

Monitoring Compositional Data using Multivariate EWMA

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Compositional Data (CoDa)

Definition

$\mathbf{x} = (x_1, x_2, \dots, x_p)$ is defined as a p -part **composition** when (i) all its components are **strictly positive real numbers** (i.e. $\mathbf{x} \in \mathbb{R}_+^p$) and (ii) they carry only **relative information**.

Example of Muesli ($p = 3$)

66% of whole-grain cereals (barley / oat / wheat flakes), 24% of dried fruits (raisin, papaya, banana), 10% of nuts (almond, hazelnut, coconut).

Compositional equivalence

- ▶ $\mathbf{x} = (0.2, 0.5, 0.3), \mathbf{y} = (20, 50, 30) \Rightarrow \mathbf{x} \neq \mathbf{y}$.
- ▶ But they are **compositionally equivalent!**
- ▶ Use of the **closure** function (in order to standardize):

$$\mathcal{C}(\mathbf{x}) = \left(\frac{\kappa x_1}{\sum_{i=1}^p x_i}, \frac{\kappa x_2}{\sum_{i=1}^p x_i}, \dots, \frac{\kappa x_p}{\sum_{i=1}^p x_i} \right),$$

$\kappa > 0$ is a constant to be fixed (usually $\kappa = 1$).

- ▶ Now, we have $\mathcal{C}(\mathbf{x}) = \mathcal{C}(\mathbf{y})$.

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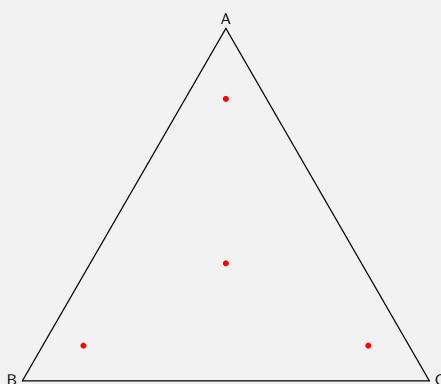
Compositional Data

Sample space

The **sample space** of compositional data is the simplex \mathcal{S}^p defined as

$$\mathcal{S}^p = \left\{ \mathbf{x} = (x_1, x_2, \dots, x_p) | x_i > 0, i = 1, 2, \dots, p \text{ and } \sum_{i=1}^p x_i = \kappa. \right\}$$

$p = 3 \Rightarrow$ Ternary diagram



Examples

- ▶ (1, 1, 1)
- ▶ (8, 1, 1)
- ▶ (1, 8, 1)
- ▶ (1, 1, 8)

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Aitchison's geometry

Euclidean geometry in \mathbb{R}^p

In \mathbb{R}^p we have an **Euclidean geometry** that defines a **vector space** with a **metric structure**:

- ▶ how to add vectors,
- ▶ how to multiply them by a scalar value,
- ▶ how to know if two vectors are orthogonal,
- ▶ how to compute the distance between two points, etc.

Cannot be used in \mathcal{S}^p

Examples: $\mathbf{x} = (0.2, 0.5, 0.3) \in \mathcal{S}^p$, $\mathbf{y} = (0.2, 0.7, 0.1) \in \mathcal{S}^p$

- ▶ $\mathbf{x} + \mathbf{y} = (0.4, 1.2, 0.4) \notin \mathcal{S}^p$,
- ▶ $3 \times \mathbf{x} = (0.6, 1.5, 0.9) \notin \mathcal{S}^p$.

A new geometry in \mathcal{S}^p

With dedicated vector space and metric structure

⇒ the **John Aitchison's geometry** and also V. Pawlowsky-Glahn (Univ. of Girona) and J.J. Egozcue (Technical Univ. of Catalonia).

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Aitchison's geometry

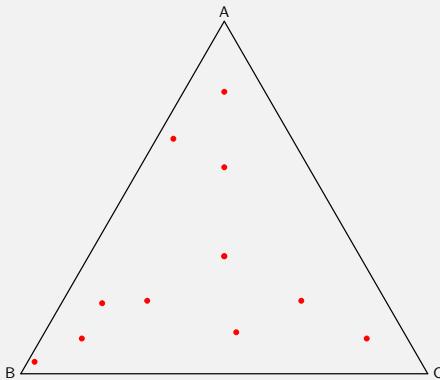
Perturbation operator \oplus (analog to the translation in \mathbb{R}^p)

If $\mathbf{x} \in \mathcal{S}^p$ and $\mathbf{y} \in \mathcal{S}^p \Rightarrow \mathbf{x} \oplus \mathbf{y} = \mathbf{y} \oplus \mathbf{x} = \mathcal{C}(x_1 y_1, x_2 y_2, \dots, x_p y_p)$.

