MATH 532: Linear Algebra

Chapter 3: Matrix Algebra

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Outline

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We will briefly go over some ideas from Chapters 1, 2 and the first half of Chapter 3 of the textbook [Mey00].

After that introduction we will start our real journey with Section 3.7 and the inverse of a matrix.

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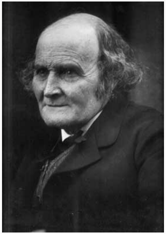

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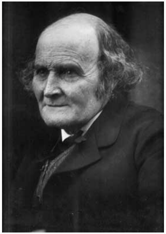

- “Modern” linear algebra is associated with Arthur Cayley (1821–1895), and many others after him.
- Recent developments have focused mostly on numerical linear algebra.

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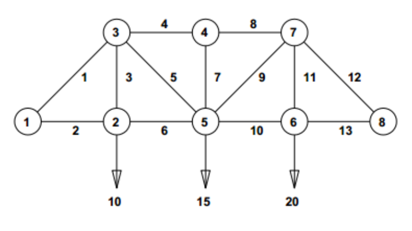

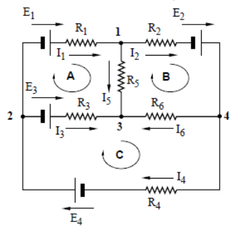

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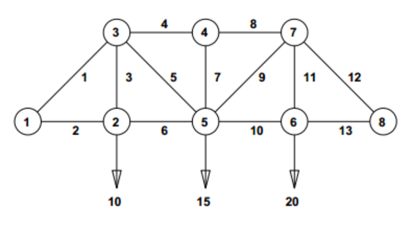

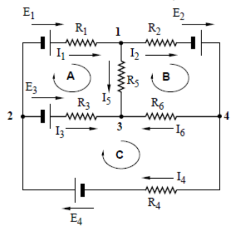

- Data science and statistics: regression

$$\min_{\boldsymbol{x}\in\mathbb{R}^m} \|A\boldsymbol{x} - \boldsymbol{b}\|_2 \quad \Longrightarrow \quad \boldsymbol{x} = (A^TA)^{-1}A^T\boldsymbol{b}$$

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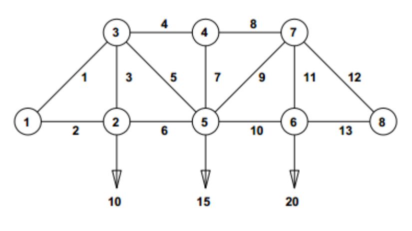

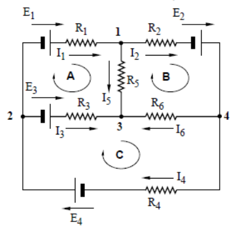

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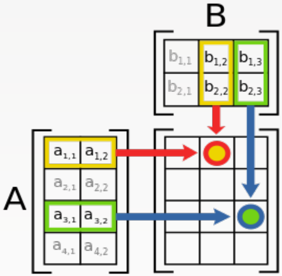
- Machine learning: regularization networks

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \left[L(\boldsymbol{b}, A\boldsymbol{x}) + \mu\|\boldsymbol{x}\|\right], \quad \text{e.g.,} \ \min_{\boldsymbol{x}\in\mathbb{R}^n} \|A\boldsymbol{x}-\boldsymbol{b}\|_2 + \mu\boldsymbol{x}^TA\boldsymbol{x}$$

Outline

Different forms of matrix products

We all know how to multiply two matrices A and B:



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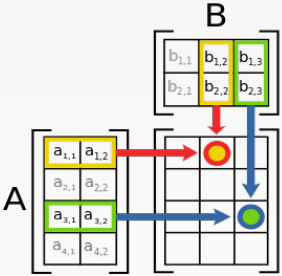

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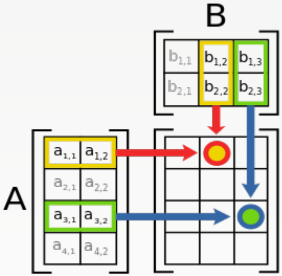

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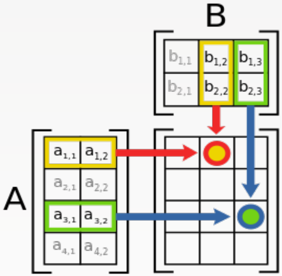


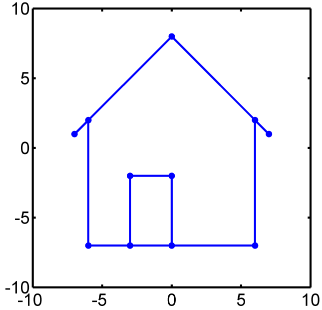
But why do we do it this way?

- Because Cayley said so.
- Because it works for systems of linear equations and for linear transformations, i.e., scalings, rotations, reflections and shear maps can be expressed as a matrix product.

Matrices as Linear Transformations

We illustrate properties of linear transformations (matrix multiplication by A) with the following “data”:

```
X = house
dot2dot(X)
```

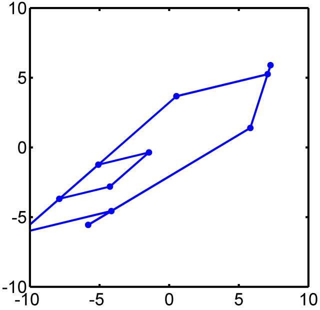


Straight lines are always mapped to straight lines.

```
A = rand(2,2)
dot2dot(A*X)
```

Sample matrix

$$A = \begin{bmatrix} 0.9357 & 0.7283 \\ 0.8187 & 0.1758 \end{bmatrix}$$

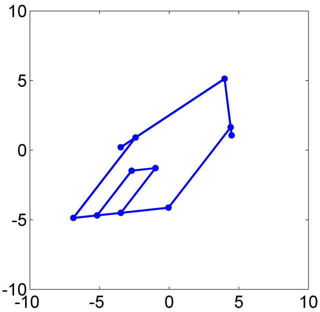


The transformation is orientation-preserving[1] if $\det A > 0$.

```
A = rand(2,2)
det(A)
dot2dot(A*X)
```

Sample matrix

$$A = \begin{bmatrix} 0.5694 & 0.4963 \\ 0.0614 & 0.6423 \end{bmatrix}$$



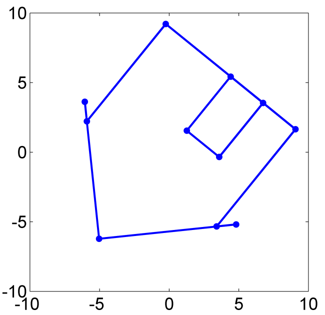
[1] The door always stays on the left.

