Session 24
May 6, 2020

Last time we finished with stating the LU decomposition:

Any invertible matrix A can be written as $PA = LU$, where P is a matrix that permutes the rows appropriately, L is lower triangular, U is upper triangular.

Note: • It turns out that any square matrix has such a decomposition (not just invertible ones).

• Often, $A = LU$ is called "LU decomposition" (does not always exist), whereas $PA = LU$ is called "LU decomposition with partial pivoting" (or "LUP").

Let us just give a very simple example for 2×2 matrices. In practice, LU decompositions are relevant for large matrices, but then computations by hand take a long time. So in most applications one uses algorithms to compute LU decompositions.

Example: $A = \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix}$

• Let us first use Gaussian elimination:

We want to add $(-2)\cdot$ row one to row two. Thus, we need to multiply with the T_3 type matrix $T = \begin{pmatrix} 1 & 0 \\ -2 & 1 \end{pmatrix}$. This gives

$$TA = \begin{pmatrix} 1 & 0 \\ -2 & 1 \end{pmatrix}\begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix} = \begin{pmatrix} 1 & 3 \\ -2+2 & -6+4 \end{pmatrix} = \begin{pmatrix} 1 & 3 \\ 0 & -2 \end{pmatrix}$$

So $A = T^{-1}\begin{pmatrix} 1 & 3 \\ 0 & -2 \end{pmatrix}$, with $T^{-1} = \begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix}$ (since $\begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ -2 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$)

$$\Rightarrow A = \begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix}\begin{pmatrix} 1 & 3 \\ 0 & -2 \end{pmatrix}$$ (double check: $\begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix}\begin{pmatrix} 1 & 3 \\ 0 & -2 \end{pmatrix} = \begin{pmatrix} 1 & 3 \\ 2 & 6-2 \end{pmatrix} = \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix}$ ✓)

• Alternatively, we could directly try to find $L = \begin{pmatrix} l_{11} & 0 \\ l_{21} & l_{22} \end{pmatrix}$ and $U = \begin{pmatrix} u_{11} & u_{12} \\ 0 & u_{22} \end{pmatrix}$ such that $A = LU$.

Then we have in general $\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{pmatrix} = \begin{pmatrix} L_{11}U_{11} & L_{11}U_{12} \\ L_{21}U_{11} & L_{21}U_{12}+L_{22}U_{22} \end{pmatrix}$

If we set all matrix elements equal, this is 4 equations for 6 unknowns, so generally this system of equations is clearly underdetermined. Thus, e.g., we can choose the diagonal of L to $\underbrace{\text{be 1's, i.e., here, } L_{11}=L_{22}=1}_{\text{this is usually the most practical choice}}$. Then, in our example, we need to solve

$$\begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} \\ L_{21}U_{11} & L_{21}U_{12}+U_{22} \end{pmatrix} \Rightarrow U_{11}=1,\ U_{12}=3,\ L_{21}=2,\ 2\cdot 3+U_{22}=4 \Rightarrow U_{22}=-2$$

$$\Rightarrow A = \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix} = LU = \begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} 1 & 3 \\ 0 & -2 \end{pmatrix} \quad \text{(same as before)}$$

Note: We can always choose the diagonal elements of L equal to 1. But this is a convention. In our example, other LU decompositions are, e.g., $A = \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 2 & -2 \end{pmatrix} \begin{pmatrix} 1 & 3 \\ 0 & 1 \end{pmatrix}$, or $A = \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 2 & 2 \end{pmatrix} \begin{pmatrix} 1 & 3 \\ 0 & -1 \end{pmatrix}$.

LU decompositions can be used to solve systems of linear equations $A\vec{x}=\vec{b}$. Suppose $A=LU$ (no row permutation necessary). Then we need to solve $LU\vec{x}=\vec{b}$. If we define $U\vec{x}=\vec{y}$, we have $L\vec{y}=\vec{b}$. Now $\underbrace{L\vec{y}=\vec{b} \text{ can directly be solved for } \vec{y}}_{\text{"from top to bottom"}}$, since L is lower triangular. But given $\vec{y}$, $\underbrace{U\vec{x}=\vec{y} \text{ can then easily be solved for } \vec{x}}_{\text{"from bottom to top"}}$, since U is upper triangular.

