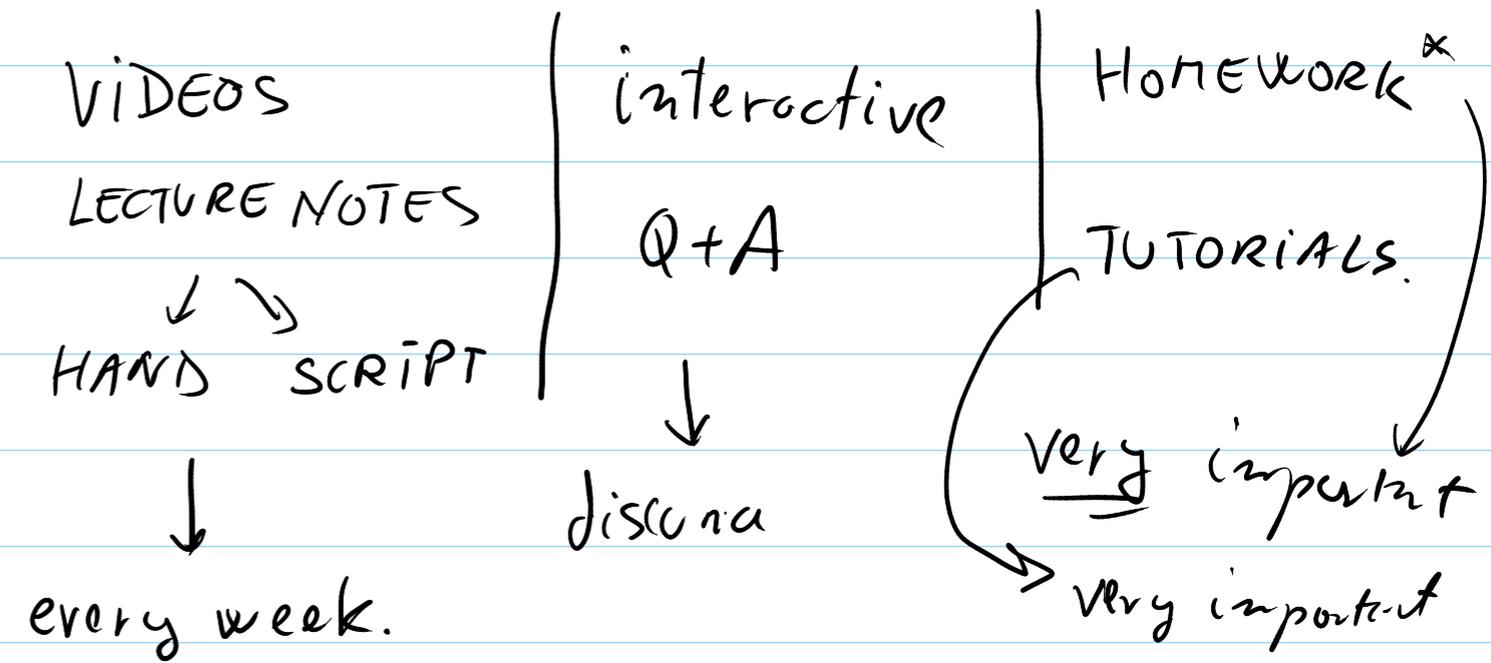


Numerical Methods for CSE

AUTUMN 2023

Q+A

22.09.2023



NO BONUS

A MOCK EXAM "BYOD" + "DIY" NOVEMBER

"CODE EXPERT"

Def Kronecker produkt of two matrices

$$\underline{A} \in \mathbb{R}^{m \times n} \quad \underline{B} \in \mathbb{R}^{l \times k}$$

$$m, n, l, k \in \mathbb{N}$$

$$\underline{A} \otimes \underline{B} \in \mathbb{R}^{(ml) \times (nk)}$$

Block of size $l \times k$

$$\begin{bmatrix} A_{11} \underline{B} & A_{12} \underline{B} & \dots & A_{1n} \underline{B} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} \underline{B} & A_{m2} \underline{B} & \dots & A_{mn} \underline{B} \end{bmatrix}$$

