Convolutional neural networks for classification of transmission electron microscopy imagery

Sergii Gryshkevych

Uppsala University
Supervisor: Max Pihlström
Reviewer: Ida-Maria Sintorn
Examinator: Justin Pearson
Opponent: Christopher Lagerhult

December 14, 2016

Introduction

This MSc project is done in cooperation with Vironova AB.

Objective

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

Objective

- Discuss the suitability of applying CNN method for classification of electron microscopy images
- Benchmark CNN models against SVM classifier for the selected problems

Objective

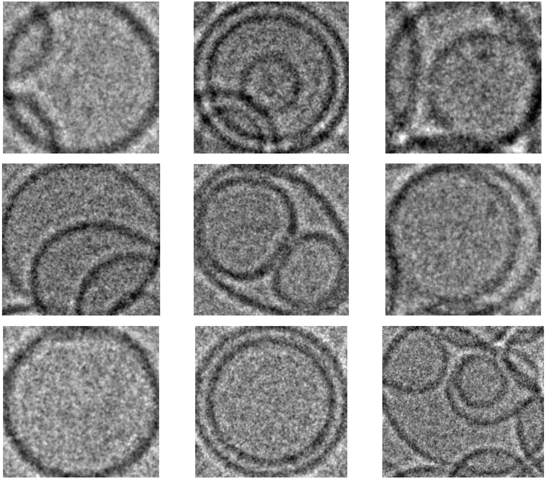
- Discuss the suitability of applying CNN method for classification of electron microscopy images
- Benchmark CNN models against SVM classifier for the selected problems
- Discuss Deep Learning software:
  - OS availability
  - Licenses
  - Performance
  - Community support

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%



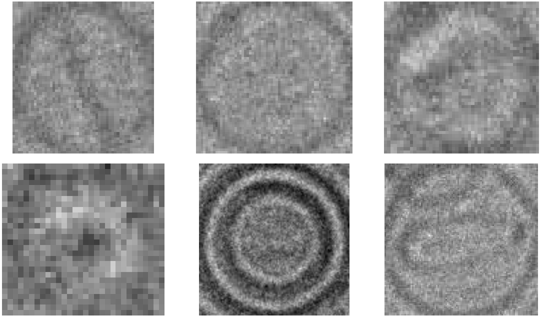
Unilamellar Multilamellar Uncertain

Problem description: Encapsulation

Determine presence of a liposomal encapsulation.

There are 24918 EM images and three classes:

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



Full Empty Uncertain

The data set of image features

Definition

In computer vision and image processing, a feature 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

Definition

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

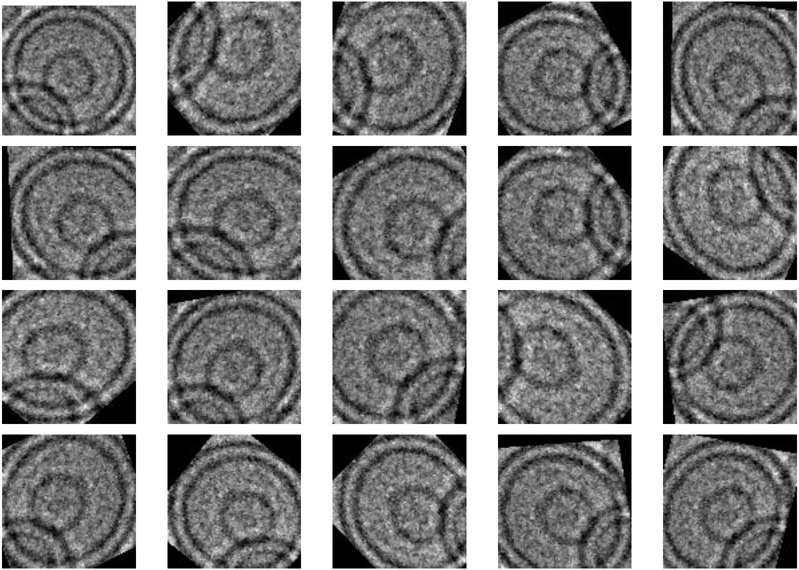
- Weight decay
- Noise injection: label smoothing
- Dropout
- Early stopping
- Data augmentation

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: $TPR = \frac{TP}{TP+FN}$

Performance measures

True positive rate (TPR)

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

True negative rate (TNR)

AKA specificity: $TNR = \frac{TN}{TN+FP}$

Performance measures

True positive rate (TPR)

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

True negative rate (TNR)

AKA specificity: $TNR = \frac{TN}{TN+FP}$

Positive predicted value (PPV)

AKA precision: $PPV = \frac{TP}{TP+FP}$

Performance measures

True positive rate (TPR)

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

True negative rate (TNR)

AKA specificity: $TNR = \frac{TN}{TN+FP}$

Positive predicted value (PPV)

AKA precision: $PPV = \frac{TP}{TP+FP}$

Negative predicted value (NPV)

$NPV = \frac{TN}{TN+FN}$

Performance measures

True positive rate (TPR)

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

True negative rate (TNR)

AKA specificity: $TNR = \frac{TN}{TN+FP}$

Positive predicted value (PPV)

