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Advanced algorithms

computer arithmetic:
number encodings and operations,
LUP decomposition, finding inverse matrix

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Natural Number Encodings

- The most common representation of natural numbers is the following binary encoding:

$$\text{value of a number} = \sum_{i=0}^{n} b_i \times 2^i$$

  where n is a number of bits of the number and b_i is a value of i-th bit.

- BCD (Binary Coded Decimal) representation with each decimal digit represented by its own four-bit binary sequence (nibble)
  - It is not as effective as the previous representation (all combinations of binary bit sequences are not used)
  - BCD format are still important and continue to be used in financial, commercial, and industrial computing.

Integer Number Encodings

- **complement representation of negative numbers (the most common):**

$$\text{value of a number } N = \begin{cases} \sum_{i=0}^{n-1} b_i \times 2^i & \text{for } b_n = 0, \text{ thus } N \in \langle 0; 2^{n-1} - 1 \rangle \\ -1 - \sum_{i=0}^{n-1} (1 - b_i) \times 2^i & \text{for } b_n = 1, \text{ thus } N \in \langle -2^{n-1}; -1 \rangle \end{cases}$$

most-significant bit									
0	1	1	1	1	1	1	1	=	127
0	1	1	1	1	1	1	0	=	126
0	0	0	0	0	0	1	0	=	2
0	0	0	0	0	0	0	1	=	1
0	0	0	0	0	0	0	0	=	0
1	1	1	1	1	1	1	1	=	−1
1	1	1	1	1	1	1	0	=	−2
1	0	0	0	0	0	0	1	=	−127
1	0	0	0	0	0	0	0	=	−128

8-bit two's-complement integers

- For additions and subtractions we can use the same algorithms as for the previous binary numbers representation of natural numbers.
- +/- sign can be detected from the most-significant bit.
- There is only encoding for zero.

Floating-point Data and Encodings

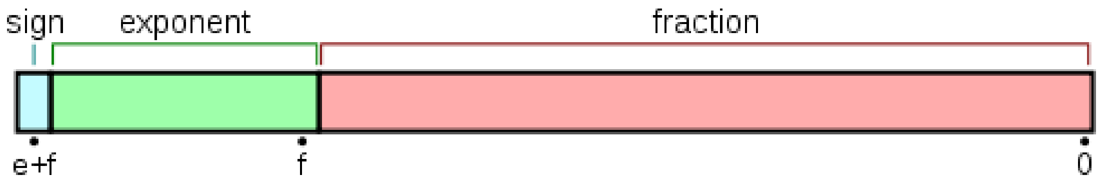
- representation:
  - $$s \times \frac{c}{b^{p-1}} \times b^e$$

  where s is the sign (signum +/-)
  c is the significand (fraction)
  b is the base (typically 2 or 10)
  p is the precision (the number of digits in the significand)
  e is the integer exponent

  - We want to encode also +∞ a -∞.
- If b=2 (the most common case) then there can arise some problems when inputs and outputs are converted from/to decimal base.

Floating-point Data and Encodings

- IEEE 754:



type	exponent field	significand (fraction field)
+/- zero	0	0
denormalized numbers	0	non zero
normalized numbers	1 až 2^e - 2	any
+/- ∞	2^e - 1	0
NaN (Not a Number)	2^e - 1	non zero

- normalized value:
  - value = $(-1)^{\text{sign}} \times 2^{\text{exponent-exponent bias}} \times (1.\text{fraction})$
- denormalized value:
  - value = $(-1)^{\text{sign}} \times 2^{\text{exponent-exponent bias+1}} \times (0.\text{fraction})$

Floating-point Data and Encodings

- IEEE 754:
  - **NaN** (Not a Number) is used for encodings of numbers that were a result of arithmetical operations with nonstandard inputs:
    - operations with a NaN as at least one operand
    - the divisions: $0/0$, ∞/∞, $\infty/-\infty$, $-\infty/\infty$, and $-\infty/-\infty$
    - the multiplications: $0\times\infty$ and $0\times-\infty$
    - the additions: $\infty + (-\infty)$, $(-\infty) + \infty$ and equivalent subtractions
    - calling functions with arguments out of its domain:
      - the square root of a negative number
      - the logarithm of a negative number
      - triginometric functions …
  - NaNs have two types:
    - **Quiet** (qNaN)
      - do not raise any additional exceptions as they propagate through most operations)
    - **Signalling** (sNaN)
      - should raise an invalid exception as underflow or overflow).
  - NaNs may also be explicitly assigned to variables, typically as a representation for missing values.

