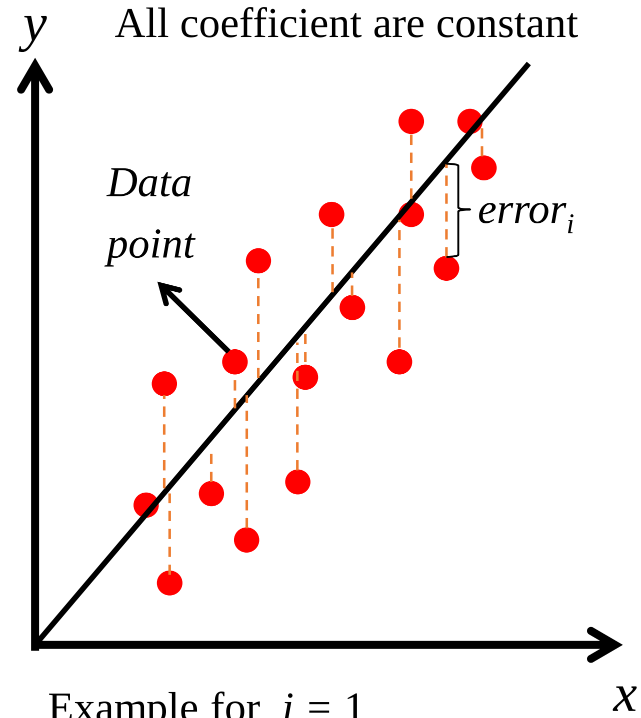
Numerical methods for Regression

Concept for Least-Square

$$y = \sum_{j=0}^{n} a_j x^j \quad n = 2, 4$$

Fitting curve: $y = a_1 x + a_0$

All coefficient are constant



Example for $j = 1$

- **Concept**: There are many data (x_i, y_i), after setting on the x-y plane, the distribution may be fitted by some curve $y = f(x)$ or $f(x, y) = k$, k is some constant, $\forall\, x, y, k \in \mathbb{R}$.
- Define $error_i = y_i - y$
- Total error $E = \sum_{i=1}^{n} (y_i - y)^2$
- **Want**: E is minimum value.

Derive the Mathematical Eq.

Existence and Uniqueness

- For linear regression, we use $y = bx + a$ to fit our data. If there are n group of data (x_i, y_i), $i = 1, 2, \ldots, n$, then, we have n group of linear equations system

$$\begin{cases} y_1 = \boxed{b}x_1 + \boxed{a} \\ \vdots \\ y_n = \boxed{b}x_n + \boxed{a} \end{cases} \xrightarrow[\text{representation}]{\text{Matrix}} \underbrace{\overset{\boldsymbol{Y}}{\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}}}_{n\times 1} = \underbrace{\overset{\boldsymbol{A}}{\begin{bmatrix} x_1 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix}}}_{n\times 2} \underbrace{\overset{\boldsymbol{x}}{\begin{bmatrix} b \\ a \end{bmatrix}}}_{2\times 1} \to \boldsymbol{Y} = \boldsymbol{A}\boldsymbol{x}$$

- In this case, there are 2 unknown parameters, so n must be bigger than 2 so that there **may** **exist** a and b **uniquely**.
- Lemma 1: Let $\boldsymbol{A} \in M_{m\times n}(F)$, $\boldsymbol{x} \in F^n$, $\boldsymbol{y} \in F^m$, $m \geq n$ then

$$\langle \boldsymbol{Ax}, \boldsymbol{y} \rangle_m = \langle \boldsymbol{x}, \boldsymbol{A}^T\boldsymbol{y} \rangle_n, \quad \langle\ ,\ \rangle\text{: inner product}$$

- Lemma 2: Let $\boldsymbol{A} \in M_{m\times n}(F)$, rank($\boldsymbol{A}$) = rank($\boldsymbol{A}^T\boldsymbol{A}$)
- Corollary: Let $\boldsymbol{A} \in M_{m\times n}(F)$ and rank($\boldsymbol{A}$) = n, then $\boldsymbol{A}^T\boldsymbol{A}$ is invertible

Derive the Mathematical Eq.
Existence and Uniqueness

Theorem of Least-square approximation:

Let $\boldsymbol{A} \in M_{m\times n}(F)$, $m \geq n$, $\boldsymbol{y} \in F^m$, then $\exists\, x_0 \in F^n$ s.t.

