Convolutional neural networks for classification of transmission electron microscopy imagery

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- Motivation of applying CNN method for classification of electron microscopy images

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- Pitfalls
- Deep Learning software:
    - OS availability
    - Licenses
    - Performance
    - Community support

Convolutional neural networks (CNN)

Convolutional neural network (CNN)

It is a special kind of neural network for processing data that has a known, grid-like topology. CNN are simply neural networks that use convolution in place of general matrix multiplication in at least one of their layers.

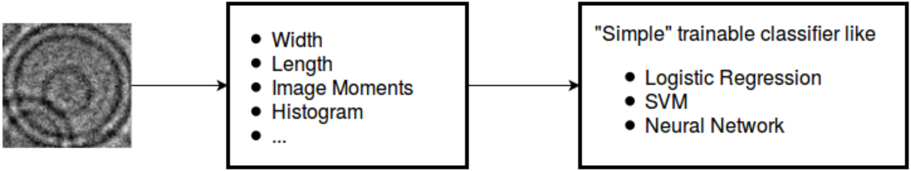
Why CNN?

- CNN operate on raw pixel data, i.e. minimum preprocessing
- CNN learn image features themselves, i.e. do not need expert knowledge for selecting feature
- Scalability due to the following assumptions:
  - Local connectivity
  - Parameter sharing
- Documented success

Motivation

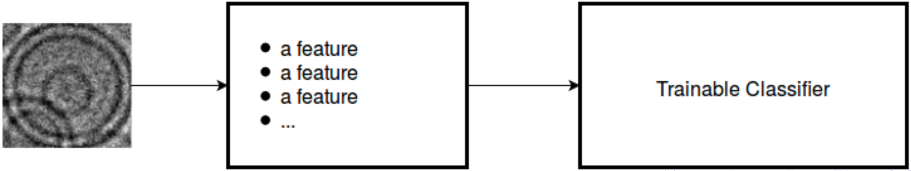
Traditional Approach

Extract a number of features and then train a "simple" classifier.



CNN Approach

Feed raw pixel data to a model that trains both feature extractor and classifier.



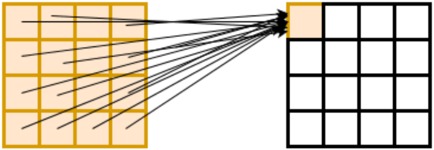
Local connectivity and parameter sharing

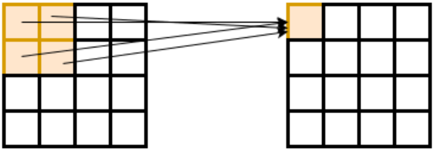
Full Connectivity

All nodes in input layer are connected to all nodes in the next layer. All weights are unique.

Local Connectivity

Each node in a layer is connected only to a small number of nodes from the previous one. All neurons in the convolutional layer share their weights.





Why now?

CNN are being successfully used for

- Classification
- Segmentation
- Super Resolution
- A lot of other examples

Three reasons why CNN have become so useful right now

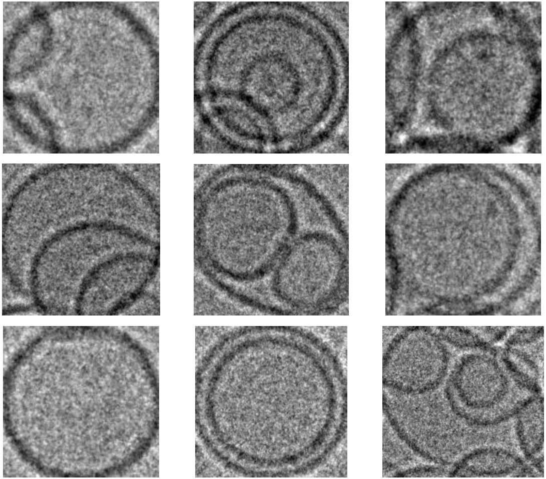
- Big datasets
- Powerful enough hardware
- Software

Problem description: Lamellarity

Determine structure of a liposome according to the number of lamellae.

There are 14169 EM images and three classes:

- Unilamellar
  12368, 87.29%
- Multilamellar
  1717, 12.12%
- Uncertain
  84, 0.5%



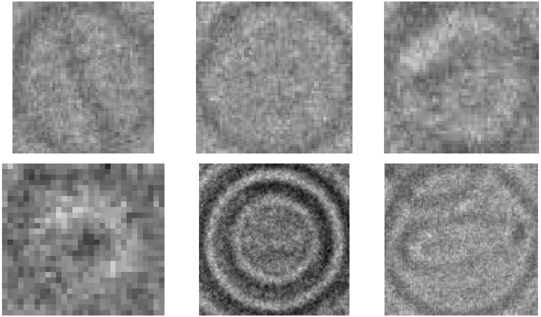
Unilamellar Multilamellar Uncertain

Problem description: Encapsulation

Determine presence of a liposomal encapsulation.

