Numerical methods for Surface Regression

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Introduction

- In experiments, we want to verify the relationship of two or more quantities, we plot the data in the plan, and the figure is seem with some trend, then we can use some function to fit the data. For example, Hook's law indicates the force is proportional to the displacement(in some linear regime), as we design a experiment to verify the law, and plot our data on Cartesian coordinate, the distribution will be like a straight line, and its slope represents the elastic constant.
- If there are more quantities, then we need to use surface regression. So our goal is extending linear regression to surface regression, and use computer to solve it.

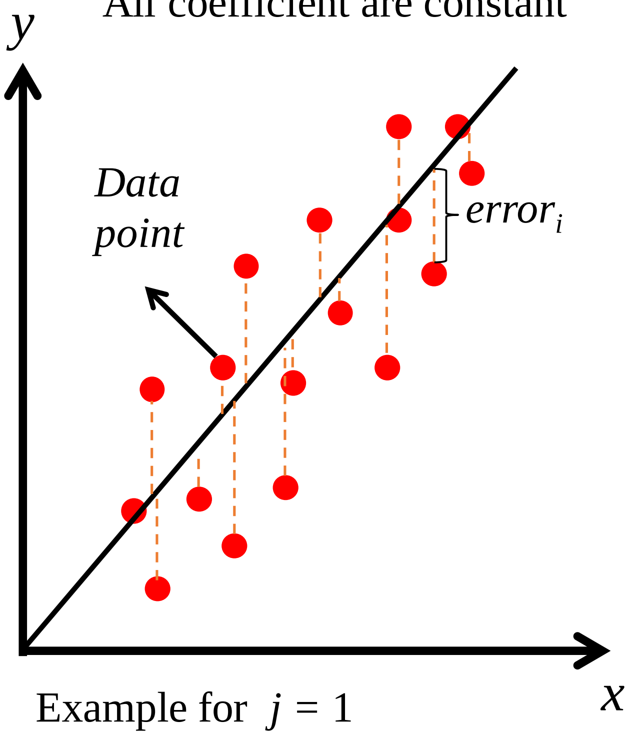
Concept for Least-Square Approximation

- **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.

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

Fitting curve: $y = a_1 x + a_0$

All coefficient are constant



Example for $j = 1$

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

$$\begin{cases} y_1 = bx_1 + a \\ \quad\vdots \\ y_n = bx_n + a \end{cases} \xrightarrow[\text{representation}]{\text{Matrix}} \underset{n\times 1}{\overset{\boldsymbol{Y}}{\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}}} = \underset{n\times 2}{\overset{\boldsymbol{A}}{\begin{bmatrix} x_1 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix}}} \underset{2\times 1}{\overset{\boldsymbol{x}}{\begin{bmatrix} b \\ a \end{bmatrix}}} \to \boldsymbol{Y} = \boldsymbol{Ax}$$

- 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

$$<\boldsymbol{Ax}, \boldsymbol{y}>_m = <\boldsymbol{x}, \boldsymbol{A}^T\boldsymbol{y}>_n, <\,,\,>: \text{inner product}$$

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

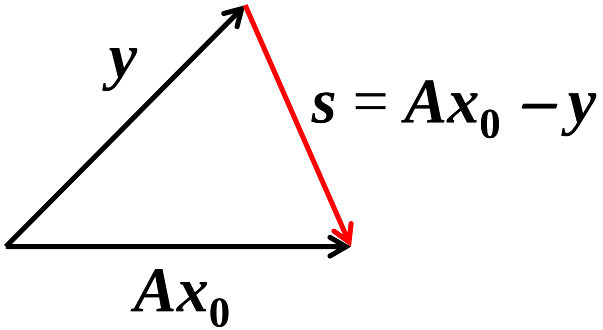
If $\boldsymbol{Ax} = \boldsymbol{y}$ is consistent, then ∃! solution $\boldsymbol{s}$

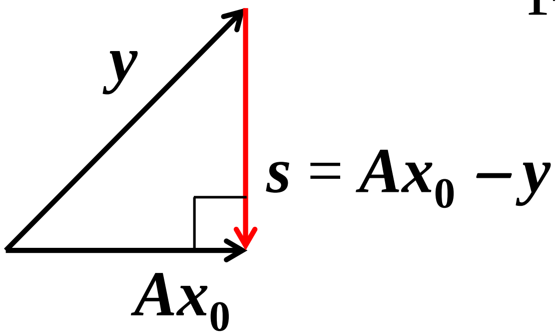
pf : In the view point of geometry, if ∃ 2 vectors $\boldsymbol{y}$ and $\boldsymbol{Ax_0}$, $\boldsymbol{s} = \boldsymbol{Ax_0} - \boldsymbol{y}$, when $\boldsymbol{s} \perp \boldsymbol{Ax_0}$, then $\|\boldsymbol{s}\|$ is minimum and exactly one