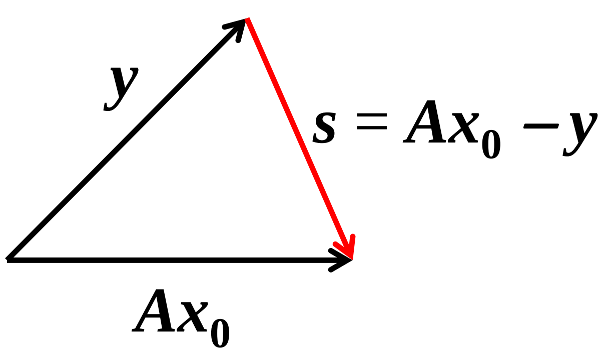
$$(\boldsymbol{A}^T\boldsymbol{A})\,\boldsymbol{x_0} = \boldsymbol{A}^T\boldsymbol{y} \text{ and } \|\boldsymbol{Ax_0} - \boldsymbol{y}\| \leq \|\boldsymbol{Ax} - \boldsymbol{y}\|,\ \boldsymbol{x} \in F^n$$

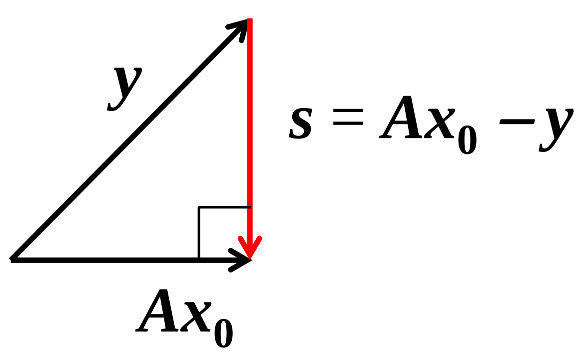
Furthermore, if rank($\boldsymbol{A}$) = n (full rank), then $\boxed{\boldsymbol{x_0} = (\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T\boldsymbol{y}}$

If $\boldsymbol{Ax} = \boldsymbol{y}$ is consistent, then $\exists!$ solution $\boldsymbol{s}$

pf : In the view point of geometry, if there exists 2 vectors $\boldsymbol{y}$ and $\boldsymbol{Ax_0}$, $\boldsymbol{s} = \boldsymbol{Ax_0} - \boldsymbol{y}$, when $\boldsymbol{s} \perp \boldsymbol{Ax_0}$, then $\|\boldsymbol{s}\|$ is minimum and exactly one

$\rightarrow \langle \boldsymbol{Ax}, \boldsymbol{s}\rangle = \langle \boldsymbol{x}, \boldsymbol{A}^T\boldsymbol{s}\rangle = \langle \boldsymbol{x}, \boldsymbol{A}^T(\boldsymbol{Ax_0} - \boldsymbol{y})\rangle = \boldsymbol{0} \rightarrow$





For $\boldsymbol{x} \neq 0$, $\boldsymbol{A}^T\boldsymbol{Ax_0} = \boldsymbol{A}^T\boldsymbol{y}$

$$\boxed{\boldsymbol{x_0} = (\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T\boldsymbol{y}}$$

Derive the Mathematical Eq. Extend to monomial Regression

- Total error $E=\sum_{i=1}^{n}(y-y_i)^2=\sum_{i=1}^{n}(y-bx_i-a)^2$, just a **parabolic eq.** with concave up, so there exists a minimum value. By calculus,

$$\begin{cases}\dfrac{\partial E}{\partial b}=0=\sum_{i=1}^{n}-2(x_i)(y_i-bx_i-a)\\ \dfrac{\partial E}{\partial a}=0=\sum_{i=1}^{n}-2(y_i-bx_i-a)\end{cases}\rightarrow\begin{cases}\sum_{i=1}^{n}x_iy_i=\sum_{i=1}^{n}(bx_i^{\ 2}+ax_i)\\ \sum_{i=1}^{n}y_i=\sum_{i=1}^{n}(bx_i+ax_i)\end{cases}$$

$$\downarrow$$

$$\underbrace{\begin{bmatrix}x_1 & \cdots & x_n\\ 1 & \cdots & 1\end{bmatrix}^T}_{\boldsymbol{A^T}}\underbrace{\begin{bmatrix}y_1\\ \vdots\\ y_n\end{bmatrix}}_{\boldsymbol{Y}}=\underbrace{\begin{bmatrix}x_1 & \cdots & x_n\\ 1 & \cdots & 1\end{bmatrix}^T}_{\boldsymbol{A^T}}\underbrace{\begin{bmatrix}x_1 & 1\\ \vdots & \vdots\\ x_n & 1\end{bmatrix}}_{\boldsymbol{A}}\underbrace{\begin{bmatrix}b\\ a\end{bmatrix}}_{\boldsymbol{x_0}}\leftarrow\begin{bmatrix}\sum_{i=1}^{n}x_iy_i\\ \sum_{i=1}^{n}y_i\end{bmatrix}=\begin{bmatrix}\sum_{i=1}^{n}x_i^{\ 2} & \sum_{i=1}^{n}x_i\\ \sum_{i=1}^{n}x_i & 1\end{bmatrix}\begin{bmatrix}b\\ a\end{bmatrix}$$

