# Convolutional neural networks for classification of transmission electron microscopy imagery


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# Introduction

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

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- A very short introduction to CNN
- Benchmarking of CNN models against the SVM classifier for the selected problems
- 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.

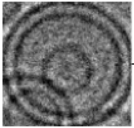
Why CNN?

- 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.



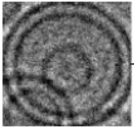
- Width
- Length
- Image Moments
- Histogram
- ...

"Simple" trainable classifier like

- Logistic Regression
- SVM
- Neural Network

## CNN Approach

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



- a feature
- a feature
- a feature
- ...

Trainable Classifier

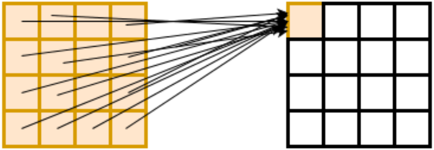
# Local connectivity and parameter sharing

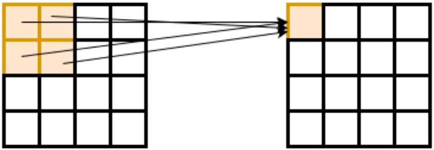
## Full Connectivity

All nodes (pixels) 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 (pixels) from the previous one. Weight are shared within each layer.





# 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

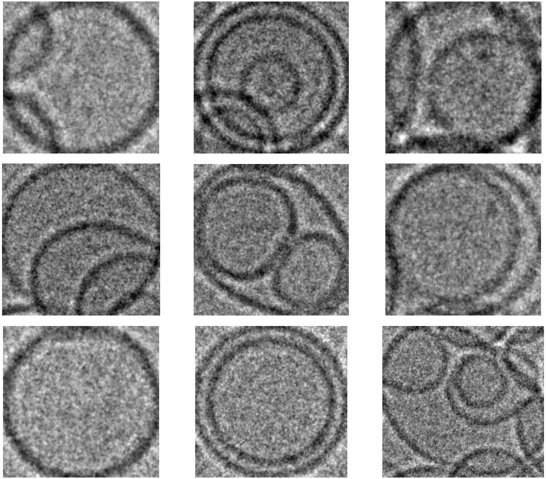
- Big datasets
- Powerful enough hardware
- Software

# 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%



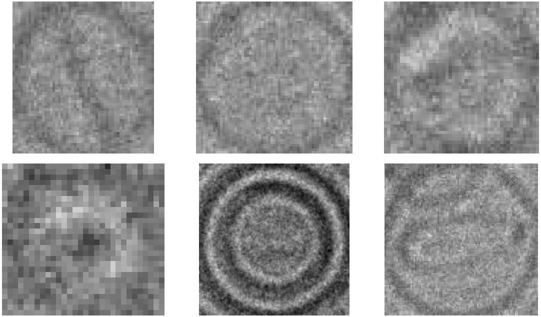
Unilamellar Multilamellar Uncertain

# Problem description: Encapsulation

Determine presence of a liposomal encapsulation.

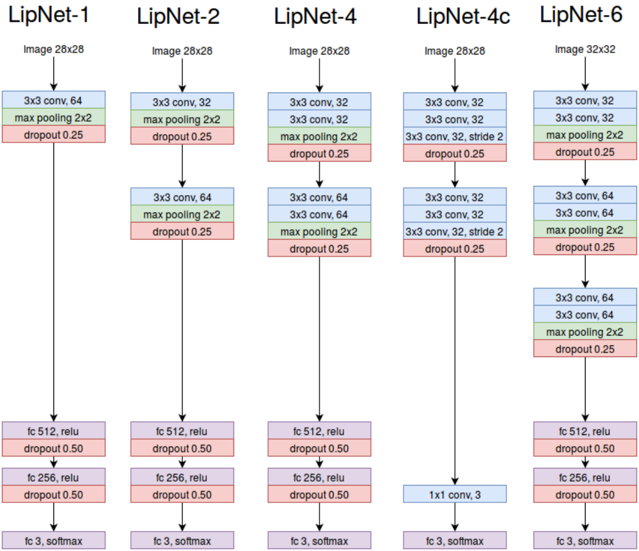
There are 24918 EM images and three classes:

- 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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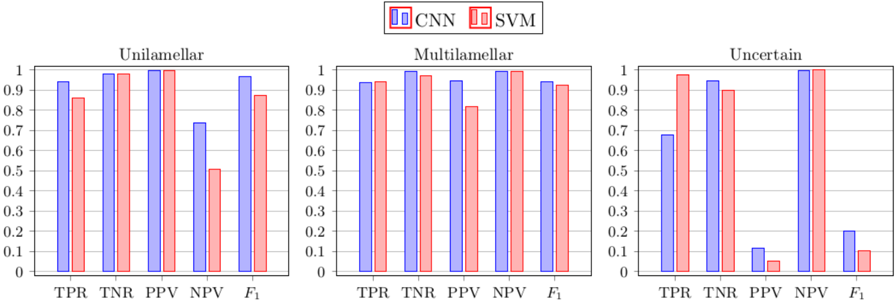
# Which LipNet model is the best?