In the example from before, we had $A = \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix} = LU = \begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} 1 & 3 \\ 0 & -2 \end{pmatrix}$.

Given $\vec{b} \in \mathbb{R}^2$, $L\vec{y}=\vec{b}$ becomes $\begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$, so $y_1=b_1$, $2y_1+y_2=b_2$, i.e., $y_2=b_2-2b_1$.

Then we still need to solve $U\vec{x}=\vec{y}$, i.e., $\begin{pmatrix} 1 & 3 \\ 0 & -2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2-2b_1 \end{pmatrix} \Rightarrow -2x_2 = b_2-2b_1$, i.e.,

$x_2 = b_1 - \frac{1}{2} b_2$, and $x_1 + 3x_2 = b_1$, i.e., $x_1 + 3\left(b_1 - \frac{1}{2} b_2\right) = b_1 \Rightarrow x_1 = -2b_1 + \frac{3}{2} b_2$.

$$\Rightarrow \vec{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} -2b_1 + \frac{3}{2} b_2 \\ b_1 - \frac{1}{2} b_2 \end{pmatrix}.$$

(Let us double check with Cramer's rule: $x_1 = \dfrac{\det\begin{pmatrix} b_1 & 3 \\ b_2 & 4 \end{pmatrix}}{\det\begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix}} = \dfrac{4b_1 - 3b_2}{4-6} = -2b_1 + \frac{3}{2} b_2 \checkmark$

$$x_2 = \frac{\det\begin{pmatrix} 1 & b_1 \\ 2 & b_2 \end{pmatrix}}{\det\begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix}} = \frac{b_2 - 2b_1}{-2} = b_1 - \frac{1}{2} b_2 \checkmark \;)$$

For this 2×2 example, Cramer's rule is much faster to apply, but for large matrices this might not be so.

A few more remarks:

- If A is Hermitian, we could try to decompose $\overbrace{A = LL^+}^{\text{then } A^+ = (LL^+)^+ = (L^+)^+ L^+ = LL^+ = A}$, where L is lower triangular, and thus L^+ upper triangular. This is called **Cholesky decomposition**. This is interesting in practice, because there are stable and efficient numerical algorithms to compute it.
  But note that $\langle \vec{x}, A\vec{x} \rangle = \langle \vec{x}, LL^+\vec{x} \rangle = \langle L^+\vec{x}, L^+\vec{x} \rangle \geq 0$, so this only works if $\langle \vec{x}, A\vec{x} \rangle \geq 0$, i.e., if A is positive definite, i.e., if all eigenvalues are ≥ 0.

- Given $A = LU$, we can easily compute

$$\det A = \det(LU) = \det L \det U = \prod_{j=1}^{n} L_{jj} \prod_{i=1}^{n} U_{ii}.$$

det of upper/lower triangular matrix is product of diagonal entries

If we decompose $A = LU$ with L having 1's on the diagonal, the formula simplifies to $\det A = \prod_{i=1}^{n} U_{ii}$.

- Given $A = LU$ for A invertible, we can solve $A\vec{x} = LU\vec{x} = \overbrace{\vec{e}_j}^{= \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \leftarrow j\text{-th entry}}$ to find the j-th column of A^{-1}!

E.g., $A\vec{x} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$ gives $\vec{x} = A^{-1} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} (A^{-1})_{11} & \cdots & (A^{-1})_{1n} \\ \vdots & & \\ (A^{-1})_{n1} & \cdots & (A^{-1})_{nn} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} (A^{-1})_{11} \\ \vdots \\ (A^{-1})_{n1} \end{pmatrix}.$

Or directly, $A^{-1} = (LU)^{-1} = U^{-1}L^{-1}$ and U^{-1}, L^{-1} can be computed very easily, since they have only 0's below or above the diagonal.

4.7.2 QR Decomposition

In the QR decomposition, Q refers to an orthogonal matrix, and R to an upper (=right) triangular matrix.

