### 18.303 Problem Set 2

Due Monday, 22 September 2014.

## Problem 2: Modified inner products for column vectors

Consider the inner product $\langle\mathbf{x}, \mathbf{y}\rangle=\mathbf{x}^{*} B \mathbf{y}$ from class (lecture 5.5 notes), where the vectors are in $\mathbb{C}^{N}$ and $B$ is an $N \times N$ Hermitian positive-definite matrix.
(a) Show that this inner product satisfies the required properties of inner products from class: $\langle\mathbf{x}, \mathbf{y}\rangle=\overline{\langle\mathbf{y}, \mathbf{x}\rangle},\langle\mathbf{x}, \mathbf{x}\rangle>0$ except for $\mathbf{x}=0$. (Linearity $\langle\mathbf{x}, \alpha \mathbf{y}+\mathbf{z}\rangle=\alpha\langle\mathbf{x}, \mathbf{y}\rangle+\langle\mathbf{x}, \mathbf{z}\rangle$ is obvious from linearity the of matrix operations; you need not show it.)
(b) If $M$ is an arbitrary (possibly complex) $N \times N$ matrix, define the adjoint $M^{\dagger}$ by $\langle\mathbf{x}, M \mathbf{y}\rangle=$ $\left\langle M^{\dagger} \mathbf{x}, \mathbf{y}\right\rangle$ (for all $\mathbf{x}, \mathbf{y}$ ). (In this problem, we use $\dagger$ instead of $*$ for the adjoint in order to avoid confusion with the conjugate transpose: for this inner product, the adjoint $M^{\dagger}$ is not the conjugate transpose $M^{*}=\overline{M^{T}}$.) Give an explicit formula for $M^{\dagger}$ in terms of $M$ and $B$.
(c) Using your formula from above, show that $M^{\dagger}=M$ (i.e., $M$ is self-adjoint/Hermitian for this inner product) if $M=B^{-1} A$ for some $A=A^{*}$.

## Problem 2: Finite-difference approximations

For this question you may find it helpful to refer to the notes and readings from lecture 3. Suppose that we want to compute the operation

$$
\hat{A} u=\frac{d}{d x}\left[c \frac{d u}{d x}\right]
$$

for some smooth function $c(x)$ (you can assume $c$ has a convergent Taylor series everywhere). Now, we want to construct a finite-difference approximation for $\hat{A}$ with $u(x)$ on $\Omega=[0, L]$ and Dirichlet boundary conditions $u(0)=u(L)=0$, similar to class, approximating $u(m \Delta x) \approx u_{m}$ for $M$ equally spaced points $m=1,2, \ldots, M, u_{0}=u_{M+1}=0$, and $\Delta x=\frac{L}{M+1}$.
(a) Using center-difference operations, construct a finite-difference approximation for $\hat{A} u$ evaluated at $m \Delta x$. (Hint: use a centered first-derivative evaluated at grid points $m+0.5$, as in class, followed by multiplication by $c$, followed by another centered first derivative. Do not separate $\hat{A} u$ by the product rule into $c^{\prime} u^{\prime}+c u^{\prime \prime}$ first, as that will make the factorization in part (d) more difficult.)
(b) Show that your finite-difference expressions correspond to approximating $\hat{A} u$ by $A u$ where $\mathbf{u}$ is the column vector of the $M$ points $u_{m}$ and $A$ is a real-symmetric matrix of the form $A=-D^{T} C D$ (give $C$, and show that $D$ is the same as the 1st-derivative matrix from lecture).
(c) In Julia, the diagm (c) command will create a diagonal matrix from a vector c. The function $\operatorname{diff} 1(M)=[[1.0 \operatorname{zeros}(1, M-1)] ; \operatorname{diagm}(o n e s(M-1), 1)-\operatorname{eye}(M)]$
will allow you to create the $(M+1) \times M$ matrix $D$ from class via $D=\operatorname{diff} 1$ (M) for any given value of $M$. Using these two commands, construct the matrix $A$ from part (d) for $M=100$ and $L=1$ and $c(x)=e^{3 x}$ via
$\mathrm{L}=1$
$M=100$
D $=\operatorname{diff} 1(M)$
$d x=L /(M+1)$
$x=d x * 0.5: d x: L \#$ sequence of $x$ values from $0.5 * d x$ to $<=$ L in steps of $d x$ $C=\ldots$ something from $c(x) \ldots$ hint: use diagm...
$\mathrm{A}=-\mathrm{D}, * \mathrm{C} * \mathrm{D} / \mathrm{dx}^{\wedge} 2$
You can now get the eigenvalues and eigenvectors by $\lambda, U=\operatorname{eig}(A)$, where $\lambda$ is an array of eigenvalues and $U$ is a matrix whose columns are the corresponding eigenvectors (notice that all the $\lambda$ are $<0$ since $A$ is negative-definite).
(i) Plot the eigenvectors for the smallest-magnitude four eigenvalues. Since the eigenvalues are negative and are sorted in increasing order, these are the last four columns of $U$. You can plot them with:
using PyPlot
plot(dx:dx:L-dx, U[:,end-3:end])
xlabel("x"); ylabel("eigenfunctions")
legend(["fourth", "third", "second", "first"])
(ii) Verify that the first two eigenfunctions are indeed orthogonal with $\operatorname{dot}(\mathbb{U}[:$, end , $\mathrm{U}\left[\right.$ : ,end-1]) in Julia, which should be zero up to roundoff errors $\lesssim 10^{-15}$.
(iii) Verify that you are getting second-order convergence of the eigenvalues: compute the smallest-magnitude eigenvalue $\lambda_{M}$ [end] for $M=100,200,400,800$ and check that the differences are decreasing by roughly a factor of 4 (i.e. $\left|\lambda_{100}-\lambda_{200}\right|$ should be about 4 times larger than $\left|\lambda_{200}-\lambda_{400}\right|$, and so on), since doubling the resolution should multiply errors by $1 / 4$.
(d) For $c(x)=1$, we saw in class that the eigenfunctions are $\sin (n \pi x / L)$. How do these compare to the eigenvectors you plotted in the previous part? Try changing $c(x)$ to some other function (note: still needs to be real and $>0$ ), and see how different you can make the eigenfunctions from $\sin (n \pi x / L)$. Is there some feature that always remains similar, no matter how much you change $c$ ?