$\hookrightarrow (ml) \times (nk)$

exempl

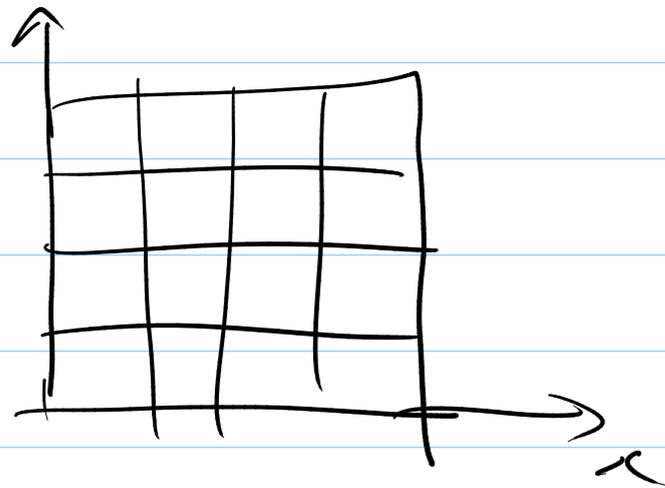
$$\underline{I}_m \otimes \underline{A} = \begin{bmatrix} \underline{A} & & 0 \\ 0 & \dots & \underline{A} \\ & & \dots & \underline{A} \end{bmatrix}$$

$$\underline{A} \times \underline{I}_m = \begin{bmatrix} a_{11} \underline{I} & a_{12} \underline{I} & \dots & a_{1k} \\ \vdots & a_{22} \underline{I} & & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nk} \underline{I} \end{bmatrix}$$

$\underline{A} \text{ } n \times k$

$$\begin{bmatrix} a_{11} & 0 & \dots & 0 \\ 0 & a_{11} & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \dots & a_{11} & \end{bmatrix} \quad \begin{bmatrix} a_{12} & 0 & \dots & 0 \\ 0 & a_{12} & & 0 \\ \vdots & & \ddots & 0 \\ 0 & \dots & a_{12} & \end{bmatrix}$$

Partial Differential Equations



$$\begin{pmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} \end{pmatrix}$$

↓
Matrix

$$\frac{\partial}{\partial x} \quad \frac{\partial}{\partial y}$$

$$\underline{D}_x \otimes \underline{D}_y$$



$x_{i-1} \quad x_i \quad x_{i+1}$

$$\underline{u} = \begin{pmatrix} u(x_0) \\ \vdots \\ u(x_{N-1}) \end{pmatrix} \quad \underline{A} \cdot \underline{D}_x$$

$$\underline{D}_y$$

$$\frac{\partial}{\partial x} u(x_i) \approx \frac{u_{i+1} - u_{i-1}}{2h}$$

(Q3.1.1.14.C) Given a matrix $B \in \mathbb{R}^{m,n}$, a vector $c \in \mathbb{R}^m$, and $\lambda > 0$, define

$$\{x^*\} := \operatorname{argmin}_{x \in \mathbb{R}^n} \|Bx - c\|_2^2 + \lambda \|x\|_2^2 \subset \mathbb{R}^n.$$

looks like a penalisation:

$\lambda \neq 0 \Rightarrow \lambda \|x\|_2^2$ does increase!

but actually no deeper meaning than for trick

State an overdetermined linear system of equations $Ax = b$, of which x^* is a least-squares solution.

↳ a method to address linear least squares problem for B with B not full rank

(i.e. ~~some of~~ the columns of B are linear dependant)

Pick a small $\lambda > 0$

$$A = \begin{bmatrix} B \\ \sqrt{\lambda} I_n \end{bmatrix} \quad b = \begin{bmatrix} c \\ 0 \end{bmatrix} \in \mathbb{R}^{m+n}$$

↳ linear independant columns of A

$$\lambda \|x\|_2^2 = \langle \sqrt{\lambda} I x, \sqrt{\lambda} I x \rangle$$

$$\operatorname{argmin}_{x \in \mathbb{R}^n} \|Ax - b\|_2^2$$

$$x \in \mathbb{R}^n$$

$(m+n) \times n$ has Rank n .

