Series 2

Notation: 1_A denotes the indicator function of the set A.

1. A Céa-type estimate for the heat equation

Let $G = (a, b)$ and $T > 0$. Denote $V := H_0^1(G)$ and $H := L^2(G)$. Consider the heat equation with homogeneous Dirichlet boundary conditions:

$$\begin{cases} \partial_t u - \Delta u = f & \text{in } G \times (0,T), \\ u = 0 & \text{on } \partial G \times (0,T), \\ u(\cdot, 0) = u_0 & \text{in } G, \end{cases}$$

where $f \in L^2((0,T); H)$ and $u_0 \in H$. On V we define the bilinear form and *energy norm*

$$a(v,w) := \int_G v'w' \mathrm{d}x, \quad \|v\|_a := a(v,v)^{1/2} = \|v'\|_H, = \left(\int_G |v'(x)|^2 \mathrm{d}x \right)^{1/2}, \quad \forall v, w \in V.$$

For time-dependent functions, define

$$\|w\|_{L^\infty((0,T);H)} := \operatorname*{ess\,sup}_{t \in (0,T)} \|w(t)\|_H,$$

$$\|w\|^2_{L^2((0,T);V)} := \int_0^T \|w(t)\|_a^2 \, \mathrm{d}t.$$

Weak formulation: Find $u \in L^2((0,T); V)$ such that $\partial_t u \in L^2((0,T); H)$ and for a.e. $t \in (0,T)$

$$(\partial_t u(t), v)_H + a(u(t), v) = (f(t), v)_H, \quad \forall v \in V.$$

Semi-discrete Galerkin discretization: Let $V_N \subseteq V$ be a finite-dimensional subspace. Find $u_N : (0,T) \to V_N$ such that

$$(\partial_t u_N(t), v_N)_H + a(u_N(t), v_N) = (f(t), v_N)_H, \quad \forall v_N \in V_N,$$

with $u_N(0) = u_{N,0} \in V_N$.

a) Show that the error $e := u - u_N$ satisfies

$$(\partial_t e(t), v_N)_H + a(e(t), v_N) = 0, \quad \forall v_N \in V_N.$$

b) Let $v_N : (0,T) \to V_N$ be any function with $\partial_t v_N \in L^2((0,T); H)$ and define

$$\rho := u - v_N, \qquad \theta := u_N - v_N, \qquad e = \rho - \theta.$$

(i) Show that for a.e. $t \in (0,T)$

$$(\partial_t \theta(t), w_N)_H + a(\theta(t), w_N) = (\partial_t \rho(t), w_N)_H + a(\rho(t), w_N), \quad \forall w_N \in V_N.$$

(ii) Choose $w_N = \theta(t)$ and prove

$$\frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} \|\theta(t)\|_H^2 + \|\theta(t)\|_a^2 \leq C \big(\|\partial_t \rho(t)\|_H^2 + \|\rho(t)\|_a^2 \big).$$

Hint: Use Cauchy-Schwarz and Young's inequality.

(iii) Integrate in time and conclude that

$$\|\theta\|^2_{L^\infty((0,T);H)} + \|\theta\|^2_{L^2((0,T);V)} \leq C\left(\|\theta(0)\|^2_H + \|\partial_t\rho\|^2_{L^2((0,T);H)} + \|\rho\|^2_{L^2((0,T);V)}\right).$$

Hint: Use Gronwall's lemma for $y(t) := \|\theta(t)\|^2_H$.

(iv) Use $e = \rho - \theta$ and the triangle inequality to show the Céa-type estimate

$$\begin{aligned}&\|u - u_N\|^2_{L^\infty((0,T);H)} + \|u - u_N\|^2_{L^2((0,T);V)} \\ &\quad\leq C\Big(\|u_N(0) - v_N(0)\|^2_H + \|\partial_t(u - v_N)\|^2_{L^2((0,T);H)} + \|u - v_N\|^2_{L^2((0,T);V)} + \|u - v_N\|^2_{L^\infty((0,T);H)}\Big).\end{aligned}$$

(v) Assume $u_{N,0} = v_N(0)$ and take the infimum over all possible v_N. Explain why this shows that the Galerkin solution is quasi-optimal in the parabolical energy norm.

