Università della Svizzera italiana

Efficient Computational Algorithms 2021

Final Project Report

Decomposition Algorithms

Abstract

This project outlines the factorisation of matrices with the six most widely used decomposition algorithms.

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1 Introduction

We use the terms decomposition and factorization interchangeably to mean writing a matrix as a product of two or more other simpler matrices, generally with some defined properties (such as lower/upper triangular).
The underlying principle of the decompositional approach to matrix computation is that to construct **computational platforms** from which a variety of problems can be solved. The article deals primarily with dense matrix computations. Although the decompositional approach has greatly influenced iterative and direct methods for sparse matrices.

Benefits of the decompositional approach :

• Matrix decomposition solves not one but many problems.
• Matrix decomposition, which is generally expensive to compute, can be reused to solve new problems involving the original matrix.
• The decompositional approach facilitates rounding-error analysis.

We will focus on six most widely used decompositions namely; Cholesky, LU, Spectral, SVD, Schur, QR. For sure these are not the only used decompositions.

2 Cholesky

If a matrix M is symmetric ($\mathbf{M}^\mathsf{T} = \mathrm{M}$), positive semi-definite (all eigenvalues are non-negative) or a complex Hermitian matrix ($\mathrm{M} = \overline{M}^\mathsf{T}$) then we can use $\mathbf{LL}^\mathsf{T}$ factorization such that L is a lower triangular matrix.

$$\mathrm{M} = \mathrm{L} * \mathbf{L}^\mathsf{T} \qquad \longrightarrow \qquad \begin{bmatrix} m_{1,1} & m_{1,2} & m_{1,3} \\ m_{2,1} & m_{2,2} & m_{2,3} \\ m_{3,1} & m_{3,2} & m_{3,3} \end{bmatrix} = \begin{bmatrix} l_{1,1} & 0 & 0 \\ l_{2,1} & l_{2,2} & 0 \\ l_{3,1} & l_{3,2} & l_{3,3} \end{bmatrix} * \begin{bmatrix} l_{1,1} & l_{1,2} & l_{1,3} \\ 0 & l_{2,2} & l_{2,3} \\ 0 & 0 & l_{3,3} \end{bmatrix}$$

$$= \begin{bmatrix} l_{1,1}^2 & l_{1,1} * l_{2,1} & l_{1,1} * l_{3,1} \\ l_{2,1} * l_{1,1} & l_{2,1}^2 + l_{2,2}^2 & l_{2,1} * l_{3,1} + l_{2,2} * l_{3,2} \\ l_{3,1} * l_{1,1} & l_{3,1} * l_{2,1} + l_{3,2} * l_{2,2} & l_{3,1}^2 + l_{3,2}^2 + l_{3,3}^2 \end{bmatrix}$$

So we can generalize the formulas for higher dimensional matrices...

$l_{i,i} = \sqrt{m_{i,i} - \sum_{j=1}^{i-1} l_{i,j}^2}$ for i = 1,2,... n and for i > j $l_{i,j} = \frac{m_{i,j} - \sum_{k=1}^{j-1} l_{i,k} * l_{j,k}}{l_{j,j}}$ with i = 1,2,... n and j = 1,2,... i-1

The Computational Cost: Computing diagonal element $l_{i,i}$ requires

- i subtractions
- i - 1 multiplications, and
- one square root,

which adds up to 2i operations so overall diagonal element calculation costs us $\sum_{i=1}^{n} 2i = 2\,\frac{n*(n+1)}{2} = n^2 + n$

