

Chapter 05 Linear Least-squares

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- Prerequisites
 - Matrix Differentiation
 - Lagrange Multiplier
 - Singular Value Decomposition
- Homography estimation—Modeled as a homogeneous linear LS problem
- Homography estimation—Modeled as an inhomogeneous linear LS problem
 - Problem Formulation
 - Method 1 (requires that A has a full column rank)
 - Method 2—A more general and accurate approach
- Summary of solvers for the linear LS problem



Function is a vector and the variable is a scalar

$$f(t) = [f_1(t), f_2(t), ..., f_n(t)]^T$$

Definition

$$\frac{d\mathbf{f}}{dt} = \left[\frac{df_1(t)}{dt}, \frac{df_2(t)}{dt}, \dots, \frac{df_n(t)}{dt}\right]^T$$



Function is a matrix and the variable is a scalar

$$\boldsymbol{F}(t) = \begin{bmatrix} f_{11}(t) & f_{12}(t), ..., f_{1m}(t) \\ f_{21}(t) & f_{22}(t), ..., f_{2m}(t) \\ \vdots & & \\ f_{n1}(t) & f_{n2}(t), ..., f_{nm}(t) \end{bmatrix} = \left[f_{ij}(t) \right]_{n \times m}$$

Definition

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$$\frac{dF}{dt} = \begin{bmatrix} \frac{df_{11}(t)}{dt} & \frac{df_{12}(t)}{dt}, ..., \frac{df_{1m}(t)}{dt} \\ \frac{df_{21}(t)}{dt} & \frac{df_{22}(t)}{dt}, ..., \frac{df_{2m}(t)}{dt} \\ \vdots & & \\ \frac{df_{n1}(t)}{dt} & \frac{df_{n2}(t)}{dt}, ..., \frac{df_{nm}(t)}{dt} \end{bmatrix} = \begin{bmatrix} \frac{df_{ij}(t)}{dt} \end{bmatrix}_{n \times m}$$



Function is a scalar and the variable is a vector

$$f(\mathbf{x}), \mathbf{x} = (x_1, x_2, ..., x_n)^T$$

Definition

$$\frac{df}{d\mathbf{x}} = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \dots, \frac{\partial f}{\partial x_n} \right]^T$$

In a similar way,

$$f(\mathbf{x}), \mathbf{x} = (x_1, x_2, ..., x_n)$$

$$\frac{df}{d\mathbf{x}} = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \dots, \frac{\partial f}{\partial x_n}\right]$$



Function is a vector and the variable is a vector

$$\mathbf{x} = [x_1, x_2, ..., x_n]^T, \mathbf{y} = [y_1(\mathbf{x}), y_2(\mathbf{x}), ..., y_m(\mathbf{x})]^T$$

Definition

$$\frac{d\mathbf{y}}{d\mathbf{x}^{T}} = \begin{bmatrix}
\frac{\partial y_{1}(\mathbf{x})}{\partial x_{1}}, \frac{\partial y_{1}(\mathbf{x})}{\partial x_{2}}, \dots, \frac{\partial y_{1}(\mathbf{x})}{\partial x_{n}} \\
\frac{\partial y_{2}(\mathbf{x})}{\partial x_{1}}, \frac{\partial y_{2}(\mathbf{x})}{\partial x_{2}}, \dots, \frac{\partial y_{2}(\mathbf{x})}{\partial x_{n}} \\
\vdots \\
\frac{\partial y_{m}(\mathbf{x})}{\partial x_{1}}, \frac{\partial y_{m}(\mathbf{x})}{\partial x_{2}}, \dots, \frac{\partial y_{m}(\mathbf{x})}{\partial x_{n}}
\end{bmatrix}_{\mathbf{m} \times \mathbf{n}}$$



Function is a vector and the variable is a vector

$$\mathbf{x} = [x_1, x_2, ..., x_n]^T$$
, $\mathbf{y} = [y_1(\mathbf{x}), y_2(\mathbf{x}), ..., y_m(\mathbf{x})]^T$
In a similar way,

$$\frac{d\mathbf{y}^{T}}{d\mathbf{x}} = \begin{bmatrix}
\frac{\partial y_{1}(\mathbf{x})}{\partial x_{1}}, \frac{\partial y_{2}(\mathbf{x})}{\partial x_{1}}, ..., \frac{\partial y_{m}(\mathbf{x})}{\partial x_{1}} \\
\frac{\partial y_{1}(\mathbf{x})}{\partial x_{2}}, \frac{\partial y_{2}(\mathbf{x})}{\partial x_{2}}, ..., \frac{\partial y_{m}(\mathbf{x})}{\partial x_{2}} \\
\vdots \\
\frac{\partial y_{1}(\mathbf{x})}{\partial x_{n}}, \frac{\partial y_{2}(\mathbf{x})}{\partial x_{n}}, ..., \frac{\partial y_{m}(\mathbf{x})}{\partial x_{n}}
\end{bmatrix}_{n \times m}$$