## Problem 3: Discrete diffusion

In this problem, you will examine thermal conduction in a system of a finite number $N$ of pieces, and then take the $N \rightarrow \infty$ limit to recover the heat equation. In particular:

- You have a metal bar of length $L$ and cross-sectional area $a$ (hence a volume $L a$ ), with a varying temperature $T$ along the rod. We conceptually subdivide the rod into $N$ (touching) pieces of length $\Delta x=L / N$.
- If $\Delta x$ is small, we can approximate each piece as having a uniform temperature $T_{n}$ within the piece $(n=1,2, \ldots, N)$, giving a vector $\mathbf{T}$ of $N$ temperatures.
- Suppose that the rate $q$ (in units of W ) at which heat flows across the boundary from piece $n$ to piece $n+1$ is given by $q=\frac{\kappa a}{\Delta x}\left(T_{n}-T_{n+1}\right)$, where $\kappa$ is the metal's thermal conductivity (in units of $\mathrm{W} / \mathrm{m} \cdot \mathrm{K}$ ). That is, piece $n$ loses energy at a rate $q$, and piece $n+1$ gains energy at the same rate, and the heat flows faster across bigger areas, over shorter distances, or for larger temperature differences. Note that $q>0$ if $T_{n}>T_{n+1}$ and $q<0$ if $T_{n}<T_{n+1}$ : heat flows from the hotter piece to the cooler piece.
- If an amount of heat $\Delta Q$ (in J ) flows into a piece, its temperature changes by $\Delta T=$ $\Delta Q /(c \rho a \Delta x)$, where $c$ is the specific heat capacity (in $\mathrm{J} / \mathrm{kg} \cdot \mathrm{K}$ ) and $\rho$ is the density $\left(\mathrm{kg} / \mathrm{m}^{3}\right)$ of the metal.
- The rod is insulated: no heat flows out the sides or through the ends.

Given these assumptions, you should be able to answer the following:
(a) "Newton's law of cooling" says that that the temperature of an object changes at a rate (K/s) proportional to the temperature difference with its surroundings. Derive the equivalent here: show that our assumptions above imply that $\frac{d T_{n}}{d t}=\alpha\left(T_{n+1}-T_{n}\right)+\alpha\left(T_{n-1}-T_{n}\right)$ for some constant $\alpha$, for $1<n<N$. Also give the (slightly different) equations for $n=1$ and $n=N$.
(b) Write your equation from the previous part in matrix form: $\frac{d \mathbf{T}}{d t}=A \mathbf{T}$ for some matrix $A$.
(c) Let $T(x, t)$ be the temperature along the rod, and suppose $T_{n}(t)=T([n-0.5] \Delta x, t)$ (the temperature at the center of the $n$-th piece). Take the limit $N \rightarrow \infty$ (with $L$ fixed, so that $\Delta x=L / N \rightarrow 0$ ), and derive a partial differential equation $\frac{\partial T}{\partial t}=\hat{A} T$. What is $\hat{A}$ ? (Don't worry about the $x=0, L$ ends until the next part.)
(d) What are the boundary conditions on $T(x, t)$ at $x=0$ and $L$ ? Check that if you go backwards, and form a center-difference approximation of $\hat{A}$ with these boundary conditions, that you recover the matrix $A$ from above.
(e) How does your $\hat{A}$ change in the $N \rightarrow \infty$ limit if the conductivity is a function $\kappa(x)$ of $x$ ?
(f) Suppose that instead of a thin metal bar (1d), you have an $L \times L$ thin metal plate (2d), with a temperature $T(x, y, t)$ and a constant conductivity $\kappa$. If you go through the steps above dividing it into $N \times N$ little squares of size $\Delta x \times \Delta y$, what PDE do you get for $T$ in the limit $N \rightarrow \infty$ ? (Many of the steps should be similar to above.)

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