



$$z := \begin{bmatrix} b_1 x_1 \\ \vdots \\ b_n x_n \end{bmatrix}$$

Efficient multiplication  $Tz$ ?  $\Theta(n^2)$  worst case

$$Tz = \begin{bmatrix} \sum_{i=1}^n z_i \\ \sum_{i=2}^n z_i \\ \vdots \\ z_{n-1} + z_n \\ z_n \end{bmatrix}$$

Can be implemented in  $\Theta(n)$

using partial-sum

(backwards computation from last entry)

$p > 1$  ?

$$AB^T = \sum_{l=1}^p \underbrace{(A)_{:,l} \cdot (B)_{:,l}^T}_{\text{outer product of 2 vectors ("p=1" case)}}$$

$\Rightarrow$  overall complexity:  $\Theta(pn)$ !

C++11 code 1.4.16: Efficient multiplication with the upper diagonal part of a rank- $p$ -matrix in EIGEN [→ GITLAB](#)

```

2  ///! Computation of y = triu(AB^T)x
3  ///! Efficient implementation with backward cumulative sum
4  ///! (partial_sum)
5  template<class Vec, class Mat>
6  void ltrimulteff(const Mat& A, const Mat& B, const Vec& x, Vec& y){
7      const int n = A.rows(), p = A.cols();
8      assert( n == B.rows() && p == B.cols()); // size mismatch
9      for(int l = 0; l < p; ++l){
10         Vec tmp = (B.col(l).array() * x.array()).matrix().reverse();
11         std::partial_sum(tmp.data(), tmp.data()+n, tmp.data());
12         y += (A.col(l).array() * tmp.reverse().array()).matrix();
13     }
14 }

```

Example: Kronecker product  $A \otimes B$

$$A \in \mathbb{K}^{m,n}, B \in \mathbb{K}^{l,k}$$

$$A \otimes B := \begin{bmatrix} (A)_{1,1}B & (A)_{1,2}B & \dots & \dots & (A)_{1,n}B \\ (A)_{2,1}B & (A)_{2,2}B & & & \vdots \\ \vdots & \vdots & & & \vdots \\ \vdots & \vdots & & & \vdots \\ (A)_{m,1}B & (A)_{m,2}B & \dots & \dots & (A)_{m,n}B \end{bmatrix} \in \mathbb{K}^{ml,nk}$$

$$(A \otimes B)x \quad x \in \mathbb{K}^{n \cdot k}$$

$$A \otimes B \quad \Theta(ml, nk)$$

Reshape  $x = \begin{bmatrix} x^1 \\ x^2 \\ \vdots \\ x^n \end{bmatrix} \quad x^d \in \mathbb{K}^k$

$$X = \begin{bmatrix} x^1 & x^2 & \dots & x^n \end{bmatrix} \in \mathbb{K}^{k,n}$$

$$(A \otimes B)x = \begin{bmatrix} (A)_{1,1}Bx^1 + (A)_{1,2}Bx^2 + \dots + (A)_{1,n}Bx^n \\ (A)_{2,1}Bx^1 + (A)_{2,2}Bx^2 + \dots + (A)_{2,n}Bx^n \\ \vdots \\ \vdots \\ (A)_{m,1}Bx^1 + (A)_{m,2}Bx^2 + \dots + (A)_{m,n}Bx^n \end{bmatrix} \leftarrow \in \mathbb{K}^l$$

m such entries

$$BXA^T = \left[ \sum_{j=1}^n Bx^j \cdot (A)_{1,j}, \dots, \sum_{j=1}^n Bx^j \cdot (A)_{m,j} \right]$$

$$BX = [Bx^1 \dots Bx^n]$$

$$A^T = \left[ ((A)_{1,:})^T \dots ((A)_{m,:})^T \right]$$

reshaping  $BXA^T$  to a column vector:  $(A \otimes B)x$

$$B \in \mathbb{K}^{l,k}, X \in \mathbb{K}^{k,n}, A^T \in \mathbb{K}^{n,m}$$

$$Y = BX \quad \Theta(lkn) \quad Y \in \mathbb{K}^{l,n} \quad YA^T: \Theta(lnm)$$

⇒ overall complexity:  $\Theta(lkn + lnm)$

[compared to  $\Theta(lknm)$ ]

Other examples: divide-and-conquer algorithms

Strassen's algorithm: for multiplication of 2  
 $n \times n$  matrices:  $\Theta(n^{\log_2 7}) \approx 2.81$   
(compared to  $\Theta(n^3)$ )

## 1.5.4. Cancellation

Example: Roots of quadratic polynomial

$$p(z) = z^2 + \alpha z + \beta$$

$$p(z_{1/2}) = 0$$

$$z_{1/2} = -\frac{\alpha}{2} \pm \frac{1}{2} \sqrt{\alpha^2 - 4\beta} \quad (*)$$

