

(Pr 1)

Consider the 2 sets

$$X_1 = \{a_1=1, a_2=2, a_3=8\}$$

$$X_2 = \{b_1=1.5, b_2=2, b_3=-1\}$$

with uniform probability mass:

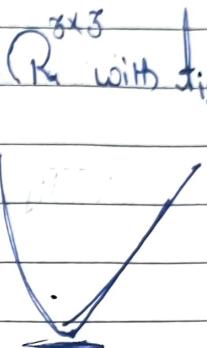
$$P(a_i) = P(b_i) = 1/3 \text{ for } i=1, 2, 3.$$

A coupling is defined by a matrix $T \in \mathbb{R}^{3 \times 3}$ with $t_{ij} \geq 0$

$$\text{and } \sum_{i=1}^3 t_{ij} = \sum_{j=1}^3 t_{ij} = 1/3$$

Find a coupling that minimizes

$$J(t) = \sum_{i,j=1}^3 |t_{ij}|(b_i - a_j)^2$$



What do you notice about sparsity structure of the optimal coupling matrix T^* ?

→ This problem is a special case of transport problems i.e. assignment problem

$a_1 \quad a_2 \quad a_3$

$b_1 \quad \begin{matrix} 1 & 4 & 1 & 3 \end{matrix}$

$b_2 \quad \begin{matrix} 1 & 1 & 3 \end{matrix}$

$b_3 \quad \begin{matrix} 1 & 3 & 1 & 2 \end{matrix}$

$\frac{1}{3} \quad \frac{1}{3} \quad \frac{1}{3}$

$$D_{11} = (b_1 - a_1)^2 = 1/4 = 0.25$$

$$D_{12} = (1/4)^2 = 0.25$$

$$D_{13} = (1.5)^2 = 9/4 = 2.25$$

$$D_{21} = 1$$

$$D_{22} = 0$$

$$D_{23} = 1$$

$$D_{31} = 1/4$$

$$D_{32} = 9/4$$

$$D_{33} = 1/6$$

To minimise T_{ij} we can begin by setting $\frac{1}{3}$ probability to every element to a row at a time in a row. & then get respective probabilities of other elements. Doing this we will have 3 matrices & we can choose the minimal T_{ij} value yielding one as optimum.

Let's take the 1st row

$$T_1 = \begin{bmatrix} 1/3 & 0 & 0 \\ 0 & t_{22} & t_{23} \\ 0 & t_{32} & t_{33} \end{bmatrix}, T_2 = \begin{bmatrix} 0 & 1/3 & 0 \\ t_{21} & 0 & t_{23} \\ t_{31} & 0 & t_{33} \end{bmatrix}, T_3 = \begin{bmatrix} 0 & 0 & 1/3 \\ t_{21} & t_{22} & 0 \\ t_{31} & t_{32} & 0 \end{bmatrix}$$

We can represent

every other element wrt a single element in a matrix.

$$\text{For } T_1, t_{23} = -t_{22} + 1/3 \quad | \quad t_{23} = 1/3 - t_{22} \quad | \quad t_{21} = 1/3 - t_{22}$$