 Function is a vector and the variable is a vector Example:

$$\mathbf{y} = \begin{bmatrix} y_1(\mathbf{x}) \\ y_2(\mathbf{x}) \end{bmatrix}, \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}, y_1(\mathbf{x}) = x_1^2 - x_2, y_2(\mathbf{x}) = x_3^2 + 3x_2$$

$$\frac{d\mathbf{y}^{T}}{d\mathbf{x}} = \begin{bmatrix}
\frac{\partial y_{1}(\mathbf{x})}{\partial x_{1}} & \frac{\partial y_{2}(\mathbf{x})}{\partial x_{1}} \\
\frac{\partial y_{1}(\mathbf{x})}{\partial x_{2}} & \frac{\partial y_{2}(\mathbf{x})}{\partial x_{2}} \\
\frac{\partial y_{1}(\mathbf{x})}{\partial x_{3}} & \frac{\partial y_{2}(\mathbf{x})}{\partial x_{3}}
\end{bmatrix} = \begin{bmatrix}
2x_{1} & 0 \\
-1 & 3 \\
0 & 2x_{3}
\end{bmatrix}$$



Function is a scalar and the variable is a matrix

$$f(X), X \in \mathbb{R}^{m \times n}$$

Definition

$$\frac{df(X)}{dX} = \begin{bmatrix}
\frac{\partial f}{\partial x_{11}} & \frac{\partial f}{\partial x_{12}} & \cdots & \frac{\partial f}{\partial x_{1n}} \\
\cdots & & \\
\frac{\partial f}{\partial x_{m1}} & \frac{\partial f}{\partial x_{m2}} & \cdots & \frac{\partial f}{\partial x_{mn}}
\end{bmatrix}$$



• Useful results

Then,
$$x, a \in \mathbb{R}^{n \times 1}$$

$$\frac{da^T x}{dx} = a, \frac{dx^T a}{dx} = a$$
 How to prove?



Useful results

(2)
$$x \in \mathbb{R}^{n \times 1}$$
 Then, $\frac{dx^T x}{dx} = 2x$

(3)
$$y(x) \in \mathbb{R}^{m \times 1}$$
, $x \in \mathbb{R}^{n \times 1}$, $\frac{dy^{T}(x)}{dx} = \left(\frac{dy(x)}{dx^{T}}\right)^{T}$

(4)
$$A \in \mathbb{R}^{m \times n}, x \in \mathbb{R}^{n \times 1}$$
 Then, $\frac{dAx}{dx^T} = A$

(5)
$$A \in \mathbb{R}^{m \times n}, x \in \mathbb{R}^{n \times 1}$$
 Then, $\frac{dx^T A^T}{dx} = A^T$

(6)
$$A \in \mathbb{R}^{n \times n}, x \in \mathbb{R}^{n \times 1}$$
 Then, $\frac{dx^T Ax}{dx} = (A + A^T)x$

(7)
$$X \in \mathbb{R}^{m \times n}, a \in \mathbb{R}^{m \times 1}, b \in \mathbb{R}^{n \times 1}$$
 Then, $\frac{da^T X b}{dX} = ab^T$



Useful results

(8)
$$X \in \mathbb{R}^{n \times m}, \boldsymbol{a} \in \mathbb{R}^{m \times 1}, \boldsymbol{b} \in \mathbb{R}^{n \times 1}$$
 Then, $\frac{d\boldsymbol{a}^T \boldsymbol{X}^T \boldsymbol{b}}{d\boldsymbol{X}} = \boldsymbol{b} \boldsymbol{a}^T$

(9)
$$X \in \mathbb{R}^{m \times n}$$
, $B \in \mathbb{R}^{n \times m}$ Then, $\frac{d(tr(XB))}{dX} = B^T$

(10)
$$X \in \mathbb{R}^{n \times n}$$
, X is invertible, $\frac{d|X|}{dX} = |X|(X^{-1})^T$



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Single-variable function

f(x) is differentiable in (a, b). At $x_0 \in (a, b)$, f(x) achieves an extremum

$$\longrightarrow \frac{df}{dx}\big|_{x_0} = 0$$

Two-variables function

f(x, y) is differentiable in its domain. At (x_0, y_0) , f(x, y) achieves an extremum

$$\longrightarrow \frac{\partial f}{\partial x}|_{(x_0,y_0)} = 0, \frac{\partial f}{\partial y}|_{(x_0,y_0)} = 0$$



In general case

If f(x), $x \in \mathbb{R}^{n \times 1}$ achieves a local extremum at x_0 and it is derivable at x_0 , then x_0 is a stationary point of f(x), i.g.,

$$\frac{\partial f}{\partial x_1}\big|_{x_0} = 0, \frac{\partial f}{\partial x_2}\big|_{x_0} = 0, \dots, \frac{\partial f}{\partial x_n}\big|_{x_0} = 0$$

