

Numerical methods for Surface Regression

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Methods for Surface Regression

- For example, the 4th order surface

$$f(x, y) = a_0 + a_1x + a_2y + a_3x^2 + a_4xy + a_5y^2 + a_6x^3 + a_7x^2y + a_8xy^2 + a_9y^3 \\ + a_{10}x^4 + a_{11}x^3y + a_{12}x^2y^2 + a_{13}xy^3 + a_{14}y^4$$

- Here x , y are independent variables
- This problem can be solved by 3 methods:
 1. Spline
 - a. Thin Plate Spline approximation
 - b. Multilevel B-Spline approximation
 - 2. Least-square approximation**

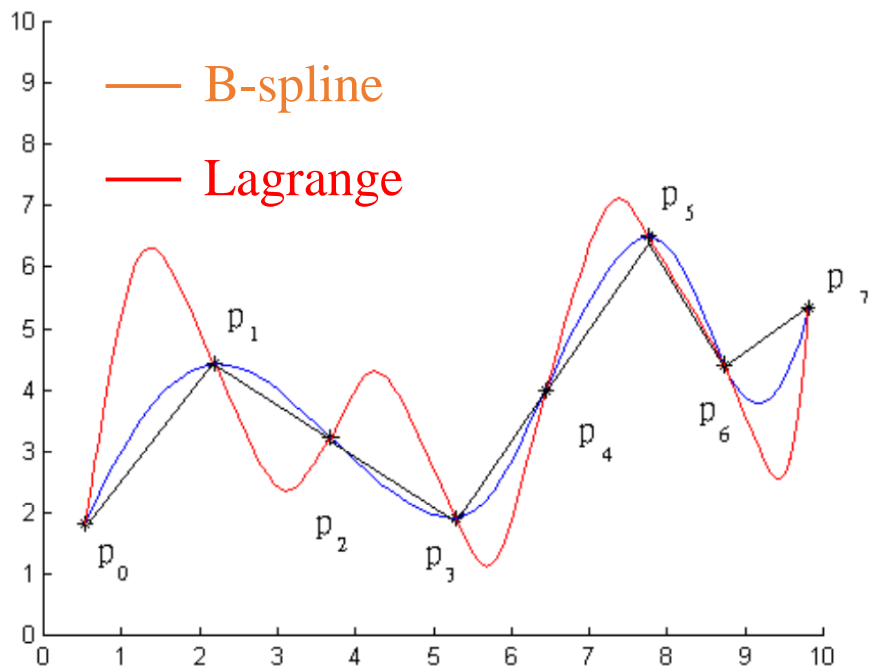
Methods for Monitoring CD Signatures

Concept for B-Spline

- For n distinct points, there exists a polynomial f with $\deg(f) = n - 1$ uniquely