Useful results:
Cauchy-Schwarz inequality: For all $w, z \in H$

$$|(w, z)_H| \leq \|w\|_H \|z\|_H$$

Young's inequality: For all $a, b \geq 0$ and every $\varepsilon > 0$,

$$ab \leq \frac{1}{2\varepsilon}a^2 + \frac{\varepsilon}{2}b^2.$$

Gronwall's lemma: Let $y : [t_0, T] \to \mathbb{R}$ be a differentiable function and $B : [0, T] \to \mathbb{R}$ be a integrable function. Assume that for all $t \in [0, T]$,

$$y'(t) \leq y(t) + B(t).$$

Then, for all $t \in [0, T]$,

$$y(t) \leq e^{t-t_0}\, y(t_0) + \int_{t_0}^{t} e^{t-s}\, B(s)\, ds.$$

2. Finite element method for the heat equation

Let $J = (0, T)$, $T > 0$, $G = (a, b) \subset \mathbb{R}$ and $f \in C(\overline{J}; L^2(G))$. We want to solve the heat equation with a variable diffusion coefficient $\kappa(x) \in C(\overline{G})$, zero Dirichlet boundary conditions and initial value $u_0 \in L^2(G)$,

$$\begin{cases} \partial_t u(t,x) - \partial_x(\kappa(x)\partial_x u(t,x)) & = f(t,x) \qquad \text{in } J \times G\,, \\ u(t,x) & = 0 \qquad \text{on } J \times \partial G\,, \\ u(0,x) & = u_0(x) \qquad \text{in } G. \end{cases} \tag{1}$$

Note that, for $\kappa \equiv 1$, this corresponds to the heat equation from the lecture.

a) Show that if u is a smooth solution of this problem, then for all $v \in H^1_0(G)$, there holds

$$\frac{d}{dt}\,(u(t), v)_{L^2(G)} + a(u(t), v) = (f(t), v)_{L^2(G)}\,, \quad \forall t \in J \tag{2}$$

for a suitable bilinear form a, where $(\varphi, \psi)_{L^2(G)} := \int_G \varphi(x)\psi(x)\,dx$.

The variational formulation to problem (1) is: find a solution $u \in C(J; H^1_0(G)) \cap C^1(J; L^2(G))$ to (2). It can be shown that this problem exhibits a unique solution if $\kappa(x) > 0$ for all $x \in \overline{G}$.

b) Assume that $\kappa(x) > 0$ for all $x \in \overline{G}$. Let V_N be a subspace of $H_0^1(G)$ of finite dimension N. We seek an approximation u_N of the solution of system (1) as the element of $C^1([0,T];V_N)$ satisfying the variational problem

$$\frac{d}{dt}\left(u_N(t), v_N\right)_{L^2(G)} + a(u_N(t), v_N) = (f(t), v_N)_{L^2(G)} \ , \quad \forall v_N \in V_N \ , \ \forall t \in J \, ,$$

with initial condition $u_N(0,x) = u_{0,N}$ where $u_{0,N}$ is some approximation of u_0 in V_N (this is sometimes called the "method of lines"). Given a basis $\{\phi_{N,j}\}_{1\leq j\leq N}$ of V_N, write

$$u_N(t,\cdot) = \sum_{j=1}^{N} u_{N,j}(t)\phi_{N,j} \ , \quad \underline{u}_N(t) = \begin{pmatrix} u_{N,1}(t) \\ \vdots \\ u_{N,N}(t) \end{pmatrix} .$$

Show that the vector $\underline{u}_N(t)$ satisfies a system of coupled ordinary differential equations of the form:

$$\mathbf{M}\frac{d}{dt}\underline{u}_N + \mathbf{A}\underline{u}_N = \underline{F} \, . \tag{3}$$

Give the expression of the matrices $\mathbf{M}$, $\mathbf{A}$ and the vector $\underline{F}$. Why are $\mathbf{M}$, $\mathbf{A}$ nonsingular?

c) We seek approximations $u_{N,i}^m$ of the values of the coefficients $u_{N,i}(t_m)$ at each time $t_m = km$ where $k > 0$ is the time step and $m \in \mathbb{N}$. Let

$$\underline{u}_N^m := \begin{pmatrix} u_{N,1}^m \\ \vdots \\ u_{N,N}^m \end{pmatrix} .$$

Starting from Eq. (3), proceed as in the case of the finite difference scheme and derive a fully discrete scheme for (2) of the form

$$\mathbf{B}_\theta \underline{u}_N^{m+1} = \mathbf{C}_\theta \underline{u}_N^m + \underline{F}_\theta^m \, ,$$

with suitable matrices $\mathbf{B}_\theta$, $\mathbf{C}_\theta$ and $\underline{F}_\theta^m$.