Or in other words,

$$\left. \nabla f(\mathbf{x}) \right|_{\mathbf{x} = \mathbf{x}_0} = \mathbf{0}$$



• Lagrange multiplier is a strategy for finding all the possible extremum points of a function subject to equality constraints

Problem: find all the possible extremum points for $y = f(x), x \in \mathbb{R}^{n \times 1}$

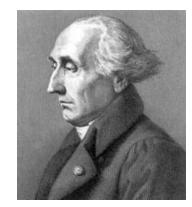
under
$$m$$
 constraints $g_k(x) = 0, k = 1, 2, ..., m$

Solution:
$$F(\mathbf{x}; \lambda_1, ..., \lambda_m) = f(\mathbf{x}) + \sum_{k=1}^m \lambda_k g_k(\mathbf{x})$$

If x_0 is an extremum point of f(x) under constraints

$$\exists \lambda_{10}, \lambda_{20}..., \lambda_{m0}, \text{ making } (\mathbf{x}_0, \lambda_{10}, \lambda_{20}..., \lambda_{m0})$$
 a stationary point of F

Thus, by identifying the stationary points of F, we can get all the possible extremum points of f(x) under equality constraints



Joseph-Louis Lagrange Jan. 25, 1736~Apr.10, 1813



 Lagrange multiplier is a strategy for finding all the possible extremum points of a function subject to equality constraints

Problem: find all the possible extremum points for $y = f(x), x \in \mathbb{R}^{n \times 1}$

under *m* constraints
$$g_k(\mathbf{x}) = 0, k = 1, 2, ..., m$$

Solution:
$$F(\mathbf{x}; \lambda_1, ..., \lambda_m) = f(\mathbf{x}) + \sum_{k=1}^m \lambda_k g_k(\mathbf{x})$$

$$(\mathbf{x}_0, \lambda_{10}, ..., \lambda_{m0})$$
 is a stationary point of F

$$\frac{\partial F}{\partial x_1} = 0, \frac{\partial F}{\partial x_2} = 0, \dots, \frac{\partial F}{\partial x_n} = 0, \frac{\partial F}{\partial \lambda_1} = 0, \frac{\partial F}{\partial \lambda_2} = 0, \dots, \frac{\partial F}{\partial \lambda_m} = 0$$

at that point

n + m equations!

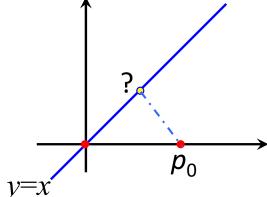
 x_0 is a possible extremum point of f(x) under equality constraints



Example

Problem: for a given point $p_0 = (1, 0)$, among all the points lying on the line y=x, identify the one having the least

distance to p_0 .



The distance is

$$f(x,y) = (x-1)^2 + (y-0)^2$$

Now we want to find the global minimizer of f(x, y) under the constraint

$$g(x,y) = y - x = 0$$

According to Lagrange multiplier method, construct the Lagrange function

$$F(x, y, \lambda) = f(x, y) + \lambda g(x, y) = (x-1)^{2} + y^{2} + \lambda (y-x)$$

Find the stationary point of $F(x, y, \lambda)$



• Example
$$\begin{cases} \frac{\partial F}{\partial x} = 0 \\ \frac{\partial F}{\partial y} = 0 \end{cases} \Rightarrow \begin{cases} 2(x-1) + \lambda = 0 \\ 2y - \lambda = 0 \\ x - y = 0 \end{cases} \end{cases} \begin{cases} x = 0.5 \\ y = 0.5 \\ \lambda = 1 \end{cases}$$

Thus, (0.5, 0.5, 1) is the only stationary point of $F(x, y, \lambda)$

(0.5,0.5) is the only possible extremum point of f(x,y)under constraints

The global minimizer of f(x,y)under constraints exists

(0.5,0.5) is the global minimizer of f(x,y) under constraints



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Singular Value Decomposition (SVD)

SVD decomposition theorem: Any matrix $A_{m \times n}$ can be decomposed as the following form,

$$\boldsymbol{A}_{m \times n} = \boldsymbol{U}_{m \times m} \boldsymbol{\Sigma}_{m \times n} \boldsymbol{V}_{n \times n}^{T}$$

where *U* and *V* are two orthogonal matrices, rank(A) = r,

$$\sum_{m \times n} = \begin{bmatrix} \sum_{r} & \boldsymbol{O}_{r \times (n-r)} \\ \boldsymbol{O}_{(m-r) \times r} & \boldsymbol{O}_{(m-r) \times (n-r)} \end{bmatrix}_{m \times n} = \begin{bmatrix} \boldsymbol{\sigma}_{1} \\ \boldsymbol{\sigma}_{2} \\ \vdots \\ \boldsymbol{\sigma}_{r} \end{bmatrix} \qquad \boldsymbol{O}_{r \times (n-r)} \\ \boldsymbol{O}_{(m-r) \times r} & \boldsymbol{O}_{(m-r) \times (n-r)} \end{bmatrix}_{m \times n}$$

