Chap 6-7 Solving linear systems of equations

Preliminaries: I will assume some familiarity with linear algebra, and in particular the following notions:

- matrix, vector
- matrix-matrix, matrix-vector product
- linear system
- singular, non-singular matrices
- determinants
- solving linear systems by hand (with row by row operations)

Goal of this section: solve a linear system of the form

$$Ax = b,$$

where $A \in \mathbb{R}^{n \times n}$ matrix (non singular) and

$x \in \mathbb{R}^n$, $b \in \mathbb{R}^n$.

There are two main kinds of algorithms for solving linear systems:

Direct methods

- LU factorization (Gaussian elimination)
- Cholesky factorization
- → Requires full knowledge of A
- → Solves for x up to maximal accuracy that can be expected.
- → Can be made very efficient for SPARSE matrices

Iterative methods

- Conjugate Gradient (CG)
- Generalized Minimum Residual (GMRES)
- Requires only knowledge of A (or sometimes A^T) acting on a vector
- Iterations $x_{n+1} = f(x_n)$ can be stopped when desired accuracy is reached

Direct Methods (chap 6 in classbook)

First here are some examples of systems $Ax = b$ that are easy to solve:

Diagonal systems:

$$A = \text{diag}(a_1, a_2, \dots, a_n) = \begin{bmatrix} a_1 & & & \\ & a_2 & & \\ & & \ddots & \\ & & & a_n \end{bmatrix}$$

then (if the $a_i \neq 0$):

$$x = A^{-1}b = \begin{bmatrix} b_1/a_1 \\ b_2/a_2 \\ b_3/a_3 \\ \vdots \\ b_n/a_n \end{bmatrix} = b./a \text{ in Matlab notation}$$

lower triangular systems

$$\underset{A}{(\Delta)}\underset{x}{[\ ]} = \underset{b}{[\ ]}, \quad \text{here } A = \begin{bmatrix} a_{11} & & & & 0 \\ a_{21} & a_{22} & & & \\ a_{31} & a_{32} & a_{33} & \ddots & \\ \vdots & & & & \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix}$$

How to solve such a system:

$$x_1 = b_1/a_{11}$$
$$x_2 = (b_2 - a_{21}x_1)/a_{22}$$
$$x_3 = (b_3 - a_{31}x_1 - a_{32}x_2)/a_{33}$$
$$\vdots$$
$$x_i = \left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j\right)/a_{ii} \qquad (i \leq n)$$

this is called <u>forward substitution</u> as we compute x_i "forward" (in direction of increasing i)

We can write forward substitution as a for loop.

for $i = 1 .. n$

$\quad x_i = (b_i - \sum_{j=1}^{i-1} a_{ij} x_j) / a_{ii}$

$O(n^2)$ flops.

or using Matlab notation:

for $i = 1 .. n$

$\quad x_i = (b_i - A_{i,1:i-1}\ x_{1:i-1}) / A_{ii}$

Upper triangular systems: (∇)

Algorithm for solving them is similar, it's backward substitution, because we progress backwards, from x_n to x_1:

Backward substitution

for $i = n : -1 : 1$

$\quad x_i = b_i - \sum_{j=i+1}^{n} a_{ij} x_j$

Triangular systems with permuted rows

For example consider permutation $p_1\ p_2 .. p_n$ of $\{1, 2, \dots, n\}$.

If the matrix $[a_{p_i j}]_{i,j=1..n}$ is lower (or upper) triangular

then we can apply forward (& backward) substitution with a slight modification.

for $i = 1, \ldots, n$

$$\lfloor x_i = \left(b_i - \sum_{j=1}^{i-1} a_{p_i j} x_j \right) / a_{p_i i} \qquad (n^2 \text{ flops})$$

a in Matlab notation:

```
for i = 1:n,
    x(i) = (b(p(i)) - A(p(i), 1:i-1) * x(1:i-1)) / A(p(i), i)
```

Similarly Backward substitution becomes.

```
for i = n:-1:1
    x_i = (b_i - sum_{j=i+1}^{n} a_{p_i j} x_j) / a_{p_i i}
```

Gaussian Elimination (or LU decomposition)

Recall GE transforms $n \boxed{A} \to \triangledown$ by applying simple transf on the left.

this process is equivalent to:

$$\underbrace{L_{n-1} \cdots L_2 L_1}_{L^{-1}} A = U$$

where $U = \triangledown_n^m$ upper triangular

$L = {}_n\triangleleft_n$ lower triangular with ones on diag ("unit-lower triangular").

