Machine Learning in Imaging

BME 590L
Roarke Horstmeyer

Lecture 13: CNN visualization and example applications

Post-processing of your results: a few options at different stages

Options to examine your test data after processing:

- ROC curve, Precision-Recall
- Confusion matrix
- Sliding window visualization
- Layer visualizations
- Saliency maps etc.
- tSNE visualization

ROC curve and confusion matrix

- Can set threshold for f(x,W) wherever
- Leads to sliding window between FN and FP rate
- Need to summarize both statistics as a function of sliding window

Estimated label

f(x, W)

Actual label y		+1	-1
	+1	True positive	False negative
	-1	False positive	True negative

Missed an event

Predict event when there isn't one

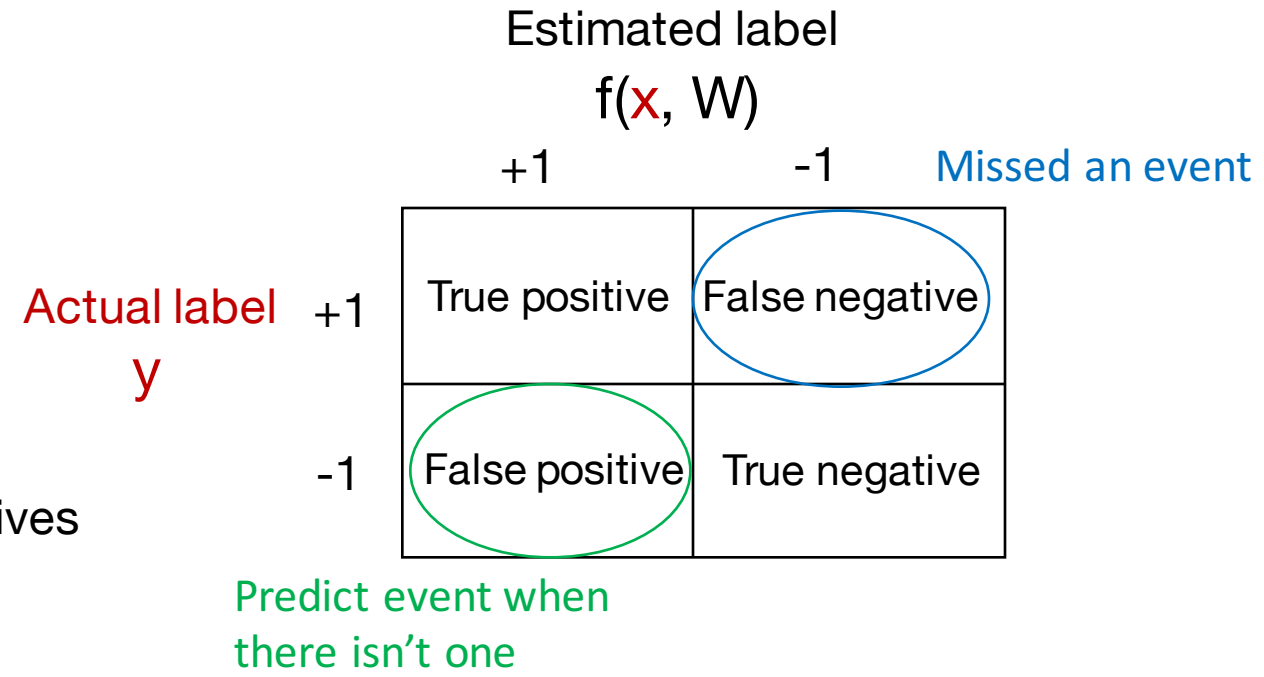
ROC curve and confusion matrix

TP Rate =

Sensitivity = TP / (TP + FN) = TP / Actual positives

False Positive Rate = FP / (TN + FP) = FP/ Actual negatives

Specificity = TN / (TN + FP) = TN / Actual negatives
= 1 – False Positive Rate



ROC curve and confusion matrix

TP Rate =

Sensitivity = TP / (TP + FN) = TP / Actual positives

False Positive Rate = FP / (TN + FP) = FP/ Actual negatives

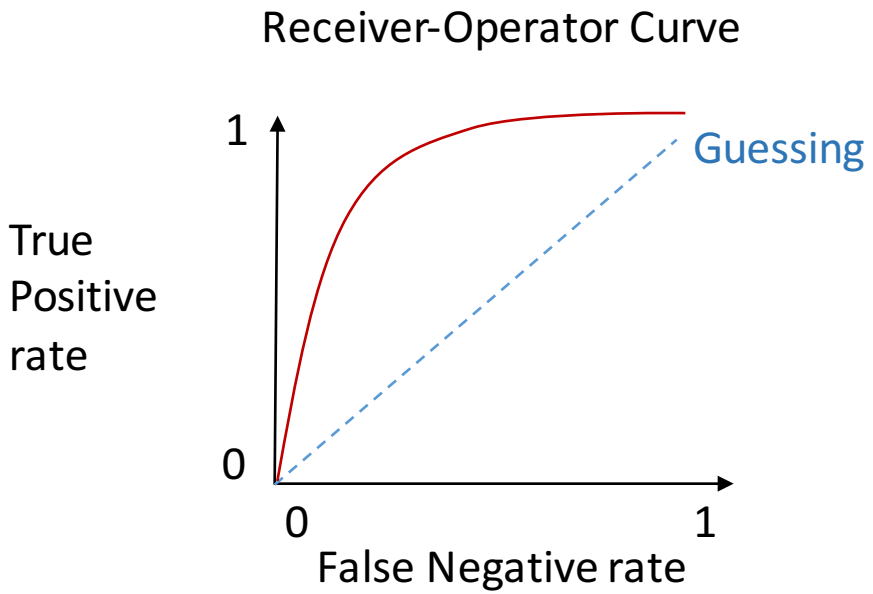
Specificity = TN / (TN + FP) = TN / Actual negatives
= 1 – False Positive Rate

Estimated label
f(x, W)

Actual label y	+1	-1
+1	True positive	False negative
-1	False positive	True negative

Missed an event

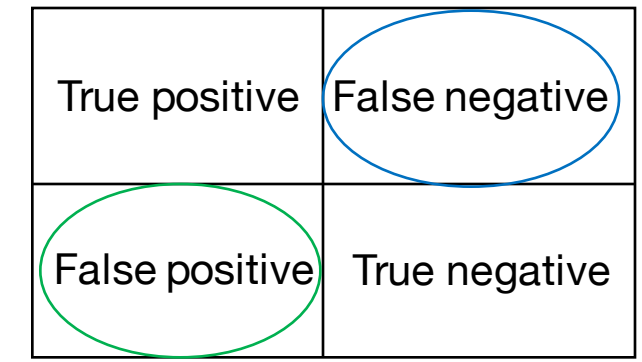
Predict event when there isn't one



ROC curve and confusion matrix

Recall =
Sensitivity = TP / (TP + FN) = TP / Actual positives

Estimated label
f(x, W)



Predict event when there isn't one

Precision = TP / (TP + FP) = TP / Estimated positives

- Sometimes, you don't care about true negatives (just want to find events)
- In this case, use Precision and Recall

ROC curve and confusion matrix

Recall =
Sensitivity = TP / (TP + FN) = TP / Actual positives

Estimated label
f(x, W)

