Homework 5 · Solutions

Posted Tuesday, October 17. Due Thursday, November 2, by 5pm.

- A note on proofs (unless otherwise stated by the problem): When asked to prove a statement this means you are to show that the requisite properties (discussed in class) for the item referenced by the statement hold true. When asked to disprove something this means you are to come up with an example that shows the proposed premise is false.
- Unless explicitly stated otherwise in the problem you are free to use MATLAB as you see fit; including for those problems that do not explicitly require it. Please submit any code that you utilize as a printout or, if it is short enough, reference your steps in your writeup directly. (example: I used MATLAB to compute the inverse to the matrix B and got...

Please write your name and instructor on your homework. There is a total of 70 points distributed among the problems below

1. [24 points: 5 points (a), 3 points (b), 8 points (c) and (d)]
   Let \( k(x) \) and \( p(x) \) be two positive-valued continuous functions on \([0,1]\).
   
   (a) Derive the weak form of the differential equation
   \[
   -\frac{d}{dx} \left( k(x) \frac{du}{dx} \right) + p(x) u = f(x), \quad 0 < x < 1,
   \]
   subject to the boundary conditions
   \[ u(0) = u(1) = 0. \]
   
   Write the full weak problem statement.
   
   (b) Verify that the bilinear form \( a(u,v) \) that you found in part (a) is an inner product.
   
   (c) Let \( p(x) = 1 \), \( k(x) = \epsilon \), and let the source function \( f(x) = 1 \). Construct the finite element system \( Au = b \), using the approximation space \( V_N \) given by the piecewise linear hat functions: for \( n \geq 1 \),
   \( h = 1/(N+1) \), and \( x_k = kh \) for \( k = 0, \ldots, N + 1 \):
   \[
   \phi_k(x) = \begin{cases} 
   (x - x_{k-1})/h, & x \in [x_{k-1}, x_k); \\
   (x_{k+1} - x)/h, & x \in [x_k, x_{k+1}); \\
   0, & \text{otherwise.} 
   \end{cases}
   \]
   
   Hint: For this specific choice of \( p(x) \) and \( k(x) \), it may be easier to show that you can express
   \[ A = \epsilon K + M, \]
   where \( K_{ij} = \int_0^1 \frac{\partial \phi_i}{\partial x} \frac{\partial \phi_j}{\partial x} \) and the form of \( M \) is that determined in Homework 3, problem 5c (the pledged problem).
   
   (d) This specific equation corresponds to the simplest steady-state reaction-diffusion equation, where \( u(x) \) is the concentration of some solvent, and the choices of \( p(x) \) model local chemical reactions that may occur due to that solvent (multiple chemicals interacting may be modeled using systems of reaction-diffusion equations).
   Use MATLAB to solve the above system with \( N = 32 \) and \( \epsilon = .1, .25, 1 \) and plot your results. In a separate figure, plot the results for \( \epsilon = .1, .01, .001 \). What do you observe about the solution as \( \epsilon \) decreases?

Solution.
(a) [5 points] Multiply the differential equation with some function $v$ from the space $V$ and integrate from $x = 0$ to $x = 1$ to obtain

$$
\int_0^1 \left( - \frac{d}{dx} \left(k(x) \frac{du}{dx}(x)\right) + p(x)u(x)v(x) \right) dx = \int_0^1 f(x)v(x) dx.
$$

Break the integral on the left into pieces to obtain

$$
\int_0^1 \left( - \frac{d}{dx} \left(k(x) \frac{du}{dx}(x)\right) \right) v(x) dx + \int_0^1 \left( p(x)u(x) \right) v(x) dx = \int_0^1 f(x)v(x) dx.
$$

Integrate the first integral by parts to obtain

$$
- \left[ k(x) \frac{du}{dx}(x)v(x) \right]_0^1 + \int_0^1 k(x) \frac{du}{dx}(x) \frac{dv}{dx} (x) dx + \int_0^1 \left( p(x)u(x) \right) v(x) dx = \int_0^1 f(x)v(x) dx.
$$

The boundary terms vanish due to the fact that $v(0) = v(1) = 0$ if $v \in V = C^2_0[0,1]$. We consolidate the integrals on the left to arrive at the weak problem:

Find $u \in V$ such that $a(u,v) = (f,v)$ for all $v \in V$,

where

$$a(u,v) = \int_0^1 \left( k(x) \frac{du}{dx}(x) \frac{dv}{dx} (x) + p(x)u(x)v(x) \right) dx.$$

(b) [3 points] To show that the form $a(u,v)$ in part (a) is an inner product, we must verify the three basic properties:

- **Symmetry** is apparent by inspection:

  $$a(u,v) = \int_0^1 \left( k(x) \frac{du}{dx}(x) \frac{dv}{dx} (x) + p(x)u(x)v(x) \right) dx
  = \int_0^1 \left( k(x) \frac{dv}{dx}(x) \frac{du}{dx} (x) + p(x)v(x)u(x) \right) dx = a(v,u).$$

- **Linearity** follows from the linearity of differentiation and integration:

  $$a(\alpha u + \beta v, w) = \int_0^1 \left( k(x) \frac{d(\alpha u(x) + \beta v(x))}{dx} \right) \frac{dw}{dx}(x) + p(x)(\alpha u(x) + \beta v(x))w(x) dx
  = \int_0^1 \left( k(x) \frac{du}{dx}(x) + \beta \frac{dv}{dx}(x) \right) \frac{dw}{dx}(x) + p(x)(\alpha u(x) + \beta v(x))w(x) dx
  = \alpha a(u,w) + \beta a(v,w).$$

- **Positivity** requires that $a(u,u) \geq 0$ and $a(u,u) = 0$ only when $u = 0$. Note that

  $$a(u,u) = \int_0^1 \left( k(x) \frac{du}{dx}(x) \frac{du}{dx}(x) + p(x)u(x)u(x) \right) dx
  = \int_0^1 \left( k(x) \left( \frac{du}{dx}(x) \right)^2 + p(x)(u(x))^2 \right) dx.$$  

Since $k(x)$ and $p(x)$ are both positive for all $x \in [0,1]$, each integrand is non-negative, and hence $a(u,u) \geq 0$. To have $a(u,u) = 0$, we must have $u(x) = 0$ for all $x \in [0,1]$, and $du(x)/dx = 0$ for all $x \in [0,1]$, which is only possible if $u(x) = 0$ for all $x \in [0,1]$, i.e., $u = 0$. 

(c) [8 points] If \( p(x) = 1 \) and \( k(x) = \epsilon \), our formulation reduces down to \( a(u, v) = (f, v) \) where

\[
a(u, v) = \int_0^1 u(x)v(x)dx + \epsilon \int_0^1 \frac{\partial u}{\partial x} \frac{\partial v}{\partial x} dx.
\]

Then, if \( A_{ij} = a(\phi_j, \phi_i) \), we have

\[
A_{ij} = \int_0^1 \phi_j(x)\phi_i(x)dx + \epsilon \int_0^1 \frac{\partial \phi_j}{\partial x} \frac{\partial \phi_i}{\partial x} dx = M_{ij} + \epsilon K_{ij}
\]

where \( M_{ij} = \int_0^1 \phi_j(x)\phi_i(x)dx \) is the Gram matrix for hat functions using the \( L^2 \) inner product. The entries of \( M \) and \( K \) are known to be

\[
M_{ij} = \begin{cases} 
2h/3 & i = j \\
h/6 & i + 1 = j \\
0 & |i - j| > 1
\end{cases}, \\
K_{ij} = \begin{cases} 
2/h & i = j \\
-1/h & i + 1 = j \\
0 & |i - j| > 1
\end{cases}
\]

It is known that \( b_i = h \) for all \( i \).