\Rightarrow QR-decomposition will work.!

Possible advantage:
if B is sparse,
so is A , so QR-dec
via Givens-Rotations
might be much
less expensive
than $\operatorname{svd}(B)$.

Question: difference in advantages CSC / CRS

CSS: good for slicing columns

CRS: good for slicing rows

both are good for interval $+$, $*$ (pointwise)
 Matrix * vector
 (might be faster)

Remark other formats are better for a fast construction.

(Q2.7.1.5.E) For a given matrix $A \in \mathbb{R}^{m,n}$, $m, n \in \mathbb{N}$, we define the square matrix

$$W_A := \begin{bmatrix} O_{m,m} & A \\ A^T & O_{n,n} \end{bmatrix} \in \mathbb{R}^{m+n, m+n}.$$

Outline the implementation of an efficient C++ function

```
void crsAtoW(std::vector<double> &val,
            std::vector<unsigned int> &col_ind,
            std::vector<unsigned int> &row_ptr);
```

whose arguments supply the three vectors defining the matrix A in CRS format and which overwrites them with the corresponding vectors of the CRS-format description of W_A .

Remember that the CRS format of a matrix $A \in \mathbb{R}^{m,n}$ is defined by

$$\text{val}[k] = (A)_{ij} \Leftrightarrow \begin{cases} \text{col_ind}[k] = j, \\ \text{row_ptr}[i] \leq k < \text{row_ptr}[i+1], \end{cases} \quad 1 \leq k \leq \text{nnz}(A).$$

It may be convenient to use `std::vector::resize(n)` that resizes a vector so that it contains n elements. If n is smaller than the current container size, the content is reduced to its first n elements, removing those beyond (and destroying them). If n is greater than the current container size, the content is expanded by inserting at the end as many elements as needed to reach a size of n using their default value.

Most important: how to implement A^T ?

This function does it:

```
CRSMatrix sparse_transpose(const CRSMatrix& input) {
    CRSMatrix res{
        input.m,
        input.n,
        input.nz,
        std::vector<double>(input.nz, 0.0),
        std::vector<int>(input.nz, 0),
        std::vector<int>(input.m + 2, 0) // one extra
    };

    // count per column
    for (int i = 0; i < input.nz; ++i) {
        ++res.rowPtr[input.colIndex[i] + 2];
    }

    // from count per column generate new rowPtr (but shifted)
    for (int i = 2; i < res.rowPtr.size(); ++i) {
        // create incremental sum
        res.rowPtr[i] += res.rowPtr[i - 1];
    }

    // perform the main part
    for (int i = 0; i < input.n; ++i) {
        for (int j = input.rowPtr[i]; j < input.rowPtr[i + 1]; ++j) {
            // calculate index to transposed matrix at which we should p
            
            const int new_index = res.rowPtr[input.colIndex[j] + 1]++;
            res.val[new_index] = input.val[j];
            res.colIndex[new_index] = i;
        }
    }
    res.rowPtr.pop_back(); // pop that one extra

    return res;
}
```

(Q2.6.0.25.F) [Loss of stability] By direct block-wise Gaussian elimination we found the following solution formulas for a block-partitioned linear system of equations with $D \in \mathbb{R}^{n,n}$, $c, b \in \mathbb{R}^n$, $\alpha \in \mathbb{R}$, $y \in \mathbb{R}^{n+1}$:

$Ax = \begin{bmatrix} D & c \\ b^T & \alpha \end{bmatrix} \begin{bmatrix} x_1 \\ \zeta \end{bmatrix} = y := \begin{bmatrix} y_1 \\ \eta \end{bmatrix}$, (2.6.0.7)

$\zeta = \frac{\eta - b^T D^{-1} y_1}{\alpha - b^T D^{-1} c}$, (2.6.0.8)
 $x_1 = D^{-1} (y_1 - \zeta c)$.

Use these formulas to compute the solution of the 2×2 linear system of equations

$\begin{bmatrix} \delta & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ \zeta \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$,

assuming $|\delta| < \frac{1}{2}EPS$ and using floating point arithmetic.

