Challenges of Virtual Testing in Statistical Quality Control of Railway Ballast

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Why SPC of railway ballast?

Source: www.erdwissen.ch

- Technical aspect
  - Forces act on the track bed
  - Attrition

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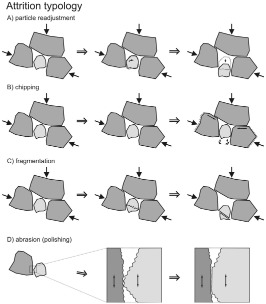

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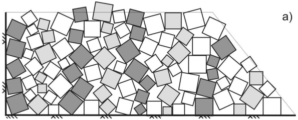
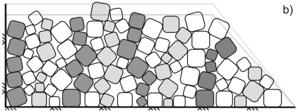


perfectly angular particles



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- Volume loss of particles 5,4%
- Volume loss of heap 10,5%

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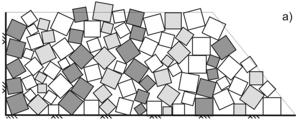

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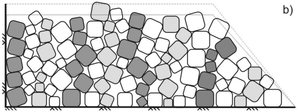

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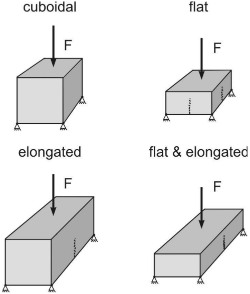

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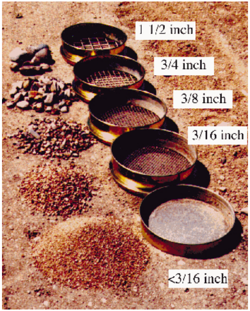

Problem of determining geometry, rock type, mechanical properties (abrasion, fragmentation, resistence to wear)

- Manual tests time consuming and expensive
- Laboratory for mechanical properties (LA value, other measures)

Why SPC of railway ballast?

www.pavementinteractive.org

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Objective: Replace manual tests by statistical prediction (= “virtual testing”)

Virtual testing

www.pavementinteractive.org

Major task:

- Prediction of mechanical properties Y (for example LA value)
  - Rock type X_1
  - Shape X_2
  - Size X_3
  - Angularity X_4

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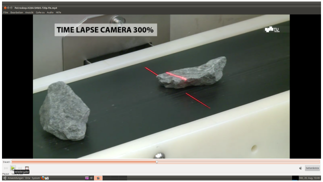

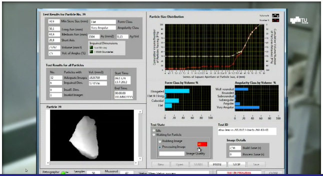

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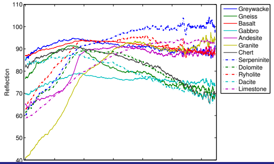

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  - Mechanical properties Y are measured samplewise (several hundered particles

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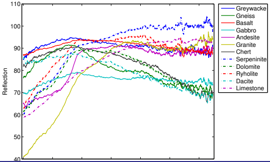

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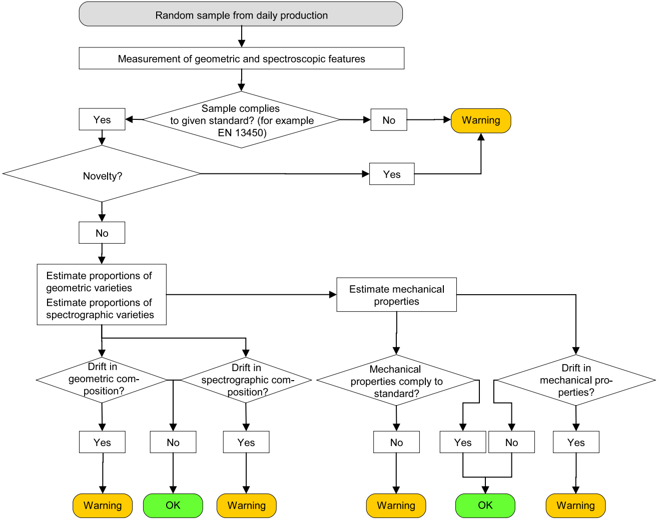
Statistical monitoring system



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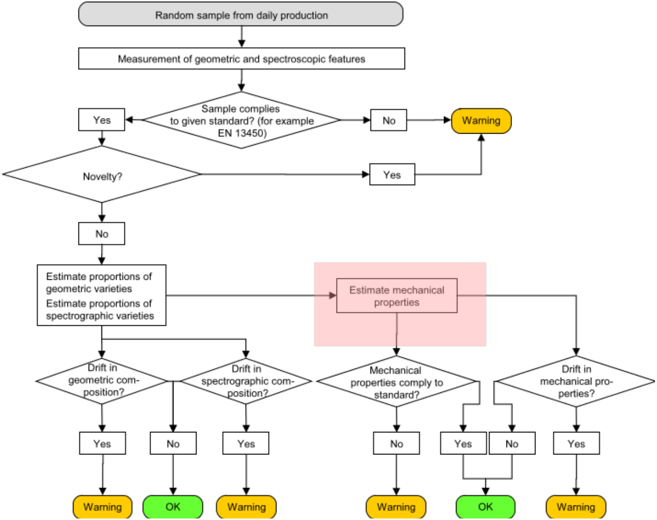