Scenario:  $z_1$  large,  $z_2$  small

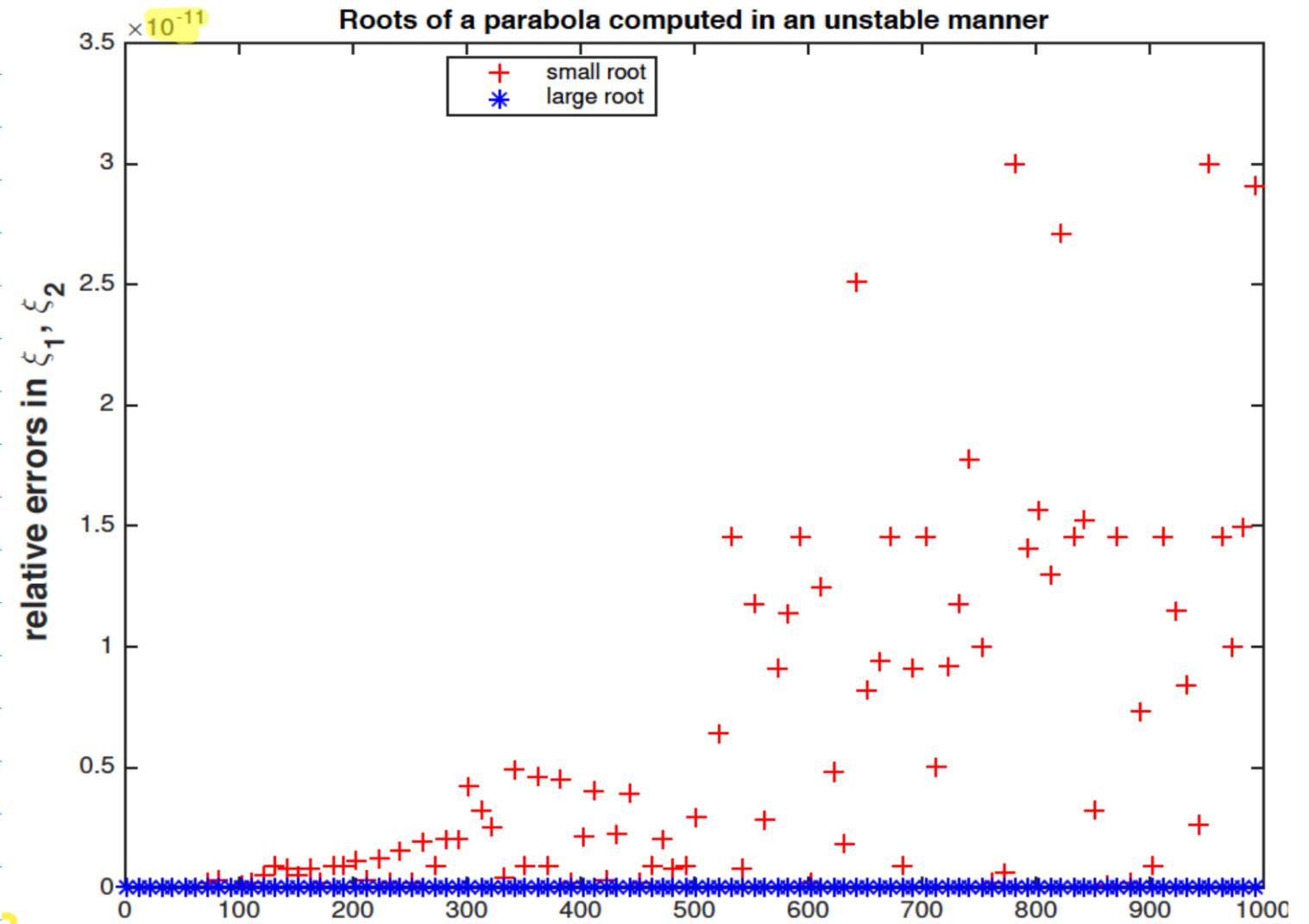
for example:  $p(z) = (z - \mu)(z - \frac{1}{\mu})$

$$p(z) = z^2 - (\mu + \frac{1}{\mu})z + 1 \quad (\alpha = \mu + \frac{1}{\mu}, \beta = 1)$$

Use (\*) to compute the roots & compare the errors made in  $z_1, z_2$

**C++11-code 1.5.41: Discriminant formula for the real roots of  $p(\xi) = \xi^2 + \alpha\xi + \beta \rightarrow$  GITLAB**

```
2  /// C++ function computing the zeros of a quadratic polynomial
3  ///  $\xi \rightarrow \xi^2 + \alpha\xi + \beta$  by means of the familiar discriminant
4  /// formula  $\xi_{1,2} = \frac{1}{2}(-\alpha \pm \sqrt{\alpha^2 - 4\beta})$ . However
5  /// this implementation is vulnerable to round-off! The zeros are
6  /// returned in a column vector
7  Vector2d zerosquadpol(double alpha, double beta){
8      Vector2d z;
9      double D = std::pow(alpha,2) - 4*beta; // discriminant
10     if (D < 0) throw "no real zeros";
11     else{
12         // The famous discriminant formula
13         double wD = std::sqrt(D);
14         z << (-alpha-wD)/2, (-alpha+wD)/2; //
15     }
16     return z;
17 }
```



Large errors in  $z_2$  compared to EPS!

$$\zeta_2 = -\frac{\alpha}{2} + \frac{1}{2}\sqrt{\alpha^2 - 4}$$

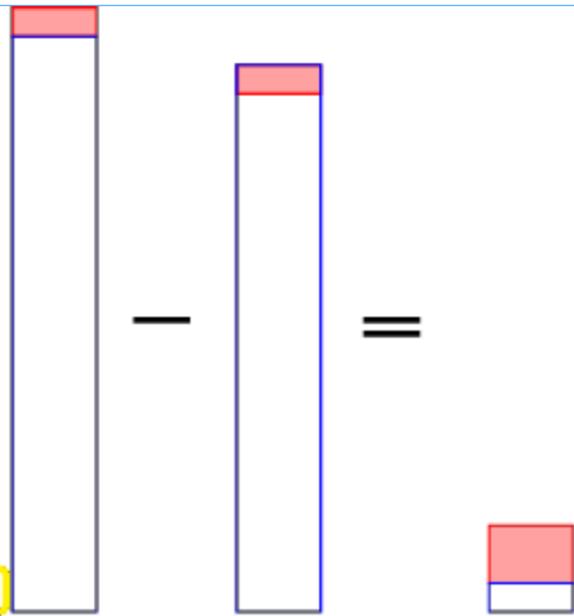
$\alpha$  large  
 $\alpha \gg 1$

$$\sqrt{\alpha^2 - 4} \approx \alpha$$

errors get amplified  
as we subtract 2 numbers  
that are about the same

size : cancellation

Fig. 41



Stable computation of roots?

Step 1 :  $\zeta_1 = -\frac{\alpha}{2} - \frac{1}{2}\sqrt{\alpha^2 - 4\beta}$  (stable)

Idea:  $\zeta_2 = -\frac{\alpha}{2} + \frac{1}{2}\sqrt{\alpha^2 - 4\beta}$

$\zeta_1 + \zeta_2 = -\alpha$

$\zeta_2 = -\alpha - \zeta_1$

BUT  $\alpha = \mu + \frac{1}{\mu}$   
 $\zeta_1 \approx \alpha$   
 $\mu = \zeta_1$

Vieta's formula:  $\beta = \zeta_1 \cdot \zeta_2$

Step 2:  $\zeta_2 = \beta / \zeta_1$  (stable)

C++11-code 1.5.57: Stable computation of real root of a quadratic polynomial → [GITLAB](#)

```

2  /// C++ function computing the zeros of a quadratic polynomial
3  ///  $\zeta \rightarrow \zeta^2 + \alpha\zeta + \beta$  by means of the familiar discriminant
4  /// formula  $\zeta_{1,2} = \frac{1}{2}(-\alpha \pm \sqrt{\alpha^2 - 4\beta})$ .
5  /// This is a stable implementation based on Vieta's theorem.
6  /// The zeros are returned in a column vector
7  VectorXd zerosquadpolstab(double alpha, double beta){
8      Vector2d z(2);
9      double D = std::pow(alpha,2) - 4*beta; // discriminant
10     if(D < 0) throw "no real zeros";
11     else{
12         double wD = std::sqrt(D);
13         // Use discriminant formula only for zero far away from 0
14         // in order to avoid cancellation. For the other zero
15         // use Vieta's formula.
16         if(alpha >= 0){
17             double t = 0.5*(-alpha-wD); //
18             z << t, beta/t;
19         }
20         else{
21             double t = 0.5*(-alpha+wD); //
22             z << beta/t, t;
23         }
24     }
25     return z;
26 }