The angles between straight lines are preserved if the matrix is orthogonal[2].

```
A = orth(rand(2,2));   % creates orthogonal matrix
A = A(:,randperm(2))   % randomly permute columns of A
det(A)
dot2dot(A*X)
```

Sample matrix

$$A = \begin{bmatrix} -0.7767 & -0.6299 \\ 0.6299 & -0.7767 \end{bmatrix}$$



[2] An orthogonal matrix A has det A $\pm$ 1 and represents either a rotation or a reflection.

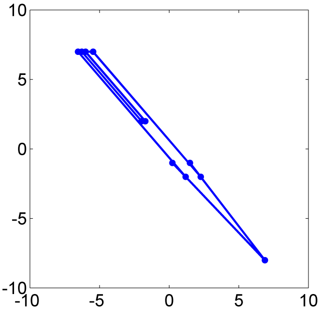
A linear transformation is invertible[3] only if $\det A \neq 0$.

```
a22 = randi(3,1,1)-2  % creates random {-1,0,1}
A = triu(rand(2,2)); A(2,2) = a22
det(A)
dot2dot(A*X)
```

Sample matrix

$$A = \begin{bmatrix} 0.0903 & 0.8586 \\ 0 & -1.0000 \end{bmatrix}$$

$$\det A = -0.0903$$



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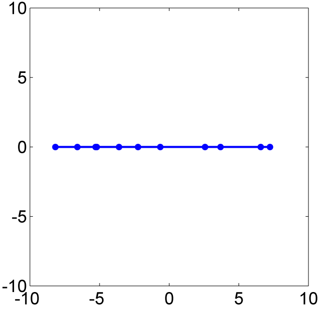
Sample matrix

$$A = \begin{bmatrix} 0.9884 & 0.3209 \\ 0 & 0 \end{bmatrix}$$

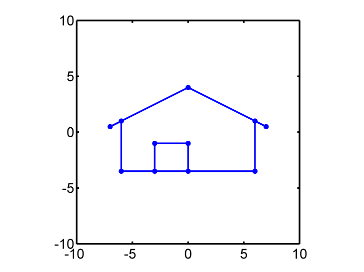
$$\det A = 0$$



[3] If the transformation is not invertible, then the 2D image collapses to a line or even a point.

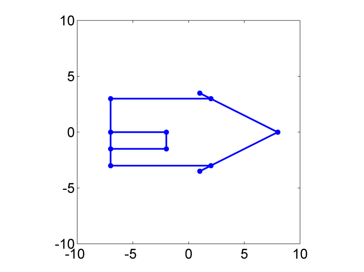
A diagonal matrix stretches the image or reverses its orientation.

$$A = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{2} \end{bmatrix}, \quad \det A = \frac{1}{2}$$



A anti-diagonal matrix in addition interchanges coordinates.

$$A = \begin{bmatrix} 0 & 1 \\ \frac{1}{2} & 0 \end{bmatrix}, \quad \det A = -\frac{1}{2}$$



The action of a diagonal matrix provides an interpretation of the effect of eigenvalues. Note that these matrices have orthogonal columns, but their determinant is not ± 1, so they are **not** orthogonal matrices. These matrices preserve right angles only.

Any rotation matrix can be expressed in terms of trigonometric functions:
The matrix

$$G(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

represents a counter-clockwise rotation by the angle θ (measured in radians).

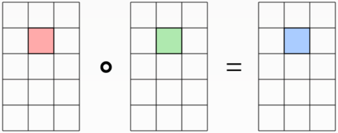
Look at `wiggle.m`.

Matrix multiplication: Why we do it the way we do it

- Because the most obvious way, i.e.,

$$[A \circ B]_{ij} = [A]_{ij}[B]_{ij},$$

known as Hadamard[4] (or Schur) product, doesn't work for linear systems and linear transformations.



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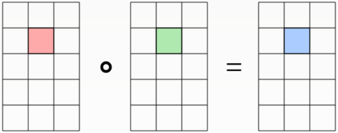


- It's also defined only for matrices of the same size.
- But it does commute.

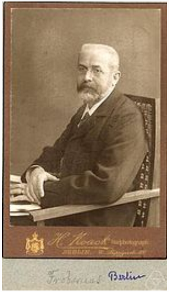
[4] Jacques Hadamard (1865–1963) and Issai Schur (1875–1941)

Matrix multiplication: Why we do it the way we do it

- Because the Frobenius[5] (inner) product,

$$\langle A, B \rangle_F = \sum_{i,j} [A]_{ij}[B]_{ij},$$

doesn't work for linear systems or linear transformations either.



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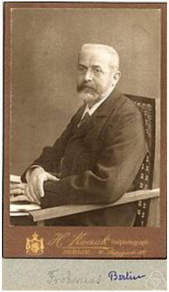

  - It is also requires $\text{size}(\mathsf{A}) = \text{size}(\mathsf{B})$.
  - It does, however, induce a useful matrix norm (see HW).

