Final Project

STAT – 517

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Abstract

Microstructure plays a very important role in determining the properties (like strength, ductility, formability etc.) of a material. The final microstructure of a material depends upon a number of variables such as elasticity constant of matrix and precipitate, direction of strain applied on the material, temperature and so on. The experimental determination of the microstructure of a material is a very tedious task and requires a lot of effort. In this work we use machine learning methods to train a convolutional neural network over a range of different microstructures and using the trained model to predict the microstructure of a material under different circumstances. We have also performed clustering, seriation and association over the microstructures.

Introduction

The study of microstructure of a material is very helpful in designing a material for a given purpose. For different purposes different materials are required. For example, we need a material which is having high strength and high toughness for defense purposes. The final properties of a material depends upon the microstructure of that material which further depends upon a lot of variables like elasticity constants, applied strain and many more. This makes study of the properties of a material a very tedious task.

Machine learning can be a useful tool in such a case where there are a lot of parameters involved in determining the final output. Through convolutional neural network we can make the machine learn the characteristic properties of the material under different processing conditions. Further the developed model can be used to predict the microstructure of the material at any arbitrary set of parameters (processing conditions). This methodology can drastically reduce the efforts of experiments as the developed model is used for analyzing the properties of the material.

Methodology

In this work, we have used a convolutional neural network to study the abstract features from the microstructure of a material. We have used eight features to define a particular microstructure keeping all other parameters constant. These eight parameters include the elasticity constants of the matrix in the three directions (c110, c120 and c440), the difference between the elasticity constants of the matrix and the elasticity constants of the precipitate in the three directions (c111, c121 and c441) and externally applied strain in the x-direction (xs) and in the y-direction (ys). The network used to store the convolved feature of the input image is 5 layers deep. We have used leaky ReLU to model the negative parts of the input image. The image of the microsturcture is represented by a 512 × 512 size pixel data as shown in Figure 1. The pixel data is normalized between -1 and 1 where -1 represent black and 1 represent white.

	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
0	0.94521	0.94482	0.94345	0.94062	0.93494	0.92255	0.89305	0.81464	0.6249	0.25632	-0.23545	-0.61991	-0.81814	-0.89578	-0.92235	-0.9303	-0.93127	-0.93026
1	0.92889	0.93104	0.9281	0.91902	0.8972	0.84273	0.71303	0.44516	0.01341	-0.43482	-0.72441	-0.85864	-0.90896	-0.92654	-0.93147	-0.93191	-0.93081	-0.92877
2	0.84741	0.86251	0.85127	0.80772	0.70715	0.50777	0.16643	-0.26283	-0.60714	-0.80133	-0.88556	-0.91722	-0.92875	-0.93183	-0.93227	-0.93135	-0.92967	-0.9276
3	0.46445	0.51316	0.47922	0.35371	0.11155	-0.21881	-0.52792	-0.74113	-0.85391	-0.9021	-0.92183	-0.92923	-0.93153	-0.93221	-0.93169	-0.93062	-0.92903	-0.92686
4	-0.33994	-0.28963	-0.32634	-0.4371	-0.58849	-0.73312	-0.83342	-0.8867	-0.91218	-0.92408	-0.92885	-0.93092	-0.9319	-0.93183	-0.93147	-0.93043	-0.92893	-0.9267
5	-0.78989	-0.77549	-0.78734	-0.81922	-0.8564	-0.88656	-0.90682	-0.91928	-0.92572	-0.92876	-0.93073	-0.93173	-0.9321	-0.93223	-0.93175	-0.93088	-0.92937	-0.92717
6	-0.90007	-0.89866	-0.90117	-0.9069	-0.91408	-0.92091	-0.9256	-0.92823	-0.93007	-0.93158	-0.93226	-0.93289	-0.93313	-0.93309	-0.93259	-0.93184	-0.93015	-0.92808
7	-0.92601	-0.92653	-0.92763	-0.92914	-0.93038	-0.93118	-0.93199	-0.93299	-0.93355	-0.93388	-0.93431	-0.93451	-0.93448	-0.93434	-0.93376	-0.93283	-0.93132	-0.92879
8	-0.93365	-0.93465	-0.93531	-0.93571	-0.93612	-0.9365	-0.93658	-0.93633	-0.93633	-0.93638	-0.93629	-0.93614	-0.93602	-0.93548	-0.93495	-0.93374	-0.93233	-0.9294
9	-0.93857	-0.9395	-0.94014	-0.94041	-0.94026	-0.93976	-0.93939	-0.93912	-0.93878	-0.93829	-0.93807	-0.93761	-0.93719	-0.93651	-0.93577	-0.93438	-0.93291	-0.92978
10	-0.94106	-0.942	-0.94247	-0.94255	-0.94246	-0.94224	-0.94175	-0.94103	-0.94045	-0.93993	-0.93929	-0.93866	-0.938	-0.9371	-0.93611	-0.93467	-0.93285	-0.92992
11	-0.9433	-0.9441	-0.94452	-0.94465	-0.94429	-0.9437	-0.94301	-0.94245	-0.94165	-0.94085	-0.94006	-0.93928	-0.93826	-0.93734	-0.93595	-0.93451	-0.9323	-0.92965
12	-0.94441	-0.94513	-0.94541	-0.94535	-0.94509	-0.94469	-0.944	-0.94311	-0.94222	-0.94138	-0.94035	-0.93936	-0.93823	-0.937	-0.93549	-0.93382	-0.9315	-0.92883
13	-0.94536	-0.94587	-0.94613	-0.9461	-0.94569	-0.94496	-0.94419	-0.94338	-0.94243	-0.9413	-0.94026	-0.93905	-0.93778	-0.93634	-0.93473	-0.93278	-0.93055	-0.92766
14	-0.94556	-0.94603	-0.94611	-0.94588	-0.9455	-0.94499	-0.94419	-0.94316	-0.94209	-0.94103	-0.93975	-0.93845	-0.93704	-0.93546	-0.9337	-0.93169	-0.92933	-0.92663
15	-0.94559	-0.94581	-0.94589	-0.94575	-0.94525	-0.94445	-0.94356	-0.94267	-0.94157	-0.94029	-0.93903	-0.93763	-0.93608	-0.93445	-0.93259	-0.93052	-0.92821	-0.9256
16	-0.94506	-0.94531	-0.94518	-0.94479	-0.9443	-0.94374	-0.94291	-0.9418	-0.94064	-0.93947	-0.93808	-0.93662	-0.93507	-0.93333	-0.93148	-0.92942	-0.92716	-0.92475

Figure 1: Part of the microstructure data (original data is 512 × 512 size)

We have used 2048 microstructures in the whole process out of which 1648 is used for training the network while 400 is used for testing purpose. Mean squared error loss is used to compute the loss function which indicates how well the machine is learning through the given input images. The training of the convolutional neural network is done by feeding the images of the microstructures into the network in mini-batches of size 64. The network is trained for 8000 epochs during which the weights and losses are updated after every epoch.

Supervised learning

We have done a thorough analysis of the phase field and machine generated images. This exercise is being done in order to monitor the efficiency of machine generated images. Basically we have used three methods for analyzing and predicting the efficiency of machine generated images.

