

Least Squares

Background: $Hx \stackrel{\text{Symbol for inconsistency}}{\approx} y$ $H \in \mathbb{R}^{N \times n}$ $N > n$

$$\begin{matrix} \left[\right] & \left[\right] & = & \left[\right] \\ \downarrow & \downarrow & & \downarrow \\ N \times n & n \times 1 & & N \times 1 \end{matrix} \rightarrow \text{Overdetermined inconsistent}$$

$y \notin R(H)$ [$R(H)$: column space of H]
 So $y = Hx + v$ for some $v \in \mathbb{R}^{N \times 1}$
 \hookrightarrow residual

Least square solⁿ: \hat{x} is one that minimizes $\|v\|^2$.

i.e. $\|y - H\hat{x}\|^2 \leq \|y - Hx\|^2 \quad \forall x \in \mathbb{R}^n$

If $y \in R(H)$, then \hat{x} is an exact solⁿ.
 Then \exists infinitely many (\hat{x}) \hookrightarrow not unique exact solutions.

Q. If $y \notin R(H)$ then is \hat{x} unique?

FACT: A vector \hat{x} is a minimizer of the cost function $J(x) = \|y - Hx\|^2$ iff it satisfies the (always consistent) normal eqns:

$$H^T H \hat{x} = H^T y$$

The minimum is $J(\hat{x}) = \|y\|^2 - \|H\hat{x}\|^2$

Proof: $0 = \frac{\partial}{\partial x} J = \frac{\partial}{\partial x} (x^T H^T H x - x^T H^T y - y^T H x + y^T y)$

$$= \hat{x}^T H^T H - y^T H = 0$$

Also $\frac{\partial^2 J}{\partial x^2} = H^T H \geq 0 \Rightarrow$ local minimum.

$$J(\hat{x}) = \|y\|^2 - \|H\hat{x}\|^2 \rightarrow \text{Exercise}$$

Q. Why are the normal equations always consistent?
 \rightarrow i.e. why will it have solutions always?

FACT: $H \in \mathbb{R}^{n \times n}$. Then $R(H^T H) = R(H^T)$: Proof: Exercise

FACT: Consider $H^T H \hat{x} = H^T y$

a) When H is full rank, the unique solution is given by $\hat{x} = (H^T H)^{-1} H^T y$

b) When H is not full-rank, the normal eqns always have more than one solution, where any two solutions \hat{x}_1 & \hat{x}_2 satisfy:

$$H(\hat{x}_1 - \hat{x}_2) = 0$$

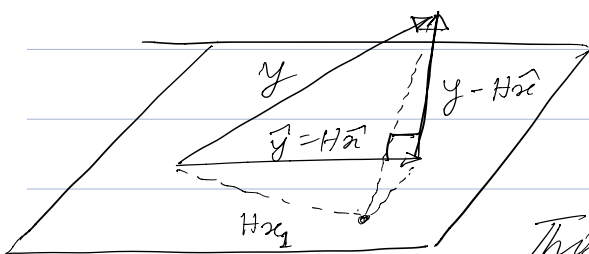
c) The projection of y onto $R(H)$ is unique & is defined as $\hat{y} := H\hat{x}$, where \hat{x} is any solution to the normal eqns. When H has full rank, $\hat{y} = H(H^T H)^{-1} H^T y$

Proof: (a) $\rightarrow H$ full rank $\Leftrightarrow H^T H$ is non-singular
(Proof: Exercise)

$$(b) \left. \begin{aligned} R(H^T H) &= R(H) \\ \Leftrightarrow N(H^T H) &= N(H) \end{aligned} \right\} \Leftrightarrow \begin{cases} H^T H(\hat{x}_1 - \hat{x}_2) = 0 \\ \Leftrightarrow H(\hat{x}_1 - \hat{x}_2) = 0 \end{cases}$$

(c) From (b) $\hat{y}_1 = H\hat{x}_1$, $\hat{y}_2 = H\hat{x}_2$
 $\hat{y}_1 - \hat{y}_2 = H(\hat{x}_1 - \hat{x}_2) = 0$.