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- Because the Kronecker[6] product,

$$\mathsf{A} \otimes \mathsf{B} = \begin{pmatrix} [\mathsf{A}]_{11}\mathsf{B} & \cdots & [\mathsf{A}]_{1n}\mathsf{B} \\ \vdots & & \vdots \\ [\mathsf{A}]_{m1}\mathsf{B} & \cdots & [\mathsf{A}]_{mn}\mathsf{B} \end{pmatrix},$$

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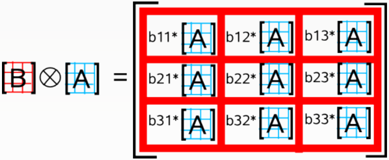

- Works for matrices of arbitrary size, i.e., A is $m \times n$, B is $p \times q$.
- Ideal for working with tensor products $\rightsquigarrow$ multilinear algebra

[6] Leopold Kronecker (1823–1891)

Modern research on matrix multiplication

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- Special algorithms for general matrices:
  - Strassen's algorithm [Str69] $\mathcal{O}(n^{2.807})$,
  - Coppersmith–Winograd algorithm [CW90] $\mathcal{O}(n^{2.375})$,
  - Stothers' algorithm [DS13] $\mathcal{O}(n^{2.374})$,
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- Exploiting structure (banded, block, hierarchical) — often implied by application
- Using factorizations, into products of structured matrices
- Exploiting sparsity
- Exploiting new hardware

Outline

Definition (Matrix inverse)

For any $n \times n$ matrix A, the $n \times n$ matrix B that satisfies

$$\mathsf{AB} = \mathsf{I} \quad \text{and} \quad \mathsf{BA} = \mathsf{I}$$

is called the *inverse* of A.
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2. *Sometimes one can find the notion of a left- and right-inverse. However, we consider only inverses of square matrices, so these notions don't apply (see also [Mey00, Ex. 3.7.2]).*

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Example

Compute the inverse of

$$A = \begin{pmatrix} 2 & 2 & 6 \\ 2 & 1 & 7 \\ 2 & -6 & -7 \end{pmatrix}.$$

Solution

$$\left(\begin{array}{ccc|ccc} 2 & 2 & 6 & 1 & 0 & 0 \\ 2 & 1 & 7 & 0 & 1 & 0 \\ 2 & -6 & -7 & 0 & 0 & 1 \end{array}\right)$$

Solution

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$$\left(\begin{array}{ccc|ccc} 2 & 2 & 6 & 1 & 0 & 0 \\ 2 & 1 & 7 & 0 & 1 & 0 \\ 2 & -6 & -7 & 0 & 0 & 1 \end{array}\right) \longrightarrow \left(\begin{array}{ccc|ccc} 2 & 2 & 6 & 1 & 0 & 0 \\ 0 & -1 & 1 & -1 & 1 & 0 \\ 0 & -8 & -13 & -1 & 0 & 1 \end{array}\right)$$

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Gauss–Jordan elimination is not good for solving linear systems, but useful for some theoretical purposes.

How to check if A is invertible

Theorem

For any $n \times n$ matrix A, the following statements are equivalent:

1. A^{-1} *exists*
2. $\operatorname{rank}(\mathsf{A}) = n$
3. *Gauss–Jordan elimination reduces* A *to* I
4. $\mathsf{A}\boldsymbol{x} = \mathbf{0}$ *has only the trivial solution* $\boldsymbol{x} = \mathbf{0}$
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Proof.

Items (1)–(4) are proved in [Mey00]. Items (5)–(7) are discussed later (but should probably be familiar concepts). □

Inverse of a matrix product

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If A *and* B *are invertible, then* AB *is also invertible and*

$$(AB)^{-1} = B^{-1}A^{-1}.$$

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Just use the definition to verify invertibility:

$$(\mathsf{AB})\,\mathsf{B}^{-1}\mathsf{A}^{-1} =$$

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$$(AB)\,B^{-1}A^{-1} = A\left(BB^{-1}\right)A^{-1}$$

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Since the inverse is unique we are done. $\square$

Inverse of a matrix sum

A simple example shows that — just because A and B are invertible — the inverse of $A + B$ need not exist!

Example

Let

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \text{and} \qquad B = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

Then $A + B$ is the zero matrix, which is obviously not invertible.

Inverse of a matrix sum (cont.)

Moreover, the inverse is not a linear function.

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Let $a = 2$ and $b = 3$.

Inverse of a matrix sum (cont.)

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Let $a = 2$ and $b = 3$. Then

- $a + b = 5$, and so $(a + b)^{-1} = \frac{1}{5}$;

Inverse of a matrix sum (cont.)

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And now we see/know that

$$(a + b)^{-1} \neq a^{-1} + b^{-1} \qquad \text{since} \qquad \frac{1}{5} \neq \frac{1}{2} + \frac{1}{3}.$$

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So, how do we compute the inverse of $\mathsf{A} + \mathsf{B}$?

It can be done if one assumes that A and B are such that the inverse exists. The following theorem was proved only in 1981 [HS81].

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Theorem (Henderson–Searle)

Suppose the $n \times n$ *matrix* A *is invertible, and let* C *be* $n \times p$, B *be* $p \times q$ *and* D *be* $q \times n$*. Also assume that* $(\mathsf{A} + \mathsf{CBD})^{-1}$ *exists. Then*

1. $(\mathsf{A} + \mathsf{CBD})^{-1} = \mathsf{A}^{-1} - \left(\mathsf{I}_n + \mathsf{A}^{-1}\mathsf{CBD}\right)^{-1} \mathsf{A}^{-1}\mathsf{CBDA}^{-1}$,
2. $(\mathsf{A} + \mathsf{CBD})^{-1} = \mathsf{A}^{-1} - \mathsf{A}^{-1} \left(\mathsf{I}_n + \mathsf{CBDA}^{-1}\right)^{-1} \mathsf{CBDA}^{-1}$,
3. $(\mathsf{A} + \mathsf{CBD})^{-1} = \mathsf{A}^{-1} - \mathsf{A}^{-1}\mathsf{C} \left(\mathsf{I}_p + \mathsf{BDA}^{-1}\mathsf{C}\right)^{-1} \mathsf{BDA}^{-1}$,
4. $(\mathsf{A} + \mathsf{CBD})^{-1} = \mathsf{A}^{-1} - \mathsf{A}^{-1}\mathsf{CB} \left(\mathsf{I}_q + \mathsf{DA}^{-1}\mathsf{CB}\right)^{-1} \mathsf{DA}^{-1}$,
5. $(\mathsf{A} + \mathsf{CBD})^{-1} = \mathsf{A}^{-1} - \mathsf{A}^{-1}\mathsf{CBD} \left(\mathsf{I}_n + \mathsf{A}^{-1}\mathsf{CBD}\right)^{-1} \mathsf{A}^{-1}$,
6. $(\mathsf{A} + \mathsf{CBD})^{-1} = \mathsf{A}^{-1} - \mathsf{A}^{-1}\mathsf{CBDA}^{-1} \left(\mathsf{I}_n + \mathsf{CBDA}^{-1}\right)^{-1}$.

