Doing statistics of (grain size) distributions

(or why doing it easy if it can be infinitely complicated?)

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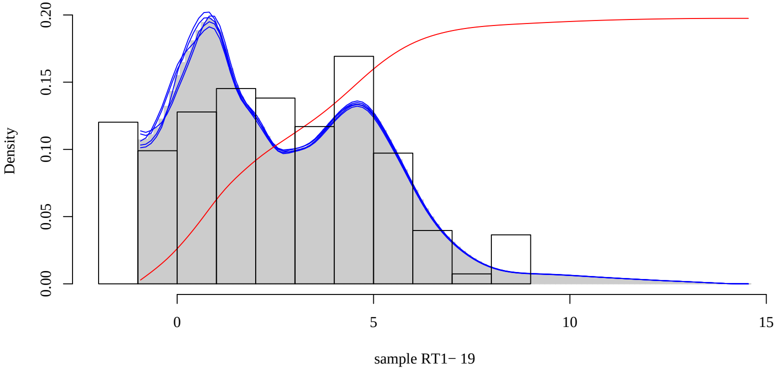
Sedi-Seminar
6 November 2007

outline

1. grain-size distribution characterization
2. geometry and statistics of distributions
   - characteristics
   - CoDa analysis
   - Hilbert space
3. application
   - generalities
   - a glacial data set from the Aar-Gotthard massif (Alps)
   - the Darss sill data set
4. final comments

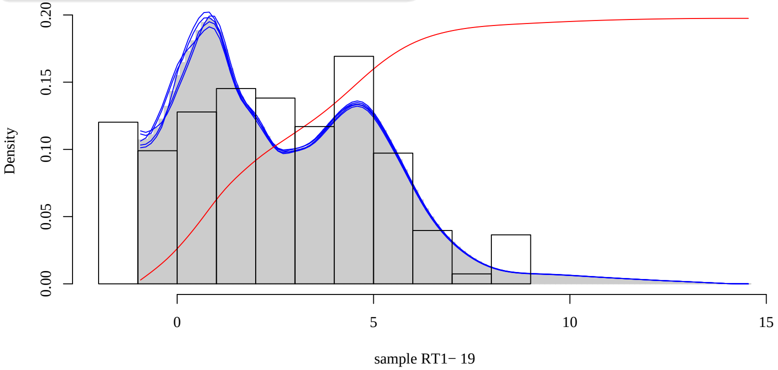
a grain-size distribution example



a grain-size distribution example

two measurement types

- quasi continuous LPS (x 5)
- binned sieve data



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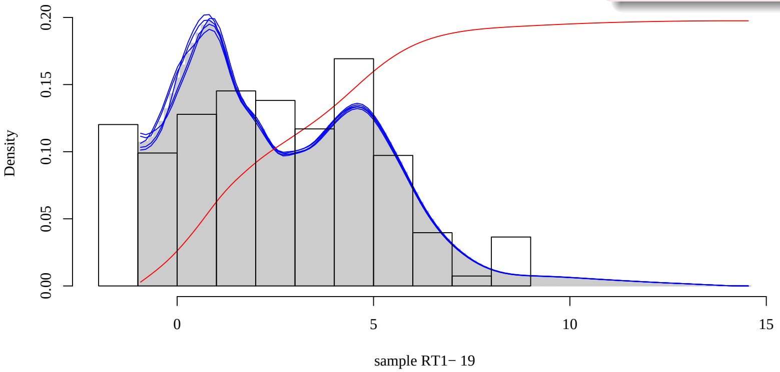

distribution!

- increasing
- bounded in [0,1]

traditional procedure (Folk, 1979; *Petrology of Sedimentary Rocks*)

1. compute the cummulative curve (distribution)
2. read some quantiles form the line, and derive distribution measures:

- central tendency
  - mode: most frequent ϕ
  - median: ϕ_{50}
  - $\frac{1}{2}(\phi_{16} + \phi_{84})$
  - combined $\frac{1}{3}(\phi_{16} + \phi_{84} + \phi_{50})$
- sorting
  - interquartile range: $\frac{1}{2}(\phi_{75} - \phi_{25})$ (bad)
  - $\frac{1}{2}(\phi_{84} - \phi_{16})$
  - combined $\frac{1}{4}(\phi_{84} - \phi_{16}) + \frac{1}{6.6}(\phi_{95} - \phi_{5})$
- skewness
- kurtosis

Argument: *statistics require many calculations* !