Geometry: Recall: $\min J = \|y - H\hat{x}\|^2 = \|y\|^2 - \|H\hat{x}\|^2$
Pythagoras thm $\leftarrow \|y - H\hat{x}\|^2 + \|H\hat{x}\|^2 = \|y\|^2$
 OR



$$H^T(y - H\hat{x}) = 0$$

i.e. $(y - H\hat{x})$ is \perp to $R(H)$

$R(H)$ This argument extends for arbitrary dimensions for inner-product spaces:

Defⁿ: Let L be a linear subspace of a inner product space V & let $y \in V$.

The projection of y onto L , denoted by the unique $\hat{y}_L \in L$ s.t. $\langle y - \hat{y}_L, a \rangle = 0$
 $\forall a \in L$.

Proof of Uniqueness & Existence: Exercise.

FACT: $\|y - \hat{y}_L\|^2 \leq \|y - a\|^2 \quad \forall a \in L$

Proof: $\|y - ay\|^2 = \|y - \bar{y}_L + \bar{y}_L - ay\|^2 \dots$ Rest: Exercise.

If H has full rank, an explicit projection matrix can be written:

$$\hat{y} = H\hat{x} = H \underbrace{(H^T H)^{-1} H^T}_{P_H} y =: P_H y$$

Verify: (i) $P_H^T = P_H$ (ii) $P_H = P_H^2$ (iii) $P_H^\perp = I - P_H$
projects only $R^\perp(H)$

Application of Geometric approach: Order Recursion
(Size of x increases)

Let $\hat{x}_{n,N} \in \mathbb{R}^{n \times 1}$ denote the LS solⁿ for $Hx \cong y$
where $H \in \mathbb{R}^{N \times n}$ has full column rank.

Suppose we add one column to H & one entry to x .

$$\begin{bmatrix} H & \underline{h}_n \end{bmatrix} \begin{bmatrix} x \\ x(n) \end{bmatrix} \cong y$$

Assume full col. rank.

Denote solⁿ by $\hat{x}_{n+1,N} \in \mathbb{R}^{(n+1) \times 1}$

Q. Is $\hat{x}_{n+1,N}$ related to $\hat{x}_{n,N}$?

$$\hat{x}_{n+1,N} = \left(\begin{bmatrix} H^T \\ \underline{h}_n^T \end{bmatrix} \begin{bmatrix} H & \underline{h}_n \end{bmatrix} \right)^{-1} \begin{bmatrix} H^T \\ \underline{h}_n^T \end{bmatrix} y$$

Denote $\hat{h}_n = P_H \underline{h}_n = H \underbrace{(H^T H)^{-1} H^T}_{\alpha} \underline{h}_n$ (Projection onto $R(H)$)
 $= H\alpha$

Residual: $\tilde{h}_n = h_n - \hat{h}_n = h_n - Ha$

$[H \tilde{h}_n]$ provides a new basis for $R\{[H h_n]\}$

But \tilde{h}_n is \perp to H

Projection of y onto $R\{[H h_n]\} \equiv$ Projection of y onto $R\{[H \tilde{h}_n]\}$