$$f(x) = a_0 + a_1x^1 + a_2x^2 + \dots + a_nx^n$$

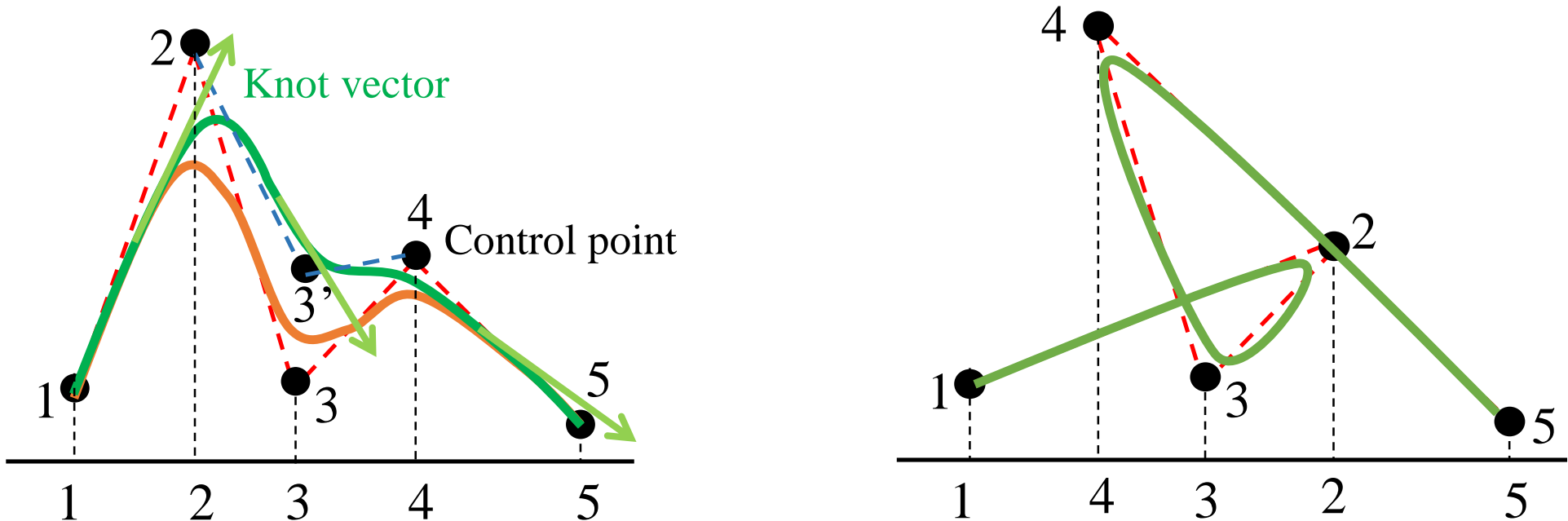
- But sometimes we want to use lower order polynomial to interpolate, or just n distinct points, but wants to use f with $\deg(f) = n+1$



Methods for Monitoring CD Signatures

Concept for B-Spline

Then we can add some constraints like $f'(x)$, $f''(x)$ to determine the curve uniquely. For continuity and piecewise, $f''(x)$ is also differentiable. In B-spline, the points are called **control points**, and $f'(x)$ are called the **knot vectors**. Suppose there are n distinct points, and m knot vectors, the $deg(f) = n + m - 1$



Methods for Monitoring CD Signatures

Concept for Least-Square

- Some of our spec are polynomial now, eg:
- I call the curve regression.

■ **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 $error_i = y_i - y$

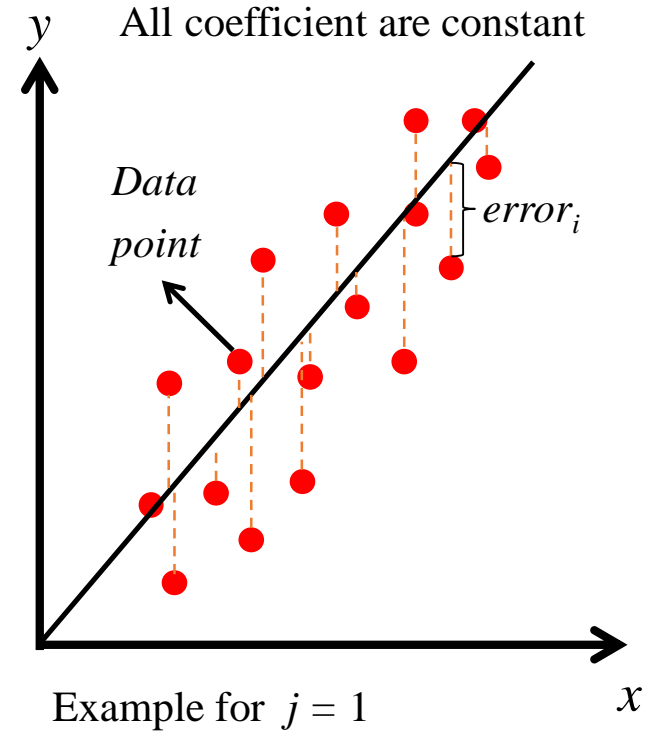
■ Total error $E = \sum_{i=1}^n (y_i - y)^2$