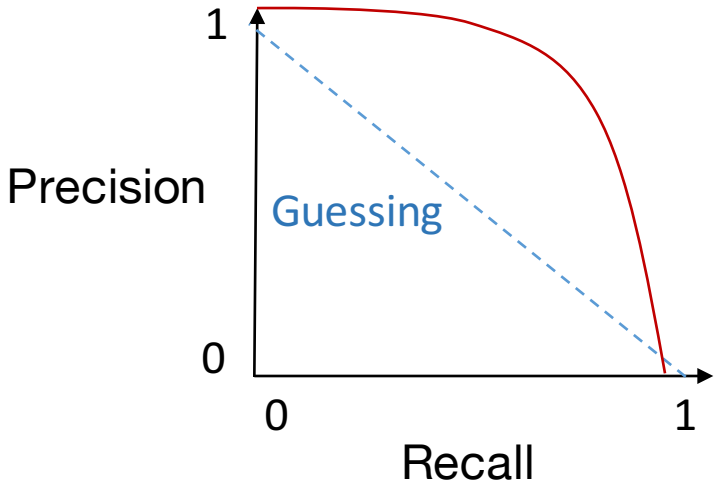
Actual label y	+1	-1
+1	True positive	False negative
-1	False positive	True negative

Missed an event

Predict event when there isn't one

Precision = TP / (TP + FP) = TP / Estimated positives

Precision-Recall curve



F1 Metric: $(1/\text{precision} + 1/\text{recall})^{-1}$

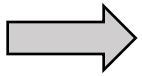
ROC curve and confusion matrix

Just 2 categories

Estimated label

f(x, W)

y \	+1	-1
+1	True positive	False negative
-1	False positive	True negative



Confusion Matrix: 2+ categories

Estimated label

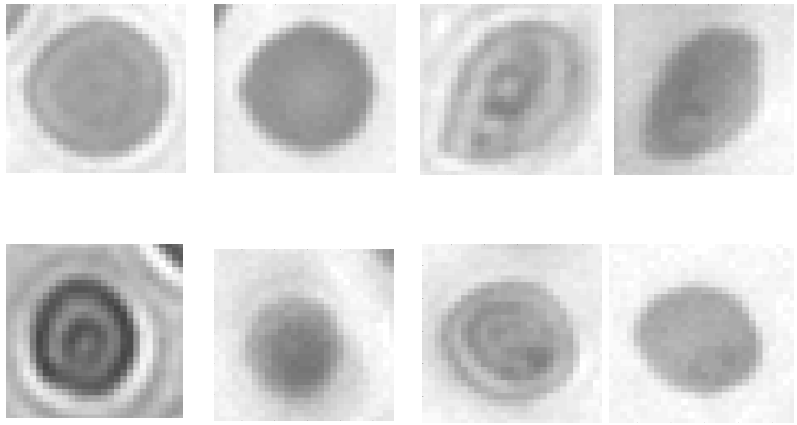
f(x, W)

y

Actual ↓	State1 (Predicted)	State2 (Predicted)	State3 (Predicted)	State4 (Predicted)	State5 (Predicted)	State6 (Predicted)	State7 (Predicted)	State8 (Predicted)
State1 (Actual)	90.12 %	0.00 %	9.88 %	0.00 %	0.00 %	0.00 %	0.00 %	0.00 %
State2 (Actual)	0.00 %	100.00 %	0.00 %	0.00 %	0.00 %	0.00 %	0.00 %	0.00 %
State3 (Actual)	0.00 %	0.00 %	92.66 %	0.00 %	0.00 %	7.34 %	0.00 %	0.00 %
State4 (Actual)	0.00 %	0.00 %	0.00 %	100.00 %	0.00 %	0.00 %	0.00 %	0.00 %

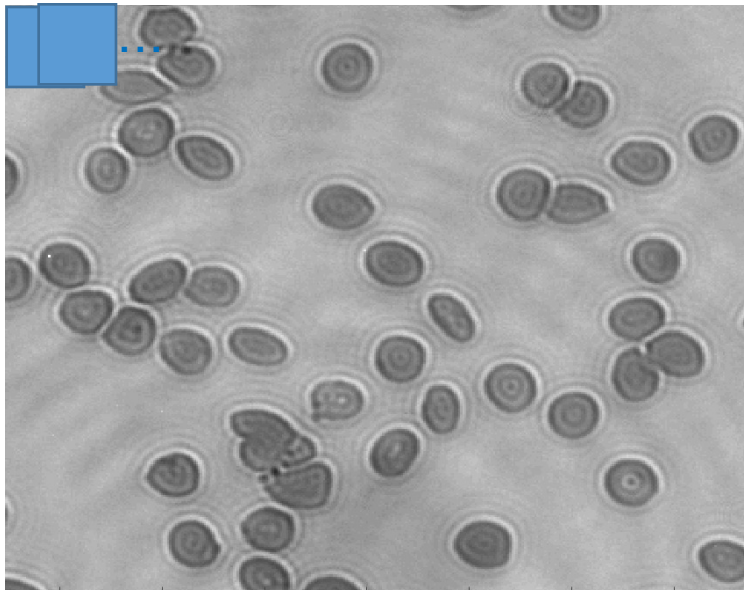
How can we visualize performance?

Training dataset



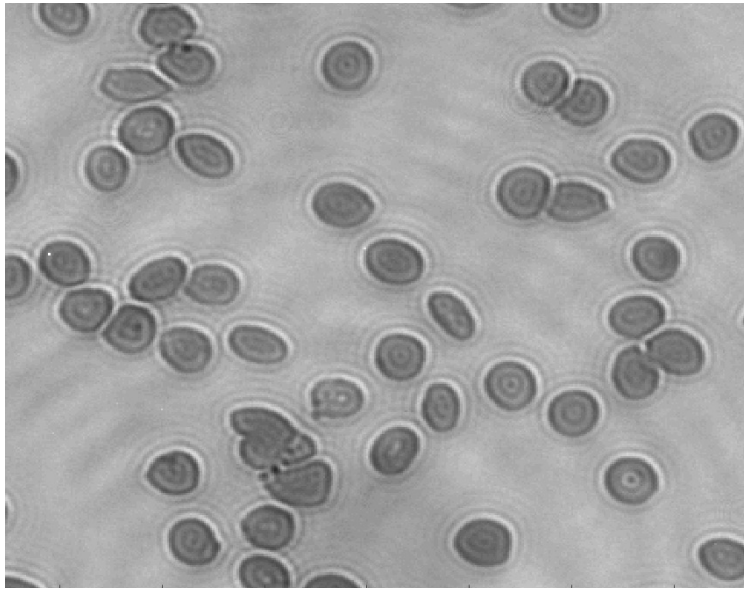
Trained CNN

Real data is big…what to do??



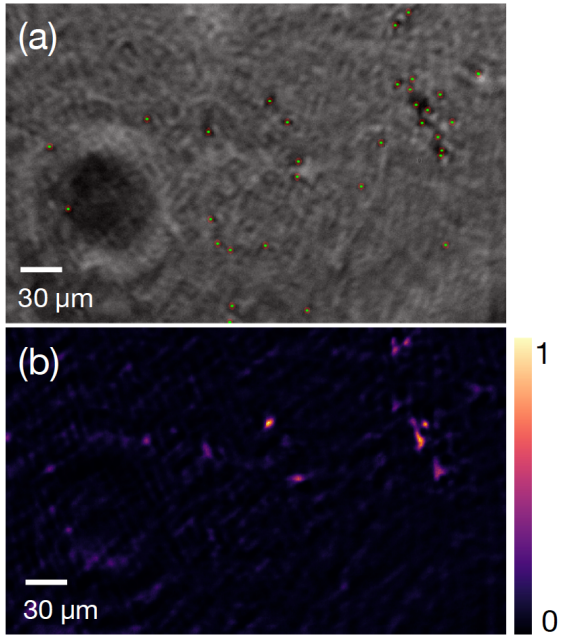
Use sliding window!

How can we visualize performance?