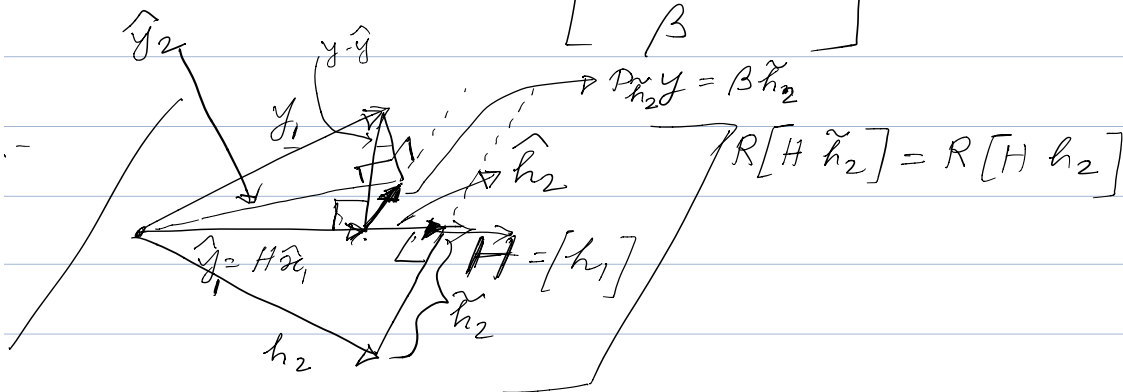
$$\hat{y}_{n+1} = P_H y + \underbrace{P_{\tilde{h}_n} y}_{\text{since } \tilde{h}_n \perp H} = H \hat{x}_{n,N} + P_{\tilde{h}_n} y \quad (1)$$

$$\text{Now, } P_{\tilde{h}_n} y = \frac{h_n^T y}{\|h_n\|^2} \tilde{h}_n = \beta \tilde{h}_n \quad \leftarrow \text{scalar}$$

$$\text{So from (1), } \hat{y}_{n+1} = H \hat{x}_{n,N} + \beta \tilde{h}_n = H \hat{x}_{n,N} + \beta [h_n - Ha] \\ = [H \tilde{h}_n] \begin{bmatrix} \hat{x}_{n,N} - \beta a \\ \beta \end{bmatrix}$$

But $\hat{y}_{n+1} = [H \tilde{h}_n] \hat{x}_{n+1,N}$ & $\hat{x}_{n+1,N}$ is unique.

$$\text{Hence } \hat{x}_{n+1,N} = \begin{bmatrix} \hat{x}_{n,N} - \alpha \beta \\ \beta \end{bmatrix}$$



Regularized Least Squares

$$J(\alpha) = (\alpha - \alpha_0)^T \Pi_0^{-1} (\alpha - \alpha_0) + \|y - H\alpha\|^2$$

$\Pi_0 > 0$. Clearly, if $\Pi_0 = \infty I$, then we recover earlier problem.

$\{\Pi_0, x_0\}$ can be tuned to factor in prior information about solution.

unique \hat{x} guaranteed, even when H is rank deficient
 # If H is already full rank, Π_0 can be used to improve condition no. (in normal eqn)

Define $x' = x - x_0$, $y' = y - Hx_0$

Then $\min_{x'} [x'^T \Pi_0^{-1} x' + \|y' - Hx'\|^2]$

$$= \min_{x'} \left\| \begin{bmatrix} 0 \\ y' \end{bmatrix} - \begin{bmatrix} \Pi_0^{-1/2} \\ H \end{bmatrix} x' \right\|^2 \quad \boxed{\Pi_0 = \Pi_0^{-1/2} \Pi_0^{1/2}}$$

Same form as before

Solution

$$\hat{x} = x_0 + \left[\Pi_0^{-1} + H^T H \right]^{-1} H^T [y - Hx_0]$$

Always invertible - so explicit form always possible.

Recursive Least Square: N increases sequentially.

$$H_{i-1} x \cong y_{i-1}$$

Let $x_0 = 0$. Then LS at $i-1$:

$$\min_x [x^T \Pi_0^{-1} x + \|y_{i-1} - H_{i-1} x\|^2]$$

Solⁿ is \hat{x}_{i-1} .

$$H_{i-1} = \begin{bmatrix} h_0 \\ \vdots \\ h_{i-1} \end{bmatrix} \in \mathbb{R}^{i \times n}$$

$$y_{i-1} = \begin{bmatrix} y(0) \\ \vdots \\ y(i-1) \end{bmatrix}$$

Now, we get another data

pt. $h_i, y(i)$: we aim to find

$$\min_x [x^T \Pi_0^{-1} x + \|y_i - H_i x\|^2] \rightarrow \text{solⁿ is } \hat{x}_i$$

