UC DAVIS, NUMERICAL SOLUTIONS OF DIFFERENTIAL EQUATIONS (MAT 228A), FALL 2016

Homework #1

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Problem 1

Let L be the linear operator $Lu = u_{xx}$, $u_x(0) = u_x(1) = 0$.

(a) Find the eigenfunctions and corresponding eigenvalues of L.

(b) Show that the eigenfunctions are orthogonal in the $L^2[0,1]$ inner product

$$\langle u, v\rangle = \int_0^1 u(x)v(x)\mathrm{d}x.$$

(c) It can be shown that the eigenfunctions $\phi_j(x)$, form a complete set in $L^2[0,1]$. This means that for any $f \in L^2[0,1]$, $f(x) = \sum_j \alpha_j \phi_j(x)$. Express the solution to

$$u_{xx} = f, u_x(0) = u_x(1) = 0,$$

as a series solution of the eigenfunctions.

(d) Note that this BVP does not have a solution for all f. Express the condition for existence of a solution in terms of the eigenfunctions of L.

(a) Let $Lu = \lambda u$. Then

$$\begin{aligned} u_{xx} - \lambda u &= 0 \\ \implies u(x) &= A\exp\left[\sqrt{\lambda}x\right] + B\exp\left[-\sqrt{\lambda}x\right] \end{aligned}$$

If $\lambda > 0$ then $u_x(x) = \sqrt{\lambda}\left[A\exp\left[\sqrt{\lambda}x\right] - B\exp\left[\sqrt{-\lambda}x\right]\right]$ and the boundary condition $u_x(0) = 0$ implies $A = B$ and so $u_x(x) = A\sqrt{\lambda}\left[\exp\left[\sqrt{\lambda}x\right] - \exp\left[-\sqrt{\lambda}x\right]\right]$. Then the boundary condition $u_x(1) = 0$ implies $A = 0$, thus there are no solutions.

If $\lambda = 0$ then $u(x) = A + Bx$ and the boundary conditions implies $B = 0$. Thus $u(x) = A$ where A is a constant is an eigenfunction.

If $\lambda < 0$ then $u(x) = A\sin\left(\sqrt{-\lambda}x\right) + B\cos\left(\sqrt{-\lambda}x\right)$ and thus $u_x(x) = \sqrt{-\lambda}\left[A\cos\left(\sqrt{-\lambda}x\right) - B\sin\left(\sqrt{-\lambda}x\right)\right]$. Then the boundary conditions imply $A = 0$ and $\sqrt{-\lambda} = k\pi$ for $k \in \mathbb{N}$. Thus the eigenfunctions are

$$u_k(x) = \cos(k\pi x) \qquad \text{for } k = 0, 1, 2, \ldots \text{ with corresponding eigenvalues } \lambda_k = -k^2\pi^2$$

(b) Assume $k \neq j$. Then

$$\begin{aligned} \left\langle \cos(k\pi x), \cos(j\pi x)\right\rangle &= \int_0^1 \cos(k\pi x)\cos(j\pi x)\mathrm{d}x \\ &= \frac{1}{2}\int_0^1 \cos\big((k+j)\pi x\big) + \cos\big((k-j)\pi x\big)\mathrm{d}x \\ &= \frac{1}{2}\left[\left.\frac{\sin\big(k+j\big)\pi x}{(k+j)\pi}\right|_0^1 + \left.\frac{\sin\big(k-j\big)\pi x}{(k-j)\pi}\right|_0^1\right] \\ &= \frac{1}{2(k+j)\pi}\left[\sin\big(k+j\big)\pi\right] + \frac{1}{2(k-j)\pi}\left[\sin\big(k-j\big)\pi\right] \end{aligned}$$

Since $k \neq j$ then $k + j$ and $k - j$ are nonzero integers and thus $\left\langle u_k, u_j\right\rangle = 0$. If $k = j$, then

$$\langle \cos(k\pi x), \cos(k\pi x)\rangle = \int_0^1 \cos^2(k\pi x)\mathrm{d}x = \frac{1}{2}\int_0^1 1 + \cos(2k\pi x)\mathrm{d}x = \frac{1}{2}$$

Thus $\sqrt{2}u_k$ are orthonormal.

