

CME 302: NUMERICAL LINEAR ALGEBRA
FALL 2005/06
LECTURE 1

GENE H. GOLUB

1. INTRODUCTION

The purpose of this course is to develop and analyze numerical algorithms for solving problems with a linear algebra component. The most common sources of such problems are:

- Solution of problems arising in physical modeling
- Data analysis

2. NUMERICAL SOLUTION OF DIFFERENTIAL EQUATIONS

Suppose that we wish to solve the differential equation

$$-y'' + \sigma y' = f, \quad 0 < x < 1,$$

with boundary conditions

$$y(0) = \alpha, \quad y(1) = \beta.$$

Let

$$h = \frac{1}{N+1}, \quad x_i = ih, \quad i = 0, 1, \dots, N+1.$$

Then

$$-y''(x_i) \approx \frac{-y_{i-1} + 2y_i - y_{i+1}}{h^2},$$

and for the first derivative, we use a *centered difference* approximation,

$$y'(x_i) \approx \frac{y_{i+1} - y_{i-1}}{2h}.$$

Alternatively, we can use the *forward difference*

$$y'(x_i) \approx \frac{y_{i+1} - y_i}{h}.$$

In other words, the difference approximation becomes

$$\frac{-y_{i-1} + 2y_i - y_{i+1}}{h^2} + \sigma \left(\frac{y_{i+1} - y_{i-1}}{2h} \right) = f_i, \quad i = 1, 2, \dots, N,$$

or

$$-\left(1 + \frac{\sigma h}{2}\right)y_{i-1} + 2y_i - \left(1 - \frac{\sigma h}{2}\right)y_{i+1} = h^2 f_i \equiv g_i$$

Date: October 18, 2005, version 1.0.

Notes originally due to James Lambers. Minor editing by Lek-Heng Lim.

where $f_i := f(x_i)$. We therefore have a system of linear equations for the points y_i . This system can be described using matrix notation as

$$\begin{bmatrix} a & b & & & \\ c & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & b \\ & & & c & a \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ \vdots \\ y_N \end{bmatrix} = \mathbf{g}$$

or

$$T\mathbf{y} = \mathbf{g},$$

where the matrix T is *tridiagonal*. While systems involving tridiagonal matrices are easy to solve in general, this particular system is even simpler because the entries of T are constant along each diagonal. We call such a matrix a *Toeplitz matrix*. When $\sigma = 0$, then $T = T^\top$ and it is also positive definite.

Having solved the above system for \mathbf{y} , a question of major concern is: what can we say about the error

$$\max_i |y_i - y(x_i)|?$$

This will be discussed later.

3. DATA FITTING

We shall consider a simple problem which will illustrate many of the issues associated with numerical linear algebra.

Suppose that we are given a set of observations $\{y_j, x_j\}_{j=1}^n$. We would like to fit this data by a model. For instance, we might write

$$p_\ell(x) = b_0 + b_1x + \cdots + b_\ell x^\ell.$$

Now, let's choose the $\ell + 1$ parameters $\{b_j\}_{j=0}^\ell$ to minimize the modeling error

$$\phi(\mathbf{b}) = \sum_{j=1}^N (y_j - p_\ell(x_j))^2$$

over all coefficient vectors \mathbf{b} . We introduce the following notation:

$$X = \begin{bmatrix} 1 & x_1 & \cdots & x_1^\ell \\ 1 & x_2 & \cdots & x_2^\ell \\ \vdots & \vdots & & \vdots \\ 1 & x_N & \cdots & x_N^\ell \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}$$

and

$$\|x\|_2 = \left(\sum_{i=1}^N \|x_i\|^2 \right)^{1/2}.$$

Then

$$\phi(\mathbf{b}) = (\mathbf{y} - X\mathbf{b})^\top (\mathbf{y} - X\mathbf{b})$$

so

$$\begin{aligned} \phi(\mathbf{b}) &= \mathbf{y}^\top \mathbf{y} - \mathbf{y}^\top X\mathbf{b} - \mathbf{b}^\top X^\top \mathbf{y} + \mathbf{b}^\top X^\top X\mathbf{b} \\ &= \mathbf{y}^\top \mathbf{y} - 2\mathbf{b}^\top X^\top \mathbf{y} + \mathbf{b}^\top X^\top X\mathbf{b}. \end{aligned}$$

Differentiating with respect to each b_i , we obtain

$$\nabla_{\mathbf{b}}\phi(\mathbf{b}) = \left[\frac{\partial\phi}{\partial b_1}(\mathbf{b}), \dots, \frac{\partial\phi}{\partial b_N}(\mathbf{b}) \right]^\top = -2X^\top \mathbf{y} + 2X^\top X\mathbf{b}.$$

Setting $\nabla_{\mathbf{b}}\phi = 0$ to obtain the minimizing value of \mathbf{b} , we have

$$X^\top X\mathbf{b} = X^\top \mathbf{y}.$$

This system of linear equations is known as the *normal equations*.