Before we prove (part of) this theorem, let's see what this says about $(A+B)^{-1}$.

Corollary

In the theorem, let all matrices be $n \times n$ and let $C = D = I$. Then

1. $(A+B)^{-1} = A^{-1} - \left(I + A^{-1}B\right)^{-1} A^{-1}BA^{-1}$,
2. $(A+B)^{-1} = A^{-1} - A^{-1}\left(I + BA^{-1}\right)^{-1} BA^{-1}$,
3. $(A+B)^{-1} = A^{-1} - A^{-1}B\left(I + A^{-1}B\right)^{-1} A^{-1}$,
4. $(A+B)^{-1} = A^{-1} - A^{-1}BA^{-1}\left(I + BA^{-1}\right)^{-1}$.

Note that only four formulas are left.

To prove this theorem one needs

Lemma

Suppose A *is an* $n \times n$ *matrix such that* $\mathsf{I} + \mathsf{A}$ *is invertible. Then*

$$\begin{aligned}(\mathsf{I}+\mathsf{A})^{-1} &= \mathsf{I} - \mathsf{A}(\mathsf{I}+\mathsf{A})^{-1} && (1a)\\ &= \mathsf{I} - (\mathsf{I}+\mathsf{A})^{-1}\mathsf{A}. && (1b)\end{aligned}$$

In particular,

$$\mathsf{A}(\mathsf{I}+\mathsf{A})^{-1} = (\mathsf{I}+\mathsf{A})^{-1}\mathsf{A}. \tag{2}$$

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Proof.

(2) follows immediately from (1).

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(2) follows immediately from (1).
To prove (1), we start with

$$\mathsf{I} = (\mathsf{I} + \mathsf{A}) - \mathsf{A}.$$

Now multiply by $(\mathsf{I} + \mathsf{A})^{-1}$ from either the right (to get (1a)), or from the left (to get (1b)). $\square$

Proof of the theorem.

We prove only the first identity.
We note that $\mathsf{I}_n + \mathsf{A}^{-1}\mathsf{CBD} = \mathsf{A}^{-1}(\mathsf{A} + \mathsf{CBD})$, where both factors are invertible by assumption. Therefore $\left(\mathsf{I}_n + \mathsf{A}^{-1}\mathsf{CBD}\right)^{-1}$ exists.

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Then

$$(\mathsf{A}+\mathsf{CBD})^{-1} = \left(\mathsf{A}\left(\mathsf{I}_n + \mathsf{A}^{-1}\mathsf{CBD}\right)\right)^{-1} \qquad \text{from above}$$

□

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We note that $I_n + A^{-1}CBD = A^{-1}(A + CBD)$, where both factors are invertible by assumption. Therefore $\left(I_n + A^{-1}CBD\right)^{-1}$ exists.
Then

$$\begin{aligned}
(A + CBD)^{-1} &= \left(A\left(I_n + A^{-1}CBD\right)\right)^{-1} && \text{from above} \\
&= \left(I_n + A^{-1}CBD\right)^{-1} A^{-1} && \text{since } (A\widetilde{B})^{-1} = \widetilde{B}^{-1}A^{-1}
\end{aligned}$$

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&= \mathsf{A}^{-1} - \left(\mathsf{I}_n + \mathsf{A}^{-1}\mathsf{CBD}\right)^{-1}\mathsf{A}^{-1}\mathsf{CBDA}^{-1}.
\end{aligned}
$$

Note that the other identities are not proven analogously. They require extra work. $\square$

Sherman–Morrison formula

The following formula is older (from 1949–50), but can also be derived as a corollary from the Henderson–Searle theorem.

Corollary

Suppose that the $n \times n$ matrix A is invertible, and also suppose that $\alpha \in \mathbb{R}$ and the column n-vectors $\boldsymbol{c}$ and $\boldsymbol{d}$ are such that $1 + \alpha \boldsymbol{d}^T \mathsf{A}^{-1} \boldsymbol{c} \neq 0$. Then $\mathsf{A} + \alpha \boldsymbol{c}\boldsymbol{d}^T$ is invertible and

$$\left(\mathsf{A} + \alpha \boldsymbol{c}\boldsymbol{d}^T\right)^{-1} = \mathsf{A}^{-1} - \frac{\alpha \mathsf{A}^{-1} \boldsymbol{c}\boldsymbol{d}^T \mathsf{A}^{-1}}{1 + \alpha \boldsymbol{d}^T \mathsf{A}^{-1} \boldsymbol{c}}.$$

Note that $\alpha \boldsymbol{c}\boldsymbol{d}^T$ is a rank-1 update of A.

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Remark

The Sherman–Morrison–Woodbury formula follows analogously and is stated in [Mey00].

Proof.

We use the fourth identity of the Henderson–Searle theorem with $\mathsf{B} = \alpha$, $\mathsf{C} = \boldsymbol{c}$ and $\mathsf{D} = \boldsymbol{d}^T$ (so that $p = q = 1$).
Then

$$(\mathsf{A} + \mathsf{CBD})^{-1} = \mathsf{A}^{-1} - \mathsf{A}^{-1}\mathsf{CB}\left(\mathsf{I}_q + \mathsf{DA}^{-1}\mathsf{CB}\right)^{-1}\mathsf{DA}^{-1}$$

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since $\boldsymbol{d}^T A^{-1}\boldsymbol{c}$ is a scalar. $\square$

If $A = I$, $\alpha = -1$ and $\boldsymbol{c}$, $\boldsymbol{d}$ such that $\boldsymbol{d}^T\boldsymbol{c} \neq 1$ in the Sherman–Morrison formula, then we get

$$\left(I - \boldsymbol{c}\boldsymbol{d}^T\right)^{-1} = I - \frac{\boldsymbol{c}\boldsymbol{d}^T}{\boldsymbol{d}^T\boldsymbol{c} - 1}.$$

If $\mathsf{A} = \mathsf{I}$, $\alpha = -1$ and $\boldsymbol{c}, \boldsymbol{d}$ such that $\boldsymbol{d}^T\boldsymbol{c} \neq 1$ in the Sherman–Morrison formula, then we get

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- $\left(\mathsf{I} - \boldsymbol{c}\boldsymbol{d}^T\right)^{-1}$ is also an elementary matrix, i.e.,

  the inverse of an elementary matrix is an elementary matrix.