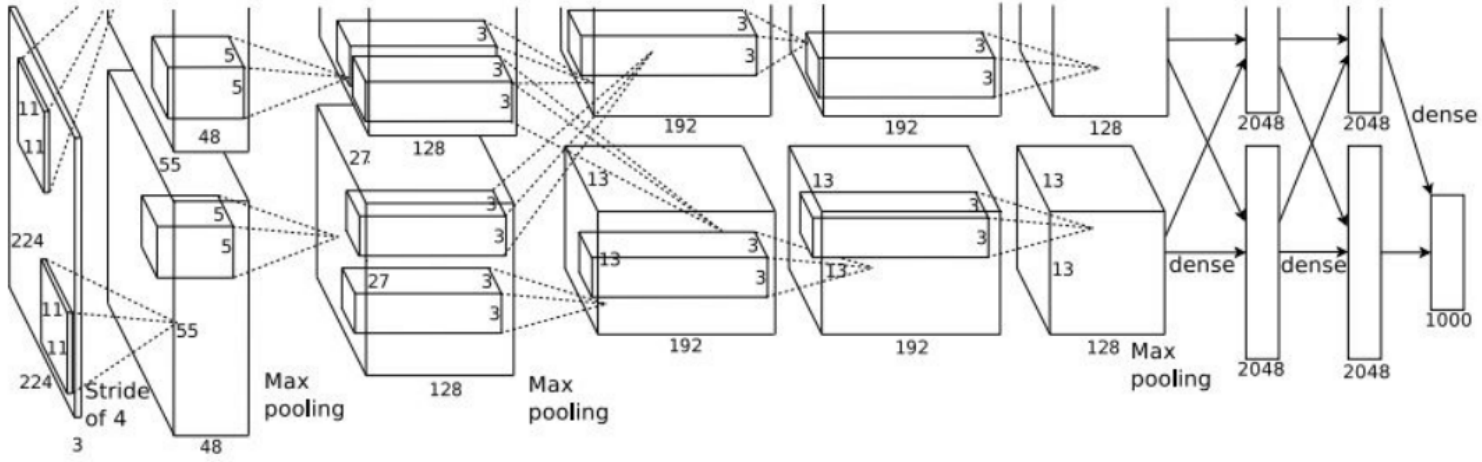


Use sliding window

Trained CNN



How can we visualize what's in the network?

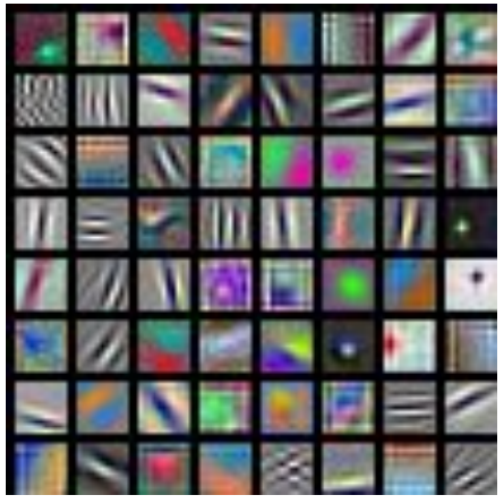


Class Scores:
1000 numbers

Input Image:
3 x 224 x 224

What are the intermediate features looking for?

First Layer: Visualize Filters

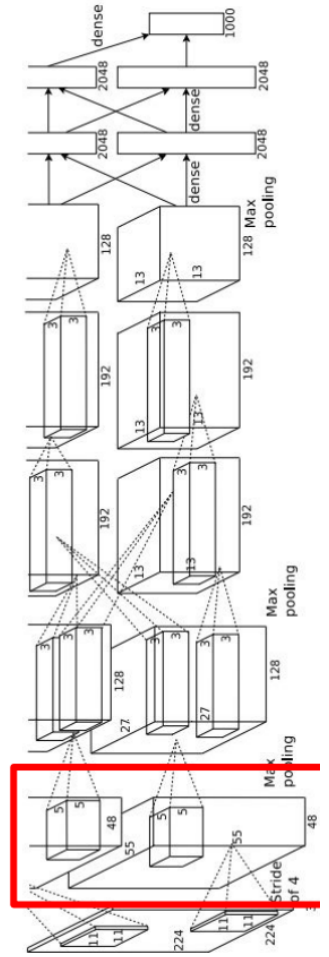


AlexNet:
64 x 3 x 11 x 11

ResNet-18:
64 x 3 x 7 x 7

ResNet-101:
64 x 3 x 7 x 7

DenseNet-121:
64 x 3 x 7 x 7



Krizhevsky, “One weird trick for parallelizing convolutional neural networks”, arXiv 2014
He et al, “Deep Residual Learning for Image Recognition”, CVPR 2016
Huang et al, “Densely Connected Convolutional Networks”, CVPR 2017

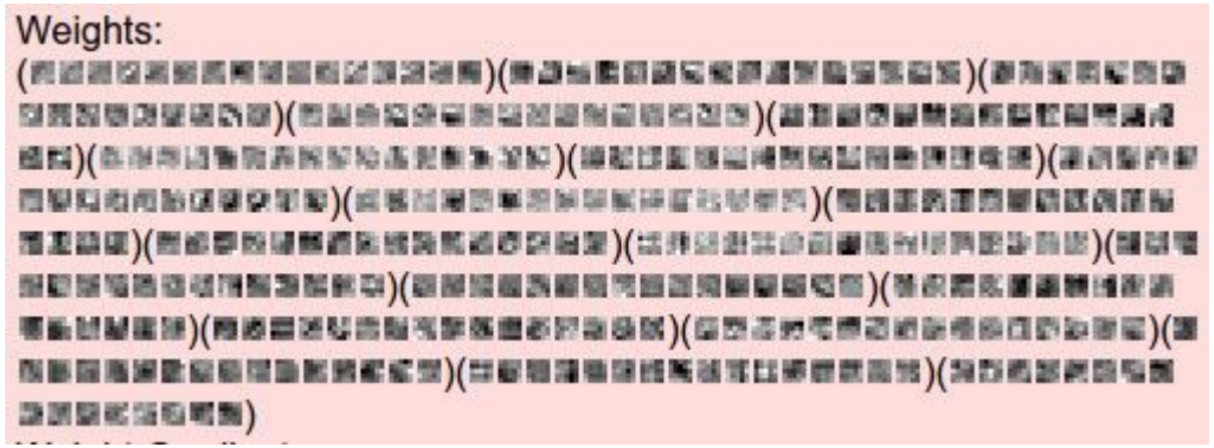
Visualize the filters/kernels (raw weights)

We can visualize filters at higher layers, but not that interesting

(these are taken from ConvNetJS CIFAR-10 demo)

layer 1 weights

16 x 3 x 7 x 7



layer 2 weights

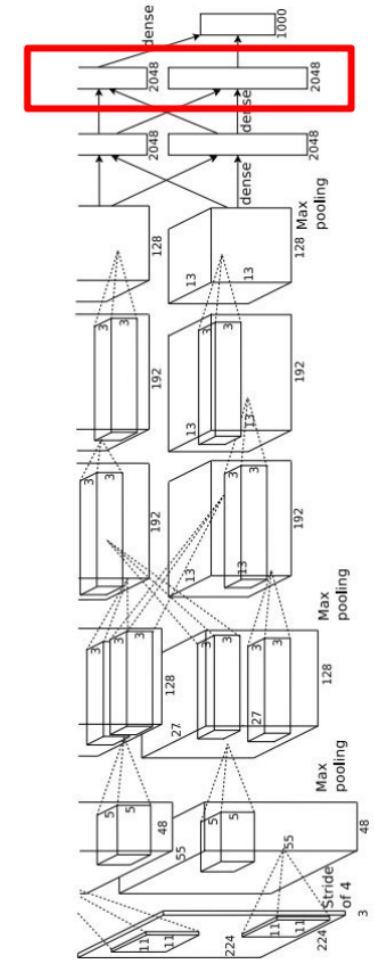
20 x 16 x 7 x 7

layer 3 weights

20 x 20 x 7 x 7

Last Layer

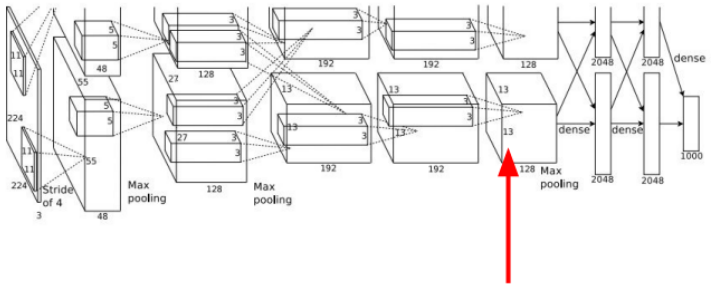
FC7 layer



4096-dimensional feature vector for an image (layer immediately before the classifier)