Q. Is it possible to calculate \hat{x}_p without re-inverting the matrix $(\Pi_0^{-1} + H_i^T H_i)$ again?

$$\hat{x}_p = \overbrace{(\Pi_0^{-1} + H_i^T H_i)^{-1}}^{P_i} H_i^T y_i$$

$$= (\Pi_0^{-1} + H_{i-1}^T H_{i-1} + h_i^T h_i)^{-1} \left[H_{i-1}^T y_{i-1} + h_i^T y(i) \right]$$

①

Define: $P_i = (\Pi_0^{-1} + H_i^T H_i)^{-1}$ $P_{-1} = \Pi_0$

Then: $P_i^{-1} = P_{i-1}^{-1} + h_i^T h_i$ $P_{-1}^{-1} = \Pi_0^{-1}$

Use: $[A + BCD]^{-1} = A^{-1} - A^{-1} B (C^{-1} + D A^{-1} B)^{-1} D A^{-1}$

Identify: $A = P_{i-1}^{-1}$; $B = h_i^T$; $C = 1$; $D = h_i$

Then;

$$P_i = P_{i-1} - \frac{P_{i-1} h_i^T h_i P_{i-1}}{1 + h_i P_{i-1} h_i^T} \quad P_{-1} = \Pi_0$$

So, from ①: $\hat{x}_i = P_{i-1} H_{i-1}^T y_{i-1} - \dots$ Exercise

$$= \hat{x}_{i-1} + \frac{P_{i-1} h_i^T}{1 + h_i P_{i-1} h_i^T} (y(i) - h_i \hat{x}_{i-1})$$

Lemma: Solution of RLS \hat{x}_p satisfies:

$$\hat{x}_p = \hat{x}_{i-1} + K_{p,i} (y(i) - h_i \hat{x}_{i-1}) \quad \hat{x}_{-1} = 0$$

where $K_{p,i} = P_{i-1} h_i^T r_{e,i}^{-1}(i)$;

$$r_{e,i} = 1 + h_i P_{i-1} h_i^T$$

$$P_i = P_{i-1} - P_{i-1} h_i^T (1 + h_i P_{i-1} h_i^T)^{-1} h_i P_{i-1}$$

$$P_{-1} = \Pi_0$$

Effort Required for 1-step recursion is $O(n^2)$ flops. (as compared to $O(n^3)$ for the matrix inversion)

Surprising observation: The above solⁿ is the (Kalman filter) solution for:

$$x_{j+1} = x_j \quad x_0 = x \in \mathbb{R}^n$$

$$y_j = h_j^T x_j + v(j)$$

$$E x_0 x_0^T = \Pi_0 \quad ; \quad E v(i) v^T(j) = \delta_{ij}$$

Q. Why? $\rightarrow y_i = \begin{bmatrix} y(0) \\ \vdots \\ y(i) \end{bmatrix} \quad v_i = \begin{bmatrix} v(0) \\ \vdots \\ v(i) \end{bmatrix} \Rightarrow y_i = H x + v_i$

STOCHASTIC LEAST SQUARES

X, Y are two vector valued random variables with joint density $f_{X,Y}(i,j)$.

Problem: Given $Y=y$, find an estimate \hat{x}

of x . i.e. find $h(\cdot)$ s.t.

$\hat{x} = h(y)$ is a "good" estimate of x .

FACT: The estimator $\hat{x} = h(y)$ that solves:

$\min_{h(\cdot)} E([x - \hat{x}][x - \hat{x}]^T)$ (least mean square (lms) estimator of r.v. x given the value of

y is $\hat{x} = E(x|y)$.

Note: As opposed to the parameter estimation problem, x & y are both random variables.

