Exercice 2: a finite volume scheme for the Laplace equation with Neumann boundary conditons

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Sections 2, 4 (question 2) and 5 (question 2) have priority.

Let Ω be a Lipschitz bounded domain in $\mathbb{R}^d$ (with $d = 1$ or $d = 2$) and $f \in L^2(\Omega)$. We consider the following problem:

$$\begin{cases} -\Delta u = f & \text{in } \Omega \\ \partial_n u = \nabla u \cdot n = 0 & \text{on } \partial\Omega, \end{cases} \tag{1}$$

where n denotes the outward norm of $\partial\Omega$. The objective of this exercice is to investigate Problem (1) and to study several numerical methods to solve it numerically .

1 Analysis of the continuous problem

In this section we prove that providing that compatibility condition (3) is fulfilled, Problem (1) has a unique solution satisfying the null average condition (2).

We consider the subspace H^1_Δ of $H^1(\Omega)$ defined by

$$H^1_\Delta = \{v \in H^1(\Omega), \Delta v \in L^2(\Omega)\}.$$

We admit that as soon as $u \in H^1_\Delta(\Omega)$, then the normal derivative $\partial_n u$ is well defined: In fact, we can prove that $\partial_n u$ belongs to the space $H^{-1/2}(\partial\Omega)$, which is the dual space of $H^{1/2}(\Omega)$ ($H^{1/2}(\Omega)$ the space made of the traces of the $H^1(\Omega)$ functions on $\partial\Omega$). Moreover, the Green's formula for the Laplacian is valid:

$$\forall u \in H^1_\Delta(\Omega),\ \ \forall v \in H^1(\Omega), \qquad \int_\Omega \Delta u\, v\, dx = -\int_\Omega \nabla u \cdot \nabla v\, dx \ + \ \langle \partial_n u, v\rangle,$$

where $\langle \cdot, \cdot\rangle$ stands for the duality pairing between $H^{-1/2}(\partial\Omega)$ and $H^{1/2}(\Omega)$. This duality pairing extends the L^2 scalar product on $\partial\Omega$.

1. Prove that $u_0 = 1$ is a non trivial solution to Problem (1) with $f = 0$. Note that u_0 belongs to $H^1(\Omega)$. To restore the uniqueness, we shall impose that u satisfies the null-average condition

$$\overline{u} = \frac{1}{|\Omega|}\int_\Omega u\, dx = 0. \tag{2}$$

In the sequel, we denote by $L^2_0(\Omega)$ the subspace of $L^2(\Omega)$ made of the functions of $L^2(\Omega)$ satisfying the null-average condition:

$$L^2_0(\Omega) = \{v \in L^2(\Omega) \text{ such that } \frac{1}{|\Omega|}\int_\Omega v\, dx = 0\}.$$

2. By integrating the first equation of Problem (1) over Ω, show that f has to satisfy the following compatibility condition:

$$\int_\Omega f(x)\, dx = 0. \tag{3}$$

3. Prove that if $u \in H^1_\Delta(\Omega)$ satisfies (1) and (2), then it satisfies the following variational problem: find $u \in H^1(\Omega) \cap L^2_0(\Omega)$ such that,

$$\forall v \in H^1(\Omega) \cap L^2_0(\Omega), \qquad \int_\Omega \nabla u \cdot \nabla v\, dx = \int_\Omega f\, v\, dx. \tag{4}$$

Conversely, prove that if $u \in H^1(\Omega) \cap L^2_0(\Omega)$ is solution to the variational Problem (4) and if f satisfies the compatibility condition (3), then u belongs to $H^1_\Delta(\Omega)$ and satisfies Problem (1).