If $A = I$, $\alpha = -1$ and $\boldsymbol{c}, \boldsymbol{d}$ such that $\boldsymbol{d}^T\boldsymbol{c} \neq 1$ in the Sherman–Morrison formula, then we get

$$\left(I - \boldsymbol{c}\boldsymbol{d}^T\right)^{-1} = I - \frac{\boldsymbol{c}\boldsymbol{d}^T}{\boldsymbol{d}^T\boldsymbol{c} - 1}.$$

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- $\left(I - \boldsymbol{c}\boldsymbol{d}^T\right)^{-1}$ is also an elementary matrix, i.e.,

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We will use such elementary matrices in the next section.

Example

Assume we have worked hard to calculate A^{-1}, and now we change one entry, $[A]_{ij}$, of A. What is the new inverse?

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We can apply the Sherman–Morrison formula with $\boldsymbol{c} = \boldsymbol{e}_i, \boldsymbol{d} = \boldsymbol{e}_j$:

$$\left(A + \alpha \boldsymbol{e}_i \boldsymbol{e}_j^T\right)^{-1} = A^{-1} - \frac{\alpha A^{-1} \boldsymbol{e}_i \boldsymbol{e}_j^T A^{-1}}{1 + \alpha \boldsymbol{e}_j^T A^{-1} \boldsymbol{e}_i}$$

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$$= A^{-1} - \alpha \frac{[A^{-1}]_{*i} [A^{-1}]_{j*}}{1 + \alpha [A^{-1}]_{ji}}.$$

Note that there's no need to recompute the entire inverse (an $\mathcal{O}(n^3)$ effort). All we need to compute is one outer product, two scalar multiplications and a division (which is $\mathcal{O}(n^2)$).

Outline

Elementary Matrices and Equivalence

Our goals for the next two sections are to

- obtain a matrix factorization of a nonsingular $n \times n$ matrix A into elementary matrices,
- obtain a representation of Gaussian elimination as a matrix factorization.

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Remark

Right-multiplication will result in similar column operations.

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Example (cont.)

Recall that elementary matrices are of the form $\mathsf{I} - \boldsymbol{c}\boldsymbol{d}^T$.

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1. E_1 can be written as

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = \mathsf{I} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}$$

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Example

Gaussian elimination with elementary matrices

Earlier we had

$$\begin{pmatrix} 2 & 2 & 6 \\ 2 & 1 & 7 \\ 2 & -6 & -7 \end{pmatrix} \xrightarrow[-R_1+R_3]{-R_1+R_2} \begin{pmatrix} 2 & 2 & 6 \\ 0 & -1 & 1 \\ 0 & -8 & -13 \end{pmatrix} \xrightarrow{-8R_2+R_3} \begin{pmatrix} 2 & 2 & 6 \\ 0 & -1 & 1 \\ 0 & 0 & -21 \end{pmatrix}$$

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So

$$\begin{aligned} \begin{pmatrix} 2 & 2 & 6 \\ 0 & -1 & 1 \\ 0 & 0 & -21 \end{pmatrix} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -8 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 2 & 2 & 6 \\ 2 & 1 & 7 \\ 2 & -6 & -7 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 7 & -8 & 1 \end{pmatrix} \begin{pmatrix} 2 & 2 & 6 \\ 2 & 1 & 7 \\ 2 & -6 & -7 \end{pmatrix} \end{aligned}$$

Note that this is of the form $U = LA$.

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Now, since the inverse of an elementary matrix is an elementary matrix (of the same type) we have

$$\mathsf{A} = \mathsf{E}_1^{-1} \mathsf{E}_2^{-1} \cdots \mathsf{E}_k^{-1} \qquad \text{as desired.}$$

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"$\Longleftarrow$": Assume $A = E_1 E_2 \cdots E_k$. Then A is nonsingular since elementary matrices are nonsingular, and so is their product. $\square$

Equivalent matrices

Definition

Two matrices A and B are called equivalent, i.e., $A \sim B$, if

$$PAQ = B$$

for some nonsingular matrices P and Q.

Moreover, A and B are row equivalent, i.e., $A \overset{\text{row}}{\sim} B$, if $PA = B$, and A and B are column equivalent, i.e., $A \overset{\text{col}}{\sim} B$, if $AQ = B$

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Remark

Note that P *performs row operations, and* Q *performs column operations on* A.

The following theorem ensures that row operations preserve column relations (an analogous theorem holds for column operations).

Theorem

If A $\overset{row}{\sim}$ B, *then*

$$[\mathsf{B}]_{*k} = \sum_{j=1}^{n} \alpha_j [\mathsf{B}]_{*j} \quad \Longleftrightarrow \quad [\mathsf{A}]_{*k} = \sum_{j=1}^{n} \alpha_j [\mathsf{A}]_{*j}.$$

The following theorem ensures that row operations preserve column relations (an analogous theorem holds for column operations).

Theorem

If $\mathsf{A} \overset{row}{\sim} \mathsf{B}$*, then*

$$[\mathsf{B}]_{*k} = \sum_{j=1}^{n} \alpha_j [\mathsf{B}]_{*j} \iff [\mathsf{A}]_{*k} = \sum_{j=1}^{n} \alpha_j [\mathsf{A}]_{*j}.$$

Before we prove the theorem, we state

Corollary

Since $\mathsf{A} \overset{row}{\sim} \mathsf{E}_{\mathsf{A}}$[a]*, the nonbasic columns of* A *are the same linear combinations of the basic columns of* A *as those of* E_{A}*.*

[a] Here E_{A} is the unique row-reduced echelon form of A (produced via Gauss–Jordan elimination). This equivalence is proved in [Mey00] with a rather long and technical proof.