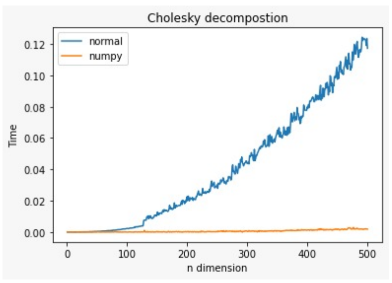
On the other hand $l_{i,j}$ requires

- j subtractions
- j - 1 multiplications, and
- one division,

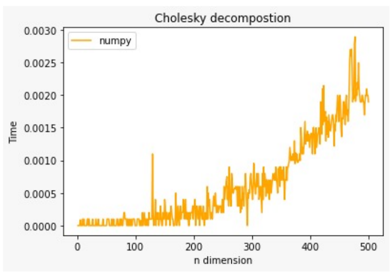
so totally 2j operations, then for n dimensional matrix it will require $\sum_{i=1}^{n} \sum_{j=1}^{i-1} 2j = \sum_{i=1}^{n} 2\frac{(i-1)*i}{2} = \frac{n^3}{3} - \frac{n}{3}$ floating-point operations.

Finally summing up those two costs results by the domination of $\frac{n^3}{3}$ Flops

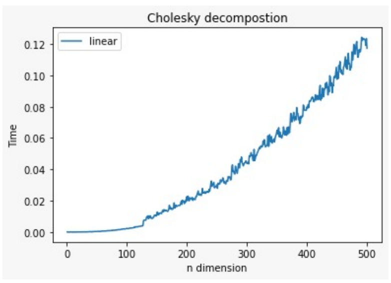
Note : if M is very sparse, most of elements of the matrix are zero , L is often (but not always) sparse then if L is sparse, the cost of the factorization is much less than $\frac{n^3}{3}$
Cholesky factorization is numerically stable; instability is characterized by significant changes in the predicted dynamical behaviour induced by only small changes in the specification of the system.



Custom vs Numpy



Numpy



Custom

3 LU

An invertible matrix M has an LU decomposition , L is an lower-triangular matrix with all diagonal entries equal to 1 and U is an upper-triangular matrix, provided that all its leading sub-matrices are non-singular (with non-zero determinants).
The k^{th} leading sub-matrix of M is denoted M_k and is the k×k matrix found by looking only at the top k rows and leftmost k columns.
Thanks to Pivoting (so called row interchange); it is always possible to re-order the rows of an invertible matrix so that all of the sub-matrices have non-zero determinants. That is why this decomposition is also called LUP factorization, P is the permutation matrix.
Let us assume there is no pivoting so the P = I

$$M = L * U * P \qquad \longrightarrow \qquad \begin{bmatrix} m_{1,1} & m_{1,2} & m_{1,3} \\ m_{2,1} & m_{2,2} & m_{2,3} \\ m_{3,1} & m_{3,2} & m_{3,3} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_{2,1} & 1 & 0 \\ l_{3,1} & l_{3,2} & 1 \end{bmatrix} * \begin{bmatrix} u_{1,1} & u_{1,2} & u_{1,3} \\ 0 & u_{2,2} & u_{2,3} \\ 0 & 0 & u_{3,3} \end{bmatrix} * \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} u_{1,1} & u_{1,2} & u_{1,3} \\ l_{2,1} * u_{1,1} & l_{2,1} * u_{1,2} + u_{2,2} & l_{2,1} * u_{1,3} + u_{2,3} \\ l_{3,1} * u_{1,1} & l_{3,1} * u_{1,2} + l_{3,2} * u_{2,2} & l_{3,1} * u_{1,3} + l_{3,2} * u_{2,3} + u_{3,3} \end{bmatrix}$$

Generalized formulas :
$u_{ij} = m_{ij} - \sum_{k=1}^{i-1} u_{kj} * l_{ik} \qquad for \quad j = 1,2,...n \quad i = 1,2,...j+1 \quad k = 1,2,...i$
$l_{ij} = \frac{1}{u_{jj}} * (m_{ij} - \sum_{k=1}^{j-1} u_{kj} * l_{ik} \quad and \quad l_{j,j} = 1 \qquad for \quad j = 1,2,...n \quad i = j, j+1,...n \quad k = 1,2,...j$
The total cost is $\frac{2}{3}n^3$ Flop

Some features of LU Decomposition:

• For some choices of P, small rounding errors in the algorithm cause very large errors in the solution (numerical instability).
• when P permutes the largest element (absolute value) of first column of M to the 1,1-position.