1. **Particle analysis** (using ImageJ software)

In this method we have used ImageJ software for particle analysis. We essentially calculate the area fraction of the matrix and precipitate for both phase field (*PF*) and machine generated (*M*) image. The error is calculated by using following equation:

$$\%Error_{Matrix} = \frac{\left|\%Matrix_{PF} - \%Matrix_{M}\right|}{\%Matrix_{PF}} \times 100$$

$$\%Error_{\mathrm{Pr}ecipitate} = \frac{\left|\%\mathrm{Pr}ecipitate_{PF} - \%\mathrm{Pr}ecipitate_{M}\right|}{\%\mathrm{Pr}ecipitate_{PF}} \times 100$$

We have also defined an efficiency term (η) in order to monitor the predicting capacity of machine after learning through the neural network model. This is shown as follows:

$$\eta = 1 - \frac{\left|\%Matrix_{PF} - \%Matrix_{M}\right|}{\%Matrix_{PF}}$$

$$\eta = 1 - \frac{\left|\%\mathrm{Pr}ecipitate_{PF} - \%\mathrm{Pr}ecipitate_{M}\right|}{\%\mathrm{Pr}ecipitate_{PF}}$$

2. **Using the random lines method.**

In this method, we use ImageJ software. We draw 5 random lines (can draw more or less random lines) over the image and calculate the number of intersection for each line with the black and white region of the image. Then we get the average of the length of those 5 random lines (l_{avg}) and the average of the number of intersections for each random line (I_{avg}). Then we report the number of intersections per unit length of random line (ρ) as follows:

$$\rho = \frac{I_{avg}}{l_{avg}}$$

Further the %Error and efficiency (η) is calculated using the following equations:

$$\%Error = \frac{\left|\rho^{PF} - \rho^{M}\right|}{\rho^{PF}} \times 100$$

$$\eta = 1 - \frac{\left|\rho^{PF} - \rho^{M}\right|}{\rho^{PF}}$$

3. **Using Aquami software**

   This package, written in python, is used for microstructure analysis such as bright field area, dark field area, ligament diameter etc.

   We have used Aquami over Phase field generated image and Machine generated image.

Results & Discussions

The training and testing loss curve is shown in Figure 2 as a function of number of epoch. It can be observed that the training as well as testing loss is decreasing with the number of epochs. This clearly reflects that the network is adjusting its weights and biases through learning process after each epoch.

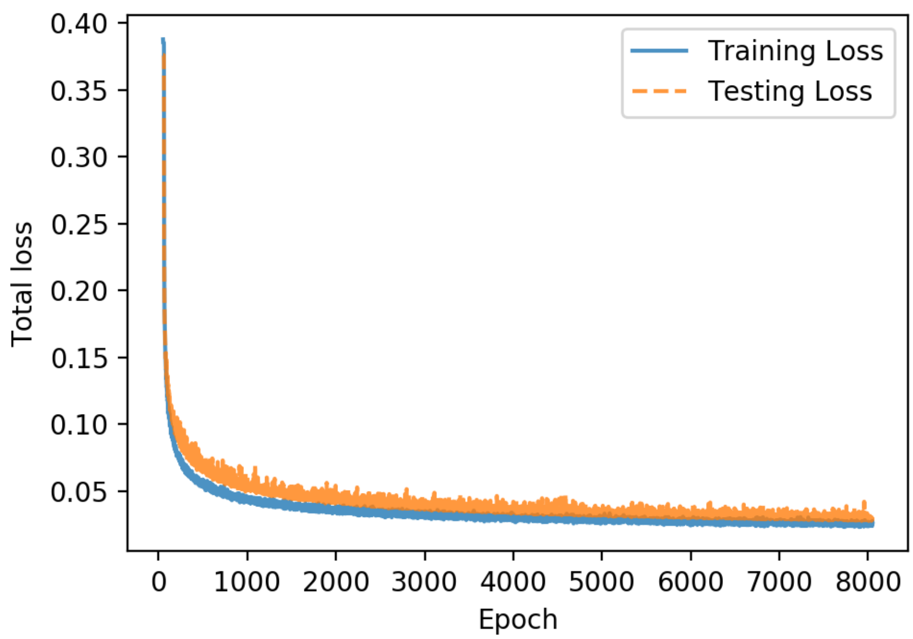


Figure 2: Training and testing loss as a function of number of epoch.

The result of the three methods that we have done in order to calculate the efficiency of machine learning algorithm is discussed below:

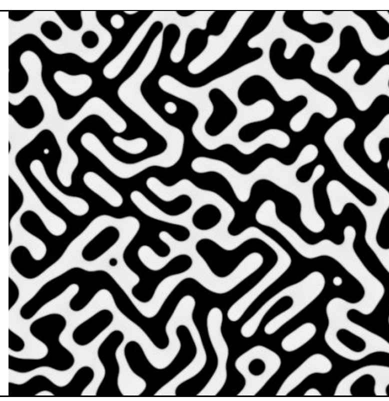
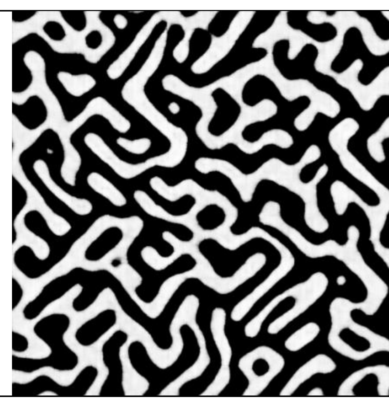
Particle analysis (using composition data)

We have discussed earlier that the composition data is scaled between -1 and 1 where -1 represents dark pixel while 1 represents bright pixel. We have done an analysis for calculating the amount of the precipitate and the matrix for both the library image and the machine generated image to quantify the efficiency of machine generated image. The negative part (from -1 to 0) represents matrix while the positive part (from 0 to 1) represents the precipitate. The calculated percentage of matrix and precipitate are in good agreement for a particular microstructure for both library and the machine generated one (see Figure 3).

Particle analysis (using ImageJ software)

TRAINING

c110: 501, c120: 208, c440: 117, c111: 0, c121: 0, c441: 0, xs = 0.0, ys = 0.0

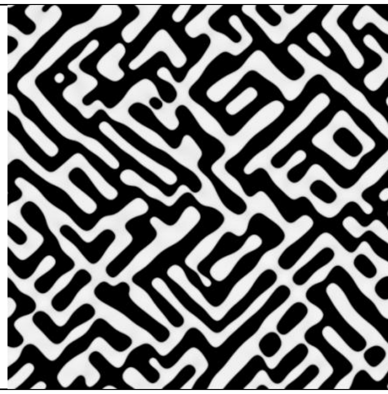
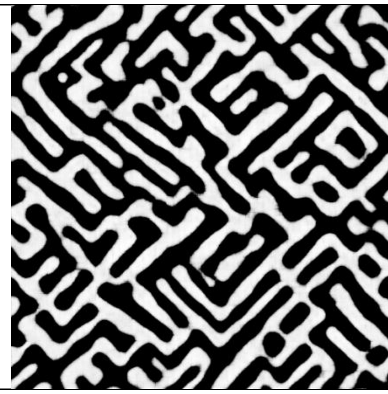
	Phase Field	Machine	%Error	Average %Error
				
%Matrix	54.4	56.668	4.169	**4.572**
%Precipitate	45.6	43.332	4.974	

***η* = 0.9602**

TESTING

c110: 742, c120: 336, c440: 96, c111: 0, c121: 0, c441: 0

	Phase Field	Machine	%Error	Average %Error

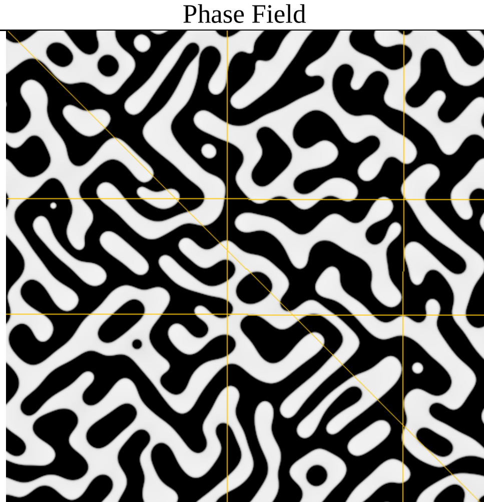
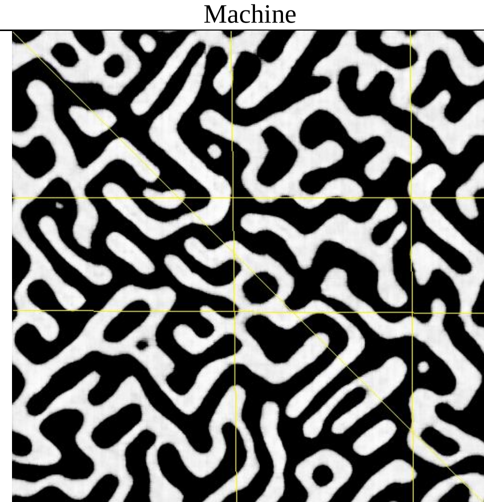
				
%Matrix	55.335	57.738	4.343	**4.862**
%Precipitate	44.665	42.262	5.380	

η = 0.9502

Using the random lines method.

