STOCHASTICS FOR MATERIAL SCIENCE

PROGRAMMING ASSIGMENT

TECHNISCHE UNIVERSITÄT
BERGAKADEMIE FREIBERG
Die Ressourcenuniversität. Seit 1765.

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COMPUTATIONAL MATERIAL SCIENCE

65074

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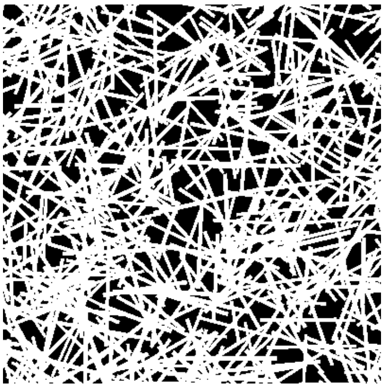
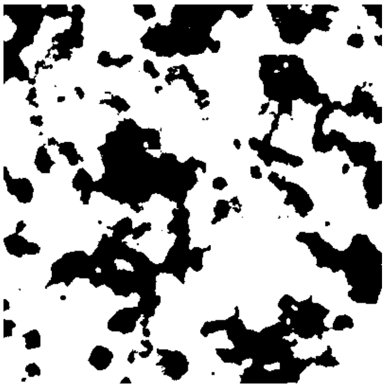
1. **Task-1** :Consider the realizations of 2D random sets given by image1_S04 and by image2_S04 (The dimensions of the images are both 400 by 400 pixels; the pixel length (spacing) is 0.025 mm.)



(a) image1_S04



(b) image2_S04

Figure 1: Realizations of 2D Random sets

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

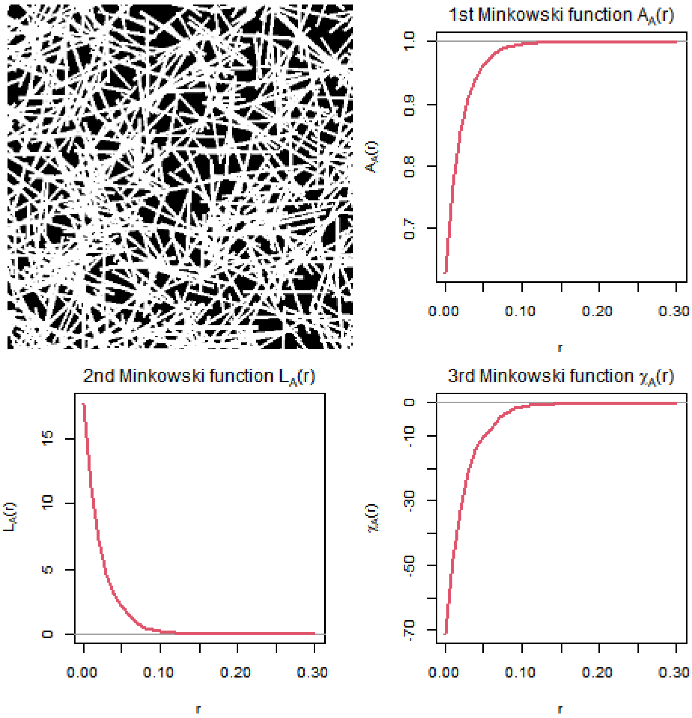
      i. Both the random realizations are compact and are non-convex sets.

      ii. Image1_S04[1] is the realization of 2D random set which represent a material model with cylindrical fibres. Generally composite materials have these structure. The structure is homogeneous set.