AKA precision: $PPV = \frac{TP}{TP+FP}$

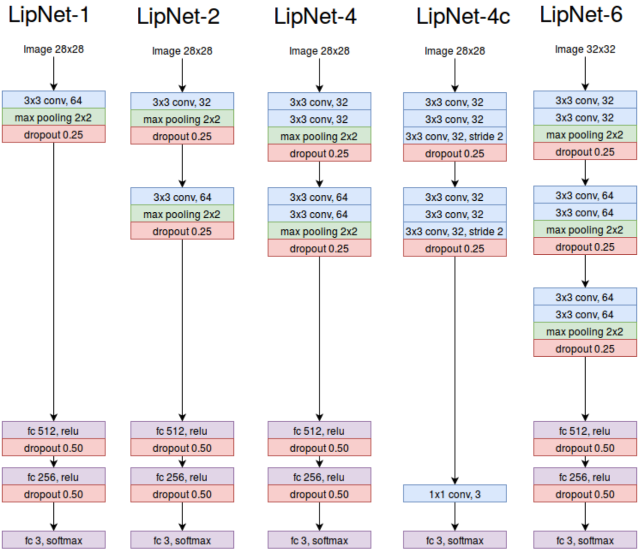
Negative predicted value (NPV)

$NPV = \frac{TN}{TN+FN}$

F_1 score

It is a harmonic mean of TPR and TNR

Network architectures



Which LipNet model is the best?

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

Which LipNet model is the best?

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

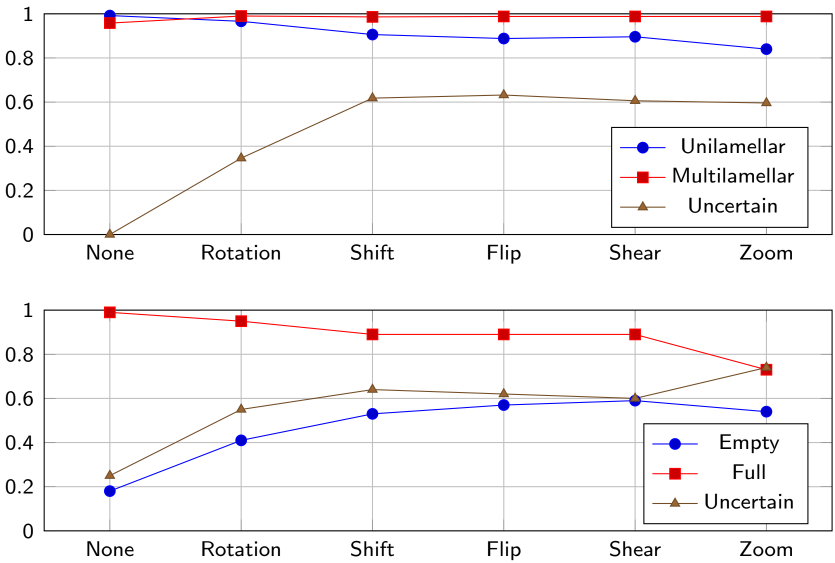
- The Lamellarity Problem: **LipNet-4** is the best

Which LipNet model is the best?

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

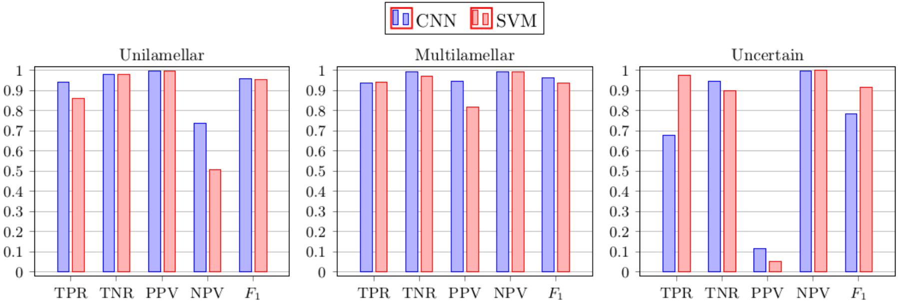
Input images: surrounding and masking

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

Three choices:

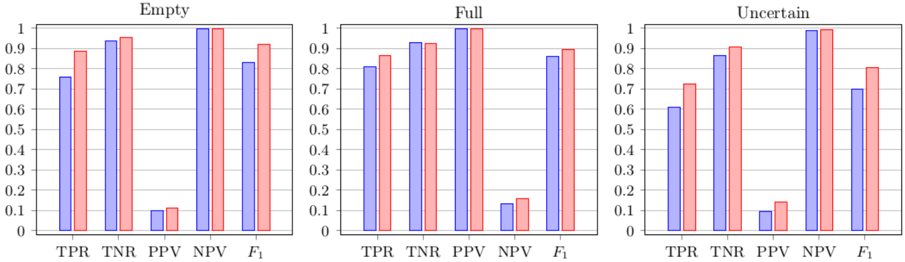
- Images with surrounding
- Cropped images
- Cropped and masked

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*.

Popularity of deep learning software as of October 2016