4. Prove that Problem (4) is well posed and conclude. You may used the so-called Poincare-Wirtinger inequality: There is a constant $C > 0$ such that, for any $u \in H^1(\Omega)$,

$$\|u - \overline{u}\|_{L^2(\Omega)} \ \leq\ C\, \|\nabla u\|_{L^2(\Omega)}.$$

2 Construction of the finite volume scheme in the one dimensional case

In this section, we assume that $\Omega = (0,1)$. We consider a mesh of N intervals (or control volumes) $T_i = (x_{i-1/2}, x_{i+1/2})$, $i \in [1:N]$ ($i \in \mathbb{N}$, $1 \le i \le N$), where the subdivision $(x_{i+1/2})_{i\in[0:N]}$ satisfies:

$$0 = x_{1/2} < x_{3/2} < \cdots < x_{i-1/2} < x_{i+1/2} < \cdots < x_{N+1/2} = 1.$$

For $i \in [1:N]$, we choose a point $x_i \in T_i$ (not necessarily the midpoint), and we denote by u_i the associated discrete unknown (note that u_i is expected to be a good approximation of $u(x_i)$ but u_i **is not equal to** $u(x_i)$). Moreover, we set $x_0 = x_{1/2} = 0$ and $x_{N+1} = x_{N+1/2} = 1$. We associate with x_0 and x_{N+1} the unknowns u_0 and u_{N+1}.

1. Imitating the approach used for the Dirichlet problem, construct a set of N linear equations associated with the N discrete unknowns u_i, $i \in [1:N]$. Do not omit to take into account the Neumann boundary conditions. Write the problem under the matricial form:

$$\mathbf{M}\mathbf{u} = \tilde{\mathbf{f}} \tag{5}$$

where $\mathbf{M} \in \mathcal{M}_N(\mathbb{R})$, $\mathbf{u} = (u_1, u_1, \cdots, u_N)^T$, and

$$\tilde{\mathbf{f}} = (|T_1| f_1, |T_2| f_2, \cdots, |T_N| f_N)^T \quad \text{with } \mathbf{f} = (f_i)_{i\in[1:N]} \text{ and } f_i = \frac{1}{|T_i|}\int_{T_i} f\,dx,\ i \in [1:N]. \tag{6}$$

Show that the matrix $\mathbf{M}$ is symmetric.

The remainder of this part consists in proving that Problem (5) has a solution.

2. Prove the following discrete variational formulation: For any $\mathbf{w} = (w_j)_{j\in[0:N+1]} \in \mathbb{R}^{N+2}$,

$$(g\mathbf{u}, g\mathbf{w})_D = (\mathbf{f}, \mathbf{w})_T.$$

where $\mathbf{f}$ is defined by (6). Here, for any $\mathbf{u} = (u_{j+1/2})_{j\in[0:N]} \in \mathbb{R}^{N+1}$ and $\mathbf{v} = (v_{j+1/2})_{j\in[0:N]} \in \mathbb{R}^{N+1}$,

$$(u, v)_D = \sum_{j=0}^{N} |D_{j+1/2}|\, u_{j+1/2}\, v_{j+1/2}.$$

for any $\mathbf{u} = (u_j)_{j\in[0:N+2]} \in \mathbb{R}^{N+2}$ and $\mathbf{v} = (v_j)_{j\in[0:N+2]} \in \mathbb{R}^{N+2}$,

$$(u, v)_T = \sum_{j=1}^{N} |T_j|\, u_j\, v_j.$$

The operator $g : \mathbb{R}^{N+2} \mapsto \mathbb{R}^{N+1}$ is the discrete gradient operator: for any $\mathbf{v} = (v_j)_{j\in[0:N+1]} \in \mathbb{R}^{N+2}$, the vector $g\mathbf{v} = \big((g\mathbf{v})_{j+1/2}\big)_{j\in[0:N]} \in \mathbb{R}^{N+1}$

$$(g\mathbf{u})_{j+1/2} = \frac{u_{j+1} - u_j}{|D_{j+1/2}|}.$$

3. Deduce from the previous question that Ker$(\mathbf{M})$ = span$\{\mathbf{u}_0\}$, where $\mathbf{u}_0 \in \mathbb{R}^N$ the constant vector such that

$$(\mathbf{u}_0)_j = 1 \quad \forall j \in [1:N]. \tag{7}$$

4. Using the result of the previous question, the fact that $\mathbf{M}$ is symmetric, and the compatibility condition (3), prove that Problem (5) has a solution (defined up to a constant).