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

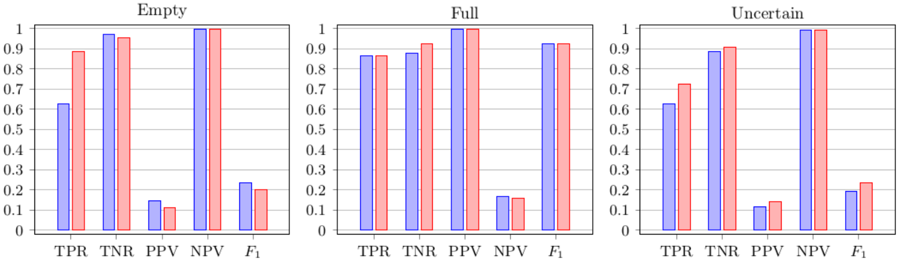
- The Lamellarity Problem: **LipNet-4** is the best
- The Encapsulation Problem: There is no clear leader. **LipNet-4** is selected.

# 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

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- Poor diversity of the training data
  - Data augmentation

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  - Undersampling
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- Poor diversity of the training data
  - Data augmentation
- Regularization
  - Weight decay
  - Noise injection, for example label smoothing
  - Dropout
  - Early stopping

# Deep learning software

## OS and API

The path of least resistance:

- Linux
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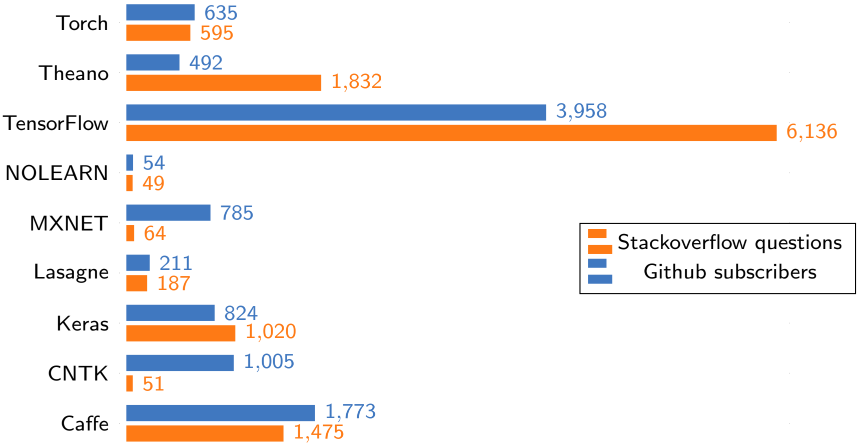
## GPU

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

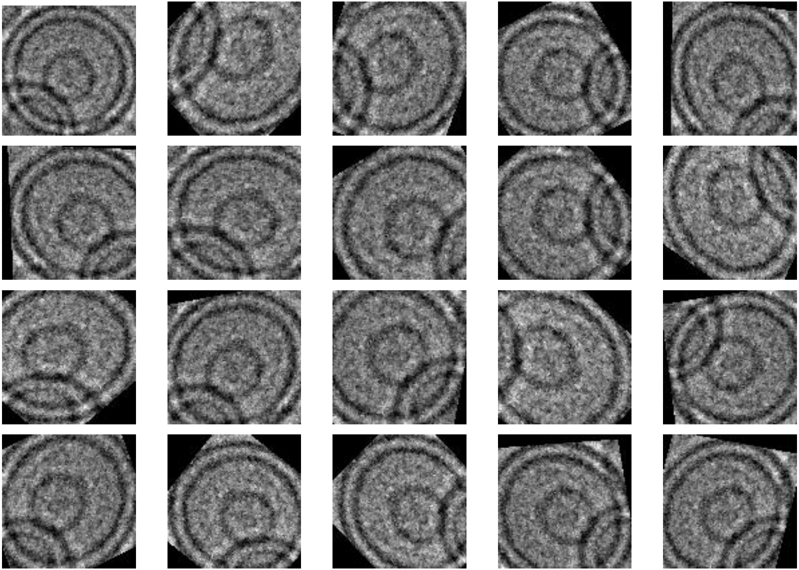
- ~~Limited support for Windows~~

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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