Convolutional neural networks for classification of transmission electron microscopy imagery

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This MSc project is done in cooperation with Vironova AB.

Objective

- Discuss the suitability of applying CNN method for classification of electron microscopy images

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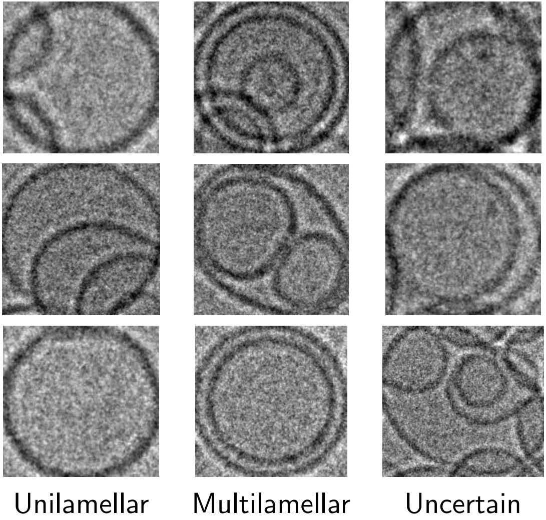
- Discuss Deep Learning software:
  - OS availability
  - Licenses
  - Performance
  - Community support

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%

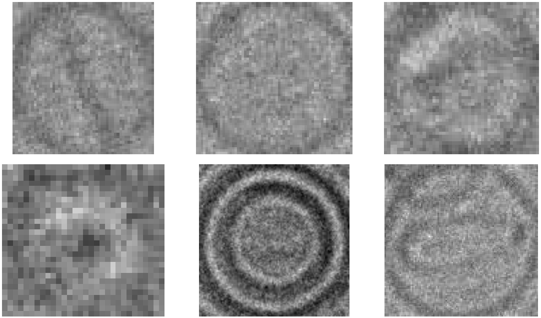


Problem description: Encapsulation

Determine presence of a liposomal encapsulation.

There are 24918 EM images and three classes:

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



Full Empty Uncertain

The data set of image features

Image Feature

It is a piece of information which is relevant for solving the computational task related to a certain application. Features may be specific structures in the image such as points, edges or objects. Features may also be the result of a general neighborhood operation or feature detection applied to the image.

- Maximum width
- Diameter
- Length
- Histogram
- Image Moments
- Radial Density Profile
- Edge Density Profile
- Signal to noise

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?

- Scalability due to the following assumptions:
  - Local connectivity
  - Parameter sharing
- 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
- Documented success

The Class Imbalance Problem

Lamellarity and Encapsulation data sets are imbalanced and it is a problem!

How to mitigate the class imbalance problem?

- Oversampling
- Undersampling
- SMOTE (Synthetic Minority Oversampling Technique)
- Artificial data
- Higher penalties for misclassification of minority classes

Regularization

Definition

Regularization is any modification we make to a learning algorithm that is intended to reduce its generalization error but not its training error

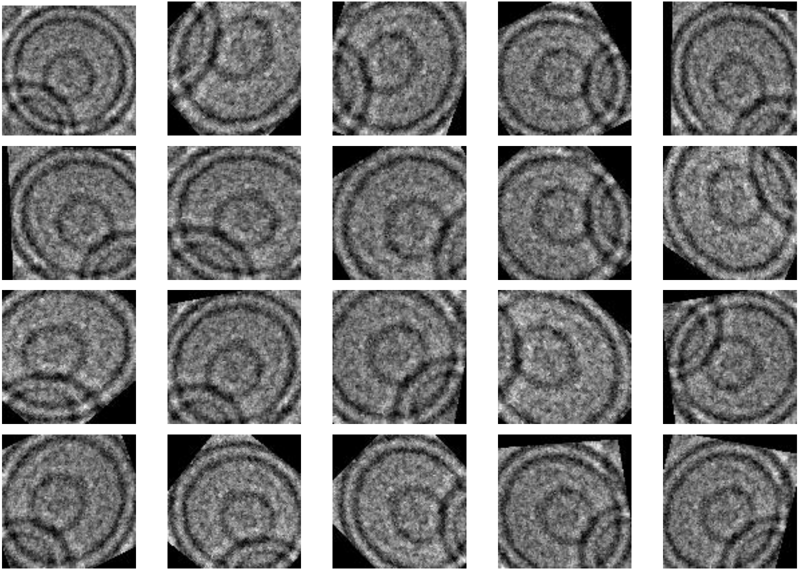
- Weight decay
- Noise injection: label smoothing
- Dropout
- Early stopping
- Data augmentation

Data augmentation techniques

Data augmentation introduces additional diversity in the training set by applying different transformations to the existing examples.

