Linear Systems – Part 2

Intensive Computation

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Methods for solving linear equations

- Direct methods: find the exact solution in a finite number of steps
- Iterative methods: produce a sequence of approximate solutions hopefully converging to the exact solution

Cholesky factorization Method for solving A x = b

- A direct method
- The idea is:
 - every **positive definite matrix** A can be factored as $A=LL^T$

A complex matrix *A* is called positive definite if for all nonzero complex vectors $x \in C$, where x^* denotes the conjugate transpose

If A is a real matrix then A is positive definite if $x^T A x > 0$ where denotes x^T the transpose

Cholesky factorization Method for solving A x = b

- A direct method
- The idea is:
 - every **positive definite matrix** A can be factored as $A=LL^T$
 - where L is lower triangular with positive diagonal elements
 - L is called the Cholesky factor of A
 - L can be interpreted as 'square root' of a positive define matrix
- The method:
 - Provides an exact result (*ignoring roundoff*)
 - Is computationally expensive

We partition matrix A as LL^T as follows

$$\begin{bmatrix} a_{11} & A_{12}^T \\ & & \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 \\ & & \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} l_{11} & L_{21}^T \\ & & \\ 0 & L_{22}^T \end{bmatrix}$$

We have the following steps:

• Step 1 - Determine l_{11} and L_{21}

$$l_{11} = \sqrt{a_{11}} \qquad \qquad L_{21} = \frac{1}{l_{11}} A_{21}$$

• Step 2 - Compute L_{22} from

$$A_{22} - L_{21}L_{21}^T = L_{22}L_{22}^T$$

This is a Cholesky factorization of order n-1

 $\begin{bmatrix} a_{11} & A_{12}^T \\ & & \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 \\ & & \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} l_{11} & L_{21}^T \\ & & \\ 0 & L_{22}^T \end{bmatrix}$

Proof that the algorithm works for positive definite A of order n

- if A is positive definite then $a_{11} > 0$
- if A is positive definite then

$$A_{22} - L_{21}L_{21}^{T} = A_{22} - \frac{1}{l_{11}}A_{21}A_{21}^{T}$$

is positive definite

• Hence we can apply again the factorization on the

Example

$$\begin{bmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{11} & l_{32} & l_{31} \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{bmatrix}$$

Example

$$\begin{bmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{11} & l_{32} & l_{31} \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{bmatrix}$$

First column of L
$$l_{11} = \sqrt{a_{11}} = 5$$
 $L_{21} = \frac{1}{l_{11}}A_{21}$

$$\begin{bmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{bmatrix} = \begin{bmatrix} 5 & 0 & 0 \\ 3 & l_{22} & 0 \\ -1 & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} 5 & 3 & -1 \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{bmatrix}$$

Example

$$\begin{bmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{11} & l_{32} & l_{31} \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{bmatrix}$$

Second column of L – Apply the same procedure to $A_{22} - L_{21}L_{21}^T$

$$A_{22} - L_{21}L_{21}^{T} = \begin{bmatrix} 18 & 0 \\ 0 & 11 \end{bmatrix} - \begin{bmatrix} 3 \\ -1 \end{bmatrix} \begin{bmatrix} 3 & -1 \end{bmatrix} = \begin{bmatrix} l_{22} & 0 \\ l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{22} & l_{32} \\ 0 & l_{33} \end{bmatrix}$$

$$\begin{aligned} l_{22} &= \sqrt{a_{22}} = 3 \\ L_{32} &= \frac{1}{l_{22}} A_{32} \end{aligned} \begin{bmatrix} 9 & 3 \\ 3 & 10 \end{bmatrix} = \begin{bmatrix} 3 & 0 \\ 1 & l_{33} \end{bmatrix} \begin{bmatrix} 3 & 1 \\ 0 & l_{33} \end{bmatrix} \end{aligned}$$

 $(=L_{22}L_{22}^T)$

Example

$$\begin{bmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{11} & l_{32} & l_{31} \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{bmatrix}$$

Third column of L $l_{33}^2 = 10 - 1$ $l_{33} = 3$

$$\begin{bmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{bmatrix} = \begin{bmatrix} 5 & 0 & 0 \\ 3 & 3 & 0 \\ -1 & 1 & 3 \end{bmatrix} \begin{bmatrix} 5 & 3 & -1 \\ 0 & 3 & 1 \\ 0 & 0 & 3 \end{bmatrix}$$