■ **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



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) , $i = 1, 2, \dots, n$, then, we have n group of linear equations system

$$\begin{cases} y_1 = bx_1 + a \\ \vdots \\ y_n = bx_n + a \end{cases} \xrightarrow[\text{matrix representation}]{\text{Matrix}} \begin{matrix} \mathbf{Y} \\ \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \\ n \times 1 \end{matrix} = \begin{matrix} \mathbf{A} \\ \begin{bmatrix} x_1 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \\ n \times 2 \end{matrix} \begin{matrix} \mathbf{x} \\ \begin{bmatrix} b \\ a \end{bmatrix} \\ 2 \times 1 \end{matrix} \rightarrow \mathbf{Y} = \mathbf{A}\mathbf{x}$$

- 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 $A \in M_{m \times n}(F)$, $\mathbf{x} \in F^n$, $\mathbf{y} \in F^m$, $m \geq n$ then
$$\langle \mathbf{A}\mathbf{x}, \mathbf{y} \rangle_m = \langle \mathbf{x}, \mathbf{A}^T \mathbf{y} \rangle_n, \quad \langle, \rangle: \text{inner product}$$
- Lemma 2: Let $A \in M_{m \times n}(F)$, $\text{rank}(A) = \text{rank}(A^T A)$
- Corollary: Let $A \in M_{m \times n}(F)$ and $\text{rank}(A) = n$, then $A^T A$ is invertible

Derive the Mathematical Eq.

Existence and Uniqueness

Theorem of Least-square approximation:

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

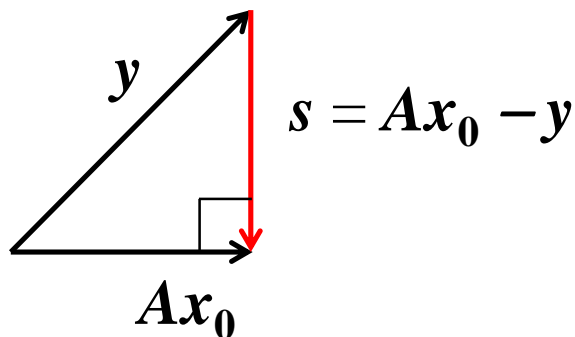
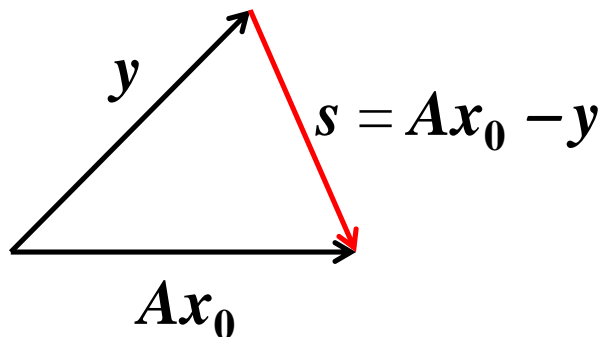
$$(A^T A) x_0 = A^T y \text{ and } \|Ax_0 - y\| \leq \|Ax - y\|, x \in F^n$$

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

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

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

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



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

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

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,

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



$$\underbrace{\begin{bmatrix} x_1 & \cdots & x_n \\ 1 & \cdots & 1 \end{bmatrix}^T}_{\mathbf{A}^T} \underbrace{\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}}_{\mathbf{Y}} = \underbrace{\begin{bmatrix} x_1 & \cdots & x_n \\ 1 & \cdots & 1 \end{bmatrix}^T}_{\mathbf{A}^T} \underbrace{\begin{bmatrix} x_1 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} b \\ a \end{bmatrix}}_{\mathbf{x}_0} \leftarrow \begin{bmatrix} \sum_{i=1}^n x_i y_i \\ \sum_{i=1}^n y_i \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^n x_i^2 & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & 1 \end{bmatrix} \begin{bmatrix} b \\ a \end{bmatrix}$$

- 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

$$CD(x, y) = a_0 + a_1x + a_2y + a_3x^2 + a_4xy + a_5y^2 + a_6x^3 + a_7x^2y + a_8xy^2 + a_9y^3 \\ + a_{10}x^4 + a_{11}x^3y + a_{12}x^2y^2 + a_{13}xy^3 + a_{14}y^4$$

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

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

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

$$\begin{matrix} \begin{bmatrix} CD_1 \\ \vdots \\ CD_n \end{bmatrix} \\ n \times 1 \end{matrix} = \begin{matrix} \begin{bmatrix} 1 & x_1 & \cdots & y_1^4 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & \cdots & y_n^4 \end{bmatrix} \\ n \times 15 \end{matrix} \begin{matrix} \begin{bmatrix} a_0 \\ \vdots \\ a_{14} \end{bmatrix} \\ 15 \times 1 \end{matrix}$$

So we complete the derivation.