Differences Between Computer and Standard Arithmetic

- in both worlds (computer and standard arithmetic) holds:
  - $1 \cdot x = x$
  - $x \cdot y = y \cdot x$
  - $x + x = 2 \cdot x$
- in computer arithmetic needs not hold:
  - $x \cdot (1/x) = 1$
  - $(1 + x) - 1 = x$
  - $(x + y) + z = x + (y + z)$
- a common programmer's mistake is
  - addition of one (or another different number) in float type inside some loop with the stop condition with equality to some arbitrary number. Typically, such loop will never finish.
  - If conditions with exact equality to float constant. Such constructions need not be satisfied.

Summary of Matrix Algebra I

- An $m \times n$ **matrix** A is a rectangular array of numbers with m rows and n columns. The numbers m and n are the dimensions of A.

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{pmatrix}$$

- *Example:* 2×3 matrix A.

$$= \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}$$

- The **transpose**, A^T, of a matrix A is the matrix obtained from A by writing its rows as columns. If A is an $m \times n$ matrix and $B = A^T$, then B is the $n \times m$ matrix with $b_{ij} = a_{ji}$.

$$A^T = \begin{pmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{pmatrix}$$

- A **vector** is a matrix with the second dimension always 1.

$$x = \begin{pmatrix} 2 \\ 3 \\ 5 \end{pmatrix}$$

- The **unit vector** e_i is the vector whose i-th element is 1 and all of whose other elements are 0. Usually, the size of a unit vector is clear from the context.
- A **Square** matrix is an $n \times n$ matrix.
- A **diagonal matrix** has $a_{ij} = 0$ whenever $i \neq j$.

$$\mathrm{diag}(a_{11}, a_{22}, \ldots, a_{nn}) = \begin{pmatrix} a_{11} & 0 & \ldots & 0 \\ 0 & a_{22} & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & a_{nn} \end{pmatrix}$$

- The $n \times n$ **identity matrix** I_n is a diagonal matrix with 1's along the diagonal.

$$I_n = \mathrm{diag}(1, 1, \ldots, 1) = \begin{pmatrix} 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 1 \end{pmatrix}$$

Summary of Matrix Algebra II

- An **upper-triangular matrix** U is one for which $u_{ij} = 0$ if $i > j$. All entries below the diagonal are zero:
- An upper-triangular matrix is **unit upper-triangular** if it has all 1's along the diagonal.

$$U = \begin{pmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ 0 & u_{22} & \dots & u_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & u_{nn} \end{pmatrix}$$

- A **lower-triangular matrix** L is one for which $l_{ij} = 0$ if $i < j$. All entries above the diagonal are zero:
- A lower-triangular matrix is **unit lower-triangular** if it has all 1's along the diagonal.

$$L = \begin{pmatrix} l_{11} & 0 & \dots & 0 \\ l_{21} & l_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & \dots & l_{nn} \end{pmatrix}$$

- A **permutation matrix** P has exactly one 1 in each row or column, and 0's elsewhere. An example of a permutation matrix is:

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

- An **inverse matrix** for $n \times n$ matrix A is a matrix $n \times n$, we denote it as A^{-1} (if it exists), that holds:

$$A A^{-1} = I_n = A^{-1} A$$

LUP Decomposition

- **solving systems of linear equations**
  - Consider systems of n linear equations $Ax = b$, letting $A = (a_{ij})$, $x = (x_j)$ a $b = (b_i)$

$$a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n = b_1$$
$$a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n = b_2$$
$$\ldots$$
$$a_{n1}x_1 + a_{n2}x_2 + \ldots + a_{nn}x_n = b_n$$

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

  - If the rank of A is less than n-then the system is *underdetermined*. An underdetermined system typically has infinitely many solutions, although it may have no solutions at all if the equations are inconsistent.
  - If the number of equations exceeds the number n of unknowns, the system is *overdetermined*, and there may not exist any solutions.
  - If A is nonsingular, it possesses an inverse A^{-1} and $x = A^{-1}b$ is the solution vector, because

    $x = I_n x = A^{-1} A x = A^{-1}b$.
  - Thus we have only one solution.

LUP Decomposition

- **solving systems of linear equations**
  - one possible solution:
    - Compute A^{-1} and then multiply both sides by A^{-1}, yielding $A^{-1} Ax$ = $A^{-1}b$, or $x = A^{-1}b$. This approach suffers in practice from numerical instability.
  - a solution using LUP decomposition:
    - The idea behind LUP decomposition is to find three $n \times n$ matrices L, U, and P such that

$$PA = LU$$

where

- L is a unit lower-triangular matrix,
- U is an upper-triangular matrix, and
- P is a permutation matrix.

