Numerical Approximation of PDEs

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1 Ellipticity

(1a) Show that the quadratic form

$$\langle L\mathbf{u}, \mathbf{v}\rangle = v_1\,(1 + x_1x_2)\,u_1 + x_1v_1u_2 + x_2v_2u_1 + v_2u_2 \tag{1}$$

is coercive in $\Omega = \{x \in \mathbb{R}^2 \mid 0 < x_1 < \frac{1}{2}, 0 < x_2 < 1\}$.

(1b) Show that the quadratic form $\langle L\mathbf{u}, \mathbf{v}\rangle = \sum_{i,j=1}^{3} u_i\,(a_{ij}v_j)$, with

$$\{a_{ij}\} = \begin{pmatrix} 1 & -x_3 & x_2 \\ x_3 & 1 + x_1^2 & x_1 \\ -x_2 & x_2 & 1 + x_3^2 \end{pmatrix} \tag{2}$$

is coercive in $\Omega = \{x \in \mathbb{R}^3 \mid |x| < 1\}$.

HINT for both exercises: We call a quadratic form $\langle L\mathbf{u}, \mathbf{v}\rangle = \mathbf{v}^T A\mathbf{u}$ coercive if $\langle L\mathbf{u}, \mathbf{u}\rangle > 0$ for $\mathbf{u} \neq \mathbf{0}$. First show that a matrix A is positive definite if and only if all eigenvalues of $\frac{A+A^T}{2}$ are strictly positive.

Solution:

Note that:

$$\left(v, \frac{A + A^T}{2}v\right) = \frac{1}{2}\,(v, Av) + \frac{1}{2}\left(v, A^T v\right) = \frac{1}{2}\,(v, Av) + \frac{1}{2}\,(Av, v) = (v, Av)\,.$$

Furthermore, note that $\frac{A+A^T}{2}$ is symmetric and hence positive definite if and only if all eigenvalues are strictly positive.

(1a) *We have*

$$A = \begin{pmatrix} 1 + x_1x_2 & x_1 \\ x_2 & 1 \end{pmatrix}$$

and hence

$$\frac{A + A^T}{2} = \begin{pmatrix} 1 + x_1x_2 & \frac{1}{2}(x_1 + x_2) \\ \frac{1}{2}(x_1 + x_2) & 1 \end{pmatrix}.$$

The smallest eigenvalue satisfies

$$\lambda_{min} = \frac{1}{2}\left(2 + x_1x_2 - \sqrt{x_1^2x_2^2 + (x_1+x_2)^2}\right).$$

For $a \geq 0$ *and* $b \geq 0$*, we have* $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$ *and thus*

$$\lambda_{min} \geq 1 - \frac{x_1+x_2}{2} \geq \frac{1}{4}, \quad \textit{for } x \in \overline{\Omega}.$$

(1b) *We have*

$$\frac{A+A^T}{2} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1+x_1^2 & \frac{1}{2}(x_1+x_2) \\ 0 & \frac{1}{2}(x_1+x_2) & 1+x_3^2 \end{pmatrix}.$$

Hence, one of the eigenvalues equals one, while the minimum of the other two is given by

$$\lambda_{min} = \frac{1}{2}\left(2 + x_1^2 + x_3^2 - \sqrt{(x_1^2 - x_3^2)^2 + (x_1+x_2)^2}\right).$$

Using $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$ *again, we find*

$$\lambda_{min} \geq \frac{1}{2}\left(2 + x_1^2 + x_3^2 - |x_1^2 - x_3^2| - |x_1+x_2|\right) \geq \frac{1}{2}\left(2 - |x_1+x_2|\right) \geq 1 - \frac{\sqrt{2}}{2}, \quad \textit{for } x \in \overline{\Omega}.$$

2 Reaction-diffusion equation in 1D

Consider the elliptic boundary value problem that reads:

$$-\left(K(x)u'(x)\right)' + c(x)u(x) = f(x), \quad x \in \Omega \tag{3}$$

subject to

$$u(0) = u(1) = 0. \tag{4}$$

where:

- $\Omega = (0,1)$.
- $K(x)$ is bounded and strictly positive scalar function on Ω.
- $c(x)$ is a bounded scalar function on Ω.
- $f \in L^2(\Omega)$ is a given function.

Derive the weak formulation and give a sufficient condition on $c(x)$ to obtain the existence and uniqueness of the weak solution.