TRAINING

c110: 501, c120: 208, c440: 117, c111: 0, c121: 0, c441: 0

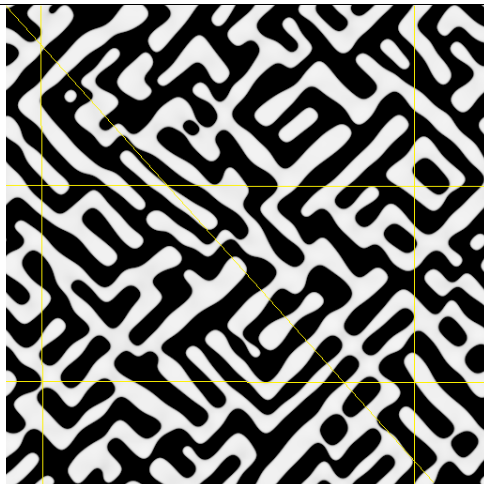
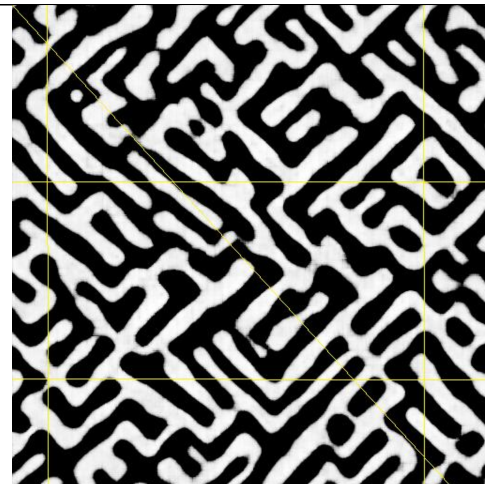
Phase Field		Machine	
			
l_{avg}^{PF}	551.05	l_{avg}^{M}	552.28
i_{avg}^{PF}	19.3	i_{avg}^{M}	19.4
ρ^{PF}	0.03502	ρ^{M}	0.03513

%Error = 0.314

η = 0.9969

TESTING

c110: 742, c120: 336, c440: 96, c111: 0, c121: 0, c441: 0

Phase Field		Machine	
			
l_{avg}^{PF}	546.04	l_{avg}^{M}	545.68
i_{avg}^{PF}	22.1	i_{avg}^{M}	22.3
ρ^{PF}	0.04047	ρ^{M}	0.04087

%Error = 0.988

***η* = 0.9901**

The efficiency scores obtained using each of the above discussed model is represented in a bar plot as shown in Figure 3.

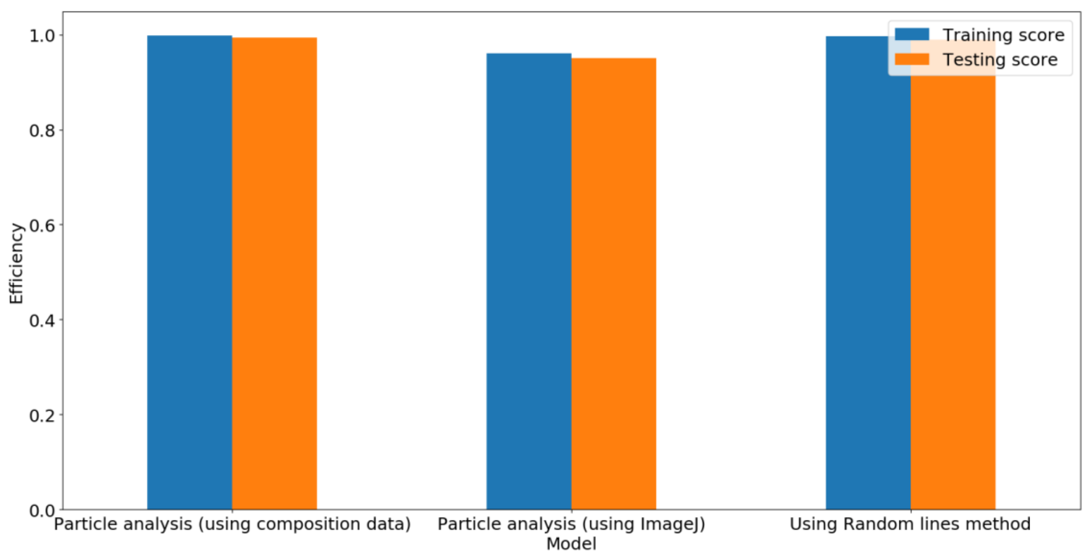


Figure 3: The efficiency of different methods used for analyzing the quality of machine generated image.

Receiver Operating Characteristic (ROC) curve

Further, the efficiency of machine generated image is quantified using ROC curve which is generally used in statistical modeling to study the accuracy of statistical models. The ROC curve is the sensitivity as a function of fallout. Since the composition of the material in our dataset varies between -1 and 1 (where -1 to 0 represents precipitate or second phase while 0 to 1 represents matrix), we represent the negative composition with 0 and positive composition to 1 (including 0). The ROC curve for a particular training and testing microstructure is shown in Figure 2 and 3 respectively.

Training (c110 = 1064, c120 = 532, c440 = 266, c111 = c121 = c441 = 0, x-strain = y-strain = 0, t = 1800)

Accuracy Score = 97.34%

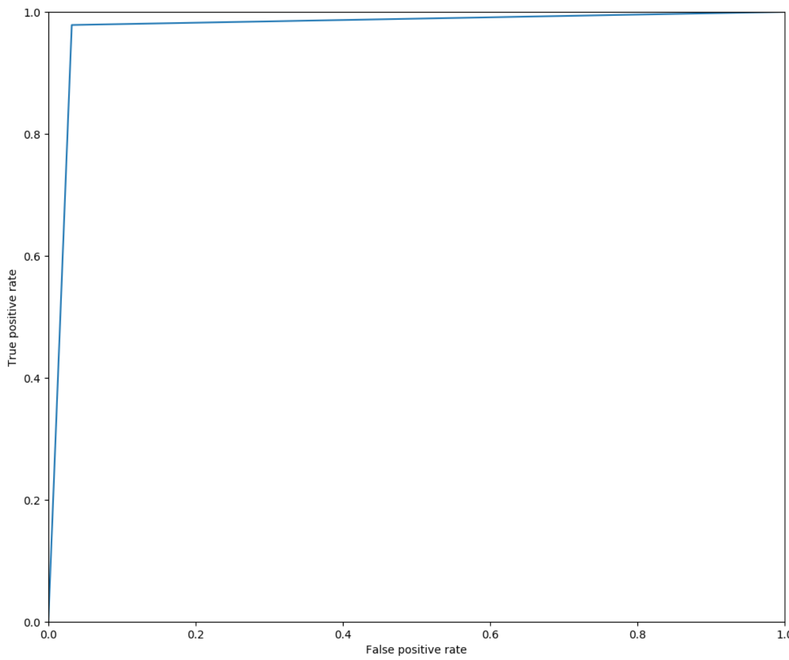


Figure 2: ROV curve for a training microstructure dataset.