(d) [8 points] The code to generate the figures for this problem is given below.

```matlab
iter = 1;
C = hsv(3);
for ep = [1 .25 .1];
N = 32;
h = 1/(N+1);
x = [1:N]*h;
M = (2/3)*diag(ones(N,1)) + (1/6)*diag(ones(N-1,1),1) + (1/6)*diag(ones(N-1,1),-1);
M = h*M;
K = 2*diag(ones(N,1)) - diag(ones(N-1,1),1) - diag(ones(N-1,1),-1);
K = (1/h)*K;
A = M + ep*K;
b = h*ones(N,1);
c = A\b;
xx = linspace(0,1,500)';
hold on
% plot the approximation solution
uN = zeros(size(xx));
for j=1:N
uN = uN + c(j)*hat(xx,j,N);
end
plot(xx,uN,'color',C(iter,:),'linewidth',2)
iter = iter + 1;
end
legend('\epsilon = 1','\epsilon = .25','\epsilon = .1')
set(gca,'fontsize',14)
xlabel('x','fontsize',15)
ylabel('Solution u(x)','fontsize',15)
print(gcf,'-depsc','../ep1.eps')
```
As $\epsilon$ decreases, the temperature in the bar increases. It is difficult to see with $\epsilon \geq .1$, but as $\epsilon$ gets small, the solution actually develops additional characteristics called boundary layers, where the solution becomes very steep near the boundaries. \textit{Graders: please give credit just for noting the temperature increases, as the boundary layer phenomena was not visible for the range of $\epsilon$ specified in the problem.}

2. [26 points: 8 points (a) and (d); 5 points (b) and (c)]

A classical problem in quantum mechanics models a particle moving in an infinite square well, subject to an infinite potential at a point. The result is a Schrödinger operator posed on $C^2_D[0,1]$ of the form

$$Lu = -u'' + \delta_{1/2}u,$$

where

$$\delta_{1/2}(x) = \delta(x - 1/2) = \begin{cases} 1 & \text{if } x = 1/2 \\ 0 & \text{otherwise} \end{cases}$$

Note, for any function $g \in C[0,1]$,

$$\int_0^1 \delta_{1/2}(x)g(x) \, dx = g(1/2).$$

The equivalent weak problem is: Find $u \in C^2_D[0,1]$ such that for all $w \in V = C^2_D[0,1]$

$$a(u, w) = (f, w)$$

where

$$a(u, w) = \int_0^1 \left( u'(x)w'(x) + \delta_{1/2}(x)u(x)w(x) \right) \, dx.$$

and $(f, w)$ is simply the $L^2$ inner product of $f$ and $w$.

Let $V_N = \text{span}\{\phi_1, \ldots, \phi_N\} \subset C^2_D[0,1]$ where

$$\phi_k(x) = \sqrt{2} \sin(k\pi x), \quad k = 1, \ldots, N$$

denote our finite dimensional subspace.

(a) Compute a general formula for $a(\phi_j, \phi_k)$ for $1 \leq j \leq N$ and $1 \leq k \leq N$. 
(b) Write out (by hand) the stiffness matrix for $N = 5$.

(c) Write down a general formula for the $k^{th}$ entry in the load vector, $(f, \phi_k)$, when $f(x) = 1$.

(d) Plot your approximate solutions to $-u''(x) + \delta_{1/2}(x)u(x) = 1$ for $N = 5, 10, 20, 35, 100$ in five separate plots (one for each value of $N$). Explain what you see as you increase $N$. Note: To see some of the differences between higher values of $N$, you may need to zoom in on the plots.

Solution.

(a) [8 points] Compute
\[
a(\phi_j, \phi_k) = \int_0^1 \left( \phi_j'(x)\phi_k'(x) + \delta_{1/2}(x)\phi_j(x)\phi_k(x) \right) dx \\
= 2kj\pi^2 \int_0^1 \cos(j\pi x)\cos(k\pi x) dx + 2\int_0^1 \delta_{1/2}(x)\sin(j\pi x)\sin(k\pi x) \\
= 2kj\pi^2 \int_0^1 \cos(j\pi x)\cos(k\pi x) dx + 2\sin(j\pi/2)\sin(k\pi/2).
\]

The integral in this last expression is $1/2$ when $j = k$, and zero otherwise. The second term will be zero if either $j$ or $k$ is even (since in that case one of the sine terms must be zero). If both $j$ and $k$ are odd, this term will be nonzero, $\pm 2$. In general, we can write
\[
a(\phi_j, \phi_k) = \begin{cases} 
   j^2\pi^2 + 2\sin^2(j\pi/2), & \text{if } j = k; \\
   2\sin(j\pi/2)\sin(k\pi/2), & \text{otherwise}.
\end{cases}
\]