- computers are here to do some dirty work

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- it must be positive
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- continuous vs. discontinuous
- smooth curve vs. fractal character (extreme irregularity)
- symmetry vs. skewness
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  - a *subjective* assessment of the difference between two values
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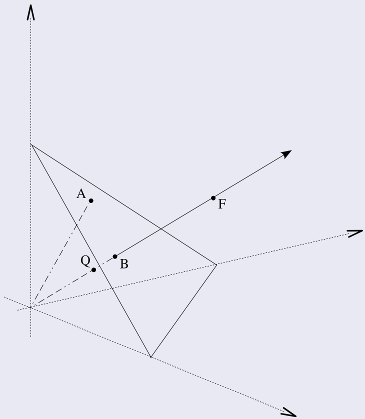

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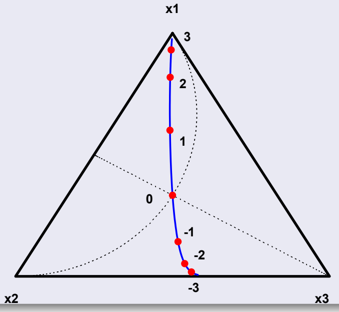

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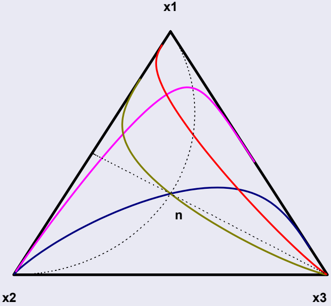
parallel and orthogonal lines



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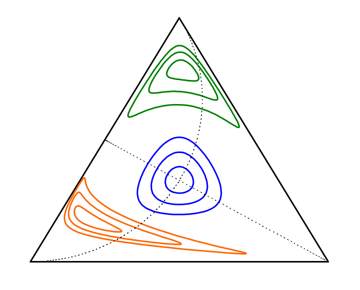
ellipses and circles



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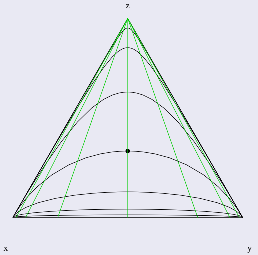

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  - centered log-ratio transformation:
    $\mathrm{clr}(\mathbf{x}) = \ln \frac{\mathbf{x}}{\sqrt[D]{\prod_i x_i}} = \ln(\mathbf{x}) - \frac{1}{D} \sum_i \ln x_i$

from compositions to distributions

distributions: *compositions of infinite parts*

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- its scale is ?

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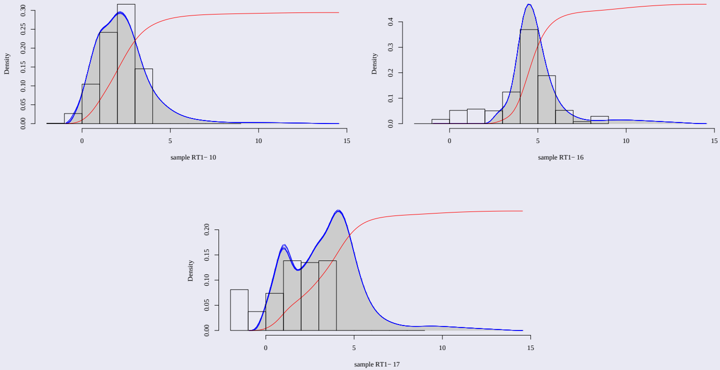
how do we compare grain-size curves?