$$t_{32} = \frac{1}{3} - t_{22}$$

$$t_{31} = 1/3 - t_{21} \quad | \quad t_{31} = t_{22}$$

$$t_{33} = t_{22}$$

$$t_{33} = t_{21}$$

$$t_{32} = \frac{1}{3} - t_{22}$$

$$J(T) = \frac{1}{3} (b_1 - a_1)^2$$

$$\therefore J(T_2) = \frac{1}{3} (b_1 - a_2)^2$$

$$\therefore J(T) = \frac{1}{3} (b_1 - a_3)^2$$

$$+ t_{22} (b_2 - a_2)^2$$

$$+ t_{23} (b_2 - a_3)^2$$

$$+ t_{32} (b_3 - a_2)^2$$

$$+ t_{33} (b_3 - a_3)^2$$

$$+ t_{21} (b_2 - a_1)^2$$

$$+ t_{23} (b_2 - a_3)^2$$

$$+ t_{31} (b_3 - a_1)^2$$

$$+ t_{33} (b_3 - a_3)^2$$

$$+ t_{21} (b_2 - a_2)^2$$

$$+ t_{22} (b_2 - a_2)^2$$

$$+ t_{31} (b_3 - a_2)^2$$

$$+ t_{32} (b_3 - a_2)^2$$

Now we simply assign values of b_i & a_i

$$\begin{aligned}
 J(T_1) &= \frac{1}{3} \times 0.25 + 0 + \left(\frac{1}{3} - t_{22}\right)(1) + \left(\frac{1}{3} - t_{22}\right)(9) \\
 &\quad + t_{22} \times (16) \\
 &= \frac{0.25}{3} + 0 + \frac{1}{3} - t_{22} + 3 - 9t_{22} + 16t_{22} \\
 &= \frac{1.25}{3} + 3 + 6t_{22} \\
 &= \frac{10.25}{3} + 6t_{22} \Rightarrow \text{Min}(J(T_1)) \text{ for } t_{22} = 0 \text{ is } 3.42
 \end{aligned}$$

$$\begin{aligned}
 J(T_2) &= \frac{1}{3} \cdot D_{12} + t_{21} \cdot D_{21} + \left(\frac{1}{3} - t_{21}\right) \cdot D_{23} \\
 &\quad + \left(\frac{1}{3} - t_{21}\right) \cdot D_{31} + t_{21} \cdot D_{33} \\
 &= \frac{1}{3} \times 0.25 + t_{21} + \frac{1}{3} - t_{21} + \frac{4}{3} - 4t_{21} \\
 &\quad + 16t_{21} \\
 &= \frac{5.25}{3} + 12t_{21} \quad \text{Min}(J(T_2)) \text{ is for } t_{21} = 0 \text{ is } 1.75
 \end{aligned}$$

$$\begin{aligned}
 J(T_3) &= \frac{1}{3} D_{13} + \left(\frac{1}{3} - t_{22}\right) (D_{21}) + t_{22} \cdot D_{22} \\
 &\quad + t_{22} \cdot D_{31} + \left(\frac{1}{3} - t_{22}\right) D_{32} \\
 &= \frac{1}{3} \times 2.25 + \frac{1}{3} - t_{22} + t_{22} \cdot 4 + 3 - 9t_{22} \\
 &= \frac{12.25}{3} - 6t_{22}
 \end{aligned}$$

$$\begin{aligned}
 J(T_3) \text{ is min if } t_{22} \text{ is max i.e. } \frac{1}{3} \\
 \therefore J(T_3) = \frac{12.25}{3} - \frac{6}{3} = \frac{6.25}{3} \approx 2.08
 \end{aligned}$$

\therefore We have most min for $T(T_2)$ for $t_{22} = 0$

\therefore By Putting respective elements w.r.t
 t_{21}

$$t_{23} = 1/3, t_{31} = 1/3, t_{33} = 0$$

& T_2 optimal is $\begin{bmatrix} 0 & 1/3 & 0 \\ 0 & 0 & 1/3 \\ 1/3 & 0 & 0 \end{bmatrix}$

EXERCISE 2A

$$X \sim \text{Unif}([0, 1]), \quad \pi_X(x) = \frac{1}{[0, 1]}(x)$$

$\forall f: \mathbb{R} \rightarrow \mathbb{R}$ ($f(x) \in L^1$)

$$\mathbb{E}[f(X)] = \int_{\mathbb{R}} f(x) \pi_X(x) dx = \int_0^1 f(x) dx$$

Given $M \in \mathbb{N}$ a quadrature rule is

$$\int_b^1 f(x) dx \approx \sum_{i=1}^M b_i f(c_i)$$

$b_i, c_i \in \mathbb{R} \quad \forall i \in \{1, \dots, M\}$

Gauss - Legendre quadrature rule

$$\int_{-1}^1 f(x) dx \approx \sum_{i=1}^M \tilde{b}_i f(\tilde{c}_i),$$

where $\{\tilde{c}_i, \tilde{b}_i\}_{i=1}^M$ are the roots of $P_M(x)$, M -degree