```

Example: Difference quotients

$$f'(x) \underset{\substack{\uparrow \\ \text{approximation}}}{\approx} \frac{f(x+h) - f(x)}{h}$$

Analysis: if  $f$  is suff. smooth e.g.  $f \in C^2$

$$f'(x) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h)$$

$$f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}$$

(approximation error tends to 0 as  $h \rightarrow 0$ )

BUT:  $f(x+h) - f(x)$ : subtraction of 2 close-by numbers

→ cancellation happens + amplified by  $\frac{1}{h}$  (large)

Ex:  $f(x) = e^x$

C++11-code 1.5.48: Difference quotient approximation of the derivative of exp → [GITLAB](#)

```
2 /// Difference quotient approximation
3 /// of the derivative of exp
4 void diffq(){
5     double h = 0.1, x = 0.0;
6     for(int i = 1; i <= 16; ++i){
7         double df = (exp(x+h) - exp(x))/h;
8         cout << setprecision(14) << fixed;
9         cout << setw(5) << -i
10            << setw(20) << df-1 << endl;
11         h /= 10;
12     }
13 }
```

Measured relative errors ▷

| $\log_{10}(h)$ | relative error    |
|----------------|-------------------|
| -1             | 0.05170918075648  |
| -2             | 0.00501670841679  |
| -3             | 0.00050016670838  |
| -4             | 0.00005000166714  |
| -5             | 0.00000500000696  |
| -6             | 0.00000049996218  |
| -7             | 0.00000004943368  |
| -8             | -0.00000000607747 |
| -9             | 0.00000008274037  |
| -10            | 0.00000008274037  |
| -11            | 0.00000008274037  |
| -12            | 0.00008890058234  |
| -13            | -0.00079927783736 |
| -14            | -0.00079927783736 |
| -15            | 0.11022302462516  |
| -16            | -1.00000000000000 |

We observe an initial decrease of the relative approximation error followed by a steep increase when  $h$  drops below  $10^{-8}$ .

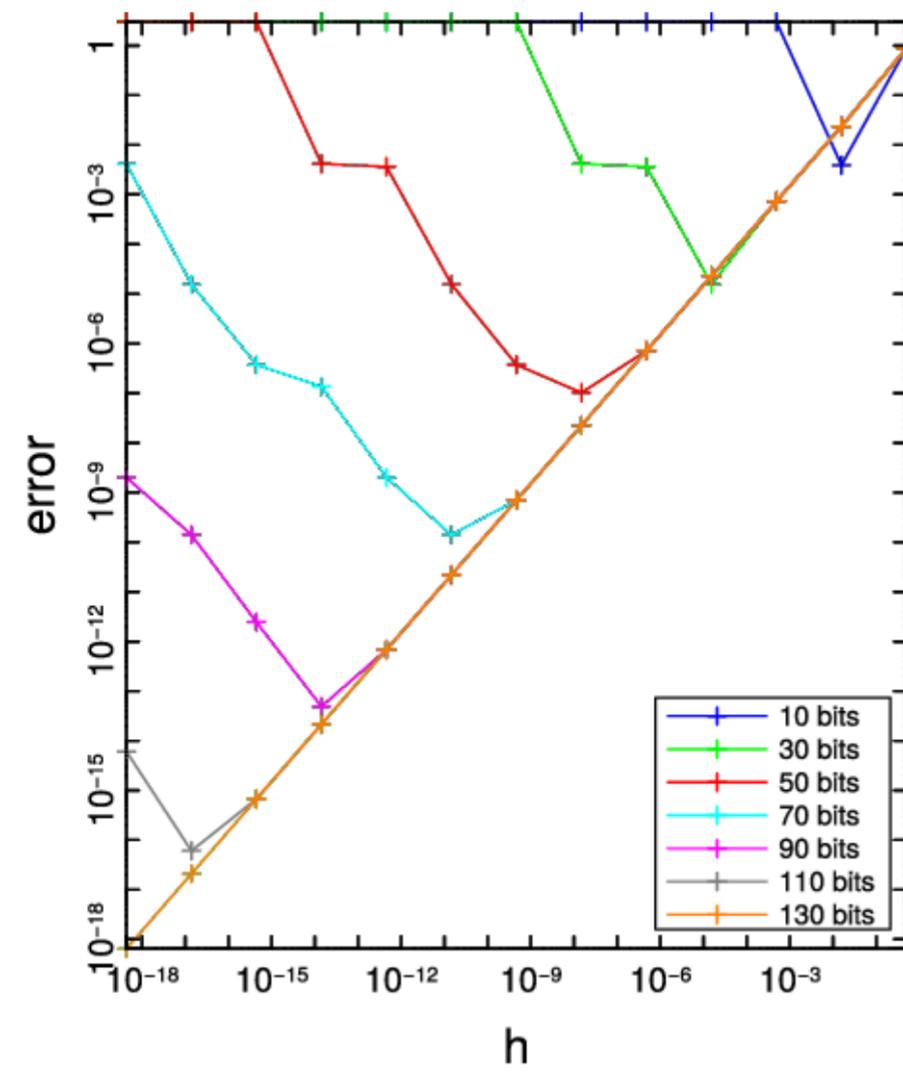


Fig. 42

Use the axiom of roundoff analysis (to compute choice of  $h$ ):

$$\text{difference quotient } dq = \frac{e^{x+h}(1+\delta_1) - e^x(1+\delta_2)}{h} \quad |\delta_1|, |\delta_2| \leq \text{EPS}$$

Choose  $h$  s.t. relative error  $\left| \frac{e^x - dq}{e^x} \right|$  is minimized

$$dq = e^x \left( \frac{e^h - 1}{h} + \frac{\delta_1 e^h - \delta_2}{h} \right)$$

$$\frac{dq - e^x}{e^x} = \underbrace{\frac{e^h - 1}{h} - 1}_{\approx h/2} + \frac{\delta_1 e^h - \delta_2}{h} \leq \frac{2\text{EPS}}{h}$$

Use  $\frac{e^{x+h} - e^x}{h} - e^x = \frac{1}{2} h e^\xi$  for some  $\xi \in [x, x+h]$