Example (for the corollary)

$$A = \begin{pmatrix} 1 & 2 & 2 & 3 & 1 \\ 2 & 4 & 4 & 6 & 2 \\ 3 & 6 & 6 & 9 & 6 \\ 1 & 2 & 4 & 5 & 3 \end{pmatrix} \quad \xrightarrow{\text{G–J}} \quad E_A = \begin{pmatrix} 1 & 2 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

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Since columns 1, 3 and 5 of E_A are basic columns, the same holds for A and

$$\begin{aligned} [E_A]_{*2} &= 2[E_A]_{*1} & \iff && [A]_{*2} &= 2[A]_{*1} \\ [E_A]_{*4} &= [E_A]_{*1} + [E_A]_{*3} & \iff && [A]_{*4} &= [A]_{*1} + [A]_{*3} \end{aligned}$$

Proof of theorem.

The definition of $A \overset{\text{row}}{\sim} B$ implies the existence of a nonsingular P so that $PA = B$.

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Therefore, if $[\mathsf{A}]_{*k} = \sum_{j=1}^{n} \alpha_j [\mathsf{A}]_{*j}$, then

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The definition of $A \overset{\text{row}}{\sim} B$ implies the existence of a nonsingular P so that $PA = B$. Then,

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$\square$

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Therefore, if $[\mathsf{A}]_{*k} = \sum_{j=1}^{n} \alpha_j [\mathsf{A}]_{*j}$, then

$$\mathsf{P}[\mathsf{A}]_{*k} = \sum_{j=1}^{n} \alpha_j \mathsf{P}[\mathsf{A}]_{*j} \quad \overset{(3)}{\Longleftrightarrow} \quad [\mathsf{B}]_{*k} = \sum_{j=1}^{n} \alpha_j [\mathsf{B}]_{*j}.$$

To prove the reverse implication we multiply the identity $[\mathsf{B}]_{*k} = \ldots$ by P^{-1}. $\square$

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Row and column operations reduce A to rank-normal form.

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Row and column operations reduce A to rank-normal form.

Theorem

If A is an $n \times n$ matrix with $\operatorname{rank}(A) = r$, then

$$A \sim N_r = \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix}.$$

N_r is called the rank-normal form of A.

Proof.

We already know $A \overset{\text{row}}{\sim} E_A$, so that $PA = E_A$ with P nonsingular.

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We already know $A \overset{\text{row}}{\sim} E_A$, so that $PA = E_A$ with P nonsingular. Now, if $\operatorname{rank}(A) = r$, then E_A has r basic (unit) columns, and we can reorder the columns of E_A via an appropriate nonsingular Q_1, so that

$$PAQ_1 = E_AQ_1 = \begin{pmatrix} I_r & J \\ 0 & 0 \end{pmatrix}$$

for an appropriate matrix J.

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for an appropriate matrix J.

Finally, define $Q_2 = \begin{pmatrix} I_r & -J \\ 0 & I \end{pmatrix}$ so that

$$PAQ_1Q_2 = E_AQ_1Q_2 = \begin{pmatrix} I_r & J \\ 0 & 0 \end{pmatrix} \begin{pmatrix} I_r & -J \\ 0 & I \end{pmatrix} = \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix}$$

and $PA\underbrace{Q_1Q_2}_{=Q} = N_r$, i.e., $A \sim N_r$. $\square$

Block matrix version

Corollary

If $\operatorname{rank}(A) = r$ *and* $\operatorname{rank}(B) = s$, *then* $\operatorname{rank}\begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} = r + s.$

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If $\operatorname{rank}(\mathsf{A}) = r$ *and* $\operatorname{rank}(\mathsf{B}) = s$, *then* $\operatorname{rank}\begin{pmatrix} \mathsf{A} & 0 \\ 0 & \mathsf{B} \end{pmatrix} = r + s$.

Proof.

Just note that $\mathsf{A} \sim \mathsf{N}_r$ and $\mathsf{B} \sim \mathsf{N}_s$ so that

$$\begin{pmatrix} \mathsf{A} & 0 \\ 0 & \mathsf{B} \end{pmatrix} \sim \begin{pmatrix} \mathsf{N}_r & 0 \\ 0 & \mathsf{N}_s \end{pmatrix},$$

where $\mathsf{P} = \begin{pmatrix} \mathsf{P}_r & 0 \\ 0 & \mathsf{P}_s \end{pmatrix}$ and $\mathsf{Q} = \begin{pmatrix} \mathsf{Q}_r & 0 \\ 0 & \mathsf{Q}_s \end{pmatrix}$. $\square$

Theorem

Let A *and* B *be* $n \times n$ *matrices. Then*

1. $\mathsf{A} \sim \mathsf{B} \iff \operatorname{rank}(\mathsf{A}) = \operatorname{rank}(\mathsf{B})$,
2. $\mathsf{A} \overset{row}{\sim} \mathsf{B} \iff \mathsf{E}_{\mathsf{A}} = \mathsf{E}_{\mathsf{B}}$,
3. $\mathsf{A} \overset{col}{\sim} \mathsf{B} \iff \mathsf{E}_{\mathsf{A}^T} = \mathsf{E}_{\mathsf{B}^T}$,

so that multiplication by a nonsingular matrix does not change rank.

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2. $A \overset{row}{\sim} B \iff E_A = E_B$,
3. $A \overset{col}{\sim} B \iff E_{A^T} = E_{B^T}$,

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Proof of (1).

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Let A *and* B *be* $n \times n$ *matrices. Then*

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Proof of (3).

This follows from (2) using the transpose since

$$A \overset{\text{col}}{\sim} B \iff AQ = B \iff (AQ)^T = B^T$$
$$\iff Q^T A^T = B^T \iff A^T \overset{\text{row}}{\sim} B^T.$$

$\square$

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Then

$$(\mathsf{PAQ})^T = \mathsf{N}_r^T \quad \Longleftrightarrow \quad \mathsf{Q}^T\mathsf{A}^T\mathsf{P}^T = \mathsf{N}_r^T$$

so that $\mathsf{A}^T \sim \mathsf{N}_r^T$.