LUP Decomposition

- **solving systems of linear equations with a LUP decomposition knowledge**
  - Multiplying both sides of $Ax = b$ by P yields the equivalent equation:

    $P\,Ax = Pb$, which only permutes the original linear equations.
  - Using our LUP decomposition equality $PA=LU$, we obtain

    $LUx = Pb$.
  - We can now solve this equation by solving two triangular linear systems.
  - Let us define $y = Ux$, where x is the desired solution vector.
  - First, we solve the lower-triangular system:

    $Ly = Pb$ for the unknown vector y by a method called ***forward substitution***.
  - Having solved for y, we then solve the upper-triangular system

    $Ux = y$ for the unknown x by a method called ***back substitution***.
  - The vector x is our solution to $Ax = b$, since the permutation matrix P is invertible:

    $Ax = P^{-1}LUx = P^{-1}Pb = b$.

LUP Decomposition

- **forward substitution**
  - can solve the lower-triangular system in $\Theta(n^2)$ given L, P, and b.
  - Let us define $c = Pb$ as permutation of a vector b (in detail: $c_i = b_{\pi(i)}$).
  - Since L is unit lower-triangular, equation $Ly = Pb$ can be rewritten as

$$\begin{array}{lllllllll} y_1 & & & & & & & = & c_1 \\ l_{21}y_1 & + & y_2 & & & & & = & c_2 \\ l_{31}y_1 & + & l_{32}y_2 & + & y_3 & & & = & c_3 \\ \vdots & & & & & \ddots & & & \vdots \\ l_{n1}y_1 & + & l_{n2}y_2 & + & l_{n3}y_3 & + \cdots + & y_n & = & c_n \end{array}$$

  - We can solve for y_1 directly (from the 1st equation). Having solved for y_1, we can substitute it into the second equation, yielding

$$y_2 = c_2 - l_{21}y_1$$

  - In general, we substitute $y_1, y_2, \ldots, y_{i-1}$ "forward" into the i-th equation to solve for y_i:

$$y_i = c_i - \sum_{j=1}^{i-1} l_{ij}\, y_j$$

- **back substitution**
  - is similar to *forward substitution*. It solves the upper-triangular system in $\Theta(n^2)$ given U and y.
  - Since U is upper-triangular, we can rewrite the system $Ux = y$ as

$$\begin{array}{ccccccccc}
u_{11}x_1 & + & u_{12}x_2 & +\cdots+ & u_{1,n-1}x_{n-1} & + & u_{1n}x_n & = & y_1 \\
 & & u_{22}x_2 & +\cdots+ & u_{2,n-1}x_{n-1} & + & u_{2n}x_n & = & y_2 \\
 & & & \ddots & & & & \vdots & \\
 & & & & u_{n-1,n-1}x_{n-1} & + & u_{n-1,n}x_n & = & y_{n-1} \\
 & & & & & & u_{nn}x_n & = & y_n
\end{array}$$

  - We can solve for x_n from the last equation as $x_n = y_n / u_{nn}$. Having solved for x_n, we can substitute it into the previous equation, yielding $x_{n-1} = (y_{n-1} - u_{n-1,n}x_n) / u_{n-1,n-1}$.
  - In general, we substitute $x_n, x_{n-1}, \ldots, x_{i+1}$ "back" into the i-th equation to solve for x_i:

$$x_i = \left(y_i - \sum_{j=i+1}^{n} u_{ij}\, x_j \right) \Big/ u_{ii}$$

LUP Decomposition

- **solving systems of linear equations with a LUP decomposition knowledge**
  - We represent the permutation P compactly by a permutation array $\pi[1..n]$.

    For $i = 1, 2, \ldots, n$, the entry $\pi[i]$ indicates that $P_{i,\pi[i]} = 1$ and $P_{ij} = 0$ for $j \neq \pi[i]$.
  - We have now shown that if an LUP decomposition can be computed for a nonsingular matrix A, *forward* and *back substitution* can be used to solve the system $Ax = b$ of linear equations in $\Theta(n^2)$ time.
  - It remains to show how an LUP decomposition for A can be found efficiently.
  - We start with the case in which A is an $n \times n$ nonsingular matrix and P is absent (or, equivalently, $P = I_n$). We call it *LU decomposition*.