Powering operator \odot (analog to the scalar multiplication in \mathbb{R}^p)

If $a \in \mathbb{R}$ and $\mathbf{x} \in \mathcal{S}^p \Rightarrow a \odot \mathbf{x} = \mathbf{x} \odot a = \mathcal{C}(x_1^a, x_2^a, \dots, x_p^a)$.

Ternary diagram



Examples

- ▶ $\mathbf{x} \oplus (0.2, 0.7, 0.1)$
- ▶ $\mathbf{x} \odot 0.5$

Aitchison's geometry

(\mathcal{S}^p, \oplus) is a commutative group structure

If \mathbf{x}, \mathbf{y} and \mathbf{z} in \mathcal{S}^p

- ▶ $\mathbf{x} \oplus \mathbf{y} = \mathbf{y} \oplus \mathbf{x}$ (commutativity),
- ▶ $(\mathbf{x} \oplus \mathbf{y}) \oplus \mathbf{z} = \mathbf{x} \oplus (\mathbf{y} \oplus \mathbf{z})$ (associativity),
- ▶ $\mathbf{0}_{\mathcal{S}^p} = \mathcal{C}(1, 1, \dots, 1) = (\frac{1}{p}, \frac{1}{p}, \dots, \frac{1}{p})$ (neutral element for \oplus),
- ▶ $-\mathbf{x} = \mathcal{C}(x_1^{-1}, x_2^{-1}, \dots, x_p^{-1})$ (inverse) such that $\mathbf{x} \oplus (-\mathbf{x}) = \mathbf{0}_{\mathcal{S}^p}$,
- ▶ $\mathbf{x} \ominus \mathbf{y} = \mathbf{x} \oplus (-\mathbf{y})$ (perturbation difference).

\odot satisfies the properties of an external product

If \mathbf{x}, \mathbf{y} in \mathcal{S}^p and a, b in \mathbb{R}

- ▶ $a \odot (b \odot \mathbf{x}) = (ab) \odot \mathbf{x}$ (associativity),
- ▶ $a \odot (\mathbf{x} \oplus \mathbf{y}) = (a \odot \mathbf{x}) \oplus (a \odot \mathbf{y})$ and $(a + b) \odot \mathbf{x} = (a \odot \mathbf{x}) \oplus (b \odot \mathbf{x})$ (distributivity),
- ▶ $1 \odot \mathbf{x} = \mathbf{x} \odot 1 = \mathbf{x}$ (neutral element for \odot).

Aitchison's geometry

Centered logratio

$$\text{clr}(\mathbf{x}) = \left(\ln \frac{x_1}{\bar{x}_G}, \ln \frac{x_2}{\bar{x}_G}, \dots, \ln \frac{x_p}{\bar{x}_G} \right),$$

- \bar{x}_G is the componentwise geometric mean of \mathbf{x}

$$\bar{x}_G = \left(\prod_{i=1}^p x_i \right)^{\frac{1}{p}} = \exp \left(\frac{1}{p} \sum_{i=1}^p \ln x_i \right).$$

- If $\text{clr}(\mathbf{x}) = \boldsymbol{\xi} = (\xi_1, \xi_2, \dots, \xi_p) \Rightarrow \xi_1 + \xi_2 + \dots + \xi_p = 0$.
- Remark: $\boldsymbol{\xi} \notin \mathcal{S}^p$.

Inverse centered logratio

If $\boldsymbol{\xi}$ satisfies $\xi_1 + \xi_2 + \dots + \xi_p = 0$ then

$$\text{clr}^{-1}(\boldsymbol{\xi}) = \mathcal{C}(\exp(\xi_1), \exp(\xi_2), \dots, \exp(\xi_p))$$

Aitchison's geometry

We already have \oplus, \odot . Now we need

Aitchison's inner product

$$\langle \mathbf{x}, \mathbf{y} \rangle_A = \langle \text{clr}(\mathbf{x}), \text{clr}(\mathbf{y}) \rangle,$$

$\langle \cdot, \cdot \rangle$ is the inner product in \mathbb{R}^p . Remark: \mathbf{x} and \mathbf{y} are **compositionally orthogonal** if $\langle \mathbf{x}, \mathbf{y} \rangle_A = 0$.