Solution:

As seen in class, the resulting weak formulation is:

$$\textit{Find} \quad u \in H_0^1(\Omega) \quad \textit{such that} \quad a(u,v) = L(v), \quad \forall v \in H_0^1(\Omega). \tag{5}$$

where

$$a(u,v) = \int_\Omega (Ku'v' + cuv)dx, \tag{6}$$

$$L(v) = \int_\Omega fv dx. \tag{7}$$

It is easy to see that the linear form $L(\cdot)$ *is continuous on* $H_0^1(\Omega)$*. We now verify the assumptions of the Lax-Milgram theorem for the bilinear form* $(u,v) \to a(u,v)$ *in* $H_0^1(\Omega) \times H_0^1(\Omega)$*.*

- *Continuity:*

$$\begin{aligned} a(u,v) &\le \|Ku'\|_{L^2(\Omega)}\|v'\|_{L^2(\Omega)} + \|cu\|_{L^2(\Omega)}\|v\|_{L^2(\Omega)}, \qquad \textit{(Cauchy-Schwartz)} \\ &\le \|K\|_{L^\infty(\Omega)}\|v\|_{H^1(\Omega)}\,\|u\|_{H^1(\Omega)} + \|c\|_{L^\infty(\Omega)}\|u\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)}, \\ &= \left(\|K\|_{L^\infty(\Omega)} + \|c\|_{L^\infty(\Omega)}\right)\|u\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)}. \end{aligned}$$

- *Coercivity: Denote* $K_0 = \min_{x\in\Omega} K(x)$ *and* $c_0 = \min_{x\in\Omega} c(x)$*. Using the Poincaré inequality, we obtain*

$$\begin{aligned} a(u,u) &= \int_\Omega \left(K(u')^2 + cu^2\right) dx \\ &\ge K_0\|u'\|^2_{L^2(\Omega)} + c_0\|u\|^2_{L^2(\Omega)} \\ &\ge \frac{K_0}{C_p^2+1}\|u\|^2_{H^1(\Omega)} + c_0\|u\|^2_{L^2(\Omega)} \end{aligned}$$

  This leads to two possible cases:

  Case 1: If $c_0 \ge 0$*, then*

$$a(u,u) \ge \min\left(\frac{K_0}{C_p^2+1}, c_0\right)\|u\|^2_{H^1(\Omega)}.$$

  Case 2: If $c_0 < 0$*, then*

$$a(u,u) \ge \left(\frac{K_0}{C_p^2+1} + c_0\right)\|u\|^2_{H^1(\Omega)}.$$

  A sufficient condition for coercivity is

$$c_0 > -\frac{K_0}{C_p^2+1}.$$

3 Reaction-diffusion equation in 2D (bonus)

Consider the elliptic boundary value problem that reads:

$$-\nabla \cdot (A(x)\nabla u(x)) + c(x)u(x) = f(x), \quad x \in \Omega \tag{8}$$

subject to

$$u(x) = 0, \quad \text{on } \partial\Omega \tag{9}$$

where:

- $\Omega \subset \mathbb{R}^2$ is a bounded open domain with a Lipschitz boundary $\partial\Omega$.
- $A(x)$ is bounded, symmetric and positive definite.
- $c(x) \geq 0$ is a bounded scalar function on Ω.
- $f \in L^2(\Omega)$ is a given function.

(2a)
Derive the weak form of the given boundary value problem.
Hint: As in 1D, multiply by a test function and integrate over the domain. In two spatial dimensions, the product rule reads:

$$\phi\nabla \cdot \mathbf{F} = -\nabla\phi \cdot \mathbf{F} + \nabla \cdot (\phi\mathbf{F})\,. \tag{10}$$

(2b)
Define the bilinear form $a(u, v)$ and the linear form $L(v)$ based on the weak formulation.

(2c)
Verify that $a(u, v)$ and $L(v)$ satisfy the boundedness and coercivity conditions necessary for the Lax-Milgram lemma.

(2d)
Use the Lax-Milgram Lemma to argue the existence and uniqueness of the solution to the weak formulation.

(2e)
Explore how the solution's properties might change if $c(x)$ is allowed to take negative values in parts of Ω. Derive a lower bound on $c(x)$ in terms of the smallest eigenvalue of $A(x)$ such that Lax-Milgram remains applicable.
Hint: You can use the Poincaré inequality to derive a lower bound.

Solution:
(2a)
We multiply by $v \in H_0^1(\Omega)$ and integrate over the domain:

$$\int_\Omega -v\nabla \cdot (A\nabla u) + vcu \,\mathrm{d}\Omega = \int_\Omega vf \,\mathrm{d}\Omega. \tag{11}$$

We use the product rule with $\phi = v$ and $\mathbf{F} = A\nabla u$ to derive

$$\int_\Omega -v\nabla \cdot (A\nabla u) + vcu \,\mathrm{d}\Omega = \int_\Omega \nabla v \cdot (A\nabla u) - \nabla \cdot (vA\nabla u) + vcu \,\mathrm{d}\Omega. \tag{12}$$