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Finally,

$$\operatorname{rank}(\mathsf{A}^T) = \operatorname{rank}(\mathsf{N}_r^T) = \begin{pmatrix} \mathsf{I}_r & \mathsf{0}_{r\times m-r} \\ \mathsf{0}_{n-r\times r} & \mathsf{0}_{n-r\times m-r} \end{pmatrix} = r.$$

□

Outline

LU Factorization/Decomposition

Recall our earlier example with the matrix

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$$\underbrace{\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -8 & 1 \end{pmatrix}}_{E_3} \underbrace{\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix}}_{=E_2} \underbrace{\begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{=E_1} A = \begin{pmatrix} 2 & 2 & 6 \\ 0 & -1 & 1 \\ 0 & 0 & -21 \end{pmatrix}$$

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lower triangular

We would, however, like a factorization of the form $A = LU$.

What we need is the inverse of the lower triangular matrix $\begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 7 & -8 & 1 \end{pmatrix}$, i.e.,

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Note that the entries below the diagonal in L correspond to the negatives of the multipliers in E_1, E_2, E_3.

If we remember that the inverse of a (lower) triangular matrix is (lower) triangular then we can be optimistic about this approach working in general.

General Discussion

Consider the $n \times n$ lower-triangular elementary matrix

$$\mathsf{T}_k = \mathsf{I} - \boldsymbol{c}_k \boldsymbol{e}_k^T,$$

where

$$\boldsymbol{c}_k = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \mu_{k+1} \\ \vdots \\ \mu_n \end{pmatrix}, \quad i.e., \qquad \boldsymbol{c}_k \boldsymbol{e}_k^T =$$

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$$\mathsf{T}_k = \begin{pmatrix} 1 & & & & & \\ & \ddots & & & 0 & \\ & & 1 & & & \\ & & -\mu_{k+1} & 1 & & \\ & 0 & \vdots & & \ddots & \\ & & -\mu_n & & & 1 \end{pmatrix}.$$

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Thus,

$$\mathsf{T}_k^{-1} = \mathsf{I} + \boldsymbol{c}_k \boldsymbol{e}_k^T$$

and we see that we always get the negatives of the multipliers $\mu_{k+1}, \ldots, \mu_n$ below the diagonal in the k^{th} column of T_k.

We now consider what happens during the k^{th} step of Gaussian elimination, i.e., we start with

$$A_{k-1} = \begin{pmatrix} \star & \star & \cdots & \alpha_1 & \star & \cdots & \star \\ 0 & \star & & \alpha_2 & & & \\ \vdots & \ddots & \ddots & \vdots & \vdots & & \vdots \\ 0 & \cdots & 0 & \alpha_k & \star & \cdots & \star \\ 0 & \cdots & 0 & \alpha_{k+1} & \star & \cdots & \star \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \alpha_n & \star & \cdots & \star \end{pmatrix}$$

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&= \mathsf{A}_{k-1} - \begin{pmatrix} 0 & \cdots & 0 & \alpha_k\boldsymbol{c}_k & \star & \cdots & \star \end{pmatrix}_{n\times n} \\
&= \begin{pmatrix}
\star & \star & \cdots & \alpha_1 & \star & \cdots & \star \\
0 & \star & & \alpha_2 & & & \\
\vdots & \ddots & \ddots & \vdots & \vdots & & \vdots \\
0 & \cdots & 0 & \alpha_k & \star & \cdots & \star \\
0 & \cdots & 0 & 0 & \star & \cdots & \star \\
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\end{pmatrix}
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From above we remember that

$$\mathsf{T}_k^{-1} = \mathsf{I} + \boldsymbol{c}_k \boldsymbol{e}_k^T$$

Therefore, using $\mathsf{T}_k^{-1} = \mathsf{I} + \boldsymbol{c}_k \boldsymbol{e}_k^T$, we have

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where

$$\boldsymbol{c}_k\boldsymbol{e}_k^T = \begin{pmatrix} 0 & \cdots & 0 & \boldsymbol{c}_k & 0 & \cdots & 0 \end{pmatrix}_{n\times n} = \begin{pmatrix} & & & 0 & & & \\ & & & \vdots & & & \\ 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ & & & \alpha_{k+1}/\alpha_k & & & \\ & & & \vdots & & & \\ & & & \alpha_n/\alpha_k & & & \end{pmatrix}$$

Finally,

$$\mathsf{T}_1^{-1}\mathsf{T}_2^{-1}\cdots\mathsf{T}_{n-1}^{-1} = \mathsf{I} + \boldsymbol{c}_1\boldsymbol{e}_1^T + \boldsymbol{c}_2\boldsymbol{e}_2^T + \ldots + \boldsymbol{c}_{n-1}\boldsymbol{e}_{n-1}^T$$
$$= \begin{pmatrix} 1 & & & & \\ \ell_{2,1} & \ddots & & 0 & \\ & \ell_{3,2} & 1 & & \\ \vdots & \vdots & \ddots & \ddots & \\ \ell_{n,1} & \ell_{n,2} & \cdots & \ell_{n,n+1} & 1 \end{pmatrix} = \mathsf{L}$$

with

$$\ell_{i,k} = \alpha_i/\alpha_k, \quad i = k+1, \ldots, n,$$

due to the form of $\boldsymbol{c}_k\boldsymbol{e}_k^T$.

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2. *By not keeping track of the (known) 1s on the diagonal of* L *we can store — on a computer — the entries of both* L *and* U *in the space previously allocated for* A. *Thus, no additional memory is required.*

How to solve linear systems using the LU factorization

Consider the linear system

$$\mathsf{A}\boldsymbol{x} = \boldsymbol{b}.$$

To solve it we first compute the factorization $\mathsf{A} = \mathsf{LU}$, so that

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Solving multiple linear systems with the same A

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The linear system can then be thought of as

$$AX = B,$$

and we compute the LU factorization of A only once, and then obtain each column of X by the forward-back substitution procedure above from the corresponding column in B.

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This forward-back substitution procedure is embarrassingly parallel.

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Namely, we solve

$$\mathsf{A}\boldsymbol{x}_j = \boldsymbol{e}_j, \qquad j = 1, \ldots, n.$$

Since $\boldsymbol{e}_j$ *is the* j^{th} *column of* I *this implies that* $\boldsymbol{x}_j$ *is the* j^{th} *column of* A^{-1}, *i.e.,*

$$\boldsymbol{x}_j = (\mathsf{A}^{-1})_{:j} \quad \Longleftrightarrow \quad \mathsf{X} = \mathsf{A}^{-1}.$$

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How do we do this in our matrix formulation?