Solve A x = b A positive definite of order n

<u>Step 1</u> $A = LL^T \rightarrow LL^T$ factorization

<u>Step 2</u> $Ly = b \rightarrow$ Solve by forward substitution

<u>Step 3</u> $L^T x = y \rightarrow$ Solve by backward substitution

LL^{T} decomposition – Algorithm cost

We have:

- Multiplication and division operations for the factorization:
 O(n³)
- Multiplication and division operations for solving the triangular systems: $O(n^2)$
- Addition and subtraction operations: **O(n³)**
- Anyway usually we consider the number of floating point operations FLOPs

Inverse of a positive definite matrix

Suppose A is positive definite with Cholesky factorization LL^{T}

- *L* is invertible (its diagonal elements are nonzero)
- $X = L^{-T}L^{-1}$ is a **right inverse** of A:

$$AX = LL^{T}L^{-T}L^{-1} = LL^{-1} = I$$

• $X = L^{-T}L^{-1}$ is a **left inverse** of A:

$$XA = L^{-T}L^{-1}LL^{T} = L^{-T}L^{T} = I$$

• hence **A** is invertible with inverse:

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

- If A is very sparse, then L is often (but not always) sparse
- If L is sparse, the cost of the factorization is less than (1/3)n³
- Exact cost depends on:
 - n
 - *#nonzero* elements
 - sparsity pattern
- Very large sets of equations (*n* ~ 10⁶) are solved by exploiting sparsity

Consider a *sparse systems*

$$\begin{bmatrix} 1 & a^T \\ a & I \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} b \\ c \end{bmatrix}$$

Factorization

$$\begin{bmatrix} 1 & a^T \\ & \\ a & I \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ & \\ a & L_{22} \end{bmatrix} \begin{bmatrix} 1 & a^T \\ & \\ 0 & L_{22}^T \end{bmatrix}$$

• Fill-in effect

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• Factorization can produce a 100% fill-in

• We can reorder the equations of the systems

$$\begin{bmatrix} 1 & a^T \\ a & I \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} b \\ c \end{bmatrix} \implies \begin{bmatrix} I & a \\ a^T & 1 \end{bmatrix} \begin{bmatrix} v \\ u \end{bmatrix} = \begin{bmatrix} c \\ b \end{bmatrix}$$

Factorization

$$\begin{bmatrix} I & a \\ a^T & 1 \end{bmatrix} = \begin{bmatrix} I & 0 \\ a^T & \sqrt{1 - a^T a} \end{bmatrix} \begin{bmatrix} I & a \\ 0 & \sqrt{1 - a^T a} \end{bmatrix}$$

We can reorder the equation of the systems



• Factorization with zero fill-in

Permutation matrix - identity matrix with rows reordered

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

The vector Ax is a permutation of x

$$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_2 \\ x_3 \\ x_1 \end{bmatrix}$$

 $A^{T}x$ is the inverse permutation applied to x

$$\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_3 \\ x_1 \\ x_2 \end{bmatrix}$$

 $A^{T}A = A A^{T} = I$ then **A** is invertible and $A^{-1} = A^{T}$

Permutation matrices

Solving *Ax=b* when *A* is a permutation matrix

The solution of Ax=b is vector $x=A^Tb$

Example

$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3.5 \\ -3.2 \\ 8.0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 3.5 \\ -3.2 \\ 8.0 \end{bmatrix} = \begin{bmatrix} 8.0 \\ 3.5 \\ -3.2 \end{bmatrix}$$

The solution is $x = [8.0, 3.5, -3.2]^T$

Sparse Cholesky factorization

- If A is sparse and positive definite, it is usually factored as $A = PLL^{T}P^{T}$
 - where *P* is a permutation matrix and *L* is lower triangular with positive diagonal elements
- Interpretation: we permute the rows and columns of A and factor

$$P^{T}AP = LL^{T}$$

- Note that:
 - choice of P greatly affects the sparsity L
 - many heuristic methods exist for selecting good permutation matrices P

Solving sparse positive definite eqs

 If A is sparse and positive definite, we solve Ax = b via factorization

$$A = PLL^{\mathsf{T}}P^{\mathsf{T}}$$

Algorithm

- b' = P^T b
- solve Lz =b' by forward substitution
- solve $L^T y = z$ by backward substitution
- 4. x = Py:
- That is we solve $(P^{T}AP)y = b'$ using the Clolesky factorization of $P^{T}AP$