Run the network on many images, collect the feature vectors

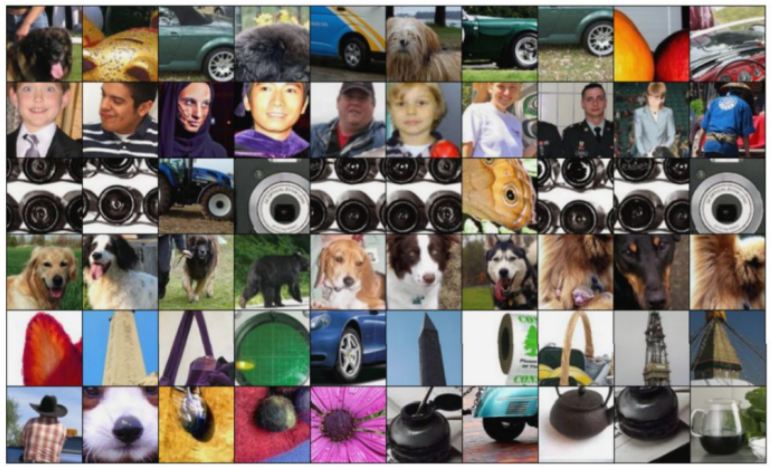
Maximally Activating Patches



Pick a layer and a channel; e.g. conv5 is 128 x 13 x 13, pick channel 17/128

Run many images through the network, record values of chosen channel

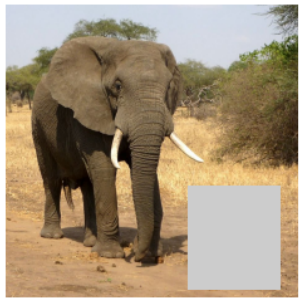
Visualize image patches that correspond to maximal activations

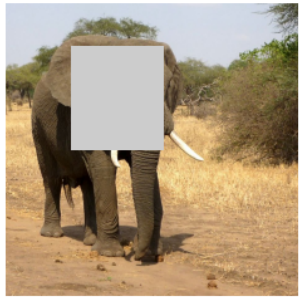


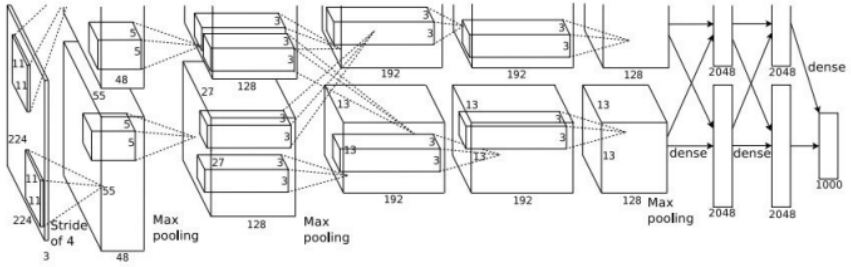
Springenberg et al, "Striving for Simplicity: The All Convolutional Net", ICLR Workshop 2015
Figure copyright Jost Tobias Springenberg, Alexey Dosovitskiy, Thomas Brox, Martin Riedmiller, 2015; reproduced with permission.

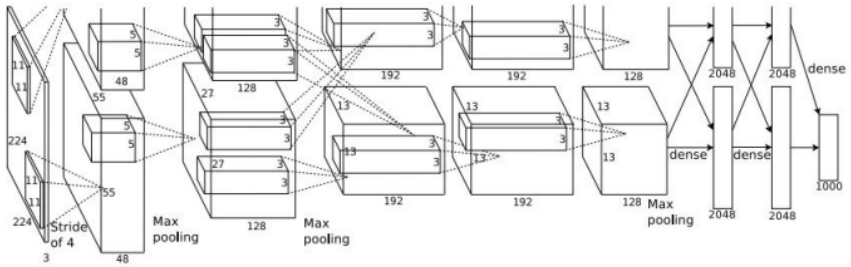
Which pixels matter: Saliency vs Occlusion

Mask part of the image before feeding to CNN, check how much predicted probabilities change

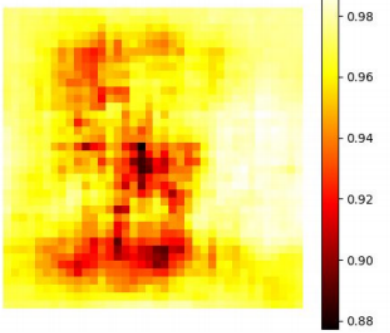




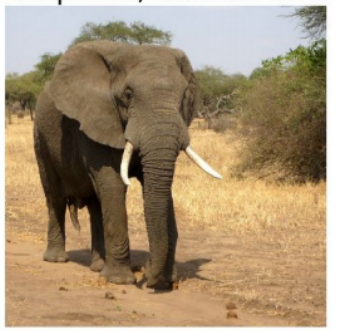


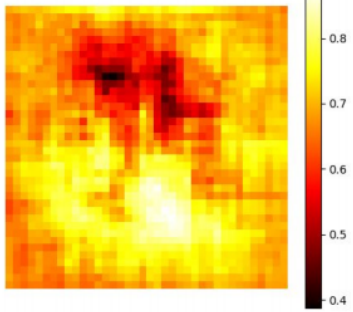


schooner

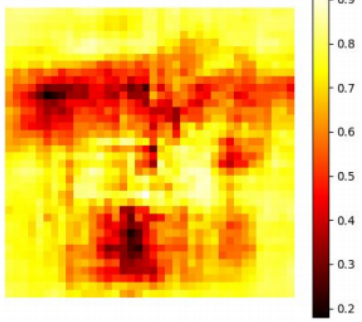


African elephant, Loxodonta africana





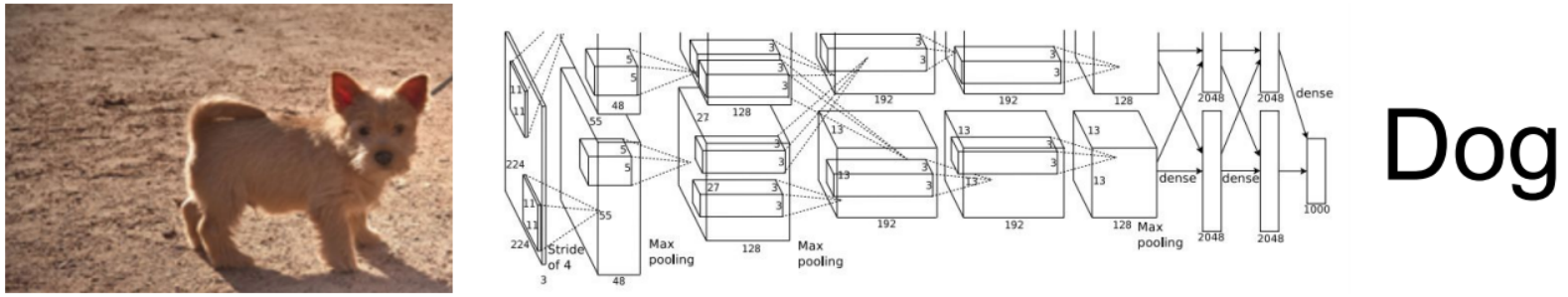
go-kart



Zeiler and Fergus, "Visualizing and Understanding Convolutional Networks", ECCV 2014