Hint. Remember that, if $|\delta| < \frac{1}{2}EPS$, in floating point arithmetic

$1 \uparrow \delta = 1$ and $2 \uparrow \delta^{-1} = \delta^{-1}$.

This is compatible with the "Axiom" of roundoff and Ass. 1.5.3.11

$$\zeta = \frac{2 - \frac{1}{\delta}}{1 - \frac{1}{\delta}} = \frac{1}{1 - \delta^{-1}} + 1$$

$1 + \delta = 1$
 $2 - \frac{1}{\delta} = -\frac{1}{\delta^{-1}} \Rightarrow 1 - 2 - \frac{1}{\delta} = 1 - \frac{1}{\delta}$

$2 - \delta^{-1} = 2 - (2 + \delta^{-1}) = -\delta^{-1}$

$1 - \delta^{-1} = 1 - (2 + \delta^{-1})$

$\zeta = \frac{-\delta^{-1}}{-\delta^{-1} - 1} = \frac{+1}{+1 + \delta} = \frac{1}{1} = 1$

$x_1 = \delta^{-1} (1 - 1) = 0 \Rightarrow \begin{bmatrix} -1 \\ 0 \end{bmatrix}$

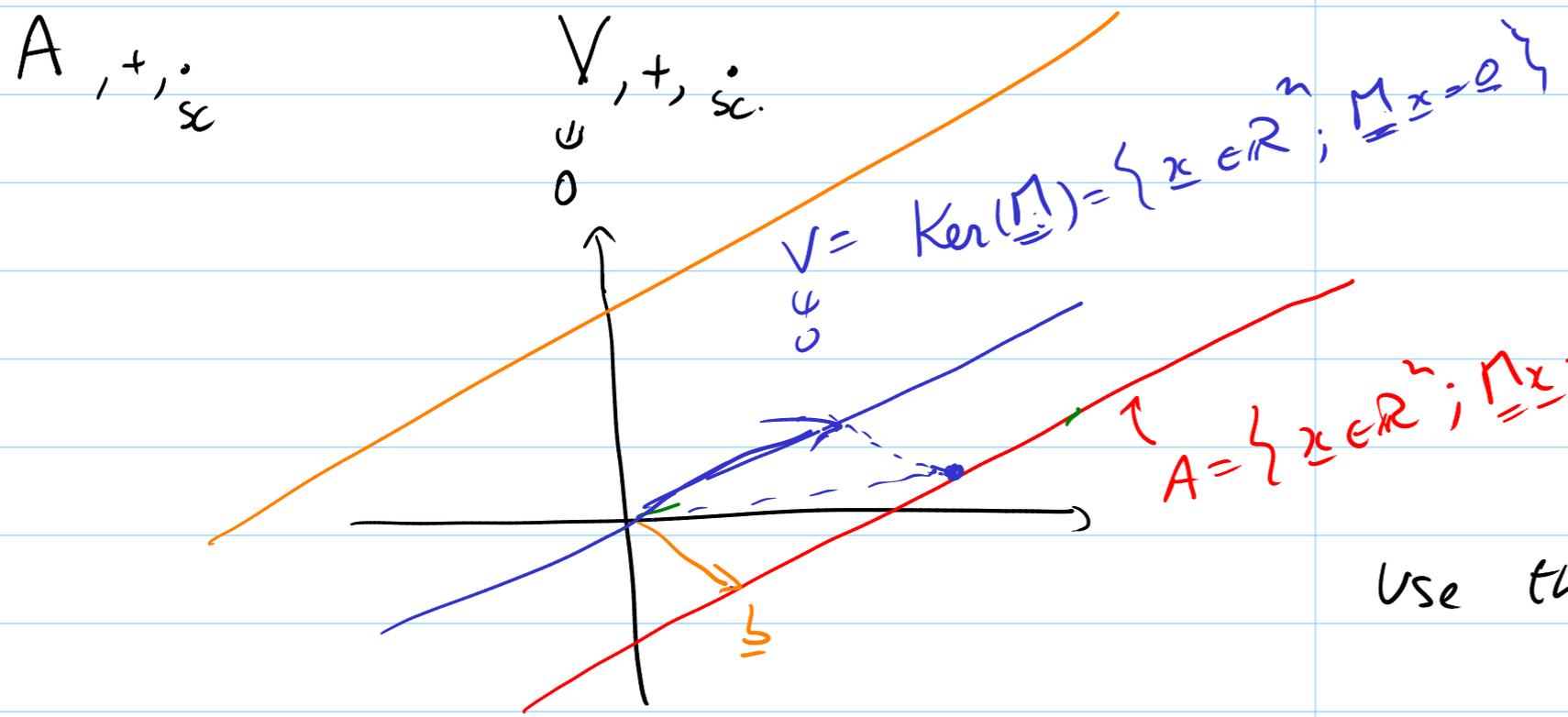
$\begin{bmatrix} \delta & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$;