$= L_1^{-1} \cdots L_{n-1}^{-1}$

$$\boxed{A = LU}$$ LU-factorization.

Example:

$$\begin{bmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{bmatrix} \xrightarrow{L_1} \begin{bmatrix} x & x & x & x \\ 0 & x & x & x \\ 0 & x & x & x \\ 0 & x & x & x \end{bmatrix} \xrightarrow{L_2} \begin{bmatrix} x & x & x & x \\ x & x & x & \\ 0 & x & x & \\ 0 & x & x & \end{bmatrix} \xrightarrow{L_3} \begin{bmatrix} x & x & x & x \\ x & x & x & \\ & x & x & \\ & 0 & x & \end{bmatrix}$$

A $\quad L_1 A$ $\quad L_2 L_1 A$ $\quad L_3 L_2 L_1 A$

gray = not updated at this step

k-Th transf. introduces zeros below diagonal in column k, by subtracting multiples of row k from rows $k+1, \cdots, m$

Another example :

$$A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$$

$$L_1 A = \begin{bmatrix} 1 & & & \\ -2 & 1 & & \\ -4 & & 1 & \\ -3 & & & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix} = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ & 3 & 5 & 5 \\ & 4 & 6 & 8 \end{bmatrix}$$

$$L_2 L_1 A = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & -3 & 1 & \\ & -4 & & 1 \end{bmatrix} L_1 A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & & 2 & 2 \\ & & 2 & 4 \end{bmatrix}$$

$$L_3 L_2 L_1 A = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & -1 & 1 \end{bmatrix} L_2 L_1 A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & & 2 & 2 \\ & & 0 & 2 \end{bmatrix} = U$$

Now we need $L = L_1^{-1} L_2^{-1} L_3^{-1}$

$$L_1^{-1} = \begin{bmatrix} 1 & & & \\ -2 & 1 & & \\ -4 & & 1 & \\ -3 & & & 1 \end{bmatrix}^{-1} = \begin{bmatrix} 1 & & & \\ 2 & 1 & & \\ 4 & & 1 & \\ 3 & & & 1 \end{bmatrix}$$

same for L_2, L_3 inverse obtained by negating entries below diag.

Also $L_1^{-1} L_2^{-1} L_3^{-1}$ can be obtained by simply putting entries in right pl

$$A = \begin{bmatrix} 1 & & & \\ 2 & 1 & & \\ 4 & 3 & 1 & \\ 3 & 4 & 1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & & 2 & 2 \\ & & 0 & 2 \end{bmatrix}$$

L $\quad$ U

In general:

Let x_k be k-th column of matrix at beginning of step k.

then transf L_k is s.t.

$$x_k = \begin{bmatrix} x_{1k} \\ \vdots \\ x_{kk} \\ x_{k+1,k} \\ \vdots \\ x_{nk} \end{bmatrix} \xrightarrow{L_k} L_k x_k = \begin{bmatrix} x_{1k} \\ \vdots \\ x_{kk} \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$L_k = \begin{bmatrix} 1 & & & \\ & \ddots & & \\ & 1 & & \\ & -l_{k+1,k} & 1 & \\ & \vdots & & \ddots \\ & -l_{n,k} & & 1 \end{bmatrix}$$

where: $l_{jk} = \frac{x_{jk}}{x_{kk}}$, $j = k+1, \dots, n$

(L_k = subtract from j-th row $\frac{x_{jk}}{x_{kk}} \times$ k-th row)