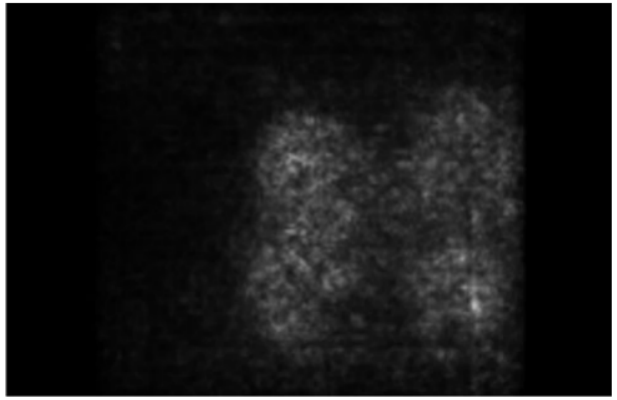
Which pixels matter: Saliency via Backprop

Forward pass: Compute probabilities



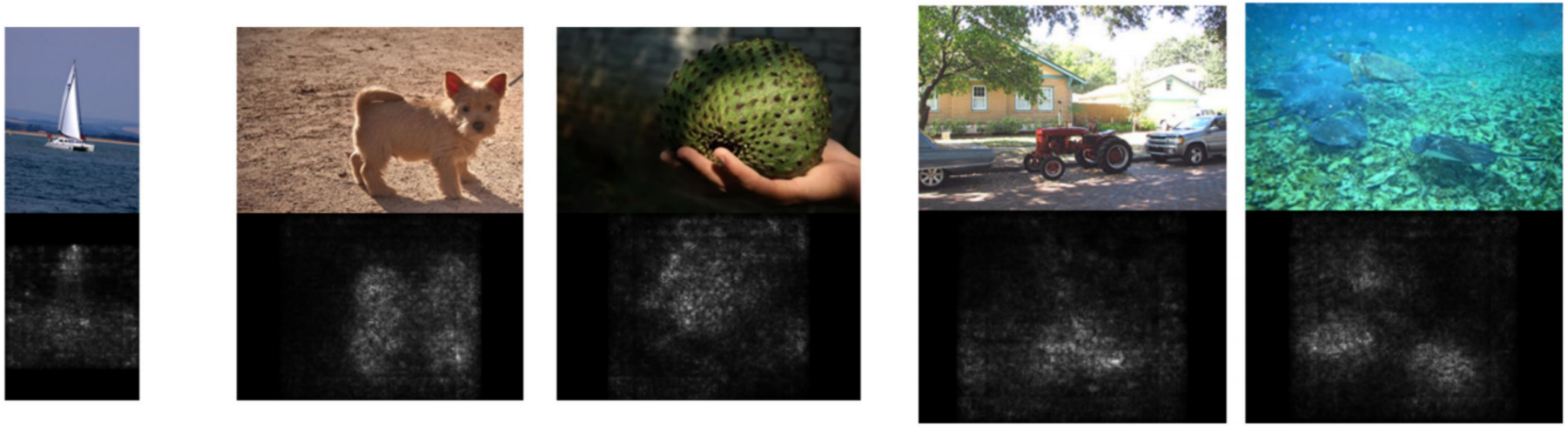
Dog

Compute gradient of (unnormalized) class score with respect to image pixels, take absolute value and max over RGB channels



Simonyan, Vedaldi, and Zisserman, "Deep Inside Convolutional Networks: Visualising Image Classification Models and Saliency Maps", ICLR Workshop 2014.

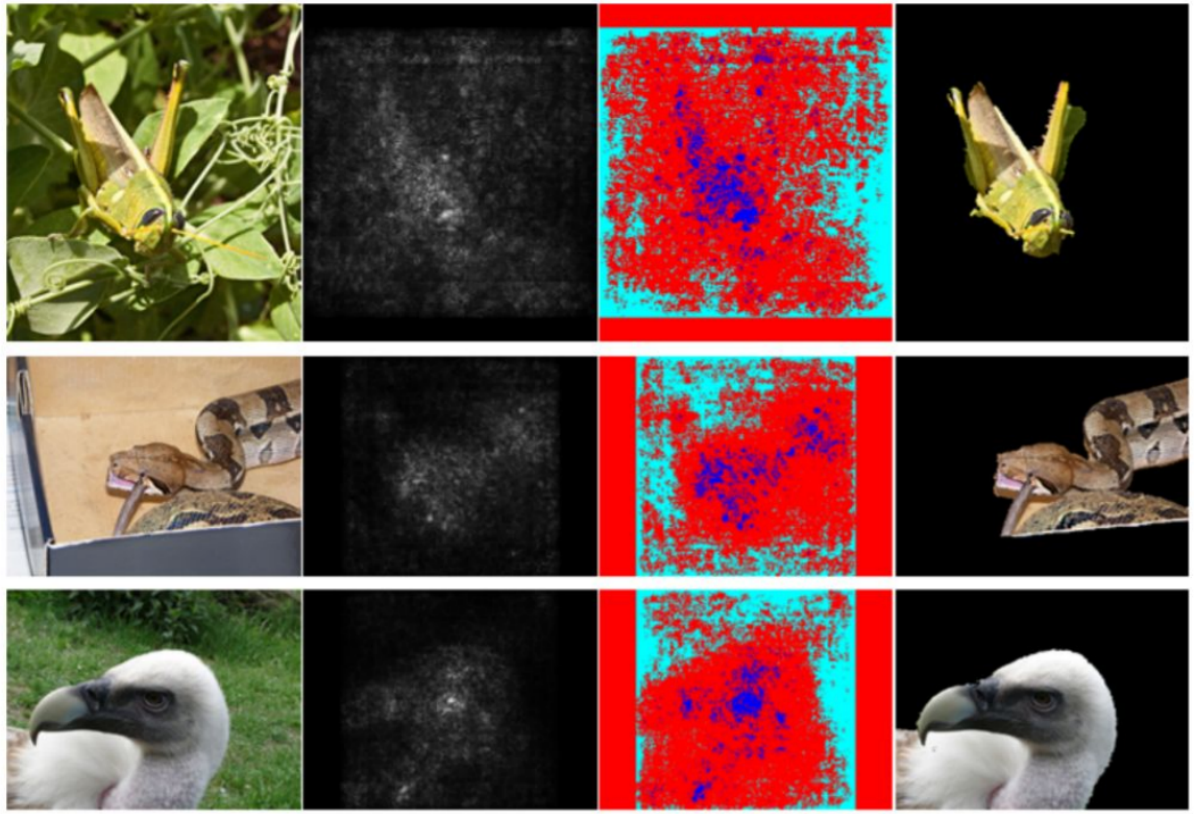
Saliency Maps



Simonyan, Vedaldi, and Zisserman, "Deep Inside Convolutional Networks: Visualising Image Classification Models and Saliency Maps", ICLR Workshop 2014.