The crucial idea for a QR decomposition is the $\boxed{\text{Gram-Schmidt orthonormalization.}}$

This is a procedure to turn n linearly independent vectors $\vec{u}_1, \dots, \vec{u}_n$ into n orthonormal vectors $\vec{v}_1, \dots, \vec{v}_n$ which span the same subspace, i.e., $\text{span}\{\vec{v}_1, \dots, \vec{v}_n\} = \text{span}\{\vec{u}_1, \dots, \vec{u}_n\}$.

E.g., $\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 2 \\ 1 \\ 0 \end{pmatrix}$ span the x-y-plane, but they are <u>not</u> orthonormal.

But $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$ and $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$ also span the x-y-plane, and they <u>are</u> orthonormal.

in $\mathbb{R}^n$ we often write $|\vec{x}| = \|\vec{x}\|$

Let us consider a general vector space with scalar product $\langle \vec{x}, \vec{y} \rangle$ and norm $\|\vec{x}\|^2 = \langle \vec{x}, \vec{x} \rangle$.

The general process goes as follows:

Step 1: We normalize the first vector: $\vec{v}_1 := \frac{\vec{u}_1}{\|\vec{u}_1\|}$ $\quad \left(\text{s.t. } \|\vec{v}_1\| = \frac{\|\vec{u}_1\|}{\|\vec{u}_1\|} = 1\right)$.

Clearly, $\text{span}\{\vec{u}_1\} = \text{span}\{\vec{v}_1\}$.

Step 2: How can we then construct a $\vec{v}_2$ with $\langle \vec{v}_1, \vec{v}_2 \rangle = 0$ using $\vec{u}_2$?

We have $\vec{u}_2 = \langle \vec{v}_1, \vec{u}_2 \rangle \vec{v}_1 + \underbrace{\left(\vec{u}_2 - \langle \vec{v}_1, \vec{u}_2 \rangle \vec{v}_1\right)}_{=:\tilde{\vec{v}}_2}$

with $\langle \vec{v}_1, \tilde{\vec{v}}_2 \rangle = \langle \vec{v}_1, \left(\vec{u}_2 - \langle \vec{v}_1, \vec{u}_2 \rangle \vec{v}_1\right) \rangle$

$$= \langle \vec{v}_1, \vec{u}_2 \rangle - \langle \vec{v}_1, \vec{u}_2 \rangle \underbrace{\langle \vec{v}_1, \vec{v}_1 \rangle}_{=1 \text{ by step 1}}$$

$$= 0$$

Thus, we set $\vec{v}_2 = \frac{\tilde{\vec{v}}_2}{\|\tilde{\vec{v}}_2\|}$ with $\tilde{\vec{v}}_2 = \vec{u}_2 - \langle \vec{v}_1, \vec{u}_2 \rangle \vec{v}_1$.

Then $\vec{v}_1$ and $\vec{v}_2$ are orthonormal.

And again, $\operatorname{span}\{\vec{v}_1, \vec{v}_2\} = \operatorname{span}\{\vec{u}_1, \vec{v}_2\} = \operatorname{span}\{\vec{u}_1, \vec{u}_2\}$ by construction.

$\vdots$

Step j: We repeat what we did in step 2 in the following way.

Given $\vec{v}_1, \dots, \vec{v}_{j-1}$, we set $\vec{\tilde{v}}_j = \vec{u}_j - \sum_{k=1}^{j-1} \langle \vec{v}_k, \vec{u}_j \rangle \vec{v}_k$.

Then for $m<j$, we have
$$\langle \vec{v}_m, \vec{\tilde{v}}_j \rangle = \langle \vec{v}_m, \vec{u}_j \rangle - \sum_{k=1}^{j-1} \langle \vec{v}_k, \vec{u}_j \rangle \underbrace{\langle \vec{v}_m, \vec{v}_k \rangle}_{= \delta_{mk} = \begin{cases} 1 & \text{for } m=k \\ 0 & \text{for } m \neq k \end{cases}}$$

only k=m term survives

$$= \langle \vec{v}_m, \vec{u}_j \rangle - \langle \vec{v}_m, \vec{u}_j \rangle$$
$$= 0,$$

so we have indeed constructed a $\tilde{v}_j$ orthogonal to all previously constructed $\vec{v}_m, m<j$.

