Partial Differential Equation Solving, vol 2.

Marcin Chrząszcz
mchrzasz@cern.ch

University of Zurich[UZH]

Monte Carlo methods,
12 May, 2016

Announcement

There will be no lectures and class on 19^{th} of May

Dirichlet conditions:expected number of steps

⇛ find the function $u(x_1, x_2, ..., x_k)$ such that if fulfils the Laplace equation:

$$\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} + ... + \frac{\partial^2 u}{\partial x_k^2} = 0, \quad (x_1, x_2, ..., x_k) \in D \subset \mathbb{R}^k$$

In the domain D, on the the $\Gamma(D)$ the u function is given by:

$$U(x_1, x_2, ..., x_k) = f(x_1, x_2, ..., x_k), \quad (x_1, x_2, ..., x_k) \in \Gamma(D)$$

⇛ Now lets assume that the domain D is a hyperball:

$$0 \leqslant \sum_{i=1}^{k} x_i^2 \leqslant r^2, \quad r = \mathrm{const}$$

⇛ Now $\pi_\nu(x_1, x_2, ..., x_k)$ is a probability that a particle starting from $(x_1, x_2, ..., x_k)$ will end up on the edge after ν steps. The $\kappa(x_1, x_2, ..., x_k)$ is the estimated number of steps for this trajectory.

$$\pi_0 = \begin{cases} 1, & (x_1, x_2, ..., x_k) \in \Gamma(D) \\ 0, & (x_1, x_2, ..., x_k) \in D \end{cases} \tag{1}$$

$$\pi_\nu = \frac{1}{2k} \sum{}' \pi_\nu(x_1{\prime}, x_2{\prime}, ..., x_k{\prime})$$

Dirichlet conditions:expected number of steps

⇛ From Eq. 1 and 2 one gets:

$$\kappa(x_1, x_2, ..., x_k) = \sum_{\nu=1}^{\infty} \nu \pi_\nu (x_1, x_2, ..., x_k)$$

one gets:

$$\kappa(x_1, x_2, ..., x_k) = \frac{1}{2k} \sum_{\nu=1}^{\infty} \left[\nu \sum{}' \pi_{\nu-1}(x_1, x_2, ..., x_k) \right]$$

$$= \frac{1}{2k} \sum_{\nu=1}^{\infty} \left[(\nu-1) \sum{}' \pi_{\nu-1}(x_1\prime, x_2\prime, ..., x_k\prime) \right] + \frac{1}{2k} \sum_{\nu=1}^{\infty} \sum{}' \pi_{\nu-1} x_1\prime, x_2\prime, ..., x_k\prime)$$

⇛ From which we get:

$$\kappa(x_1, x_2, ..., x_k) = \frac{1}{2k} \sum{}' \kappa(x_1\prime, x_2\prime, ..., x_k\prime) + 1$$

⇛ Now this is equivalent of the Poisson differential equation:

$$\frac{\partial^2 \kappa}{\partial x_1^2} + \frac{\partial^2 \kappa}{\partial x_2^2} + ... + \frac{\partial^2 \kappa}{\partial x_k^2} = -2k, \text{ b. con. } \kappa(x_1, x_2, ..., x_k) = 0, \quad (x_1, x_2, ..., x_k) \in \Gamma(D)$$

Dirichlet conditions:expected number of steps

$\Rightarrow$ From previous equation: $\kappa(x_1, x_2, ..., x_k) = \psi(x_1, x_2, ..., x_k) - \sum_{i=1}^{k} x_i^2$ we get the for the ψ function the Laplace equation:

$$\frac{\partial^2 \psi}{\partial x_1^2} + \frac{\partial^2 \psi}{\partial x_2^2} + ... + \frac{\partial^2 \psi}{\partial x_k^2} = 0$$

because on the border ($\Gamma(D)$):

$$\psi(x_1, x_2, ..., x_k) = r^2 = \text{const}$$

so also inside the D: $\psi(x_1, x_2, ..., x_k) = r^2 = \text{const}$ $\Rightarrow$ From which we can estimate the number steps in the random walk:

$$\kappa(x_1, x_2, ..., x_k) = r^2 - \sum_{i=1}^{k} \leqslant r^2$$

Important conclusion:

The expected number of steps in the random walk (the time of walk) from the point $(x_1, x_2, ..., x_k)$ till the edge od the domain can be estimated by r number (the LINEAR! size). It is completly independent of the k!