We can now explain the recipes we used:

$$L_k = I - l_k e_k^T \quad \text{where: } l_k = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ l_{k+1,k} \\ \vdots \\ l_{n,k} \end{bmatrix}, \quad e_k = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \leftarrow k \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Because first k entries of l_k are zero:

$$e_k^T l_k = 0$$

$$\Rightarrow (I - l_k e_k^T)(I + l_k e_k^T) = I$$

For the reason that we need to memorize entries to perform multiplication $L_1^{-1} L_2^{-1} \cdots L_{n-1}^{-1}$:

Look at $L_k^{-1} L_{k+1}^{-1}$:

$$(I + \ell_k e_k^T)(I + \ell_{k+1} e_{k+1}^T)$$
$$= I + \ell_k e_k^T + \ell_{k+1} e_{k+1}^T + \ell_k \underbrace{e_k^T \ell_{k+1}}_{=0} e_{k+1}$$

$$\Rightarrow \quad L = L_1^{-1} L_2^{-1} \cdots L_{n-1}^{-1} = \begin{bmatrix} 1 & & & \\ \ell_{21} & 1 & & \\ \ell_{31} & \ell_{32} & 1 & \\ \vdots & \vdots & & \ddots \\ \ell_{n1} & \ell_{n2} & & \ell_{n,n-1} \; 1 \end{bmatrix}$$

Note: in practice matrices L_k are never computed, we just keep track of multipliers by storing them directly in L.

Gaussian Elimination (no pivoting)

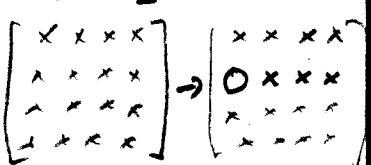
$U = A, \quad L = I$

for $k = 1 \cdots n-1$

  for $j = k+1, \ldots, n$ — compute multipliers for row j

    $\ell_{jk} = u_{jk} / u_{kk}$

    $u_{j,k:n} = u_{j,k:n} - \ell_{jk} u_{k,k:n}$ — compute updated row j



note: A, L, U are not needed, everything can be stored in same memory as $A = [L\backslash U]$

Operation count: $O(n^3)$ (three nested loops of length n)

$\approx \frac{2}{3} n^3$ flops. (if we do a more careful count of flops)

When can Gaussian elimination break down?

Here are some 2×2 examples, where the row op. involved in GE break down or give inaccurate answers.

(E1) $\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$ $\rightsquigarrow$ can't add a multiple of (1st eq) to introduce zeros in (2nd eq) (but we know that it admits solution $x_1 = 1, x_2 = 1$)

(E2) $\begin{bmatrix} \varepsilon & 1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$

$\downarrow$ GE

$\begin{bmatrix} \varepsilon & 1 \\ 0 & 1-\varepsilon^{-1} \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2-\varepsilon^{-1} \end{bmatrix}$ $\Rightarrow \begin{cases} x_2 = \dfrac{2-\varepsilon^{-1}}{1-\varepsilon^{-1}} \approx 1 \\ x_1 = (1-x_2)\varepsilon^{-1} \approx 0 \text{ (WRONG!)} \end{cases}$

Since in floating point arithmetic x_2 could be so close to 1 that $fl(1-x_2) = 0$, where $fl(x)$ = floating point repr of x.

The problem is not only smallness of a_{11}, but how small it is compared to other elements in its row.

(E3) $\begin{bmatrix} 1 & \varepsilon^{-1} \\ 1 & 1 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \varepsilon^{-1} \\ 2 \end{bmatrix}$ (same as (E2) but rescaling first row by ε)

$\xrightarrow{GE}$ $\begin{bmatrix} 1 & \varepsilon^{-1} \\ 0 & 1-\varepsilon^{-1} \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \varepsilon^{-1} \\ 2-\varepsilon^{-1} \end{bmatrix}$ $\rightsquigarrow \begin{cases} x_2 = \dfrac{2-\varepsilon^{-1}}{1-\varepsilon^{-1}} \approx 1 \\ x_1 = \varepsilon^{-1} - \varepsilon^{-1}x_2 \approx 0 \text{ (WRONG!)} \end{cases}$

Solution to this problem is to permute rows:

$$(E4)\quad \begin{pmatrix} 1 & 1 \\ \varepsilon & 1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \end{pmatrix} \xrightarrow{GE} \begin{pmatrix} 1 & 1 \\ 0 & 1-\varepsilon \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 2 \\ 1-2\varepsilon \end{pmatrix}$$

$$\Rightarrow \quad x_2 = \frac{1-2\varepsilon}{1-\varepsilon} \approx 1 \qquad \text{(correct solution)}$$

$$x_1 = 2 - x_1 \approx 1$$

Morale of these examples: We need to permute rows in general.