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- clr transformation

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the Hilbert space of distributions: basis and coordinates

- infinite dimension $\Rightarrow$ infinite coordinates, infinite elements in a basis
- orthonormal:

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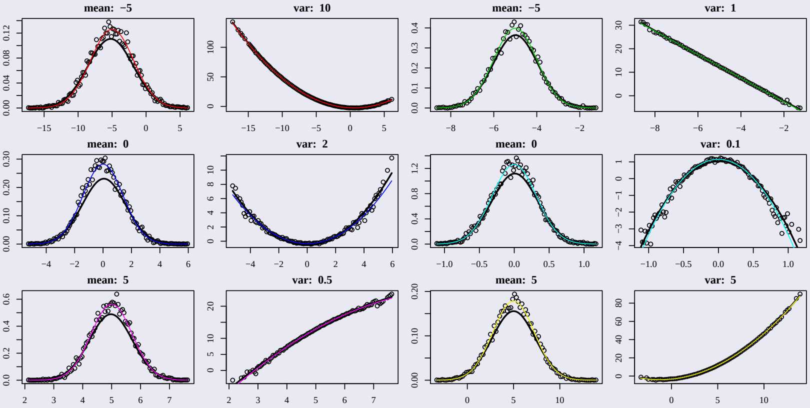
- coordinates
  - Hermite polynomials: $\frac{\mu}{\sigma^2}$, $\frac{\sigma^2-1}{\sqrt{2}\sigma^2}$, etc. (deviation from normality)
  - Laguerre polynomials: $\lambda - 1$

example of Hermite polynomials

- polynomials: $H_0 = 1,\ H_1 = x,\ H_2 = \frac{1}{\sqrt{2}}(1 - x^2)$
- decomposition: $\phi(x;\mu,\sigma) = \phi(x;0,1) \oplus \frac{\mu}{\sigma^2} \odot e^{H_1} \oplus \frac{\sigma^2 - 1}{\sqrt{2\sigma^2}} \odot e^{H_2}$



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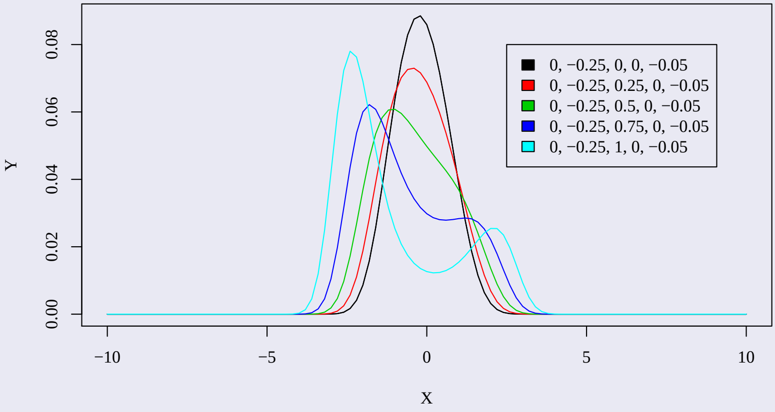

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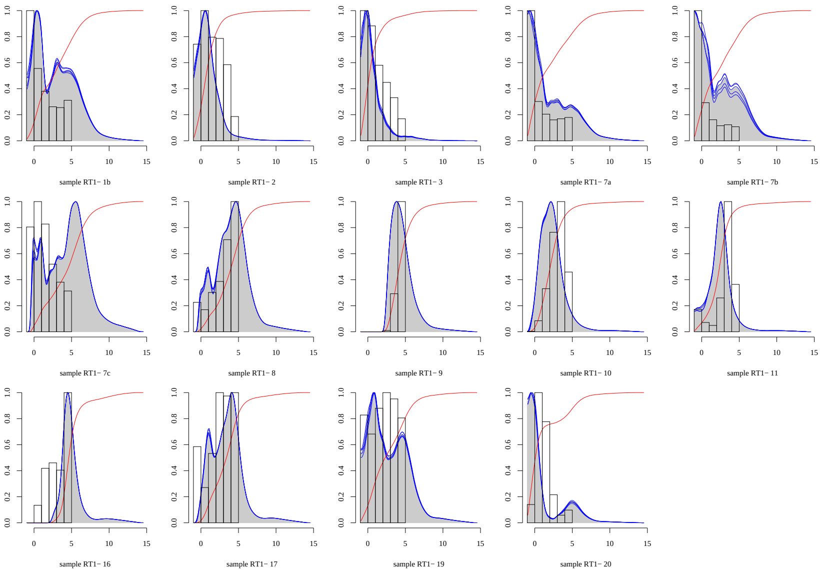
6. apply the method you want to $\hat{\beta}$
   - principal component analysis, non-supervised classification
   - mapping