Testing (c110 = 1000, c120 = 462, c440 = 269, c111 = c121 = c441 = 0, x-strain = y-strain = 0, t = 1800)
Accuracy Score = 92.75%

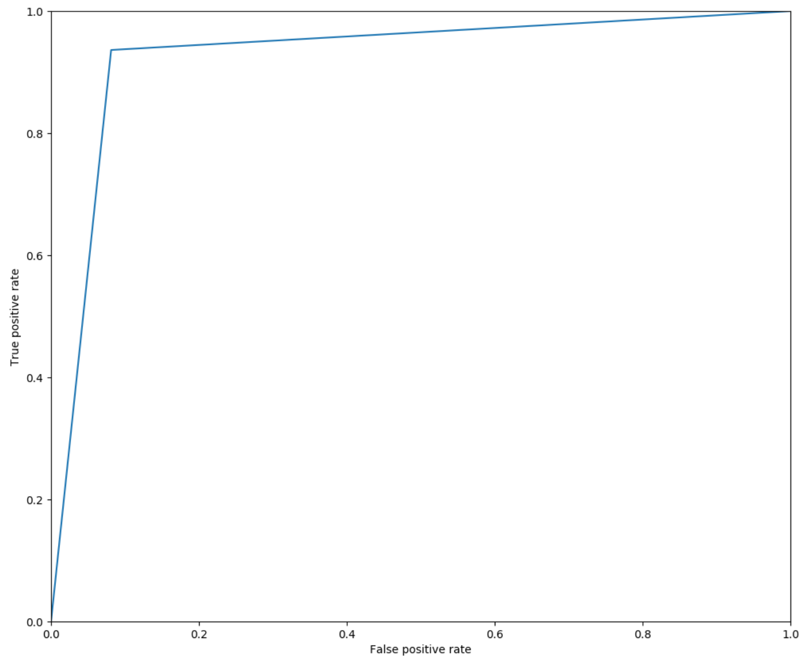
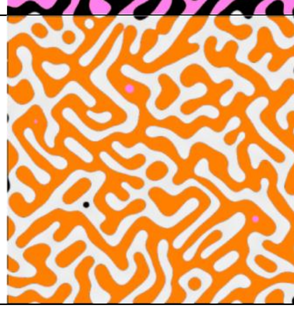
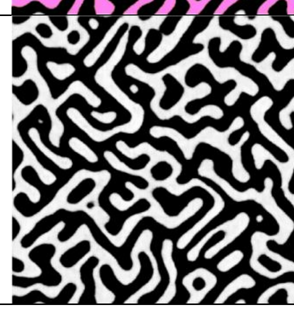


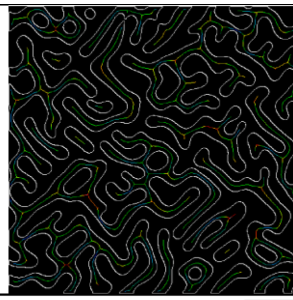
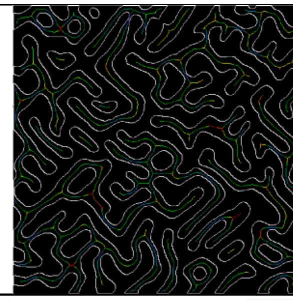
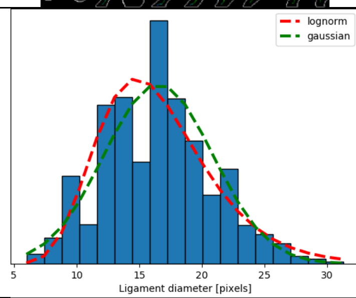
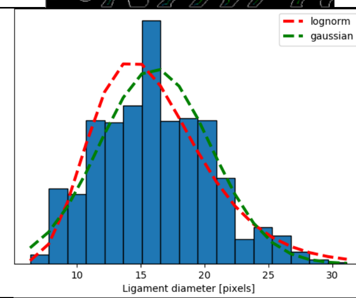
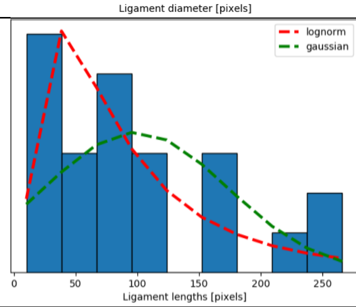
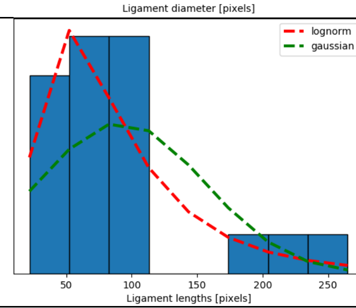
Figure 3: ROC curve for a testing microstructure dataset.

Using Aquami software

TRAINING

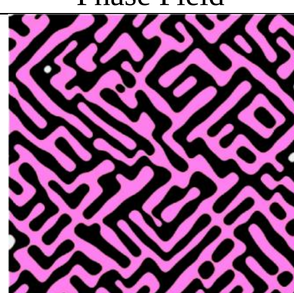
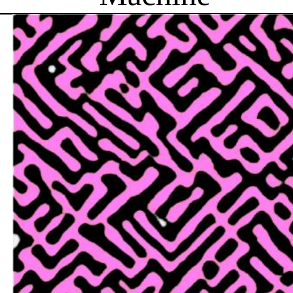
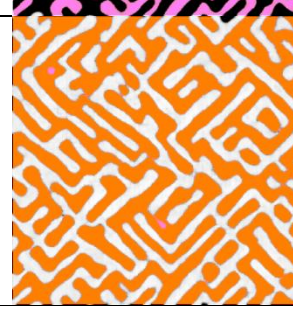
c110: 501, c120: 208, c440: 117, c111: 0, c121: 0, c441: 0

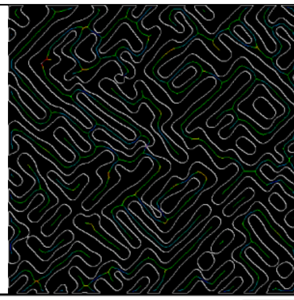
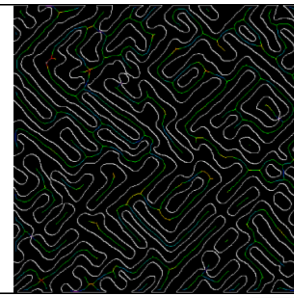
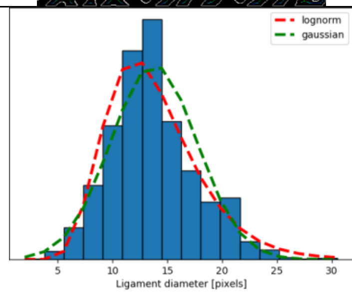
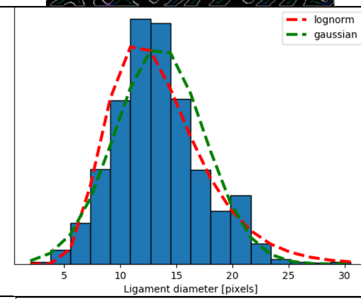
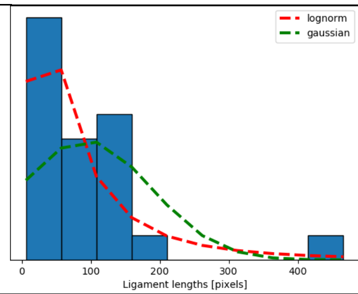
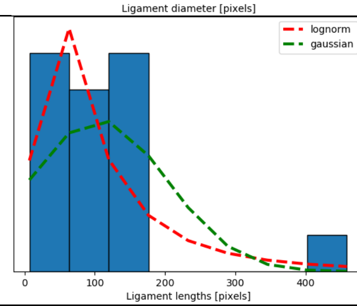
	Phase Field	Machine
Bright phase mask		
Dark phase mask		