4 SPECTRAL

The Spectral Decomposition also called Jordan Decomposition recasts a matrix in terms of its eigenvalues and eigenvectors. This representation turns out to be enormously useful.
Each symmetric M (nxn) matrix can be written as PDP^{-1} or PDP^{T}, where D is $diag(\lambda_1, ..., \lambda_n)$, λ_i is the corresponding eigenvalue and where P (Jordan canonical form)is an orthogonal matrix, $(v_1, ..., v_n)$, consisting of the orthonormal eigenvectors v_i. One important side note is orthogonal matrices have unit norm.

$$\mathrm{M = P * D *} P^T \qquad \longrightarrow \qquad \begin{bmatrix} m_{1,1} & m_{1,2} & m_{1,3} \\ m_{2,1} & m_{2,2} & m_{2,3} \\ m_{3,1} & m_{3,2} & m_{3,3} \end{bmatrix} = \begin{bmatrix} \uparrow & \uparrow & \uparrow \\ v_1 & v_2 & v_3 \\ \downarrow & \downarrow & \downarrow \end{bmatrix} * \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} * \begin{bmatrix} \leftarrow & v_1 & \rightarrow \\ \leftarrow & v_2 & \rightarrow \\ \leftarrow & v_3 & \rightarrow \end{bmatrix}$$

Generalized formula :

$$\mathrm{M} = \sum_{i=1}^{n} \lambda_i * v_i * v_i^T \qquad for \quad i = 1, 2, ...n$$

Some Usefull features of Spectral Factorization:
$*$ The Jordan decomposition gives a representation of a symmetric matrix in terms of eigenvalues and eigenvectors.
$*$ The eigenvectors belonging to the largest eigenvalues indicate the “main direction” of the data.
$*$ The Jordan decomposition allows one to easily compute the power of a symmetric matrix $M^{\alpha} = P * D^{\alpha} * P^T$

5 SVD

Let m and n be arbitrary ; we don't not require $m \geqslant n$. Given M ϵ C^{mxn}, not necessarily of full rank, a SVD of M is a factorization

$$M = U\Sigma V^* \qquad \longrightarrow \qquad \begin{bmatrix} \uparrow & & \uparrow \\ m_1 & \dots & m_n \\ \downarrow & & \downarrow \end{bmatrix} = \begin{bmatrix} \uparrow & & \uparrow \\ u_1 & \dots & u_n \\ \downarrow & & \downarrow \end{bmatrix} \begin{bmatrix} \sigma_1 & & \\ & \sigma_2 & \\ & & \sigma_p \end{bmatrix} \begin{bmatrix} \uparrow & & \uparrow \\ v_1 & \dots & v_n \\ \downarrow & & \downarrow \end{bmatrix}^{-T}$$

with $U \epsilon C^{mxn}$ unitary, $V \epsilon C^{nxn}$ unitary, $\Sigma \epsilon R^{mxn}$ diagonal.
In addition, it is assumed that the diagonal entries σ_j of Σ are non-negative and in non-increasing order; that is, $\sigma_1 \geqslant \sigma_2 \geqslant \dots \geqslant \sigma_p \geqslant 0$ where p = min(m,n) The diagonal matrix Σ has the same shape as M even when M is not square, but U and V are always square unitary matrices.

Different between Eigenvalue(Spectral) Decomposition and SVD:
$A \epsilon C^{mxn}, B \epsilon C^{mxm}$
$B = PDP^{-1}$; P is collection of eigenvectors of B ,D is diagonal matrix with eigenvalue
$A = U\Sigma V^*$; u is left eigenvector in m dimension, v is right eigenvector in n dimension , Σ is diagonal matrix with singular value.
$AA^* = U\Sigma V^*(U\Sigma V^*)^T = U\Sigma V^*(V\Sigma U^*) = U\Sigma(\Sigma U^*) = U\Sigma^2 U^*$ U is eigenvector of AA^*, Σ^2 is eigenvalue of AA^*