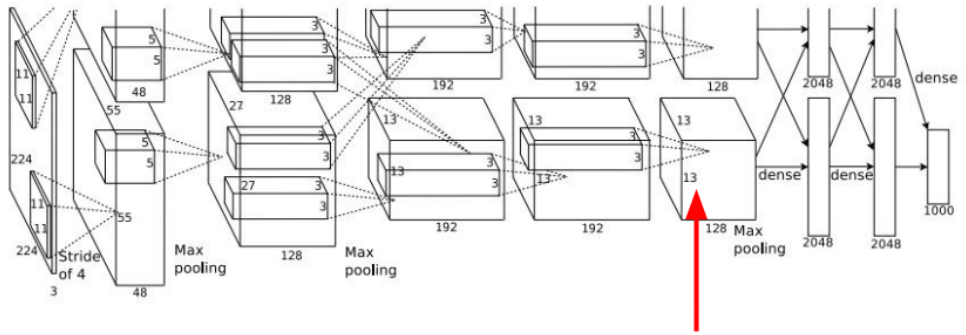
Saliency Maps: Segmentation without supervision

Use GrabCut on saliency map



Simonyan, Vedaldi, and Zisserman, "Deep Inside Convolutional Networks: Visualising Image Classification Models and Saliency Maps", ICLR Workshop 2014.
Figures copyright Karen Simonyan, Andrea Vedaldi, and Andrew Zisserman, 2014; reproduced with permission.
Rother et al. "Grabcut: Interactive foreground extraction using iterated graph cuts". ACM TOG 2004

Intermediate Features via (guided) backprop



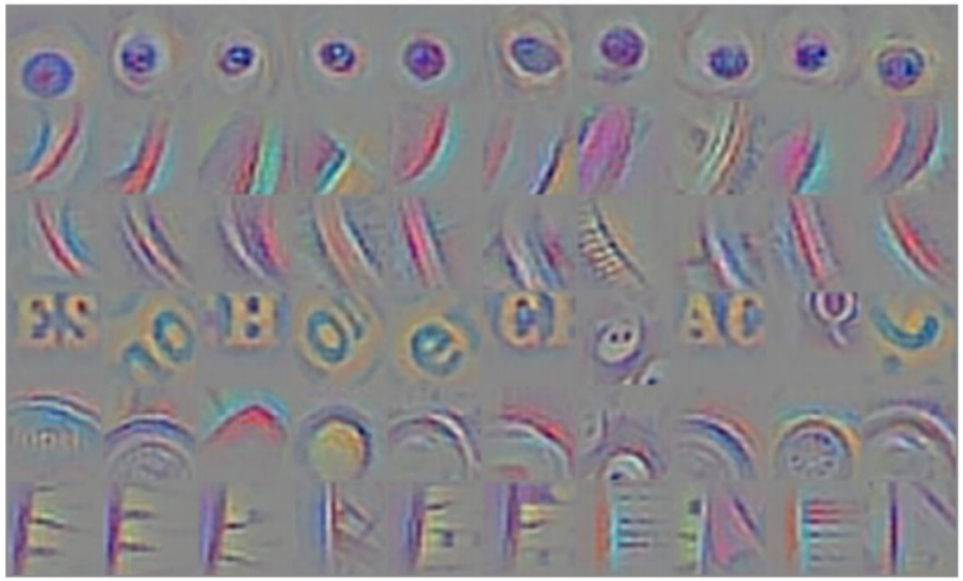
Pick a single intermediate neuron, e.g. one value in 128 x 13 x 13 conv5 feature map

Compute gradient of neuron value with respect to image pixels

Zeiler and Fergus, "Visualizing and Understanding Convolutional Networks", ECCV 2014
Springenberg et al, "Striving for Simplicity: The All Convolutional Net", ICLR Workshop 2015

Intermediate features via (guided) backprop

Maximally activating patches
(Each row is a different neuron)



Guided Backprop

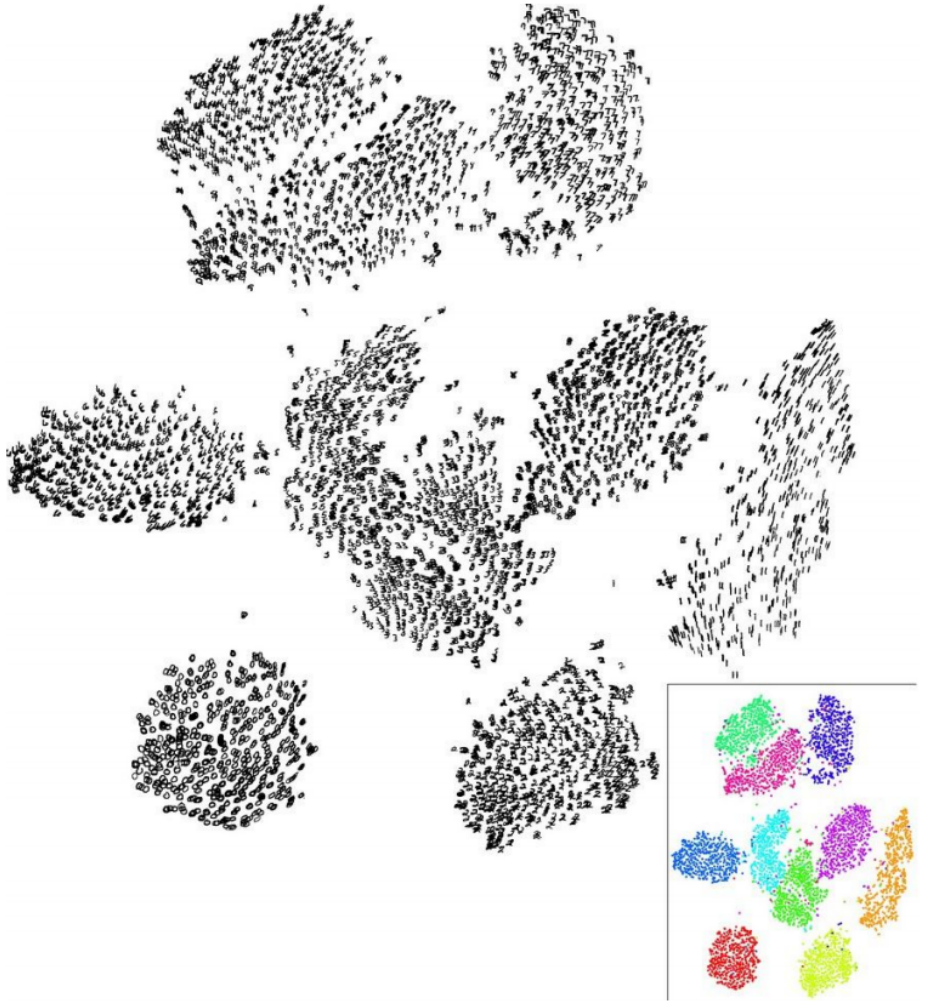
Zeiler and Fergus, "Visualizing and Understanding Convolutional Networks", ECCV 2014
Springenberg et al, "Striving for Simplicity: The All Convolutional Net", ICLR Workshop 2015

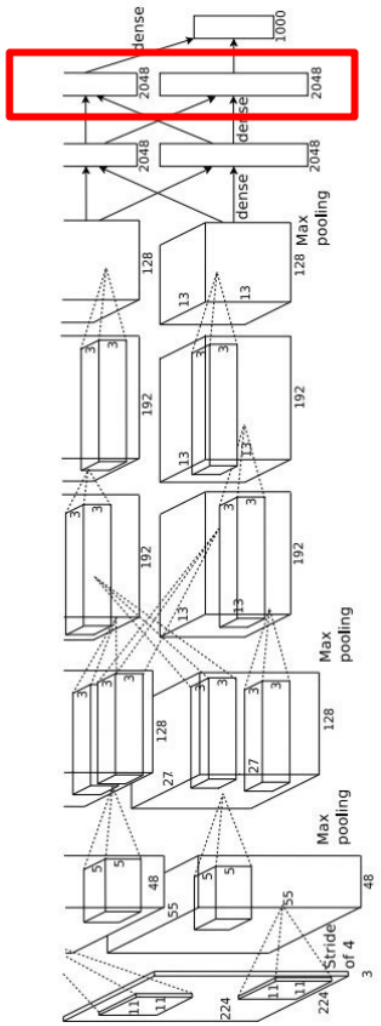
Last Layer: Dimensionality Reduction

Visualize the “space” of FC7 feature vectors by reducing dimensionality of vectors from 4096 to 2 dimensions