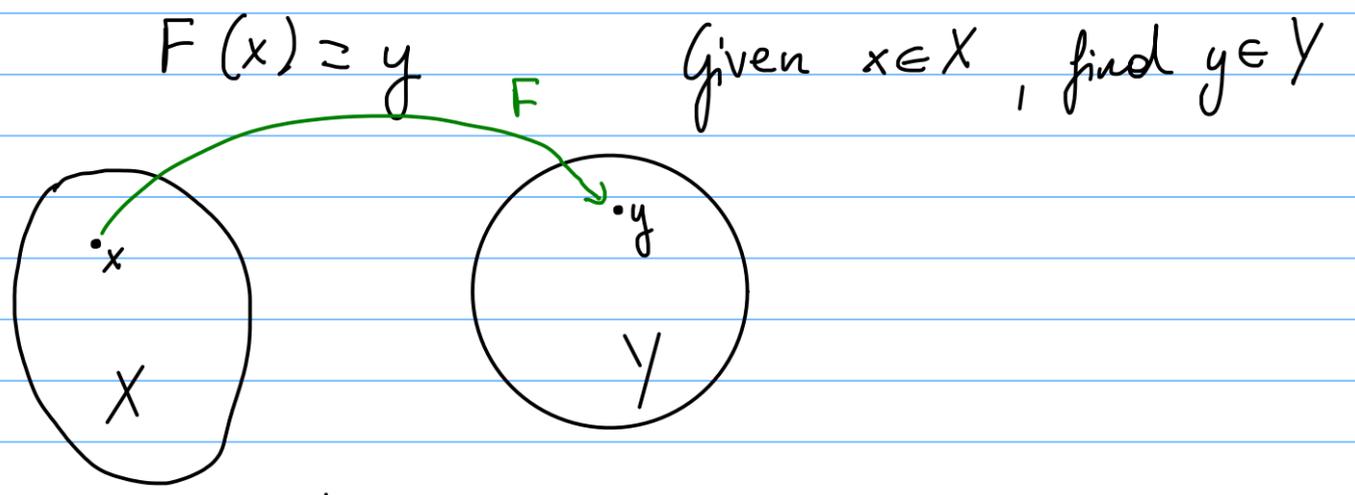
with  $x=0$ :  $\frac{e^h - 1}{h} - 1 = \frac{1}{2} h e^\xi$   $\xi \in [0, h]$

$$\left| \frac{dq - e^x}{e^x} \right| \approx \frac{h}{2} + \frac{2 \text{EPS}}{h} \quad \leftarrow \text{minimize}$$

$$\frac{1}{2} - \frac{2 \text{EPS}}{h^2} \approx 0 \quad \Rightarrow \quad h \approx 2 \sqrt{\text{EPS}}$$

### 1.5.5. Numerical stability

Mathematical problem: data space  $X$  with  $\|\cdot\|_X$   
 solution space  $Y$  with  $\|\cdot\|_Y$   
 mapping  $F: X \rightarrow Y$



$F$  is well-defined: for any  $x \in X$  there exists a solution  $y \in Y$

|                      |                                                  |
|----------------------|--------------------------------------------------|
| Problem              | Algorithm                                        |
| $F: X \rightarrow Y$ | $\tilde{F}: X \rightarrow \tilde{Y} \subset M^m$ |

Example: Solving a linear system (LSE)

$$F: \begin{cases} X = \mathbb{R}_{\text{reg}}^{n,n} \times \mathbb{R}^n & \longrightarrow & Y = \mathbb{R}^n \\ (A, b) & \longmapsto & x \end{cases}$$

well-defined? Need to restrict to set of regular matrices  $\mathbb{R}_{\text{reg}}^{n,n}$

Given problem  $F$  and an algorithm  $\tilde{F}$

$$\tilde{F}: X \rightarrow \tilde{Y} \subseteq M^m$$

When is  $\tilde{F}$  numerically stable?

**Definition 1.5.85. Stable algorithm** [backward stable]

An algorithm  $\tilde{F}$  for solving a problem  $F: X \mapsto Y$  is **numerically stable** if for all  $x \in X$  its result  $\tilde{F}(x)$  (possibly affected by roundoff) is the exact result for "slightly perturbed" data:

$$\exists C \approx 1: \forall x \in X: \exists \tilde{x} \in X: \|x - \tilde{x}\|_X \leq C \omega(x) \text{EPS} \|x\|_X \wedge \tilde{F}(x) = F(\tilde{x})$$

comp. effort

machine precision

$$\frac{\|x - \tilde{x}\|_X}{\|x\|_X} \leq C \omega(x) \text{EPS}$$

$$\tilde{F}(x) = F(\tilde{x})$$

$\tilde{F}$  is outputting the exact solution to nearly the right question

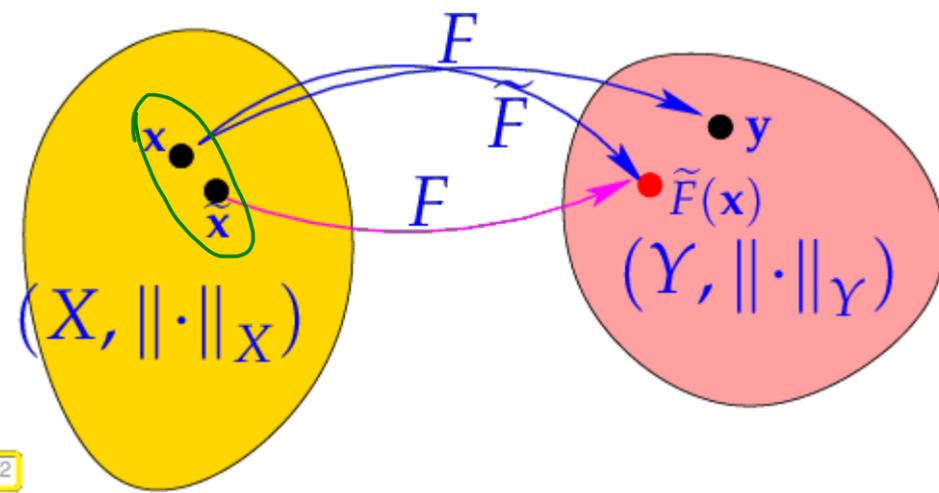


Fig. 52

Sloppily speaking, the impact of roundoff (\*) on a *stable algorithm* is of the same order of magnitude as the effect of the inevitable perturbations due to rounding the input data.

More general: (mixed) stability

there is  $\tilde{x}$  with  $\frac{\|x - \tilde{x}\|}{\|x\|} \leq \Theta(\text{EPS})$  s.t.

$$\frac{\|\tilde{F}(x) - F(\tilde{x})\|}{\|F(\tilde{x})\|} \leq \Theta(\text{EPS})$$

backward stability  $\Rightarrow$  mixed stability

Q: How close is  $\tilde{F}(x)$  to  $F(x)$ ?

