Stat 517 Final project

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Introduction

Materials microstructure plays a very important role in determining the properties of a material which has applications in various fields including infrastructure, computing systems, space technology and many more. This project work is based on materials system in which we are employing machine learning technologies to predict the microstructure of a material under different conditions.

Initially we generate a number of different microstructures (20,000 in this case) by varying the elastic constants (C110, C120, C440, C111, C121 and C441) of the matrix and the precipitate in the alloy system (for example Steel). We split the generated microstructures into training and testing groups. Further we are using a Convolutional neural network to train the machine on the training microstructures and then test the efficiency of model on testing microstructures.

Microstructural dataset

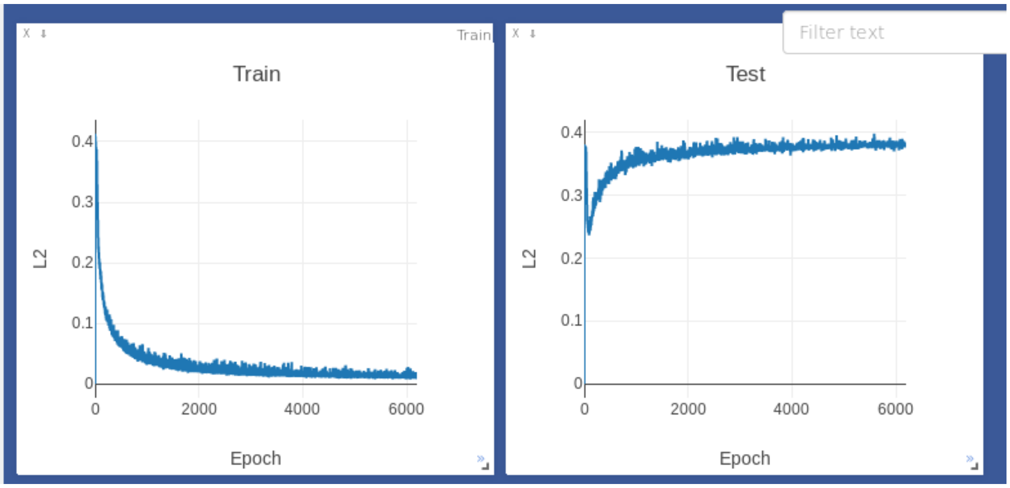
The formation of each of the 20,000 microstructure is governed by the 6 elastic constant values as mentioned above. Each of the microstructural image is of 512 × 512 pixel size and is represented in the form of composition distribution as follows:

	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

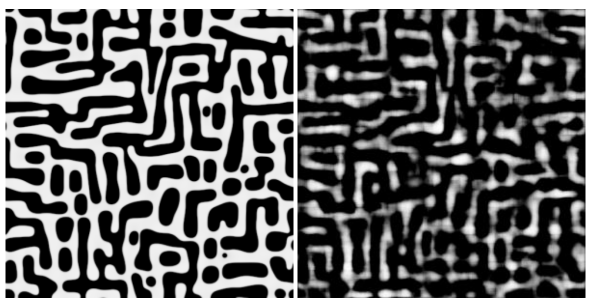
We can easily observe that each value is normalized and is in the range of -1 to 1.

Preliminary Results

Training and Testing curves

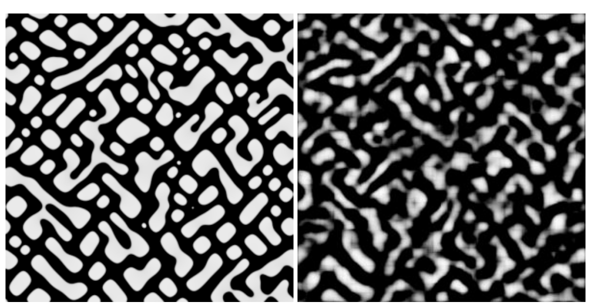


For Training Data (C110 = 501, C120 = 275, C440 = 181, C111 = 11, C121 = 17, C441 = -30)



Phase Field Data		Machine Generated Data	
% Matrix	50.137	% Matrix	52.211
% Precipitate	49.862	% Precipitate	47.788

For Testing Data (C110 = 749, C120 = 310, C440 = 185, C111 = 44, C121 = 22, C441 = 35)



Phase Field Data		Machine Generated Data	
% Matrix	50.039	% Matrix	52.204
% Precipitate	49.961	% Precipitate	47.796