(c) Let $u = \sum_j \alpha_j \cos(j\pi x)$, and let $f = \sum_j \beta_j \cos(j\pi x)$. Then $u_{xx} = -\sum_j \alpha_j j^2\pi^2 \cos(j\pi x)$. Then

$$-\sum_j \alpha_j j^2\pi^2 \cos(j\pi x) = \sum_j \beta_j \cos(j\pi x)$$

Since $\cos(j\pi x)$ are orthonormal, each term in the series must match, and thus

$$\alpha_j = -\frac{\beta_j}{j^2\pi^2}$$

So, the solution to $Lu = f$ where $f = \sum_j \beta_j \cos(j\pi x)$ is

$$u(x) = -\sum_j \frac{\beta_j}{j^2\pi^2} \cos(j\pi x)$$

(d) Since L is self-adjoint, then $Lu = f$ is solvable if $f \perp \ker L$ where $\ker L = [1]$, that is, the kernel of L is spanned by the constant function 1. $f \perp \ker L$ if

$$\langle f, 1\rangle = \int_0^1 f(x)\mathrm{d}x = 0$$

that is, the mean of $f(x)$ is zero. In terms of the eigenfunctions,

$$\langle f, \cos(0\pi x)\rangle = 0.$$

Problem 2

Define the functional $F : X \to \mathbb{R}$ by

$$F(u) = \int_0^1 \frac{1}{2}(u_x)^2 + fu\,\mathrm{d}x,$$

where X is the space of real-valued functions on $[0,1]$ that have at least one continuous derivative and are zero at $x=0$ and $x=1$. The Frechet derivative of F at a point u is defined to be the linear operator $F'(u)$ for which

$$F(u+v) = F(u) + F'(u)v + R(v),$$

where

$$\lim_{\|v\|\to 0} \frac{\|R(v)\|}{\|v\|} = 0.$$

One way to compute the derivative is

$$F'(u)v = \lim_{\varepsilon\to 0} \frac{F(u+\varepsilon v) - F(u)}{\varepsilon}.$$

Note that this looks just like a directional derivative.

(a) Compute the Frechet derivative of F.

(b) $u \in X$ is a critical point of F if $F'(u)v = 0$ for all $v \in X$. Show that if u is a solution to the Poisson eqution $u_{xx} = f$, $u(0) = u(1) = 0$, then it is a critical point of F.

(c) Let X_h be a finite dimensional subspace of X, and let $\{\phi_i(x)\}$ be a basis for X_h. This means that all $u_h \in X_h$ can be expressed as $u_h(x) = \sum_i u_i\phi_i(x)$ for some constants u_i. Thus we can identify the elements of X_h with vectors $\vec{u}$ that have components u_i. Let $G(\vec{u}) = F(u_h)$. Show that the gradient of G (whos components are $(\nabla G)_j = \frac{\partial G}{\partial u_j}$) is of the form $\nabla G(\vec{u}) = A\vec{u} + \vec{b}$, and write expressions for the elements of the matrix A and the vector $\vec{b}$.

(d) Divide the unit interval into a set of $N+1$ equal length intervals $I_i = (x_i, x_{i+1})$ for $i = 0,\dots,N$. The enpoints of the intervals are $x_i = ih$, where $h = \frac{1}{N+1}$. Let X_h be the subspace of X such that the elements u_h of X_h are linear on each interval, continuous on $[0,1]$, and satisfy $u_h(0) = u_h(1) = 0$. X_h is an N dimensional space with basis elements

$$\phi_i(x) = \begin{cases} 1 - h^{-1}|x - x_i| & \text{if } |x - x_i| < h, \\ 0 & \text{otherwise} \end{cases}$$

for $i = 1,\dots,N$. Compute the matrix A from the previous problem that appears in the gradient.

Finite element methods are based on these "weak formulations" of the problem. The Ritz method is based on minimizing F and the Galerkin method is based on finding the critical points of $F'(u)$.

(a)

$$\begin{aligned}
F'(u)v &= \lim_{\varepsilon\to 0} \frac{F(u+\varepsilon v) - F(u)}{\varepsilon} \\
&= \lim_{\varepsilon\to 0} \frac{\int_0^1 \frac{1}{2}(u_x + \varepsilon v_x)^2 + f(u+\varepsilon v) - \frac{1}{2}u_x^2 - fu\,\mathrm{d}x}{\varepsilon} \\
&= \lim_{\varepsilon\to 0} \int_0^1 u_x v_x + \frac{1}{2}\varepsilon v_x^2 + fv\,\mathrm{d}x \\
&= \int_0^1 u_x v_x + fv\,\mathrm{d}x \\
&= [vu_x]_0^1 + \int_0^1 v(f - u_{xx})\,\mathrm{d}x
\end{aligned}$$