a glacial data set from the Aar-Gotthard massif (Alps)

goal and location

- characterize the effect of (weathering and) comminution on grain-size/geochemistry/mineralogy compositions
- focus: comminution $\sim$ glacial comminution (fluvial sorting)
- Aar-Gotthard granitic massif, central Alps (Switzerland); Rhone Gletscher, Damma Gletscher, Tiefer Gletscher
- fluvial sediments, recent central morraines, older lateral morraines
- grain size analyses:
  - laser particle sizer (LPS), 116 classes of $\phi \in [-0.865, 14.61]$
  - sieves, 11 classes from $\phi < -1$ to $\phi > 8$
- analyses of major oxides and trace element geochemistry (not now)

measured densities



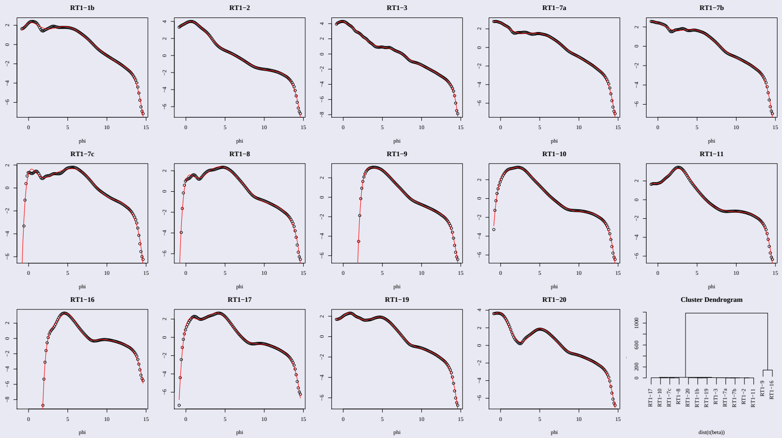
measured densities

summary of characteristics

sample	glacier	placement	coarsest	modes	finest
1b	Rhone	side	yes	2	yes
2	Rhone	side	yes	1	no
3	Rhone	side	yes	1	no
7a	Damma	side (older)	yes	3	yes
7b	Damma	side (older)	yes	3	no
7c	Damma	side (older)	yes	many	yes
8	Damma	side (older)	yes	2	yes
9	Damma	front	no	1	yes
10	Damma	front	yes	1	no
11	Damma	front	yes	1	no
16	Rhone	washed	no	1	yes
17	Rhone	washed	yes	2	yes
19	Tiefer	front	yes	2	yes
20	Tiefer	front	yes	2	no

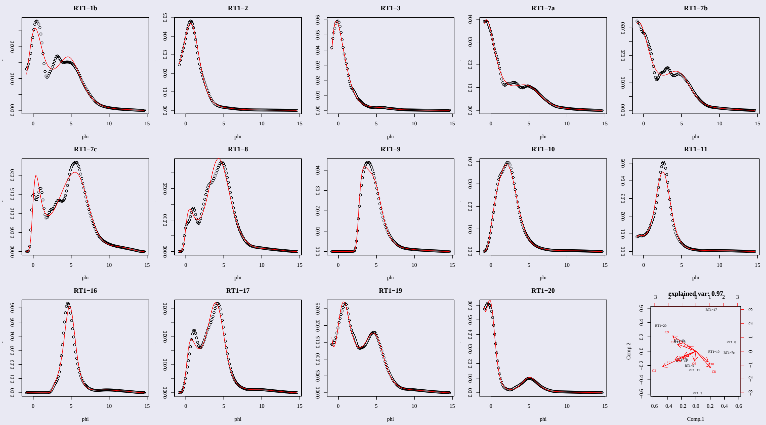
clr-transformed densities

fitted model: 11 Laguerre polynomials (exponential reference)



