Scientific Computing I

(Wissenschaftliches Rechnen I)

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1st excercise sheet

Submission on October 15 or 17, before the lecture

Excercise 1. (3+2=5 points)

Let $I = (0,1)$ be the unit intervall. The eigenfunctions of the one dimensional Laplacian (with homogeneous Dirichlet boundary conditions) are those functions $u \in C^2(I)$ fulfilling

$$\begin{aligned} -u''(x) &= \lambda u(x) \qquad \forall x \in I, \\ u(0) &= 0, \\ u(1) &= 0, \end{aligned}$$

with a corresponding eigenvalue $\lambda \in \mathbb{R}$.

a) Determine all eigenvalues and corresponding eigenfunctions of the one dimensional Laplacian and show that eigenfunctions corresponding to different eigenvalues are pairwise orthogonal w.r.t. $L^2(I)$-scalar product.

Now, choose $n \in \mathbb{N}$ and let $x_i = i/n$, $i = 0, \dots, n$ be the standard partition of I. A function $u \in C^2(I)$ fulfilling $u(0) = u(1) = 0$ can be discretized by the vector $\mathbf{u} \in \mathbb{R}^{n-1}$ such that $\mathbf{u}_i = u(x_i)$, $i = 1, \dots, n-1$. (The boundary condition $u(0) = u(1) = 0$ is encoded in the choice of the space!)

b) Determine the corresponding discretization of the Laplacian, i.e. determine the matrix $\mathbf{A} \in \mathbb{R}^{(n-1)\times(n-1)}$ such that it holds for $u \in C^2(I)$, $u(0) = u(1) = 0$, and its discretization $\mathbf{u} \in \mathbb{R}^{n-1}$:

$$(\mathbf{Au})_i \approx u''(x_i) \qquad \forall i = 1, \dots, n-1.$$

At "$\approx$", use the second order central difference scheme.

Excercise 2. (4+3=7 points)

We consider the tridiagonal matrix

$$\mathbf{K} := \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \in \mathbb{R}^{d\times d}.$$

a) Show that the vectors $v_k := \left(\sin\left(\frac{ik\pi}{d+1}\right)\right)_{i=1,\dots,d} \in \mathbb{R}^d$, $k = 1, \dots, d$ are eigenvectors of $\mathbf{K}$ and compute the corresponding eigenvalues.

Give an interpretation with respect to excercise 1.

b) Show that the condition number of $\mathbf{K}$ fulfills: $\kappa_2(\mathbf{K}) = \mathcal{O}(d^2)$ as $d \longrightarrow \infty$.

We recall the *divergence theorem* resp. *Gauss' theorem*:

Theorem. For a continuously differentiable vector field $F : \Omega \longrightarrow \mathbb{R}^n$ on a bounded open set $\Omega \subset \mathbb{R}^n$ with smooth boundary $\partial\Omega$ it holds:

$$\int_\Omega \operatorname{div} F(x)dx = \int_{\partial\Omega} F(x) \cdot n(x)ds$$

Here, $n : \partial\Omega \longrightarrow \mathbb{R}^n$ denotes the outer normal vector, dx is the Lebesgue measure on Ω and ds the corresponding surface measure on the submanifold $\partial\Omega$.

Excercise 3. (1+1+1=3 points)

Prove the following identities for $u, v \in C^2(\Omega)$:

a) $\int_\Omega \Delta u(x)dx = \int_{\partial\Omega} \nabla u(x) \cdot n(x)ds$

b) $\int_\Omega v(x)\Delta u(x)dx = \int_\Omega \nabla u(x) \cdot \nabla v(x)dx + \int_{\partial\Omega} v(x)\nabla u(x) \cdot n(x)ds$

c) $\int_\Omega (u(x)\Delta v(x) - v(x)\Delta u(x))dx = \int_{\partial\Omega}(u(x)\nabla v(x) \cdot n(x) - v\nabla u(x) \cdot n(x))ds$

Excercise 4. (2+3=5 points)

Given $A : \mathbb{R}^n \longrightarrow \mathbb{R}^{n\times n}$ continuously differentiable, such that $A(x)$ is symmetric and uniformly positive definite[1] for every $x \in \mathbb{R}^n$, we define for $u \in C^2(\mathbb{R}^n)$:

$$(Lu)(x) := -\operatorname{div}_x (A(x)\nabla_x u(x))$$

Such L is a so called second order elliptic differential operator in divergence form.
The subscripts x in div_x resp. ∇_x indicate that divergence resp. gradient are computed with respect to the x-coordinates. Further, let $B \in \mathbb{R}^{n\times n}$ be invertible. We consider the associated coordinate transform $x = By$. With the subscripts y in div_y resp. ∇_y we will indicate that the differential operators are computed with respect to the y-coordinates now.
Define $v(y) := u(By)$ for a scalar function $u \in C^2(\mathbb{R}^n)$ and $V(y) := U(By)$ for a vector field $U \in C^1(\mathbb{R}^n, \mathbb{R}^n)$.

a) Express $\nabla_y v(y)$ resp. $\operatorname{div}_y(V(y))$ in terms of B, u and x.

b) Find an operator $\hat{L}$ of the same structure as L that fulfills $(\hat{L}v)(y) = (Lu)(x)$.

c) (2 bonus points) Show that a function $u \in C^2(\mathbb{R}^n)$ that fulfills $(Lu)(x) < 0$ for all x has no strict local maximum.

Programming excercise 1. (5 bonus programming points)

Implement the finite difference approximation from excercise 1 in python utilizing numpy resp. scipy. Compute approximations for the eigenvalues and plot the corresponding approximations of the eigenfunctions. Compare with the exakt solutions from excercise 1. Which convergence order (w.r.t. n) can you observe?

This first programming excercise is optional, but we recommend to get familiar with python, numpy, matplotlib etc. to be prepared for future programming excercises.

[1] i.e. there is $a > 0$ such that $v^T A(x)v > a\|v\|_2^2$ for all $v \in \mathbb{R}^n$ and $x \in \mathbb{R}^n$.