If we compute "correctly", we get the wrong answer! ;)

06.10.2023

Could you please explain what the algorithm 2.10.1 from the exercise sheet does?
I don't quite understand why we can use the Sherman-Morris-Woodbury Formula for sub-problem c)

affine space \neq linear space
vektor



$x \in A \Leftrightarrow x = \underline{b} + \underline{v}$ with $\underline{v} \in V$

Use SMW-Formula in order to avoid solving.

$Mx = \underline{e}$ with a full matrix M

Use the fact that $M = \text{diag}(d) + \underline{u}\underline{v}^T$
Sparse \swarrow Rank 1-modification \uparrow

$\text{diag}(d)x = \underline{b}$ is solvable directly in $O(n)$ operations

Hence $O(n)$ instead of $O(n^3)$.

13.10.2023

(Q3.4.4.13.A) Let $M \in \mathbb{R}^{n,n}$ be symmetric and positive definite (s.p.d.) and $A \in \mathbb{R}^{m,n}$. Devise an algorithm for computing

$\operatorname{argmax}_{x \in B} \|Ax\|$, $B := \{x \in \mathbb{R}^n, x^T M x = 1\}$,

also based on the SVD of M .

$M = U \Sigma U^T$ $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n > 0$
 $D = \sqrt{\Sigma}$

Write the condition: $x^T M x = 1$

$x^T U \Sigma U^T x = 1$

$x^T U D^T D U^T x = 1$
 $y^T y = 1$

orthonormal.

$y^T y = 1$ with $y = D U^T x \Leftrightarrow U D^{-1} y = x$

$\operatorname{argmax}_{x \in \mathbb{R}^n, x^T M x = 1} \|Ax\| =$

$\operatorname{argmax}_{y \in \mathbb{R}^2, y^T y = 1} \|A U D^{-1} y\| = U D^{-1} \operatorname{argmax}_{y \in \mathbb{R}^2, y^T y = 1} \|B y\|$

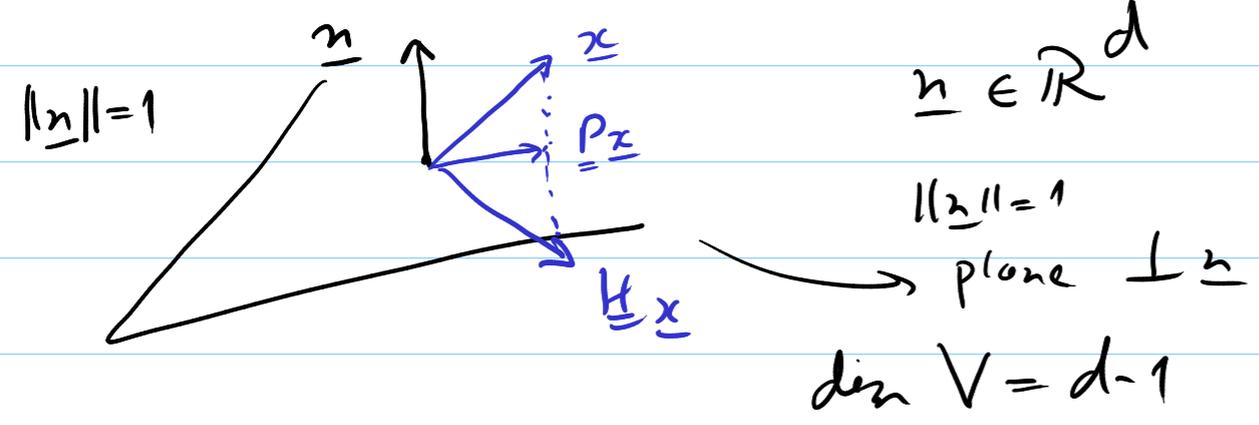
Which x makes $\|Ax\| = \min$

See (3.4.4.3) for the solution of this problem.