 $\sigma_1, \sigma_2, ..., \sigma_r > 0$ are called the **singular values** of A

In general case, $\sum_{m \times n}$ is not unique. However, if $\{\sigma_i\}_{i=1}^r$ are arranged in order, $\sum_{m \times n}$ is uniquely determined by A. In the following, we require that $\sigma_1 \ge \sigma_2 \ge ,..., \ge \sigma_r > 0$



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Suppose that by matching keypoints on I_1 and I_2 , we get $S = \{x_i \leftrightarrow x_i^{'}\}_{i=1}^{p}$

where $x_i \leftrightarrow x_i'$ means that the point x_i from I_1 and the point x_i' from I_2 matches, and p is the number of correspondence pairs

temporarily suppose there is no outliers in ${\cal S}$

All the pairs can be linked via a universal 2D linear geometric transformation $H_{3\times3}$

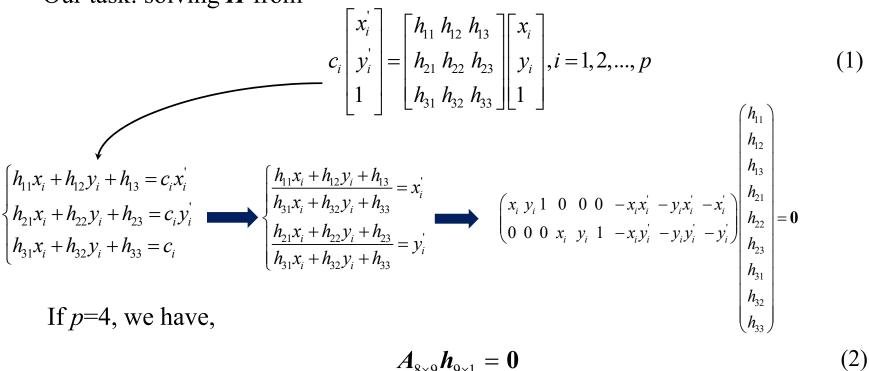
If there is no prior knowledge about the geometric transformation between I_1 and I_2

H can take the most general form, the 2D projective transformation,

$$\forall \boldsymbol{x}_{i} \leftrightarrow \boldsymbol{x}_{i}' \in \mathcal{S}, \quad c_{i} \boldsymbol{x}_{i}' = \boldsymbol{H}_{3\times 3} \boldsymbol{x}_{i}$$



Our task: solving *H* from



$$A_{8\times9}h_{9\times1}=\mathbf{0} \tag{2}$$

Normally, rank(A)=8; thus (2) has 1 linear independent solution vector in its solution space

4 correspondence pairs can uniquely determine a 2D projective transformation (Homography)



Our task: solving *H* from

$$c_{i}\begin{bmatrix}x_{i}\\y_{i}\\1\end{bmatrix} = \begin{bmatrix}h_{11} & h_{12} & h_{13}\\h_{21} & h_{22} & h_{23}\\h_{31} & h_{32} & h_{33}\end{bmatrix}\begin{bmatrix}x_{i}\\y_{i}\\1\end{bmatrix}, i = 1, 2, ..., p$$

$$\begin{cases}h_{11}x_{i} + h_{12}y_{i} + h_{13} = c_{i}x_{i}\\h_{21}x_{i} + h_{22}y_{i} + h_{23} = c_{i}y_{i}\\h_{31}x_{i} + h_{32}y_{i} + h_{33} = c_{i}\end{cases}$$

$$\begin{cases}h_{11}x_{i} + h_{12}y_{i} + h_{13}\\h_{21}x_{i} + h_{22}y_{i} + h_{23}\\h_{31}x_{i} + h_{32}y_{i} + h_{33}\\h_{31}x_{i} + h_{32}y_{i} + h_{33}\\h_{32}h_{33}\\h_{34}\\h_{35}\\h_$$

Normally, rank(A)=8; thus (2) has 1 linear independent solution vector in its solution space

However, in most cases p>4





$$A_{2p\times 9}h_{9\times 1}=0, p>4$$
 (3)

Normally, rank(A)=9; thus (3) **only has a zero solution**, which is of no use for us!

