0.04 & 0.15 & 0.07 & 0.02 & -0.03 & 9.95 \end{bmatrix}, \boldsymbol{B} = \begin{bmatrix} 9.98 & -10.28 & -0.11 & 9.32 \\ 10.06 & 10.38 & 10.68 & 24.18 \\ 10.45 & -10.05 & 21.46 & 45.75 \\ 10.38 & 10.12 & 30.99 & 82.85 \\ 10.00 & -10.16 & 39.70 & 158.06 \\ 10.12 & 10.12 & 49.98 & 318.62 \end{bmatrix}, \boldsymbol{X} = \begin{bmatrix} 1 & -1 & 0 & 1 \\ 1 & 1 & 1 & 2 \\ 1 & -1 & 2 & 4 \\ 1 & 1 & 3 & 8 \\ 1 & -1 & 4 & 16 \\ 1 & 1 & 5 & 32 \end{bmatrix}.$$

.....(G2)

We now take $q = \dfrac{1}{10.49}$, $\boldsymbol{L} = q\boldsymbol{B}$, and $\boldsymbol{H} = \mathbf{I} - q\boldsymbol{A}$. The results of three independent runs, carried out exactly as for the first example, are tabulated below. The notation is the same.

PLAIN MONTE CARLO			SEQUENTIAL MONTE CARLO				WORK RATIO
w	STEPS_1	ε	ν	w	STEPS_2	ε	$\text{STEPS}_1/\text{STEPS}_2$
478,447	1,911,350	0.002 666	3	16	47	0.003 004	40,667.02
476,542	1,907,739	0.006 363	3	16	67	0.001 938	28,473.72
479,328	1,918,531	0.002 150	4	20	73	0.000 049	26,281.25

Further experimentation (not shown here) indicates that one should work with minimal values of w_ν (we take $w_\nu = 4$ here) and rather large stopping probabilities (we have $\varpi = 0.25$). The worst-of-three estimate, from the above results, of the work ratio $\text{STEPS}_1/\text{STEPS}_2$ is greater than 4,710 for the first example, and greater than 26,281 for the (larger) second example.

The improvement in efficiency derived from the use of the sequential method is quite remarkably impressive.

By (B3), $$\mathbb{T}_{\text{ITER}}(m, n, s_0) = O(m^2 n s_0), \qquad \text{(G3)}$$

Since we use uniform probabilities,[33] the time needed to determine any random index γ_r is $O(1)$;[52] so the time to determine Γ_u is $O(s)$. The time for computing each component estimate by summing (C8) or (C11) over s

[52] We use (A13). If we use the general formula (A12), the time is $O(m)$ instead. See Footnote[29].

steps of Γ_u is also $O(s)$.[53] Thus, for *plain MC*, over cn components and w random walks, the total time is[54]

$$\mathbb{T}_{\text{MC,PLAIN}}(m, c, n, s_1, w_1) \;=\; O(cns_1w_1) \;=\; O(cn\ \text{STEPS}_1). \tag{G4}$$

For *sequential MC*, most of this is the same. The estimates for one sequential stage take time $O(mnsw) = O(mn\ \text{STEPS})$, because we are now forced to take $c = m$, so as to have the complete matrix $\boldsymbol{Y}^{(\nu)}$ available to compute the matrix $\boldsymbol{D}^{(\nu)}$.[55] This computation takes time $O(m^2n)$. Thus, the total time for the sequential process with ν improvements is[36]

$$\begin{aligned}\mathbb{T}_{\text{MC,SEQ}}(m, c, n, s_2, w_2, \nu) \;&=\; O\big(mn\nu(m + s_2w_2)\big)\\ &=\; O\big(mn(\nu m + \text{STEPS}_2)\big).\end{aligned} \tag{G5}$$

H. APPROXIMATIVE SEQUENTIAL MONTE CARLO

When one considers problems with large values of m — those for which [by (G3) and (G4), even if $c = m$] the Monte Carlo method is more efficient than the classical methods—it becomes difficult to make (G5) competitive, because of the first term, which is due to the computation of $\boldsymbol{D}^{(\nu)}$.

There are two ways to reduce the necessary labor:

(i) We can use Monte Carlo sampling to estimate the sums in $\boldsymbol{H}\boldsymbol{Y}^{(\nu)}$, which, by (D3), are the principal contributors to the labor of computing $\boldsymbol{D}^{(\nu)}$. The question is then whether the number of samples required can be kept to $o(m)$, thus effecting a saving.

