Exercise 1. Neumann boundary conditions and Dirichlet boundary conditions

Let us consider the rectangle $A = [|1, n|] \times [|1, m|]$ in \mathbb{Z}^2 , and its boundary ∂A which is the set of vertices in $\mathbb{Z}^2 \setminus A$ adjacent to a vertex of A. We define the normal derivative at $y \in \partial A$ as:

$$\partial_n f(y) = f(x) - f(y),$$

where x is the unique neighbour of y in A. We denote by $\underline{\partial A}, \partial A|, \overline{\partial A}$ and $|\partial A|$ the 4 parts of the boundary, respectively the lower horizontal, the right most vertical, the upper horizontal and the left-most vertical parts of ∂A .

(1) Prove that the problem

$$\begin{cases} \Delta f(x) = 0 & \text{in } A \\ f(y) = 0 & \text{on } \underline{\partial A} \\ f(y) = 1 & \text{on } \overline{\partial A} \\ \partial_n f(y) = 0 & \text{on } \partial A | \cup |\partial A| \end{cases}$$

has a unique solution if any.

Solution. Let us consider two solutions f and g, then h = f - g is a solution of the problem

$$\begin{cases} \Delta h(x) = 0 & \text{in } A \\ h(y) = 0 & \text{on } \underline{\partial A} \cup \overline{\partial A} \\ \partial_n h(y) = 0 & \text{on } \partial A | \cup |\partial A \end{cases}$$

and we apply the maximum principle: by harmonicity the maximum of h can only be attained on the boundary if h is not constant, but it can not be on $\partial A|\cup|\partial A$ since h(x)=h(y) if $y\in\partial A|\cup|\partial A$ and $y\sim x\in A$. Thus the maximum of h must be attained in A.

(2) Let us consider the simple random walk on $A \cup \partial A$ ($x \in A$ and $y \in \partial A$ are linked by an edge if y is adjacent to x in \mathbb{Z}^2 , two points of ∂A are not linked by an edge). Is $\tau_{\underline{\partial A} \cup \overline{\partial A}}$, the hitting time for $\underline{\partial A} \cup \overline{\partial A}$, finite almost surely?

Solution. Yes since $A \cup \partial A$ is finite, the simple random walk is recurrent, and thus for any $y \in \underline{\partial A} \cup \overline{\partial A}$, τ_y is finite almost surely. This implies that $\tau_{\partial A \cup \overline{\partial A}}$, the hitting time for $\underline{\partial A} \cup \overline{\partial A}$, is finite almost surely.

(3) Give an explicit formulation of the unique solution of the discrete PDE in terms of random walks. What is the difference with the pure Dirichlet conditions?

Solution. The unique solution is given by $f(x) = \mathbb{E}^x \left(\mathbbm{1}_{S_{\tau_{\underline{\partial A} \cup \overline{\partial A}}} \in \overline{\partial A}} \right)$: it is the probability that the simple random walk on $A \cup \partial A$ hits $\overline{\partial A}$ before $\underline{\partial A}$. (In fact $f((a,b)) = \frac{b}{m+1}$ satisfies each equations and this shows that it is the explicit expression for f). The difference with the pure Dirichlet condition is that here we consider the simple random walk on $A \cup \partial A$ and we do not stop it when we hit the boundary: some part of the boundary is thus a "reflecting boundary".

Let us prove that the given solution does indeed solve the problem:

- (a) using the usual arguments it is harmonic in A,
- (b) it is equal to 0 on ∂A trivially,
- (c) it is also equal to 1 on $\overline{\partial A}$ trivially,
- (d) and for the normal derivative condition: if the random walk goes from $y \in \partial A$, the only place it can go for the first step is the unique $x \sim y$. Thus if $y \in \partial A | \cup |\partial A|$, $\mathbb{E}^x \left(\mathbbm{1}_{S_{\tau_{\underline{\partial A} \cup \overline{\partial A}}} \in \overline{\partial A}} \right) = \mathbb{E}^y \left(\mathbbm{1}_{S_{\tau_{\underline{\partial A} \cup \overline{\partial A}}} \in \overline{\partial A}} \right)$ which is exactly the Neumann boundary conditions.