Sol. is. the first right singular vector of B

Sol $x = U D^{-1} y$

Q Why $\det H = -1$ for any Householder Matrix?



Take basis (orthonormal) $\underline{v}_1, \dots, \underline{v}_{d-1} \in V$

$$H \underline{v}_1 = \underline{v}_1, \dots, H \underline{v}_{d-1} = \underline{v}_{d-1}$$

$$H \underline{n} = -\underline{n}$$

$\rightarrow 1$ is EW of H of multiplicity $d-1$
 -1 is EW of H of multiplicity 1

$$\det H = \lambda_1 \lambda_2 \dots \lambda_n = (1)^{d-1} (-1) = -1$$

Q How do we solve Linear Systems of Eq.?

- 1) Want good precision? \neq Moderate precision.
- 2) how expensive?

good precision, not too big Matrix \Rightarrow LU-decomp.

Asymmetric pos. def \Rightarrow Cholesky-decomp.

big Matrix, sparse (banded)

\rightarrow there might be some direct methods

that keep sparsity, so might be

feasible QR; LU

in general LU would be not feasible.

less precision or large sparse Matrix A

\Rightarrow iterative methods \rightarrow symmetric $\bar{C}b$
 Krylov-type Method, \rightarrow non-sym others

Krylov-type methods use only

$$\Rightarrow \text{if } \underline{A} \text{ is sparse} \Rightarrow O(n, n^2)$$

Note: CG slow if $\text{cond}(\underline{A})$ is big.

\Rightarrow use pre-conditioning

$$\underline{A} \underline{x} = \underline{b} \Rightarrow \underline{B}^{-1} \underline{A} \underline{x} = \underline{B}^{-1} \underline{b}$$

$$\text{if } \underline{B}^{-1} = \underline{A}^{-1} \Rightarrow \underline{x} = \underline{B}^{-1} \underline{b} \quad (\odot)$$

$$\text{use } \underline{B}^{-1} \approx \underline{A}^{-1}$$

ex $\underline{B} = \text{diag}(\underline{A}) \Rightarrow \underline{B}^{-1}$ cheap
 \Rightarrow solve (CG) for $\underline{B}^{-1} \underline{A} \underline{x} = \underline{B}^{-1} \underline{b}$

(Q) Polar decomposition

$$\underline{A} = \underbrace{U}_{\substack{\uparrow \\ \underline{I} = V^T V}} \underbrace{\Sigma}_{\substack{\underline{Q} \\ \underline{H} \text{ spd.}}} V^T = \underbrace{UV^T}_{\substack{\underline{Q} \\ \underline{H} \text{ spd.}}} \underbrace{V \Sigma V^T}_{\substack{\underline{H} \text{ spd.}}}$$

$$= U \underbrace{\Sigma U^T}_{\substack{\underline{H} \text{ spd.}}} \underbrace{UV^T}_{\substack{\underline{Q}}}$$

$m \geq n$ economical SVD

$$\underline{U} \in \mathbb{R}^{m \times n}, \quad \underline{\Sigma} = \begin{bmatrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_n \\ & & & 0 \end{bmatrix}$$
$$\underline{V} \in \mathbb{R}^{n \times n}$$

$$\underline{V} \underline{\Sigma} \underline{V}^T \sim n^2 \text{ Operations (Storage)}$$

$$\underline{U} \sim m \cdot n \text{ Operations (Storage)}$$

$$\Rightarrow \text{not cheaper } O(mn + n^2)$$

$+n \rightarrow$ dominates!

3.12.d. Main messages:

- ① avoid using economical QR-decomposition,
- ② if using it, then be aware of dimensions!