- Example of a sparse system
- Consider an electric circuit with only resistors



To solve an electric circuit with only resistors, we can write the equations describing the circuit where:

- Unknowns are
 - B branch currents (i)
 - N node voltages (e)
 - B branch voltages (v)
- Equations are
 - N+B Conservation Laws
 - B Constitutive Equations

For our circuit

- v1, v2, v3, v4, v5, v6, v7 branch voltages
- î1, i2, i3, i4, i5, i6, i7 *branch currents*
- ê1, e2, e3, e4 *node voltages* with voltage of node 5 equal to 0



Branch Constitutive Equations

- -v1 = V 1
- v2 R1 x i2 = 0
- v3 R2 x i3 = 0
- v4 R3 x i4 = 0
- v5 R4 x i5 = 0
- v6 R5 x i6 = 0
- v7 R6 x i7 = 0

Kirchhoff's Current Law (KCL)

- -i1 + i2 = 0 (node 1)
- -i2 + i3 + i4 = 0 (node 2)
- -i3 + i5 + i6 = 0 (node 3)
- -i4 i5 + i7 = 0 (node 4)



Kirchhoff's Voltage Law (KVL)

- v1 + e1 = 0
- v2 e1 + e2 = 0
- v3 e2 + e3 = 0
- v4 e2 + e4 = 0
- v5 e3 + e4 = 0
- v6 e3 = 0
- v7 e4 = 0

In matrix form



Iterative methods

Iterative methods for solving Ax = b

- Begin with an **approximation** to the solution x_0
- Then provide a series of improved approximations x_1, x_2, \ldots
- That converge to the exact solution

Iterative methods

The method can be stopped as soon as the approximations
 x_i have converged to an acceptable precision (which might also be something as 10⁻³)

 With a direct method, the process of elimination and backsubstitution has to be carried right through to completion, or else abandoned altogether

Iterative methods

 The main attraction of iterative methods is that for certain problems (particularly those where the matrix A is large and sparse) they are much faster than direct methods

 On the other hand, iterative methods can be unreliable: for some problems they may exhibit very slow
 convergence, or they may not converge at all

Consider the system

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \dots + a_{2n}x_n = b_2$$

.....

$$a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \dots + a_{nn}x_n = b_n$$

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The Jacobi Method

• Rewrite the system in the form:

 $a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n = b_1$ $a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \dots + a_{2n}x_n = b_2$

 $a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \dots + a_{nn}x_n = b_n$



.



• Consider $x^{(0)} = (x_1^{(0)}, x_2^{(0)}, x_3^{(0)}, \dots, x_n^{(0)})$ as an initial

approximation of the solution and **substitute** $x_i^{(0)}$ in the eqs



$$x_n^{(1)} = -\frac{a_{n1}}{a_{nn}} x_1^{(0)} - \frac{a_{n2}}{a_{nn}} x_2^{(0)} - \dots - \frac{a_{nn-1}}{a_{nn}} x_{n-1}^{(0)} + \frac{b_n}{a_{nn}}$$

• Iterate the substitution of $x^{(k)} = (x_1^{(k)}, x_2^{(k)}, x_3^{(k)}, \dots, x_n^{(k)})$ such

that at each step a new solution approximation is obtained

$$x_{1}^{(k+1)} = -\frac{a_{12}}{a_{11}} x_{2}^{(k)} - \frac{a_{13}}{a_{11}} x_{3}^{(k)} - \dots - \frac{a_{1n}}{a_{11}} x_{n}^{(k)} + \frac{b_{1}}{a_{11}}$$
$$x_{2}^{(k+1)} = -\frac{a_{21}}{a_{22}} x_{1}^{(k)} - \frac{a_{23}}{a_{22}} x_{3}^{(k)} - \dots - \frac{a_{2n}}{a_{22}} x_{n}^{(k)} + \frac{b_{2}}{a_{22}}$$
$$\dots$$
$$x_{n}^{(k+1)} = -\frac{a_{n1}}{a_{nn}} x_{1}^{(k)} - \frac{a_{n2}}{a_{nn}} x_{2}^{(k)} - \dots - \frac{a_{nn-1}}{a_{nn}} x_{n-1}^{(k)} + \frac{b_{n}}{a_{nn}}$$