Recall toy example  $3 \times 3$ :

$$\frac{\|b - b^\delta\|_2}{\|b\|_2} \text{ small } \sim 10^{-4}$$

$$\frac{\|x - x^\delta\|_2}{\|x\|_2} \text{ large } \sim 10^2$$

Condition number of  $F$ :

$$F: X \rightarrow Y$$

$$C_F(x) = \sup_{\Delta x} \left( \frac{\|F(x + \Delta x) - F(x)\|}{\|F(x)\|} / \frac{\|\Delta x\|}{\|x\|} \right)$$

$\rightarrow$  sensitivity of the output to changes in the input

Condition number of a matrix

$$C_A(x) = \sup_{\Delta x} \left( \frac{\|A \Delta x\|}{\|Ax\|} / \frac{\|\Delta x\|}{\|x\|} \right)$$

$$C_A(x) = \sup_{\Delta x} \left( \frac{\|A \Delta x\|}{\|\Delta x\|} \cdot \frac{\|x\|}{\|Ax\|} \right)$$

$$= \|A\| \cdot \frac{\|x\|}{\|Ax\|} \quad \|A\| := \sup_x \frac{\|Ax\|}{\|x\|}$$

$$= \sup_{\|x\|=1} \|Ax\|$$

$$C_A := \|A\| \cdot \|A^{-1}\|$$

$$= \frac{\sigma_{\max}}{\sigma_{\min}}$$

$\leftarrow$  if small: well-conditioned  
 $\leftarrow$  if large: ill-cond.

$$\frac{\|\tilde{F}(x) - F(x)\|_y}{\|F(x)\|_y} \leq \mathcal{O}(C_F(x) \cdot \text{EPS})$$

If the problem is well-conditioned:

backward stability guarantees accurate results

No guarantee when  $C_F$  is large

We can't expect  $\frac{\|\tilde{F}(x) - F(x)\|}{\|F(x)\|} \leq \mathcal{O}(\text{EPS})$

## II. Direct Methods for Solving LSE

Solve an LSE  $Ax = b$   $A \in \mathbb{K}^{n,n}, b \in \mathbb{K}^n$   
}  
given

solve for  $x$

If  $A$  is regular/invertible:

existence & uniqueness of a solution  $x$

$A$  invertible:  $\exists B \in \mathbb{K}^n$  s.t.  $AB = I_n = BA$

$\Leftrightarrow \text{rank}(A) = n \Leftrightarrow \det(A) \neq 0$

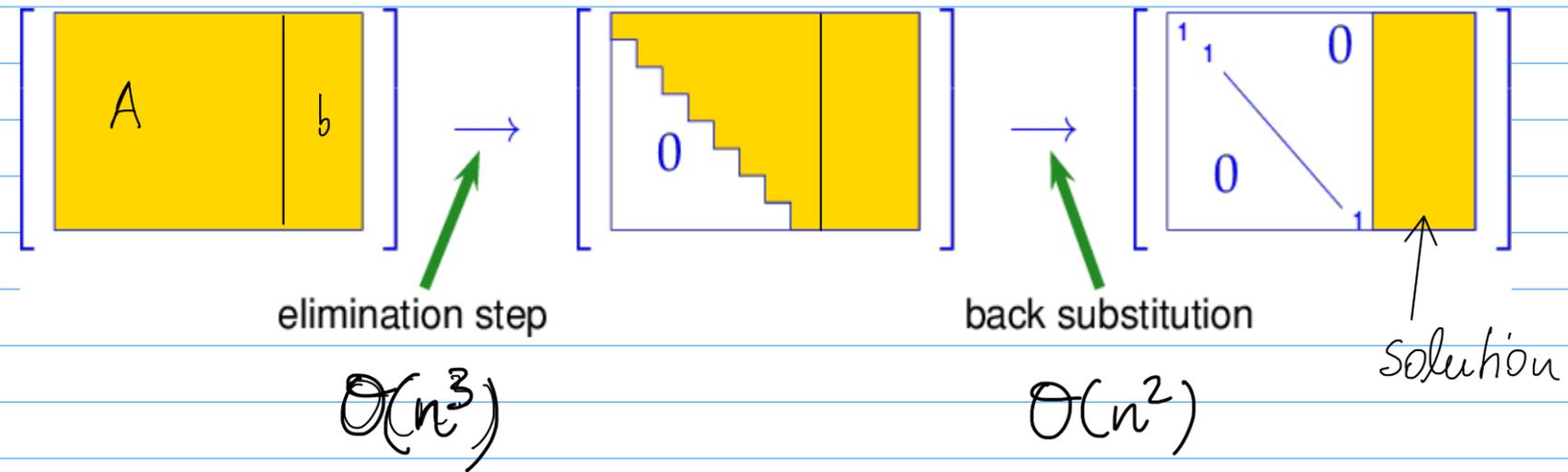
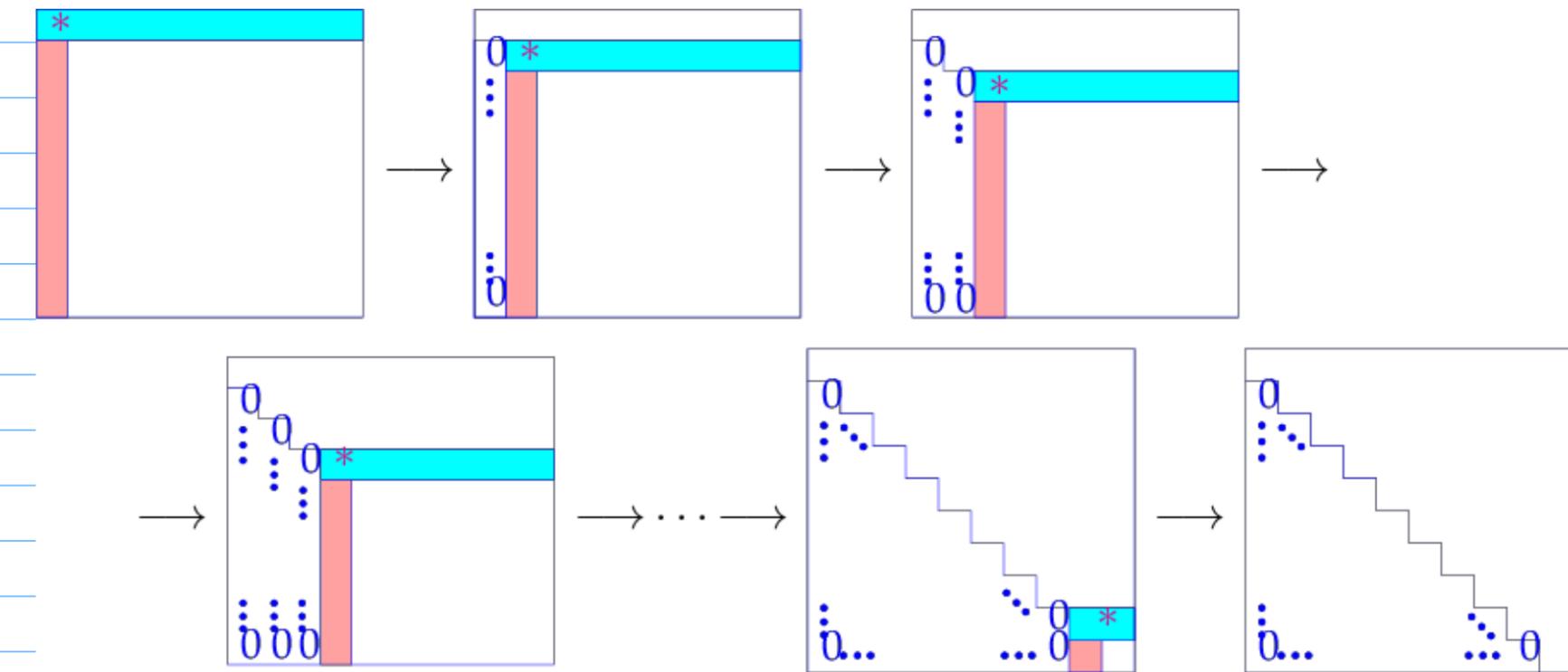
$\Leftrightarrow \mathcal{N}(A) = \{x : Ax = 0\} = \{0\}$