3.10. $X_1 = A_1 B_1^T \in \mathbb{R}^{m \times n}$ $X_2 = A_2 B_2^T$

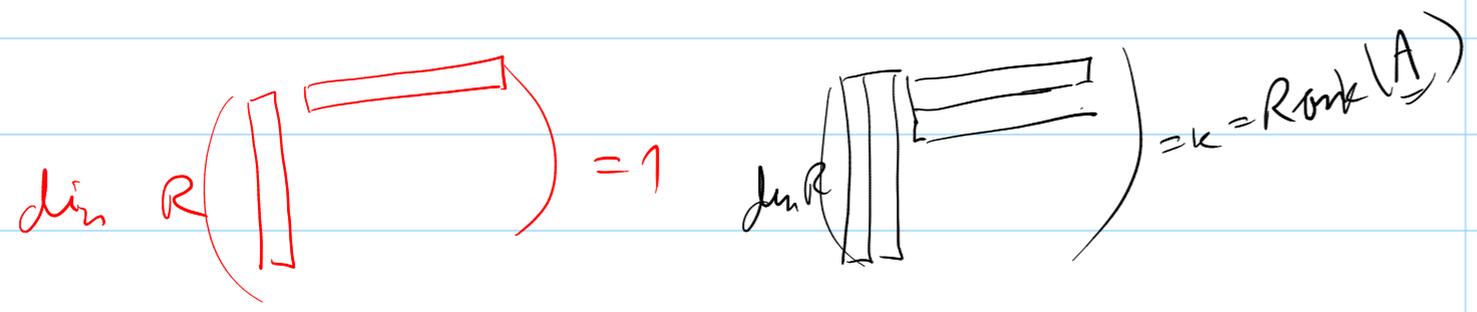
$A_1, A_2 \in \mathbb{R}^{m \times k}$ $B_1, B_2 \in \mathbb{R}^{n \times k}$

$\underline{X} = [X_1 \ X_2] \in \mathbb{R}^{m \times 2n}$

$R(\underline{X}) = R(X_1) + R(X_2)$

$\Rightarrow \dim R(\underline{X}) \leq \dim R(X_1) + \dim R(X_2) = 2k \Rightarrow$

$\dim R(\underline{X}) \leq m$



$\dim R(\underline{X}) \leq \min\{m, 2k\}$

SVD of \underline{X} without assembling \underline{X} ?
 i.e. by using only the factors
 A_1, B_1, A_2, B_2 .

economical!

$B_1 = Q_1 R_1$ $B_2 = Q_2 R_2$

$\underline{X} = [A_1 R_1^T Q_1^T \quad A_2 R_2^T Q_2^T] =$

$= \underbrace{[A_1 R_1^T \quad A_2 R_2^T]}_{\in \mathbb{R}^{m \times 2n}} \underbrace{\begin{bmatrix} Q_1^T & 0 \\ 0 & Q_2^T \end{bmatrix}}_{\in \mathbb{R}^{2k \times 2n}}$

$\underline{Z} = \tilde{U} \tilde{\Sigma} \tilde{V}^T$ $\tilde{U} \in \mathbb{R}^{m, 2k}$ $\tilde{V} \in \mathbb{R}^{2k \times 2n}$

Which b_1, \dots, b_n to choose?

$$V = P_n \Rightarrow b_k(t) = t^{k-1} \quad ;$$

↓

Linear system bad conditioned!

+ better basis!

+ suitable space.

$$b_k(t) = e^{ikt} = \cos(kt) + i \sin(kt)$$

→ trigonometric polynomials

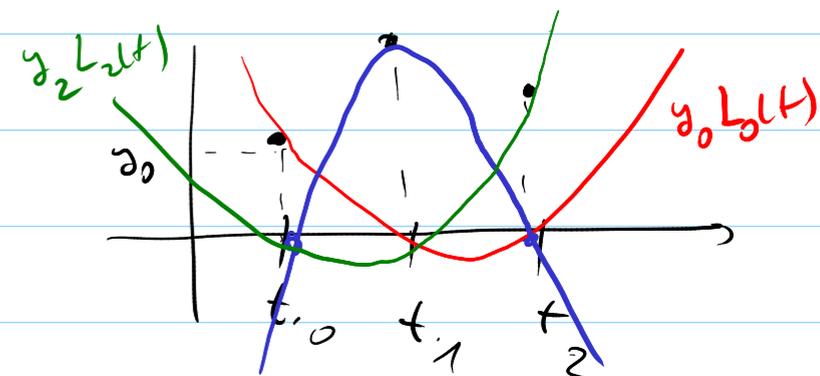
→ very fast and accurate algorithms via FFT.