Remark. We used a mix of conditions in order to have a finite stopping time. Yet, one can solve the Neumann problem with pure Neumann boundary conditions. In this case, the boundary conditions must satisfy some additional conditions for a solution to exist, and the solution is unique only up to a constant. This is slightly more technical. (Section 6.7 of https://www.math.uchicago.edu/~lawler/srwbook.pdf)

Remark. Actually we considered a rectangle for simplicity, but one can do the same with any discretisation of any domain Ω with 4 points marked on the boundary in counterclockwise order a,b,c and d and with Dirichlet boundary conditions on [a,b],[c,d] and Neumann conditions on [b,c],[d,e]. Then the solution would be the imaginary part of the discretisation of the conformal mapping which sends the domain Ω to a rectangle $[0,L] \times [0,i]$ (for some L) which sends a,b,c,d to the corners of the rectangle.

Exercise 2. Green's function representation by determinant

We consider $A \subseteq \mathbb{Z}^d$ finite. The goal of this exercise is to prove that if $x_1, \dots, x_n \in A$ and $A_k = A \setminus \{x_1, \dots, x_k\}$ then

$$G_A(x_1, x_1) G_{A_1}(x_2, x_2) \cdots G_{A_{n-1}}(x_n, x_n)$$

is independent of the order of x_1, \ldots, x_n .

Remark. For this exercise sheet, we will consider:

$$\Delta^{+} f(x) = f(x) - \frac{1}{2d} \sum_{y \sim x} f(y)$$

 $(\Delta^+ = -\Delta \text{ is the positive definite operator}).$

(1) We can consider Δ^+ as a linear operator $\Delta_A^+: \mathbb{R}^A \to \mathbb{R}^A$, by considering a vector on A as a function on $A \cup \partial A$ such that $f \upharpoonright_{\partial A} = 0$. Show that :

$$G_A(x,x) = \frac{\det \Delta_{A\setminus \{x\}}^+}{\det \Delta_A^+}.$$

Solution. We know that $G_A = (\Delta_A^+)^{-1}$. Thus, we can use Cramer's theorem to compute the inverse. If $\Delta_A^{x,x}$ is the matrix obtained after removing the line and the column x to Δ_A , we have

$$G_A(x,x) = (\Delta_A^+)^{-1}(x,x) = \frac{\det(\Delta_A^+)^{x,x}}{\det \Delta_A^+}$$

but $(\Delta_A^+)^{x,x}$ is the same matrix as $\Delta_{A\setminus\{x\}}^+$ since removing the row associated to x correspond to not evaluating Δ^+f at x and removing the column to x correspond to put the constraint f(x) = 0. This is the minus Laplacian operator on $A\setminus\{x\}$ (since boundary values are set to zero). Thus the desired formula holds.

(2) If $x_1, \dots, x_n \in A$ and $A_k = A \setminus \{x_1, \dots, x_k\}$, give the value of $G_A(x_1, x_1) G_{A_1}(x_2, x_2) \cdots G_{A_{n-1}}(x_n, x_n)$

and prove that it is independent of the order of x_1, \dots, x_n .

Solution. Using the previous equality:

$$G_A(x_1, x_1) G_{A_1}(x_2, x_2) \cdots G_{A_{n-1}}(x_n, x_n) = \prod_{i=0}^{n-1} \frac{\det \Delta_{A_{i+1}}^+}{\det \Delta_{A_i}^+},$$

where $A_0 = A$. Thus it is equal to $\frac{\det \Delta_{A_n}^+}{\det \Delta_A^+}$. This last value is clearly independent of the order of x_1, \dots, x_n .

Exercise 3. Determinant of Laplacian and uniform spanning trees: Kirchhoff's theorem

Remark. If M is a matrix, we denote by $M^{i,j}$ the matrix obtained by deleting the i-th row and j-column of M. We also denote by $M^{i,j}$ the matrix obtained by deleting only the i-th row of M. The cofactor $\det^{i,j} M$ is $(-1)^{i+j} \det M^{i,j}$.

Let G be a connected graph with n vertices and m edges (here an edge is a couple of vertices, in particular, we do not consider the case where two vertices are related by two or more edges). Recall that a spanning tree of G is a connected subgraph of G with no loop and which covers all vertices of G. Let us give a unique number between 1 and n to each vertex and a unique number between 1 and m to each edge. For this exercise, we denote by $\tilde{\Delta}_G$ the matrix defined by:

$$\tilde{\Delta}_G(i,j) = \delta_{i,j} \deg(i) - \delta_{j \sim i},$$

where $1 \le i, j \le n$ denote vertices of G and deg(i) is the degree of i.