# 2.3 Gauss elimination

idea:  $Ax=b, T \in K^{n \times n}$  reg.

$$\Leftrightarrow TAX = Tb$$

$\hat{=}$  row transformations & permutations

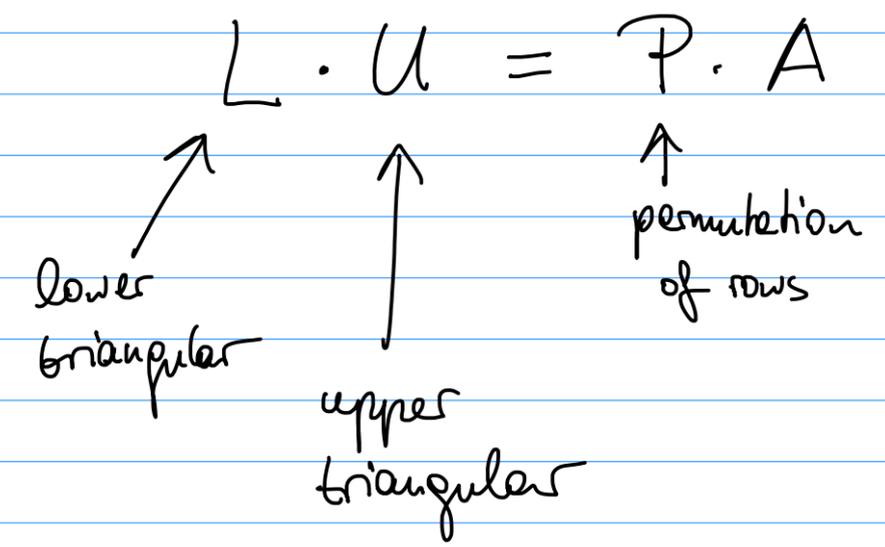


→ overall complexity:  $\Theta(n^3)$

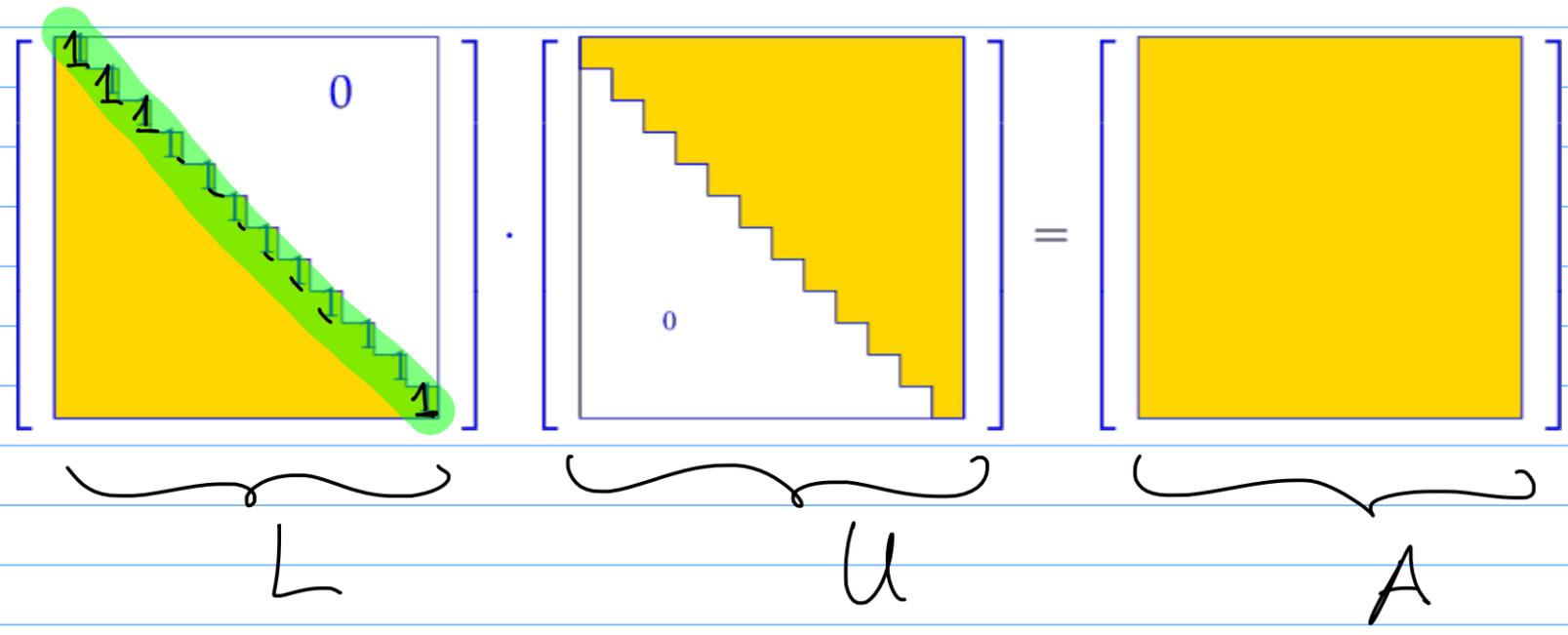
[solving LSE triangular matrix:  $\Theta(n^2)$ ]