Aitchison's norm

$$\|\mathbf{x}\|_A = \|\text{clr}(\mathbf{x})\|_2,$$

$\|\cdot\|_2$ is the L^2 -norm in \mathbb{R}^p .

Aitchison's distance

$$d_A(\mathbf{x}, \mathbf{y}) = d_2(\text{clr}(\mathbf{x}), \text{clr}(\mathbf{y})),$$

$d_2(\cdot, \cdot)$ is the L^2 -distance in \mathbb{R}^p .

Aitchison's geometry

Orthonormal decomposition

- ▶ Since \mathbf{x} is constrained by $\sum_{i=1}^p x_i = \kappa \Rightarrow$ dimension of \mathcal{S}^p is $p - 1$.
- ▶ Let $\{\mathbf{b}_1, \mathbf{b}_2, \dots, \mathbf{b}_{p-1}\}$ be an orthonormal basis of $\mathcal{S}^p \Rightarrow \langle \mathbf{b}_i, \mathbf{b}_j \rangle_A = \langle \text{clr}(\mathbf{b}_i), \text{clr}(\mathbf{b}_j) \rangle = 0$ (1) when $i \neq j$ ($i = j$).
- ▶ Decomposition of $\mathbf{x} = (x_1^* \odot \mathbf{b}_1) \oplus (x_2^* \odot \mathbf{b}_2) \oplus \dots \oplus (x_{p-1}^* \odot \mathbf{b}_{p-1})$ where $x_i^* = \langle \mathbf{x}, \mathbf{b}_i \rangle_A = \langle \text{clr}(\mathbf{x}), \text{clr}(\mathbf{b}_i) \rangle$.

Isometric logratio (and inverse)

$$\text{ilr}(\mathbf{x}) = \mathbf{x}^* = (x_1^*, x_2^*, \dots, x_{p-1}^*)$$

- ▶ If \mathbf{B} is the $(p - 1, p)$ matrix in which rows are $\text{clr}(\mathbf{b}_i)$, then

$$\text{ilr}(\mathbf{x}) = \text{clr}(\mathbf{x})\mathbf{B}^\top.$$

- ▶ The composition coordinates \mathbf{x} can be obtained from the ilr-coordinates \mathbf{x}^* using

$$\text{ilr}^{-1}(\mathbf{x}^*) = \text{clr}^{-1}(\mathbf{x}^*\mathbf{B}) = \mathcal{C}(\exp(\mathbf{x}^*\mathbf{B})).$$

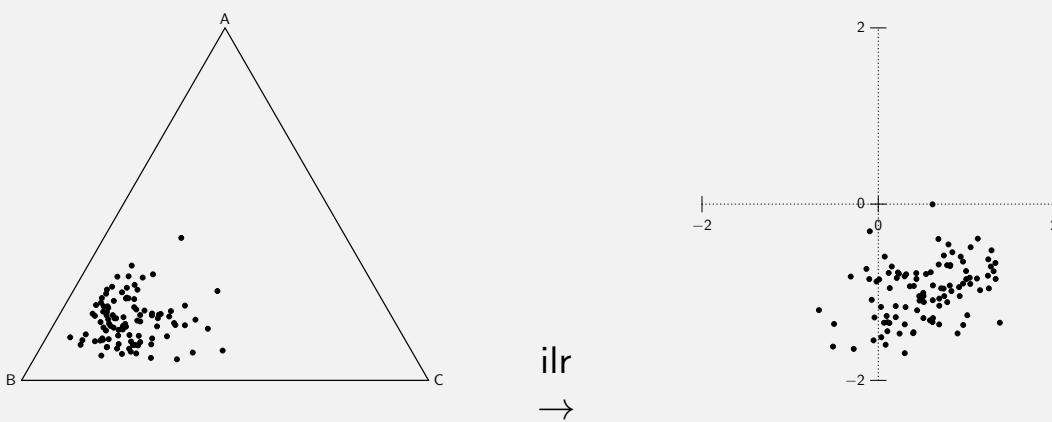
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Aitchison's geometry

Matrix \mathbf{B}

Many possible choices... A possible one is

$$B_{i,j} = \begin{cases} \sqrt{\frac{1}{(p-i)(p-i+1)}} & j \leq p-i \\ -\sqrt{\frac{p-i}{p-i+1}} & j = p-i+1 \\ 0 & j > p-i+1 \end{cases}$$