- Notice two facts
 - What we want is a non-zero solution h^* that can roughly satisfy Eq. (3)
 - h^* actually represents a projective transformation; and $\forall k \neq 0, kh^*$ represents the same projective transformation with h^* . Without loss of generality, we can require that $\|h^*\|_2^2 = 1$



Thus, our problem can be formulated as,

$$h^* = \underset{h}{\operatorname{arg min}} \|Ah\|_{2}^{2}$$
, subject to $\|h\|_{2}^{2} = 1$, $A \in \mathbb{R}^{2p \times 9}$, $h \in \mathbb{R}^{9 \times 1}$, $rank(A) = 9$

A more general form (the homogeneous linear least-squares problem),

$$\boldsymbol{x}^* = \arg\min_{\boldsymbol{x}} \|\boldsymbol{A}\boldsymbol{x}\|_2^2, \text{ subject to } \|\boldsymbol{x}\|_2^2 = 1, \boldsymbol{A} \in \mathbb{R}^{m \times n}, \boldsymbol{x} \in \mathbb{R}^{n \times 1}, rank(\boldsymbol{A}) = n$$
 (4)

→ Let's solve it!



Construct the Lagrange function,

$$L(\mathbf{x},\lambda) = \|\mathbf{A}\mathbf{x}\|_{2}^{2} + \lambda \left(1 - \|\mathbf{x}\|_{2}^{2}\right)$$

Solving the stationary points of $L(x, \lambda)$. (x_0, λ_0) is a stationary of $L(x, \lambda)$, if only if,

$$\begin{cases}
\frac{\partial L}{\partial x}\big|_{\mathbf{x}=\mathbf{x}_{0},\lambda=\lambda_{0}} = \mathbf{0} \\
\frac{\partial L}{\partial \lambda}\big|_{\mathbf{x}=\mathbf{x}_{0},\lambda=\lambda_{0}} = 0
\end{cases}
\Rightarrow
\begin{cases}
\frac{\partial \left(\mathbf{x}^{T}A^{T}A\mathbf{x} + \lambda\left(1-\mathbf{x}^{T}\mathbf{x}\right)\right)}{\partial \mathbf{x}}\big|_{\mathbf{x}=\mathbf{x}_{0},\lambda=\lambda_{0}} = \mathbf{0} \\
\frac{\partial \left(\mathbf{x}^{T}A^{T}A\mathbf{x} + \lambda\left(1-\mathbf{x}^{T}\mathbf{x}\right)\right)}{\partial \lambda}\big|_{\mathbf{x}=\mathbf{x}_{0},\lambda=\lambda_{0}} = 0
\end{cases}
\Rightarrow
\begin{cases}
A^{T}A\mathbf{x}_{0} = \lambda_{0}\mathbf{x}_{0} \\
\mathbf{x}_{0}^{T}\mathbf{x}_{0} = 1
\end{cases}$$
Note: the stationary point of $L(\mathbf{x},\lambda)$ is not unique

Suppose that (x_i, λ_i) is a stationary point of $L(x, \lambda)$, then x_i is a possible extremum point of $f(x) = ||Ax||_2^2$ under the equality constraint and we have,

$$f(\mathbf{x}_i) = ||A\mathbf{x}_i||_2^2 = \mathbf{x}_i^T A^T A \mathbf{x}_i = \mathbf{x}_i^T \lambda_i \mathbf{x}_i = \lambda_i$$

Thus, the minimum of f(x) (under the equality constraint) is $\min \{\lambda_i\}_{i=1}^n$, that is, the least eigenvalue of A^TA . And the minimizer of f(x) is the unit eigen-vector of A^TA associated with its least eigen value



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We know that a 3×3 matrix \boldsymbol{H} , representing a valid 2D projective transform, has 8 DoF. Thus, when optimizing a 9d vector representing a projective transform, we need to constrain its DoF to 8. When the problem is modeled as a homogeneous linear LS problem, such a goal is achieved by imposing a constraint $\|\boldsymbol{h}\|_2^2 = 1$

In practical applications, another method can be used to constrain the DoF of \boldsymbol{H} to 8, that is by fixing an element of \boldsymbol{H} to a non-zero constant (such an element in the ground-truth \boldsymbol{H} should be non-zero). Usually, we can fix $h_{33}=1$



Our task: solving *H* from

$$c_{i} \begin{bmatrix} x'_{i} \\ y'_{i} \\ 1 \end{bmatrix} = \begin{bmatrix} h_{11} & h_{12} & h_{13} \\ h_{21} & h_{22} & h_{23} \\ h_{31} & h_{32} & h_{33} \end{bmatrix} \begin{bmatrix} x_{i} \\ y_{i} \\ 1 \end{bmatrix}, i = 1, 2, ..., p$$
(1)
fixed to 1



$$\frac{c_{i} \begin{bmatrix} x_{i} \\ y_{i} \\ 1 \end{bmatrix} = \begin{bmatrix} h_{11} & h_{12} & h_{13} \\ h_{21} & h_{22} & h_{23} \\ h_{31} & h_{32} & 1 \end{bmatrix} \begin{bmatrix} x_{i} \\ y_{i} \\ 1 \end{bmatrix}, i = 1, 2, ..., p$$

