TU Bergakademie Freiberg
Institute of Stochastics
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WiSe 2020/21

Programming project

within the module

Stochastic Methods for Materials Science

Preliminaries

The programming project is an essential part of the module *Stochastic Methods for Materials Science*, it is marked and contributes 50% to the final grade. It has to be finished and submitted via OPAL **not later than 23rd March, 2021, 23:59**.

The programming project contains **four tasks** addressing several aspects of the lecture, in particular its application. You can use all code of the R script files provided during the lectures. In so far it would be natural that you use R for solving the tasks.

For the examination of your solution of the project tasks it is expected that you **provide one (compressed) file** including

- the self-written code pieces (`.r` script files), and,
- the answers of the tasks (beyond programming) in text form (`.pdf` file) including requested plots.

Please read the tasks carefully in order that you do not miss to answer everything.

In case that you feel that the formulation of a task is not precise enough or that you need some advice for realizing the tasks, please, **do not hesitate to contact me for a consultation**.

Along with the tasks you find three individual images of random structures as `.png` images. In the below tasks the placeholder `ID` in the image file names has to be replaced by your individual two-digits number. In all images the phase of white pixels / pixels of value 1 represent the set of interest.

You also find two R script files which contain needed R packages (`libs.r`) as well as needed R functions (`fcts.r`) (covers a part of the R script files provided during the lectures but contains also further functions).

If you want to save a plot in R you can either use the export button in the graphics window in RStudio or directly write it into (for instance) a `.png` file by running

```
png(file = "myplot.png", width = 480, height = 480)
plot(...)
dev.off()
```

see also the help `?png` for further options.

Task 1 (2+5+3 points + 2 points for suitable R code)

Consider the realizations of 2D random sets given by `image1_ID.png` and by `image2_ID.png`. (The dimensions of the images are both 400 by 400 pixels; the pixel length (`spacing`) is 0.025 mm.)

a) Write down at least two discernible similarities or differences.

b) Estimate each the three Minkowski functions, plot each the first Minkowski function, the second Minkowski function and the third Minkowski function of both sets jointly in one plot and add the plots to your report.

c) Describe important similarities or differences between the Minkowski functions of both structures and explain by means of the images possible reasons for that.

Useful R functions: `readImage` (package `EBImage`), `display` (`EBImage`), `estALXFct`, `plotALXFct`

Task 2 (4+8 points + 2 points for suitable R code)

Someone claims that the structure in the first image `image1_ID.png` can be modelled by a Boolean model with a uniformly oriented deterministic rectangular typical grain. This sounds reasonable. Denote by λ the intensity of the Boolean model, by a the length of the longer side and by b the length of the shorter side of the rectangular typical grain.

a) In order get some idea of b do the following. Apply morphological openings to the image with a disc for several radii. Start with the smallest possible radius (unit: number of pixels) and increase it stepwise. Each time inspect the morphological opening. The (true) disc diameter (unit: number of pixels multiplied by pixel length) where a considerable part of the supposed rectangular grains vanishes for the first time is a good measure of the length of the shorter side. Report the morphological openings and your guess for b.

b) Two persons determine estimates of the model parameters of the Boolean model with a uniformly oriented deterministic rectangular typical grain:

   Person A: $\hat{\lambda} = 4.7$, $\hat{a} = 1.71$, $\hat{b} = 0.15$

   Person B: $\hat{\lambda} = 5.1$, $\hat{a} = 1.98$, $\hat{b} = 0.11$

   Apply each the global rank envelope test with $m = 999$ repetitions with one suitable functional characteristic (and an appropriately chosen range) in order to check the goodness of the proposed models A and B. Report each the p-value. Report your decision about the goodness of the model at significance level $\alpha = 0.05$. Report also each a plot of the global envelopes for $\alpha = 0.05$ based on $m = 999$ repetitions and comment on the plots.

Useful R functions: `readImage` (`EBImage`), `makebrush` (`EBImage`), `opening` (`EBImage`), `display` (`EBImage`), `writeImage` (`EBImage`), `rBM.rect.const`, `digitizeRectSys`, `estALXFct`, `globalTest`, `globalEnvelopes`

Task 3 (2+6+4+2 points + 2 points for suitable R code)

Consider the random set realization given by `image3_ID.png` (1400 by 1400 pixels). It is known that this image represents a 2D section of a 3D structure consisting of spherical grains. (Although not important you might assume that the length of one pixel corresponds to 0.001 mm.)

a) Estimate the volume fraction V_V and (under the assumption of isotropy) the specific surface area S_V of the underlying 3D structure and report the values.

b) Apply a segmentation algorithm and, considering the segmented components as ideal discs, determine their centres and diameters. Determine the range of diameters and report it. For further processing apply the idea of minus sampling and restrict to those discs which are completely inside the original window and have their centre inside some previously specified rectangular sub-window. Report the number of all such discs, the histogram of their diameters for a reasonable binning as well as the empirical mean and the empirical standard deviation of these diameters.

c) Apply Saltykov's method. That is, determine the absolute frequencies of disc diameters in 2D per unit area for an appropriate choice of equal-sized bins. Use then Saltykov's method to obtain the absolute frequencies per unit volume for the (unobservable) diameters of the underlying balls in 3D. Report a plot of the obtained (3D) frequencies.

d) Provide estimates of the intensity λ_V (mean number of balls per unit volume) and the mean ball diameter μ_V.

Useful R functions: `readImage` (EBImage), `estALX`, `bwlabel` (EBImage), `computeFeatures.moment` (EBImage), `range`, `hist`, `sum`, `saltykov`, `barplot`

Task 4 (6 points + 2 points for suitable R code)

Consider the Matérn III hard-disc model (in 2D) with parameters λ_{Poi} (intensity of the underlying Poisson point process) and R (radius of the equal-sized discs). Unfortunately, no analytical expression for any of the usual characteristics in dependence of λ_{Poi} and R is known. Because of that a Monte Carlo approach is appropriate to get information on the three quermass densities A_A, L_A and χ_A.

Choose a window of size 10 by 10 and a radius $R = 0.05$.
Each for the values 5, 10 and 15 for λ_{Poi}

- generate 100 realizations of the Matérn III hard-disc model,
- digitize them with a pixel length of 0.01 (`spacing=0.01`),
- estimate from the digitized images each A_A, L_A and χ_A (leading to each 100 estimates $\hat{A}_{A,i}$, $\hat{L}_{A,i}$, $\hat{\chi}_{A,i}$, $i = 1, \ldots, 100$),
- determine each from the 100 estimates the empirical mean (= Monte Carlo estimate) and the empirical standard deviation and report the values,
- determine each from the 100 estimates a boxplot and report it.

Useful R functions: `rM3.disc.const`, `digitizeDiscSys`, `estALX`, `mean`, `sd`, `sapply`, `boxplot`