We will prove Kirchhoff's theorem :

Kirchhoff's theorem : #{spanning trees of G} =
$$\det^{i,j} \left(\tilde{\Delta}_G \right)$$

Actually, we will only show that $\#\{\text{spanning trees of G}\}=\det^{1,1}\left(\tilde{\Delta}_{G}\right)$, the general case can be deduced using elementary linear algebra arguments.

(1) Let the $n \times m$ incidence matrix E such that the only non zero elements are given by the following: if the k-th edge goes between i and j and i < j then $E_{ik} = 1$ and $E_{jk} = -1$. Show that $\tilde{\Delta}_G = EE^{\mathrm{T}}$, where E^{T} is the transpose of E.

Solution. Let E be the incidence matrix, we have

$$(EE^{T})_{x,y} = \sum_{e} E_{x,e} E_{e,y}^{T} = \sum_{e} E_{x,e} E_{y,e}.$$

If x=y then for any edge e adjacent to x, $E_{x,e}^2=1$ and for any edge non adjacent to x, $E_{x,e}^2=0$: thus $\sum_e E_{x,e} E_{y,e} = \deg(x)$ in this case. If $x \neq y$, then $E_{x,e} E_{y,e} = -1$ if and only if x and y are adjacent, if not it is equal to 0. This is exactly the definition of $\tilde{\Delta}_G$.

(2) Show that $\tilde{\Delta}_{G}^{1,1} = E^{1,.} (E^{1,.})^{\mathrm{T}}$.

Solution. This is obvious from the last question. In order to remove a vertex from $\tilde{\Delta}_G$, we need to remove the same vertex to E: vertices in E are the lines.

(3) Prove that $m \ge n-1$ i.e. the matrix $E^{1,.}$ has a horizontal shape more than a vertical shape.

Solution. The graph G being connected, to connect n vertices one needs at least n-1 edges. Thus $m \ge n-1$.

(4) Recall the Cauchy-Binet formula which says that if A and B are two matrices of size $l \times k$ and $k \times l$ then

$$\det\left(AB\right) = \sum_{S \subset [k], \#S = l} \det\left(A_{[l],S}\right) \det\left(B_{S,[l]}\right)$$

where $[k] = \{1, ..., k\}$, $A_{S,[k]}$ is the matrix obtained by choosing the rows in S and the columns in [k]. Use this formula to show that

$$\det \tilde{\Delta}_G^{1,1} = \sum_{S \subset [m], \#S = n-1} \det \left(\left(E^{1,\cdot} \right)_{[n-1],S} \right)^2.$$

Solution. This is an application of the Cauchy-Binet Formula:

$$\begin{split} \det \tilde{\Delta}_G^{1,1} &= \sum_{S \subset [m], \#S = n-1} \det \left(\left(E^{1,\cdot} \right)_{[n-1],S} \right) \det \left(\left(E^{1,\cdot} \right)_{S,[n-1]}^{\mathrm{T}} \right) \\ &= \sum_{S \subset [m], \#S = n-1} \det \left(\left(E^{1,\cdot} \right)_{[n-1],S} \right)^2. \end{split}$$

(5) What represents a choice of $S \subset [m]$ in the original graph G? We want to show that S forms a spanning tree of G if and only if $\det\left(\left(E^{1,\cdot}\right)_{[n-1],S}\right) = \pm 1$, and if it does not form a spanning tree then $\det\left(\left(E^{1,\cdot}\right)_{[n-1],S}\right) = 0$.

Solution. The choice S is a choice of edges of G: it is thus a subgraph of S.

(a) Show that if S is not a spanning tree, then there exists a cycle in S.

Solution. We recall two facts :

- (i) trees are the connected graphs with number of edges which is equal to the number of vertices minus one
- (ii) trees are the connected graphs without cycles.

Thus if S is not a spanning tree then it must have more than one connected component (since if not it would be connected and would satisfy the condition i. above). For one of the component, the number of edges must be strictly greater than the number of vertices minus one (if not, by summing all the inequalities for all the connected components, we would find a contradiction with the fact that the total number of edges is n-1). This connected component is

- connected

- its number of edges must is strictly greater than the number of vertices minus one it can not be a tree thus there exists a cycle.