$$\begin{cases} h_{11}x_{i} + h_{12}y_{i} + h_{13} = c_{i}x_{i}' \\ h_{21}x_{i} + h_{22}y_{i} + h_{23} = c_{i}y_{i}' \\ h_{31}x_{i} + h_{32}y_{i} + 1 = c_{i} \end{cases}$$

$$\begin{cases} h_{11}x_{i} + h_{12}y_{i} + h_{13} = x_{i}' \\ h_{31}x_{i} + h_{32}y_{i} + 1 = y_{i}' \end{cases}$$

$$\begin{cases} x_{i} & y_{i} & 1 & 0 & 0 & 0 & -x_{i}x_{i}' - y_{i}x_{i}' \\ 0 & 0 & 0 & x_{i} & y_{i} & 1 & -x_{i}y_{i}' - y_{i}y_{i}' \\ h_{22} \\ h_{23} \\ h_{31} \\ h_{31} \\ h_{32} \end{cases}$$

$$\begin{cases} x_{i} & y_{i} & 1 & 0 & 0 & 0 & -x_{i}x_{i}' - y_{i}x_{i}' \\ 0 & 0 & 0 & x_{i} & y_{i} & 1 & -x_{i}y_{i}' - y_{i}y_{i}' \\ h_{22} \\ h_{23} \\ h_{31} \\ h_{32} \\ \end{cases}$$

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$$\begin{cases} x_{i} & y_{i} & 1 & 0 & 0 & 0 & -x_{i}x_{i}' - y_{i}x_{i}' \\ h_{22} \\ h_{23} \\ h_{31} \\ h_{32} \\ \end{cases}$$

If p=4, we have,

$$\boldsymbol{A}_{8\times8}\boldsymbol{h}_{8\times1}=\boldsymbol{b}_{8\times1} \tag{6}$$

Normally, rank(A) = rank([A; b]) = 8; thus (6) has 1 unique solution

4 correspondence pairs can uniquely determine a 2D projective transformation (Homography)



$$\frac{c_{i} \begin{bmatrix} x_{i} \\ y_{i} \\ 1 \end{bmatrix} = \begin{bmatrix} h_{11} & h_{12} & h_{13} \\ h_{21} & h_{22} & h_{23} \\ h_{31} & h_{32} & 1 \end{bmatrix} \begin{bmatrix} x_{i} \\ y_{i} \\ 1 \end{bmatrix}, i = 1, 2, ..., p$$

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$$\begin{cases} h_{11}x_{i} + h_{12}y_{i} + h_{13} = x_{i}' \\ h_{31}x_{i} + h_{32}y_{i} + 1 = y_{i}' \end{cases}$$

$$\begin{cases} x_{i} & y_{i} & 1 & 0 & 0 & 0 & -x_{i}x_{i}' - y_{i}x_{i}' \\ 0 & 0 & 0 & x_{i} & y_{i} & 1 & -x_{i}y_{i}' - y_{i}y_{i}' \\ h_{22} \\ h_{23} \\ h_{31} \\ h_{31} \\ h_{32} \end{cases}$$

$$\begin{cases} x_{i} & y_{i} & 1 & 0 & 0 & 0 & -x_{i}x_{i}' - y_{i}x_{i}' \\ 0 & 0 & 0 & x_{i} & y_{i} & 1 & -x_{i}y_{i}' - y_{i}y_{i}' \\ h_{22} \\ h_{23} \\ h_{31} \\ h_{32} \\ \end{cases}$$

$$\begin{cases} x_{i} & y_{i} & 1 & 0 & 0 & 0 & -x_{i}x_{i}' - y_{i}x_{i}' \\ 0 & 0 & 0 & x_{i} & y_{i} & 1 & -x_{i}y_{i}' - y_{i}y_{i}' \\ h_{22} \\ h_{23} \\ h_{31} \\ h_{32} \\ \end{cases}$$

$$\begin{cases} x_{i} & y_{i} & 1 & 0 & 0 & 0 & -x_{i}x_{i}' - y_{i}x_{i}' \\ h_{22} \\ h_{23} \\ h_{31} \\ h_{32} \\ \end{cases}$$

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However, in most cases p>4





$$A_{2p\times 8}h_{8\times 1} = b_{2p\times 1}, p > 4 \tag{7}$$

Normally, rank(A) = 8, rank([A; b]) = 9, $rank(A) \neq rank([A; b])$, and thus Eq. 7 does not have a solution!