→ solving without computing  $A^{-1}$   
 avoid computing  $A^{-1}$

Alternative way : LU-decomposition



$a_{11} = l_{11} u_{11}$   
 if  $a_{11} = 0$   
 $\rightarrow$  permutation needed



Solve for  $Ax = B$  using

LU decomposition :

- $Ax = b$  :
- ① LU-decomposition  $A = LU$ , #elementary operations  $\frac{1}{3}n(n-1)(n+1)$   $\rightarrow \Theta(n^3)$
  - ② forward substitution, solve  $Lz = b$ , #elementary operations  $\frac{1}{2}n(n-1)$   $\leftarrow$
  - ③ backward substitution, solve  $Ux = z$ , #elementary operations  $\frac{1}{2}n(n+1)$   $\uparrow$

$Ax = b$

- ①  $L \underbrace{U}_z x = b$
- ②  $Lz = b$  solve for  $z$
- ③  $Ux = z$  solve for  $x$

Remark: Overall complexity is  $\Theta(n^3)$   
 (same as Gauss elimination)

Q: What's the benefit?

Benefit if we solve for multiple  
RHS!

Suppose  $A$   $n \times n$ ,  $N$  different RHS  
complexity  $\Theta(n^3 + Nn^2) \leftarrow$  LU decomp

Gauss elimination:  $\Theta(Nn^3)$

C++11 code 2.5.11: Wasteful approach!  
→ [GITLAB](#)

```

2 // Setting:  $N \gg 1$ ,
3 // large matrix  $A \in \mathbb{K}^{n,n}$ 
4 for(int j = 0; j < N; ++j){
5     x = A.lu().solve(b);
6     b = some_function(x);
7 }

```

computational effort  $O(Nn^3)$

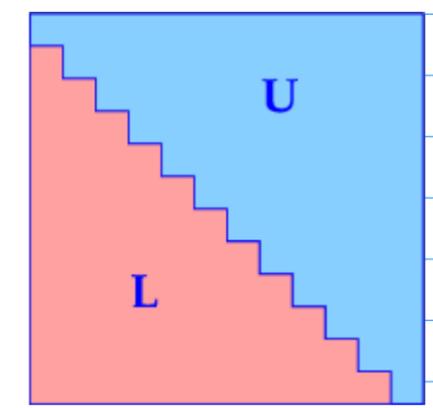
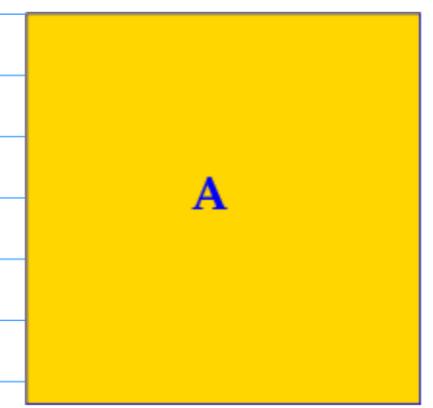
C++11 code 2.5.12: Smart approach!  
→ [GITLAB](#)

```

2 // Setting:  $N \gg 1$ ,
3 // large matrix  $A \in \mathbb{K}^{n,n}$ 
4 auto A_lu_dec = A.lu();
5 for(int j = 0; j < N; ++j){
6     x = A_lu_dec.solve(b);
7     b = some_function(x);
8 }

```

computational effort  $O(n^3 + Nn^2)$



(EIGEN)  
↑  
one matrix  
containing  $L$  &  $U$   
[without storing  
 $\text{diag}(L)$ ]

Use existing general solvers (for LSE)  
that are built-in

# 2.6 Exploiting structure when solving / LSE

some entries vanish

matrix entries fulfill some formula

simple example: LSE with triangular matrix  $\mathcal{O}(n^3) \rightarrow \mathcal{O}(n^2)$

## 2.6.2. Block elimination

Block matrix multiplication

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} = \begin{bmatrix} A_{11}B_{11} + A_{12}B_{21} & A_{11}B_{12} + A_{12}B_{22} \\ A_{21}B_{11} + A_{22}B_{21} & A_{21}B_{12} + A_{22}B_{22} \end{bmatrix}$$

## Block elimination

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}, \quad \begin{matrix} A_{11} \in \mathbb{K}^{k,k}, A_{12} \in \mathbb{K}^{k,l}, A_{21} \in \mathbb{K}^{l,k}, A_{22} \in \mathbb{K}^{l,l}, \\ x_1 \in \mathbb{K}^k, x_2 \in \mathbb{K}^l, b_1 \in \mathbb{K}^k, b_2 \in \mathbb{K}^l. \end{matrix}$$