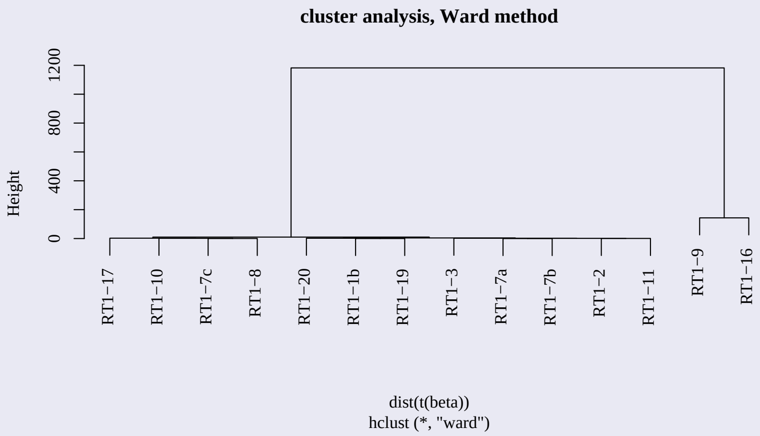
original densities

fitted model: 11 Laguerre polynomials (exponential reference)

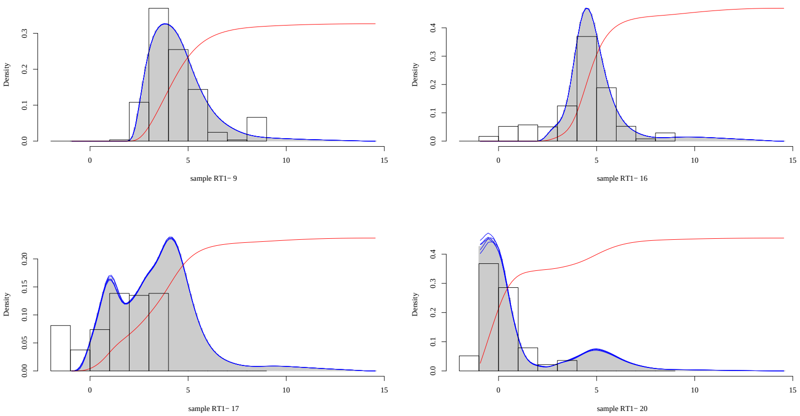


comparing densities: cluster analysis of $\hat{\beta}$'s

non-supervised classification: Ward cluster analysis



comparing densities: 9 and 16 against the other?

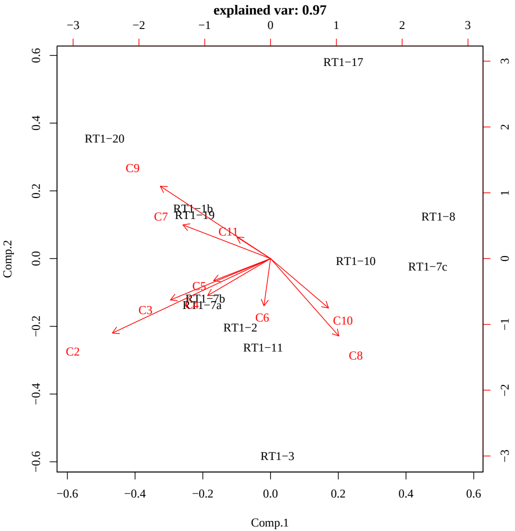


comparing densities: a "map" of differences

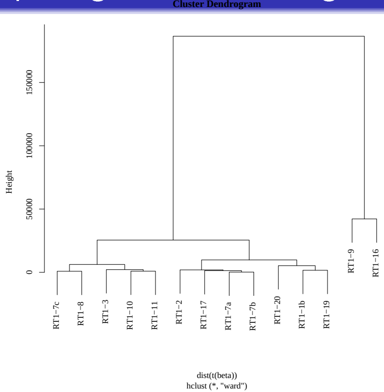
characteristics

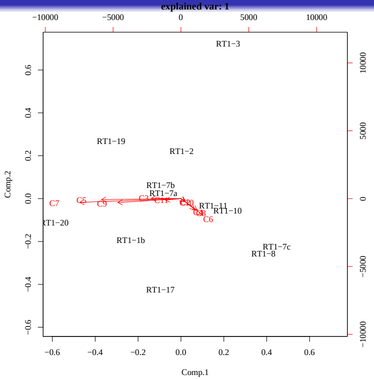
- morraines:
  - old side: 7(a,b,c), 8
  - recent side: 1b, 2, 3
  - front: (9) 10, 11, 19, 20
  - washed sediment: (16) 17
- unimodal: 2, 3, 10, 11
- tail to finest:
  - heavy: 7c, (16), 17, 19
  - yes: 1b, 7a, 8, (9)
  - no: 2, 3, 7b, 10, 11, 20

