PDE and Boundary-Value Problems
Winter Term 2014/2015

Lecture 21

Saarland University

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Purpose of Lesson

- To explain the basic philosophy of Monte Carlo methods and suggest how they can be used to solve various problems.
- To show how random games (Monte Carlo methods) can be designed whose outcomes approximate solutions to differential equations. A specific game (tour du wino) is described whose outcome is the finite-difference approximation to a Dirichlet problem inside a square. The game is extended to include solutions to other problems as well.

Monte Carlo Methods (an Introduction)

- The basic idea here is that games of chance can be played (generally on a computer) whose outcomes approximate solutions to real-word problems.
- First of all Monte Carlo methods are procedures for solving nonprobabilistic-type problems (problems whose outcome does not depend on chance) by probabilistic-type methods (methods whose outcome depends on chance).
- The general philosophy of Monte-Carlo methods is illustrated on the next page.

Probabilistic game

The outcome of the game $\hat{p}$

(Like the fraction of heads in tossing a coin, throwing darts, and so forth)

Deterministic problem

The answer to the problem is p

(Like evaluation an integral, solving a PDE, and so forth)

$$\text{Outcome} = \hat{p} \xrightarrow[\text{Approximation}]{} \text{Answer} = p$$

Evaluating an Integral

- To illustrate the method, suppose we wanted to evaluate the integral
$$I = \int_a^b f(x)dx$$
(a nonprobabilistic problem).
- To use the Monte Carlo method, we would devise a game of chance whose outcome was the value of the integral (or approximates the integral).
- There are, of course, many games that we could devise; the actual game we used would depend on the accuracy of the approximation, simplicity of the game, and so on.

Evaluating an Integral (cont.)

- An obvious game to evaluate the integral would be throwing darts at the rectangle

$$R = \{(x, y) : a \leqslant x \leqslant b, 0 \leqslant y \leqslant \max f(x)\}.$$

- It's fairly obvious that if we randomly toss 100 or so darts at the rectangle R enclosing the graph, then the fraction of darts hitting below the curve times the area of R will estimate the value of the integral.

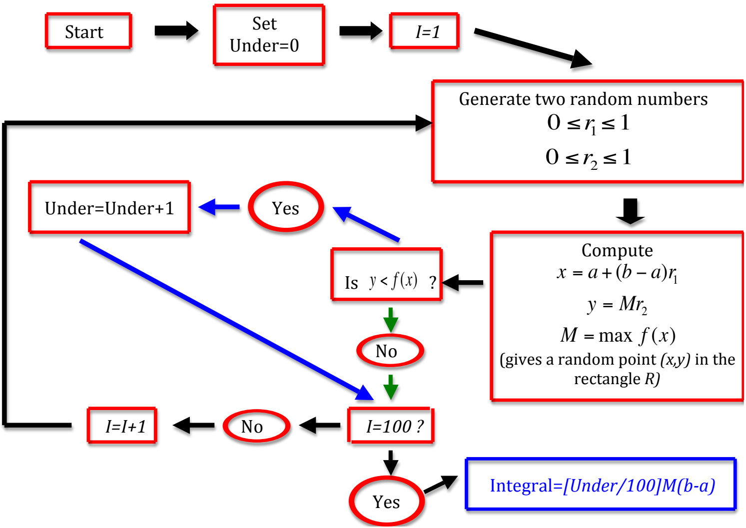
- Hence, our outcome of the game

$$\widehat{I} = [\text{fraction of tosses under } f(x)] \times (\text{area of } R)$$

is used to estimate the true value of the integral I.

Evaluating an Integral (cont.)

- To carry out the actual computation on a computer, we would have to generate the sequence of random points in some way (we'll discuss this shortly) and have the computer play the dart tossing game.
- Let us assume for the time being that we have a sequence of random points. The flow diagram on the next page illustrates how the computer would attack this problem. (See flow diagram to evaluate $\int_a^b f(x)dx$ by the Monte Carlo method (100 tosses)).


Start
Set Under=0
I=1
Generate two random numbers
$0 \le r_1 \le 1$
$0 \le r_2 \le 1$
Compute
$x = a + (b - a) r_1$
$y = M r_2$
$M = \max f(x)$
(gives a random point (x,y) in the rectangle R)
Is $y < f(x)$?
Yes
Under=Under+1
No
I=100 ?
No
I=I+1
Yes
Integral=[Under/100]M(b-a)

Random Numbers

- Before going on to apply this technique to the solution of PDEs, we discuss the important topic of random numbers.
- In the integral just considered, it was necessary to generate a sequence of random points $P_i = (x_i, y_i)$ that fell inside rectangle R. In other words, the x-coordinate would have to be a random number in the interval $[a, b]$, while y_i must be in $[0, M]$.

Random Numbers (cont.)

- To find random numbers inside specific intervals, we start with a basic sequence of random numbers r_i (uniformly distributed) inside $[0, 1]$.
- It's obvious then that if we want a random number x_i inside $[a, b]$, we just compute
$$x_i = a + (b - a)r_i$$
- So everything comes down to the question, how do we generate a sequence of random numbers $\{r_i, i = 1, 2, \dots\}$ uniformly distributed in $[0, 1]$.