LUP Decomposition

- **computing an LU decomposition**
  - the idea is based on ***Gaussian elimination***:
    - We start by subtracting multiples of the first equation from the other equations so that the first variable is removed from those equations.
    - Then, we subtract multiples of the second equation from the third and subsequent equations so that now the first and second variables are removed from them.
    - We continue this process until the system that is left has an upper-triangular form-in fact, it is the matrix U. The matrix L is made up of the row multipliers that cause variables to be eliminated.
  - the recursive algorithm:

1. Divide A into following parts according the picture:

$$A = \left(\begin{array}{c|cccc} a_{11} & a_{12} & \cdots & a_{1n} \\ \hline a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{array}\right) = \begin{pmatrix} a_{11} & w^{\mathrm{T}} \\ v & A' \end{pmatrix},$$

A' is $(n-1) \times (n-1)$ matrix,

v is a column vector, and

w^{T} is a row vector.

computing an LU decomposition

2. Then we decompose the matrix:

$$
\begin{aligned}
A &= \begin{pmatrix} a_{11} & w^{\mathrm{T}} \\ v & A' \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \\ v/a_{11} & I_{n-1} \end{pmatrix} \begin{pmatrix} a_{11} & w^{\mathrm{T}} \\ 0 & A' - vw^{\mathrm{T}}/a_{11} \end{pmatrix} .
\end{aligned}
$$

- The submatrix $A'\text{-}vw^{\mathrm{T}}/a_{11}$ with dimensions $(n-1) \times (n-1)$ is called *Schur complement* A with respect to a_{11}.
- Because the *Schur complement* is nonsingular, we can now recursively find an LU decomposition of it (= $L'U'$).
- where L' is unit lower-triangular and U' is upper-triangular. Then, using matrix algebra, we have

$$
\begin{aligned}
A &= \begin{pmatrix} 1 & 0 \\ v/a_{11} & I_{n-1} \end{pmatrix} \begin{pmatrix} a_{11} & w^{\mathrm{T}} \\ 0 & A' - vw^{\mathrm{T}}/a_{11} \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \\ v/a_{11} & I_{n-1} \end{pmatrix} \begin{pmatrix} a_{11} & w^{\mathrm{T}} \\ 0 & L'U' \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \\ v/a_{11} & L' \end{pmatrix} \begin{pmatrix} a_{11} & w^{\mathrm{T}} \\ 0 & U' \end{pmatrix} \\
&= LU ,
\end{aligned}
$$

LUP Decomposition

- **computing an LU decomposition** (nonrecursive)

```
Procedure LU-DECOMPOSITION(matrix A)
n = rows[A] ;
for k = 1 to n do {
    u_kk = a_kk ;
    for i = k + 1 to n do {
        l_ik = a_ik/u_kk ;        // l_ik represents v_i
        u_ki = a_ki ;             // u_ki represents w^T_i
    }
    for i = k + 1 to n do
        for j = k + 1 to n do
            a_ij = a_ij - l_ik u_kj ;
}
return L and U
```

- The asymptotic time complexity is $\Theta(n^3)$.

LUP Decomposition

- **computing an LU decomposition** (Example)

$$\begin{array}{cccc} 2 & 3 & 1 & 5 \\ 6 & 13 & 5 & 19 \\ 2 & 19 & 10 & 23 \\ 4 & 10 & 11 & 31 \end{array} \qquad \begin{array}{c|ccc} 2 & 3 & 1 & 5 \\ \hline 3 & 4 & 2 & 4 \\ 1 & 16 & 9 & 18 \\ 2 & 4 & 9 & 21 \end{array} \qquad \begin{array}{cc|cc} 2 & 3 & 1 & 5 \\ \hline 3 & 4 & 2 & 4 \\ 1 & 4 & 1 & 2 \\ 2 & 1 & 7 & 17 \end{array} \qquad \begin{array}{ccc|c} 2 & 3 & 1 & 5 \\ 3 & 4 & 2 & 4 \\ \hline 1 & 4 & 1 & 2 \\ 2 & 1 & 7 & 3 \end{array}$$

(a) (b) (c) (d)

$$\underbrace{\begin{pmatrix} 2 & 3 & 1 & 5 \\ 6 & 13 & 5 & 19 \\ 2 & 19 & 10 & 23 \\ 4 & 10 & 11 & 31 \end{pmatrix}}_{A} = \underbrace{\begin{pmatrix} 1 & 0 & 0 & 0 \\ 3 & 1 & 0 & 0 \\ 1 & 4 & 1 & 0 \\ 2 & 1 & 7 & 1 \end{pmatrix}}_{L} \underbrace{\begin{pmatrix} 2 & 3 & 1 & 5 \\ 0 & 4 & 2 & 4 \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & 3 \end{pmatrix}}_{U}$$

(e)

- Of course, if it holds $a'_{11} = 0$ for a currently processed sub-matrix A', then this method doesn't work, because it attempts to divide by 0.
- Thus, if $|a'_{11}|$ is near to 0, then this algorithm can produce big errors.