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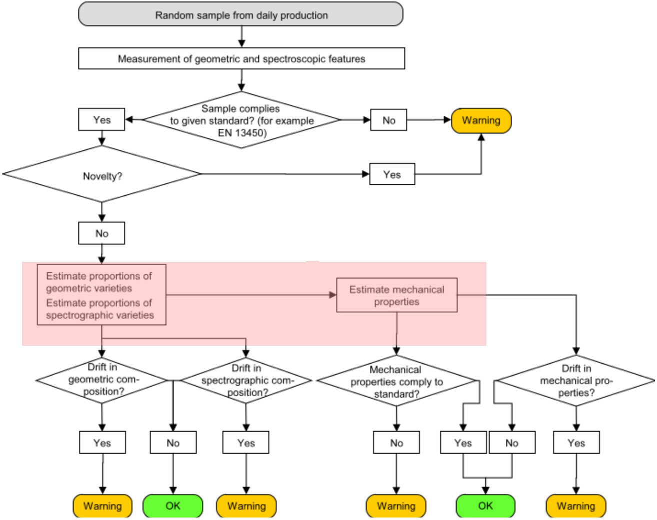

Compositional data approach

- Aggregation of particlewise geometric property X_i for sample $j = 1, 2, \ldots$ to the samplewise feature $\mathbf{p}_i = (p_{i1}, p_{i2}, \ldots, p_{iL})$ with

$$\sum_{j=1}^{L} p_{ij} = 1$$

- Raw data are continuous features: no direct aggregation!
  - Cluster analysis to determine geometric similarity classes and classification of new sample into these classes
  - Classification of spectroscopic data into rock classes
  - Determine distribution vectors $\mathbf{q}_i$ for rock composition and $\mathbf{p}_i$ for geometric composition

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Compositional data versus multivariate data

- Negative bias: For $X = (X_1, \ldots, X_L)$ with $\sum_{i=1}^{L} X_i = 1$

$$
\begin{aligned}
Cov(X_1, \sum_{i=1}^{L} X_i) &= Cov(X_1, 1) = 0 \\
\sum_{i=2}^{L} Cov(X_1, X_i) &= -Var(X_1)
\end{aligned}
$$

- Spurious correlation

Compositional data versus multivariate data

- Negative bias
- Spurious correlation: correlation of the ratios X/Z and Y/Z of three uncorrelated random variables will not be uncorrelated (Pearson, 1897)
- Euclidean distance can be larger in a subspace than for the full composition

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Compositional data analysis!

Pioneer

Prof. Aitchison

Source: Wikipedia

Isometric log-ratio (ilr) transform

- Let **p** be a compositional data vector in the simplex

$$\mathbb{S}^L = \left\{ \mathbf{p} = (p_1, \ldots, p_L) \in [0,\, 1]^L \;\middle|\; \sum_{i=1}^{L} p_i = 1 \right\}$$

- ilr transformation: $ilr : \mathbb{S}^L \longrightarrow \mathbb{R}^{L-1}$

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where $\boldsymbol{\Psi}$ is the $L \times (L-1)$ Helmert matrix with normalised columns

$$\boldsymbol{\Psi} = \begin{pmatrix} \frac{L-1}{\sqrt{L(L-1)}} & 0 & \cdots & 0 & 0 \\ -\frac{1}{\sqrt{L(L-1)}} & \frac{L-2}{\sqrt{(L-1)(L-2)}} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{-1}{\sqrt{L(L-1)}} & \frac{-1}{\sqrt{(L-1)(L-2)}} & \cdots & \frac{-1}{\sqrt{6}} & \frac{-1}{\sqrt{2}} \end{pmatrix}$$

