Monte Carlo Methods & Virtual Photonics

Tuesday-Thursday 9 – 10:30
Room 3201, Nat. Sci. II
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Please help yourselves to refreshments at the back of the room and leave your name, affiliation and contact information on the sign-in sheet.
Classes Posted

You may view the first five (9/18, 9/20, 9/25, 9/27, 0/2) class presentations at

http://lammp.bli.ucl.edu/education/mcm

Click on “lectures”

Today’s presentation will also be posted there very soon
The Basic Problem

- Statistical error reduces (for conventional MC) as \((N)^{-1/2}\) where \(N\) = number of (independent) photon biographies generated
  - More precisely, \(\sigma_N(\xi) = \sigma_1(\xi)/N^{1/2}\) where
    \[
    \sigma_1^2 = \int_{\Omega} (\xi - \bar{\xi})^2 dM = \int_{\Omega} \xi^2 dM - \bar{\xi}^2
    \]
  - Variance reduction methods, e.g., use of
    \[
    \int_{\Omega} \xi dM = \int_{\Omega} \xi \frac{dM}{dN} dN
    \]
    where
    \[
    \int_{\Omega} \left(\xi \frac{dM}{dN}\right)^2 dN < \int_{\Omega} \xi^2 dM
    \]
    help, but do not affect rate of convergence
Fuel-Efficient Monte Carlo Engines: Adaptive Algorithms

**First Idea:** Why not apply variance reduction sequentially, or adaptively?

**Second Idea:** Monte Carlo is best at estimating *averages*

**Third Idea:** Expansion coefficients are (weighted) solution averages

Can these ideas be combined?
Putting This Plan Into Action

**Mechanism for Global Learning:** Expand solution \( \Psi(P) = \sum_{i=1}^{\infty} a_i B_i(P) \) in basis functions \( B_i \)

and truncate \( \tilde{\Psi}(P) = \sum_{i=1}^{M} a_i B_i(P) \approx \Psi(P) \)

where \( \Psi(P) = \int_{\Gamma} K(P, P') \Psi(P')dP' + S(P) \) \hspace{1cm} \text{(RTE)}

Then estimate \( a_i = \int_{\Gamma} B_i(P) \Psi(P)dP \) (if \( B_i \) are orthonormal) in adaptive stages of ever-increasing accuracy.
What is Geometric Convergence?

Let \( \tilde{\Psi}_n(P) \) be the approximation to the solution from adaptive stage \( n \) : \( \tilde{\Psi}_n \approx \Psi \). We want

\[
\Pr \left\{ \| \Psi - \tilde{\Psi}_n \|_\infty \leq \lambda \| \Psi - \tilde{\Psi}_{n-1} \|_\infty \right\} > 1 - \varepsilon \quad (GC)
\]

where

\[
\| \Psi - \Phi \|_\infty = \max_{P \in \Gamma} | \Psi(P) - \Phi(P) |
\]

Our convergence theorems state that for any \( \varepsilon > 0 \) and any \( \lambda \)

\[
0 < \lambda < 1,
\]

there exists a threshold number of random walks per stage \( W_0 \) so that the inequality (GC) is satisfied for any \( W \geq W_0 \).
1st Generation (Global) Methods

Residual MC (Reduced Source):
SCS Algorithm
Adaptive Importance Sampling:
AIS Algorithm
Generalized Weighted Analog Sampling:
GWAS Algorithm
IDEA: The adaptive feature is embodied in the reduced source

\[ S^{n+1}(P) = S^n(P) + K\tilde{\Psi}^n(P) - \tilde{\Psi}^n(P) \quad S^0(P) = S(P) \]

where \( \tilde{\Psi}^n(P) \) is the approximate solution from stage \( n \).

As the approximation improves, \( S^n(P) \to 0 \) so \( \tilde{\Psi}^n(P) \to 0 \) also.
Qualities of SCS

**SCS is**

- Fast – uses analog kernel, $\mathcal{K}$
- Relatively easy to implement
- Forgiving (robust)

**But** reduced source $S^n$ is complicated (usually requires numerical integration, resulting in loss of control of accuracy)
Adaptive Importance Sampling (AIS)

**IDEA:** Use RTE reciprocity and take advantage of the fact that $\Psi(P)$ is the perfect (dual) importance function for the adjoint RTE:

$$\Psi_i^*(P) = \int_{\Gamma} K^*(P, P') \Psi_i^*(P') dP' + S_i^*(P)$$  \hspace{1cm} \text{(RTE}_{i*}\text{)}$$

where $K^*(P, P') = K(P', P)$

Then

$$\int_{\Gamma} S_i^*(P) \Psi(P) dP = \int_{\Gamma} \Psi_i^* (P) S(P) dP$$
AIS (cont’d)