6 SCHUR

Consider this matrix:
$A = \begin{bmatrix} 13 & 8 & 8 \\ -1 & 7 & -2 \\ -1 & -2 & 7 \end{bmatrix}$ How do we get A^{60} ?
Easiest way is using A $= PDP^{-1}$ $\quad A^{60} = PD^{60}P^{-1}$ (eigenvalue decomposition), in fact that does not work for this matrix. However we can do something almost as good For any given matrix, the Schur decomposition allows to find another matrix that is similar to the given one and is upper triangular.
A $=$ UTU^* $\quad U_2U_1AU_1U_2 = \begin{bmatrix} \lambda_1 & . & . \\ 0 & \lambda_2 & . \\ 0 & 0 & \lambda_3 \end{bmatrix} = U^*TU$
where T is upper triangular, with the eigenvalues of A on its diagonal, and U was a unitary matrix.
The Schur decomposition is not unique we choose an eigenvalue arbitrarily; as a consequence, there are different possible orderings of the eigenvalues of A on the main diagonal of T.
More in general, if $\quad U^*AU = T$
is a Schur decomposition of A, we can take any unitary matrix Q such that Q^*TQ
is upper triangular, and use it to construct another Schur decomposition $(UQ)^*A(UQ) = Q^*TQ$

7 QR

QR factorization is often used to solve the linear least squares problem. Assume that M $\epsilon C^{mxn} (m \geq n)$ has full rank n.

$$\text{M} = \text{Q * R} \quad \longrightarrow \quad \begin{bmatrix} \uparrow & & \uparrow \\ m_1 & \dots & m_n \\ \downarrow & & \downarrow \end{bmatrix} = \begin{bmatrix} \uparrow & & \uparrow \\ q_1 & \dots & q_n \\ \downarrow & & \downarrow \end{bmatrix} * \begin{bmatrix} r_{1,1} & \cdots & r_{1,n} \\ & \ddots & \vdots \\ & & r_{n,n} \end{bmatrix}$$

Written out these equations as linear combination of $m_1, m_2, ...m_n$ and take the form;
$m_1 = r_{11} * q_1$
$m_2 = r_{12} * q_1 + r_{22} * q_2$
.
.
.
$m_n = r_{1n} * q_1 + r_{2n} * q_2 + ... + r_{nn} * q_n$
As a matrix formula, we have M = $\hat{Q} * \hat{R}$ called reduced QR Factorization
Q-factor:

- Q is mxn matrix with orthogonal columns ($Q^T * Q = I$)
- If M ıs a square (m=n) matrix, then Q is orthogonal ($Q^T * Q = Q * Q^T = I$)

R-factor:

- Q is nxn upper triangular matrix with non zero diagonal elements ($r_{kk} \neq 0$)
- R is non-singular (diagonal elements are non-zero)

Full QR Factorization:
QR factorization of a matrix M ϵC^{mxn}, appending an additional m-n orthogonal to columns so $\hat{Q}$ becomes an mxn matrix.
2 Group: :
Orthogonal triangularization-Householder $Q_n ... Q_2 Q_1 A = R$
Triangular orthogonalization- Gram-Schmidt $A R_1 R_2 ... R_n = Q$

Algorithms for QR factorization
Modified Gram-Schmidt algorithm: complexity for mxn dimensional matrix;

$$\sum_{k=1}^{n} (4m-1)(k-1) - 3m) = (4m-1)\frac{n(n-1)}{2} + 3mn$$
$$= 2mn^2 \text{ Flops}$$

Householder Algorithm:

$$\sum_{k=1}^{n} 4(m-k+1)(n-k+1) = \int_0^n 4(m-t)(n-t)\,dt$$
$$= 2mn^2 - \frac{2}{3}n^3 \text{ Flops}$$

SVD $\sim 2mn^2 + 11n^3$ flops
Normal equation $\sim mn^2 + \frac{1}{3}n^3$ flops