If we write

$$\mathbf{x}^r = \begin{bmatrix} x_1^r \\ x_2^r \\ \vdots \\ x_N^r \end{bmatrix}$$

then $X = (\mathbf{x}^0, \mathbf{x}^1, \dots, \mathbf{x}^\ell)$ and for $i, j = 0, 1, \dots, \ell$, we have

$$[X^\top X]_{ij} = (\mathbf{x}^i)^\top \mathbf{x}^j = \sum_{r=1}^N x_r^i x_r^j = \sum_{r=1}^N x_r^{i+j} =: \mu_{i+j}$$

and therefore

$$X^\top X = \begin{bmatrix} \mu_0 & \mu_1 & \mu_2 & \cdots & \mu_\ell \\ \mu_1 & \mu_2 & & & \mu_{\ell+1} \\ \mu_2 & & & & \vdots \\ \vdots & & & & \\ \mu_\ell & \mu_{\ell+1} & \cdots & & \mu_{2\ell} \end{bmatrix}.$$

Matrices of this form arise quite often and are known as *Hankel matrices*. It has $2\ell + 1$ parameters, namely the values μ_j for $j = 0, 1, \dots, 2\ell$.

Does the solution $\tilde{\mathbf{b}}$ to the normal equations yield a minimum value for $\phi(\mathbf{b})$? Suppose $\hat{\mathbf{b}} = \tilde{\mathbf{b}} + \boldsymbol{\delta}$. Then

$$\begin{aligned} \phi(\hat{\mathbf{b}}) &= (\mathbf{y} - X\hat{\mathbf{b}})^\top (\mathbf{y} - X\hat{\mathbf{b}}) \\ &= (\mathbf{y} - X\tilde{\mathbf{b}} - X\boldsymbol{\delta})^\top (\mathbf{y} - X\tilde{\mathbf{b}} - X\boldsymbol{\delta}) \\ &= (\mathbf{y} - X\tilde{\mathbf{b}})^\top (\mathbf{y} - X\tilde{\mathbf{b}}) - \boldsymbol{\delta}^\top X^\top (\mathbf{y} - X\tilde{\mathbf{b}}) - (\mathbf{y} - X\tilde{\mathbf{b}})X\boldsymbol{\delta} + \boldsymbol{\delta}^\top X^\top X\boldsymbol{\delta} \\ &= (\mathbf{y} - X\tilde{\mathbf{b}})^\top (\mathbf{y} - X\tilde{\mathbf{b}}) + \boldsymbol{\delta}^\top X^\top X\boldsymbol{\delta}. \end{aligned}$$

Since $\boldsymbol{\delta}^\top X^\top X\boldsymbol{\delta} = \|X\boldsymbol{\delta}\|_2^2 \geq 0$, it follows that

$$\phi(\hat{\mathbf{b}}) \geq (\mathbf{y} - X\tilde{\mathbf{b}})^\top (\mathbf{y} - X\tilde{\mathbf{b}}) = \phi(\tilde{\mathbf{b}})$$

and therefore $\tilde{\mathbf{b}}$ is a vector that minimizes ϕ . Is the solution $\tilde{\mathbf{b}}$ unique? If X has full column rank, then $\boldsymbol{\delta}^\top X^\top X\boldsymbol{\delta} > 0$ for all nonzero $\boldsymbol{\delta}$ and therefore we must have $\boldsymbol{\delta} = 0$ for $\phi(\hat{\mathbf{b}})$ to be a minimum. Otherwise, $\hat{\mathbf{b}}$ is a solution whenever $X\boldsymbol{\delta} = 0$, so the solution is not unique. In such cases, a unique solution $\tilde{\mathbf{b}}$ is often determined by requiring that a solution must be of minimum length; i.e.

$$\tilde{\mathbf{b}}^\top \tilde{\mathbf{b}} \leq \hat{\mathbf{b}}^\top \hat{\mathbf{b}}$$

for any solution $\hat{\mathbf{b}}$. Later we shall discuss how such a solution can be found.

4. ISSUES IN DATA FITTING

In the previous section, we followed a three-step process to fit the original data to a function:

- (1) We chose to model the data using a polynomial approximation
- (2) We formed the normal equations, whose solution would yield the best approximation possible given the chosen model
- (3) We solved the linear system to obtain the approximation.

We will now discuss some issues that commonly arise from these three stages of data fitting.

4.1. Modeling with Polynomial Approximations. Implicitly we assumed that we know x_i exactly. We can drop this assumption and use the statistical model

$$y_j = p_\ell(x_j) + \varepsilon_j$$

where ε_j is noise, and

$$x_j = \xi_j + \eta_j$$

where η_j is noise, uncorrelated to the noise ε_j . We might want to consider minimizing both

$$(\mathbf{y} - X\mathbf{b})^\top (\mathbf{y} - X\mathbf{b})$$

and

$$(\mathbf{x} - \boldsymbol{\xi})^\top (\mathbf{x} - \boldsymbol{\xi}).$$

4.2. Forming the Normal Equations. We have assumed that $X^\top X$ is formed exactly, but we need to consider error in computing the entries of $X^\top X$. For example, if we need to compute x_i^5 where $x_i \approx 10^3$, $x_i^5 \approx 10^{15}$, and therefore we need 15 places to compute the matrix $X^\top X$ exactly. Because precision is limited, roundoff error must be taken into account when computing the entries.