Dirichlet conditions as linear system

⇛ In the discrete form we can write the Dirichlet conditions as (2-dim case):

$$u(x,y) = \frac{1}{4}\left[u(x-1,y) + u(x+1,y) + u(x,y-1) + u(x,y+1)\right], \quad (x,y) \in D$$
$$u(x,y) = f(x,y), \quad (x,y) \in \Gamma(D)$$

⇛ Now we can order the grid ($(x,y) \in D \cup D$), we can represente the above equations as a linear system:

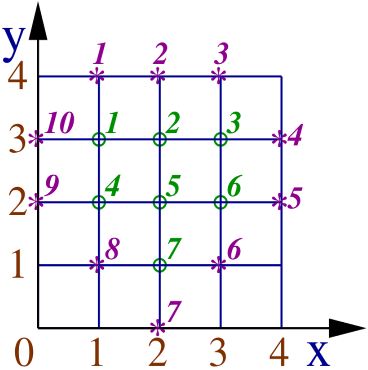
$$u_i = a_i + \sum_{j=1}^{n} h_{ij} u_j, \quad i = 1, 2, ..., n$$

The trick:

So to solve a differential equation with Dirichlet boundary condition we can use all the methods of solving linear equation systems such as Neumann-Ulam or Wassow.

Dirichlet conditions as linear system - example

- To do this we act as following: we number separately the points inside the D domain and on the border $\Gamma(D)$.
- We write for each point inside the domain the Laplace equation as system of linear equations:



$$
\begin{array}{llllllll}
u_1 & -u_2/4 & & -u_4/4 & & & & = (f_1 + f_{10})/4 \\
-\,u_1/4 & u_2 - u_3/4 & & -\,u_5/4 & & & & = (f_2)/4 \\
& -u_2/4 \quad u_3 & & & -u_6/4 & & & = (f_3 + f_4)/4 \\
-\,u_1/4 & & & u_4 - u_5/4 & & & & = (f_8 + f_9)/4 \\
-\,u_1/4 & & & -u_4/4 \quad u_5 & -u_6/4 - u_7/4 & & & = 0 \\
& -\,u_3/4 & & -\,u_5/4 & u_6 & & & = (f_5 + f_6)/4 \\
& & & -\,u_5/4 & & u_7 & & = (f_5 + f_6)/4
\end{array}
$$

Dirichlet conditions as linear system - example

$\Rrightarrow$ The above equation we can transform the above equation into the iterative representation:

$$\overrightarrow{u} = \overrightarrow{a} + \mathbf{H}\overrightarrow{u}$$

where $\overrightarrow{u} = (u_1, u_2, ..., u_7)$ is the vector which represent the values of the function inside the D domain, $\overrightarrow{a}$ is the linear combinations of the boundary values. In our example:

$$\mathbf{H} = \begin{pmatrix} 0 & \frac{1}{4} & 0 & \frac{1}{4} & 0 & 0 & 0 \\ \frac{1}{4} & 0 & \frac{1}{4} & 0 & \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 & 0 & \frac{1}{4} & 0 \\ \frac{1}{4} & 0 & 0 & 0 & \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{4} & 0 & \frac{1}{4} & 0 & \frac{1}{4} & \frac{1}{4} \\ 0 & 0 & \frac{1}{4} & 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{4} & 0 & 0 \end{pmatrix}$$

$\Rrightarrow$ To find the solution to aka $\overline{u}$ one can use the methods we already know: Neumann-Ulam and Wasow, etc.

$\Rrightarrow$ There are tricks and tips one can use to make this problem faster as each of the entry is $\frac{1}{4}$.

Neumann-Ulam method

⇛ We put the particle in (x, y).
⇛ We observe the trajectory of the particle until it reaches the boundary. Point P_k is the last point before hitting the boundary.
⇛ For each trajectory we assign a value that the arithmetical mean of the boundary points that are neighbours of the point P_k.
⇛ We repeat the above n times and calculate the mean.
⇛ The example solution for 20 trajectories:

$$u(2,2) = 1.0500 \pm 0.2756$$

⇛ E 10.1 Solve the above linear system using the Neumann-Ulam method for an assumed boundary conditions.

Dual Wasow method

⇛ We choose the boundary conditions with arbitrary chosen probability p.d.f. $p(Q)$ the starting point.
⇛ We choose with equal probability the point inside D where the particle goes.
⇛ With equal probability we choose the next positions and so on until the particle hits the boundary in the point Q'.
⇛ We count all trajectories $N((x_1, x_2, x_3, ..., x_k)$ that that have passed the point $(x_1, x_2, x_3, ..., x_k)$.
⇛ For the point $(x_1, x_2, ..., x_k)$ we calculate:

$$w(x_1, x_2, ..., x_k) = \frac{1}{2k} N(x_1, x_2, ..., x_k) \frac{f(Q)}{p(Q)}$$

⇛ The above steps we repeat N times.
⇛ After that we take the arithmetic mean of w.