Simple algorithm: Principal Component Analysis (PCA)

More complex: **t-SNE**



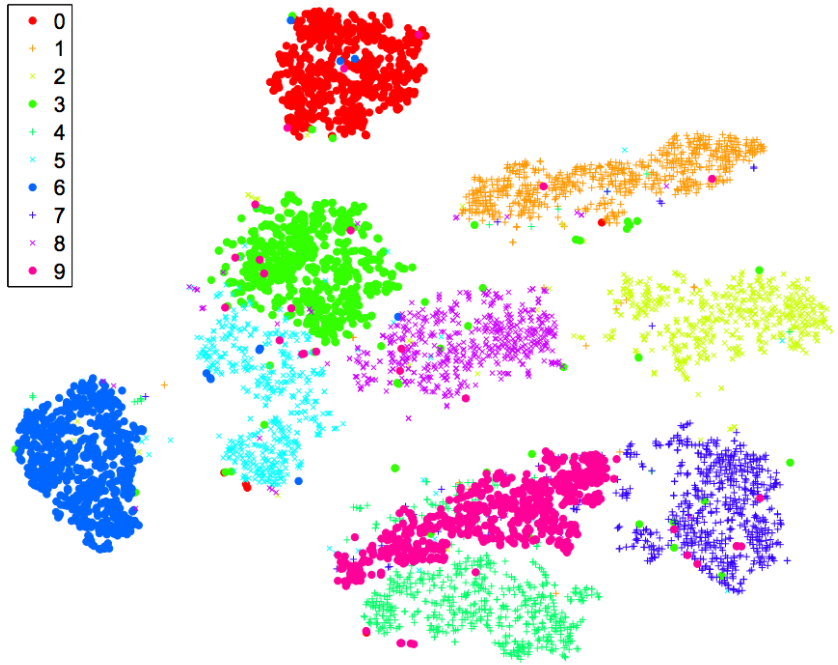


Van der Maaten and Hinton, “Visualizing Data using t-SNE”, JMLR 2008
Figure copyright Laurens van der Maaten and Geoff Hinton, 2008. Reproduced with permission.

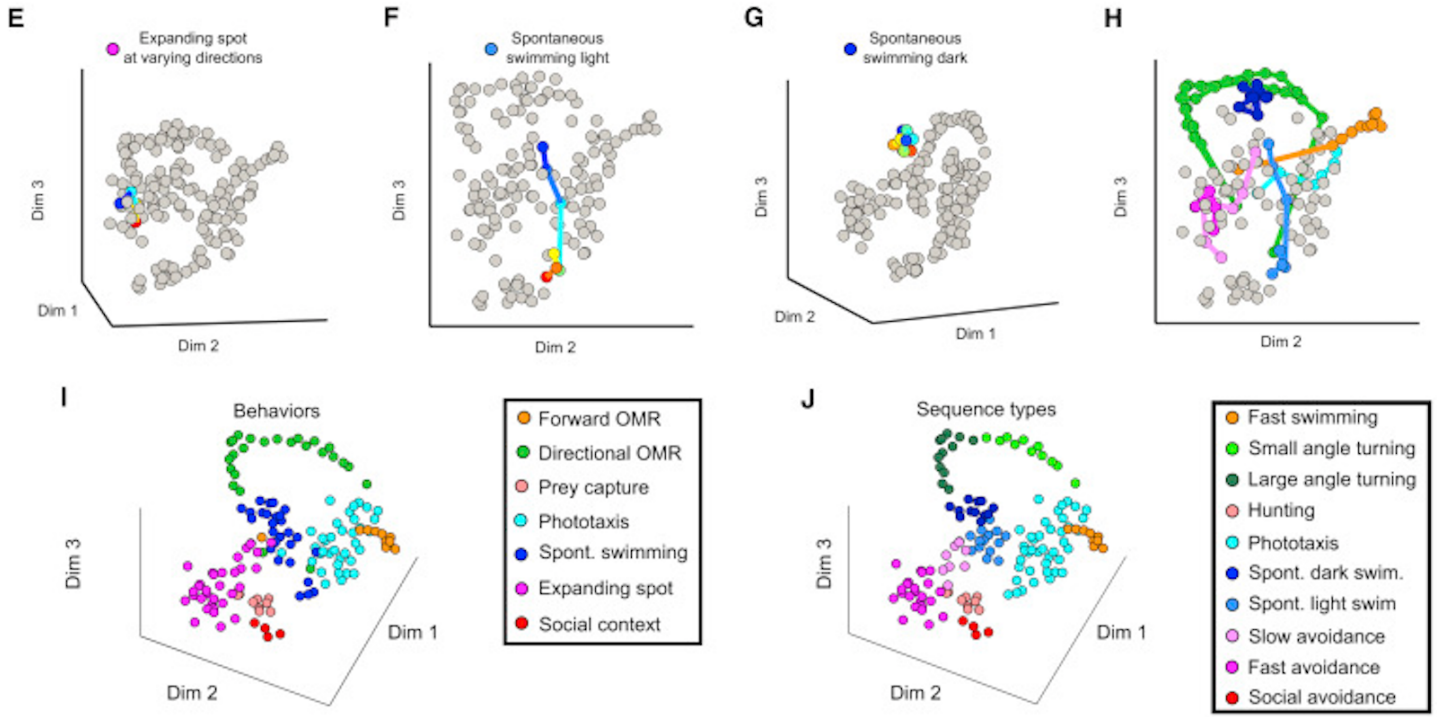
TSNE for data visualization

- Reduce data dimensions to enable visualization in 2D or 3D
  - nD -> 2D or 3D
  - Preserve local structure of data to highlight groups
  - Unsupervised – clusters unlabeled data