Can we reduce the effect of roundoff error by choosing another basis? Suppose that we know our values of x_i are approximately some value a . Then we can shift by a to obtain the representation

$$p_\ell(x) = a_0 + a_1(x - a) + \cdots + a_\ell(x - a)^\ell,$$

resulting in entries of smaller magnitude in $X^\top X$. Another strategy is to use the approximation

$$p_\ell(x) = c_0 q_0(x) + \cdots + c_\ell q_\ell(x)$$

where $q_\ell(x)$ is a polynomial of degree ℓ and

$$\sum_{i=1}^N q_r(x_i) q_s(x_i) = 0$$

whenever $r \neq s$. Such polynomials are called *orthogonal polynomials*. Using

$$Q = \begin{bmatrix} q_0(x_1) & q_1(x_1) & \cdots & q_\ell(x_1) \\ \vdots & & & \vdots \\ q_0(x_N) & \cdots & \cdots & q_\ell(x_N) \end{bmatrix},$$

we obtain

$$X^\top X = Q^\top Q = \begin{bmatrix} d_0 & & \\ & \ddots & \\ & & d_\ell \end{bmatrix}$$

where

$$d_r = \sum_{i=1}^N q_r(x_i)^2.$$

In forming the normal equations, we need to consider the situation where the value of the degree ℓ is increased. In other words, we want to increase the order of the approximating polynomial so $X_{\ell+1} = [X_\ell \mid \mathbf{x}^{\ell+1}]$ and

$$\begin{aligned} X_{\ell+1}^\top X_{\ell+1} &= \begin{bmatrix} X_\ell^\top \\ (\mathbf{x}^{\ell+1})^\top \end{bmatrix} \begin{bmatrix} X_\ell & \mathbf{x}^{\ell+1} \end{bmatrix} \\ &= \begin{bmatrix} X_\ell^\top X_\ell & X_\ell^\top \mathbf{x}^{\ell+1} \\ (\mathbf{x}^{\ell+1})^\top X_\ell & (\mathbf{x}^{\ell+1})^\top \mathbf{x}^{\ell+1} \end{bmatrix}, \end{aligned}$$

resulting in the updated normal equations

$$X_{\ell+1}^\top X_{\ell+1} \mathbf{b}_{\ell+1} = X_{\ell+1}^\top \mathbf{y}_{\ell+1}.$$

Note that in the case of orthogonal polynomials, $Q_{\ell+1}^\top Q_{\ell+1}$ is a diagonal matrix so that the coefficients c_0, \dots, c_ℓ do not change.

Another common scenario is that we might add one more observation

$$\mathbf{x}_N^r \rightarrow \mathbf{x}_{N+1}^r = \begin{bmatrix} x_1^r \\ \vdots \\ x_N^r \\ x_{N+1}^r \end{bmatrix}.$$

These modifications are examples of *updating problems*, where we seek to obtain the solution of a modified problem more efficiently by updating the solution to the original problem, rather than recomputing the solution to the modified problem from the beginning. It is also not uncommon to have to solve *downdating problems*, where the solution is affected by the removal of data from the original problem. The above discussion shows that orthogonal polynomials are particularly well-suited to updating and downdating, which is just one reason why they are used so frequently in data-fitting applications.

4.3. Solving Linear Equations. In solving systems of linear equations, the following questions arise:

- How can we perform computations accurately?
- Are there alternative methods of solution?
- Can specialized methods for structured matrices such as Hankel matrices or Toeplitz matrices be used?

In many applications, systems involving *sparse* matrices must be solved, and as a result many methods, some of which we will discuss, have been developed for these cases. Furthermore, the advent of vector and parallel architectures have led to the development of new methods for solving linear systems.

A common difficulty is the occurrence of an *ill-posed problem*. The question that must be answered when solving any linear system is, can small changes in data make a large change in solution? A priori bounds and a posteriori bounds can be used to help answer this question.

Another consideration is that many linear systems must be solved subject to constraints such as

$$C^\top \mathbf{b} = 0$$

for some given matrix C , or

$$\mathbf{b}^\top \mathbf{b} = \alpha^2$$

for some known constant α . For example, one may wish to fit data using different functions on different intervals, in which case such constraints can be used to make the composite function smooth. This is the idea behind cubic splines.

Finally, it makes sense to ask, why minimize $\phi(\mathbf{b}) = \sum_{j=1}^N (y_j - p_\ell(x_j))^2$? Instead, why not minimize

$$\phi(\mathbf{b}) = \sum_{j=1}^N |y_j - p_\ell(x_j)|?$$

Minimizing alternative measures of error such as this is possible, but the sum of squares lends itself to minimization more naturally than these other measures, as will be discussed later.

DEPARTMENT OF COMPUTER SCIENCE, GATES BUILDING 2B, ROOM 280, STANFORD, CA 94305-9025
E-mail address: `golub@stanford.edu`