Derive the Mathematical Eq. Extend to Surface Regression

- If some costumers want to use higher order , just extend the matrix and to calculate the new spec.
- For example, 2D, 6th order surface, there are 28 coefficients.

$$CD(x, y) = a_0 + a_1x + a_2y + \cdots + a_{27}y^6$$

$$\begin{array}{ccc} \left[\begin{array}{c} CD_1 \\ \vdots \\ CD_n \end{array} \right] & = & \left[\begin{array}{cccc} 1 & x_1 & \cdots & y_1^6 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & \cdots & y_n^6 \end{array} \right] \left[\begin{array}{c} a_0 \\ \vdots \\ a_{27} \end{array} \right] \\ n \times 1 & & n \times 28 \quad \quad 28 \times 1 \end{array}$$

Error and Stability Issues in Computation

- Computer **CANNOT** store all digits in memory, and the number will round automatically
- For example: $1/3 = 0.33333\dots = 0.\overline{3} \rightarrow$ **Infinity** digits in our brain
- In computer, the most digits computer can store is **finite**, so

$\frac{1}{3}$ in computer is 0.333333333333333333333333.....

finite digits

- $2/3$ in computer is 0.6666666666666666**7**666666666.....
- This error is called the **Rounding error**, it makes the algorithm unstable
- Because of the rounding error, as we times a number bigger than 1, the error is enlarged.

Algorithm Selecting

- Solve $(A^T A) x_0 = A^T y \rightarrow$ The worst method
- Solve $x_0 = (A^T A)^{-1} A^T y$ by getting $(A^T A)^{-1}$
 1. Gaussian elimination \rightarrow Backward unstable
 2. LU decomposition (LUD) \rightarrow More stable than the former

Easy to write

Less stable

- QR Decompose $A = QR = [Q_1 \ Q_2]$ $\begin{bmatrix} R_+ \\ 0 \end{bmatrix} Q_1 R_1 \rightarrow R_1 x = Q_1^T y$

(QRD)

1. Modified Gram-schmidt process
2. Givens Rotation
3. Householder transform \rightarrow **Candidate**

Highest CP value

**Matlab algorithm
for this problem**

$x = A \backslash Y$

- **SV Decomposition (SVD) $A = U \Sigma V^T$ \rightarrow **Candidate****

Most stable

Most expensive

Algorithm Selecting

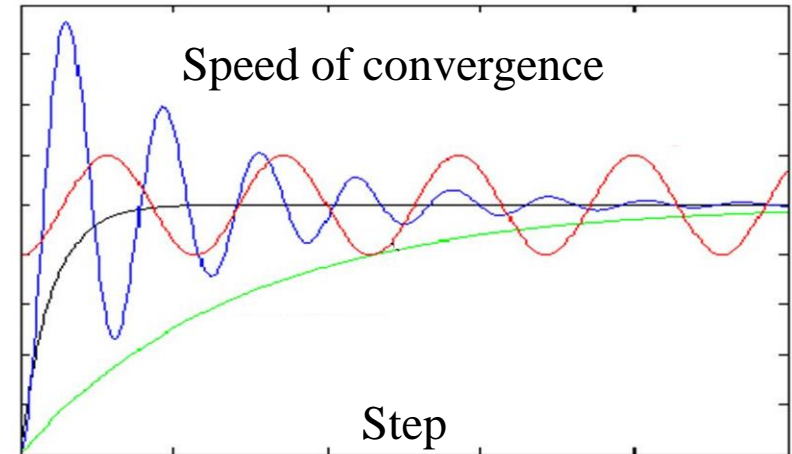
Criterion for selecting an algorithm

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



<http://slideplayer.com/slide/6029362/20/images/6/Damping+Summary.jpg>

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

Algorithm

Matrix decomposition (LUD)

