Monte Carlo Methods

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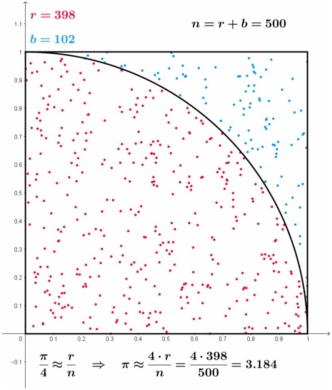
These slides are available at
https://github.com/dstndstn/MCMC-talk

Monte Carlo

- A set of computational approaches that uses *repeated random simulations*
- Often: *numerical integration*, *optimization*, and *sampling from probability distributions*
- *Monte Carlo* is a casino in Monaco – a reference to the *randomness* used in these algorithms
- Developed at the very beginning of computing: 1940s, Los Alamos, nuclear bomb work (diffusion of neutrons in fissionable material)
- Compute *Expectation values* over probability distributions:
- $\mathbb{E}(\phi(X)) = \int p(X)\phi(X)dX \sim \frac{1}{N}\sum_i^N \phi(X_i)$

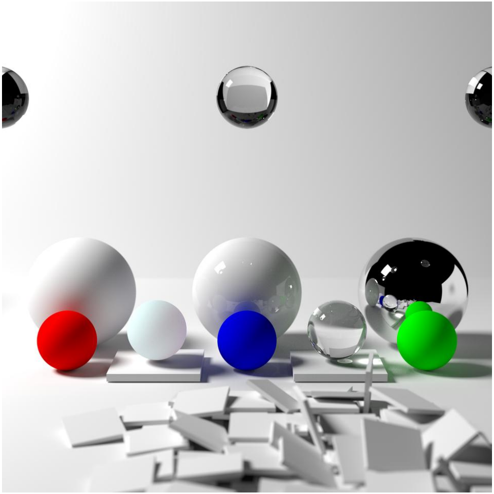
Monte Carlo: Examples

From *https://en.wikipedia.org/wiki/Monte_Carlo_method*



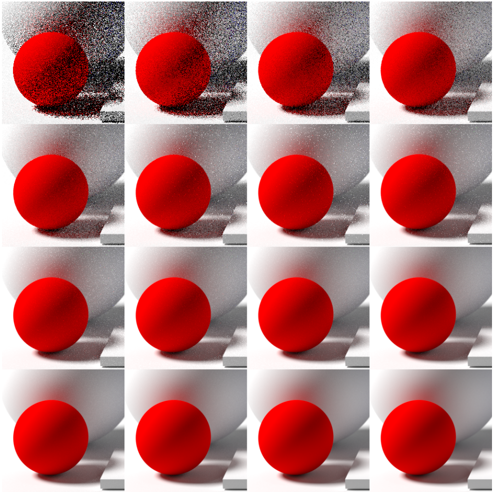
- Monte Carlo estimator: $\hat{\theta} = \frac{1}{N} \sum_{i=1}^{N} \phi(x_i)$
- Variance: $\mathrm{var}(\hat{\theta}) = \frac{1}{N} \mathrm{var}(\phi(X))$ (of the *distribution* X)
- Sample v: $\mathrm{var}(\hat{\theta}) \simeq \frac{1}{N} \left(\frac{1}{N-1} \sum (\phi(x_i) - \hat{\theta})^2 \right)$
- see *https://mpaldridge.github.io/math5835/lectures* for proofs

Monte Carlo examples: Path Tracing



Credit: Wikimedia,
https://commons.wikimedia.org/wiki/File:Path_tracing_001.png

Monte Carlo examples: Path Tracing

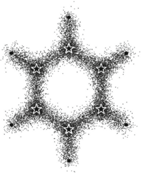


Credit: Wikimedia,

https://en.wikipedia.org/wiki/Path_tracing#/media/File:Path_tracing_sampling_values.p

Monte Carlo examples: Quantum Monte Carlo

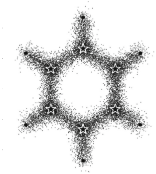
- Dealing with multi-particle wavefunctions often involves many-dimensional integrals
- *The Curse of Dimensionality*
- Variational Monte Carlo: uses Monte Carlo sampling of electron positions in real space to estimate the ground-state wavefunction, given a Hamiltonian
- Parameterized wavefunction $|\psi(a)\rangle$
- Estimate $E(a) = \frac{\langle\psi(a)|H|\psi(a)\rangle}{\langle\psi(a)|\psi(a)\rangle}$
- ie, the integral $E(a) = \frac{\int |\psi(X,a)|^2 \frac{H\psi(X,a)}{\psi(X,a)}}{\int |\psi(X,a)|^2 dX}$



From *https://doi.org/10.11*

Monte Carlo examples: Quantum Monte Carlo

- ie, the integral $E(a) = \frac{\int |\psi(X,a)|^2 \frac{H\psi(X,a)}{\psi(X,a)} dX}{\int |\psi(X,a)|^2 dX}$
- Treat this term as a probability distribution function: $p(X) = \frac{|\psi(X,a)|^2}{\int |\psi(X,a)|^2 dX}$
- Then we've got $E(a) = \int p(X) \frac{H\psi(X,a)}{\psi(X,a)} dX$
- Monte Carlo it!
- $E(a) \simeq \frac{1}{N} \sum \frac{H\psi(X_i,a)}{\psi(X_i,a)}$
- with X_i drawn from the "trial wavefunction" $\psi(a)$



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