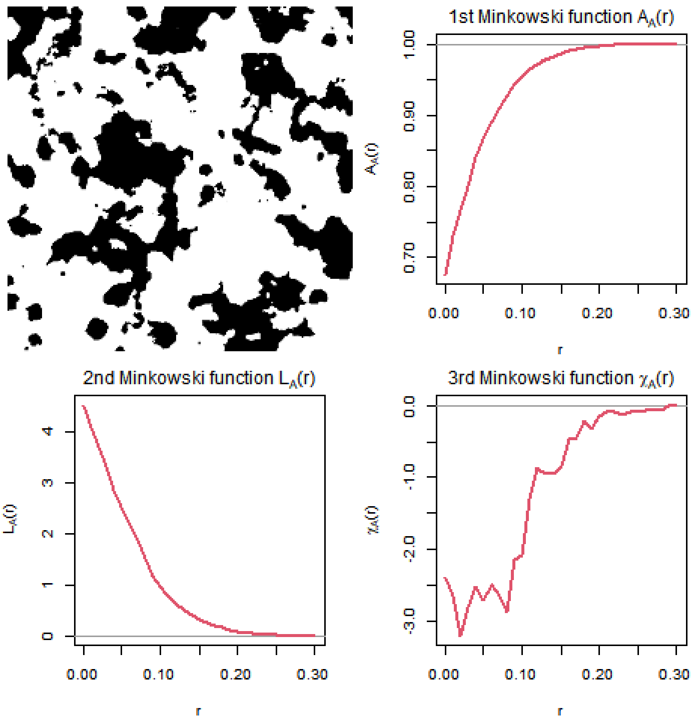
      iii. Image2_S04[1] is also the realization of 2D random set which represent a material model having two distinct phases. Generally ceramics or meta materials have these structure. The structure is non-homogeneous set.

   (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.

   Minkowski functions for the estimation of empirical characteristics. The 1^{st}, 2^{nd} and 3^{rd} Minkowski functions represent area fraction, perimeter fraction and Euler Number of the realization of random set.

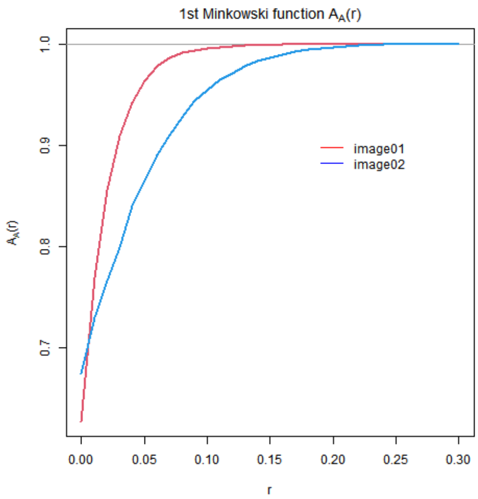


(a) image1_S04

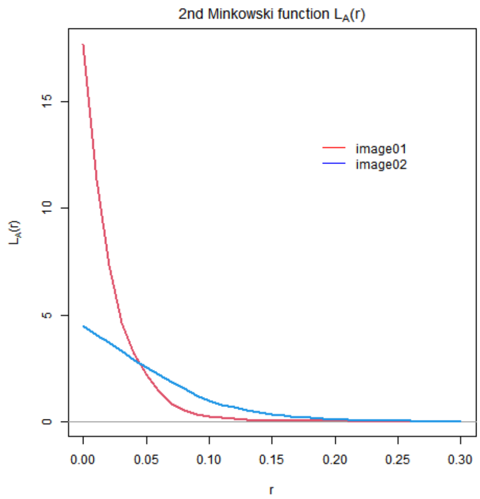


(b) image2_S04

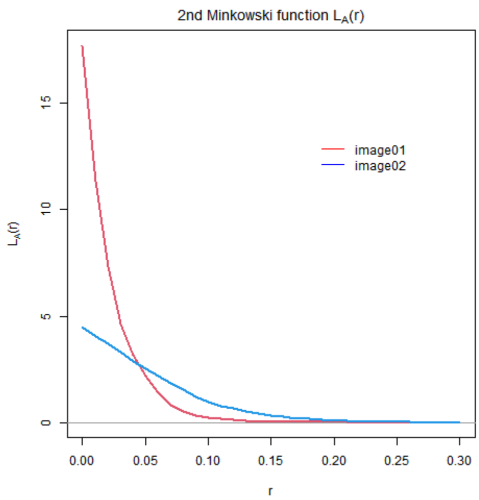
Figure 2: Minkowski functions



(a) 1^{st} Minkowski functions



(b) 2^{nd} Minkowski functions



(c) 3^{rd} Minkowski functions

Figure 3: Comparison of Minkowski functions for image01 and image02

Figure[2] contains the 1^{st}, 2^{nd} and 3^{rd} Minkowski functions for image01 and image02.