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

B

In our situation, $\mathbf{B} \in M_{15 \times 15}(F)$

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

$$\begin{array}{l} \text{Do} \\ \text{3 times} \end{array} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \ell_{2,1} & 1 & 0 & 0 \\ \ell_{3,1} & \ell_{3,2} & 1 & 0 \\ \ell_{4,1} & \ell_{4,2} & \ell_{4,3} & 1 \end{bmatrix} \begin{bmatrix} u_{1,1} & u_{1,2} & u_{1,3} & u_{1,4} \\ 0 & u_{2,2} & u_{2,3} & u_{2,4} \\ 0 & 0 & u_{3,3} & u_{3,4} \\ 0 & 0 & 0 & u_{4,4} \end{bmatrix}$$

L

U

Algorithm

Matrix decomposition (LUD)

$$\bullet Bx_0 = A^T y \rightarrow L U x_0 = A^T y \rightarrow L(Ux_0) = L(c) = b, Ux_0 = c, A^T y = b$$

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

L : Lower triangular U : Upper triangular

$\underbrace{\hspace{10em}}_c$

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

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

Solving the linear eq.

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

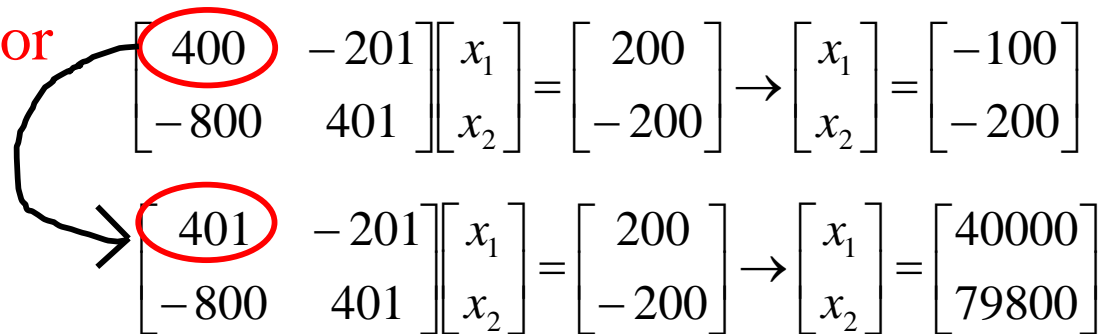
Algorithm

Matrix decomposition (QRD(Householder))

- Ill-condition

Numerical error
may cause

Mathematical
problem


$$\begin{bmatrix} 400 & -201 \\ -800 & 401 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 200 \\ -200 \end{bmatrix} \rightarrow \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -100 \\ -200 \end{bmatrix}$$
$$\begin{bmatrix} 401 & -201 \\ -800 & 401 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 200 \\ -200 \end{bmatrix} \rightarrow \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 40000 \\ 79800 \end{bmatrix}$$

- Although the result by PLUD is very close to Nanya's result, but we may encounter this problem, and the error may get larger when we calculate $\mathbf{B} = \mathbf{A}^T \mathbf{A}$. So I'll use QRD or SVD to solve this problem.

Algorithm

Matrix decomposition (QRD(Householder))