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

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 Surface 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,

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

$$\downarrow$$

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

- 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 Surface Regression

$$f(x, y) = a_0 + a_1 x + a_2 y + a_3 x^2 + a_4 xy + a_5 y^2$$

For example, if we want to fit a surface like above, and there n data, then the matrix is

$$\begin{bmatrix} f(x_1, y_1) \\ \vdots \\ f(x_n, y_n) \end{bmatrix} = \begin{bmatrix} 1 & x_1 & y_1 & x_1^2 & x_1 y_1 & y_1^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & y_n & x_n^2 & x_n y_n & y_n^2 \end{bmatrix} \begin{bmatrix} a_0 \\ \vdots \\ a_5 \end{bmatrix}$$

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

Highest CP value

Matlab algorithm for this problem

$\boldsymbol{x} = \boldsymbol{A}\backslash\boldsymbol{Y}$

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

$$\begin{tikzcd} \begin{bmatrix} 10^{-20} & 0 \\ 1 & 1 \end{bmatrix} \arrow[d, "\text{Pivoting}"'] \\ \begin{bmatrix} 1 & 1 \\ 10^{-20} & 0 \end{bmatrix} \end{tikzcd}$$

Algorithm
Matrix decomposition (LUD)

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

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

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

Algorithm
Matrix decomposition (LUD)

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

$$\begin{bmatrix} 1 & 0 & \cdots & 0 \\ \ell_{2,1} & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \ell_{15,1} & \ell_{15,2} & \cdots & 1 \end{bmatrix} \underbrace{\begin{bmatrix} u_{1,1} & u_{1,2} & \cdots & u_{1,15} \\ 0 & u_{2,2} & \cdots & u_{2,15} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & u_{15,15} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{15} \end{bmatrix}}_{\boldsymbol{c}} =$$

L : Lower triangular U : Upper triangular

$$\boxed{\begin{bmatrix} 1 & 0 & \cdots & 0 \\ \ell_{2,1} & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \ell_{15,1} & \ell_{15,2} & \ell_{15,3} & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_{15} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_{15} \end{bmatrix}}$$

Solving the linear eq.

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

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

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

Algorithm
Matrix decomposition (QRD(Householder))

- Ill-condition

Numerical error may cause Mathematical problem

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

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

- PLUD may encounter this problem, and the error may get larger when we calculate $\boldsymbol{B} = \boldsymbol{A}^T\boldsymbol{A}$. So I'll use QRD or SVD to solve this problem.

Algorithm
Matrix decomposition (QRD(Householder))