Ligament analysis		
Ligament diameter analysis		
Ligament length analysis		

TESTING

c110: 742, c120: 336, c440: 96, c111: 0, c121: 0, c441: 0

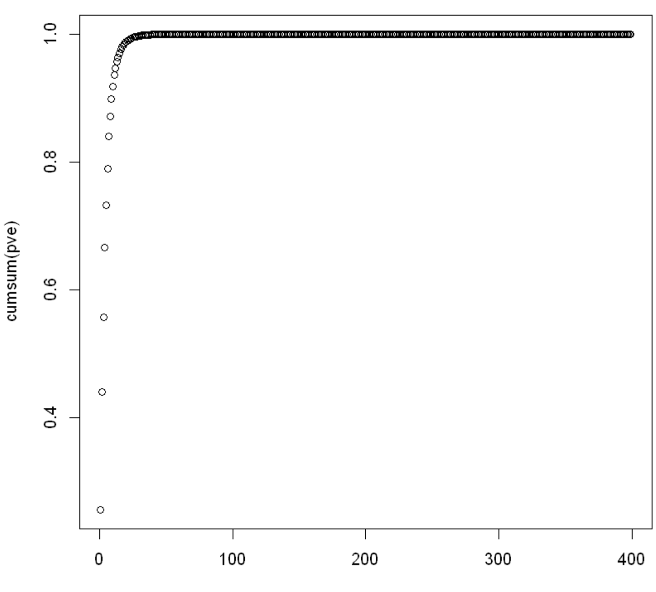
	Phase Field	Machine
Bright phase mask		
Dark phase mask		

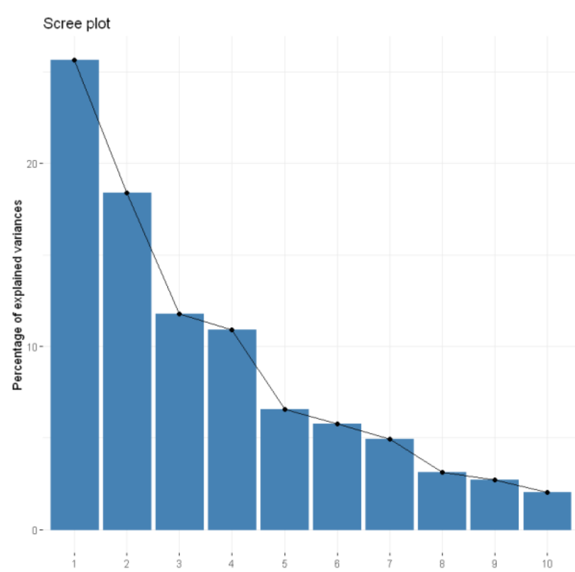
Ligament analysis		
Ligament diameter analysis		
Ligament length analysis		

The ligament length and diameter analysis by Aquami software produce similar curves for the microstructures generated through phase field and machine learning. This further reflects good efficiency of the neural network model.

Unsupervised learning

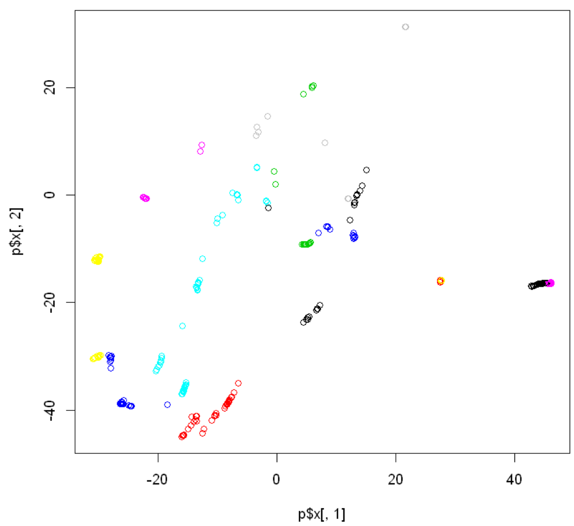
1. Principle component analysis

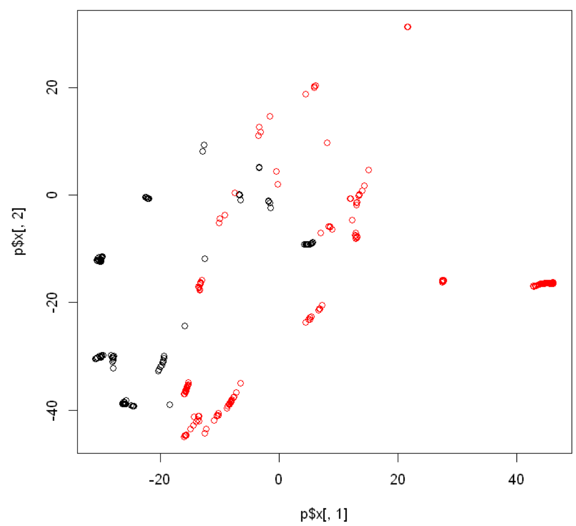




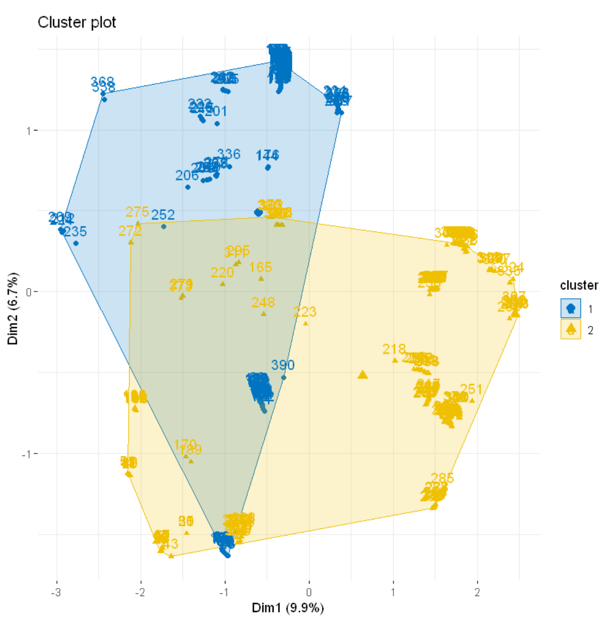
12 principle components can explain 95% of the data. 16 principle components can explain 98% of the data.