Example

Consider the system

$$10x_{1} - x_{2} + 2x_{3} = 6$$

-x₁ + 11x₂ - x₃ + 3x₄ = 25
2x₁ - x₂ + 10x₃ - x₄ = -11
3x₂ - x₃ + 8x₄ = 15

Example

Rewrite the system



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The Jacobi Method

Example

• Start iterations with $x^{(0)} = (0, 0, 0, 0)$



Example

 Continuing with iterations, we obtain the sequence of approximations shown in the Table

k 0 2 3 4 5 6 7 8 9 1 $x_1^{(k)}$ 0.0000 0.6000 1.0473 0.9326 1.0152 0.9890 1.0032 0.9981 1.0006 0.9997 $x_{2}^{(k)}$ 0.0000 2.2727 1.7159 2.0533 1.9537 2.0114 1.9922 2.0023 1.9987 2.0004 $x_{3}^{(k)}$ $0.0000 \ -1.1000 \ -0.8852 \ -1.0493 \ -0.9681 \ -1.0103 \ -0.9945 \ -1.0020 \ -0.9990$ -1.0004 $x^{(k)}$ 0.0000 1.8750 0.8852 1.1309 1.0214 0.9739 0.9944 1.0036 0.9989 1.0006

The Jacobi Method in Matrix Form

• Consider the system *Ax=b*

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

We split A into

$$A = \begin{bmatrix} a_{11} & 0 & \cdots & 0 \\ 0 & a_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{bmatrix} - \begin{bmatrix} 0 & \cdots & 0 \\ -a_{21} & \cdots & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -a_{n1} & \cdots & -a_{nn-1} & 0 \end{bmatrix} \begin{bmatrix} 0 & -a_{12} & \cdots & -a_{1n} \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \ddots & -a_{n-1n} \\ 0 & 0 & \cdots & 0 \end{bmatrix} = D - (-L - U)$$

That is Ax=b is transformed in (D-(-L-U))x=b

The Jacobi Method in Matrix Form

- Assume D⁻¹ exists $D^{-1} = \begin{bmatrix} \frac{1}{a_{11}} & 0 & \cdots & 0 \\ 0 & \frac{1}{a_{22}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{a_{nn}} \end{bmatrix}$
- Then $x = D^{-1}(-L-U)x + D^{-1}b$
- The matrix form of Jacobi iterative method is

$$x^{(k+1)} = D^{-1}(-L-U)x^{(k)} + D^{-1}b$$
 $k = 0, 1, 2, ...$

- We need a stopping criterion
- We are interested in the error **e** at each iteration between the true solution **x** and the approximation $\mathbf{x}^{(k)}$: $\mathbf{e}^{(k)} = \mathbf{x} - \mathbf{x}^{(k)}$
- Obviously, we don't usually know the true solution x
- To better understand the behavior of an iterative method, we can consider a system Ax = b for which we do know the true solution and analyze how quickly the approximations are converging to the true solution

• We can consider different ways of measuring the error:



• We use one of the previous measures asking that it is $< \mathcal{E}$

- **Theorem** The Jacobi method converges if the coefficient matrix *A* is a **strictly diagonally dominant matrix**
- An *nxn* matrix *A* is strictly diagonally dominant if the **absolute** value of each entry on the main diagonal is greater than the sum of the absolute values of the other entries in the same

row:

$$|a_{11}| > |a_{12}| + |a_{13}| + \dots + |a_{1n}|$$

$$|a_{22}| > |a_{21}| + |a_{23}| + \dots + |a_{2n}|$$

$$\dots$$

$$|a_{nn}| > |a_{n1}| + |a_{n3}| + \dots + |a_{n,n-1}|$$

Jacobi method – Algorithm cost

- Multiplication operations for each iteration: $n(n-1) \rightarrow O(n^2)$
- If we do *k* iteration the cost is: *kn(n-1)*
- We also have the divisions with a_{ii} during the first iteration \rightarrow the cost is kn^2
- To decide between Gauss and Jacobi methods we evaluate:

$$kn^2 < \frac{1}{3}n^3 \implies k < \frac{1}{3}n$$

Hence when using the Jacobi method we need to evaluate how many iterations are needed before stopping