Figure[3] contains the 1^{st}, 2^{nd} and 3^{rd} Minkowski functions for image01 and image02 plotted together for comparison.

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

i. **1^{st} Minkowski functions** The comparison as shown in fig[3(a)], the area fraction for both images increases until the whole area of the sample is considered i.e 1. For image01, the increase is steep and reach maximum area at r1=0.16. For image02, the increase is not steep and reach maximum area at r2=0.29. This indicates that image01 structure has smaller grains and image02 has some larger grains,therefore B(o,r) has to selected in range of (0,r1), (0,r2) for image01 and image02 respectively.

ii. **2^{nd} Minkowski functions**:.The comparison as shown in fig[3(b)], the perimeter fraction decreases as the radius of random set B(o,r) increases. The curve is steep for image01 and reach 0 at r1=0.15 and for image02 at r2=0.29.

iii. **3^{rd} Minkowski functions**:.The comparison as shown in fig[3(c)],the Euler number which indicates the number of holes in the system. The Euler number decreases for both the structures but rapidly for which indicates that the grain are of smaller size. As r increases, the number of connected elements in image01 are less than hole but it is relatively consistent for image02.

2. **TASK-2** :
Someone claims that the structure in the first image image1_S04.png can be modelled by a Boolean model with a uniformly oriented deterministic rectangular typical grain. This sounds reasonable. Denote by γ 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.

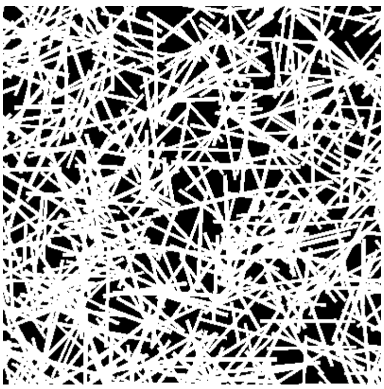
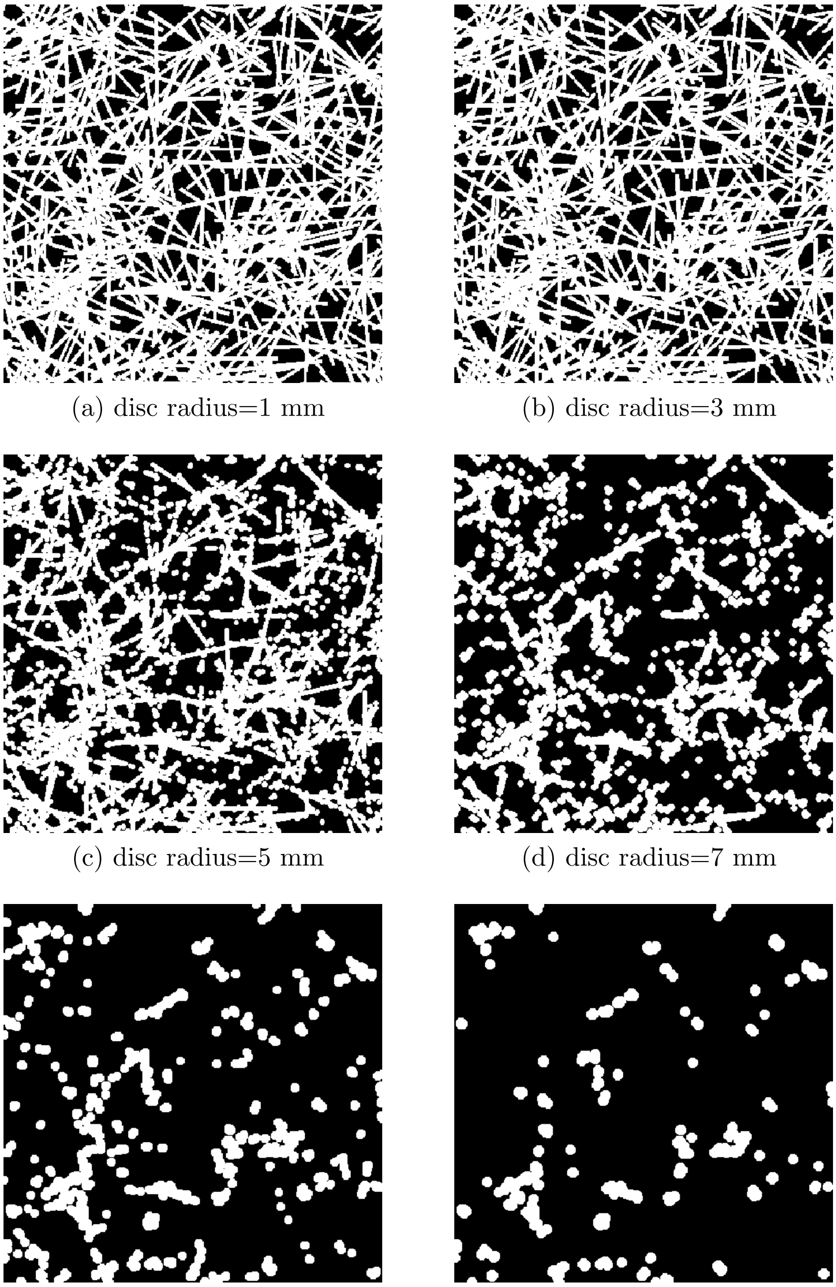