- Here we take the **derivative on the coefficient**, not x and y, so we can apply this method to our regression.

Derive the Mathematical Eq. Extend to monomial Regression

$$f(x,y) = a_0 + a_1 x + a_2 y + a_3 x^2 + a_4 xy + a_5 y^2 + a_6 x^3 + a_7 x^2 y + a_8 xy^2 + a_9 y^3$$
$$+ a_{10} x^4 + a_{11} x^3 y + a_{12} x^2 y^2 + a_{13} xy^3 + a_{14} y^4$$

Here x, y are independent. By previous derivation, our total error is

$$E = E\,(a_0,\, a_1,\, a_2,\, \ldots,\, a_{14})$$

so that we can apply our concept to find the minimum error for surface regression.

$$\underset{n\times 1}{\begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}} = \underset{n\times 15}{\begin{bmatrix} 1 & x_1 & \cdots & y_1^{\,4} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & \cdots & y_n^{\,4} \end{bmatrix}} \underset{15\times 1}{\begin{bmatrix} a_0 \\ \vdots \\ a_{14} \end{bmatrix}}$$

So we complete the derivation.

Algorithm Selecting

- Solve $(\boldsymbol{A}^T\boldsymbol{A})\,\boldsymbol{x}_0 = \boldsymbol{A}^T\boldsymbol{y}$ → The worst method
- Solve $\boldsymbol{x}_0 = (\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T\boldsymbol{y}$ by getting $(\boldsymbol{A}^T\boldsymbol{A})^{-1}$
  1. Gaussian elimination → Backward unstable
  2. LU decomposition (LUD) → More stable than the former

Easy to write

Less stable

- QR Decompose $\boldsymbol{A} = \boldsymbol{QR} = [\boldsymbol{Q}_1 \;\; \boldsymbol{Q}_2]\begin{bmatrix} \boldsymbol{R}_1 \\ 0 \end{bmatrix} = \boldsymbol{Q}_1\boldsymbol{R}_1$ → $\boldsymbol{R}_1\boldsymbol{x} = \boldsymbol{Q}_1^T\boldsymbol{y}$
  (QRD)
  1. Modified Gram-schmidt process
  2. Givens Rotation
  3. Householder transform → **Candidate**

Highest CP value

Matlab algorithm for this problem

x = A\Y

- $\boxed{\text{SV Decomposition (SVD) } \boldsymbol{A} = \boldsymbol{U\Sigma V}^T}$ → **Candidate**

  Most stable

  Most expensive

Algorithm Selecting

Criterion for selecting an algorithm

- Stability
- Time and memory cost
- Speed of convergence

In general, these 2 relation are in direct proportion.

Now I use LU Decomposition since it is easy to write.

1. Loading data and getting $\boldsymbol{A}$ and $\boldsymbol{A^T}$
2. $\boldsymbol{B} = \boldsymbol{A^T A} \rightarrow$ This step produces more error.
3. Get $\boldsymbol{B}^{-1}$ by **LU decomposition with pivoting (PLUD)**
4. Get $\boldsymbol{x_0} = (\boldsymbol{A^T A})^{-1}\boldsymbol{A^T y}$

$$\begin{bmatrix} 10^{-20} & 0 \\ 1 & 1 \end{bmatrix} \Big\downarrow \text{Pivoting} \quad \begin{bmatrix} 1 & 1 \\ 10^{-20} & 0 \end{bmatrix}$$