$$A_{11}x_1 + A_{12}x_2 = b_1$$

$$x_1 = A_{11}^{-1}(b_1 - A_{12}x_2)$$

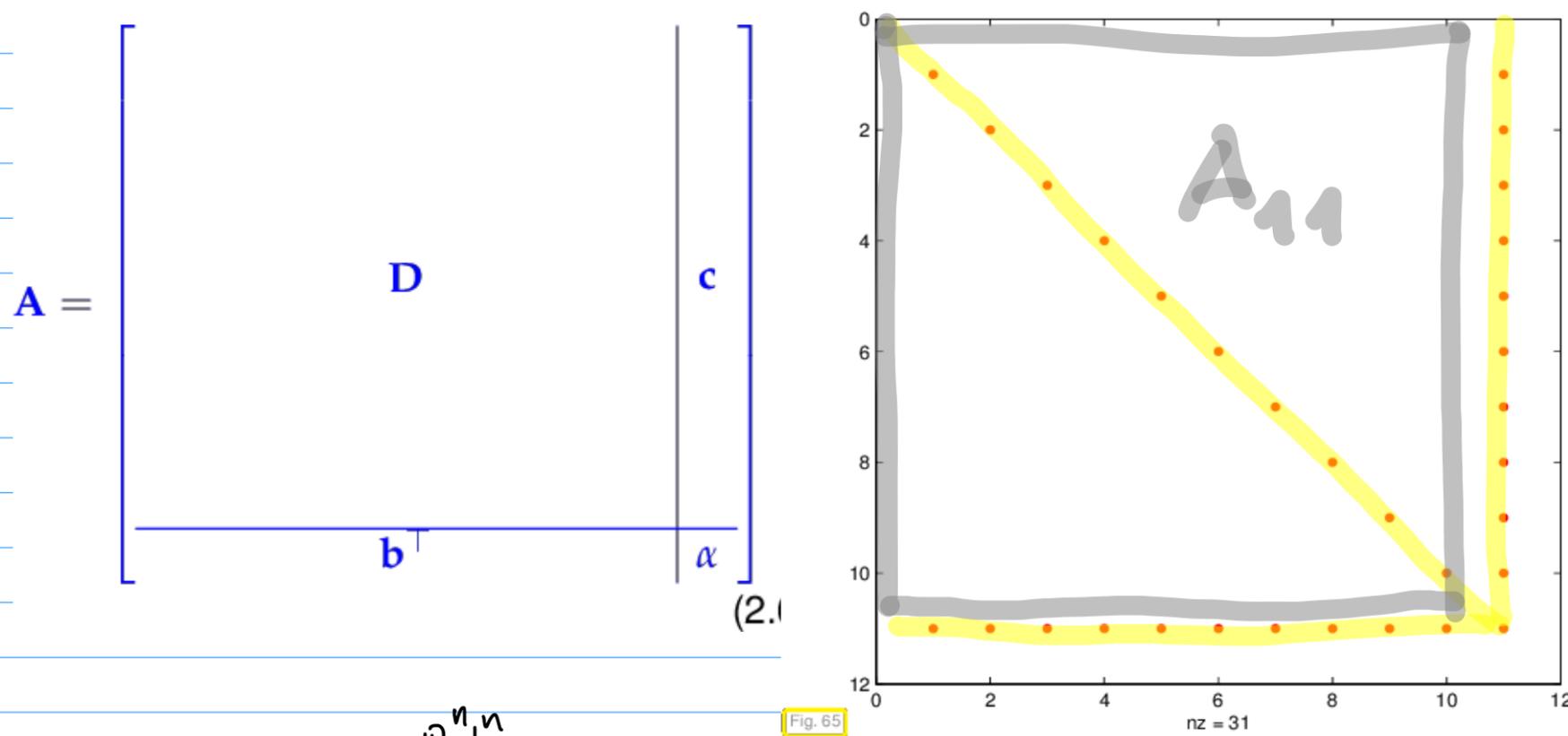
$$A_{21}x_1 + A_{22}x_2 = b_2$$

$$A_{21}A_{11}^{-1}(b_1 - A_{12}x_2) + A_{22}x_2 = b_2$$

$$(1.3.16) \quad \underbrace{(A_{22} - A_{21}A_{11}^{-1}A_{12})}_{\text{Schur complement}} x_2 = b_2 - A_{21}A_{11}^{-1}b_1$$

easy to solve if  $A_{11}^{-1}$  can be easily computed

Example:  $A_{11}$  is diagonal



$$\begin{array}{c}
 \in \mathbb{R}^{n,n} \\
 \downarrow \\
 \left[ \begin{array}{c} D \\ b^T \end{array} \right] \left[ \begin{array}{c} c \\ \alpha \end{array} \right] \left[ \begin{array}{c} x_1 \\ \zeta \end{array} \right] = \left[ \begin{array}{c} b_1 \\ \beta \end{array} \right]
 \end{array}$$

$\uparrow$  scalar       $\uparrow$  scalar

Solving with LU:  $\Theta(n^3)$

$$Dx_1 + c\zeta = b_1$$

$$(I) \quad x_1 = D^{-1}(b_1 - c\zeta)$$

$$b^T x_1 + \alpha \zeta = \beta$$

$$b^T D^{-1}(b_1 - c\zeta) + \alpha \zeta = \beta$$

$$(II) \quad (\alpha - b^T D^{-1} c) \zeta = \beta - b^T D^{-1} b_1$$

$$z := D^{-1} c : \Theta(n)$$

$$w := D^{-1} b_1 : \Theta(n)$$

$$\text{computing } \zeta : \Theta(n)$$

$$\text{computing } x : \Theta(n)$$

overall:  $\Theta(n)$

C++11 code 2.6.10: Solving an arrow system according to (2.6.8) → [GITLAB](#)

```

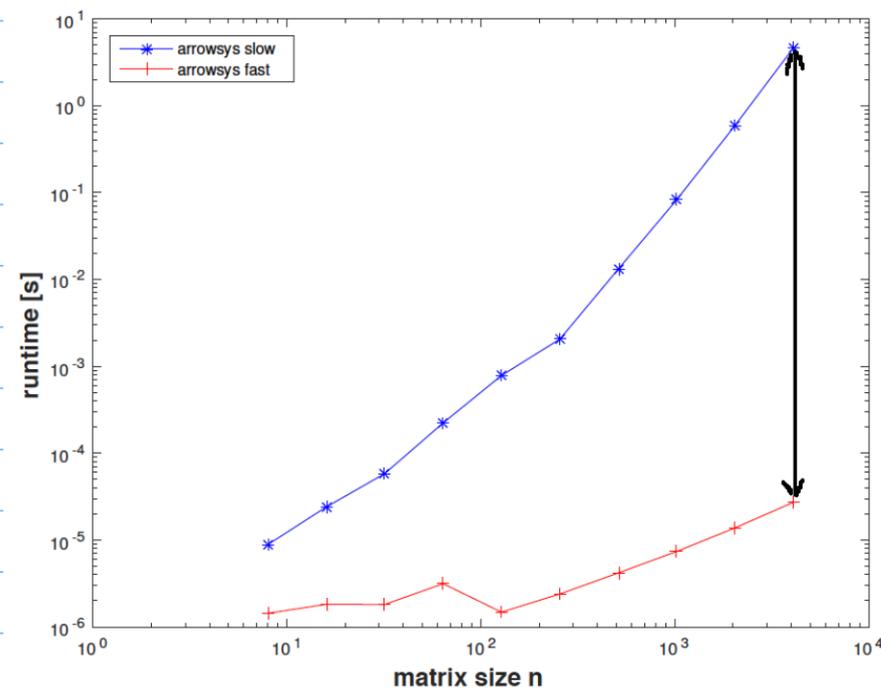
2 VectorXd arrowsys_fast(const VectorXd &d, const VectorXd &c, const
  VectorXd &b, const double alpha, const VectorXd &y){
3   int n = d.size();
4   VectorXd z = c.array() / d.array(); // z = D^{-1}c
5   VectorXd w = y.head(n).array() / d.array(); // w = D^{-1}b_1
6   double xi = (y(n) - b.dot(w)) / (alpha - b.dot(z));
7   VectorXd x(n+1);
8   x << w - xi*z, xi;
9   return x;
10 }

```

warning: Block elimination can suffer from numerical instability [equivalent to Gauss elimination without pivoting]

roughly:

- stable for s.p.d. matrices
- stable for diagonally dominant matrices



$\sim 10^6$

$$\text{for all } i \in \{1, \dots, n\}: |A_{ii}| \geq \sum_{j \neq i} |A_{ij}|$$

Example: Low-rank modifications  
of LSE