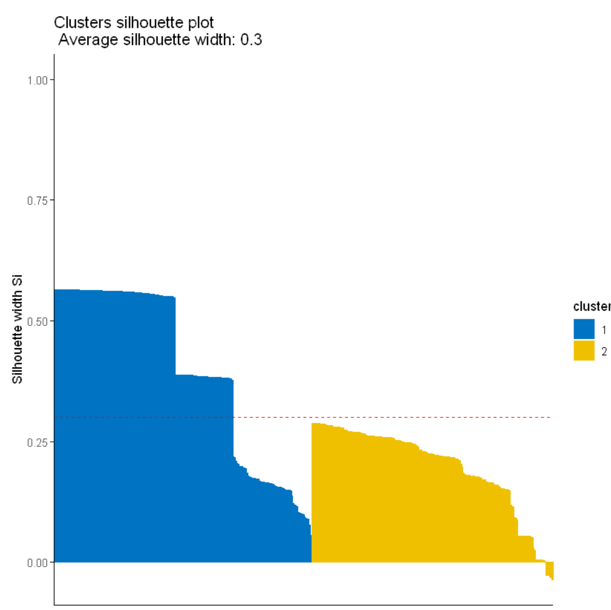
2. K-Means clustering



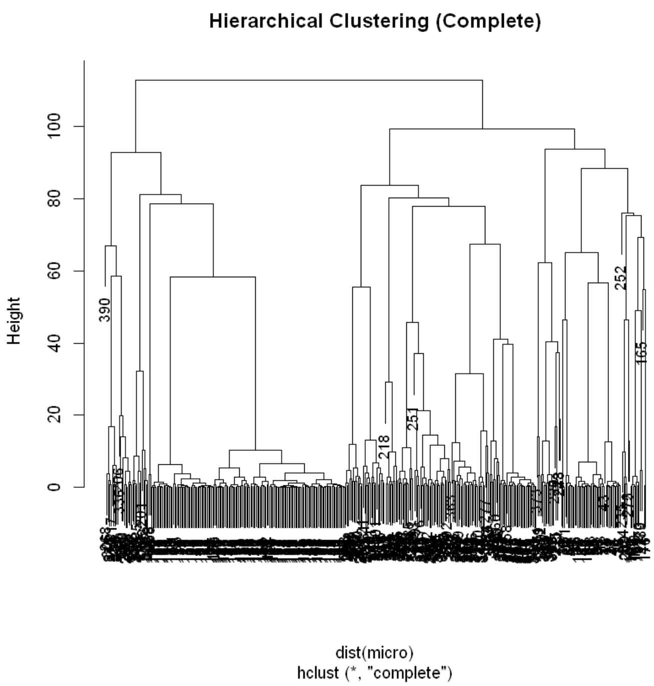


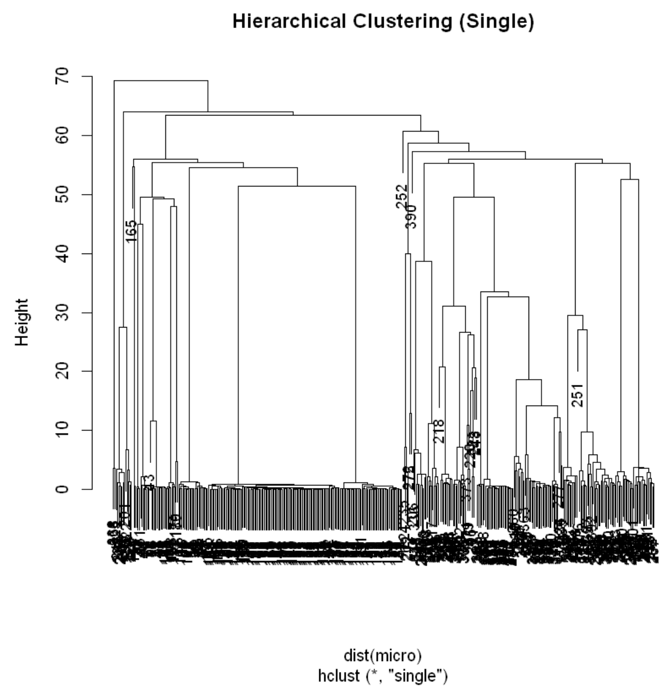
I have done kmeans clustering with 16 clusters which doesn't means much sense. Kmeans clustering with 2 clusters make some sense as it shows 2 clusters for 2 different types of microstructures i.e. homogeneous and inhomogeneous.



