3. Direct methods for linear least Squares

Introduction: Want to solve $Ax=b$ but the system is over determined. So you won't find an exact solution

$x \in lsq(A,b) \iff Ax$ is closest element in $R(A)$ to b

Note: If $\operatorname{rank}(A) = n$ you still have the problem that b just isn't in $R(A)$. Therefore Least squares and not Gauss / LU

Normal Equation: $A^T A x = A^T b$

To be a unique solution we would need: $N(A^TA) = N(A) \overset{!}{=} \{0\}$

1.) Compute $C := A^T A$ $\quad O(m \cdot n^2)$

2.) Compute $c := A^T b$ $\quad O(n \cdot m)$

3.) Solve s.p.d. LSE $Cx = c$ $\quad O(n^3)$ $\quad \Rightarrow O(n^2 m + n^3)$

Sparse A:

Problem: A^TA not sparse anymore. , Squaring $\operatorname{cond}(A)$

Fix: $\begin{bmatrix} -\alpha I & A \\ A^H & 0 \end{bmatrix} \begin{bmatrix} r \\ x \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}$ Use α to do good conditioning.
$[O(n^{3/2}), O(n^{5/2})]$

Generalized Solution:

If $N(A^TA) \neq \{0\}$ we get a unique solution by taking that x, such that:

$$x^+ := \operatorname{argmin}\{ \|x\|_2 : x \in lsq(A,b)\}$$

$$x^+ = V(V^TA^TAV)^{-1}V^TA^T$$ Moore-Penrose-Pseudoinverse A^+ of A.
↳ Does not depend on V

Note: V is a Basis for the $Kern(A)$.
Note: Alternative way to compute the Moore-Penrose-Inv. → SVD

Orthogonal Transformation (⇒ Householder QR) ($\operatorname{Rank}(A) = n$)

$A = QR$ with Q unitär, R upper Triangular.

$Rx = Q^Tb$ $\quad$ Backwards substitution: $O(n^2)$

To compute the QR factorization:

Gramm Schmidt: unstable, $O(n^3)$

Householder: stable, $O(m \cdot n^2)$

MatrixXd Q = qr.householderQ(); // applies all HH ref. m times

Singular Value Decomposition

+ If $cond(A) \gg 0$
+ Construction of Moore-Penrose

$A = U \Sigma V^H$

- Exists for all A
- U, V are unitary matrices

Get Factorization: $O(m \cdot n^2)$ S. 84

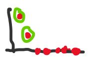
To solve least squares:

$$A = \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} \Sigma_r & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_1^H \\ V_2^H \end{bmatrix} \qquad r = Rank(A)$$

Not generalized : $\Sigma_r V_1^H x = U_1^H b$ (not unique)

generalized : $x = \underbrace{V_1 \cdot \Sigma_r^{-1} U_1^H}_{\text{Moore-Penrose-Pseudoinverse}} b$ (unique)

SVD-Based Optimization / Approximation

- $\|Ax\|_2 \to min$ with $\|x\| = 1$
  ↳ $x = (V)_{1:n} = V \cdot e_n$
- Find $\tilde{A}$ that's close to A and has Rank k.
  ↳ $\tilde{A} = \sum_{i=1}^{k} \sigma_i \cdot (U)_{:,i} \cdot (V)_{:,i}^H$
- Principle Component Analysis (PCA)
  ↳ $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_p \gg \sigma_{p+1} \approx \dots \approx \sigma_{min\{m,n\}} \approx 0$
  ↳ z.B.  ⇒ 2 diodes (electricity)