

Partial Differential Equation Solving, vol 2.

Marcin Chrzyszcz
mchrzasz@cern.ch



University of
Zurich ^{UZH}

Monte Carlo methods,
12 May, 2016

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

Dirichlet conditions: expected number of steps

⇒ find the function $u(x_1, x_2, \dots, x_k)$ such that it fulfils the Laplace equation:

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

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

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

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

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

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

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

$$\pi_\nu = \frac{1}{2k} \sum_{l=1}^{\nu} \pi_\nu(x_1^l, x_2^l, \dots, x_k^l)$$

Dirichlet conditions: expected number of steps

⇒ From Eq. 1 and 2 one gets:

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

one gets:

$$\begin{aligned} \kappa(x_1, x_2, \dots, x_k) &= \frac{1}{2k} \sum_{\nu=1}^{\infty} \left[\nu \sum_{l=1}^k \pi_{\nu-1}(x_1, x_2, \dots, x_k) \right] \\ &= \frac{1}{2k} \sum_{\nu=1}^{\infty} \left[(\nu-1) \sum_{l=1}^k \pi_{\nu-1}(x_1^l, x_2^l, \dots, x_k^l) \right] + \frac{1}{2k} \sum_{\nu=1}^{\infty} \sum_{l=1}^k \pi_{\nu-1}(x_1^l, x_2^l, \dots, x_k^l) \end{aligned}$$

⇒ From which we get:

$$\kappa(x_1, x_2, \dots, x_k) = \frac{1}{2k} \sum_{l=1}^k \kappa(x_1^l, x_2^l, \dots, x_k^l) + 1$$

⇒ Now this is equivalent of the Poisson differential equation:

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

Dirichlet conditions: expected number of steps

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

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

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

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

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

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

Important conclusion:

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

Dirichlet conditions as linear system

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

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

$$u(x, y) = f(x, y), \quad (x, y) \in \Gamma(D)$$

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

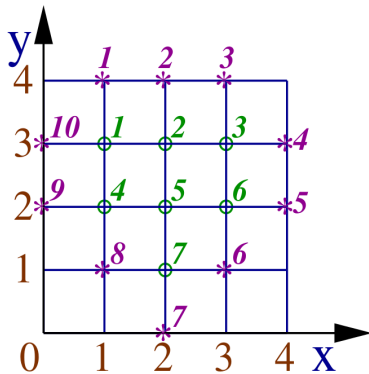
$$u_i = a_i + \sum_{j=1}^n h_{ij} u_j, \quad i = 1, 2, \dots, n$$

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:



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

Dirichlet conditions as linear system - example

⇒ The above equation we can transform the above equation into the iterative representation:

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

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

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

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

⇒ 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 is 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 $N((x_1, x_2, x_3, \dots, x_k))$ that that have passed the point $(x_1, x_2, x_3, \dots, x_k)$.
- ⇒ For the point (x_1, x_2, \dots, x_k) we calculate:

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

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

Random walk with different step size

⇒ 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:

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

⇒ The above is true for in all the dimensions.

⇒ The E.Muller method:

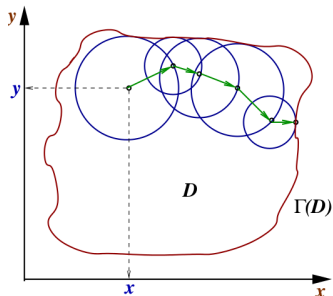
- At the begging we set the point in the initial point: (x_1, x_2, \dots, x_k) .
- We construct a k dimensional sphere with center (x_1, x_2, \dots, x_k) and radius r . The r has to be chosen in a way that the whole is inside the D : $S_r(\vec{x}) \in D$. We choose a random point from $\mathcal{U}(0,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

⇒ We repeat this N times.

⇒ The final result if the arithmetical mean of all trajectories and is equal of the $u(x_1, x_2, \dots, x_k)$.

