Lecture 1. Introduction to “Applied Stochastic Analysis”

Tiejun Li$^{1,2}$

$^1$School of Mathematical Sciences (SMS),
$^2$Center for Machine Learning Research (CMLR),
Peking University,
Beijing 100871,
P.R. China

Office: No. 1 Science Building, Room 1376E
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Stochastics: Why, What and Where

Monte Carlo Concepts

Typical Applications

Course Plan
There are still debates on whether the world is deterministic or stochastic.
Stochastics: why

There are still debates on whether the world is deterministic or stochastic. We take a practical point of view on this problem. The reason why we utilize stochastics is as below:

▶ The problem itself is stochastic (quantum mechanics).
Stochastics: why

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- The problem itself is stochastic (quantum mechanics).
- Even the problem is deterministic in nature, the degrees of freedom is too huge to be handled in a deterministic manner (statistical mechanics).
There are still debates on whether the world is deterministic or stochastic. We take a practical point of view on this problem. The reason why we utilize stochastics is as below:

- The problem itself is stochastic (quantum mechanics).
- Even the problem is deterministic in nature, the degrees of freedom is too huge to be handled in a deterministic manner (statistical mechanics).
- The considered problem is in deterministic form, but we utilize its equivalent stochastic form to do computing (Monte Carlo methods).
The course will be composed of three parts:

1. Monte Carlo methods
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2. SDEs and their simulations
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1. Monte Carlo methods
2. SDEs and their simulations
3. Applications
Stochastics: where

Main application area of the Monte Carlo methods:

- Statistical physics
Stochastics: where

Main application area of the Monte Carlo methods:
- Statistical physics
- Statistical inference
Stochastics: where

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- Data Science
Stochastics: where

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Main application area of the Monte Carlo methods:

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- etc.
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Monte Carlo method

We will show the basic idea of Monte Carlo method through two simple examples at first:

1. Buffon’s needle test
Monte Carlo method

We will show the basic idea of Monte Carlo method through two simple examples at first:

1. Buffon’s needle test
2. Monte Carlo integration
Buffon’s needle problem

Formulation: (Buffon’s needle problem)

1. Parallel lines with distance $a$ in the plane;

\[
\frac{x}{a} = \frac{\ell}{2 \sin \phi}
\]

Figure: Schematics for Buffon’s needle problem.
Buffon’s needle problem

Formulation: (Buffon’s needle problem)

1. Parallel lines with distance \( a \) in the plane;
2. Tossing a needle of length \( l \) \((l < a)\) randomly;

\[
\frac{\ell}{2} \sin \phi
\]

\( x \)

\( a \)

**Figure**: Schematics for Buffon’s needle problem.
Buffon’s needle problem

Formulation: (Buffon’s needle problem)

1. Parallel lines with distance $a$ in the plane;
2. Tossing a needle of length $l$ ($l < a$) randomly;
3. What is the probability of intersection?

Figure: Schematics for Buffon’s needle problem.
Buffon’s needle problem

Solution. This is a geometric probability problem. The admissible set is

$$
\Omega := \{0 \leq x \leq \frac{a}{2}, 0 \leq \phi \leq \pi\}.
$$

The set of intersection is

$$
G = \{x \leq \frac{l}{2}\sin \phi\},
$$

then the probability of intersection

$$
P = \frac{\text{meas}(G)}{\text{meas}(\Omega)} = \left(\int_{0}^{\pi} \frac{l}{2}\sin \phi d\phi\right) / \left(\frac{a\pi}{2}\right) = \frac{2l}{a\pi},
$$

thus

$$
\pi = \frac{2l}{aP}.
$$
Buffon’s needle problem

Another choice (taking into account more symmetry):

\[ \Omega := \left\{ 0 \leq x \leq \frac{a}{2}, 0 \leq \phi \leq \frac{\pi}{2} \right\}. \]

and

\[ G = \left\{ x \leq \frac{l}{2} \sin \phi \right\}, \]

we also have

\[ P = \frac{2l}{a\pi}. \]
Monte Carlo integration

Numerically solve

\[ I(f) = \int_0^1 f(x) \, dx. \]