5. Prove that imposing additionally the discrete null average condition

$$\sum_{i=1}^{N} |T_i| v_i = 0 \tag{8}$$

restores the uniqueness.

The new system of linear equations made Problem (5) together with the discrete null average condition (8) a system of $N+1$ equations with N unknowns. As a result, the direct methods (LU, Gauss elimination) for solving the linear square systems of equations cannot be used directly.

In the next three sections, we shall investigate three methods for the resolution of this problem. **For the numerical results, you might take $f(x) = \pi^2\cos(\pi x)$. The exact solution is this case is given by $u(x) = \cos(\pi x)$. You might use a uniform mesh.**

3 The penalization method

The first idea to deal with this problem is to replace the Neumann condition $\partial_n u$ by a mixed condition (or Robin condition)

$$\partial_n u_\varepsilon + \varepsilon u_\varepsilon = 0 \text{ on } \partial\Omega. \tag{9}$$

where ε is a small parameter.

1. Prove that if u_ε satisfies the penalized problem, the $u_\varepsilon \in H^1(\Omega)$ satisfies the modified variational formulation:

$$\forall v \in H^1(\Omega), \int_\Omega \nabla u_\varepsilon \cdot \nabla v \, dx + \varepsilon \int_{\partial\Omega} u_\varepsilon v \, dx = \int_\Omega f v dx. \tag{10}$$

We admit that the associated bilinear form is coercive on $H^1(\Omega)$, so that Problem (10) has a unique solution.

2. Under the compatibility condition (3), prove that the solution of Problem (10) satisfies the null average (2).

3. Construct a finite volume scheme associated with this method. We denote $\mathbf{u}_\varepsilon^h$ the approximation u^ε using this scheme. represent the evolution of the error

$$\frac{\|\mathbf{u}_\varepsilon^h - \Pi u\|_T}{\|u\|_{L^2(\Omega)}}, \quad \|u_\varepsilon^h - u\|_T = \sqrt{(u_\varepsilon^h - u, u_\varepsilon^h - u)_T},$$

with respect to the penalisation parameter ε in the logarithmic scale. Here $\Pi : \mathcal{C}^0(0,1) \to \mathbb{R}^N$ is defined by $(\Pi u)_i = u(x_i)$. You can take ε between 10^{-1} and 10^{-7}. You may choose h sufficiently small so that the approximation error ($\|\mathbf{u}_\varepsilon^h - \Pi u_\varepsilon\|_T$) is small compared to penalisation error ($\|u - u_\varepsilon\|_{L^2(\Omega)}$). What do you observe ? Explain.

Remark. *To improve the efficiency of your code, you may declare the discretisation matrix as a sparse matrix (e.g.* `M = sparse(1000,1000)`*).*

4 The Lagrange multiplier method

The second method presented here consists in imposing the discrete null average condition by means of a Lagrange multiplier (this method is strongly connected to the optimization theory).

1. Prove that Problem (5)-(8) is equivalent to the following linear square system : find $(\mathbf{u}, \lambda) \in \mathbb{R}^N \times \mathbb{R}$ such that

$$\begin{cases} \mathbf{M}\mathbf{u} + \lambda \mathbf{b} = \tilde{\mathbf{f}} \\ \mathbf{b}^T \mathbf{u} = 0 \end{cases} \tag{11}$$

where $\mathbf{b} = (|T_i|)_{i \in [1:N]} \in \mathbb{R}^N$ and $\tilde{\mathbf{f}}$ is defined in (6). Prove that the square linear system (11) has a unique solution.

2. Implement this method and plot the evolution of the error $\dfrac{\|\mathbf{u} - \Pi u\|_T}{\|u\|_{L^2(\Omega)}}$ with respect to h.

5 An iterative method: the conjugate gradient method

The conjugate gradient method is a very powerful iterative method to solve square linear systems of the form $\mathbf{A}\mathbf{x} = \mathbf{b}$ providing that $\mathbf{A} \in \mathcal{M}_N(\mathbb{R})$ is a symmetric definite positive matrix, $\mathbf{x} \in \mathbb{R}^N$ and $\mathbf{y} \in \mathbb{R}^N$.