$$
\underbrace{\begin{bmatrix} b_{1,1} & b_{1,2} & b_{1,3} & b_{1,4} \\ b_{2,1} & b_{2,2} & b_{2,3} & b_{2,4} \\ b_{3,1} & b_{3,2} & b_{3,3} & b_{3,4} \\ b_{4,1} & b_{4,2} & b_{4,3} & b_{4,4} \end{bmatrix}}_{\boldsymbol{B}}
=
\begin{bmatrix} 1 & 0 & 0 & 0 \\ \dfrac{b_{2,1}}{b_{1,1}} & 1 & 0 & 0 \\ \dfrac{b_{3,1}}{b_{1,1}} & 0 & 1 & 0 \\ \dfrac{b_{4,1}}{b_{1,1}} & 0 & 0 & 1 \end{bmatrix}
\begin{bmatrix} b_{1,1} & b_{1,2} & b_{1,3} & b_{1,4} \\
0 & b_{2,2} - \dfrac{b_{1,2}\times b_{2,1}}{b_{1,1}} & b_{2,3} - \dfrac{b_{1,3}\times b_{2,1}}{b_{1,1}} & b_{2,4} - \dfrac{b_{1,4}\times b_{2,1}}{b_{1,1}} \\
0 & b_{3,2} - \dfrac{b_{1,2}\times b_{3,1}}{b_{1,1}} & b_{3,3} - \dfrac{b_{1,3}\times b_{3,1}}{b_{1,1}} & b_{3,3} - \dfrac{b_{1,4}\times b_{3,1}}{b_{1,1}} \\
0 & b_{4,2} - \dfrac{b_{1,2}\times b_{4,1}}{b_{1,1}} & b_{4,3} - \dfrac{b_{1,3}\times b_{4,1}}{b_{1,1}} & b_{4,4} - \dfrac{b_{1,4}\times b_{4,1}}{b_{1,1}} \end{bmatrix}
$$

$$
= \begin{bmatrix} 1 & 0 & 0 & 0 \\ \ell_{2,1} & 1 & 0 & 0 \\ \ell_{3,1} & 0 & 1 & 0 \\ \ell_{4,1} & 0 & 0 & 1 \end{bmatrix}
\begin{bmatrix} b_{1,1} & b_{1,2} & b_{1,3} & b_{1,4} \\ 0 & b_{2,2}^{(1)} & b_{2,3}^{(1)} & b_{2,4}^{(1)} \\ 0 & b_{3,2}^{(1)} & b_{3,3}^{(1)} & b_{3,3}^{(1)} \\ 0 & b_{4,2}^{(1)} & b_{4,3}^{(1)} & b_{4,4}^{(1)} \end{bmatrix}
$$

$$
\overset{\substack{\text{Do} \\ \text{3 times}}}{=}
\underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ \ell_{2,1} & 1 & 0 & 0 \\ \ell_{3,1} & \ell_{3,2} & 1 & 0 \\ \ell_{4,1} & \ell_{4,2} & \ell_{4,3} & 1 \end{bmatrix}}_{\text{L}}
\underbrace{\begin{bmatrix} u_{1,1} & u_{1,2} & u_{1,3} & u_{1,4} \\ 0 & u_{2,2} & u_{2,3} & u_{2,4} \\ 0 & 0 & u_{3,3} & u_{3,3} \\ 0 & 0 & 0 & u_{4,4} \end{bmatrix}}_{\text{U}}
$$

Algorithm
Matrix decomposition (LUD)

- $\boldsymbol{Bx_0 = A^Ty \rightarrow LUx_0 = A^Ty \rightarrow L(Ux_0) = L(c) = b,\ Ux_0 = c,\ A^Ty = b}$

$$\begin{bmatrix} 1 & 0 & \cdots & 0 \\ \ell_{2,1} & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \ell_{15,1} & \ell_{15,2} & \cdots & 1 \end{bmatrix} \underbrace{\begin{bmatrix} u_{1,1} & u_{1,2} & \cdots & u_{1,15} \\ 0 & u_{2,2} & \cdots & u_{2,15} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & u_{15,15} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{15} \end{bmatrix}}_{\boldsymbol{c}} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ \ell_{2,1} & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \ell_{15,1} & \ell_{15,2} & \ell_{15,3} & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_{15} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_{15} \end{bmatrix}$$

L : Lower triangular U : Upper triangular

Solving the linear eq.

$$\begin{bmatrix} u_{1,1} & u_{1,2} & \cdots & u_{1,15} \\ 0 & u_{2,2} & \cdots & u_{2,15} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & u_{15,15} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{15} \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_{15} \end{bmatrix}$$

L and U matrix can be store in one matrix to reduce the memory usage.

$$\begin{bmatrix} u_{1,1} & u_{1,2} & \cdots & u_{1,15} \\ \ell_{2,1} & u_{2,2} & \cdots & u_{2,15} \\ \vdots & \vdots & \ddots & \vdots \\ \ell_{15,1} & \ell_{15,2} & \cdots & u_{15,15} \end{bmatrix}$$

Ill-condition

Numerical error may cause Mathematical problem

$$\begin{bmatrix} 400 & -201 \\ -800 & 401 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 200 \\ -200 \end{bmatrix} \rightarrow \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -100 \\ -200 \end{bmatrix}$$

$$\begin{bmatrix} 401 & -201 \\ -800 & 401 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 200 \\ -200 \end{bmatrix} \rightarrow \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 40000 \\ 79800 \end{bmatrix}$$

- This issue can be by using QRD or SVD.