Figure 4: Realizations of random set image01

(a) Reporting the morphological openings and guessing for b.



(a) disc radius=1 mm

(b) disc radius=3 mm

(c) disc radius=5 mm

(d) disc radius=7 mm

(e) disc radius=9 mm

(f) disc radius=11 mm

Figure 5: Morphological opening operation on image01

From fig[5], the vanishing of rectangular grains occurs from disc radius r=7 mm, pixel length (spacing) l=0.025 mm. Then the (true) disc diameter **b=0.175 mm**.

(b) Determining the estimates of the model parameters of the Boolean model with a uniformly oriented deterministic rectangular typical grain:

Person A:

Boolean Model parameters: λ=4.9 , a=2.5,b=0.15

For significance level α= 0.05 and m = 999

From global test analysis, the P-value obtained is 0.682

`02_Boolean_model_personA.png`

Figure 6: Global envelopes for person A

The sample fit is within the envelope limits so the data fits well to the model.

Person B:

Boolean Model parameters: λ=4.8 , a=1.8,b=0.13

For significance level α= 0.05 and m = 999

From global test analysis, the P-value obtained is 0.1

02_Boolean_model_personB.png

Figure 7: Global envelopes for person B

The sample fit is not within the envelop limits so the data does not fits well to the model.

3. **Task 3:** Consider the random set realization given by image3_S04.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.)

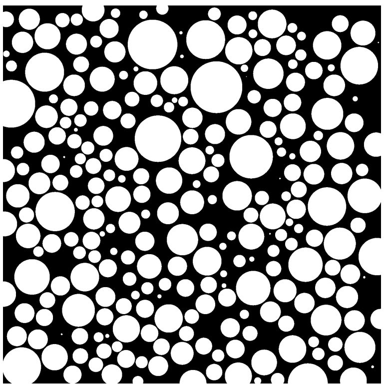


Figure 8: Realizations of random set image03

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

Empirical characteristics of the random set
Volume fraction V[r]: 0.5530623
Specific surface area S[r] : 33.72992

(b) Applying segmentation algorithm and, considering the segmented components as ideal discs, determining their centres and diameters. Determine the range of diameters and report it.