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MEWMA-CoDa chart

Assumptions

- ▶ At each sampling period $i = 1, 2, \dots$, we collect n independent observations $\{\mathbf{X}_{i,1}, \dots, \mathbf{X}_{i,n}\}$, where each $\mathbf{X}_{i,j} \in \mathcal{S}^p$, $j = 1, \dots, n$.
- ▶ $\mathbf{X}_{i,j}^* = \text{ilr}(\mathbf{X}_{i,j}) \in \mathbb{R}^{p-1}$ are the corresponding ilr coordinates.
- ▶ $\mathbf{X}_{i,j}^* \sim \text{MNor}_{p-1}(\boldsymbol{\mu}^*, \boldsymbol{\Sigma}^*)$, where $\boldsymbol{\mu}^*$ is the $(1, p-1)$ mean vector, $\boldsymbol{\Sigma}^*$ is the $(p-1, p-1)$ variance-covariance matrix.
- ▶ When the process is in-control the composition center is $\boldsymbol{\mu}_0$ (or, equivalently $\boldsymbol{\mu}_0^* = \text{ilr}(\boldsymbol{\mu}_0)$).
- ▶ When the process is out-of-control the composition center is $\boldsymbol{\mu}_1$ (or, equivalently $\boldsymbol{\mu}_1^* = \text{ilr}(\boldsymbol{\mu}_1)$).

Goal is to monitor the composition center $\boldsymbol{\mu}$ using a Multivariate EWMA control chart monitoring $\boldsymbol{\mu}^*$.

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MEWMA-CoDa chart

Monitored statistic

$$Q_i = \mathbf{Z}_i \boldsymbol{\Sigma}_Z^{-1} \mathbf{Z}_i^\top, i = 1, 2, \dots$$

with $\mathbf{Z}_i \in \mathbb{R}^{p-1}$ defined as

$$\mathbf{Z}_i = r(\bar{\mathbf{X}}_i^* - \boldsymbol{\mu}_0^*) + (1 - r)\mathbf{Z}_{i-1}, i = 1, 2, \dots$$

where $\mathbf{Z}_0 = \mathbf{0}$, $r \in (0, 1]$ is a smoothing parameter to be fixed and

$$\boldsymbol{\Sigma}_Z = \frac{r}{n(2-r)} \boldsymbol{\Sigma}^*.$$

Control limits

- ▶ Out-of-control signal when $Q_i > \text{UCL} = H$, where $H > 0$ is chosen to achieve a specified in-control ARL (difficult to compute).
- ▶ Non-centrality parameter $\delta = \sqrt{n(\boldsymbol{\mu}_1^* - \boldsymbol{\mu}_0^*)^\top (\boldsymbol{\Sigma}^*)^{-1} (\boldsymbol{\mu}_1^* - \boldsymbol{\mu}_0^*)}$.

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MEWMA-CoDa chart – Comparison with the T_C^2 chart