C2: pure exponential



comparing densities using the normal reference





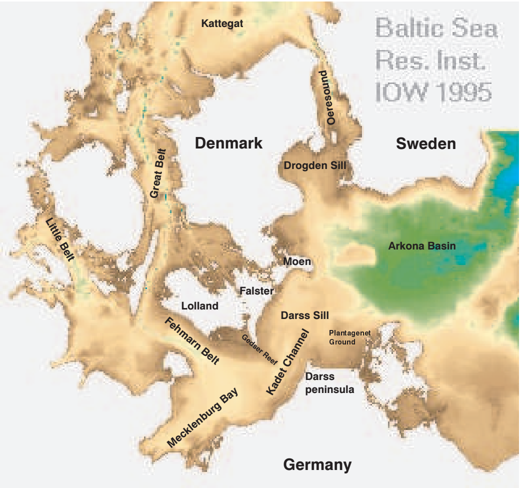
characteristics

old side morraines: 7(a,b,c), 8; recent side: 1b, 2, 3; front: (9) 10, 11, 19, 20; washed sediment: (16) 17

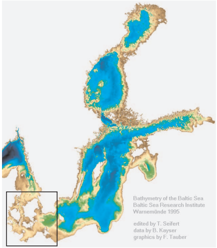
heavy tail to finest: 7c, (16), 17, 19; some fine: 1b, 7a, 8, (9); no fine: 2, 3, 7b, 10, 11, 20

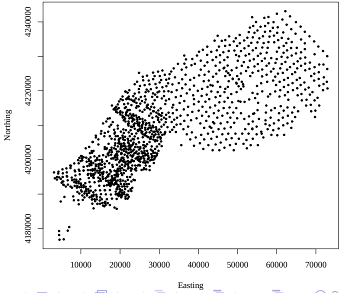
unimodal: 2, 3, 10, 11; C2: mean; C3: inverse variance

the Darss sill data set



Investigation area





the Darss sill data set

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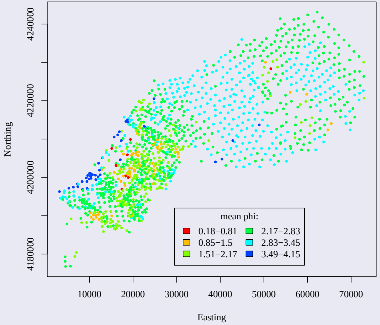
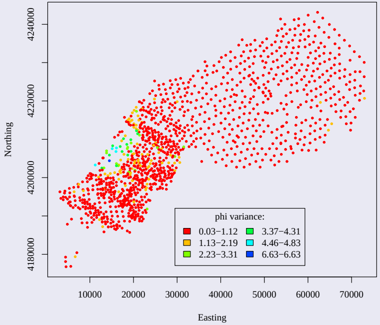
- Baltic Sea (412,560 km^2): world large brackish water bodies
- oceanographic conditions controlled by: (i) large river freshwater input, (ii) restricted ocean connections (Danish Straits)
- $\sim 73\%$ of water exchange is via the Darss Sill (minimum water depth: 18 m bsl)
    - prevailing outflow of brackish Baltic waters in the upper part of the water column usually along the Danish coast
    - inflow of more saline water in the southern part of the area and in the deeper part of the Kadet Channel
    - tidal currents are negligible; sediment-transporting bottom currents are intermittent
    - outcropping till genetically related to an ice marginal zone, short re-advance of the retreating Late Weichselian ice sheet ($\sim$ 13,500 years BP); thin cover of lag sediments (locally, stones and blocks $>$ 1 m)

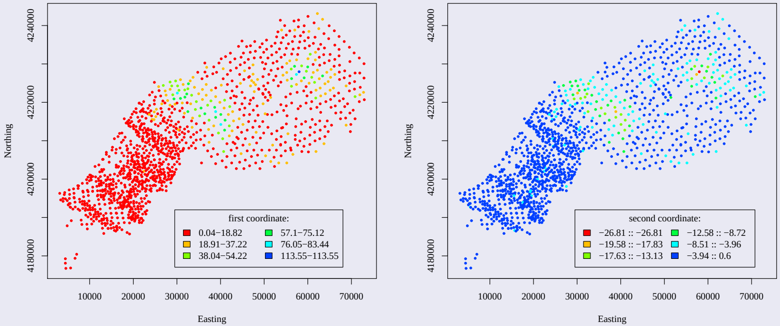
conventional analysis: average (μ) and sorting (σ^2)