$$\begin{array}{ccc}
 \begin{array}{c} \xrightarrow{\text{column}} \\ A \in M_{m \times n}(F) \end{array} & \begin{array}{c} R_1 \in M_{m \times n}(F) \\ \xrightarrow{H_1 A} \end{array} & \begin{array}{c} R_2 \in M_{m \times n}(F) \\ \xrightarrow{H_2 R_1} \end{array} \\
 \begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,15} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,15} \\ a_{3,1} & a_{3,2} & \cdots & a_{2,15} \\ a_{4,1} & a_{4,2} & \cdots & a_{2,15} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,1} & a_{m,2} & \cdots & a_{m,15} \end{bmatrix} & \begin{bmatrix} r_{1,1} & r_{1,2} & \cdots & r_{1,15} \\ 0 & r_{2,2} & \cdots & r_{2,15} \\ 0 & r_{3,2} & \cdots & r_{2,15} \\ 0 & r_{4,2} & \cdots & r_{2,15} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & r_{m,2} & \cdots & r_{m,15} \end{bmatrix} & \begin{bmatrix} r_{1,1} & r_{1,2} & \cdots & r_{1,15} \\ 0 & r_{2,2}' & \cdots & r_{2,15}' \\ 0 & 0 & \cdots & r_{2,15}' \\ 0 & 0 & \cdots & r_{2,15}' \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{m,15}' \end{bmatrix} \\
 \begin{array}{c} u_1 \\ \|u_1\| = k_1 \\ v_1 = \frac{u_1 - ke_1}{\|u_1 - ke_1\|} \\ H_1 = I_m - 2v_1v_1^T \end{array} & \begin{array}{c} u_2 \\ \|u_2\| = k_2 \\ v_2 = \frac{u_2 - ke_2}{\|u_2 - ke_2\|} \\ H_2 = I_{m-1} - 2v_2v_2^T \end{array} & \begin{array}{c} \xrightarrow{H_3 R_2} \\ \text{End the process until} \\ \text{to the last row} \end{array}
 \end{array}$$

\uparrow Row

Algorithm

Matrix decomposition (QRD(Householder))

Q is orthogonal matrix $= (H_n \dots H_2 H_1)^T$

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

$$\begin{array}{c} m \\ \left\{ \begin{array}{c} \overbrace{\hspace{2cm}}^n \\ A \in M_{m \times n}(F) \end{array} \right\} = \begin{array}{|c|c|} \hline Q_1 \in M_{m \times n}(F) & Q_2 \in M_{m \times (m-n)}(F) \\ \hline \end{array} \times \begin{array}{|c|} \hline R_1 \in M_{n \times n}(F) \\ \hline R_2 = 0 \in M_{(m-n) \times m}(F) \\ \hline \end{array} \\
 \begin{array}{c} A = QR = \\ Q_1 R_1 \rightarrow R_1 x = Q_1^T y \end{array}
 \end{array}$$

Solving the linear eq.

Algorithm

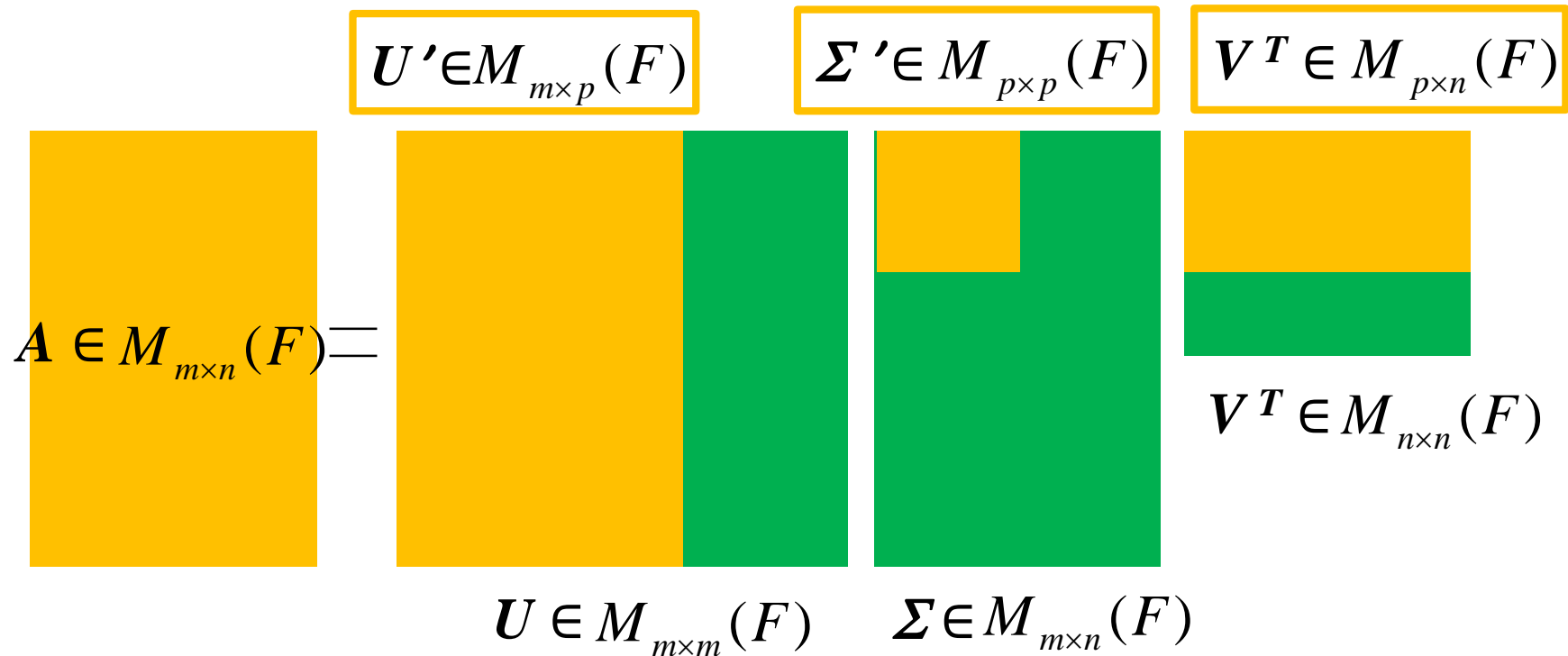
Matrix decomposition (SVD)