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

column →

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

↑ Row

$\boldsymbol{u_1}$

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

$\boldsymbol{u_2}$

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

End the process until to the last row

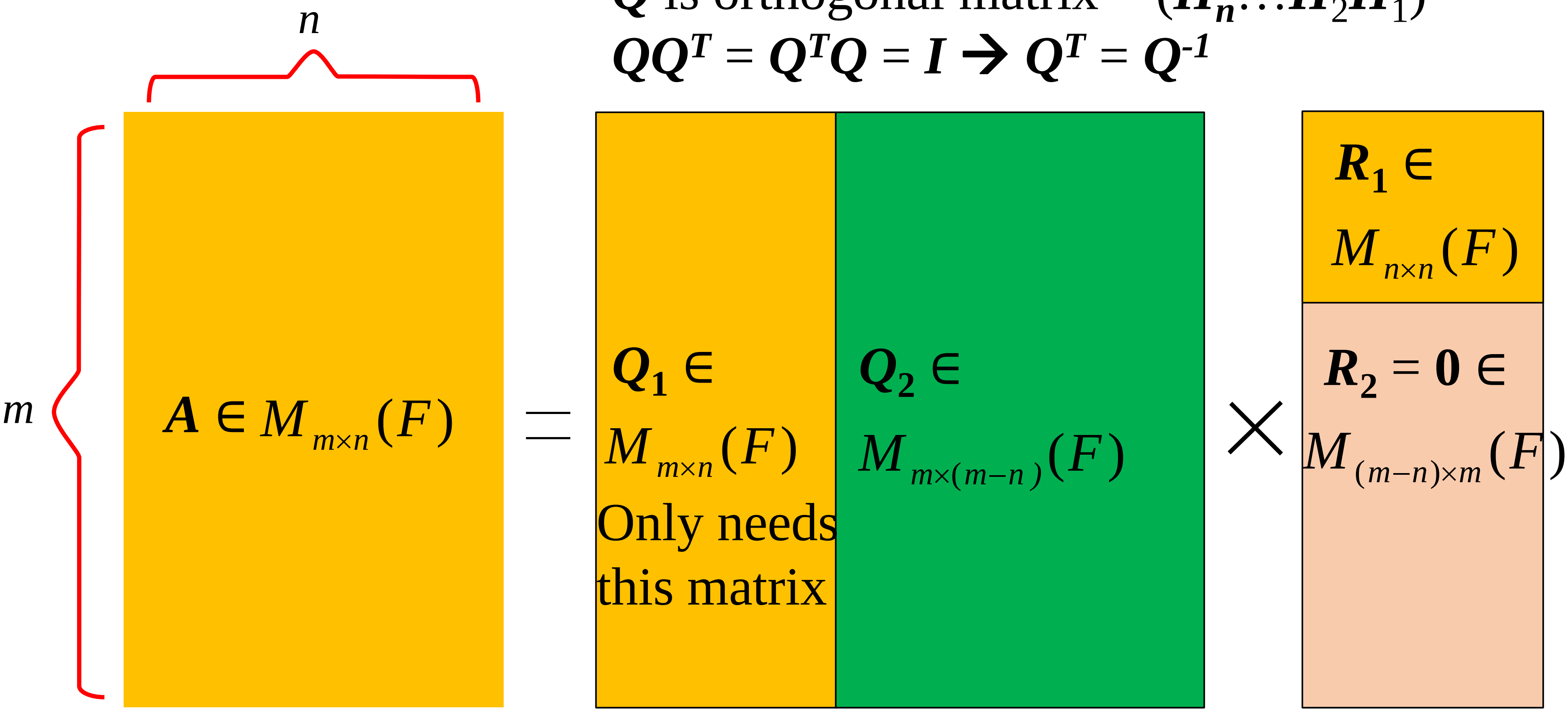
$$\boldsymbol{v_1} = \frac{\boldsymbol{u_1} - k\boldsymbol{e_1}}{\|\boldsymbol{u_1} - k\boldsymbol{e_1}\|} \qquad \boldsymbol{v_2} = \frac{\boldsymbol{u_2} - k\boldsymbol{e_2}}{\|\boldsymbol{u_2} - k\boldsymbol{e_2}\|}$$

$$\boldsymbol{H_1} = \boldsymbol{I_m} - 2\boldsymbol{v_1}\boldsymbol{v_1}^T \qquad \boldsymbol{H_2} = \boldsymbol{I_{m\text{-}1}} - 2\boldsymbol{v_2}\boldsymbol{v_2}^T$$

Algorithm
Matrix decomposition (QRD(Householder))

$\boldsymbol{Q}$ is orthogonal matrix = $(\boldsymbol{H}_{\boldsymbol{n}} \dots \boldsymbol{H}_2 \boldsymbol{H}_1)^T$