δ	$p = 3$	$p = 5$	$p = 10$	$p = 20$
$ARL_0 = 200$				
0.25	(64.6, 171.0)	(75.8, 181.0)	(91.1, 188.5)	(106.3, 192.7)
0.50	(26.4, 115.5)	(31.7, 138.1)	(39.6, 159.1)	(49.3, 172.7)
0.75	(15.1, 70.4)	(18.1, 94.4)	(22.8, 122.7)	(28.7, 145.0)
1.00	(9.9, 41.9)	(11.9, 61.0)	(15.0, 88.7)	(18.9, 115.2)
1.25	(7.1, 25.3)	(8.5, 38.7)	(10.7, 61.5)	(13.5, 87.6)
1.50	(5.4, 15.8)	(6.4, 24.6)	(8.1, 41.7)	(10.2, 64.4)
1.75	(4.3, 10.2)	(5.1, 16.0)	(6.4, 28.1)	(8.0, 46.4)
2.00	(3.5, 6.9)	(4.1, 10.6)	(5.2, 19.0)	(6.5, 33.0)
$ARL_0 = 500$				
0.25	(102.9, 416.4)	(126.1, 445.8)	(160.5, 467.4)	(197.5, 479.4)
0.50	(34.6, 265.7)	(41.8, 327.1)	(53.6, 385.5)	(69.3, 423.7)
0.75	(18.8, 151.9)	(22.6, 212.3)	(28.5, 287.3)	(36.0, 348.0)
1.00	(12.1, 84.9)	(14.4, 129.7)	(18.2, 199.1)	(23.0, 268.6)
1.25	(8.5, 48.3)	(10.1, 77.7)	(12.7, 131.8)	(16.1, 197.3)
1.50	(6.4, 28.3)	(7.6, 46.8)	(9.5, 85.1)	(11.9, 139.8)
1.75	(5.0, 17.3)	(5.9, 28.7)	(7.4, 54.5)	(9.3, 96.6)
2.00	(4.1, 11.0)	(4.8, 18.1)	(5.9, 35.1)	(7.4, 65.8)
$ARL_0 = 1000$				
0.25	(145.2, 816.8)	(184.1, 881.5)	(245.7, 929.2)	(315.8, 955.4)
0.50	(41.6, 499.9)	(50.7, 628.5)	(66.4, 753.4)	(88.9, 835.8)
0.75	(21.8, 272.9)	(26.0, 393.0)	(32.7, 547.6)	(41.6, 675.7)
1.00	(13.8, 145.9)	(16.3, 230.7)	(20.5, 368.1)	(26.0, 510.6)
1.25	(9.6, 79.4)	(11.3, 132.7)	(14.2, 235.5)	(17.9, 366.0)
1.50	(7.2, 44.6)	(8.4, 76.7)	(10.5, 146.8)	(13.2, 252.1)
1.75	(5.6, 26.1)	(6.5, 45.1)	(8.1, 90.7)	(10.2, 169.1)
2.00	(4.5, 15.9)	(5.3, 27.3)	(6.5, 56.3)	(8.1, 111.7)

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Incorporating measurement errors

In practice

- ▶ Sample reduces to $n = 1$.
- ▶ Each $\mathbf{X}_i \in \mathcal{S}^p$ cannot be observed!
- ▶ But can be measured m times $\rightarrow \mathbf{Y}_{i,1}, \dots, \mathbf{Y}_{i,m}$.

Linearly covariate measurement error model

$$\mathbf{Y}_{i,k} = \mathbf{a} \oplus (\mathbf{b} \odot \mathbf{X}_i) \oplus \varepsilon_{i,k},$$

- ▶ $\mathbf{a} \in \mathcal{S}^p$ and $\mathbf{b} \in \mathbb{R}$ are perturbation and powering constants,
- ▶ $\varepsilon_{i,k} \sim \text{MNOR}_{\mathcal{S}^p}(\mathbf{0}, \boldsymbol{\Sigma}_M^*)$ is an error term independent of \mathbf{X}_i .
- ▶ $\boldsymbol{\Sigma}_M^*$ is the known measurement error variance-covariance matrix.

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Incorporating measurement errors

Reduce the effect of measurement errors

Use

$$\begin{aligned}\bar{\mathbf{Y}}_i &= \frac{1}{m} \odot (\mathbf{Y}_{i,1} \oplus \cdots \oplus \mathbf{Y}_{i,m}) \\ &= \mathbf{a} \oplus (b \odot \mathbf{X}_i) \oplus \left(\frac{1}{m} \odot (\varepsilon_{i,1} \oplus \cdots \oplus \varepsilon_{i,m}) \right).\end{aligned}$$

We have $\bar{\mathbf{Y}}_i \sim \text{MNOR}_{\mathcal{S}^p}(\mu_{\bar{\mathbf{Y}}}^*, \Sigma_{\bar{\mathbf{Y}}}^*)$ with

$$\begin{aligned}\mu_{\bar{\mathbf{Y}}}^* &= \mathbf{a}^* + b\mu^*, \\ \Sigma_{\bar{\mathbf{Y}}}^* &= b^2\Sigma^* + \frac{1}{m}\Sigma_M^*.\end{aligned}$$

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MEWMA-CoDa chart with measurement errors

Monitored statistic

$$Q_i = \mathbf{Z}_i^* \Sigma_{\mathbf{Z}_i^*}^{-1} \mathbf{Z}_i^{*\top}$$

with $\mathbf{Z}_i^* \in \mathbb{R}^{p-1}$ defined as

$$\mathbf{Z}_i^* = r(\bar{\mathbf{Y}}_i^* - \mathbf{a}^* - b\mu_0^*) + (1-r)\mathbf{Z}_{i-1}^*$$

where $\mathbf{Z}_0 = \mathbf{0}$, $r \in (0, 1]$ is a smoothing parameter to be fixed and

$$\Sigma_{\mathbf{Z}_i^*} = \frac{r}{(2-r)} \Sigma_{\bar{\mathbf{Y}}^*} = \frac{r}{(2-r)} \left(b^2 \Sigma^* + \frac{1}{m} \Sigma_M^* \right).$$