But $v \in X$, and thus $v(0) = v(1) = 0$. So, for all v,

$$F'(u)\,v = \int_0^1 v\big(f - u_{xx}\big)\mathrm{d}x$$

(b) Let u be a solution to the Poisson equation. Then $u_{xx} = f$. Then $u_{xx} - f = 0$. Thus,

$$F'(u)v = \int_0^1 v(f - u_{xx})\mathrm{d}x = \int_0^1 v \cdot 0 \mathrm{d}x = 0$$

(c)

$$G(\vec{u}) = F(u_h) = \int_0^1 \frac{1}{2}\left(\sum_{i=1}^n u_i \phi_i'(x)\right)^2 + f(x)\sum_{i=1}^n u_i \phi_i(x)\mathrm{d}x$$

$$\implies (\nabla G)_j = \frac{\partial}{\partial u_j} G(\vec{u}) = \int_0^1 \left(\sum_{i=1}^n u_i \phi_i(x)\right)\phi_j'(x) + f(x)\phi_j(x)\mathrm{x}$$

$$= \left[\phi_j \sum_{i=1}^n u_i \phi_i'\right]_0^1 + \int_0^1 \phi_j(x)\left(f(x) - \sum_{i=1}^n u_i \phi_i''(x)\right)\mathrm{d}x$$

But the boundary conditions are 0 since $\phi_j \in X_h \subset X$ and $u(0) = u(1) = 0$ for all $u \in X$. Thus,

$$(\nabla G)_j = -\int_0^1 \left(\sum_{i=1}^n u_i \phi_i''(x)\right)\phi_j(x)\mathrm{d}x + \int_0^1 f(x)\phi_j(x)\mathrm{d}x$$
$$= A\vec{u} + \vec{b}$$

where $\vec{b} = \begin{pmatrix} \int_0^1 f(x)\phi_1(x)\mathrm{d}x \\ \int_0^1 f(x)\phi_2(x)\mathrm{d}x \\ \vdots \\ \int_0^1 f(x)\phi_n(x)\mathrm{d}x \end{pmatrix}$ and $A = (a_{ij})$ where $a_{ij} = -\int_0^1 \phi_i(x)\phi_j''(x)\mathrm{d}x$.

(d) Note that

$$\phi_i(x) = \begin{cases} 1 - h^{-1}|x - x_i| & \text{if } |x - x_i| < h, \\ 0 & \text{otherwise} \end{cases}$$

and thus

$$\phi_i'(x) = \begin{cases} \frac{1}{h} & \text{if } x_{i-1} < x < x_i \\ -\frac{1}{h} & \text{if } x_i < x < x_{i+1} \\ 0 & \text{otherwise} \end{cases} \qquad \text{and} \qquad \phi_i''(x) = \delta\left(x - \frac{i}{N+1}\right)$$

This shows

$$a_{ij} = -\int_0^1 \phi_i(x)\delta\left(x - \frac{j}{N+1}\right)\mathrm{d}x = -\phi_i\left(\frac{j}{N+1}\right) = \begin{cases} -1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

and so $A = -I$ where I is the $n \times n$ identity matrix.

Problem 3

(a) Using a Taylor expansion, derive the finite difference formula to approximate the second derivative at x using function values at $x - \frac{h}{2}$, x, and $x + h$. How accurate is the finite difference approximation?

(b) Perform a refinement study to verify the accuracy of the difference formula you derived.

(c) Derive an expression for the quadratic polynomial that interpolates the data $\left(x - \frac{h}{2}, u\left(x - \frac{h}{2}\right)\right)$, $(x, u(x))$, and $(x + h, u(x + h))$. How is the finite difference formula you derived in problem 3a related to the interpolating polynomial?

(a) Let D^2 be a finite difference formula for the secon derivative. Then

$$\begin{aligned}(D^2u)_j &= au\left(x-\frac{h}{2}\right)+bu(x)+cu(x+h)\\ &= (a+b+c)u(x)+\left(c-\frac{a}{2}\right)hu'(x)+\left(\frac{a}{8}+\frac{c}{2}\right)h^2u''(x)+\left(\frac{c}{6}-\frac{a}{48}\right)h^3u'''(x)+\dots\end{aligned}$$

