Problem Set 1: Preliminaries, and Solution of Linear Algebraic Equations
Computational Physics
Physics 480/680

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Exercise 1.1 due in five days, Monday, January 27
Remainder due in two weeks, Monday, February 3
Last correction at January 8, 2014, 10:09 pm

Reading

Numerical Recipes, preface and chapters 1 and 2, skipping the technical bits. (Which bits are technical depends on how much you already know...)

(Sherman–Morrison optional for Physics 480)

1.1 Plots. (Setup) ②

It's important that reading and writing files, generating data and plotting it be efficient and convenient for you, whatever working environment you will be using in this course and in your future researches.

Pick a working environment. Using it,

(a) *Generate a list of one hundred points* $\{x_n, \exp[-6\sin(x_n)]\}$*, with* x_n *equally spaced between zero and* 2π*. Plot these points, joined by line segments, as a thick green curve (or a dashed line), in a graph with the axes labeled with large fonts (suitable for a presentation or publication); print it. Zoom in on this plot to show just the y-axis range between zero and one, and print that.*

(b) *Download the file* `NoisyFunction.dat` *from the course Web site http://www.physics.cornell.edu/~sethna/teaching/ComputationalPhysics/ From this file, read the* $(t_n, y(t_n))$ *pairs into your working environment as two vectors* $\mathbf{t}$ *and* $\mathbf{y}$*. Calculate* $\log(y^2)$ *as a vector, and plot it versus* t*, without lines connecting the points.*

1.2 Condition Number and Accuracy.[1] (Numerical) ③

You may think this exercise, with a 2x2 matrix, hardly demands a computer. However, it introduces tools for solving linear equations, condition numbers, singular value decomposition, all while illustrating subtle properties of matrix solutions. Use whatever linear algebra packages are provided in your software environment.

Consider the equation $A\mathbf{x} = \mathbf{b}$, where

$$A = \begin{pmatrix} 0.780 & 0.563 \\ 0.913 & 0.659 \end{pmatrix} \quad \text{and} \quad \mathbf{b} = \begin{pmatrix} 0.217 \\ 0.254 \end{pmatrix}. \tag{1}$$

[1] Adapted from Saul Teukolsky, 2003.

The exact solution is $\mathbf{x} = (1, -1)$. Consider the two approximate solutions $\mathbf{x}_\alpha = (0.999, -1.001)$ and $\mathbf{x}_\beta = (0.341, -0.087)$.

(a) *Compute the residuals* $\mathbf{r}_\alpha$ *and* $\mathbf{r}_\beta$ *corresponding to the two approximate solutions.* (The residual is $\mathbf{r} = \mathbf{b} - \mathbf{A}\mathbf{x}$.) *Does the more accurate solution have the smaller residual?*

(b) *Compute the condition number*[2] *of A. Does it help you understand the result of (a)?* (Hint: V^T maps the errors $\mathbf{x}_\alpha - \mathbf{x}$ and $\mathbf{x}_\beta - \mathbf{x}$ into what combinations of the two singular values?)

(c) *Use a black-box linear solver to solve for* $\mathbf{x}$*. Subtract your answer from the exact one. Do you get within a few times the machine accuracy of* 2.2×10^{-16}*? Is the problem the accuracy of the solution, or rounding errors in calculating A and b?* (Hint: try calculating $A\mathbf{x} - \mathbf{b}$.)

1.3 **Sherman–Morrison formula.** (Numerical) ③

Consider the 5x5 matrices

$$T = \begin{pmatrix} E-t & t & 0 & 0 & 0 \\ t & E & t & 0 & 0 \\ 0 & t & E & t & 0 \\ 0 & 0 & t & E & t \\ 0 & 0 & 0 & t & E-t \end{pmatrix} \tag{2}$$

and

$$C = \begin{pmatrix} E & t & 0 & 0 & t \\ t & E & t & 0 & 0 \\ 0 & t & E & t & 0 \\ 0 & 0 & t & E & t \\ t & 0 & 0 & t & E \end{pmatrix}. \tag{3}$$

These matrices arise in one-dimensional models of crystals.[3] The matrix T is *tridiagonal*: its entries are zero except along the central diagonal and the entries neighboring the diagonal. Tridiagonal matrices are fast to solve; indeed, many routines will start by changing basis to make the array tridiagonal. The matrix C, on the other hand, has a nice periodic structure: each basis element has two neighbors, with the first and last basis elements now connected by t in the upper-right and lower-left corners. This periodic structure allows for analysis using Fourier methods (Bloch waves and **k**-space).

[2] See section 2.6.2 for a technical definition of the condition number, and how it is related to singular value decomposition. Look on the Web for the more traditional definition(s), and how they are related to the accuracy.

[3] As the Hamiltonian for electrons in a one-dimensional chain of atoms, t is the hopping matrix element and E is the on-site energy. As the potential energy for longitudinal vibrations in a one-dimensional chain, $E = -2t = K$ is the spring constant between two neighboring atoms. The tridiagonal matrix T corresponds to a kind of free boundary condition, while C corresponds in both cases to periodic boundary conditions.

For matrices like C and T which differ in only a few matrix elements[4] we can find C^{-1} from T^{-1} efficiently using the Sherman-Morrison formula (section 2.7).

Compute the inverse[5] *of* T *for* $E = 3$ *and* $t = 1$. *Compute the inverse of* C. *Compare the difference* $\Delta = T^{-1} - C^{-1}$ *with that given by the Sherman-Morrison formula*

$$\Delta = \frac{T^{-1}\mathbf{u} \otimes \mathbf{v}\mathbf{T^{-1}}}{1 + \mathbf{v} \cdot T^{-1} \cdot \mathbf{u}}. \tag{4}$$

[4]More generally, this works whenever the two matrices differ by the outer product $\mathbf{u} \otimes \mathbf{v}$ of two vectors. By taking the two vectors to each have one non-zero component $u_i = u\delta_{ia}, v_j = v\delta_{jb}$, the matrices differ at one matrix element $\Delta_{ab} = uv$; for our matrices $\mathbf{u} = \mathbf{v} = 1, 0, 0, 0, 1$ (see section 2.7.2).

[5]Your software environment should have a *solver* for tridiagonal systems, rapidly giving $\mathbf{u}$ in the equation $T \cdot \mathbf{u} = \mathbf{r}$. It likely will not have a special routine for inverting tridiagonal matrices, but our matrix is so small it's not important.