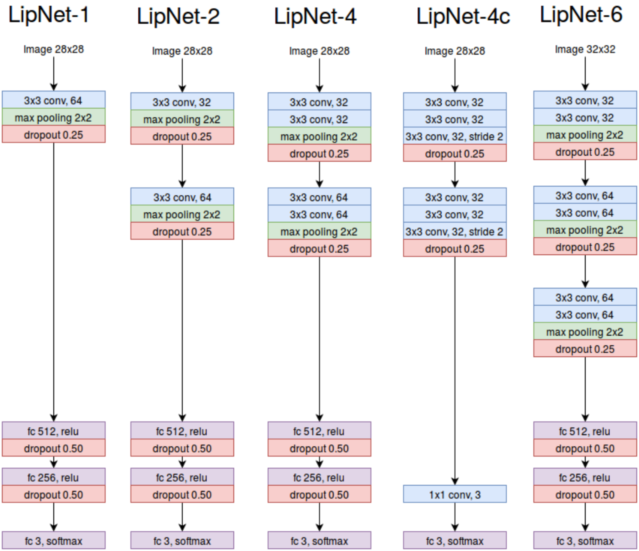
There are 24918 EM images and three classes:

- Full
  24255, 97.34%
- Empty
  161, 0.65%
- Uncertain
  502, 2.01%



Full Empty Uncertain

Network architectures



Which LipNet model is the best?

Five LipNet models are evaluated by recording their 5-fold cross validated F_1 scores. Present performance measures.

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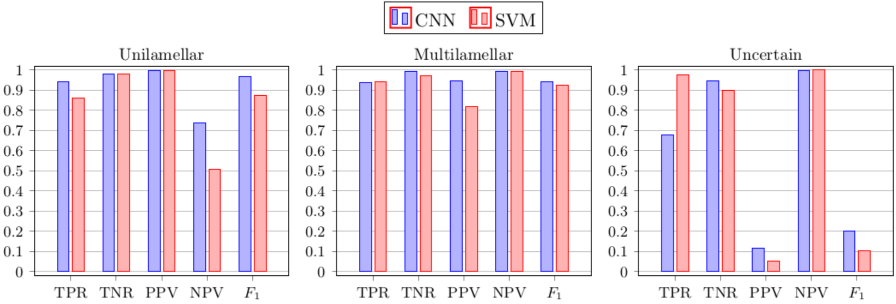
Which LipNet model is the best?

Five LipNet models are evaluated by recording their 5-fold cross validated F_1 scores. Present performance measures.

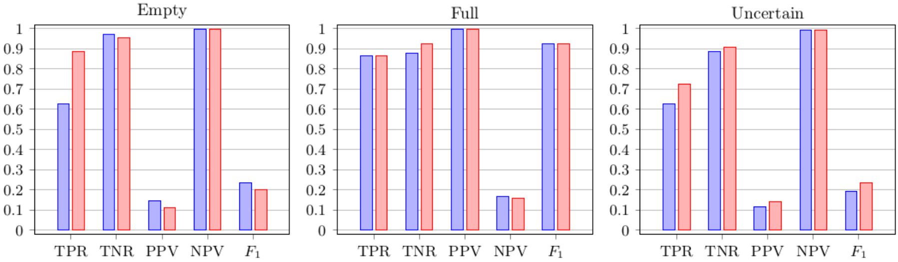
- The Lamellarity Problem: **LipNet-4** is the best
- The Encapsulation Problem: There is no clear leader. **LipNet-4** is selected.

CNN vs SVM: Lamellarity



- CNN is slightly better than SVM.
- Less false negative *unilamellar* by CNN than SVM.
- Less false positive *multilamellar* by CNN than SVM.
- Many false positive predictions of *uncertain*, mainly *unilamellar* is confused with *uncertain*.

CNN vs SVM: Encapsulation



- Almost the same performance.
- Some *full* are falsely classified as *empty* and *uncertain*
  - Low NPV for *full*
  - Poor precision (PPV) for *empty* and *uncertain*
- PPV for *full* and NPV for *empty* and *uncertain* are almost 1, so hardly any false positive of *full*.