This is called pivoting because we choose pivot (the akk by which we divide in LU algorithm) by something that is not zero (or some more elaborate rule as we will see).

In general LU factorization routines give a factorization of the form:

$$\boxed{PA = LU} \qquad (*)$$

where A, L, U are as in the LU factorization and P is a permutation matrix. This is the identity with permuted rows.

Here is an example:

$$P = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

which permutes a vector as follows:

$$P\begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix} = \begin{bmatrix} 3 \\ 4 \\ 2 \\ 1 \end{bmatrix}$$

Most of the time P is not represented as a matrix but simply as a vector p s.t.

$$e_{p(i)} = P e_i \quad , \quad \text{here } e_i = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \leftarrow i\text{th pos.}$$

= canonical basis vector

To solve a system $Ax = b$, assuming we have factorization (*) all we need to do is:

1) Solve $Lz = Pb$
2) Solve $Ux = z$

How to choose the pivot?

Our little examples (E1) - (E4) suggest two rules:

- select largest pivot (in |·|) i.e. p s.t.

$$|u_{pk}| \geq |u_{ik}| \quad \text{for } i \geq k \quad ,$$

- select largest pivot (in |·|) relative to all other elements in a row (this is the recommended pivot selection rule because of (E3), and the one given in your book) i.e. p s.t.

$$\frac{|u_{pk}|}{\max\limits_{k \leq j \leq n} |u_{pj}|} \geq \frac{|u_{ik}|}{\max\limits_{k \leq j \leq n} |u_{ij}|} \quad \text{for } i \geq k$$

Here is how Gaussian Elimination with (partial) pivoting looks like.

$U = A, \quad L = I, \quad P = I$

for $k = 1, \ldots, n-1$

1. Choose index $i \geq k$ of pivot according to one of previous rules.
2. $u_{k,k:n} \leftrightarrow u_{i,k:n}$ (switch k-th row with pivot row i)
3. $l_{k,1:k-1} \leftrightarrow l_{i,1:k-1}$ (switch rows in L, this keeps $L = (\Delta)$ structure; and is needed to be consistent w/ permutations on U).
4. $P_{k,:} \leftrightarrow P_{i,:}$ (this how we keep track of permutation, but could have done with a vector ...)

for $j = k+1, \ldots n$

$l_{jk} = u_{jk} / u_{kk}$

$u_{j,k:n} = u_{j,k:n} - l_{jk} u_{k,k:n}$

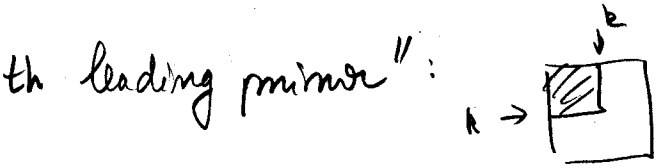
$O(n^3)$ flops

Note: There is also a complete pivoting where row and column permutations are allowed. This is much more expensive because we need to look for the pivot among a greater number of matrix elements, and the benefits in stability are not that significant compared to partial pivoting. The factorization is then:

$PAQ = LU$, where P, Q are permutation matrices.

Note that without pivoting the LU factorization of a matrix A may not even exist. Here is a sufficient condition that ensures existence:

Theorem: If all n leading (principal) minors of $A \in \mathbb{R}^{n\times n}$ are non-singular then A has an LU decomposition.

Here we call "k-th leading minor": 

$= A(1:k, 1:k)$

One can dispense from pivoting when A is diagonally dominant (which sometimes appear in applications):

$$|a_{ii}| > \sum_{\substack{j=1 \\ j\neq i}}^{n} |a_{ij}|$$ ≡ diag element larger than sum of everything else in that row.