For the sake of completeness, we remind the algorithm associated with this method (in what follows, $(\cdot,\cdot)$ denotes the euclidian scalar product of $\mathbb{R}^N$): let $\delta \geq 0$ (δ being the prescribed precision),

1. Initialization step: $\mathbf{x}_0 \in \mathbb{R}^N$ is given.
   - $k = 0$
   - $\mathbf{x}_k = \mathbf{x}_0$
   - $\mathbf{r}_k := \mathbf{y} - \mathbf{A}\mathbf{x}_k$
   - $\mathbf{p}_k := \mathbf{r}_k$
2. Reccurrent step:

- if $\sqrt{(\mathbf{r}_k, \mathbf{r}_k)} > \delta$
  - $\alpha_k := \dfrac{(\mathbf{r}_k, \mathbf{r}_k)}{(\mathbf{p}_k, \mathbf{A}\mathbf{p}_k)}$
  - $\mathbf{x}_{k+1} := \mathbf{x}_k + \alpha_k \mathbf{p}_k$
  - $\mathbf{r}_{k+1} := \mathbf{r}_k - \alpha_k \mathbf{A}\mathbf{p}_k$
  - $\beta_k := \dfrac{(\mathbf{r}_{k+1}, \mathbf{r}_{k+1})}{(\mathbf{r}_k, \mathbf{r}_k)}$
  - $\mathbf{p}_{k+1} := \mathbf{r}_{k+1} + \beta_k \mathbf{p}_k$
  - $k := k + 1$
- If $\sqrt{(\mathbf{r}_k, \mathbf{r}_k)} \leq \delta$, the convergence is reached. We set $M = k$.

By convention for $k > M$ we set $\mathbf{x}_k = \mathbf{x}_M$ and $\mathbf{r}_k = \mathbf{p}_k = 0$.

If $\delta = 0$ and $\mathbf{A}$ is a symmetric definite positive matrix, the previous algorithm converges in at most N iterations.

1. Assume that $\mathbf{A}$ is symmetric (not necessarily definite and positive), let $\{\tilde{\mathbf{u}}\} \in \mathbb{R}^N$ belong to Ker($\mathbf{A}$). Assume that that

$$(\mathbf{x}_0, \tilde{\mathbf{u}}) = 0 \quad \text{and} \quad (\mathbf{y}, \tilde{\mathbf{u}}) = 0. \tag{12}$$

Prove that the sequences $(\mathbf{x}_k)_{k\in\mathbb{N}}$, $(\mathbf{r}_k)_{k\in\mathbb{N}}$ and $(\mathbf{p}_k)_{k\in\mathbb{N}}$ defined by the previous algorithm are well defined and show that the sequence $(\mathbf{x}_k)_{k\in\mathbb{N}}$ satisfies

$$(\mathbf{x}_k, \tilde{\mathbf{u}}) = 0 \text{ for any } k \in \mathbb{N}.$$

In other words, if $\mathbf{x}_0$ is orthogonal to $\tilde{\mathbf{u}}$, all the terms $\mathbf{x}_k$ are orthogonal to $\tilde{\mathbf{u}}$.

The third method then consists in applying the conjugate gradient method to the linear system (5) (of course, in this case, $\mathbf{M}$ is symmetric and positive but not invertible), choosing $\mathbf{x}_0$ orthogonal to $\mathbf{u}_0$ (defined in (7)). We admit that, in the present case, the conjugate gradient algorithm converges to a solution of (5). This method then selects the unique solution of (5) that is orthogonal to Ker($\mathbf{M}$).

Naturally, the selected solution corresponds to the solution satisfying the discrete null average condition (8) only if the mesh is regular. But, if the mesh is not regular, we can, in a first step, compute the solution orthogonal to $\mathbf{u}_0$, the solution satisfying the discrete null average condition (8) being computed a posteriori.

2. Implement this method and plot the evolution of the error $\dfrac{\|\mathbf{u} - \Pi u\|_T}{\|u\|_{L^2(\Omega)}}$ with respect to h.