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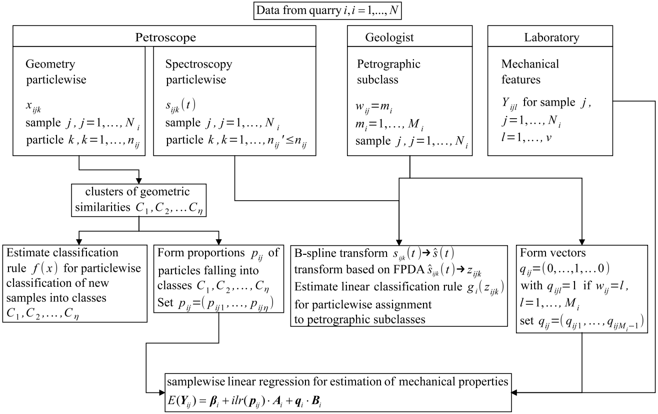
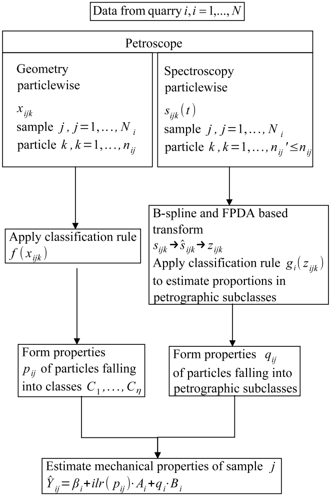
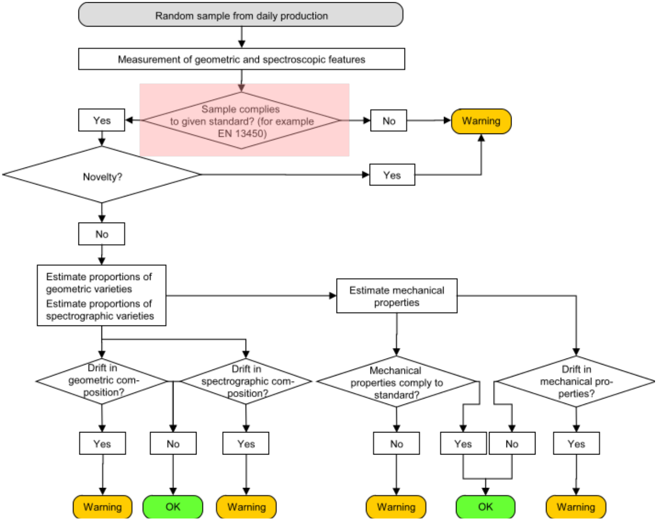
Statistical modelling



Statistical prediction



Statistical monitoring system



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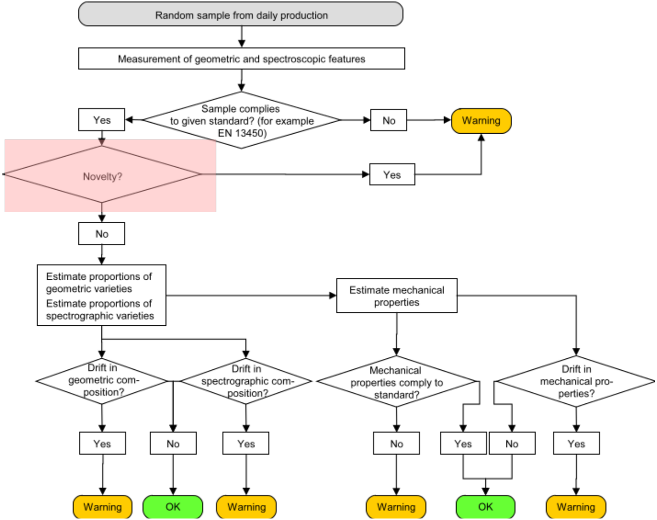

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One-class support vector machines

- Decision rule

$$g_i(\mathbf{z}) = \mathrm{sign}\left(\sum_{j=1}^{N_i}\sum_{k_2=1}^{n'_{ij}} \theta_{ijk_2} K(\mathbf{z}, \mathbf{z}_{ijk_2}) - \theta_0\right)$$

with $g_i(\mathbf{z}) = +1$ for ‘regular’ data and $g_i(\mathbf{z}) = -1$ for ‘novel’ data is estimated.

- $K(\cdot,\cdot)$ denotes the radial kernel

$$K(\mathbf{z}, \mathbf{z}_{ijk_2}) = e^{\delta \, \|\mathbf{z}-\mathbf{z}_{ijk_2}\|^2}$$

with parameter δ.

One-class support vector machines

Solve the minimisation problem

$$\min_{\boldsymbol{\theta}_\mathbf{i}} \quad \frac{1}{2} \sum_{j,j'=1}^{N_i} \sum_{k_2,k_2'=1}^{n'_{ij}} \theta_{ijk_2} \theta_{ij'k_2'} K(\mathbf{z}_{ijk_2}, \mathbf{z}_{ij'k_2'})$$

$$\text{s.t.} \quad \sum_{j=1}^{N_i} \sum_{k_2=1}^{n'_{ij}} \theta_{ijk_2} = 1$$

$$0 \leq \theta_{ijk_2} \leq \frac{1}{\rho\, n'_i} \qquad n'_i = \sum_{j=1}^{N_i} n'_{ij}$$

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$\rho \in]0,\, 1]$ is an upper bound on the number of training points outside the location of 'regular' data points.

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θ_0 is derived for a point with $0 < \theta_{ijk_2} < \frac{1}{\rho\, n'_i}$ as

$$\theta_0 = \sum_{j'=1}^{N_i} \sum_{k_2'=1}^{n'_{ij}} \theta_{ij'k_2'} K(\mathbf{z}_{ij'k_2'}, \mathbf{z}_{ijk_2}) \, .$$

Statistical monitoring system