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

$$\begin{array}{ccccccc} & & & & & & V^T \in M_{n \times n}(F) \\ A \in M_{m \times n}(F) = & U \in M_{m \times m}(F) & \Sigma \in M_{m \times n}(F) & & & & \\ & \text{Orthogonal} & \text{Diagonal} & & & & \text{Orthogonal} \end{array}$$

Algorithm

Matrix decomposition (SVD)

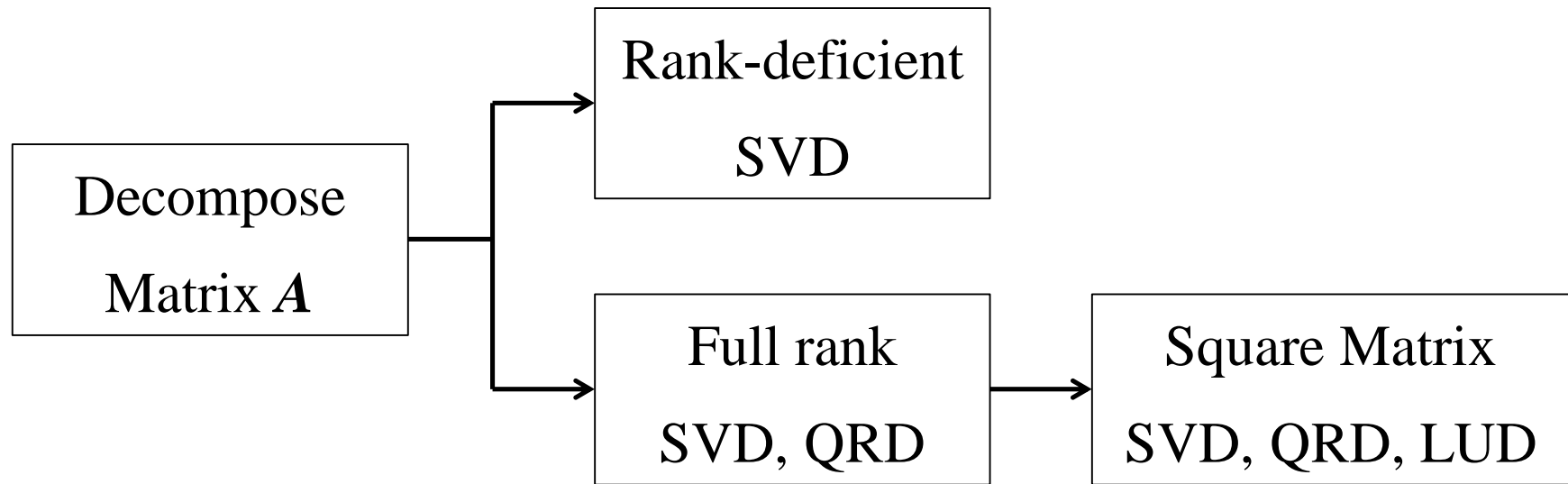


Only needs orange parts, it can reduce memory and time cost, but still costs much memory and time.