After applying segmentation algorithm

Extracted features:

Number of discs within observation window :253
Range of the disc diameter :[0.003023716 0.1918457]mm
Mean of the disc diameter :0.06618689 mm
Variance of the disc diameter : 0.03446007

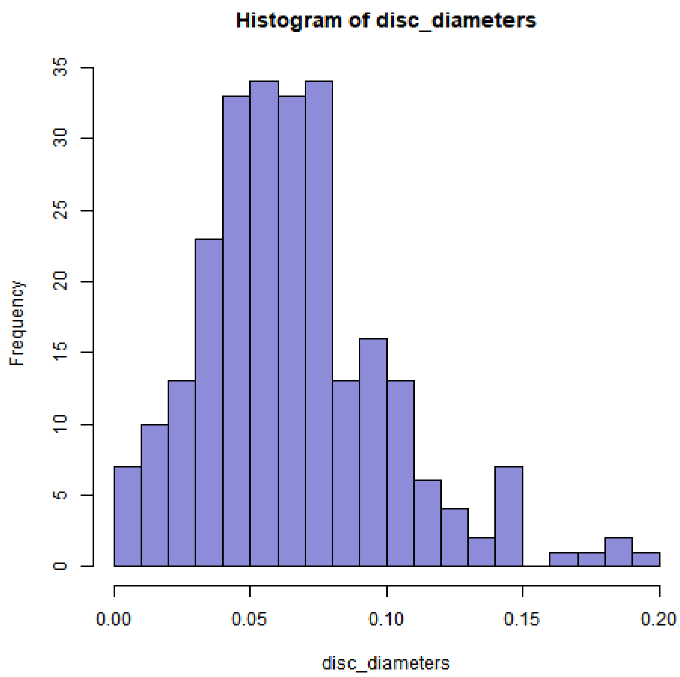


Figure 9: Distribution of disc diameter

(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. Report a plot of the obtained (3D) frequencies.

Applied Scheil Schwartz Saltykov method.
Plotting histogram for 2d and 3d diameter distributions.

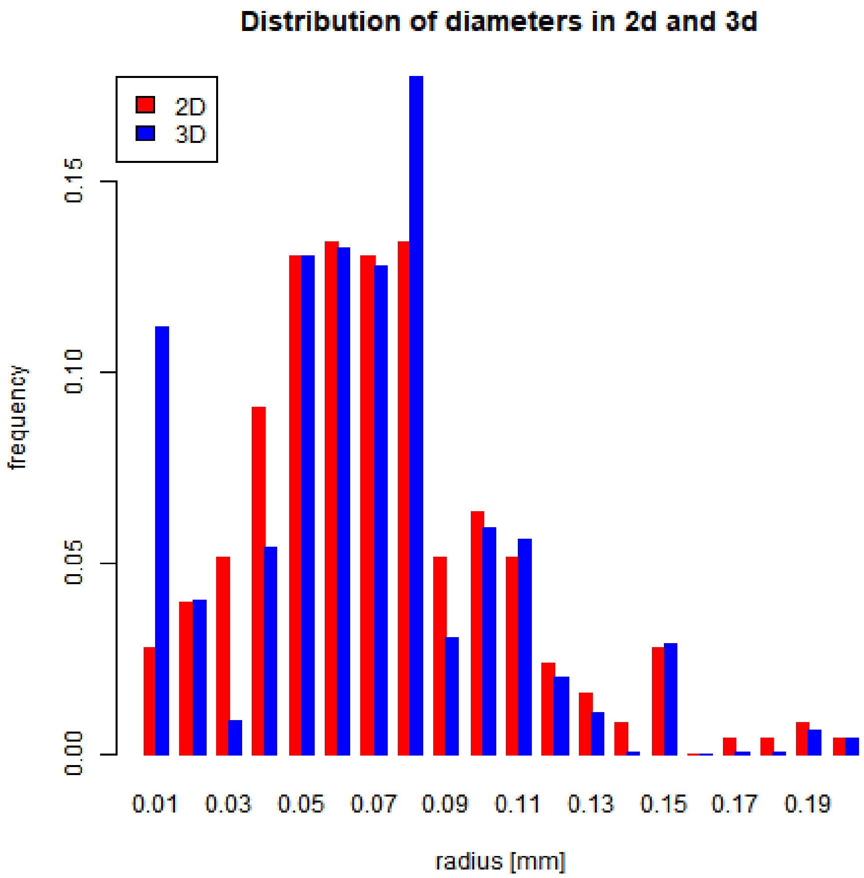


Figure 10: Distribution of disc diameter 2D and 3D

The bins are the interval present and previous radius ex-0.01-(0.00,0.01].