We multiply (from the left) by an appropriate permutation matrix.

Partial Pivoting

Since the choice of pivot is not unique we declare that we always pick that row that produces the largest pivot.

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Example

Consider

$$A = \begin{pmatrix} 2 & 4 & 6 & -2 \\ 1 & 2 & 1 & 2 \\ 0 & 2 & 4 & 2 \\ -2 & 1 & 0 & 10 \end{pmatrix}$$

and use a permutation counter.

Permutation counter in rightmost column, multipliers in blue.

$$\left(\begin{array}{cccc|c} 2 & 4 & 6 & -2 & 1 \\ 1 & 2 & 1 & 2 & 2 \\ 0 & 2 & 4 & 2 & 3 \\ -2 & 1 & 0 & 10 & 4 \end{array}\right)$$

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$$\left(\begin{array}{cccc|c} 2 & 4 & 6 & -2 & 1 \\ 1 & 2 & 1 & 2 & 2 \\ 0 & 2 & 4 & 2 & 3 \\ -2 & 1 & 0 & 10 & 4 \end{array}\right) \longrightarrow \left(\begin{array}{cccc|c} 2 & 4 & 6 & -2 & 1 \\ \color{blue}{\frac{1}{2}} & 0 & -2 & 3 & 2 \\ \color{blue}{0} & 2 & 4 & 2 & 3 \\ \color{blue}{-1} & 5 & 6 & 8 & 4 \end{array}\right)$$

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Therefore, we end up with the pivoted LU factorization

$$PA = LU,$$

where

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ \frac{1}{2} & 0 & 1 & 0 \\ 0 & \frac{2}{5} & -\frac{4}{5} & 1 \end{pmatrix}, \quad U = \begin{pmatrix} 2 & 4 & 6 & -2 \\ 0 & 5 & 6 & 8 \\ 0 & 0 & -2 & 3 \\ 0 & 0 & 0 & \frac{6}{5} \end{pmatrix}, \quad P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

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Remark

The messy details of the general derivation can be found in the book.

Now we are ready to solve any nonsingular system $A\boldsymbol{x} = \boldsymbol{b}$.

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Therefore, we can use exactly the same two-step procedure as before, but we must permute the right-hand side first.

Example

Solve $A\boldsymbol{x} = \boldsymbol{b}$, where

$$A = \begin{pmatrix} 2 & 4 & 6 & -2 \\ 1 & 2 & 1 & 2 \\ 0 & 2 & 4 & 2 \\ -2 & 1 & 0 & 10 \end{pmatrix}, \quad \boldsymbol{b} = \begin{pmatrix} 0 \\ 1 \\ 2 \\ 10 \end{pmatrix}.$$

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Now we just need to solve

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Step 1: Solve $\mathsf{L}\boldsymbol{y} = \mathsf{P}\boldsymbol{b}$ (using augmented matrix notation)

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LU Factorization for Symmetric Matrices

We begin by creating a more symmetric version of the basic LU factorization for an arbitrary nonsingular $n \times n$ matrix A.

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The trick is to factor out the diagonal of U, i.e.,

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$$\begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & & \\ \vdots & \ddots & \ddots & \\ 0 & \cdots & 0 & u_{nn} \end{pmatrix} = \begin{pmatrix} u_{11} & & & \\ & u_{22} & & \\ & & \ddots & \\ & & & u_{nn} \end{pmatrix} \begin{pmatrix} 1 & \frac{u_{12}}{u_{11}} & \cdots & \frac{u_{1n}}{u_{11}} \\ 0 & 1 & \frac{u_{23}}{u_{22}} & \\ \vdots & \ddots & \ddots & \\ 0 & \cdots & 0 & 1 \end{pmatrix}.$$

Cholesky (see [BT14]) Factorization

If A is a symmetric matrix, then the LU factorization must be symmetric as well, i.e., $\mathsf{L} = \widetilde{\mathsf{U}}^T$, so that

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Moreover, if the entries of D are all positive (so that we can take square roots), then we can split $\mathsf{D} = \sqrt{\mathsf{D}}\sqrt{\mathsf{D}}$ with

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This results in the Cholesky factorization of A

$$A = R^T R, \quad \text{with} \quad R = \sqrt{D}\widetilde{U},$$

where R is upper-triangular.

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Theorem

A matrix A *is positive definite if and only if it has a unique Cholesky factorization* $A = R^T R$ *with* R *and upper-triangular matrix with positive diagonal entries*

Proof.

The implication

$$\mathsf{A} \text{ positive definite} \Longrightarrow \mathsf{A} = \mathsf{R}^T\mathsf{R}$$

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Factoring out r_{ii} produces

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$$\mathsf{R} = \mathsf{D}\mathsf{U}, \quad \mathsf{D} = \operatorname{diag}(r_{11}, \ldots, r_{nn}).$$

So

$$\mathsf{A} = (\mathsf{D}\mathsf{U})^T\mathsf{D}\mathsf{U} = \mathsf{U}^T\mathsf{D}^2\mathsf{U} = \mathsf{L}\mathsf{D}^2\mathsf{L}^T$$

and we have an LU factorization with positive pivots.

Proof.

The implication

$$\mathsf{A} \text{ positive definite} \Longrightarrow \mathsf{A} = \mathsf{R}^T\mathsf{R}$$

follows from the discussion above.

"$\Longleftarrow$": Assume $\mathsf{A} = \mathsf{R}^T\mathsf{R}$ with $r_{ii} > 0$.

Factoring out r_{ii} produces

$$\mathsf{R} = \mathsf{DU}, \quad \mathsf{D} = \operatorname{diag}(r_{11}, \ldots, r_{nn}).$$

So

$$\mathsf{A} = (\mathsf{DU})^T\mathsf{DU} = \mathsf{U}^T\mathsf{D}^2\mathsf{U} = \mathsf{LD}^2\mathsf{L}^T$$

and we have an LU factorization with positive pivots.

Uniqueness follows from the uniqueness of the LU factorization. $\square$

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