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



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

$\boldsymbol{Q_1} \in M_{m\times n}(F)$

Only needs this matrix

$\boldsymbol{Q_2} \in M_{m\times(m-n)}(F)$

$\times$

$\boldsymbol{R_1} \in M_{n\times n}(F)$

$\boldsymbol{R_2} = \boldsymbol{0} \in M_{(m-n)\times m}(F)$

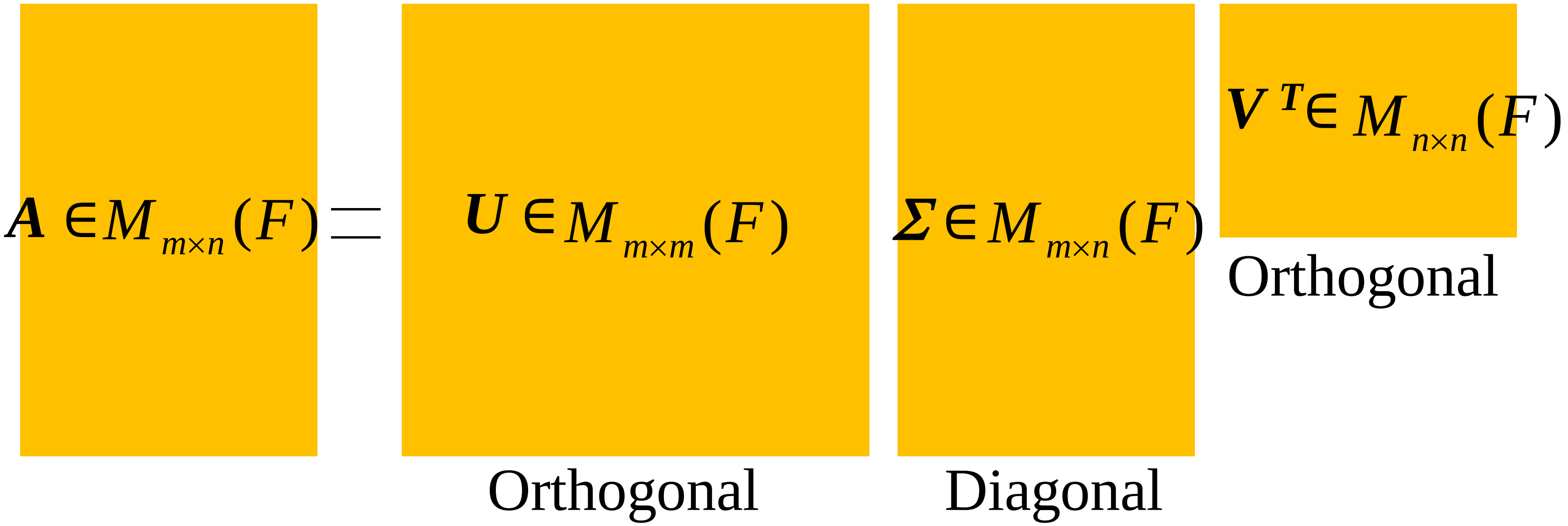
$\boldsymbol{A = QR =}$ $[\boldsymbol{Q_1}\ \ \boldsymbol{Q_2}]$ $\begin{bmatrix} \boldsymbol{R}_1 \\ 0 \end{bmatrix}$

$\boldsymbol{= Q_1 R_1 \rightarrow R_1 x = Q_1^T y}$

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.



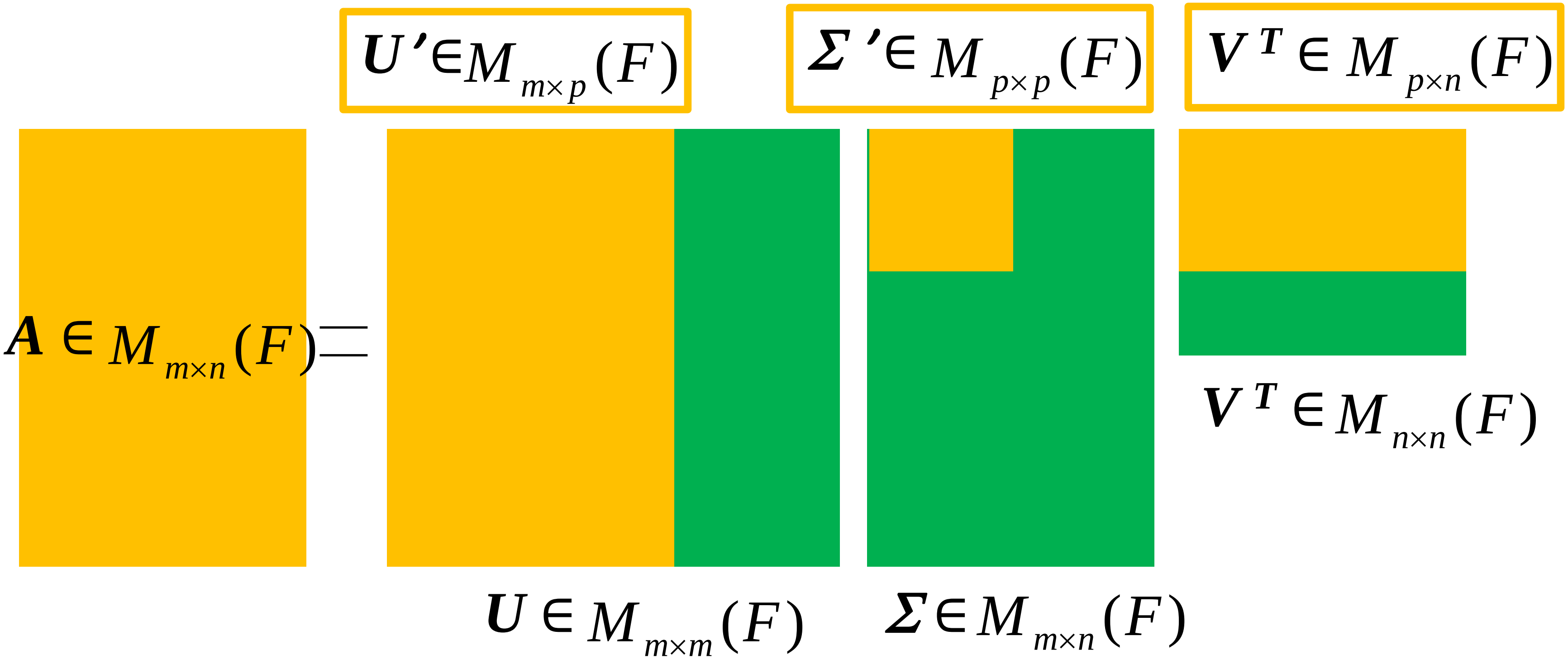
$\boldsymbol{A} \in M_{m \times n}(F) = \boldsymbol{U} \in M_{m \times m}(F) \ \boldsymbol{\Sigma} \in M_{m \times n}(F) \ \boldsymbol{V}^{\boldsymbol{T}} \in M_{n \times n}(F)$