LUP Decomposition

- **computing an LUP decomposition** (nonrecursive)

```
Procedure LUP-DECOMPOSITION(matrix A)
n = rows[A];
for i = 1 to n do π[i] = i ;
for k = 1 to n do {              // main cycle
    p = 0 ;                      // initialization of pivot
    for i = k to n do {          // selection of pivot
        if |a_ik| > p then {
            p = |a_ik| ;
            k' = i ;             // position of pivot
        }
    if p = 0 then error "singular matrix“;
    exchange π[k] ↔ π[k'] ;
    for i = 1 to n do exchange a_ki ↔ a_k'i ;
    for i = k + 1 to n do {
        a_ik = a_ik/a_kk ;       // k-th column of L
        for j = k + 1 to n do  a_ij = a_ij - a_ik a_kj ;   // U
    }
}
```

- The asymptotic time complexity is $\Theta(n^3)$.
- The resulting matrices L and U are contained in “improved” matrix A in the following way

$$a_{ij} = \begin{cases} l_{ij} & \text{if } i > j \\ u_{ij} & \text{if } i \leq j \end{cases}$$

LUP Decomposition

- **computing an LUP decomposition** (Example)

1	2	0	2	0.6
2	3	3	4	−2
3	5	5	4	2
4	−1	−2	3.4	−1

(a)

3	5	5	4	2
2	3	3	4	−2
1	2	0	2	0.6
4	−1	−2	3.4	−1

(b)

3	5	5	4	2
2	0.6	0	1.6	−3.2
1	0.4	−2	0.4	−.2
4	−0.2	−1	4.2	−0.6

(c)

3	5	5	4	2
2	0.6	0	1.6	−3.2
1	0.4	−2	0.4	−0.2
4	−0.2	−1	4.2	−0.6

(d)

3	5	5	4	2
1	0.4	−2	0.4	−0.2
2	0.6	0	1.6	−3.2
4	−0.2	−1	4.2	−0.6

(e)

3	5	5	4	2
1	0.4	−2	0.4	−0.2
2	0.6	0	1.6	−3.2
4	−0.2	0.5	4	−0.5

(f)

3	5	5	4	2
1	0.4	−2	0.4	−0.2
2	0.6	0	1.6	−3.2
4	−0.2	0.5	4	−0.5

(g)

3	5	5	4	2
1	0.4	−2	0.4	−0.2
4	−0.2	0.5	4	−0.5
2	0.6	0	1.6	−3.2

(h)

3	5	5	4	2
1	0.4	−2	0.4	−0.2
4	−0.2	0.5	4	−0.5
2	0.6	0	0.4	−3

(i)

$$\underbrace{\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix}}_{P} \underbrace{\begin{pmatrix} 2 & 0 & 2 & 0.6 \\ 3 & 3 & 4 & -2 \\ 5 & 5 & 4 & 2 \\ -1 & -2 & 3.4 & -1 \end{pmatrix}}_{A} = \underbrace{\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.4 & 1 & 0 & 0 \\ -0.2 & 0.5 & 1 & 0 \\ 0.6 & 0 & 0.4 & 1 \end{pmatrix}}_{L} \underbrace{\begin{pmatrix} 5 & 5 & 4 & 2 \\ 0 & -2 & 0.4 & -0.2 \\ 0 & 0 & 4 & -0.5 \\ 0 & 0 & 0 & -3 \end{pmatrix}}_{U}$$

(j)

Computing Inverse Matrix

- **computing inverse matrix using LUP decomposition**
  - Using LUP-DECOMPOSITION, we can solve an equation of the form $Ax = b$ in time $\Theta(n^2)$.
  - Since the LUP-DECOMPOSITION decomposition depends on *A* but not *b*, we can run LUP-DECOMPOSITION on a second set of equations of the form $Ax = b'$ in additional time $\Theta(n^2)$.
  - Using the same LUP-DECOMPOSITION, we can solve n equations of the form $Ax = e_i$ for i from 1 to n (dimensions of matrix A is $n \times n$) where e_i is a unit vector also in time $\Theta(n^2)$.
  - If we join all n vectors e_i for i from 1 to n together then we have I_n (unit matrix).
  - The task of finding an inverse matrix X for A is to find a solution of the following matrix equation $AX = I$.
  - If we join all n solutions x from $Ax = e_i$ from 1 to n together then we have a matrix to X (so it holds: $AX = I$).
  - Since the LUP decomposition of A can be computed in time $\Theta(n^3)$, the inverse A^{-1} of a matrix A can be determined in time $\Theta(n^3)$.

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