We want a solution that can *roughly* satisfy Eq. 7



Thus, our problem can be formulated as,

$$h^* = \underset{h}{\operatorname{arg min}} ||Ah - b||_2^2, A \in \mathbb{R}^{2p \times 8}, h \in \mathbb{R}^{8 \times 1}, b \neq 0 \in \mathbb{R}^{2p \times 1}$$

where rank(A)=8

A more general form (the inhomogeneous linear least-squares problem),

$$\boldsymbol{x}^* = \underset{\boldsymbol{x}}{\operatorname{arg\,min}} \left\| \boldsymbol{A} \boldsymbol{x} - \boldsymbol{b} \right\|_2^2, \boldsymbol{A} \in \mathbb{R}^{m \times n}, \boldsymbol{x} \in \mathbb{R}^{n \times 1}, \boldsymbol{b} \neq \boldsymbol{0} \in \mathbb{R}^{m \times 1}, rank(\boldsymbol{A}) = n$$
 (8)

→ Let's solve it!



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Method 1 (requires that A has a full column rank)

$$\boldsymbol{x}^* = \underset{\boldsymbol{x}}{\operatorname{arg\,min}} \left\| \boldsymbol{A} \boldsymbol{x} - \boldsymbol{b} \right\|_2^2, \boldsymbol{A} \in \mathbb{R}^{m \times n}, \boldsymbol{x} \in \mathbb{R}^{n \times 1}, \boldsymbol{b} \neq \boldsymbol{0} \in \mathbb{R}^{m \times 1}, rank(\boldsymbol{A}) = n$$
 (8)

Exercise

Please prove that the objective function in (8),

$$f(\mathbf{x}) = ||\mathbf{A}\mathbf{x} - \mathbf{b}||_{2}^{2}, \mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{x} \in \mathbb{R}^{n \times 1}, \mathbf{b} \neq \mathbf{0} \in \mathbb{R}^{m \times 1}$$

is a convex function

The stationary point of the objective function f(x) is $x_s = (A^T A)^{-1} A^T b$

Since f(x) is convex

$$\boldsymbol{x}^* = \boldsymbol{x}_s = \left(\boldsymbol{A}^T \boldsymbol{A}\right)^{-1} \boldsymbol{A}^T \boldsymbol{b} \tag{9}$$

(For a convex function, its stationary point is the global minimizer^[1]. We will discuss more about the convex optimization in Chapter 13)

[1] S. Boyd and L. Vandenberghe, Convex Optimization, Cambridge University Press, 2004, pp. 69



Method 1 (requires that A has a full column rank)

$$\boldsymbol{x}^* = \underset{\boldsymbol{x}}{\operatorname{arg\,min}} \left\| \boldsymbol{A} \boldsymbol{x} - \boldsymbol{b} \right\|_2^2, \boldsymbol{A} \in \mathbb{R}^{m \times n}, \boldsymbol{x} \in \mathbb{R}^{n \times 1}, \boldsymbol{b} \neq \boldsymbol{0} \in \mathbb{R}^{m \times 1}, rank(\boldsymbol{A}) = n$$
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nvex $\mathbf{x}^* = \mathbf{x}_{s} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{b}$

Is it really invertible?

(9)

Assignment

For the matrix $A \in \mathbb{R}^{m \times n}$, if rank(A) = n, A^TA should be invertible

The "method 1" requires that A has a full column rank. Next, we will learn a more general and accurate method to solve the inhomogeneous linear LS problem



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- For solving the linear least squares numerically with a computer, usually we do not use the form of Eq. (9) (though it is elegant) for two reasons
 - When $rank(A) < n, x^*$ can not be determined
 - Even though A^TA is invertible, the formation of A^TA can dramatically degrade the accuracy of the computation
- Instead, we can use the technique of SVD

Our problem,

$$\boldsymbol{x}^* = \underset{\boldsymbol{x}}{\operatorname{arg\,min}} \left\| \boldsymbol{A} \boldsymbol{x} - \boldsymbol{b} \right\|_2^2, \boldsymbol{A} \in \mathbb{R}^{m \times n}, \boldsymbol{x} \in \mathbb{R}^{n \times 1}, \boldsymbol{b} \neq \boldsymbol{0} \in \mathbb{R}^{m \times 1}$$
 (10)

Note that this problem is more general than Eq. 8 since its does not have additional requirements on the rank of $\cal A$



Suppose the SVD form of *A* is,

$$\boldsymbol{A}_{m \times n} = \boldsymbol{U}_{m \times m} \boldsymbol{\Sigma}_{m \times n} \boldsymbol{V}_{n \times n}^{T}$$



$$\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{T}\boldsymbol{x} - \boldsymbol{b} = \boldsymbol{U}\left(\boldsymbol{\Sigma}\boldsymbol{V}^{T}\boldsymbol{x}\right) - \boldsymbol{U}\left(\boldsymbol{U}^{T}\boldsymbol{b}\right) \triangleq \boldsymbol{U}\left(\boldsymbol{\Sigma}\boldsymbol{y}_{n\times 1} - \boldsymbol{c}_{m\times 1}\right)$$

where
$$y_{n\times 1} = V^T x, c_{m\times 1} = U^T b$$

Since U is an orthogonal matrix,

$$\|Ax - b\| = \|U(\Sigma y_{n\times 1} - c_{m\times 1})\| = \|\Sigma y_{n\times 1} - c_{m\times 1}\|$$