Lastly, we normalize: $\vec{v}_j := \dfrac{\vec{\tilde{v}}_j}{\|\vec{\tilde{v}}_j\|}$.

By construction, $\operatorname{span}\{\vec{u}_1, \dots, \vec{u}_j\} = \operatorname{span}\{\vec{v}_1, \dots, \vec{v}_j\}$.

With this procedure we have constructed orthonormal $\vec{v}_1, \dots, \vec{v}_n$ that span the same subspace as $\vec{u}_1, \dots, \vec{u}_n$.

Note: · In general, $P_W: \mathbb{R}^n \to W$, where W is a subspace of $\mathbb{R}^n$, is called a projection if $P_W(\vec{w}) = \vec{w}$ for any vector $\vec{w} \in W$.

P_W is called orthogonal projection if $\vec{u} - P_W(\vec{u})$ is orthogonal to W for any $\vec{u} \in \mathbb{R}^n$.

If $\vec{w}_1, \dots, \vec{w}_j$ is an orthonormal basis of W, then $P_W(\vec{u}) = \sum_{m=1}^{j} \langle \vec{w}_j, \vec{u} \rangle \vec{w}_j$.

Check: $\langle \vec{w}_i, (\vec{u} - P_W(\vec{u})) \rangle = \langle \vec{w}_i, \vec{u} \rangle - \langle \vec{w}_i, \sum_{m=1}^{j} \langle \vec{w}_j, \vec{u} \rangle \vec{w}_j \rangle = \langle \vec{w}_i, \vec{u} \rangle - \langle \vec{w}_i, \vec{u} \rangle = 0.$ ✓

as before, $\langle \vec{w}_i, \vec{w}_j \rangle = \delta_{ij}$

So above in the Gram-Schmidt process, we have used orthogonal projections to construct the orthonormal basis.

Now, what does this have to do with the QR decomposition?

Let us consider a real invertible $n\times n$ matrix A.

A invertible means its columns are linearly independent. Let us call them $\vec{u}_1,\dots,\vec{u}_n$, i.e.,

$A=\left(\vec{u}_1 \,|\, \vec{u}_2 \,|\, \dots \,|\, \vec{u}_n\right)$. Then we apply Gram-Schmidt and obtain orthonormal $\vec{v}_1,\dots,\vec{v}_n$.

These are the columns of an orthogonal matrix Q, i.e., $Q=\left(\vec{v}_1 \,|\, \dots \,|\, \vec{v}_n\right)$.

With Gram-Schmidt, we have expressed the $\vec{u}_j$ in terms of the $\vec{v}_j$:

$$\vec{u}_1 = \langle \vec{v}_1,\vec{u}_1\rangle \vec{v}_1 \qquad \left(\langle \vec{v}_1,\vec{u}_1\rangle = \langle \frac{\vec{u}_1}{\|\vec{u}_1\|}, \vec{u}_1\rangle = \frac{\langle \vec{u}_1,\vec{u}_1\rangle}{\|\vec{u}_1\|} = \frac{\|\vec{u}_1\|^2}{\|\vec{u}_1\|} = \|\vec{u}_1\| \right)$$

$$\vec{u}_2 = \langle \vec{v}_1,\vec{u}_2\rangle \vec{v}_1 + \langle \vec{v}_2,\vec{u}_2\rangle \vec{v}_2$$

$$\vdots$$

$$\vec{u}_n = \langle \vec{v}_1,\vec{u}_n\rangle \vec{v}_1 + \langle \vec{v}_2,\vec{u}_n\rangle \vec{v}_2 + \dots + \langle \vec{v}_n,\vec{u}_n\rangle \vec{v}_n$$