Residue Algorithm for Generating Random Numbers

To generate a sequence of random integers (between 0 and P), we use the residue algorithm.

1. Pick the first random integer any way you like between 0 and P (P was picked in advance).
2. Multiply this random integer by some fixed integer M (picked in advance).
3. Add to that product another fixed integer K (picked in advance).
4. Divide the resulting sum by P and pick the remainder as the new random integer. Now go back to step 2 and repeat steps 2-4 until you have enough random integers.

- This residue algorithm can be written as

$$r_{i+1} \equiv (Mr_1 + K) \bmod P \qquad i = 0, 1, 2, \ldots$$

which says, if we are given a random integer r_i, then to compute a new one r_{i+1}, we multiply by M, add K, divide by P, and pick the remainder.

Remarks

- If we choose, for example, $P = 100$ in our random-number generator, the remainders will be one of the integers $0, 1, 2, \ldots, 99$, and, hence, our entire process will start repeating before long.
- In fact, our random numbers might be

$$15,\ 71,\ 43,\ 7,\ 43,\ 7,\ 43,\ 7, \qquad \text{(Cycle of two numbers)}$$

  and, hence, our method is no good.
- The ideal situation is to generate the entire residue class $\{0, 1, 2, \ldots, 99\}$ in a random fashion before starting to repeat.

Remarks (cont.)

- It can be proven mathematically that if the numbers M, K, and P are chosen according to certain rules, then no matter how we pick the first random number r_0, the algorithm will generate the entire residue class.
- So, if we pick P very large (like 2^{40}), we are assured that (for practical purposes) the process will never repeat.
- It is possible to generate random samples from various statistical distributions other than the uniform distribution $f(x) = 1$, $0 < x < 1$ (the usual random-generator).
- Computer programs are available to generate random samples from the binomial, gamma, normal, and many other distributions.

Monte Carlo Solution of PDEs

We show how we can design a game to approximate solution of the Dirichlet problem:

Problem 21-1

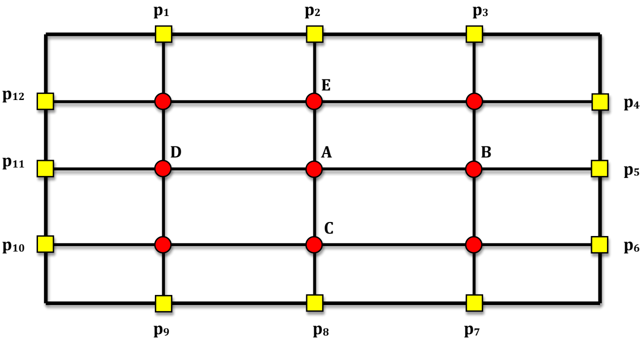
To find a function $u(x, y)$ that satisfies

$$\text{PDE:} \quad u_{xx} + u_{yy} = 0, \qquad 0 < x < 1, \quad 0 < y < 1$$

$$\text{BC:} \quad u(x, y) = g(x, y) = \begin{cases} 1, & \text{On the top of the square} \\ 0, & \text{On the sides and} \\ & \text{bottom of the square} \end{cases}$$

To illustrate the Monte Carlo method in this problem, we introduce a game called tour du wino. To play it, we need a board on which grid lines are drown (see next page).

Board for tour du wino



A = starting points for game

= interior grid points

= end points p_i

g_i = reward for ending at p_i

How Tour du Wino is Played

1. The wino starts from an arbitrary point (point A in our case).
2. At each stage of the game, the wino staggers off randomly to one of the four neighboring points. (In our case, the neighbors of A are B, C, D and E, and the probability of going to each of these neighbors is $1/4$.
3. After arriving ata neighboring point, the wino continues this process wandering from point to point until eventually hitting a boundary point p_j. He then stops, and we record that point p_i. This completes one random walk.

How Tour du Wino is Played (cont.)

4. We repeat steps 1-3 until many random walks are completed. We now compute the fraction of times the wino had ended up at each of the boundary points p_i.

5. Suppose the wino receives a reward g_i (g_i is the value of the BC at p_i) if he ends his walk at the boundary point p_i, and suppose that the goal of the game is to compute his average reward $R(A)$ for all this walks. The average reward is

$$R(A) = g_1 P_A(p_1) + g_2 P_A(p_2) + \cdots + g_{12} P_A(p_{12})$$

The game is completed with the determination of $R(A)$.

Probability of Random Walk Ending at p_i

Boundary point p_i	$P_A(p_i)$ = fraction of times the wino ends at p_i	g_i = reward for ending at p_i
1	0.04	1
2	0.15	1
3	0.03	1
4	0.06	0
5	0.17	0
6	0.05	0
7	0.06	0
8	0.15	0
9	0.03	0
10	0.06	0
11	0.16	0
12	0.04	0

Reason for Playing Tour du Wino

It turns out that the average reward is the approximate solution to our Dirichlet problem at Point A. This interesting observation is based on two facts.