The letting $a+b+c=0$, $c=\frac{a}{2}$ and $a=\frac{8}{3h^2}$, we get

$$(D^2u)_j = u''(x)+\frac{h}{6}u'''(x)+\dots$$

where $a=\frac{8}{3h^2}$, $b=-\frac{4}{h^2}$, and $c=\frac{4}{3h^2}$. Thus

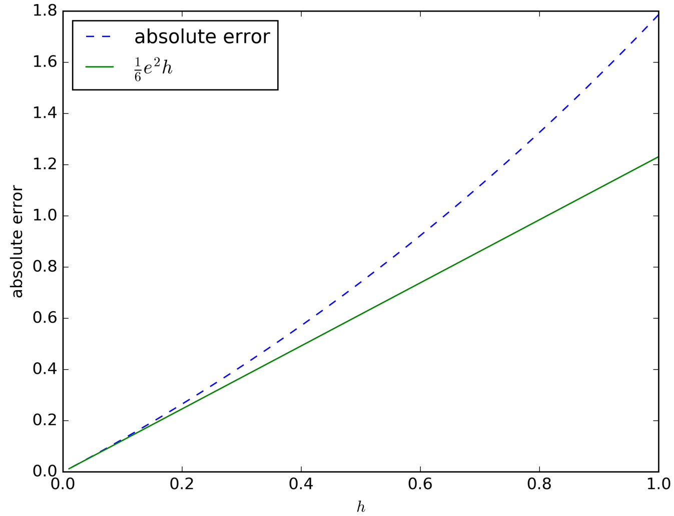
$$(D^2u)_j = \frac{8}{3h^2}u\left(x-\frac{h}{2}\right)-\frac{4}{h^2}u(x)+\frac{4}{3h^2}u(x+h)$$

Note that $\dfrac{c}{6}-\frac{a}{48}=\frac{1}{6h^2}$ and thus the $u'''(x)$ term is order h. This means D^2 has $\mathcal{O}(h)$ accuracy.

(b) I tested the accuracy of the second derivative of the function $f(x)=e^x$ at the point $x=2$. Below is the Python (version 2.7.x) code used to plot absolute error of the approximation as a function of h.

```
from __future__ import division
import numpy as np
from math import exp
import matplotlib.pyplot as plt

x = 2
true_val = exp(2)

def approximation(h):
    A = (8/(3*(h**2)))*exp(x - (h/2))
    B = (4/(h**2))*exp(x)
    C = (4/(3*(h**2)))*exp(x + h)
    return A - B + C

h = np.linspace(1, 0.01, 100)
approx_vals = [approximation(H) for H in h]
errors = [abs(i - true_val) for i in approx_vals]

plt.figure()
plt.plot(h, errors, "--", label="absolute␣error")
plt.plot(h, (1/6)*h*exp(x), label=r"$\frac{1}{6}e^2h$")
plt.legend(loc=0)
plt.xlabel(r"$h$")
plt.ylabel("absolute␣error")
plt.savefig("problem_3.png", dpi=300)
plt.close()
```

Below is the outcome of the analysis. Notice the plot is asymptotically linear near 0. The $\mathcal{O}(h)$ term in the Taylor expansion is plotted for reference.



(c) The polynomial through the points

$$(x, u(x)) \qquad (x+h, u(x+h)) \qquad \left(x-\frac{h}{2}, u\left(x-\frac{h}{2}\right)\right)$$

satisfies

$$\begin{aligned} u(x) &= A + Bx + Cx^2 \\ u(x+h) &= A + B(x+h) + C(x+h)^2 \\ u\left(x-\frac{h}{2}\right) &= A + B\left(x-\frac{h}{2}\right) + C\left(x-\frac{h}{2}\right)^2 \end{aligned}$$

This is a simple linear algebra problem that can be solved symbolically using a symbolic solver like Maple or Python (`sympy` package). We get:

$$\begin{aligned} A &= \frac{1}{3h^2}\left(3h^2u(x) + 4hu\left(x-\frac{h}{2}\right)x - 3hu(x)x - hu(x+h)x + 4u\left(x-\frac{h}{2}\right)x^2 - 6u(x)x^2 + 2u(x+h)x^2\right) \\ B &= -\frac{1}{3h^2}\left(4hu\left(x-\frac{h}{2}\right) - 3hu(x) - hu(x+h) + 8u\left(x-\frac{h}{2}\right)x - 12u(x)x + 4u(x+h)x\right) \\ C &= \frac{2}{3h^2}\left(2u\left(x-\frac{h}{2}\right) - 3u(x) + u(x+h)\right) \end{aligned}$$

Then note that since $u(x) = A + Bx + Cx^2$, then $u''(x) = 2C = \frac{8}{3h^2}u\left(x-\frac{h}{2}\right) - \frac{4}{h^2}u(x) + \frac{4}{3h^2}u(x+h)$, which exactly matches with the finite difference formula from part (a). This means the best possible second derivative approximation using three points is precisely the quadratic function through those points.