Cholesky factorization

In many applications, A is symmetric positive definite, meaning it has the properties:

i) $A = A^T$ (symmetry)

ii) For any $x \in \mathbb{R}^n, x \neq 0$ we have $x^T A x > 0$. (pos. definiteness)

Theorem:

A s.p.d $\Rightarrow$ A invertible

Proof: $Ax = 0 \Rightarrow x^T A x = 0 \Rightarrow x = 0$

Theorem: A s.p.d. always has an LU facto.

proof: All principal minors of A are s.p.d (and thus invertible) (why?):

$$(x_1 \cdots x_k\, 0 \cdots 0)\, A \begin{pmatrix} x_1 \\ \vdots \\ x_k \\ 0 \\ \vdots \\ 0 \end{pmatrix} = (x_1 \cdots x_k)\, A_k \begin{pmatrix} x_1 \\ \vdots \\ x_k \end{pmatrix} > 0 \text{ if } (x_1 \cdots x_k) \neq 0.$$

A_k: k-th principal minor of A.
$= A(1{:}k, 1{:}k)$.

Now let us see if the LU facto of A is any special.

$$\left.\begin{array}{l} A = LU \\ \| \\ A^T = U^T L^T \end{array}\right\} \Rightarrow UL^{-T} = L^{-1}U^T = \underbrace{(\diagdown)}_{\text{diagonal}} = D$$

$$\underbrace{(\nabla)(\nabla)}_{=(\nabla)} \quad \underbrace{(\triangle)(\triangle)}_{=(\triangle)}$$

here we used that:

$$(\nabla)^{-1} = (\nabla) \qquad (\nabla)(\nabla) = (\nabla)$$

$$(\triangle)^{-1} = (\triangle) \qquad (\triangle)(\triangle) = (\triangle)$$

Now write:

$$A = L \underbrace{U L^{-T}}_{=D} \overbrace{L^T}^{=I} = L D L^T$$

Notice that D must have positive entries since:

$$D = L^{-1} A L^{-T}$$

$$x^T D x = x^T L^{-1} A L^{-T} x$$

$$= (L^{-T} x)^T A (L^{-T} x) > 0 \text{ if } x \neq 0.$$

Thus:

$$A = L D^{\frac{1}{2}} D^{\frac{1}{2}} L^T, \text{ where } D^{\frac{1}{2}} = \text{diag}(d_1^{\frac{1}{2}}, \ldots, d_n^{\frac{1}{2}})$$

$$= \tilde{L} \tilde{L}^T, \text{ where } \tilde{L} = L D^{\frac{1}{2}}$$

Theorem If A s.p.d. it admits a unique Cholesky factorization

$$A = L L^T$$

Note: some routines give $L^T = (\nabla)$ instead of L.

To derive Cholesky factorization algorithm, partition

$$A = \begin{bmatrix} a_{11} & w^T \\ w & K \end{bmatrix}$$

and consider the following identity

$$A = \begin{bmatrix} a_{11} & w^T \\ w & K \end{bmatrix} = \begin{bmatrix} \alpha & 0 \\ wk & I \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & K - ww^T/a_{11} \end{bmatrix} \begin{bmatrix} \alpha & w^T/\alpha \\ & I \end{bmatrix}$$

(check)

Here we apply to A on both sides an elementary transformation so as to introduce zeros in first column and in first row simultaneously (which is what we expect since $A = A^T$)

The algorithm is: (here we compute $R = L^T = (\nabla)$ for convenience)

Cholesky

$R = A$

for $k = 1, \dots n$

  for $j = k+1, \dots, n$

    $R_{j,j:n} = R_{j,j:n} - R_{k,j:n} R_{kj} / R_{kk}$

  $R_{k,k:n} = R_{k,k:n} / \sqrt{R_{kk}}$

$\frac{1}{3} n^3$ flops

works only w/ (∇) part

- Cholesky factorization is very robust and does not have any of the stability problems that may affect LU facto
- No need for pivoting
- breaks down when $R_{kk} < 0$, but incomplete Cholesky can be used to approx an indefinite matrix by a pos semi def matrix (i.e. LL^T)