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 of Laplace equation on square ($0 \leq x \leq 1$, $0 \leq y \leq 1$) with the boundary conditions: $u(0, y) = 1$, $u(1, y) = u(x, 0) = u(x, 1) = 1$

Method	Points (x, y)	N. trajectories	Ave.n.of.steps	Time [s]	Solution
Cons. step $(h = 0.05)$	(0.3, 0.3)	2000	89.87	42.0	0.396
	(0.5, 0.1)	2000	46.05	21.5	0.075
	(0.5, 0.5)	2000	115.83	54.1	0.247
Muller met.	(0.3, 0.3)	2000	6.06	17.9	0.398
	(0.5, 0.1)	2000	6.04	18.0	0.078
	(0.5, 0.5)	2000	5.07	14.5	0.255

Other boundary conditions

⇒ Find the solution to the Laplace equation:

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

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

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

where $\frac{\partial u(x_1, x_2, \dots, x_k)}{\partial n}$ 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:

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

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:

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

⇒ 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:

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

⇒ 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 $\psi(Q)$.

Random walk for boundary points, continued

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

⇒ The algorithm:

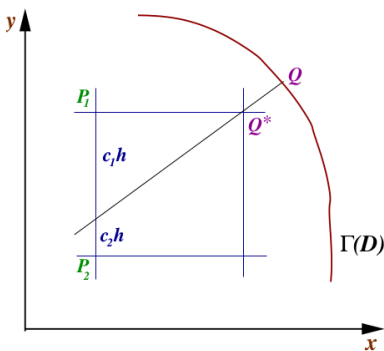
- We start the walk from an internal point (X, Y) and we assign to it a weight: $W = 1$.
- If a particle at a given moment is sitting on the boundary then with probability p it goes back to previous point P and gets a weight $W \cdot \phi(Q)$ and with probability $(1 - p)$ it finishes the walk and gets a weight of $W \cdot \psi(Q)$.
- For each trajectory we assign a value equal to the weight of the last point. So for example if the trajectory: $Q^{(1)}, Q^{(2)}, Q^{(3)}, \dots, Q^{(k)}$ we will assign the number:

$$\phi(Q^{(1)})\phi(Q^{(2)})\phi(Q^{(3)})\dots\phi(Q^{(k-1)})\psi(Q^{(k)})$$

⇒ One again this is only for 1 neighbour point P and that the normal of the boundary is parallel to the grid!

⇒ The general case is more difficult!

More general case



⇒ The boundary conditions:

$$f(Q) \frac{1}{h\sqrt{1+c_1^2}} [c_2u(P_1) + c_1u(P_2) - u(Q^*)] + g(Q)u(Q^*) = h(Q)$$

⇒ The trick:

$$\phi_1(Q^*) = \frac{c_1 f(Q)}{p_1 [f(Q) - h\sqrt{1+c_1^2}]}$$

$$\phi_2(Q^*) = \frac{c_2 f(Q)}{p_2 [f(Q) - h\sqrt{1+c_1^2}]}$$

$$\psi_3(Q^*) = -h \frac{\sqrt{c_1^2 + 1} h(Q)}{p_3 [f(Q) - h\sqrt{1+c_1^2}]}$$

⇒ Putting above new variables we get:

$$u(Q^*) = p_1 \phi_1(Q^*) u(P_1) + p_2 \phi_2(Q^*) u(P_2) + p_3 \psi_3(Q^*)$$

⇒ We will interpret the p_1, p_2, p_3 numbers as probability.

More general case, continuation

⇒ The rules of random walk:

- The particle starts in (X, Y) inside the domain with weight: $W = 1$.
- If at some point in time the particle hits the boundary in point Q^* :
 - With probability p_1 it goes to point P_1 and the weight is $W \cdot \phi_1(Q^*)$
 - With probability p_2 it goes to point P_2 and the weight is $W \cdot \phi_2(Q^*)$
 - With probability p_3 it stops the walk and the weight is $W \cdot \psi(Q^*)$
- For each trajectory we assign the weight at the end point.

Backup