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[53] Consider the *direct* estimate (the *adjoint* estimate is entirely analogous). We begin with SUM = L_{ik} and TERM = 1. At the step $\gamma_{r-1}\gamma_r$, we multiply TERM by $H_{\gamma_{r-1}\gamma_r}/P_{\gamma_{r-1}\gamma_r}$ [Note: if $r = 1$, the factor is $H_{i\gamma_r}/R_{\gamma_r}$ instead] and store TERM. Then we multiply TERM by $L_{\gamma_r k}$ and add the product to SUM. On termination of the random walk, SUM is the required estimate. This takes two multiplications, one division, and one addition per random step.

[54] Since we use the infinite series expansion with automatic termination through the augmented index set, the length s_1 or s_2 of our random walks is not necessarily related to the number of classical iterations s_0.

[55] Since the $r = 0$ term of the (i, k) component estimate is $D_{ik}^{\{\nu\}}$, this alone suffices to ensure that *all* components of $\boldsymbol{D}^{\{\nu\}}$ have to be computed for each sequential stage.

(ii) When the problem (B1) is *a discretization of a continuous problem* [such as (B4a) or (B4b)], the solution $\boldsymbol{X}$ will also be a discretization of a continuous function [such as $X(\xi, \eta, \omega)$ or $X(\eta, \omega)$]. The continuity and differentiability of the solution—and therefore of the estimates $\boldsymbol{Y}^{(\nu)}$—and the analytic properties of the operator $\boldsymbol{H}$ allow us to *approximate* each column of $\boldsymbol{Y}^{(\nu)}$ on the basis of the components in relatively few (say c) of the m rows, by any of the usual methods of numerical approximation, such as classical interpolation, piecewise-polynomial splines, or least-square fits. The computing labor will then be reduced from $O\big(mn(\nu m + \text{STEPS}_2)\big)$ to $O\big(cn(\nu c + \text{STEPS}_2)\big)$, since we no longer need $c = m$, but with the additional labor, $\mathbb{J}\nu$, of approximating, at each sequential stage, n full columns of $\boldsymbol{Y}^{(\nu)}$, each from c values. Clearly, whatever is the chosen formula, there will be a constant $\mathbb{K}_1$ (denoting setting-up labor at each of the c rows where $\boldsymbol{Y}^{(\nu)}$ is known) and another constant $\mathbb{K}_2$ (denoting work at each of the $m - c$ interpolated rows), such that

$$\mathbb{J} \;=\; n\Big[c\big(\mathbb{K}_1 - \mathbb{K}_2\big) + m\mathbb{K}_2\Big], \tag{H1}$$

whence $$\mathbb{T}^{\text{APPROX}}_{\text{MC,SEQ}}(m, c, n, s_2, w_2, \nu) \;=\; O\big(n[\nu(m + c^2) + c\ \text{STEPS}_2]\big). \tag{H2}$$

Some recent calculations by the author, using method (i)—MC sampling—have been very successful. Our *third example* has arbitrary m, and $n = 1$. Where possible, we used $c = 20$. We begin with the matrices $\boldsymbol{H}$ and $\boldsymbol{X}$:

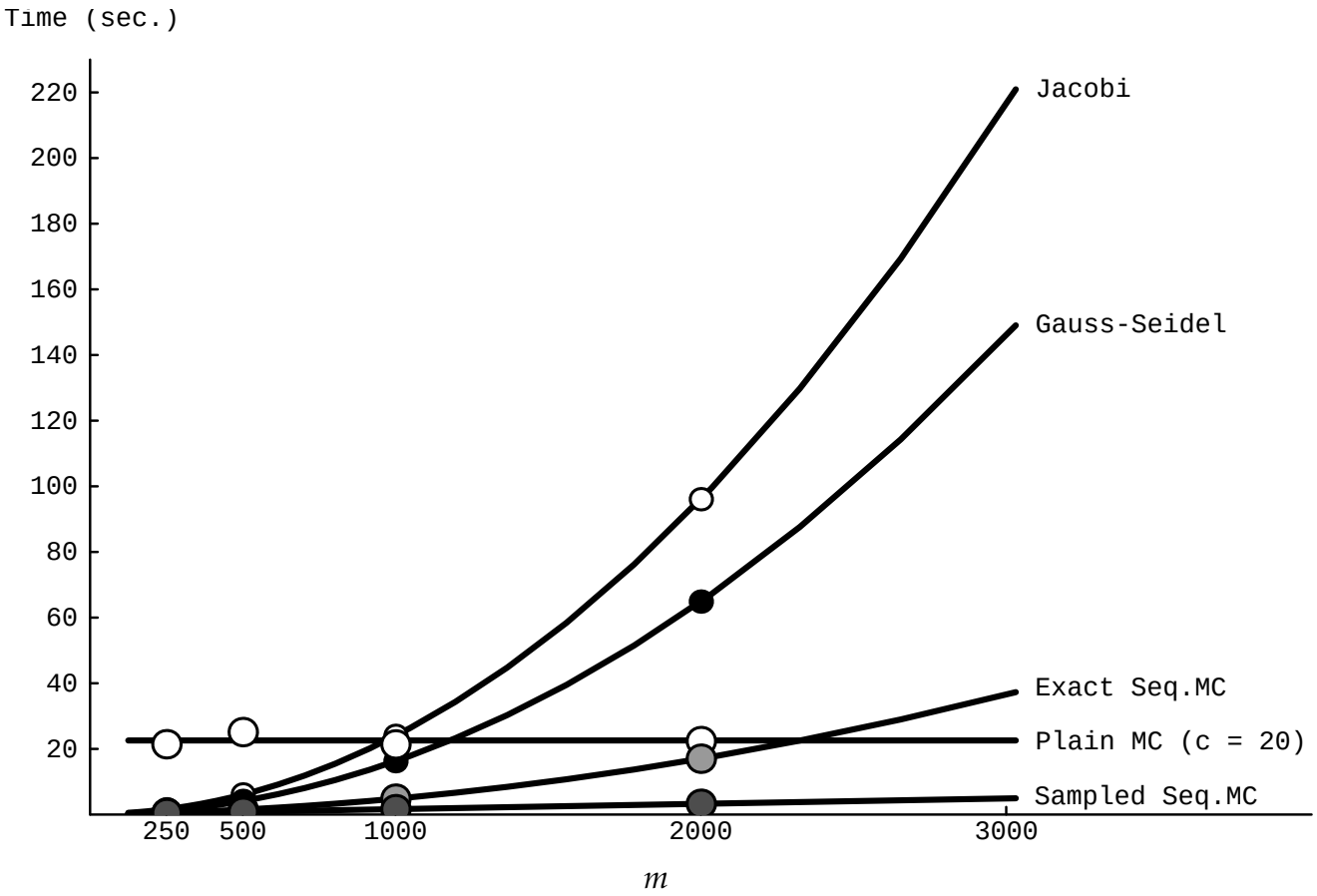
$$H_{ij} \;=\; \frac{\left(1.12 – 0.72^{\dfrac{i-1}{m}}\right)\left(1.12 – 0.72^{\dfrac{j-1}{m}}\right)}{m} \tag{H3}$$

and $$X_i \;=\; \frac{1}{2.25 – 1.45^{\dfrac{i-1}{m}}}, \tag{H4}$$

and compute the corresponding matrix $\boldsymbol{L}$ by (B7), for any given m. This yields a family of comparable linear systems. These were solved, for $m = 500$, $m = 1{,}000$, and $m = 2{,}000$, with the same accuracy of 0.1% as before, using the *Jacobi* and *Gauss-Seidel iterations*, *plain MC*, *exact sequential MC*, and the *sampling method* (i) above. The tabulated criteria were the *CPU times* used on a Cray Y-MP supercomputer to obtain the solutions. The results are tabulated below.

METHOD	$m = 250$	$m = 500$	$m = 1{,}000$	$m = 2{,}000$
JACOBI	1.5979 sec.	6.1276 sec.	23.9797 sec.	96.0721 sec.
GAUSS-SEIDEL	1.0979 sec.	4.1595 sec.	16.2632 sec.	64.8932 sec.
PLAIN MC	21.4261 sec.	25.1242 sec.	21.3617 sec.	22.3789 sec.
EXACT SEQUENTIAL MC	0.5382 sec.	1.5106 sec.	4.8386 sec.	17.0154 sec.
SAMPLING SEQUENTIAL	0.4310 sec.	0.8305 sec.	1.6382 sec.	3.2796 sec.