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

Intensity(mean number of balls per unit volume): 2128.233
Mean ball diameter 3D: 0.02616804 mm

4. **Task-4**: Consider the Matérn III hard-disc model (in 2D) with parameters λ

(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 and R is known. Because of that a Monte Carlo approach is appropriate to get information on the three quermass densities AA, LA and χA. Choose a window of size 10 by 10 and a radius R = 0.06. Each for the values 4, 8 and 12 for λ

Empirical characteristics of Matérn hard ball model 3
For λ=4:

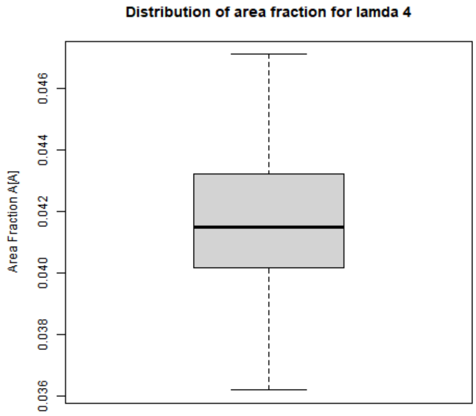
Mean of the area fraction : 0.04174134
variance of the area fraction : 0.002159334
Mean of the perimeter fraction : 1.384027
variance of the perimeter fraction : 0.0713638
Mean of the Euler Number: 3.613688
Variance of the Euler Number: 0.1824207

For λ=8:

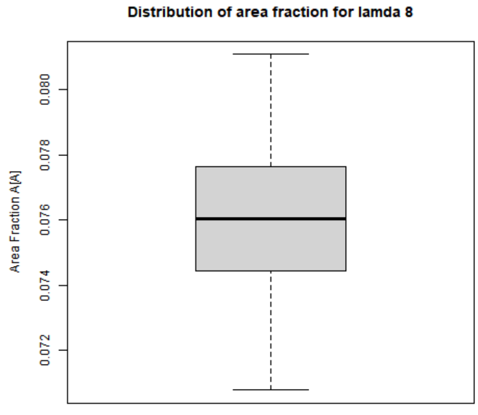
Mean of the area fraction : 0.0761337
variance of the area fraction : 0.002297063
Mean of the perimeter fraction : 2.522377
variance of the perimeter fraction : 0.07608183
Mean of the Euler Number: 6.509958
Variance of the Euler Number: 0.1914804

For λ=12:

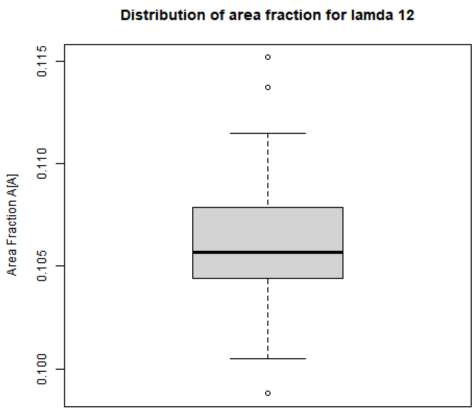
Mean of the area fraction : 0.1060161
variance of the area fraction : 0.002657377
Mean of the perimeter fraction : 3.509729
variance of the perimeter fraction : 0.08752768
Mean of the Euler Number: 8.946546
Variance of the Euler Number: 0.2268495