Assume $g(y)$

Proof: $E[(x - \hat{x})(x - \hat{x})^T] = E\left[\begin{matrix} (x - E(x/y) + E(x/y) - \hat{x}) \\ (x - E(x/y) + E(x/y) - \hat{x})^T \end{matrix}\right]$

Recall $E[xy^T(y)] = E\{E\{xg^T(y)/y\}\} = E\{E\{x/y\}g^T(y)\}$
(for any $g(y)$)

Hence here: $E[(x - E(x/y))g^T(y)] = E[xg^T(y)] - E[E(x/y)g^T(y)] = 0$

$$= E[x - E(x/y)][x - E(x/y)]^T + E[E(x/y) - \hat{x}][E(x/y) - \hat{x}]^T$$

So minimum is achieved by $\hat{x} = E(x/y)$

But we usually don't know $f(x/y)$.

So we restrict ourselves to linear estimators

of the form $\hat{x} = Ky$

$$\begin{bmatrix} \hat{x}_1 \\ \vdots \\ \hat{x}_n \end{bmatrix} = \begin{bmatrix} K_0 \\ n \times p(N+1) \end{bmatrix} \begin{bmatrix} y_0 \\ \vdots \\ y_N \end{bmatrix}$$

Find K_0 such that for every $K \in \mathbb{R}^{n \times p(N+1)}$

$y \rightarrow N$ observations of a p -dim random variable.

$y \cong Hy \rightarrow H, y$ - known find \hat{x} s.t. $\|y - H\hat{x}\|$ min.

Compare with det. L.S.: $\hat{x} \cong Hy$ then $\hat{x} \cong Ky$, more information about x, y known. Find K_0 s.t. $\|x - Ky\|$ is min.

$$P(K) := E[x - Ky][x - Ky]^T \geq P(K_0) := E[(x - \hat{x})(x - \hat{x})^T]$$

↳ P.S.-D. (1)

Thm: (Optimal LMS): Given two zero mean r.v.s x & y , the L.L.M.S estimator of x given y (i.e. satisfying ①) is given by any solution k_0 of the "normal eqn":

$$k_0 R_y = R_{xy}$$

where $R_y = Eyy^T$ & $R_{xy} = Exy^T = R_{yx}^T$

The var $P(k_0) = R_x - k_0 R_{yx} = R_x - R_{xy} k_0^T$

Proof: ① above $\Leftrightarrow aP(k)a^T \geq aP(k_0)a^T \quad \forall a \in \mathbb{R}^n$

Scalar

$$aP(k)a^T = aE[(x-ky)(x-ky)^T]a^T = a[R_x - R_{xy}k^T - kR_{yx} + kR_yk^T]a^T$$

$$= aR_x - aR_{xy}(ak)^T - (ak)R_{yx}a^T + (ak)R_y(ak)^T$$

$$\frac{\partial aP(k)a^T}{\partial (ak)} = 0 \Leftrightarrow -aR_{xy} - aR_{yx} + 2(ak_0)R_y = 0 \quad \forall a$$

$$\Leftrightarrow a[R_{xy} - k_0R_y] = 0 \quad \forall a$$

$$\Leftrightarrow R_{xy} = k_0R_y$$

Corresponding mmse: $P(k_0) = \dots = R_x - k_0 R_{yx}$

The optimal k_0 also minimizes mse in the estimator of each component of x .

If $R_y > 0$, $k_0 = R_{xy} R_y^{-1}$ & $P(k_0) = R_x - R_{xy} R_y^{-1} R_{yx}$

R_y singular is "unusual" since $\Rightarrow \exists c \in \mathbb{R}^{(N+1)P}$, $c \neq 0$
s.t. $c^T R_y = 0 \Leftrightarrow 0 = c^T R_y c = c^T (Eyy^T) c = E[c^T y]^2 = 0$

i.e. $\text{Mean}(c^T y) = 0$ & $\text{Var}(c^T y) = 0$
 $\Leftrightarrow c^T y = 0$ almost surely.

This usually means, something is wrong with the problem formulation.

Even then if Ry is assumed to be singular:

Thm: Even if Ry is singular, the normal equations

$K_0 Ry = Ry$ will be consistent, and there will be many solutions. No matter which solution

K_0 is used, the corr. lms estimator $\hat{x} = K_0 y$

& $P(K_0)$ will each be unique.