- Rotation in the range $[-180, 180]$ degrees with spline interpolation
- Shear transformation in the range $[0, 0.2]$
- Vertical shift in the range $[-10, 10]$ percent of total height
- Horizontal shift in the range $[-10, 10]$ percent of total width
- Zoom in the range $[0.8, 1.0]$ which means zoom by a maximum 20%
- Horizontal flip
- Vertical flip

Data augmentation example



Performance measures

The Accuracy Paradox

Models with a given accuracy may have greater predictive power than models with higher accuracy.

Confusion matrix

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

Performance measures

True positive rate (TPR)

AKA sensitivity or recall: $TPR = \frac{TP}{TP+FN}$

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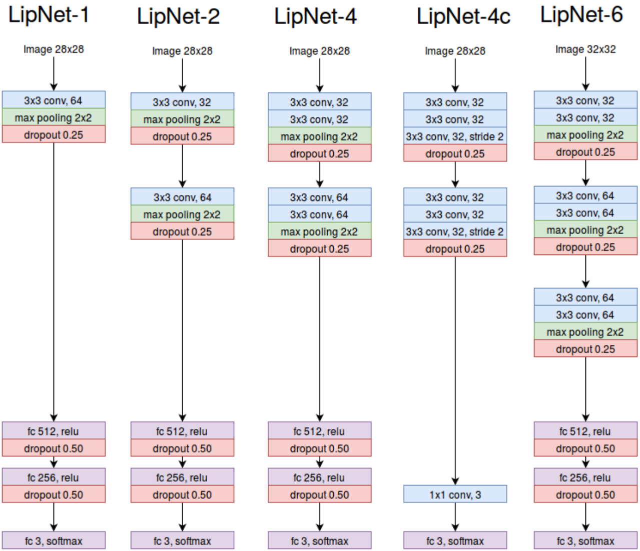
F_1 score

It is a harmonic mean of TPR and TNR

Network architectures



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

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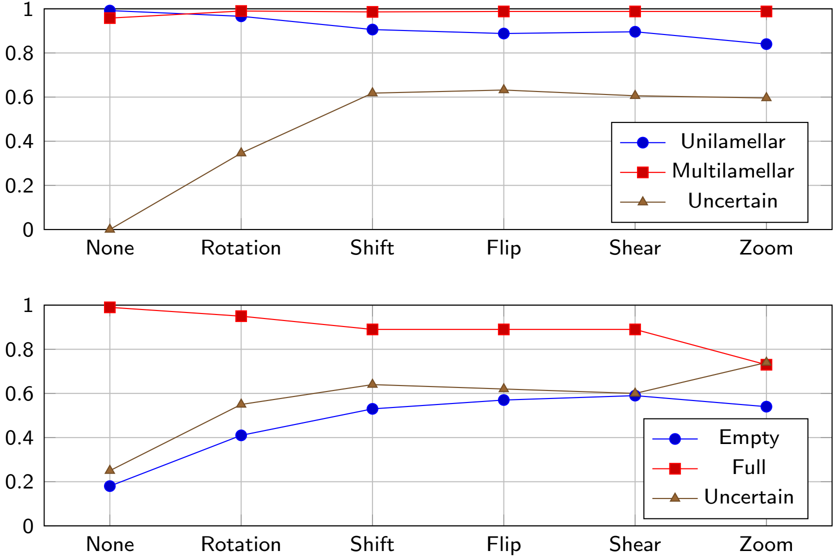
Five LipNet models are evaluated by recording their 5-fold cross validated F_1 scores.

- The Lamellarity Problem: **LipNet-4** is the best
- The Encapsulation Problem: There is no clear leader. **LipNet-2** is selected for the final experiment. LipNet-6 performed worst.