[GRADERS: the amount that students simplify $a(\phi_j, \phi_k)$ will vary. The ultimate solution need not take the precise form that we have given above, but it should be simplified beyond just writing down the definition of $a(\phi_j, \phi_k)$.]\]

(b) [8 points] For $N = 5$ we have
\[
\begin{bmatrix}
\pi^2 + 2 & 0 & -2 & 0 & 2 \\
0 & 4\pi^2 & 0 & 0 & 0 \\
-2 & 0 & 9\pi^2 + 2 & 0 & -2 \\
0 & 0 & 0 & 16\pi^2 & 0 \\
2 & 0 & -2 & 0 & 25\pi^2 + 2
\end{bmatrix}
\]

(c) [5 points] The entries of the load vector are
\[
(f, \phi_k) = \int_0^1 1 \cdot \sqrt{2}\sin(k\pi x) dx = \begin{cases} 
   2\sqrt{2}/(n\pi), & \text{if } k \text{ is odd}; \\
   0, & \text{if } k \text{ is even},
\end{cases}
\]

as computed in previous examples earlier in the semester.

[GRADERS: students do not need to show work for this formula.]\]

(d) [5 points] Approximate solutions for $N = 5, 10, 20, 35, 100$ are shown below, followed by the code that produced them.

From these plots, we see that by including higher frequency basis functions in our approximate solutions, we are able to better capture the effect of the delta function at $x = 1/2$. 

for $N = [5, 10, 20, 35, 100]$

```matlab
K = zeros(N); f = zeros(N,1);
for j=1:N, for k=1:N
    K(j,k) = 2*sin(j*pi/2)*sin(k*pi/2);
end, end
K = K + diag([1:N].^2*pi^2);
for k=1:N
    f(k) = (sqrt(2)/pi)*(1+(-1).^(k+1))./k;
end
c = K\f;
xx = linspace(0,1,1000);
uN = zeros(size(xx));
for k=1:N
```
\[ u_N = u_N + c(k) \sqrt{2} \sin(k \pi x); \]
\[ \text{end} \]
\[ \text{figure}(N), \text{clf} \]
\[ \text{plot}(x, u_N, 'r-', 'linewidth', 2) \]
\[ \text{title}('\text{Galerkin solution for } N=' N, 'interpreter','latex','fontsize', 18) \]
\[ \text{xlabel}('x', 'interpreter','latex','fontsize', 16) \]
\[ \text{ylabel}('u_N(x)', 'interpreter','latex','fontsize', 16) \]
\[ \text{set(gca, 'fontsize', 14}) \]
\[ \text{eval}(\text{sprintf('print -depsc2 delta_''d', N)}) \]
\[ \text{if } N==5, \text{disp}(K), \text{end} \]
\[ \text{end} \]

3. [10 points: 6 points (a), 4 points (b)]
Consider the following boundary value problem
\[ -(k(x)u')' + q(x)u = f(x), \quad 0 < x < \ell, \]
subject to the boundary conditions
\[ u(0) - k(0)u'(0) = \beta, \quad u'(\ell) = 0 \]
for some constant $\beta$. Assume that $q$ and $f$ are continuous on $[0, \ell]$ and $k \in C^1[0, \ell]$.

(a) Derive the weak form of the above problem. Write the variational problem statement.

(b) Show that the weak form from part (a) is equivalent to the strong form of the boundary value problem.

Solution.

(a) [6 points] Let $V = \{ v \in C^2[0, 1] : v(0) - k(0)v'(0) = \beta, v'(\ell) = 0 \}$.