Legendre polynomial, and

$$b_1 = \frac{2}{(1-\tilde{x}_1^2)(P_M'(\tilde{x}_1))^2}$$

Given $M=1$

$$\mathbb{E}[f(x)] = \int_{-1}^1 f(x) dx =$$

$$= \frac{1}{2} \int_{-1}^1 f\left(\frac{x}{2} + \frac{1}{2}\right) dx \approx$$

$$\hookrightarrow x = \frac{\tilde{x}}{2} + \frac{1}{2} \quad \tilde{x} \in [-1, 1]$$

$$dx = d\tilde{x}$$

$$\approx \frac{1}{2} b_1 \int_{-1}^1 f\left(\frac{\tilde{x}_1}{2} + \frac{1}{2}\right) d\tilde{x} = f\left(\frac{1}{2}\right)$$

GAUSS-LEGENDRE QUADRATURE

RULE $\rightarrow b_1 = 2, \tilde{x}_1 = 0$ since $P_1(\tilde{x}) = \tilde{x}$

Then, for $M=1, b_1 = 1$ and

$$c_1 = \frac{1}{2}$$

Thus quadrature rule has order $p=2$
 since $\forall f \in \bar{V}_1(\mathbb{R}) \quad \int_0^1 f(x) dx = b_1 f(c_1)$

If $f(x) = ax \in \mathbb{R}$

$$\int_0^1 f(x) dx = aw = 1 \quad f\left(\frac{1}{2}\right) = b_1 f(c_1)$$

If $f(x) = aw + a_1x \quad a_1 \in \mathbb{R}$
 $a_1 \in \{0, 1\}$

$$\begin{aligned} \int_0^1 f(x) dx &= aw + \frac{a_1}{2} = \\ &= 1 \quad f\left(\frac{1}{2}\right) = b_1 f(c_1) \end{aligned}$$

[2] If we consider $M=2$
 quadrature points by
 proceeding as in [1] we
 get

$$E[f(X)] = \int_0^1 f(x) dx \approx$$

$$\approx \frac{1}{2} \sum_{i=1}^2 b_i f\left(\frac{1}{2}c_i + \frac{1}{2}\right) \quad (*)$$

$$P_2(X) = \frac{1}{2}(3x^2 - 1) = 0$$

$$\Leftrightarrow x = -\frac{1}{\sqrt{3}} = c_1 \quad \vee \quad x = \frac{1}{\sqrt{3}} = c_2$$

$$\text{and } b_1 = b_2 = 1$$

\implies

$$(*) = \frac{1}{2} \left(f\left(\frac{1}{2}\left(-\frac{1}{\sqrt{3}}\right) + \frac{1}{2}\right) + f\left(\frac{1}{2}\frac{1}{\sqrt{3}} + \frac{1}{2}\right) \right) = \\ = \frac{1}{2} f\left(\frac{1-\sqrt{3}}{2}\right) + \frac{1}{2} f\left(\frac{\sqrt{3}+1}{2}\right)$$

$$\text{Then, } b_1 = b_2 = \frac{1}{2} \quad \text{and} \quad c_1 = \frac{1-\sqrt{3}}{2}, \quad c_2 = \frac{1+\sqrt{3}}{2}$$

The formula has order $p=3$

$$\text{since } \int_0^1 f(x) dx = \sum_{i=1}^2 b_i f(c_i) \quad \forall f \in \Pi_2(\mathbb{R})$$

If $f(x) = \omega \in \mathbb{R}$

$$\int_0^1 f(x) dx = \omega = \frac{1}{2} (2\omega) =$$
$$= b_1 f(c_1) + b_2 f(c_2)$$