Written in matrix form, this reads

$$\underbrace{\left(\vec{u}_1 \,|\, \dots \,|\, \vec{u}_n\right)}_{A} = \underbrace{\left(\vec{v}_1 \,|\, \dots \,|\, \vec{v}_n\right)}_{Q} \underbrace{\begin{pmatrix} \langle \vec{v}_1,\vec{u}_1\rangle & \langle \vec{v}_1,\vec{u}_2\rangle & \cdots & \langle \vec{v}_1,\vec{u}_n\rangle \\ 0 & \langle \vec{v}_2,\vec{u}_2\rangle & \cdots & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & 0 & \langle \vec{v}_n,\vec{u}_n\rangle \end{pmatrix}}_{R = \text{upper triangular}}$$

To summarize:

Theorem: Any real invertible $n \times n$ matrix can be written as $A = QR$, where Q is an orthogonal matrix and R is an upper triangular matrix.

Note: • If we have found such a decomposition $A = QR$, then

$$A^{-1} = (QR)^{-1} = R^{-1} \underbrace{Q^{-1}}_{= Q^T \text{ since } Q \text{ orthogonal}} = R^{-1} Q^T.$$

Q^T is directly given and R^{-1} can easily be computed since R is upper triangular.

• One can actually compute $A = QR$ for any real $n \times n$ matrix A, not just invertible ones.

• If A is a complex $n \times n$ matrix, the corresponding decomposition is $A = QR$, but where Q is a unitary matrix.

• QR decompositions even work for $m \times n$ matrices with $m > n$. In that case, Q is still an orthonormal/unitary $m \times m$ matrix, but R is an $m \times n$ upper triangular matrix. Since $m > n$, the last $m-n$ rows of R are 0.

So in block form we can write

$$A = QR = Q \begin{array}{c} n \\ \begin{pmatrix} R_1 \\ 0 \end{pmatrix} \end{array} \begin{array}{l} \}n \\ \}m-n \end{array} = m\Big\{ \Big(\underbrace{Q_1}_{n} \,\Big|\, \underbrace{Q_2}_{m-n} \Big) \begin{array}{c} n \\ \begin{pmatrix} R_1 \\ 0 \end{pmatrix} \end{array} \begin{array}{l} \}n \\ \}m-n \end{array} = Q_1 R_1$$

↳ R_1 = upper triangular $n \times n$ matrix

↳ Q_1 = $m \times n$ matrix with orthonormal columns

$\Rightarrow$ Q_2 has orthonormal columns that are also orthonormal to the columns of Q_1. These can be constructed with Gram-Schmidt as well

- One application of the QR decomposition is the least-square method. Let us consider $A\vec{x}=\vec{b}$ for an $m\times n$ matrix A with $m>n$, i.e., more equations than unknowns. This is an overdetermined system of equations, and it thus often has no solutions. But we could ask for $\|A\vec{x}-\vec{b}\|$ to be as small as possible instead.

With a QR decomposition as in the remark above, we get

$$\|A\vec{x}-\vec{b}\| = \|QR\vec{x}-\vec{b}\| \overset{\substack{Q^T \text{ is orthogonal and does not change lengths}\\ \downarrow}}{=} \|Q^T(QR\vec{x}-\vec{b})\| \underset{\substack{\uparrow\\ Q^TQ=I}}{=} \|R\vec{x}-Q^T\vec{b}\|$$

Now, $R\vec{x} = \begin{array}{c} \begin{pmatrix} R_1\vec{x} \\ 0 \\ \vdots \\ 0 \end{pmatrix} \begin{array}{l} \}n \\ \\ \}m-n \\ \end{array} \end{array}$, and $Q^T\vec{b} := \vec{c} = \begin{pmatrix} \vec{c}_1 \\ \vec{c}_2 \end{pmatrix} \begin{array}{l} \}n \\ \}m-n \end{array}$

Then $\|A\vec{x}-\vec{b}\|^2 = \|R_1\vec{x}-\vec{c}_1\|^2 + \underbrace{\|0-\vec{c}_2\|^2}_{\geq 0}$.

This expression is the smallest when $R_1\vec{x}=\vec{c}_1$, i.e., $\vec{x} = \underbrace{R_1^{-1}}_{\text{easy to compute}}\vec{c}_1$.