Pitfalls and performance improvement techniques

- The Class Imbalance Problem. It is very problematic when a data set is unbalanced. They usually are!
  - Oversampling
  - Undersampling
  - Artificial data
  - Higher penalties for minority classes

Pitfalls and performance improvement techniques

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- Poor diversity of the training data
    - Data augmentation

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  - Oversampling
  - Undersampling
  - Artificial data
  - Higher penalties for minority classes
- Poor diversity of the training data
  - <u>Data augmentation</u>
- Regularization
  - Weight decay
  - Noise injection, for example label smoothing
  - Dropout
  - Early stopping

Deep learning software

OS and API

The path of least resistance:

- Linux
- Python

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Licensing

Nearly all libraries are distributed according to some of OSI-approved licenses like Apache, BSD, MIT, etc.

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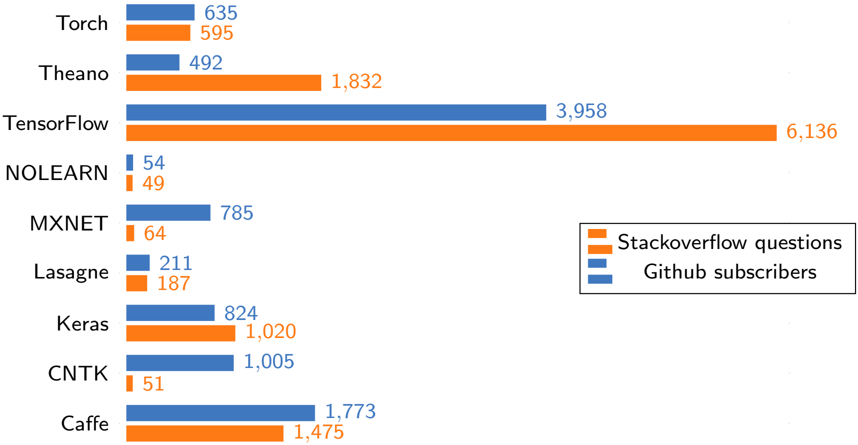
GPU

All libraries benefit from GPUs. At the moment there is no study that shows superiority of any library in terms of performance.

Popularity of deep learning software as of January 2017



Conclusion and future work

Conclusions:

- CNN is a promising tool for research and production
- Reasonable performance
- CNN does not require feature representation

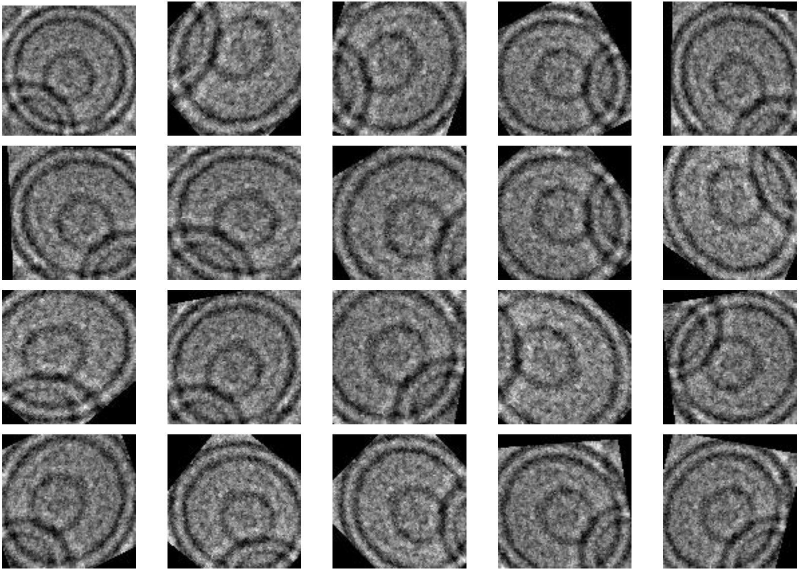
- ~~Limited support for Windows~~

Future work:

- Fully convolutional networks with input of variable size
- Alternative ways to expand the training set
- Fusing, i.e. combine LipNet and another neural network trained on image features

Thank you!

Data augmentation example go back



Performance measures go back

Accuracy is not enough when the data set is imbalanced.

Confusion matrix

	Predicted Positive	Predicted Negative
Actual Positive	True Positive	False Negative
Actual Negative	False Positive	True Negative

- True Positive Rate: $TPR = \frac{TP}{TP+FN}$ (sensitivity or recall)
- True Negative Rate: $TNR = \frac{TN}{TN+FP}$ (specificity)
- Positive Predicted Value: $PPV = \frac{TP}{TP+FP}$ (precision)
- Negative Predicted Value: $NPV = \frac{TN}{TN+FN}$
- F_1 score : harmonic mean of TPR and PPV

Input images: surrounding and masking

Each image contains a liposome object and its surrounding which goes 50 pixels in each direction. Corresponding particle masks are also available.

Three choices:

- Images with surrounding
- Cropped images
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