▶ Midpoint rule:

\[ I_N^{(1)}(f) = h \sum_{i=1}^{N} f(x_i), \quad h = \frac{1}{N}, \quad x_i = (i + \frac{1}{2})h \]

Accuracy: \( O(h^2) \).
Monte Carlo integration

- Monte Carlo:

\[ I_N^{(2)}(f) = \frac{1}{N} \sum_{i=1}^{N} f(X_i), \quad X_i \sim \text{i.i.d. } U[0, 1] \]

One has \( \mathbb{E} I_N^{(2)}(f) = I(f) \), and the mean square error

\[
\mathbb{E} |e_N|^2 = \mathbb{E} \left( I_N^{(2)}(f) - I(f) \right)^2 = \mathbb{E} \left( \frac{1}{N} \sum_{i=1}^{N} (f(X_i) - I(f)) \right)^2
\]

\[
= \frac{1}{N^2} \sum_{i,j=1}^{N} \mathbb{E} (f(X_i) - I(f))(f(X_j) - I(f))
\]

\[
= \frac{1}{N} \mathbb{E} (f(X_i) - I(f))^2 = \frac{1}{N} \text{Var}(f),
\]

One obtains \( e_N \sim \sqrt{\frac{\text{Var}(f)}{N}} \sim O(h^{1/2}) \) — half order convergence.

Question: How to generate \( X_i \)?
Monte Carlo integration

High dimensional case:

- Ensemble average in statistical mechanics

$$\langle A \rangle = \frac{1}{Z} \int_{R^{6N}} A(x) e^{-\beta H(x)} dx$$

where $Z = \int_{R^{6N}} e^{-\beta H(x)} dx$ is partition function, $\beta = (k_B T)^{-1}$, $k_B$ is Boltzmann constant, $T$ is the absolute temperature, $dx = dx_1 \cdots dx_N dp_1 \cdots dp_N$, $N$ is the number of particles.
Monte Carlo integration

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- Deterministic quadrature: 10 segments in each direction, totally \( 10^6N \) nodes!

- Monte Carlo method is the only viable approach!
Monte Carlo integration

Deterministic vs. Stochastic approach, which is better?

- Estimate of computational effort:

  Dimension — \( d \), number of quadrature points — \( N \)

  Midpoint rule \( \sim O(N^{-\frac{d}{2}}) \), Monte Carlo \( \sim O(N^{-\frac{1}{2}}) \).

  If \( d > 4 \), Monte Carlo is better.
Monte Carlo integration

Brief summary:

▶ The advantage of Monte Carlo:

[Half order convergence independent of dimensions; Parallel essentially; Versatile: If we can find a probabilistic interpretation of a problem, we can apply MC.]

▶ The disadvantage of Monte Carlo:

[Half order convergence (slow convergence); Noisy result.]
Monte Carlo integration

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Randomized linear algebra

Problem setup: Compute the matrix product

$$C = AB,$$

where $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{n \times p}$, and assume $n \gg 1$. When $n$ is huge, which is possible in many applications in big data, the following randomized matrix multiplication was proposed.
Randomized linear algebra

Given any probability distribution \( \{p_i\} \), where \( p_i > 0 \) and \( \sum_{i=1}^{n} p_i = 1 \), randomly pick \( K \) columns with the \( i_m \)th column from \( A \), \( L^{(m)} \) and the \( i_m \)th row from \( B \), \( R^{(m)} \) according to \( \{p_i\} \). Correspondingly define

\[
L^{(m)} = \frac{1}{\sqrt{K p_{i_m}}} A_{\cdot,i_m}, \quad R^{(m)} = \frac{1}{\sqrt{K p_{i_m}}} B_{i_m,\cdot}, \quad m = 1, \ldots, K
\]

then compute

\[
C \approx \sum_{m=1}^{K} L^{(m)} R^{(m)}.
\]  

Does it work? Is it possible to generalize and improve it?
Bayesian methods in statistical learning

**Problem:** Sampling the posterior distribution of the unknown parameters $\theta$.

- In statistics, we have large amount of sampling data, and we want to extract the parameters from some type of probabilistic model.
Bayesian methods in statistical learning

Problem: Sampling the posterior distribution of the unknown parameters $\theta$.