If $f(x) = \omega + \alpha_1 x \quad \omega, \alpha_1 \in \mathbb{R}$

$$\int_0^1 f(x) dx = \omega + \frac{\alpha_1}{2} \quad \text{and}$$

$$b_1 f(c_1) + b_2 f(c_2) = \frac{1}{2} \left(\omega + \alpha_1 \left(\frac{1 - \sqrt{5}}{2} \right) + \right.$$
$$+ \omega + \alpha_1 \left(\frac{1 + \sqrt{5}}{2} \right) \left. \right) =$$
$$= \frac{1}{2} (2\omega + \alpha_1) = \omega + \frac{\alpha_1}{2}$$

If $f(x) = \alpha_0 + \alpha_1 x + \alpha_2 x^2 \quad \alpha_i \in \mathbb{R}, i \in \{0, 1, 2\}$

$$\int_0^1 f(x) dx = \omega + \frac{\alpha_1}{2} + \frac{\alpha_2}{3} \quad \text{and}$$

$$\begin{aligned}
 b_1 f(c_1) + b_2 f(c_2) &= \frac{1}{2} \left(\alpha_0 + \alpha_1 \left(\frac{1 - \sqrt{\beta}}{2} \right) + \right. \\
 &+ \alpha_2 \left(\frac{1 - \sqrt{\beta}}{2} \right)^2 + \alpha_0 + \alpha_1 \left(\frac{1 + \sqrt{\beta}}{2} \right) + \\
 &\quad \left. + \alpha_2 \left(\frac{1 + \sqrt{\beta}}{2} \right)^2 \right) = \\
 &= \frac{1}{2} \left(2\alpha_0 + \alpha_1 + \frac{\alpha_2}{4} \left(\frac{8}{3} \right) \right) = \\
 &= \alpha_0 + \frac{\alpha_1}{2} + \frac{\alpha_2}{3}
 \end{aligned}$$

Problem 2b (30pts) [Problem 3.3 of the lecture notes] Determine the ANOVA decomposition for

$$f(x_1, x_2) = 12x_1 + 6x_2 - 6x_1x_2$$

and compute the associated variances σ_1^2 , σ_2 and σ_{12}^2 . The underlying measure is uniform measure on $[0, 1]^2$. (See also pp.71–72 for explanation about ANOVA decomposition.)

ANOVA decomposition:

$$1) f(x_1, x_2) = f_0 + f_1(x_1) + f_2(x_2) + f_{12}(x_1, x_2)$$

2) Let's compute each $f(x)$

$$\begin{aligned} f_0 &= \mathbb{E}[f(x)] = \int_0^1 \int_0^1 f(x_1, x_2) dx_1 dx_2 = \int_0^1 \left(\int_0^1 (12x_1 + 6x_2 - \right. \\ &\quad \left. - 6x_1x_2) dx_1 \right) dx_2 = \int_0^1 \left(6x_2^2 + 6x_1x_2 - 3x_1^2x_2 \right) dx_2 = \\ &= \int_0^1 6x_2 + \frac{3}{2}x_2^2 = \frac{15}{2} \end{aligned}$$

$$\begin{aligned} 3) f_1(x_1) &= \int_0^1 f(x_1, x_2) dx_2 - f_0 = \int_0^1 (12x_1 + 6x_2 - 6x_1x_2) dx_2 - \frac{15}{2} = \\ &= \int_0^1 (12x_1x_2 + 3x_2^2 - 3x_1x_2^2) - \frac{15}{2} = 9x_1 - \frac{9}{2} \end{aligned}$$

$$\begin{aligned} 4) f_2(x_2) &= \int_0^1 f(x_1, x_2) dx_1 - f_0 = \int_0^1 (12x_1 + 6x_2 - 6x_1x_2) dx_1 - \frac{15}{2} = \\ &= \int_0^1 (6x_1 + 6x_1x_2 - 3x_1^2x_2) - \frac{15}{2} = 6 + 6x_2 - 3x_2^2 - \frac{15}{2} = 3x_2 - \frac{3}{2} \end{aligned}$$

$$\begin{aligned} 5) f_{12}(x_1, x_2) &= f(x_1, x_2) - f_1(x_1) - f_2(x_2) - f_0 = \\ &= 12x_1 + 6x_2 - 6x_1x_2 - 9x_1 + \frac{9}{2} - 3x_2 + \frac{3}{2} - \frac{15}{2} = \\ &= 3x_1 + 3x_2 - 6x_1x_2 - \frac{3}{2} \end{aligned}$$