In AIS, we use $\text{RTE}_i^*$ to generate adjoint biographies, and estimates of $\Psi(P)$ obtained from the flux expansion coefficients are used to modify the sampling/weighting strategy (dual importance sampling). We omit the details here.
Qualities of AIS

**AIS:**
- Has high information content/biography
- Finds complete solution (not SCS-type correction)
- Should work well in problems not amenable to analog simulation

**But** is computationally intensive (transformed sampling densities are hard to calculate precisely)
Generalized Weighted Analog Sampling (GWAS)

**IDEA:** Combine *speed* of SCS with *power* of AIS. Relax rules for generating biographies (introduce bias that is negligible as the # of adaptive stages increases). GWAS is a strict generalization of AIS but has an extra degree of freedom.

Potentially, GWAS is very versatile and powerful.
Qualities of GWAS (limited trials)

**GWAS is:**

- Almost as fast as SCS with proper sampling choices
- Almost as powerful as AIS with proper sampling/weighting choices

**But** is difficult to analyze for optimality and requires considerable “customization” at present (too many choices)
Geometric Convergence: 1-D Model Problem

Comparison of AIS, SCS, and GWAS: \( B_1 = 0.1 \) -- \( B_2 = 1 \) -- 10 Trials
A More Formidable Challenge: SCS Results
Other Tests

We have achieved similar results with other model problems as well as more complex test problems. In general, these tend to support the findings made with quite simple model problems.

At present, we are working with a 1-D test problem that is the equivalent of a highly heterogeneous slab (although the independent variable is energy) and with a 2-D test that extends the 1-D test just discussed.
Pros/Cons: 1st Generation Algorithms

Pros

• Very accurate RTE solutions are possible
• Knowledge of full solution everywhere enables all possible tallies to be computed by quadrature
• Proofs reveal some, not all of the conditions needed for success
Pros/Cons: 1st Generation Algorithms

Cons

• Work involved grows geometrically with phase space dimension (more expansion coeffs needed)
• Quadrature-induced errors, truncation errors are difficult to estimate and to control
• Computational burden is large in many dimensions
Many model and test problems (1-D mono- and bi-directional, 1-D general angle + higher dimensional rectangular and spherical geometries) confirm:

• Theory is solid;
• High precision is possible, but with increasing costs in higher dimensions;
• Problems all stem from need for basis function expansion of solution
Doing Better: 2nd Generation Algorithms

**IDEA:** Focus on Tallies (Measurements)

**QUESTION:** Is it possible to estimate $D$ measurements

\[ \int_{\Gamma} S_1^* (P) \Psi(P) dP, \ldots, \int_{\Gamma} S_D^* (P) \Psi(P) dP \]

accurately without estimating $\Psi(P)$ for all $P \in \Gamma$

(or even without representing $\Psi(P)$ globally in basis functions)?
Implications

• Computational burden greatly lessened (goal: 4-6 digits of relative precision, not 10-15)
• Avoids need for flux expansion and resultant truncation error
• Precision should be easier to control
• If $D$ (# of detectors) is small (as is usual), total computational requirements should be significantly reduced
2\textsuperscript{nd} Generation (cont’d)

Decompose $\Gamma = \bigcup_{i=1}^{R} \Gamma_i$ to include all tally (detector) regions $\Gamma_1, \ldots, \Gamma_D$ and assume $\Gamma_i \cap \Gamma_j = \emptyset$, $i \neq j$.

Define a global “detector” function $S^*(P)$ to coincide with each “detector” function $S_i^*(P) = \begin{cases} 1 & \text{if } P \in \Gamma_i \\ 0 & \text{if } P \notin \Gamma_i \end{cases}$ in tally regions and take the value 1 elsewhere. If we then multiply the (RTE) by $S^*(P)$ and integrate over $\Gamma_i$.
we obtain the matrix equation $\alpha = M\alpha + q$
where $M$ is an $R \times R$ matrix.
and
$$\alpha_i = \int_{\Gamma_i} S^*(P)\Psi(P)dP, \quad q_i = \int_{\Gamma_i} S^*(P)S(P)dP$$

This implies that
$$M_{ij} = \frac{\int_{\Gamma_i} \int_{\Gamma_j} S^*(P)K(P,Q)\Psi(Q)dQdP}{\int_{\Gamma_j} S^*(Q)\Psi(Q)dQ}$$
2nd Generation (cont’d)