(b) Show that if S is not a spanning tree then $\det \left((E^{1,\cdot})_{[n-1],S} \right) = 0.$

Solution. We know that there is a cycle in S: we denote it e_1, \dots, e_k (e_i is an edge), and we can always suppose that $e_1 = (1, 2), \dots, e_k = (k, 1)$. If we look at the columns labelled by e_1, \dots, e_k it looks like

$$\begin{pmatrix}
-1 & 1 & 0 & \dots & 0 & 0 \\
0 & -1 & 1 & \dots & 0 & 0 \\
0 & 0 & -1 & \dots & 0 & 0 \\
0 & 0 & 0 & \dots & 1 & 0 \\
0 & 0 & 0 & \dots & -1 & 1 \\
0 & 0 & 0 & \dots & 0 & 0 \\
\vdots & \vdots & \vdots & \dots & \vdots & \vdots \\
0 & 0 & 0 & \dots & 0 & 0
\end{pmatrix}$$

(if 1 was not in the cycle, we would have a line at the top of the matrix of the form $(1,0,\ldots,-1)$). But if we sum these columns we get the null vector: the determinant has to be null.

(c) Let us suppose that S is a spanning tree. Consider the vertex 1 and an edge e in S connected to 1 and to a vertex i. Prove that

$$\det\left(\left(E^{1,\cdot}\right)_{[n-1],S}\right)=\pm\det\left(\left(E^{1,\cdot}\right)_{[n-1]\backslash\{i-1\},S\backslash\{e\}}\right).$$

Solution. We can consider the column corresponding to e. All its coefficients are zero except the one at position i-1 (corresponding to the vertex i). Thus, if we develop the determinant according to this column, we get $\det\left(\left(E^{1,\cdot}\right)_{[n-1],S}\right) = \pm \det\left(\left(E^{1,\cdot}\right)_{[n-1]\setminus\{i-1\},S\setminus\{e\}}\right)$.

(d) Conclude that if S is a spanning tree, then $\det\left(\left(E^{1,\cdot}\right)_{[n-1],S}\right)=\pm 1.$

Solution. Let us recall that $(E^{1,\cdot})_{[n-1],S}$ is the incidence matrix of the tree defined by S where we discard the first line corresponding to the vertex 1. Let us remark also that if we consider \hat{E} , the incidence matrix of the tree obtained by merging the vertices 1 and i keeping the index 1 for the resulting vertex and to discard the edge e, then

$$\left(E^{1,\cdot}\right)_{[n-1]\backslash\{i-1\},S\backslash\{e\}}=\hat{E}^{1,\cdot}$$

Thus

$$\det\left(\left(E^{1,\cdot}\right)_{[n-1],S}\right)=\pm\det\left(\left(E^{1,\cdot}\right)_{[n-1]\backslash\{i-1\},S\backslash\{e\}}\right)=\pm\det\left(\hat{E}^{1,\cdot}\right).$$

Thus we managed to link the determinant of the incidence matrix of the tree (minus the first line) with the incidence matrix of a tree with less vertices (since we merge 1 and i). By recursion argument, we get that

$$\det\left(\left(E^{1,\cdot}\right)_{[n-1],S}\right) = \pm \det\left(-1\right) = \pm 1$$

where the det(-1) correspond to the case where we consider the tree with 2 vertices and thus one edge.

(6) Prove Kirchhoff's theorem.

Solution. We have :

$$\det \tilde{\Delta}_{G}^{1,1} = \sum_{S \subset [m], \#S = n-1} \det \left(\left(E^{1,\cdot} \right)_{[n-1],S} \right)^{2}$$

$$= \sum_{S \subset [m], S \text{ is a spanning tree of } G} (\pm 1)^{2}$$

$$= \# \{ S \subset [m], S \text{ is a spanning tree of } G \}$$

hence Kirchhoff's theorem.

(7) How do you write the number # {spanning trees of G} using the Laplacian Δ_G ?

Solution. One just has to notice that in order to get $-\tilde{\Delta}_G$, we need to multiply each line of the Laplacian Δ_G by deg (i). Thus

$$\#\left\{\text{spanning trees of G}\right\} = \det \tilde{\Delta}_G^{1,1} = -\left(\prod_{i=2}^{\#V} \deg\left(i\right)\right) \det \Delta_G^{1,1}$$

where #V is the number of vertices of G.