1. Suppose the wino started at a point A that was on the boundary of the square. Each resulting random walk ends immediately at that point, and the wino collects the amount g_i. Thus, his average reward for starting from a boundary point is also g_i.

2. Now suppose the wino starts from an interior point. Then, the average reward $R(A)$ is clearly the average of the four average rewards of the four neighbors

$$R(A) = \frac{1}{4}\left[R(B) + R(C) + R(D) + R(E)\right]$$

- We ask why the wino's average reward $R(A)$ approximates the solution of the Dirichlet problem at A. We have seen that $R(A)$ satisfies two equations

$$R(A) = \frac{1}{4}\left[R(B) + R(C) + R(D) + R(E)\right] \quad (A \text{ an interior point})$$
$$R(A) = g_i \qquad (A \text{ a boundary point})$$

- If we let g_i be the value of the boundary function $g(x, y)$ at the boundary point p_i, then our two equations are exactly the two equations we arrived at when we solved the Dirichlet problem by the finite-difference method.

- That is, $R(A)$ corresponds to $u_{i,j}$ in the finite-difference equations

$$u_{i,j} = \frac{1}{4}\left(u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1}\right) \quad (i,j) \text{ an interior point}$$
$$u_{i,j} = g_{i,j} \quad g_{i,j} \text{ the solution at a boundary point } (i,j)$$

- Hence, $R(A)$ will approximate the true solution of the PDE at A.

Solution of Laplace's Equation by the Monte Carlo Method

These rules give the solution at one point inside the square.

1. Generate several random walks starting at some specific point A and ending once you hit a boundary point. Keep track of how many times you hit each boundary point.
2. After completing the walks, compute the fraction of times you have ended at each point p_i. Call these fractions $P_A(p_i)$.
3. Compute the approximate solution $u(A)$ from the formula

$$u(A) = g_1 P_A(p_1) + g_2 P_A(p_2) + \cdots + g_N P_A(p_N)$$

where g_i is the value of the function at p_i and N is the number of boundary points.

Solution to a Dirichlet Problem with Variable Coefficients

The game tour du wino can be modified to solve more complicated problems, as in the following example.

Problem 21-2

To find a function $u(x, y)$ that satisfies

$$\text{PDE:} \quad u_{xx} + (\sin x)\, u_{yy} = 0, \quad 0 < x < \pi, \quad 0 < y < \pi$$

$$\text{BC:} \quad u(x, y) = g(x, y) \qquad \text{on the boundary of the square}$$

- To solve Problem 21-2, we replace u_{xx}, u_{yy} and $\sin x$ by

$$\begin{aligned} u_{xx} &= \left[u_{i,j+1} - 2u_{i,j} + u_{i,j-1}\right]/h^2 \\ u_{yy} &= \left[u_{i+1,j} - 2u_{i,j} + u_{i-1,j}\right]/k^2 \\ \sin x &= \sin x_j \end{aligned}$$

  and plug them into the PDE.

- Making these substitutions and solving for $u_{i,j}$ gives

$$u_{i,j} = \frac{u_{i,j+1} + u_{i,j-1} + \sin x_j \left(u_{i+1,j} + u_{i-1,j}\right)}{2(1 + \sin x_j)} \tag{21.1}$$

- Look carefully at (21.1). The coefficients of $u_{i+1,j}$, $u_{i-1,j}$, $u_{i,j+1}$, and $u_{i,j-1}$ are positive and sum to one. In other words, $u_{i,j}$ is a weighted average of the solutions at the four neighboring points.
- Hence, we modify our game so that the wino doesn't stagger off to each neighbor with probability $1/4$, but, rather, with a probability equal to the coefficients of the respective term.

- In other words, if the wino is at the point (i, j), he then goes to the point:

$$
\begin{aligned}
(i, j+1) \text{ with probability } & \frac{1}{2(1+\sin x_J)} \\
(i, j-1) \text{ with probability } & \frac{1}{2(1+\sin x_J)} \\
(i+1, j) \text{ with probability } & \frac{\sin x_j}{2(1+\sin x_J)} \\
(i-1, j) \text{ with probability } & \frac{\sin x_j}{2(1+\sin x_J)}
\end{aligned}
$$

- Other than this slight modification, the game is exactly the same as before.

Remarks

- Observe that once the fractions $P_A(p_i)$ (the fraction of times the wino ends at p_i) are computed, we can then find the solution $u(A)$ for any other boundary conditions g_i just by plugging the $P_A(p_i)$ into the formula

$$u(A) = g_1 P_A(p_1) + g_2 P_A(p_2) + \cdots + g_N P_A(p_N).$$

  That is, we don't have to recompute new random walks.

- In many cases, a researcher wants to find the solution of a PDE at only one point. If the boundary is fairly complicated and if the PDE involves 3 or 4 dimensions, then Monte Carlo methods may come to rescue.

Remarks (cont.)

- In fact, Monte Carlo methods were originally developed to study difficult neutron-diffusion problems that were impossible to solve analytically.