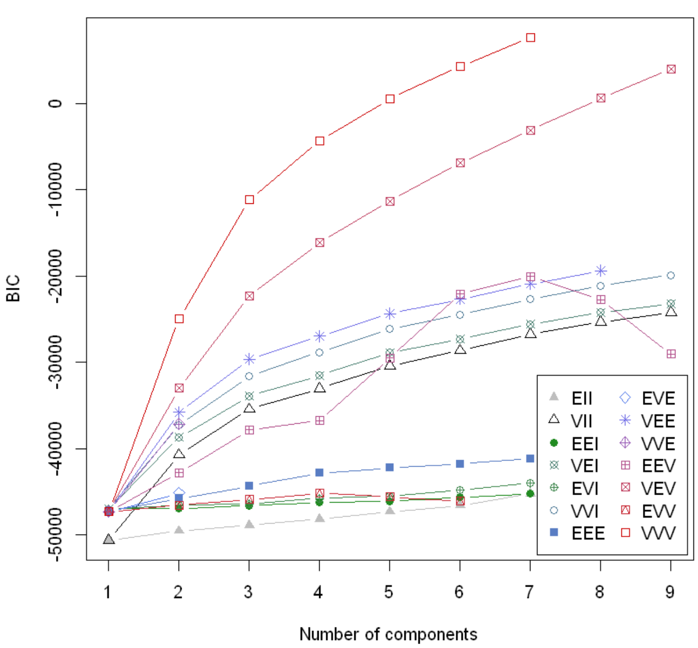


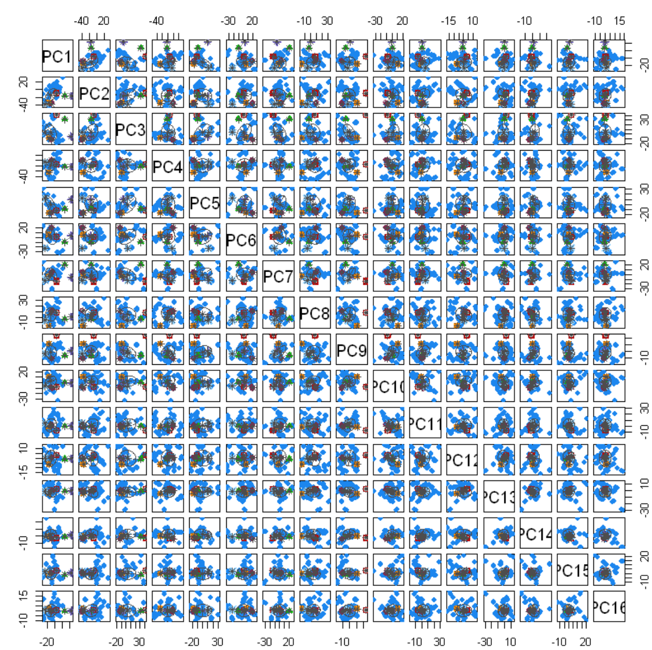
3. Hierarchical clustering

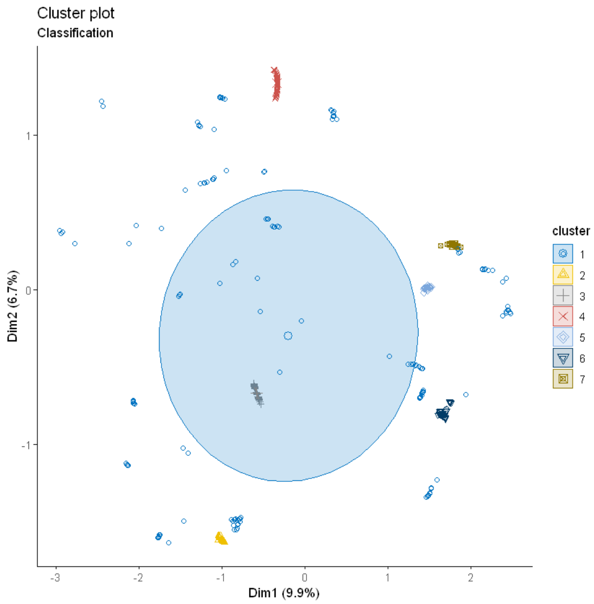


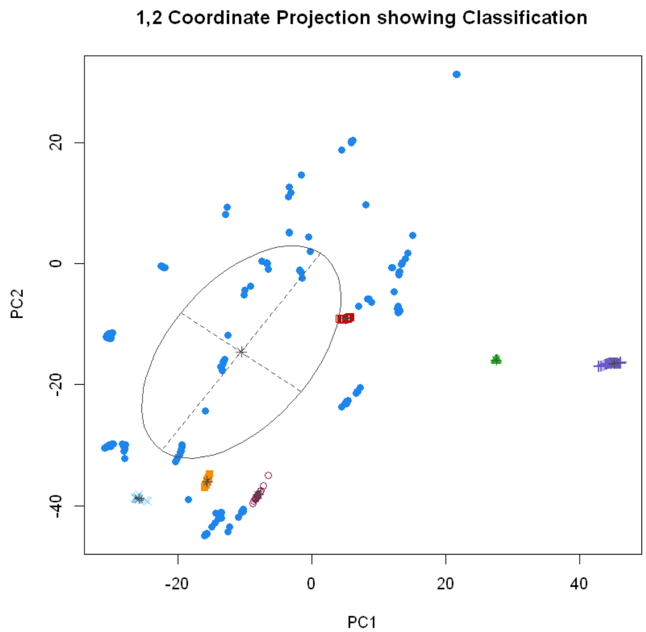


4. MClust

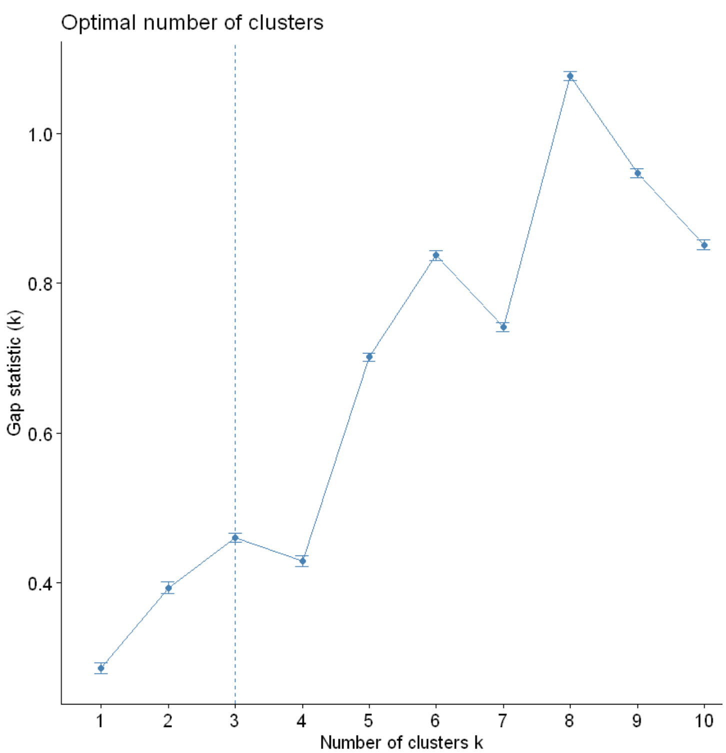


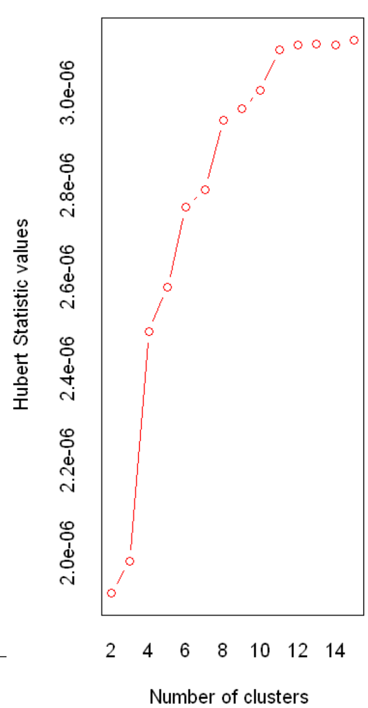


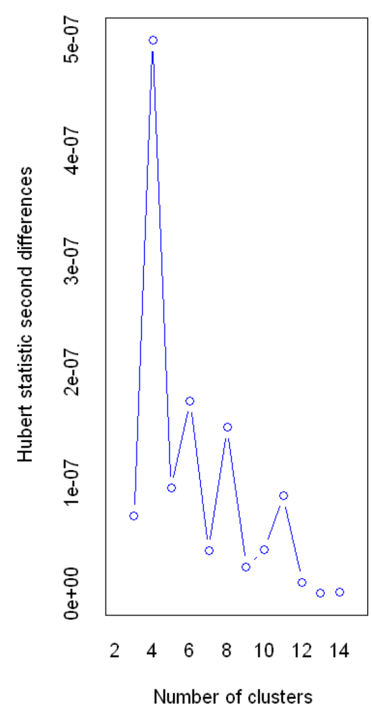

Cluster plot
Classification
Dim2 (6.7%)
Dim1 (9.9%)
cluster
1
2
3
4
5
6
7


1,2 Coordinate Projection showing Classification
PC2
PC1

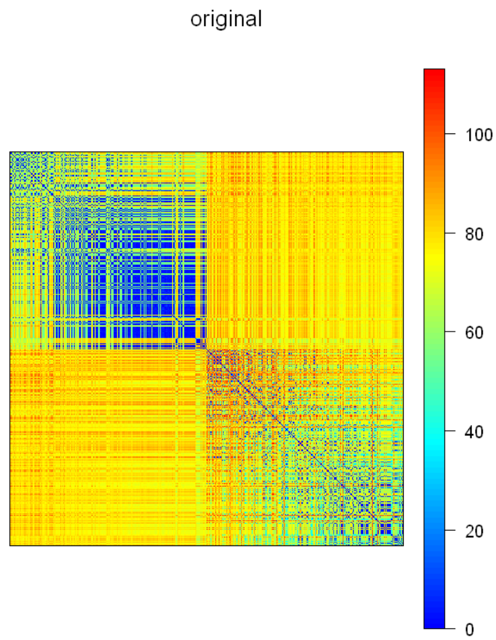
5. NbClust

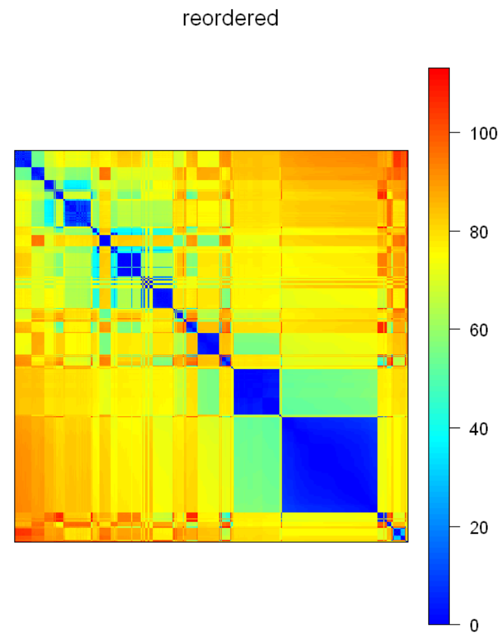

Optimal number of clusters
Gap statistic (k)
Number of clusters k


Hubert Statistic values
Number of clusters


Hubert statistic second differences
Number of clusters

Seriation analysis and heat map





get_order(o)