GRADERS: they also can use $V = \{ v \in C^2[0, 1] : v'(0) = 0, v'(\ell) = 0 \}$ or $V = \{ v \in C^2[0, 1] : v(0) = 0, v'(\ell) = 0 \}$ Take a test function $v \in V$. Multiply the differential equation by the test function $v \in V$ and integrate both sides from $x = 0$ to $x = \ell$ to obtain
\[ -\int_0^\ell (k(x)u'(x))'v(x)dx + \int_0^\ell q(x)u(x)v(x)dx = \int_0^\ell f(x)v(x)dx. \]

Use integration by parts on the left-most term to obtain
\[ \int_0^\ell k(x)u'(x)v'(x)dx + k(0)u'(0)v(0) - k(\ell)u'(\ell)v(\ell) + \int_0^\ell q(x)u(x)v(x)dx = \int_0^\ell f(x)v(x)dx. \]

Plugging in the boundary conditions, we can then consolidate the integrals on the left to arrive at the weak problem:

Find $u \in V$ such that $a(u, v) = (f, v) + \beta v(0)$ for all $v \in V$,

where
\[ a(u, v) = \int_0^\ell [k(x)u'(x)v'(x) + q(x)u(x)v(x)]dx + u(0)v(0). \]
(b) [4 points] The part "strong form to weak form" is shown above in part (a). Suppose \( u \) is a solution to the weak form in part (a). Then "weak form to strong form" can be shown by going backward in (a) and using the fact that

\[
-\int_0^\ell (k(x)u'(x))'v(x)dx + \int_0^\ell q(x)u(x)v(x)dx = \int_0^\ell f(x)v(x)dx
\]

\[
\Rightarrow \int_0^\ell [-(k(x)u'(x))' + q(x)u(x) - f(x)]v(x)dx = 0.
\]

Since this relationship holds for all test functions \( v \in V \) and we know that \( k \in C^1[0, \ell] \), \( q \in C[0, \ell] \), and \( f \in C[0, \ell] \), we can conclude that \( -(k(x)u'(x))' + q(x)u(x) - f(x) = 0 \). Hence, \( u \) must also be a solution to the strong form.

4. [10 points: 5 points each] **This problem is pledged!**

You may not discuss this with anyone but your instructor. You may not consult any source other than approved textbooks, CAAM 336 lecture notes or your in-class notes to help you with the problem.

Let \( k(x) \) and \( p(x) \) be two positive-valued continuous functions on \([0, 1]\).

(a) Derive the weak form of the differential equation

\[-\frac{d}{dx}(k(x)\frac{du}{dx}) + p(x)u = f(x), \quad 0 < x < 1,\]

subject to the boundary conditions

\[u(0) = \frac{du}{dx}(1) = 0.\]

Write the variational problem statement.

(b) Show that the bilinear form \( a(u, v) \) from the weak formulation in part (a) is an inner product for \( u, v \in V \).

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**Solution.**

(a) [5 points] The process is very similar to problem 1 (a). Multiply the differential equation with some function \( v \) from the space \( V \) and integrate from \( x = 0 \) to \( x = 1 \) to obtain

\[
\int_0^1 \left( -\frac{d}{dx}(k(x)\frac{du}{dx})v(x) + p(x)u(x)v(x) \right) dx = \int_0^1 f(x)v(x)dx.
\]

Break the integral on the left into pieces to obtain

\[
\int_0^1 \left( -\frac{d}{dx}(k(x)\frac{du}{dx}) \right) v(x) dx + \int_0^1 \left( p(x)u(x)v(x) \right) dx = \int_0^1 f(x)v(x)dx.
\]

Integrate the first integral by parts to obtain

\[
-\left[k(x)\frac{du}{dx}(x)v(x)\right]_0^1 + \int_0^1 k(x)\frac{du}{dx}(x)\frac{dv}{dx}(x) dx + \int_0^1 \left( p(x)u(x)v(x) \right) dx = \int_0^1 f(x)v(x)dx.
\]

The first term disappears because of the boundary conditions \( v(0) = 0 \) and \( du(1)/dx = 0 \). We consolidate the integrals on the left to arrive at the weak problem:

Find \( u \in V \) such that \( a(u, v) = (f, v) \) for all \( v \in V \),

where

\[
a(u, v) = \int_0^1 \left( k(x)\frac{du}{dx}(x)\frac{dv}{dx}(x) + p(x)u(x)v(x) \right) dx.
\]
(b) [5 points] The proof is identical to the proof for 1(b). *Graders: please give full credit if the student notices this.*