(a) Area fraction λ=4

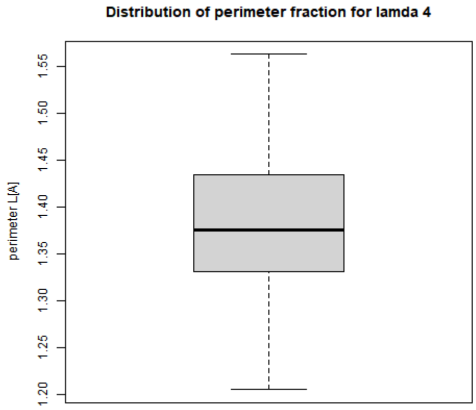


(b) Area fraction λ=8

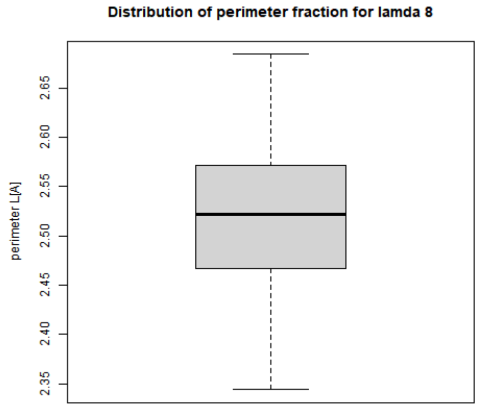


(c) Area fraction λ=12

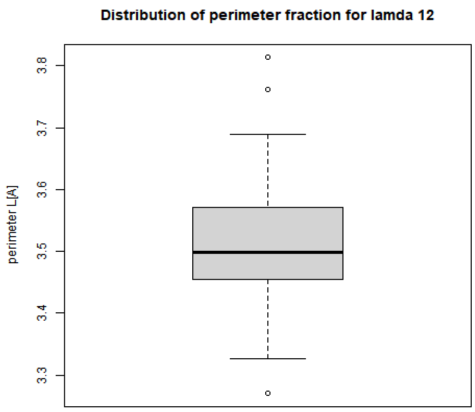
Figure 11: Distribution of empirical characteristics Area fraction



(a) perimeter fraction λ=4

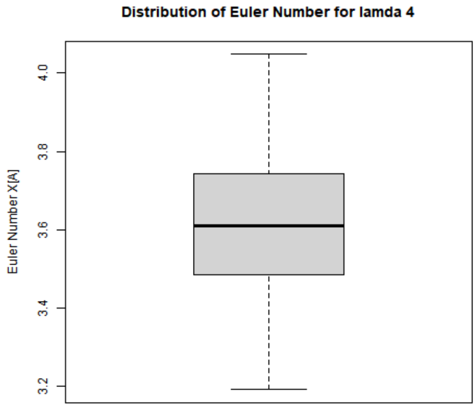


(b) perimeter fraction λ=8

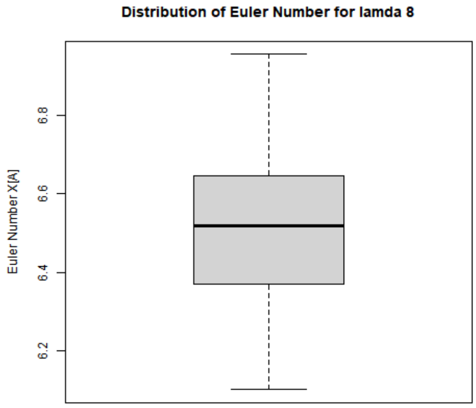


(c) perimeter fraction λ=12

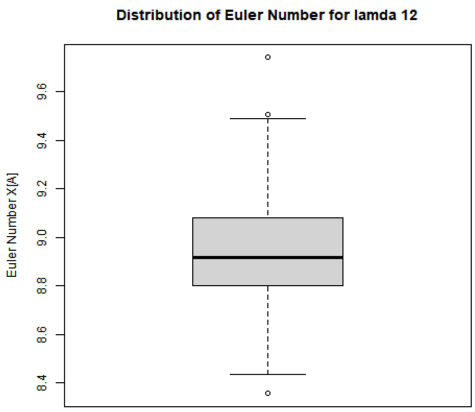
Figure 12: Distribution of empirical characteristics perimeter



(a) Euler Number λ=4



(b) Euler Number λ=8



(c) Euler Number λ=12

Figure 13: Distribution of empirical characteristics Euler Number