An SCS-type algorithm based on the reduced source is

\[ S_{\text{red}}^{n+1}(\Gamma_i) = q_i - \alpha_i^n + \int_{\Gamma_i} \int_{\Gamma} S^*(P)K(P,Q)\Psi^n(Q)dQdP \]

where

\[ q_i = \int_{\Gamma_i} S^*(P)S(P)dP, \quad \alpha_i^n = \int_{\Gamma_i} S^*(P)\Psi^n(P)dP \]

For comparison with SCS,

\[ S^{n+1}(P) = S^n(P) - \tilde{\Psi}^n(P) + K\tilde{\Psi}^n(P) \]

The resulting **ASCS algorithm** combines continuous sampling of biographies with regionwise averaging of information.
Geometric Convergence: ASCS

To illustrate the behavior of this algorithm, we solved the same 1-D RTE for a slab of thickness 100, with 1000 uniformly spaced subregions. The following graph shows the result obtained by generating only 5 photons in each subinterval; a total of 5000 for each of the 4 adaptive stages shown.
Geometric Convergence: ASCS

\[ E = \log_{10}|R| \]

-0.5
-1
-1.5
-2
-2.5
-3
-3.5
-4
-4.5
-5

stage number

B1=0.99, B2=100
RW/subinterval = 5
Num of Subintervals = 1000
Geometric Convergence: ASCS

Theorem: The ASCS algorithm converges geometrically to an estimate whose error depends only on the phase space subdivision

$$\Gamma = \bigcup_{i=1}^{R} \Gamma_i$$

This raises the questions: Can the same be done with AIS? Can geometric learning be continued with refinements in this subdivision? What is an optimal strategy for refinements? (On what does non-uniform subdivision depend?)
An importance sampling-based algorithm, AAIS, has also been developed that behaves very similarly to ASCS. We believe that ASCS and AAIS will ultimately be useful for more or less complementary classes of RTE problems (those amenable to analog sampling and those that aren’t).

We omit the AAIS numerical results for lack of time.
Next, we investigated the possibility of intelligent refinement of the decomposition

\[ \Gamma = \bigcup_{i=1}^{R} \Gamma_i \]

in order to enhance and extend geometric learning with both ASCS and AAIS.
3rd Generation Algorithms: Grid Refinement

Given a single source $S$ and a single detector (tally region) characterized by $S^*$, define an information density function by

$$C(P) = \Psi(P)\Psi^*(P)$$

where $\Psi$ is the solution of the RTE with source $S$ and $\Psi^*$ is the solution of RTE* with adjoint source $S^*$. Since $\Psi(P)$ is the density of radiation at $P$ per unit source, and $\Psi^*(P)$ is the expected contribution to the tally of a particle sourced at $P$ with weight 1, $C(P)$ seems appropriately defined.

We introduced this idea earlier and called $C(P)$ the contribution function.
Extended Geometric Convergence: Grid Refinement With ASCS

\[ E = \log_{10}|R| \]

- \( B_1 = 0.99, B_2 = 100 \)
- \( \text{RW/subintervals} = 5 \)
- Mesh 1
- Stage number

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Comparative Efficiencies

Although not strictly applicable to adaptive methods, to give at least a rough idea of computational gains, we used the same efficiency definition $E = 1/TV$ that applies when comparing conventional Monte Carlo methods to analyze gains made with our adaptive methods. Since we know the exact relative error, we replace the variance term $V$ in this formula by $|R|^2$, which recognizes that $|R|^2 \approx V$. 
## Comparative Efficiencies

| Method | $S$ | $Est.$    | $|R|   $ | $T$  | $Eff$  |
|-------|-----|-----------|--------|------|--------|
| exact | 0   | .3869022  | -      | -    | -      |
| CMC   | 1   | .3400000  | $5.77 \times 10^{-2}$ | 2.5  | $1.2 \times 10^2$ |
| G2    | 8   | .3869062  | $1.04 \times 10^{-5}$ | 16   | $5.8 \times 10^8$ |
| G3    | 8   | .3869025  | $8.16 \times 10^{-7}$ | 328  | $4.6 \times 10^{10}$ |

Table 1
Comparison of efficiencies of each method. $S =$ number of adaptive stages, $Est.$ = estimate of the average flux in a specified region, $|R|$ = absolute value of the relative error, $T =$ simulation run time (sec), $Eff =$ efficiency.
Implications

The results shown on the last slide imply that to obtain equivalent error reduction with conventional Monte Carlo would require more than $10^7$ years of computation on the same 2.80GHz processor.
Summary/Conclusions

• Expansion-free geometric learning is possible
• The theory for Generation 2 is complete for both ASCS and AAIS
• The theory for Generation 3 has yet to be fully worked out but the method seems promising
Monte Carlo Methods and Virtual Photonics

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