301 261 228 309 213 299 207 202 256 266 211 245 214 219 208 269 241 240 255 217 227 230 253 204 284 273
286 283 265 247 231 239 250 244 254 263 288 274 353 285 333 298 304 312 291 262 236 216 251 302 297 293
296 294 342 356 327 355 321 325 365 330 320 344 376 331 389 398 352 370 348 392 395 391 369 393 218 388
397 372 394 387 339 316 15 1 29 26 22 25 5 10 42 37 32 43 260 310 306 324 307 281 292 371 367 351 359
350 341 334 343 319 345 313 303 326 300 335 308 287 280 276 282 289 264 258 360 277 198 340 329 169 192
318 314 191 195 193 190 383 396 377 385 386 381 378 362 374 399 357 364 379 354 358 384 337 332 349 363
223 189 51 170 17 41 40 4 27 69 390 55 30 21 361 315 328 347 346 366 382 375 380 322 248 53 28 13 73 7
84 2 61 86 83 11 101 14 56 19 8 66 45 109 99 16 36 295 317 311 290 323 233 234 270 246 305 268 220 275
272 165 91 136 52 77 62 9 59 57 78 153 112 67 49 105 124 72 12 24 75 6 133 38 68 70 3 46 98 18 104 35
168 138 20 117 33 34 90 123 173 119 151 113 100 103 23 64 144 176 336 155 156 161 125 182 152 121 148
142 166 127 175 180 131 130 120 147 163 128 146 115 184 94 199 96 97 93 179 149 102 122 85 174 196 178
137 185 132 74 88 158 181 114 186 164 154 111 118 95 157 177 162 129 140 183 107 63 106 110 160 135 54
79 71 65 187 92 116 197 194 139 44 50 81 172 47 145 126 39 108 188 60 89 58 31 48 143 159 167 82 171
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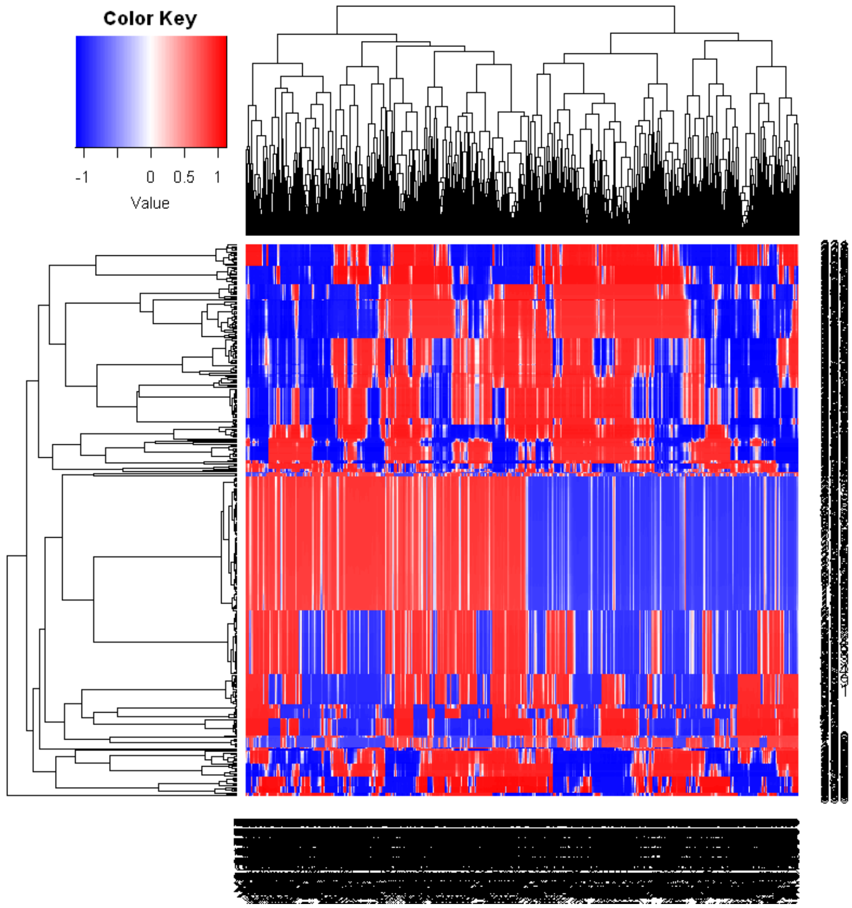
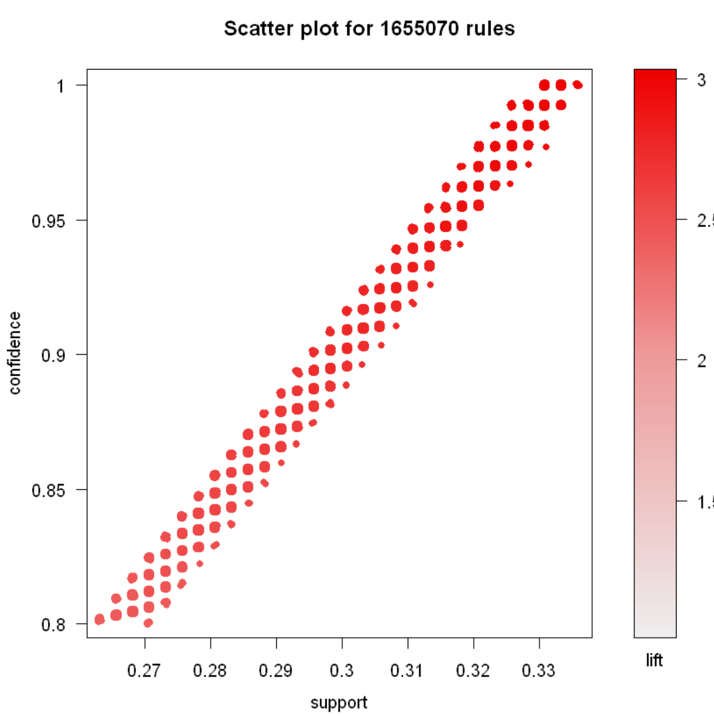
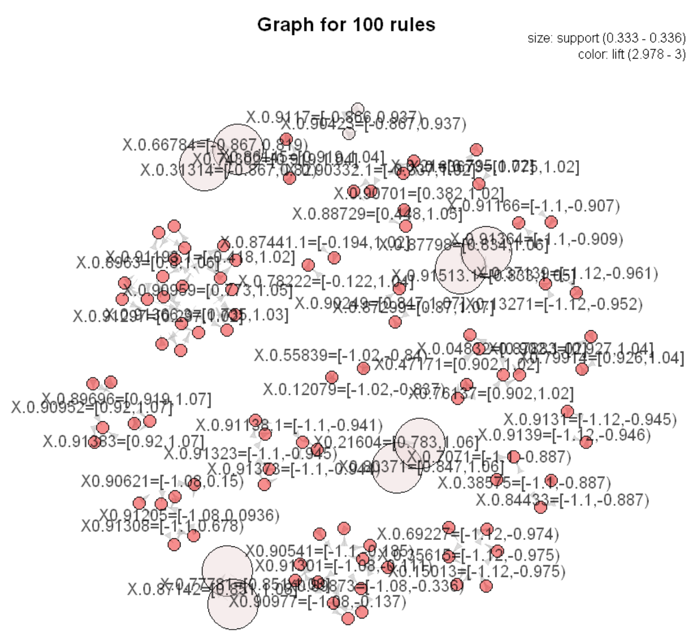
210 237 242 225 222 226 215 229 373 338 368



Association





```
set of 1655070 rules rule length distribution (lhs + rhs):sizes 2 1655070 Min. 1st Qu.
Median Mean 3rd Qu. Max. 2 2 2 2 2 2 summary of quality measures: support confidence lift
count Min. :0.2632 Min. :0.8000 Min. :2.378 Min. :105.0 1st Qu.:0.2732 1st Qu.:0.8195 1st
Qu.:2.459 1st Qu.:109.0 Median :0.2832 Median :0.8496 Median :2.549 Median :113.0 Mean
:0.2876 Mean :0.8627 Mean :2.588 Mean :114.7 3rd Qu.:0.2982 3rd Qu.:0.8947 3rd Qu.:2.684
3rd Qu.:119.0 Max. :0.3358 Max. :1.0000 Max. :3.023 Max. :134.0 mining info: data
ntransactions support confidence micro 399 0.1 0.8
```

Discussion

We have used a convolutional neural network for supervised learning on 400 microstructural images. The network has 8 hidden layers. The machine is trained well for 8000 epochs on microstructural dataset for Homogeneous and Inhomogeneous case and is used further for predicting the microstructure for different cases using the pre-trained model. We have developed 3 methods for calculating the accuracy of the predicted microstructure and the accuracy is coming greater than 95% using these methods.

We have also performed clustering analysis, seriation and association over the microstructural dataset with 64 by 64 pixel sized 400 images having 2 different types of microstructures i.e. Homogeneous and Inhomogeneous. PCA reveals that 16 components are required to cover 98% of the variance in the whole dataset. NbClust gives 15 number of optimal clusters which doesn't make much sense while Mclust gives 7 optimal clusters which is somehow explaining the matrix and precipitate in two different kind of microstructural dataset plus some noise that must have introduced while generating the microstructural dataset. We have performed clustering analysis by considering 2 clusters also and that gives some meaningful results by clustering homogeneous and inhomogeneous dataset into 2 separate clusters. Further we have done association on the dataset. We got like 1655070 rules. We have also produced the association rule's graph by considering 100 rules.

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