A geometric interpretation: Consider the normal eqns:

$$K_0 Ry = Ry \Leftrightarrow K_0 E y y^T = E x y^T$$

$$\Leftrightarrow E(x - K_0 y) y^T = 0 \quad \text{--- (1)}$$

Q. Can we consider x, y as vectors in an inner product space? with $\langle x, y \rangle := E x y^T$

Then (1) is eq. to $x - K_0 y \perp y$

Potential problems: $x: \Omega \rightarrow \mathbb{R}^m$ $y: \Omega \rightarrow \mathbb{R}^p$
 $E x y^T \in \mathbb{R}^{m \times p}$ $\begin{matrix} \text{rect. matrix} \\ \text{(not scalar)} \end{matrix}$

Check: 1) Linearity: $\langle a_1 x_1 + a_2 x_2, y \rangle = a_1 \langle x_1, y \rangle + a_2 \langle x_2, y \rangle$

2) Reflexivity: $\langle x, y \rangle = \langle y, x \rangle^T \xrightarrow{\forall a_1, a_2 \in \mathbb{R}}$ Easy to check

3) Non-degeneracy: $\|x\|^2 = \langle x, x \rangle = 0 \Leftrightarrow x = 0$

(Additional assumption: $E x x^T = 0$ near.) $\xrightarrow{\text{Equality almost surely.}}$

So $\langle x, y \rangle = E x y^T$ is a valid inner product

Then given x & $y = \begin{bmatrix} y_0 \\ \vdots \\ y_N \end{bmatrix} \rightarrow \mathbb{R}^{p \times 1}$, find $\hat{x} = Ky$ s.t.

$E[x - \hat{x}][x - \hat{x}]^T = \langle (x - \hat{x}), (x - \hat{x}) \rangle$ is minimized.

Recall V , lin subspace - L . PSD
 $\|y - \hat{y}_L\| < \|y - a\| \forall a \in L$
 iff $y - \hat{y}_L \perp L \Leftrightarrow \langle y - \hat{y}_L, a \rangle = 0 \forall a \in L$

Here \hat{x} is Ky i.e. $\hat{x} \in L := \text{col sp. of } y$

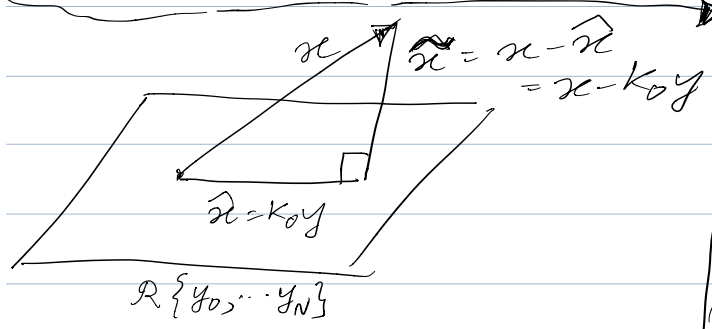
so $\|x - \hat{x}\|$ is minimized $\Leftrightarrow x - \hat{x} \perp \text{span}\{Ky\}$

$\Leftrightarrow \langle x - Ky, Ky \rangle = 0; \langle x - Ky, y \rangle K^T = 0 \forall K$

$\Leftrightarrow \langle x, y_i \rangle = k_i \langle y, y_i \rangle \quad \forall i=0, \dots, N$

$\Leftrightarrow Rxy = k_0 Ry \rightarrow$ Existence & uniqueness of projection

Valid even if Ry singular $\left\{ \begin{array}{l} \text{is guaranteed by inner prod.} \\ \text{sp. properties (complete? Hilbert sp?)} \end{array} \right.$



$$\langle x - Ky, y \rangle = E \begin{bmatrix} x \\ \vdots \\ x \end{bmatrix} \begin{bmatrix} y_0 & y_1 & \dots & 1 \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} = 0$$

(N+1)P

\Rightarrow Each $\langle x - Ky, y_i \rangle = 0$

FACT: The lms estimator of r.v. x given a set of other r.v. y is characterized by the error

\tilde{x} being orthogonal (uncorrelated with) each of the r.v.'s used to form the estimate.