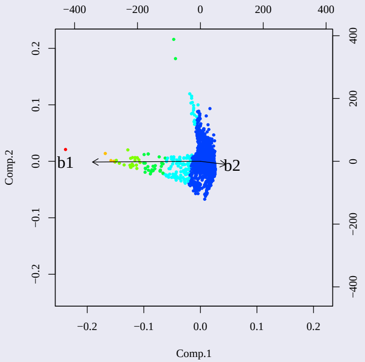
- Kadet Channel, Danish coast ($\uparrow \bar{\phi}; \uparrow \sigma^2_\phi;$)
- Kadet Channel, German coast ($\sim \bar{\phi}; \downarrow \sigma^2_\phi;$)
- Ground, Plantagenet basin? ($\uparrow \bar{\phi}; \downarrow \sigma^2_\phi;$)
- Bar, Darss Sill itself? ($\downarrow \bar{\phi}; \downarrow \sigma^2_\phi;$)

proposed analysis (I): average ($\beta_1 = \frac{\mu}{\sigma^2}$) and sorting ($\beta_2 = \frac{\sigma^2 - 1}{\sqrt{2}\sigma^2}$)



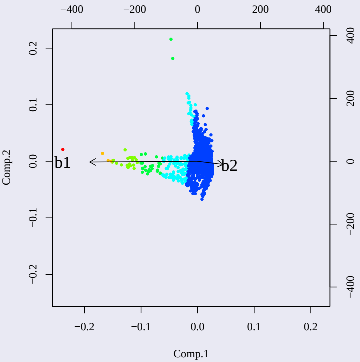
- two areas with extremely low variance ($\downarrow\downarrow \sigma^2_\phi$;)
- undiscriminated ground ($\sim \sigma^2_\phi$;)

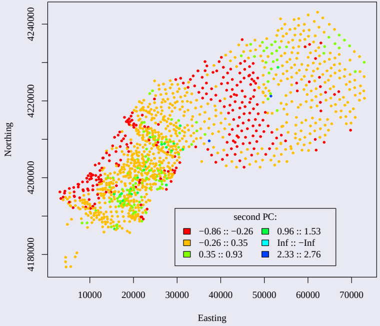
proposed analysis (II): a non-redundant characterization



- β_1 and β_2 almost proportional (inverse)

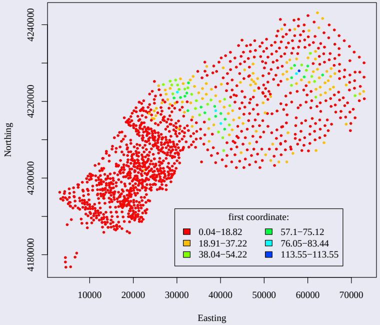
proposed analysis (II): a non-redundant characterization

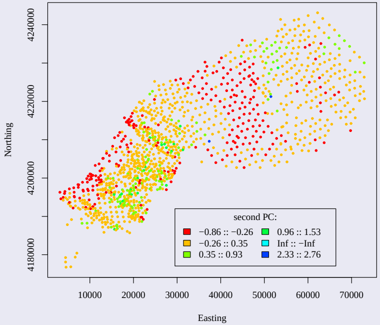




- β_1 and β_2 almost proportional (inverse)
- complementary direction to $\beta_1 || \beta_2$ (non-normality?)

proposed analysis (II): a non-redundant characterization





- Kadet Channel, Danish coast (low departure)
- Kadet Channel, German coast (average departure)
- two singular areas (extreme sorting, average-high departure)
- undiscriminated ground (low departure) $\sim$ Danish coast

final comments

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    - high-dimensional
    - further structure (ordered bins, smoothness)
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3. these parameters may be statistically treated
   - to uncover groups (cluster)
   - to display patterns of variation (biplot)
   - to explain them (regression, anova)
   - to make several measures compatible (weighted average)