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MEWMA-CoDa chart with measurement errors

Non-centrality parameter

$$\delta_M = b^2(\mu_1^* - \mu_0^*) \left(b^2 \Sigma^* + \frac{1}{m} \Sigma_M^* \right)^{-1} (\mu_1^* - \mu_0^*)^\top.$$

- ▶ Linna et al. (2001) “multivariate control charts are not equally powerful in detecting shifts in all directions in the presence of measurement errors” .
- ▶ For a fixed δ , $\delta_M \in [\delta_{\min}, \delta_{\max}]$ where $\delta_{\min} = \delta\lambda_1$ and $\delta_{\max} = \delta\lambda_{p-1}$.
- ▶ λ_1 (λ_{p-1}) is the smallest (largest) eigenvalues of the $(p-1, p-1)$ matrix $b^2 \Sigma^* (b^2 \Sigma^* + \frac{1}{m} \Sigma_M^*)^{-1}$.

Evaluation of the MEWMA-CoDa chart with measurement errors:
influence of σ_M , b and m ... Not presented here (boring).

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Illustrative example

The product

Muesli (for breakfast), where every 100 grams contain:

- A 66% of whole-grain cereals (barley flakes, oat flakes, wheat flakes),
- B 24% of dried fruits (raisin, papaya, banana),
- C 10% of nuts (almond, hazelnut, coconut).

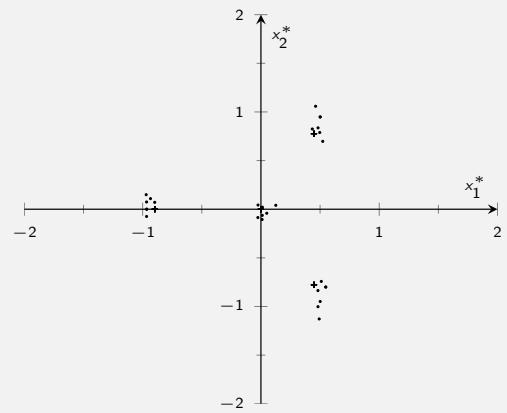
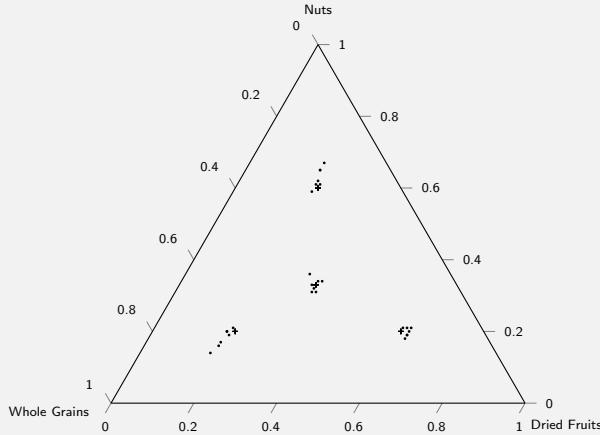
i	j	y_i			$x_{i,j}$			y_i^*		$x_{i,j}^*$	
1	1	0.33	0.33	0.33	0.34	0.33	0.33	0.0000	0.0000	0.0122	0.0211
	2				0.32	0.35	0.33			0.0115	-0.0634
	3				0.33	0.35	0.32			0.0491	-0.0416
	4				0.31	0.35	0.34			-0.0259	-0.0858
	5				0.36	0.34	0.30			0.1255	0.0404
	6				0.34	0.32	0.34			-0.0247	0.0429
	7				0.31	0.36	0.33			0.0100	-0.1057
2	1	0.60	0.20	0.20	0.62	0.19	0.19	0.4485	0.7768	0.4828	0.8363
	2				0.65	0.17	0.18			0.5009	0.9484
	3				0.59	0.22	0.19			0.5224	0.6976
	4				0.61	0.20	0.19			0.4971	0.7885
	5				0.67	0.15	0.18			0.4621	1.0583
	6				0.65	0.17	0.18			0.5009	0.9484
	7				0.61	0.19	0.20			0.4343	0.8248
3	1	0.20	0.60	0.20	0.17	0.65	0.18	0.4485	-0.7768	0.5009	-0.9484
	2				0.14	0.69	0.17			0.4926	-1.1279
	3				0.21	0.60	0.19			0.5103	-0.7423
	4				0.19	0.62	0.19			0.4828	-0.8363
	5				0.20	0.62	0.18			0.5479	-0.8000
	6				0.16	0.66	0.18			0.4823	-1.0020
	7				0.20	0.62	0.18			0.5479	-0.8000
4	1	0.20	0.20	0.60	0.18	0.20	0.62	-0.8970	0.0000	-0.9668	-0.0745
	2				0.19	0.19	0.62			-0.9657	0.0000
	3				0.21	0.19	0.60			-0.8980	0.0708
	4				0.21	0.18	0.61			-0.9336	0.1090
	5				0.20	0.18	0.62			-0.9668	0.0745
	6				0.19	0.19	0.62			-0.9657	0.0000
	7				0.21	0.17	0.62			-0.9702	0.1494