3. Implementation in Python

From now on, we assume $J = G = (0,1)$ and $\kappa(x) := x + 1$. For any $N, M \in \mathbb{N}$, we set $h = \frac{1}{N+1}, k = \frac{1}{M}$ and consider the spatial mesh points $x_i = hi, i = 1, 2, \ldots, N$. Let V_N be the vector space of continuous functions on G, vanishing at both ends of the interval, and which are linear on each (x_i, x_{i+1}). For each $i \in \{1, \ldots, N\}$, there is a unique element $\phi_{N,i}$ of V_N (the so-called hat-functions) satisfying

$$\phi_{N,i}(x_j) = \delta_{i,j} \ , \quad \forall j \in \{1, \ldots, N\}$$

and $\{\phi_{N,i}\}_{1\leq i\leq N}$ is a basis of V_N.

a) Let $K(x,y) := \int_x^y \kappa(x)\, dx$. Derive an explicit expression for K in terms of $x, y \in \mathbb{R}$. In the script "`FEM_heat.py`" provided, implement the function "`kappa_integral(x,y)`" for the calculation of $K(x,y)$ using the derived explicit expression.

b) For this choice of basis, compute the entries of $\mathbf{M}$ and $\mathbf{A}$ obtained in 2.b). In the script "`FEM_heat.py`" provided, fill the functions "`build_massMatrix(N)`" and "`build_rigidityMatrix(N)`" accordingly. The input for both functions are the discretization parameter N and the output should be the matrices $\mathbf{M}$ and $\mathbf{A}$ accordingly. You should compute the matrices $\mathbf{M}$ and $\mathbf{A}$ in closed form so that no numerical approximations are required.

For any $F \in C^4[a,b]$, one can evaluate approximately the integral $\int_a^b F(x)\,dx$ using the Simpson rule, which reads

$$\int_a^b F(x)\,dx \approx \frac{b-a}{6}\left(F(a) + 4F\left(\frac{a+b}{2}\right) + F(b)\right).$$

The order of approximation is $O(|b-a|^5)$.

c) Let $u(t,x) = e^{-t}\sin(\pi x)$. Check that $u(t,x)$ is the solution of system (1) for

$$f(t,x) = \left((x+1)\pi^2 - 1\right)e^{-t}\sin(\pi x) - \pi e^{-t}\cos(\pi x)\,, \quad u_0(x) = \sin(\pi x)\,.$$

Define the corresponding functions "`f(t,x)`", "`initial_value(x)`" and "`exact_solution_at_1(x)`" in "`FEM_heat.py`". Here "`f`" has the temporal and spatial variables (t,x) as the input and outputs the value of $f(t,x)$. "initial_value" and "exact_solution_at_1" shall receive a vector of spatial grid points and compute a vector containing the value of $u(x,0)$ and $u(x,1)$ at these points respectively.

d) Show that

$$\int_G f(t,x)\phi_{N,i}(x)\,dx = h\frac{f(t,x_i - h/2) + f(t,x_i) + f(t,x_i + h/2)}{3} + O(h^5)\,. \tag{4}$$

In the template "`FEM_heat.py`", complete the function "`build_F(t,N)`" accordingly. The parameters of this function are the time level t and the discretization parameter N. The output shall be the approximated value of the column vector $\underline{\mathrm{F}}$ at time t, using (4).

e) In the template "`FEM_heat.py`", complete the functions "`FEM_theta(N,M,theta)`" which shall implement the Finite Element Method with the fully discrete scheme derived in the previous exercise. Here $N, M, theta$ are the discretization parameters and the function returns the numerical solution on the spatial grid $x_i, i = 1, 2, \ldots, N$ at $t = 1$.

To finish the following two exercises, you first need to modify the block "error analysis" in the script. Follow the comments in this block.

f) Test your code with $\theta = 0.3, 0.5, 1$, $N = 2^l - 1$ and $M = 2^l$ with $l = \{2,3,4,5,6\}$. Do we get a convergent numerical solution for each θ? Use the template to obtain the convergence rates with respect to k and generate the plots describing the convergence rates if they converge. Comment on your results.

g) Test your code with $\theta = 0.3, 0.5, 1$, $N = 2^l - 1$ and $M = 4^l$ with $l = \{2,3,4,5,6\}$. As before, study if those numerical schemes converge and report the convergence rates if they converge. Comment on your results.

Due: Wednesday, March 11th, at 12:00.