Using the divergence theorem on the second integrand, we obtain

$$\int_\Omega \nabla v \cdot (A\nabla u) - \nabla \cdot (vA\nabla u) + vcu \,\mathrm{d}\Omega = \int_\Omega \nabla v \cdot (A\nabla u) + vcu \,\mathrm{d}\Omega - \int_{\partial\Omega} vA\nabla u \cdot \mathbf{n} \,\mathrm{d}\Gamma. \tag{13}$$

Since $v = 0$ on $\partial\Omega$, the last term vanishes and we are left with the weak form:

$$\int_\Omega \nabla v \cdot (A\nabla u) + cvu \,\mathrm{d}\Omega = \int_\Omega vf \,\mathrm{d}\Omega, \quad \forall v \in H_0^1(\Omega). \tag{14}$$

(2b)
We write the forms $a(u, v)$ and $L(v)$ concisely as:

$$\begin{aligned} a(u, v) &= (\nabla v, A\nabla u)_\Omega + (v, cu)_\Omega \\ L(v) &= (f, v)_\Omega \,. \end{aligned} \tag{15}$$

(2c)
We have

$$\begin{aligned} a(u, v) &= \int_\Omega \nabla v \cdot (A\nabla u) + cvu \,\mathrm{d}\Omega \\ &\le |\nabla v|_{L^2(\Omega)} \, |A\nabla u|_{L^2(\Omega)} + \|cu\|_{L^2(\Omega)} \, \|v\|_{L^2(\Omega)} \\ &\le \|A\|_{L^\infty(\Omega)} \, \|v\|_{H^1(\Omega)} \, \|u\|_{H^1(\Omega)} + \|c\|_{L^\infty(\Omega)} \, \|u\|_{H^1(\Omega)} \, \|v\|_{H^1(\Omega)} \\ &= \left(\|A\|_{L^\infty(\Omega)} + \|c\|_{L^\infty(\Omega)}\right) \|u\|_{H^1(\Omega)} \, \|v\|_{H^1(\Omega)} \,. \end{aligned} \tag{16}$$

Furthermore, we utilise the Poincaré inequality to bound $a(u, u)$ from below:

$$\begin{aligned} a(u, u) &= \int_\Omega \nabla u \cdot (A\nabla u) + \underbrace{cu^2}_{>0} \,\mathrm{d}\Omega \\ &\ge \int_\Omega \nabla u \cdot (A\nabla u) \,\mathrm{d}\Omega \\ &\ge \lambda_{\min}(A) \int_\Omega \|\nabla u\|^2 \,\mathrm{d}\Omega \qquad (\lambda_{\min} \text{ is the smallest eigenvalue}) \\ &\ge \frac{\lambda_{\min}(A)}{C_p^2 + 1} \, \|u\|_{H^1(\Omega)}^2 \,. \end{aligned} \tag{17}$$

As for $L(v)$, we have directly by Cauchy-Schwartz

$$L(v) = \int_\Omega fv \mathrm{d}\Omega \le \|f\|_{L^2(\Omega)} \, \|v\|_{L^2(\Omega)} \,. \tag{18}$$

(2d)

The solution of ***(2c)*** *demonstrates that all conditions for applying the Lax-Milgram theorem are satisfied which means that the weak form admits a unique solution $u \in V$, with $V = H_0^1(\Omega)$.*

(2e)

$$a(u, v) = (\nabla u, A\nabla u)_\Omega + (u, cv)_\Omega$$

We have:

$$(\nabla u, A\nabla u)_\Omega \geq \frac{\lambda_{\min}(A)}{C_p^2 + 1} \|u\|_{H^1(\Omega)}^2 .$$

Let $c_{\min} := \min_{x \in \Omega} c(x) < 0$. We have

$$(u, cu) \geq c_{\min} \|u\|_{L^2(\Omega)}^2 \geq c_{\min} \|u\|_{H^1(\Omega)}^2 < 0.$$

Therefore:

$$a(u, u) \geq \underbrace{\left(\frac{\lambda_{\min}(A)}{C_p^2 + 1} + c_{\min} \right)}_{\textit{must be} > 0} \|u\|_{H^1(\Omega)}^2$$

Therefore, a sufficient condition is:

$$c_{\min} > -\frac{\lambda_{\min}(A)}{C_p^2 + 1}.$$

4 Coding warmup

Consider the Heron method for computing square roots: starting with an initial guess $x_0 > 0$ and a number $S > 0$, we recursively define:

$$x_{n+1} = \frac{S + x_n^2}{2x_n}. \tag{19}$$

The iterates x_n converge to the square root $\sqrt{S}$.
Implement this method and plot the errors $e_i = x_i - \sqrt{S}$ of the iterates $x_0, x_1, \ldots, x_{10}$ when $S = 10000$ and $x_0 = 20000$. For plotting, you can use Matplotlib in Python.

Solution:
The solution can be found in a separate .py file.