→ complete basis in L^2

② Lagrange interpolation.

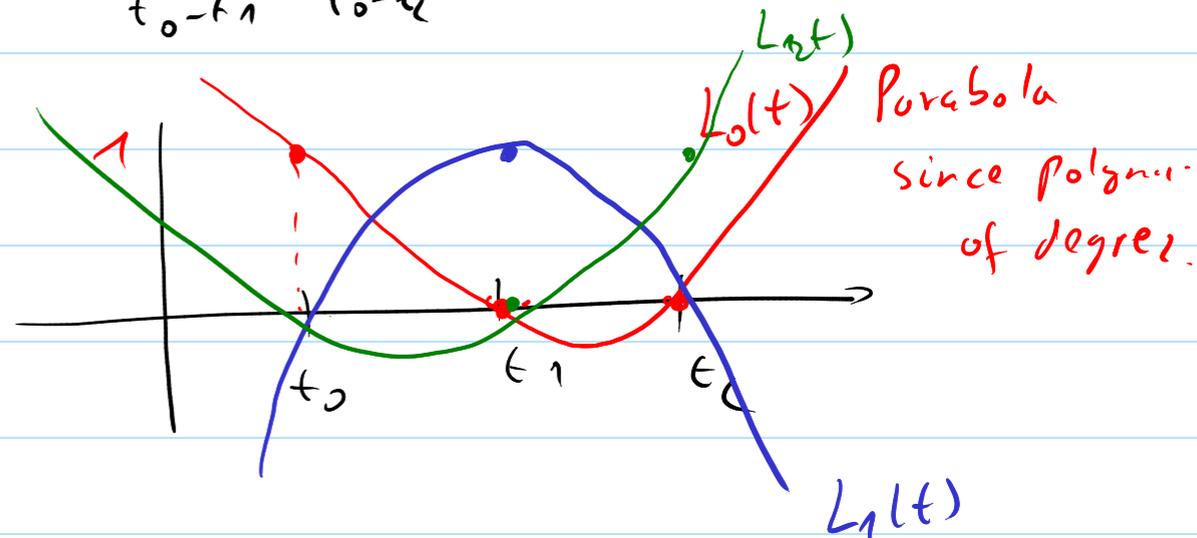
Let us take 3 measurements.

t_0	t_1	t_2
y_0	y_1	y_2



$$L_0(t) = \frac{t-t_1}{t_0-t_1} \frac{t-t_2}{t_0-t_2} \Rightarrow L_0(t_0) = \frac{t_0-t_1}{t_0-t_1} \frac{t_0-t_2}{t_0-t_2} = 1$$

$$L_0(t_1) = \frac{t_1-t_1}{t_0-t_1} \frac{t_1-t_2}{t_0-t_2} = 0 \Rightarrow L_0(t_1) = L_0(t_2) = 0$$



$$f(t) = \gamma_0 L_0(t) + \gamma_1 L_1(t) + \gamma_2 L_2(t)$$

$$f(t_0) = \gamma_0 \cdot 1 + \gamma_1 \cdot 0 + \gamma_2 \cdot 0 = \gamma_0$$

$$f(t_1) = \gamma_0 \cdot 0 + \gamma_1 \cdot 1 + \gamma_2 \cdot 0 = \gamma_1$$

$$f(t_2) = \gamma_0 \cdot 0 + \gamma_1 \cdot 0 + \gamma_2 \cdot 1 = \gamma_2$$

↑

" δ "-property.

$$L_j(t_k) = \begin{cases} 1 & \text{if } j=k \\ 0 & \text{if } j \neq k. \end{cases}$$