Algorithm Matrix decomposition (QRD(Householder))

$$A \in M_{m\times n}(F) \qquad R_1 \in M_{m\times n}(F) \qquad R_2 \in M_{m\times n}(F)$$

column

$$\begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,15} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,15} \\ a_{3,1} & a_{3,2} & \cdots & a_{2,15} \\ a_{4,1} & a_{4,2} & \cdots & a_{2,15} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,1} & a_{m,2} & \cdots & a_{m,15} \end{bmatrix} \xrightarrow{\boldsymbol{H_1A}} \begin{bmatrix} r_{1,1} & r_{1,2} & \cdots & r_{1,15} \\ 0 & r_{2,2} & \cdots & r_{2,15} \\ 0 & r_{3,2} & \cdots & r_{2,15} \\ 0 & r_{4,2} & \cdots & r_{2,15} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & r_{m,2} & \cdots & r_{m,15} \end{bmatrix} \xrightarrow{\boldsymbol{H_2R_1}} \begin{bmatrix} r_{1,1} & r_{1,2} & \cdots & r_{1,15} \\ 0 & r_{2,2}' & \cdots & r_{2,15}' \\ 0 & 0 & \cdots & r_{2,15}' \\ 0 & 0 & \cdots & r_{2,15}' \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{m,15}' \end{bmatrix} \xrightarrow{\boldsymbol{H_3R_2}}$$

Row

$\boldsymbol{u_1}$

$$\|\boldsymbol{u_1}\| = k_1$$

$$\boldsymbol{v_1} = \frac{\boldsymbol{u_1} - k\boldsymbol{e_1}}{\|\boldsymbol{u_1} - k\boldsymbol{e_1}\|}$$

$$\boldsymbol{H_1} = \boldsymbol{I_m} - 2\boldsymbol{v_1}\boldsymbol{v_1}^T$$

$\boldsymbol{u_2}$

$$\|\boldsymbol{u_2}\| = k_2$$

$$\boldsymbol{v_2} = \frac{\boldsymbol{u_2} - k\boldsymbol{e_2}}{\|\boldsymbol{u_2} - k\boldsymbol{e_2}\|}$$

$$\boldsymbol{H_2} = \boldsymbol{I_{m\text{-}1}} - 2\boldsymbol{v_2}\boldsymbol{v_2}^T$$

End the process until to the last row

Algorithm Matrix decomposition (QRD(Householder))

$\boldsymbol{Q}$ is orthogonal matrix $= (\boldsymbol{H}_n \ldots \boldsymbol{H}_2\boldsymbol{H}_1)^T$

$\boldsymbol{QQ}^T = \boldsymbol{Q}^T\boldsymbol{Q} = \boldsymbol{I} \rightarrow \boldsymbol{Q}^T = \boldsymbol{Q}^{-1}$

n

m

$\boldsymbol{A} \in M_{m\times n}(F)$ $=$ $\boldsymbol{Q_1} \in M_{m\times n}(F)$ Only needs this matrix | $\boldsymbol{Q_2} \in M_{m\times(m-n)}(F)$ $\times$ $\boldsymbol{R_1} \in M_{n\times n}(F)$ / $\boldsymbol{R_2} = \boldsymbol{0} \in M_{(m-n)\times m}(F)$

$$\boldsymbol{A} = \boldsymbol{QR} = [\boldsymbol{Q}_1 \ \ \boldsymbol{Q}_2]\begin{bmatrix}\boldsymbol{R}_1 \\ 0\end{bmatrix}$$

$$= \boldsymbol{Q}_1\boldsymbol{R}_1 \rightarrow \boldsymbol{R}_1\boldsymbol{x} = \boldsymbol{Q}_1^T\boldsymbol{y}$$

Solving the linear eq.