Phase 0 (calibration)

- ▶ $k = 4$ reference samples have been prepared with known percentages,
- ▶ measured $m = 7$ times.

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Illustrative example



Estimation of the measurement parameters

- ▶ $\hat{\mathbf{a}} = (0.3354, 0.3357, 0.3289)$ or $\hat{\mathbf{a}}^* = (0.0162972, -0.0006318)$,
- ▶ $\hat{b} = 1.1070$,
- ▶ $\hat{\Sigma}_M^* = \begin{pmatrix} 0.0014346 & 0.0007812 \\ 0.0007812 & 0.0102893 \end{pmatrix}$.

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Illustrative example

Phase 1 (in-control parameters estimation)

20 batches of muesli have been measured $m = 3$ times.

$$\hat{\mu}_{\bar{\mathbf{Y}}}^* = (1.2766, 0.7657) \quad \hat{\Sigma}_{\bar{\mathbf{Y}}}^* = \begin{pmatrix} 0.0146362 & 0.0105839 \\ 0.0105839 & 0.0510887 \end{pmatrix}$$

We deduce

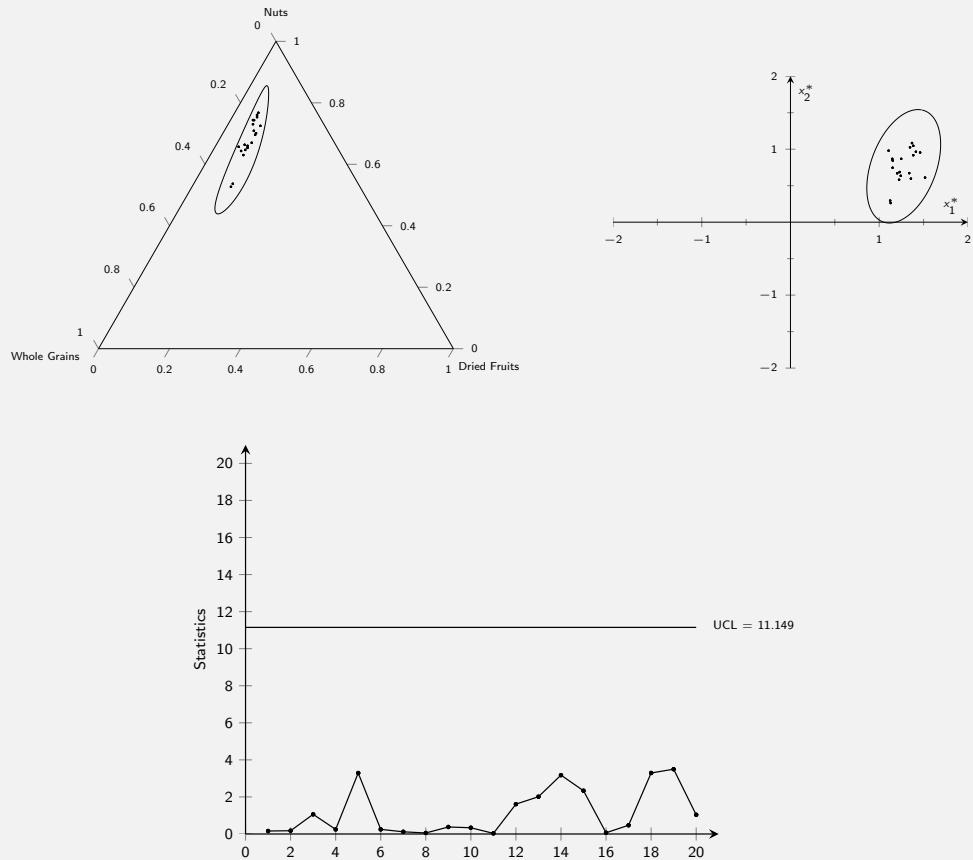
- ▶ $\hat{\mu}_0^* = \frac{1}{\hat{b}}(\hat{\mu}_{\bar{\mathbf{Y}}}^* - \hat{\mathbf{a}}^*) = (1.1385, 0.6922)$,
- ▶ $\hat{\Sigma}^* = \frac{1}{\hat{b}^2} \left(\hat{\Sigma}_{\bar{\mathbf{Y}}}^* - \frac{1}{m} \hat{\Sigma}_M^* \right) = \begin{pmatrix} 0.0115533 & 0.0084242 \\ 0.0084242 & 0.038891 \end{pmatrix}$.