Random walk with different step size

$\Rrightarrow$ If $u(x,y)$ is a harmonic function that obeys the Laplace equation and $S_r(x,y)$ is a circle in with the middle point (x,y) and radius r. Then a theorem states:

$$S_r(x,y) = \frac{1}{2\pi}\int_0^{2\pi} u(x + r\cos\phi, y + r\sin\phi)d\phi$$

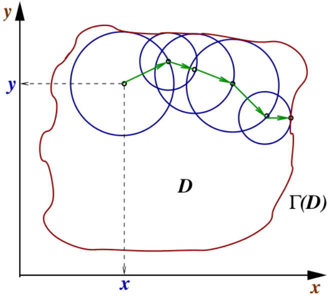
$\Rrightarrow$ The above is true for in all the dimensions.
$\Rrightarrow$ The E.Muller method:

- At the begging we set the point in the initial point: $(x_1, x_2, ..., x_k)$.
- We construct a k dimensional sphere with center $(x_1, x_2, ..., x_k)$ and radius r. The r has to be choosen in a way that the whole is inside the D: $S_r(\overrightarrow{x}) \in D$. We choose a random point from $\mathcal{U}(0, 2\pi)$ on the sphere which is our new point.
- We stop the walk when the point is on $\Gamma(D)$.

$\Rrightarrow$ We repeat this N times.
$\Rrightarrow$ The final result if the arithmetical mean of all trajectories and is equal of the $u(x_1, x_2, ..., x_k)$.

Muller method

⇛ The method is faster the faster the particle reaches the edge.
⇛ In order to do so we choose the radius that it is the maximal one that allows the sphere to be inside the domain D.



⇛ There is a problem!!!! The probability that we choose a point on the edge is 0!!!!
⇛ An approximation has to be made: we choose a small number δ and we consider that the particle reached the border when the distance is with δ.
⇛ We can always choose the δ such that the estimator error of function is smaller then a given ϵ.

Muller method, example

⇛ An example solution in the

Other boundary conditions

⇛ Find the solution to the Laplace equation:

$$\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} + .. + \frac{\partial^2 u}{\partial x_k^2} = 0, \quad (x_1, x_2, ..., x_k) \in D \subset \mathbb{R}^k$$

inside the D domain if on the edge $\Gamma(D)$ the function fulfils the equation:

$$f(x_1, x_2, ..., x_k)\frac{\partial u(x_1, x_2, ..., x_k)}{\partial n} + g(x_1, x_2, ..., x_k)u(x_1, x_2, ..., x_k) = h(x_1, x_2, ..., x_k)$$

where $\frac{\partial u(x_1,x_2,...,x_k)}{\partial n}$ is there derivative in the direction of normal to the $\Gamma(D)$ in the direction inside D.

⇛ The cases:

- $f = 0$. ⇛ Dirichlet boundary condition (1st class condition).
- $g = 0$. ⇛ Neumann boundary condition (2nd class condition).
- others. ⇛ General case (3rd class condition).

Other boundary conditions

⇛ In 2-dim:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0, \quad (x, y) \in D \subset \mathbb{R}^2$$

with the boundary condition:

$$f(x, y)\frac{\partial u(x, y)}{\partial n} + g(x, y)u(x, y) = h(x, y), \quad (x, y) \in \Gamma(D)$$

⇛ And the discrete differential equation:

$$u(x, y) = \frac{1}{4}\left[u(x-h, y) + u(x+h, y) + u(x, y-h) + u(x, y+h)\right]$$

Reminder:

If at moment t the point is in (x, y) then in the $t+1$ time the particle moves with equal probability to one of the following points: $(x-h, y)$, $(x+h, y)$, $(x, y-h)$, $(x, y+h)$.

Random walk for boundary points

⇛ The boundary point Q has only one internal neighbour point P.

- If the normal is parallel to the grid axis in the point Q:

$$f(Q)\frac{u(P)-u(Q)}{h}+g(Q)u(Q)=h(Q)$$

- Solving the above to get $u(Q)$ we get:

$$u(Q)=\frac{f(Q)u(P)}{f(Q)-hg(Q)}-\frac{h(Q)}{f(Q)-hg(Q)}$$

- To help we assign a temporary values:

$$\phi(Q)=\frac{f(Q)}{p\left[f(Q)-hg(Q)\right]},\quad \psi(Q)=-h\frac{h(Q)}{(1-p)\left[f(Q)-hg(Q)\right]}$$

⇛ So:

$$u(Q)=p\phi(Q)u(P)+(1-p)\psi(Q)$$

Random walk for boundary points

⇛ The boundary point Q has only one internal neighbour point P.

- If the normal is parallel to the grid axis in the point Q:

$$f(Q)\frac{u(P)-u(Q)}{h}+g(Q)u(Q)=h(Q)$$

- Solving the above to get $u(Q)$ we get:

$$u(Q)=\frac{f(Q)u(P)}{f(Q)-hg(Q)}-\frac{h(Q)}{f(Q)-hg(Q)}$$

- To help we assign a temporary values:

$$\phi(Q)=\frac{f(Q)}{p\left[f(Q)-hg(Q)\right]},\quad \psi(Q)=-h\frac{h(Q)}{(1-p)\left[f(Q)-hg(Q)\right]}$$

⇛ So:

$$u(Q)=p\phi(Q)u(P)+(1-p)\psi(Q)$$

⇛ Interpretation: $u(Q)$ can be seen that with probability p it is equal $\phi(Q)u(P)$ and with provability $(1-p)$ is equal to $\psi(Q)$.

Backup