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

Algorithm

Matrix decomposition



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

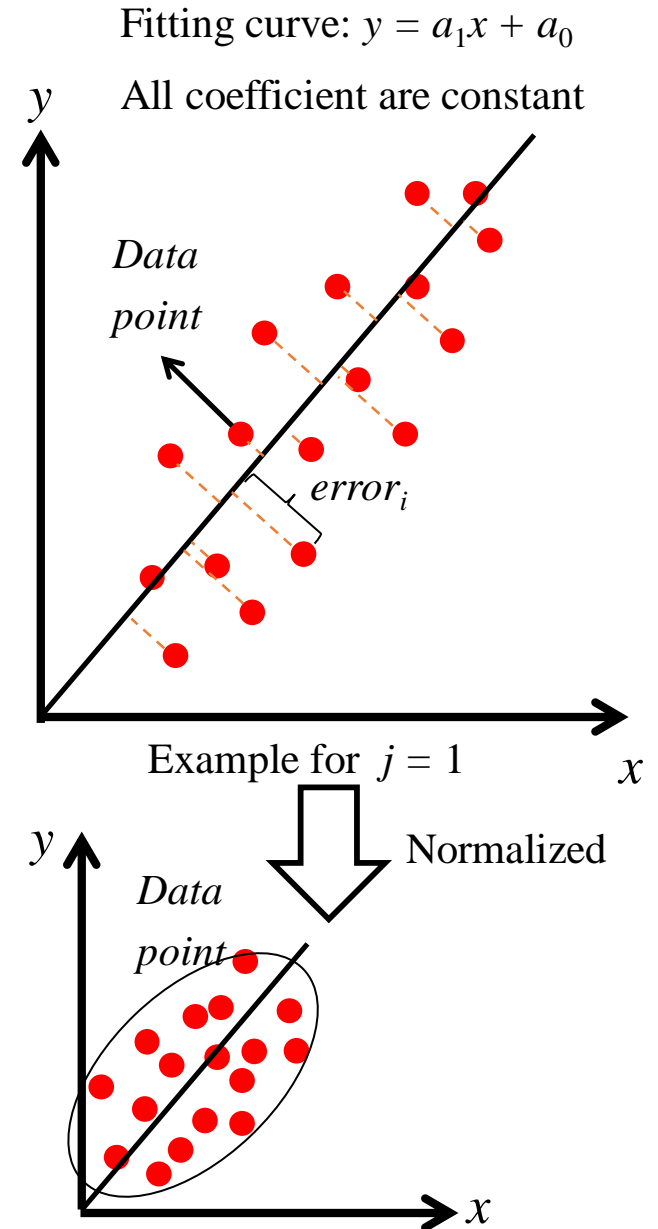
More about Regression

- Suppose the measurement data with noise

$$\eta = x + \delta, \delta \sim N(0, \sigma_\delta^2)$$

$$\xi = y + \zeta, \zeta \sim N(0, \sigma_\zeta^2)$$

- So we must redefine the errors as shown the figure on the right.
- After normalizing our data, the distribution on the 2D-plane is like an ellipse, the major axis is called the **Principle Component**, and the method is called **Principle Component Analysis (PCA)**.



More about Regression

- If many factors affect our CDU performance,

$$CD = \sum_{i=0}^n a_i x_i \quad n \geq 2 \quad 1 = \sum_{i=0}^n a_i$$

- Then we can use PCA and SVD algorithm to find the major factor.
- The key usage of the regression is **predicting** the result, less regression error, more accurate result.
- Suppose we have n data, now we add one more data in our model, then we must recalculate the coefficients to find the minimum error. The method is called **Machine Learning (ML)**.
- If we want to ask computer help us, the 1st step is derive the mathematical equation.