▶ In statistics, we have large amount of sampling data, and we want to extract the parameters from some type of probabilistic model.

▶ Suppose we have the likelihood function

$$L(\theta|x), \quad \theta \in \Theta,$$

and the prior distribution of the parameter $\theta$ is $\pi(\theta)$, we would like to sample the posteriori distribution of $\theta$

$$\pi(\theta|x) \propto L(\theta|x)\pi(\theta)$$

or compute the expectation of the parameters.
Bayesian methods in statistical learning

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- Suppose we have the *likelihood* function

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or compute the expectation of the parameters.

- Usually $\theta$ is in a high dimensional space, and $\pi(\theta|x)$ is only known up to a constant.
Bayesian methods in statistical learning

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- Suppose we have the likelihood function

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\]

and the prior distribution of the parameter \( \theta \) is \( \pi(\theta) \), we would like to sample the posteriori distribution of \( \theta \)

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\]

or compute the expectation of the parameters.
- Usually \( \theta \) is in a high dimensional space, and \( \pi(\theta|x) \) is only known up to a constant.
- We need the Monte Carlo sampling method here.
Simulated annealing for optimization

Problem: $\min_x H(x)$, $H(x)$ is an energy function.

- If $H(x)$ is convex, the problem is quite easy by steepest decent method

$$\frac{dx}{dt} = -\nabla H$$

- If $H(x)$ is non-convex, the problem is complicated. The solution by steepest descent will fall into a local minimum generally.

Introduce thermal noise

$$\frac{dx}{dt} = -\nabla H + \epsilon \dot{w}$$

$\epsilon \sim$ temperature. Let $\epsilon \to 0$ with suitable speed, one can achieve the global minimum.
Simulated annealing for optimization

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\( \epsilon \sim \text{temperature} \). Let \( \epsilon \to 0 \) with suitable speed, one can achieve the global minimum.
Kinetic Theory

Problem: Dynamics of harmonic oscillator with random forcing.

- How to describe the noise mathematically? (Potential $U(x) = \frac{1}{2} k x^2$)
Kinetic Theory

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- Conservative harmonic oscillator

\[
\begin{align*}
\dot{x} &= v \\
$m\dot{v}$ &= $-kx$
\end{align*}
\]
Kinetic Theory

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- Frictional harmonic oscillator (frictional coefficient $\gamma$)

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▶ Frictional harmonic oscillator (frictional coefficient $\gamma$)

\[
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\end{aligned}
\]

▶ White noise forcing (mesoscopic particles)

\[
\begin{aligned}
\dot{x} &= v \\
\dot{v} &= -\gamma v - kx + \sqrt{2k_B T \gamma } \dot{w}
\end{aligned}
\]

$\dot{w}$ is the temporal white noise. How to define $w$?
First exit time — Connection with PDEs

Solving the elliptic PDE

\[
\begin{align*}
\Delta u &= 0 & \text{in } D \\
u &= f & \text{on } \partial D
\end{align*}
\]

- Traditional method: FEM, FD
First exit time — Connection with PDEs

Solving the elliptic PDE

\[
\begin{cases}
\Delta u = 0 & D \\
\left. u \right|_{\partial D} = f & \partial D
\end{cases}
\]

- Traditional method: FEM, FD
- Stochastic formulation

\[ u(x) = \mathbb{E}(f(X_{\tau_D})) \]

where \( X_{\tau_D} \) is the first exit point form \( \partial D \) of the Brownian motion starting at \( x \in D \).
First exit time — Connection with PDEs

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u(x) = \mathbb{E}(f(X_{\tau_D}))
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where \(X_{\tau_D}\) is the first exit point form \(\partial D\) of the Brownian motion starting at \(x \in D\).