Orthogonal

Diagonal

Orthogonal

Algorithm
Matrix decomposition (SVD)



$\boldsymbol{U'} \in M_{m\times p}(F)$

$\boldsymbol{\Sigma'} \in M_{p\times p}(F)$

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

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

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

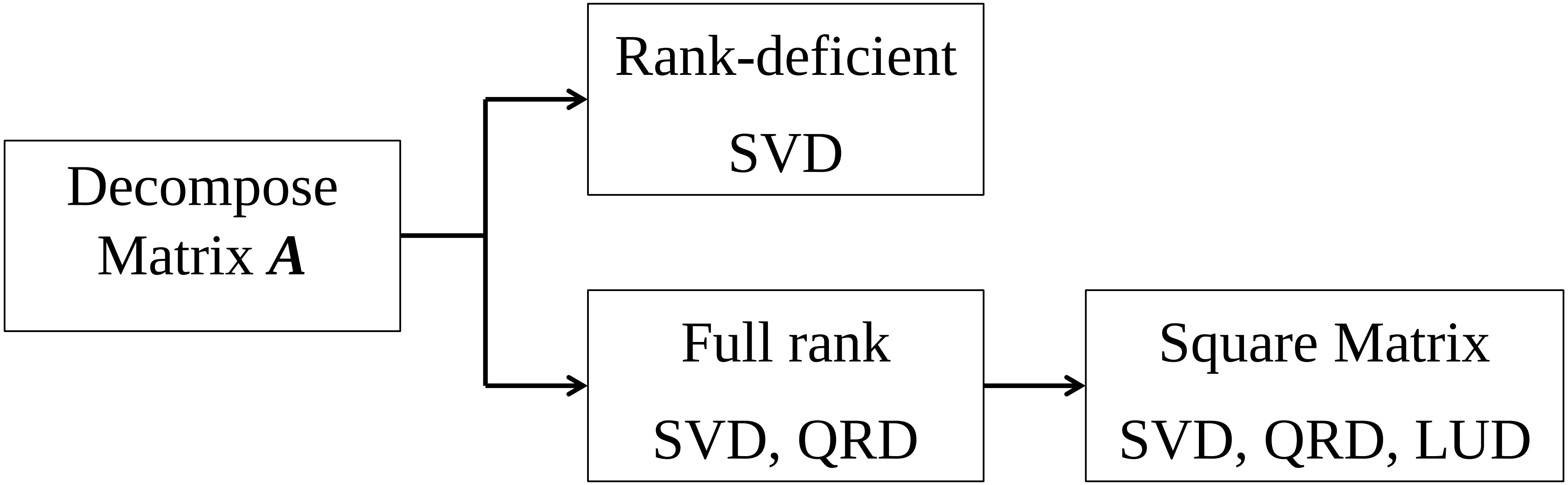
$\boldsymbol{U} \in M_{m\times m}(F)$

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

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

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

Algorithm
Matrix decomposition



Decompose Matrix ***A***

Rank-deficient

SVD

Full rank

SVD, QRD

Square Matrix

SVD, QRD, LUD

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