Effect of the data augmentation



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
- Cropped and masked

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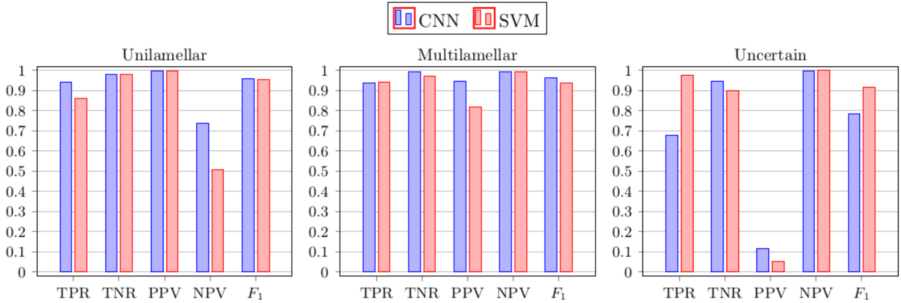
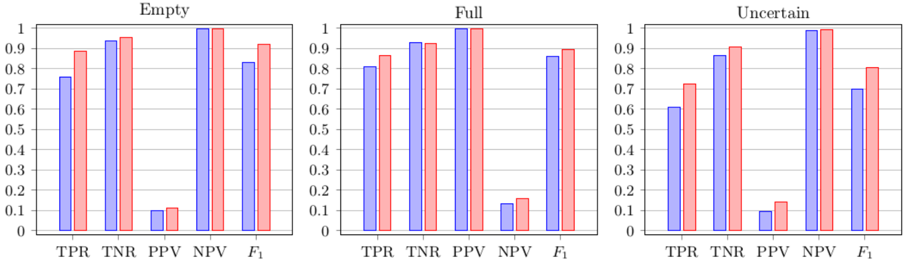
CNN vs SVM: Lamellarity



- CNN is better in predicting *unilamellar* and *multilamellar*.
- More false negative *unilamellar* by SVM than CNN.
- More false positive *multilamellar* by SVM than by CNN.
- SVM is better in predicting *uncertain*.
- Many false positive predictions of *uncertain*, mainly *unilamellar* is confused with *uncertain*.

CNN vs SVM: Encapsulation



- SVM is slightly better than CNN.
- Poor precision for *empty* and *uncertain* because some *full* are falsely classified.
- Low NPV for *full*, it is a direct consequence of the previous item.
- Precision of *full* and NPV of *empty* and *uncertain* are almost 1, so hardly any false positive of *empty*.
- Both classifiers underestimate the number of *full*.

Deep learning software

OS and API

The path of least resistance:

- Linux
- Python

Deep learning software

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

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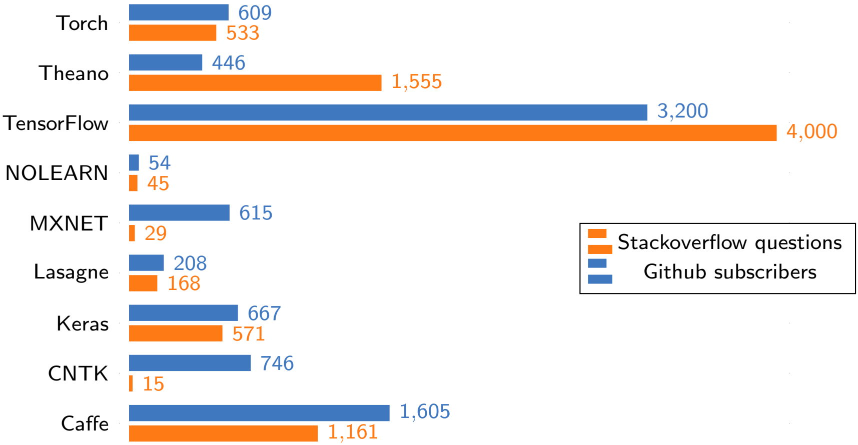
GPU

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 October 2016



Conclusion and future work

Conclusions:

- Reasonable performance
- CNN is an excellent research tool

Future work:

- Fully convolutional networks with input of variable size
- Alternative ways to expand the training set
- Late fusing