Algorithm
Matrix decomposition (SVD)

- $\boldsymbol{A} \in M_{m\times n}(F)$, $m \geq n$ and rank(A) = n → full rank.
  rank(A) < n → rank-deficient
- This method is not appropriate in our situation, but it's a strong method for much more application.
- So we decompose $\boldsymbol{A} = \boldsymbol{U\Sigma V}^{\boldsymbol{T}}$ into 3 matrix as below.

$$\boldsymbol{A} \in M_{m\times n}(F) = \boldsymbol{U} \in M_{m\times m}(F) \quad \boldsymbol{\Sigma} \in M_{m\times n}(F) \quad \boldsymbol{V}^{\boldsymbol{T}} \in M_{n\times n}(F)$$

Orthogonal (U) | Diagonal (Σ) | Orthogonal (V^T)

Algorithm
Matrix decomposition (SVD)

$\boldsymbol{U}' \in M_{m\times p}(F)$ $\quad$ $\boldsymbol{\Sigma}' \in M_{p\times p}(F)$ $\quad$ $\boldsymbol{V}^{\boldsymbol{T}} \in M_{p\times n}(F)$

$\boldsymbol{A} \in M_{m\times n}(F) =$

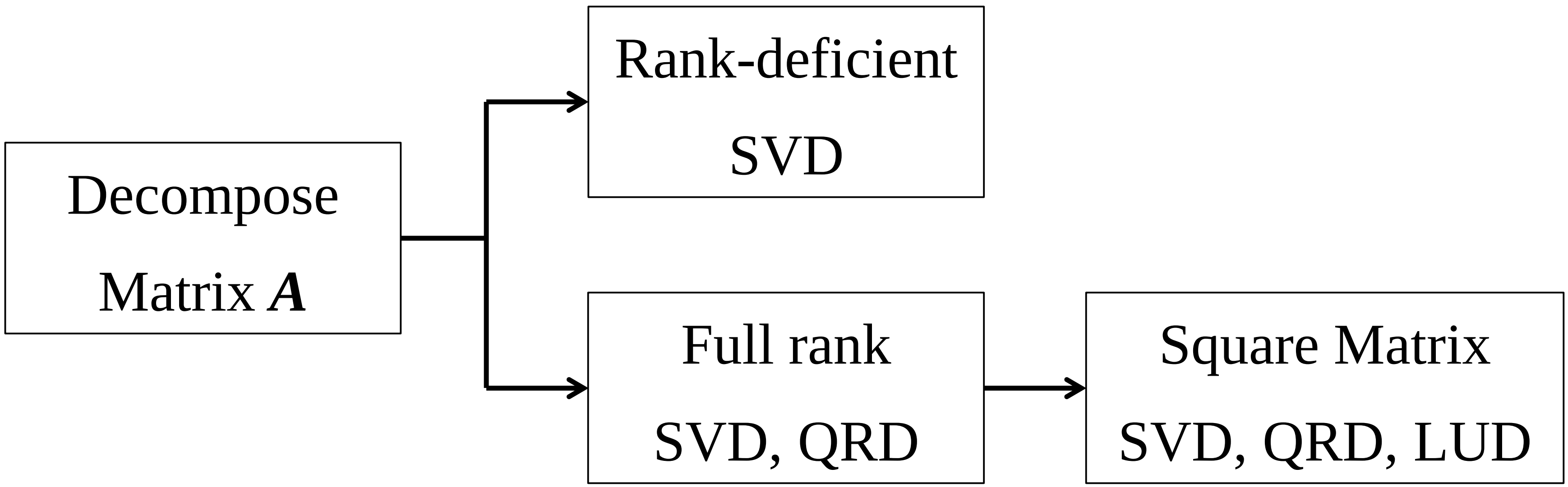
$\boldsymbol{V}^{\boldsymbol{T}} \in M_{n\times n}(F)$

$\boldsymbol{U} \in M_{m\times m}(F)$ $\quad$ $\boldsymbol{\Sigma} \in M_{m\times n}(F)$

Only needs orange parts, it can reduce memory and time cost, but still costs much memory and time.

$\boxed{\forall\, \boldsymbol{A} \in M_{m\times n}(F),\ \exists!\ \boldsymbol{U}, \boldsymbol{S} \text{ and } \boldsymbol{V} \text{ s.t. } \boldsymbol{U\Sigma V}^{\boldsymbol{T}}}$

Algorithm
Matrix decomposition



If matrix ***A*** is always full rank(should be check **mathematically**),
then **QRD** is the most appropriate algorithm for this problem.