Then, our objective is to identify y that can make $\|\Sigma y_{n\times 1} - c_{m\times 1}\|$ have the minimum length



$$\boldsymbol{\Sigma} \boldsymbol{y}_{n \times 1} = \begin{bmatrix} \boldsymbol{\sigma}_{1} & & & & \\ \boldsymbol{\sigma}_{2} & & & \\ & \ddots & & \\ & \boldsymbol{\sigma}_{r} \end{bmatrix} \quad \boldsymbol{O}_{r \times (n-r)} \quad \boldsymbol{O}_{(m-r) \times r} \quad \boldsymbol{O}_{(m-r) \times (n-r)} \end{bmatrix}_{m \times n} \begin{bmatrix} \boldsymbol{y}_{1} \\ \boldsymbol{y}_{2} \\ \vdots \\ \boldsymbol{y}_{n} \end{bmatrix} = \begin{bmatrix} \boldsymbol{\sigma}_{1} \boldsymbol{y}_{1} \\ \boldsymbol{\sigma}_{2} \boldsymbol{y}_{2} \\ \vdots \\ \boldsymbol{\sigma}_{r} \boldsymbol{y}_{r} \\ \boldsymbol{0} \\ \vdots \\ \boldsymbol{0} \end{bmatrix}_{m \times 1} \quad \boldsymbol{\Sigma} \boldsymbol{y}_{n \times 1} - \boldsymbol{c}_{m \times 1} = \begin{bmatrix} \boldsymbol{\sigma}_{1} \boldsymbol{y}_{1} - \boldsymbol{c}_{1} \\ \boldsymbol{\sigma}_{2} \boldsymbol{y}_{2} - \boldsymbol{c}_{2} \\ \vdots \\ \boldsymbol{\sigma}_{r} \boldsymbol{y}_{r} - \boldsymbol{c}_{r} \\ -\boldsymbol{c}_{r+1} \\ \vdots \\ -\boldsymbol{c}_{m} \end{bmatrix}_{m \times 1}$$

Then, we simply let $y_i = \frac{c_i}{\sigma_i}$, $1 \le i \le r$; then, $\|\Sigma y_{n \times 1} - c_{m \times 1}\|$ can get the minimum length $\sqrt{\sum_{i=r+1}^m c_i^2}$

Note that $y_{r+1} \sim y_n$ can be arbitrary



The operation $y_i = \frac{C_i}{\sigma_i}$, $1 \le i \le r$ can be simply completed by a matrix multiplication,

$$\mathbf{y} = \begin{bmatrix} \frac{1}{\sigma_1} & & \\ \frac{1}{\sigma_2} & & \\ & \ddots & \\ & \frac{1}{\sigma_r} \end{bmatrix} \quad \mathbf{o}_{r \times (m-r)} \quad \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix}_{m \times 1} = \begin{bmatrix} c_1 / \sigma_1 \\ c_2 / \sigma_2 \\ \vdots \\ c_r / \sigma_r \\ 0 \\ \vdots \\ 0 \end{bmatrix}_{n \times 1} \triangleq \mathbf{\Sigma}^+ \mathbf{c}_{m \times 1}$$

$$\mathbf{o}_{(n-r) \times r} \quad \mathbf{o}_{(n-r) \times (m-r)} \end{bmatrix}_{n \times m}$$

where Σ^+ means transposing Σ and inverting all non-zero diagonal entries Finally,

$$x = Vy_{n \times 1} = V\Sigma^{+}c_{m \times 1} = V\Sigma^{+}U^{T}b$$
 (11) Moore-Penrose inverse





Roger Penrose (born 8 August 1931) is an English mathematician, mathematical physicist, philosopher of science and Nobel Laureate in Physics. He is Emeritus Rouse Ball Professor of Mathematics in the University of Oxford.

Penrose has contributed to the mathematical physics of general relativity and cosmology. He has received several prizes and awards, including the 1988 Wolf Prize in Physics, which he shared with Stephen Hawking for the **Penrose–Hawking singularity theorems**, and the 2020 Nobel Prize in Physics for the discovery that black hole formation is a robust prediction of the general theory of relativity.



- Some notes about the Moore-Penrose inverse used in linear least squares
 - It does not have requirements for the rank of A
 - It can guarantee that the obtained solution can make ||Ax-b|| having the minimum length; but the solution may be not unique



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Summary of solvers for the linear LS problem

To solve the equation,

