Materials Informatics – Fall 2018

Final Computer Project

Due on: Dec 6

We will use the Carnegie Mellon University Ultrahigh Carbon Steel (CMU-UHCS) dataset in

> B. DeCost, T. Francis and E. Holm (2017), "Exploring the microstructure manifold: image texture representations applied to ultrahigh carbon steel microstructures." arXiv:1702.01117v2.

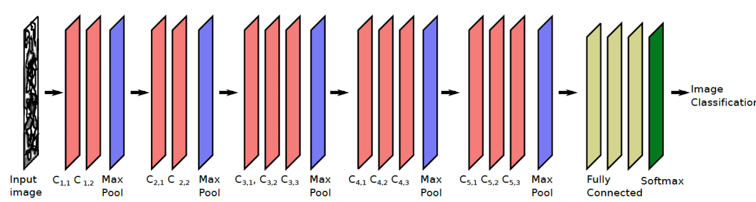
The data set is available on the TAMU Google Drive at `http://bit.ly/2jaGCkg`. There are three files: a ZIP file containing the raw images and two excel files containing the labels and sample preparation information. Please read DeCost's paper to learn more about the data set.

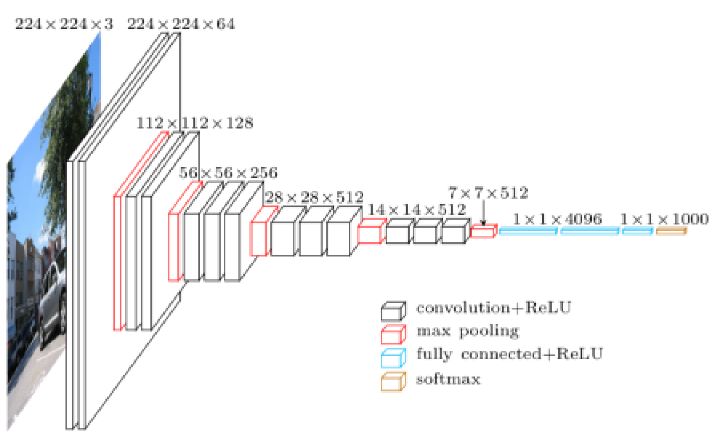
We will classify the micrographs according to **primary microconstituent**. There are a total of seven different labels, corresponding to different phases of steel resulting from different thermal processing (number of images in parenthesis): spheroidite (374), network (212), pearlite (124), pearlite + spheroidite (107), spheroidite+widmanstatten (81), martensite (36), and pearlite + widmanstatten (27).

We will use the spherodite, network, pearlite, and spheroidite+widmanstatten categories for training. The training data will be **the first 100 data points** in the spherodite, network, pearlite categories and **the first 60 points** in the spheroidite+widmanstatten category. The remaining data points will compose the various test sets (more below).

The classification rule to be used is a Radial Basis Function (RBF) nonlinear SVM classification rule. We will use a *one-vs-one* approach to deal with the multiple labels, where each of 4 choose $2 = 6$ classification problems for each pair of labels are carried out. Given a new image, each of the six classifiers is applied and then a vote is taken to achieve a consensus for the most often predicted label. If there are ties, the classifier reports multiple labels.

To featurize the images, we will use the pre-trained VGG16 deep convolutional neural network (CNN), which has the following architecture:





We will ignore the fully connected layers, and take the features from the **max pool layers** only (following the the intermediate layers **C1,2 C2,2 C3,3 C4,3 C5,3**), using the "channels" mean value as the feature vector (each channel is a 2D image corresponding to the output of a different filter). This results in feature vectors of length 64, 128, 256, 512, 512, respectively (these lengths correspond to the number of filters in each layer and are fixed, having nothing to do with the image size). In each pairwise classification experiment, we will select one of the five layers according to the best 10-fold cross-validation error estimate.

You are supposed to record the following:

(a) The convolution layer used and the cross-validated error estimate for each of the six pairwise two-label classifiers.

(b) Separate test error rates on the unused micrographs of each of the four categories, for the pairwise two-label classifiers and the multilabel one-vs-one voting classifier described previously. For the pairwise classifiers use only the test micrographs with one of the two labels used to train the classifier. For the multilabel classifier, use the test micrographs with one of the four labels in the training data.

(c) For the mixed pearlite + spheroidite and pearlite + widmanstatten micrographs, which were not used in training, apply the trained one-vs-one multilabel voting classifier and find out which label it gives to each micrograph.

(d) Now apply the pairwise classifier pearlite vs. spheroidite to the mixed pearlite + spheroidite micrographs. Compare to the results in part (c).

(e) For the martensite microstructure, which was not trained for, apply the trained one-vs-one multilabel voting classifier and find out which label it gives to each micrograph.

In each case above, interpret your results. Implementation should use the Scikit-Learn and Keras python libraries.