The agreement with the asymptotic forms of (G3)–(G5) and (H2) is remarkably good, as is illustrated by the quadratic and linear least-square fits shown in the graph below.



Both of the algebraic (iterative) methods take time $O(m^2)$. For every m, *Jacobi's method* converged in $s_0 = 13$ iterations and the *Gauss-Seidel method* in $s_0 = 9$. *Plain MC*, with $c = 20$ and stopping

probability[56] 0.02, took about the same number of steps for all three values of m, and therefore took approximately constant time (in accordance with (G4)). *Exact sequential MC* (as used for the two earlier examples) worked best with stopping probability[57] 0.33 and all $w_\nu = 100$. For every m, convergence was achieved in $\nu = 3$ sequential improvements. The time is again $O(m^2)$ (as predicted by (G5)). Finally, *sampled sequential MC* takes time $O(m)$, for fixed $c = 20$ (comparable to (H2)).

The advantage of the sampled sequential MC method over the exact sequential method is evident, even for $m \le 2{,}000$. For larger m, it becomes increasingly apparent. If we take $c = m$, as we did for the first two examples, then the time required by plain MC is multiplied by m/c; and when we compare the sampled sequential method with plain MC, we get a work-ratio of 682.37 for this problem.

The main questions remaining here are (a) *when* (i.e., under what *conditions* on the matrices $\boldsymbol{L}$ and $\boldsymbol{H}$) is sampling of the terms of $\boldsymbol{H}\boldsymbol{Y}^{(\nu)}$ effective, and (b) *how* should we adjust the number of terms sampled at each stage to *maximize the efficiency* of the sampled sequential MC scheme. Since the sequential schemes are essentially iterative methods, which tend to adapt to errors in each iterate by only slowing down the overall convergence, so long as the approximations are good enough; we have to investigate both the extent of the region of *stability* of the method and the possibility of *optimizing* any stable scheme.

Earlier calculations by the author, using method (ii) above with very rough approximations, indicate that it is quite effective.[58] This should certainly be followed up. Here we have much less detailed information, so far, but the concept is very promising, and we know that *very many practical applications* (being intrinsically *smooth* problems, usually with solutions in C^r, with $r \ge 2$) will lend themselves to this approach. It is important to develop more mathematical control of the situation, and to devise stable, efficient, optimally convergent schemes. Any progress will require an examination of various schemes for the *interpolation* of all the components of the m-vector $\boldsymbol{Y}^{(\nu)}$ from only c known component, and the corresponding *approximation* of the matrix $\boldsymbol{H}$.

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56 See Footnote[50]. For plain MC, it was found that larger probabilities were counter-productive, since they required *more* computer time.

57 See Footnote[50]. Note that large values of ϖ were effective for the first two examples (though note that $\varpi = 0.25$ is comparable to $1/m$, in these cases, with $m = 4$ and $m = 6$), and also for the sequential schemes applied to the third example; but $\varpi = 0.02$ worked better there for plain MC (but note that, in this case, we had $m = 250$, $m = 500$, $m = 1{,}000$, and $m = 2{,}000$).

58 See HALTON, **(17)** and **(26)**.

We do not know the exact criteria for the applicability of the two *approximative sequential methods* to linear problems. This needs to be investigated before valid recommendations can be made. Furthermore, in the important special case of radiation diffusion (particle transport) with reactions (e.g., fission and fusion reactions), further analysis is needed to get accurate time estimates, since the matrix $\boldsymbol{H}$ takes the form of a product of matrices corresponding to free flight between collisions and to reactions on collision.

I. SEQUENTIAL MONTE CARLO FOR NON-LINEAR SYSTEMS

It is of interest to investigate the extent to which the same approaches can be applied to *non-linear problems*. It would seem to be a relatively easy extension. There is a flavor of *Newton's method* to it. First, a local linearization yields an approximation. Unlike the classical Newtonian iterations, the Monte Carlo estimates will (and need) not be exact solutions of the linearized problem. Each step leads us to a new location (by going from $\boldsymbol{Y}^{(\nu)}$ to $\boldsymbol{Y}^{(\nu+1)}$), where the local linearized problem is essentially a change in the values of the matrices $\boldsymbol{L}$ and $\boldsymbol{H}$. There, we obtain a new Monte Carlo iterate; and so on.

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