□

6) According to the uniform distribution:

$$E(X) = \frac{\alpha + \beta}{2}, \quad \text{Var}(X) = \frac{(\beta - \alpha)^2}{12}$$

$$\hat{\sigma}_1^2 = \text{Var}(f_1(x_1)) = \text{Var}\left(9x_1 - \frac{9}{2}\right) = \text{Var}(9x_1) = \frac{(9 \cdot 1 - 0)^2}{12} = \frac{81}{12} = \frac{27}{4}$$

$$\hat{\sigma}_2^2 = \text{Var}(f_2(x_2)) = \text{Var}\left(3x_2 - \frac{3}{2}\right) = \text{Var}(3x_2) = \frac{9}{12} = \frac{3}{4}$$

$$\begin{aligned} \hat{\sigma}_{12}^2 &= \text{Var}(f_{12}(x_1, x_2)) = \text{Var}\left(3x_1 + 3x_2 - 6x_1x_2 - \frac{3}{2}\right) = \\ &= \text{Var}(3x_1 + 3x_2) + \text{Var}(6x_1x_2) - 2\text{Cov}(3x_1 + 3x_2, -6x_1x_2) = \\ &= 9\text{Var}(x_1) + 9\text{Var}(x_2) - 2\text{Cov}(3x_1, 3x_2) + 36\text{Var}(x_1x_2) - \\ &\quad - 2\text{Cov}(3x_1 + 3x_2, 6x_1x_2) = \\ &= 9\text{Var}(x_1) + 9\text{Var}(x_2) + 36\text{Var}(x_1x_2) - 36\text{Cov}(x_1 + x_2, x_1x_2) = \\ &= [9\text{Var}(x_1) + 9\text{Var}(x_2) + 36\text{Var}(x_1x_2) - 36\text{Cov}(x_1, x_1x_2) - \\ &\quad - 36\text{Cov}(x_2, x_1x_2)] \quad (*) \end{aligned}$$

f)

let's find $\hat{\sigma}_{12}^2$:

$$\begin{aligned} \text{Var}(x_1, x_2) &= E[x_1^2 x_2^2] - (E[x_1 x_2])^2 = \\ &= \int_0^1 \int_0^1 x_1^2 x_2^2 dx_1 dx_2 - E[x_1]^2 E[x_2]^2 = \frac{1}{9} - \left(\frac{1}{2} \cdot \frac{1}{2}\right)^2 = \\ &\quad \text{as independent } x_1 \text{ and } x_2 \\ &= 49 - \frac{1}{16} = \frac{7}{144} \end{aligned}$$

$$\begin{aligned} \text{Cov}(x_1, x_1 x_2) &= E[x_1 x_1 x_2] - E[x_1] E[x_1 x_2] = \\ &= \int_0^1 \int_0^1 x_1^2 x_2 dx_1 dx_2 - E[x_1] E[x_1] E[x_2] = \\ &= \frac{1}{6} - \frac{1}{2} \cdot \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{24} \end{aligned}$$

Using computed (*) formula:

$$\hat{\sigma}_{12}^2 = \frac{9}{12} + \frac{9}{12} + 36 \cdot \frac{1}{144} - 36 \cdot \frac{1}{24} - 36 \cdot \frac{1}{24} = \frac{1}{4}$$

As a result: $\hat{\sigma}_1^2 = \frac{27}{4}, \hat{\sigma}_2^2 = \frac{3}{4}, \hat{\sigma}_{12}^2 = \frac{1}{4}$