Proof: True since $(x - ky) \perp y_i \quad \forall i = 0, \dots, N$.

Example: Consider zero-mean stationary process $\{y(t)\}$ with autocovariance $\int_{-\infty}^{\infty} \langle y(t), y(t-\tau) \rangle = R_y(\tau)$. Find the estimator of $\int_0^T y(t) dt$ in terms of $y(0)$ & $y(T)$.

Let $Z = \int_0^T y(t) dt$ & $\hat{Z} = ay(0) + by(T)$ (we find a & b)

The orthogonality condition:

$$Z - \hat{Z} \perp \text{sp.}\{y(0), y(T)\}$$

i.e. $\left[\int_0^T y(t) dt - ay(0) - by(T) \right] \perp \text{sp.}\{y(0), y(T)\}$

$$\left\langle \int_0^T y(t) dt - ay(0) - by(T), y(0) \right\rangle = 0$$

$$\Leftrightarrow \int_0^T R_y(t) dt - aR_y(0) - bR_y(T) = 0 \quad \text{--- (1)}$$

Also;

$$\left\langle \int_0^T y(t) dt - ay(0) - by(T), y(T) \right\rangle = 0$$

$$\Leftrightarrow \int_0^T R_y(t-T) dt - aR_y(-T) - bR_y(0) = 0$$

$$= \int_0^T R_y(t) dt - aR_y(T) - bR_y(0) = 0 \quad \text{--- (2)}$$

$$\begin{bmatrix} R_y(0) & R_y(T) \\ R_y(T) & R_y(0) \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \int_0^T R_y(t) dt$$

Solving: $\hat{z} = \frac{\int_0^T R_y(t) dt}{R_y(0) + R_y(T)} [y(0) + y(T)]$

Linear Models

$$y = Hx + v \quad \begin{array}{l} y \in \mathbb{R}^p, \quad H = \mathbb{R}^{p \times n} \\ x \in \mathbb{R}^n \quad \rightarrow \text{known} \end{array}$$

Known: H, R_x, R_v, x & v are uncorrelated. v is zero mean random noise.

So $R_y = HR_x H^T + R_v$ (Assume $R_y > 0$)

Then, $\text{Lms e } \hat{x} = K_0 y, \quad K_0 = R_x H^T [HR_x H^T + R_v]^{-1}$

Also $P(K_0) = R_x - R_x H^T [R_v + HR_x H^T]^{-1} HR_x$

Equivalent forms: $K_0 = (R_x^{-1} + H^T R_v^{-1} H)^{-1} H^T R_v^{-1}$ sometimes useful
 (derived by using $(A+BCD)^{-1}$ formula) $P(K_0) = (R_x^{-1} + H^T R_v^{-1} H)^{-1}$

Gauss Markov Thm:

x is not a r.v. but unknown constant.

Equivalently, $R_x = \alpha R$ with $\alpha \rightarrow \infty$.

From above, $\hat{x}_0 := (H^T R_v^{-1} H)^{-1} H^T R_v^{-1} y$

$= (H^T H)^{-1} H^T y$ if $R_v = I$

$P_0(K_0) := (H^T R_v^{-1} H)^{-1} = (H^T H)^{-1}$

(Assume H full rank)

G-M Thm (again) Consider $y = Hx + v$, where

v is zero mean r.v. with unit variance $\langle v, v \rangle = I$

x is a deterministic vector, & H has full

column rank. Then $\hat{x}_{LS} = (H^T H)^{-1} H^T y$ is the optimum unbiased linear least-mean-square estimator of x .

Proof: Exercise (without this trade of $R_{xx} = \alpha R$ with $\alpha \rightarrow \infty$)

Q. Is it MVUE? Refer to previous statement of GM then.