- One can compute the value of \(u\) at any point in \(\Omega\) separately.
Particle system —- Mckean-Vlasov equation

Problem: Particle system — Macroscopic behavior from microscopic movements

▸ Deterministic case (without interaction): Liouville equation.
\[
\frac{d\mathbf{x}_i}{dt} = b(x_i) \quad \rightarrow \quad \psi_t + \nabla \cdot (b\psi) = 0
\]

▸ Stochastic case (without interaction): Fokker-Planck equation.

▸ Stochastic case (with interaction): Mckean-Vlasov equation.
\[
\frac{d\mathbf{x}_i}{dt} = \frac{1}{N} \sum_{j=1}^{N} b(x_i - x_j) + \dot{w}_i \quad \rightarrow \quad \psi_t + \nabla \cdot (U\psi) = \frac{1}{2} \Delta \psi
\]
where
\[
U = \int b(x - y) \psi(y) dy
\]
Particle system — Mckean-Vlasov equation

**Problem:** Particle system — Macroscopic behavior from microscopic movements

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  \frac{dx_i}{dt} = b(x_i) \rightarrow \psi_t + \nabla \cdot (b\psi) = 0
  \]

- **Stochastic case (without interaction):** Fokker-Planck equation.
  \[
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**Problem:** Particle system — Macroscopic behavior from microscopic movements

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\]

- **Stochastic case (with interaction):** McKeane-Vlasov equation.

\[
\frac{dx_i}{dt} = \frac{1}{N} \sum_{j=1}^{N} b(x_i - x_j) + \dot{w}_i \rightarrow \psi_t + \nabla \cdot (U\psi) = \frac{1}{2} \Delta \psi
\]

where \( U = \int b(x - y)\psi(y)dy. \)
Traditional modeling of chemical reaction: reaction rate equation (RRE):

\[
\frac{dx}{dt} = a(x)
\]

where \(x\) is the concentration of the reactants, \(a\) is the reaction rate.
Traditional modeling of chemical reaction: reaction rate equation (RRE):

\[ \frac{dx}{dt} = a(x) \]

where \( x \) is the concentration of the reactants, \( a \) is the reaction rate.

In biological reactions, the population of some species are very few. The concept concentration does not make any sense there. The reaction also shows the random character. How to model the chemical reaction kinetics?
Diffusion-Limited Aggregation (DLA) model

Fractal growth of crystallization.

Figure: DLA model. Adapted from PRL 47(1981), 1400.
Complex fluids

Complex fluids: Such as the suspensions, colloids and liquid crystals, etc.

Figure: Schematics of flexible, semi-flexible and rigid polymers.

How to describe the behavior of the fluids through describing the polymers?
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Course plan

The following topics will be covered in this course:

- Generation of pseudo random variables,
- Variance reduction methods,
- Simulated annealing and quasi-Monte Carlo,
- Large deviation principle,
- Metropolis algorithm (Markov chain Monte Carlo method),
- Multilevel sampling and kinetic MC,
- Wiener Process and its construction,
- Stochastic differential equations and Ito’s formula,
- Fokker-Planck equation and diffusion process,
- Numerical solution of SDEs,
- Path integral methods and Girsanov transformation,
- Applications in material science (rare events),
- Applications in biology,
- Applications in networks,
- Applications in fluids.

We will have 2 numerical projects which will account for 15 pts. The homeworks will account for 15 pts, and the final exam will
Course plan

We will have 2 numerical projects which will account for 15 pts. The homeworks will account for 15 pts, and the final exam will account for 70 pts.
Main references

▶ P.E. Kloeden and E. Platen, Numerical Solution of Stochastic Differential Equations, Springer-Verlag, Berlin and Heidelberg,
TA Info

TA information:

Qiangwei Peng, qiangwei_peng@stu.pku.edu.cn

The HW will be collected on Monday per two weeks.