Neural Network for Nanoscience: Scanning Electron Microscope Image Recognition

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NFFA-Europe project

Nano Foundries and Fine Analysis

- Network for multidisciplinary research at the nanoscale, from synthesis to nanocharacterization to theory and numerical simulation.
- 20 partners
- The widest range of tools for research at the nanoscale
Nanoscience needs

- Manage and store high volume/variety of data generated
- High Performance data access
- Data Sharing: reuse and interoperability
- Identify and organize Metadata associated to data
- Metadata search engine: data accessible and searchable
Nanoscience needs

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Datascience in NFFA

- Develop the first distributed Information and Data Repository Platform (IDRP) for the nanoscience community
- Employ deep learning to classify scientific images
- Integrate a SEM image classifier to provide additional metadata
- Produce a semi-automatic workflow from the instrument to the repository
- Allow semantic search on the database
Glossary

● Training from scratch: the weights of all the layers are re-initialized

● Transfer learning: the weights of all layers have been trained on a different dataset

● Fine tuning: all weights are initialized to the last check point and are allowed to vary (with small learning rate)

● Feature extraction: last layer(s) re-initialized, previous layers frozen to checkpoint
Supervised learning

We created and manually annotated the first sample of classified SEM images (for a total of \(\sim 20,000\) images)

Figure 1. Categories chosen for SEM images. The dimensionality of nanoscience objects provided the basis for the choice. Other categories, such as Biological and Tips were added as these were common images found in the SEM database.

Modarres et al. 2017, Scientific Report, in press
Machine learning tools

- Tensorflow, Tensorflow-Slim
- Network architectures
  - Inception v3, v4
  - ResNet v2
  - DenseNet (preliminary results)
- 85/15 splitting of the dataset
Computational resources

Cosilt Cloud Computing Environment

Eurotech AURORA system with 8 GPU nodes
- 2 Intel Xeon E5-2697 (12 cores each)
- 2 NVIDIA K20s GPUs (2496 CUDA cores, 5GB ram)
Transfer Learning from ImNet to NFFA - Feature Extraction

- **ResNetv2** (lr0.009-exp-dec, bs32)
- **Incv3** (lr0.007-exp-dec, bs32)
- **Incv4** (lr0.007-exp-dec, bs32)

Accuracy vs Hours

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Transfer Learning from ImNet to NFFA - Fine-Tuning

- Incv4 (lr0.007-exp-dec, bs16)
- Incv3 (lr0.007-exp-dec, bs16)
Train from scratch

Training on NFFA

Accuracy vs Hours

- Inc_v4 (lr0.01-exp-dec, bs16)
- Inc_v3 (lr0.01-exp-dec, bs16)
- Inc_v3 (lr0.01-exp-dec, bs32)
Train from scratch

Training on NFFA

Accuracy vs Epochs

- Inc_v4 (lr=0.01-exp-dec, bs=16)
- Inc_v3 (lr=0.01-exp-dec, bs=16)
- Inc_v3 (lr=0.01-exp-dec, bs=32)
Inception V3: Training vs Transfer Learning

- Training from scratch (lr0.01-exp-dec, bs32)
- ImNet-Fine-Tuning (lr0.007-exp-dec, bs32)
- ImNet-Features-Extr (lr0.007-exp-dec, bs32)
Traning vs Transfert Learning

Inception V3: Training vs Transfer Learning

Accuracy

Epochs

Training from scratch (lr0.01-exp-dec, bs32)
ImNet-Fine-Tuning (lr0.007-exp-dec, bs32)
ImNet-Features-Extr (lr0.007-exp-dec, bs32)
Refining further

Transfert Learning + Fine-Tuning + Feature Extraction

Better accuracy and faster time to solution!

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Accuracy vs. time

- Trans. learn. + Fine tuning + Feature extraction
- Training from scratch + Feature extraction
- Trans. learn. + Fine tuning
- Training from scratch
- Trans. learn. + Feature extraction
DenseNet

Transfer Learning from ImNet to NFFA - Fine-Tuning

Accuracy

Hours

- Incv3 (lr0.007-exp-dec, bs16)
- Incv4 (lr0.007-exp-dec, bs16)
- Dnet121 (lr0.007-exp-dec, bs16)

WORK IN PROGRESS
<table>
<thead>
<tr>
<th>Image</th>
<th>Processing page</th>
<th>Nanowires</th>
<th>MEMS devices electrodes</th>
<th>Biological</th>
<th>Films Coated Surface</th>
<th>Porous Sponge</th>
<th>Patterned surface</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.jpg" alt="Image 237" /></td>
<td>237</td>
<td>0.2%</td>
<td>4.1%</td>
<td>0.03%</td>
<td>0.9%</td>
<td>93.6%</td>
<td>Predicted</td>
</tr>
<tr>
<td><img src="image2.jpg" alt="Image 238" /></td>
<td>238</td>
<td>0.07%</td>
<td>0.00%</td>
<td>99.9%</td>
<td>0.00%</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
</tbody>
</table>
The complete Workflow
Conclusions

- Very high accuracy (>96%) on a specific dataset
- Best approach (both for accuracy and time to solution) → Transf. Learning + Fine Tuning + Feature Extraction
- Automatic metadata generation
- Semi-automatic workflow for SEM scientist, which allows to further improve the training