Upper control limit

The optimal couple for $\delta = 1.5$ is ($r = 0.226$, UCL = $H = 11.149$).

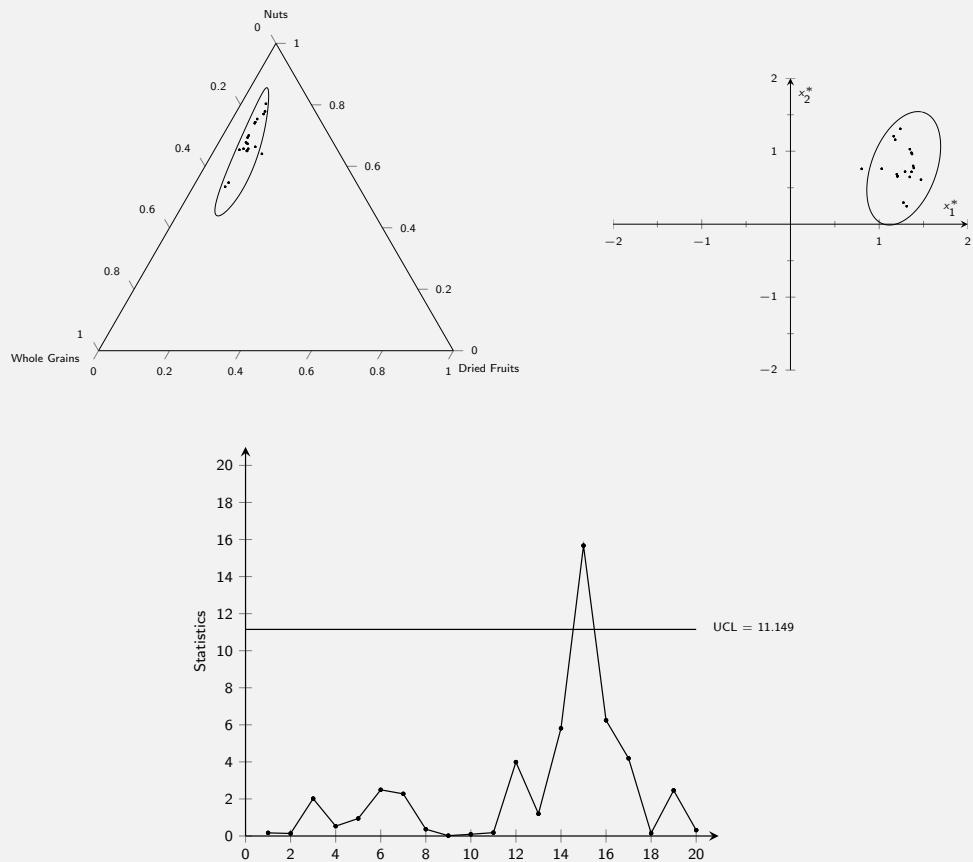
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Illustrative example



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Illustrative example



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THANK YOU FOR YOUR ATTENTION



K.P. Tran, P. Castagliola, G. Celano, M.B.C Khoo. Monitoring Compositional Data using Multivariate Exponentially Weighted Moving Average Scheme. Quality and Reliability Engineering International, 34(3):391-402, 2018.