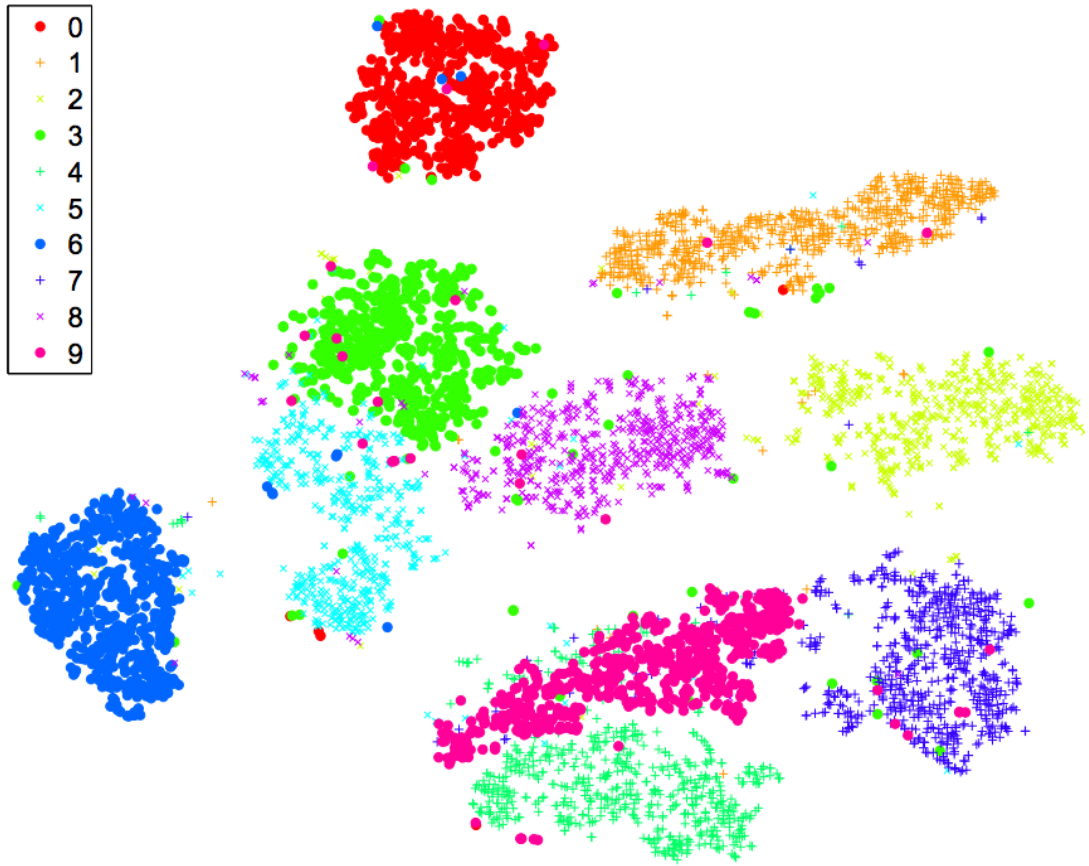
Applied to MNIST digits



Applied to movies of zebrafish behavior



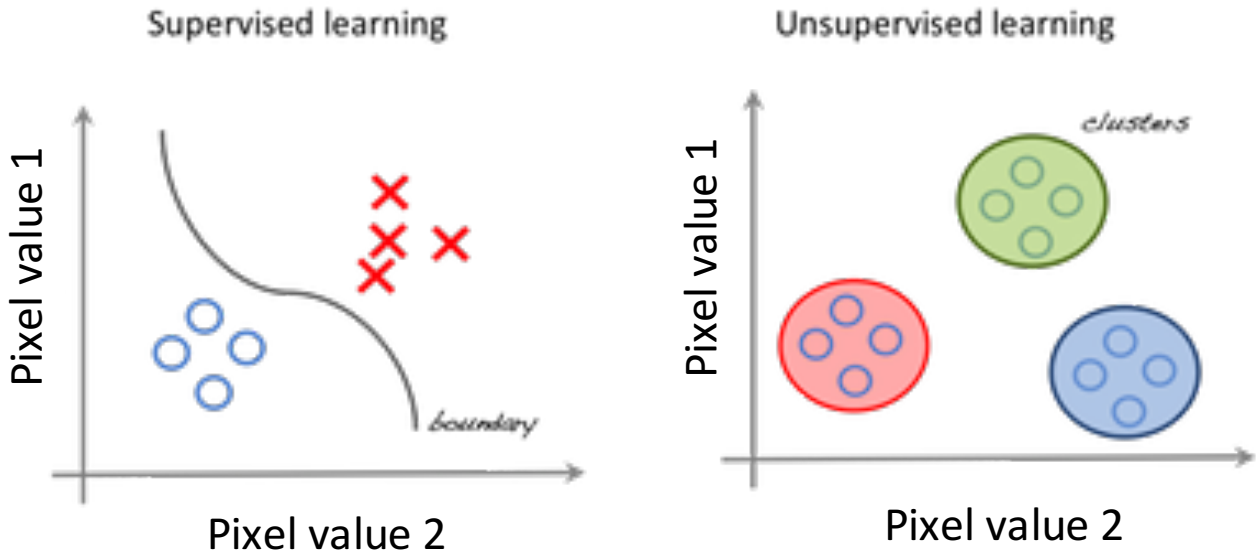
Aside about clustering data – why do we need deep learning at all?



Isn't this good enough?

Unsupervised learning in a nutshell

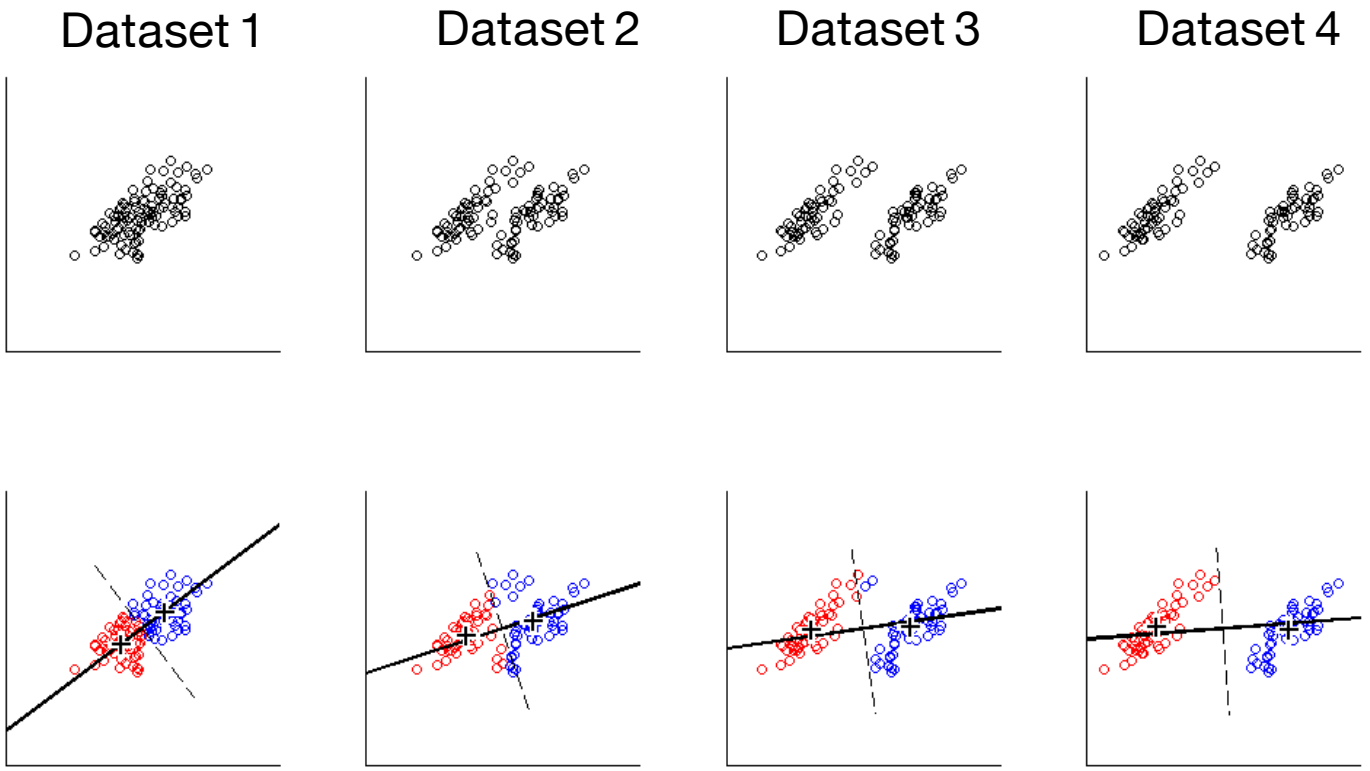
Definition of Unsupervised Learning:
Learning useful structure *without* labeled classes, optimization criterion, feedback signal, or any other information beyond the raw data



Unsupervised learning in a nutshell

Mathematical tools for finding patterns in data:

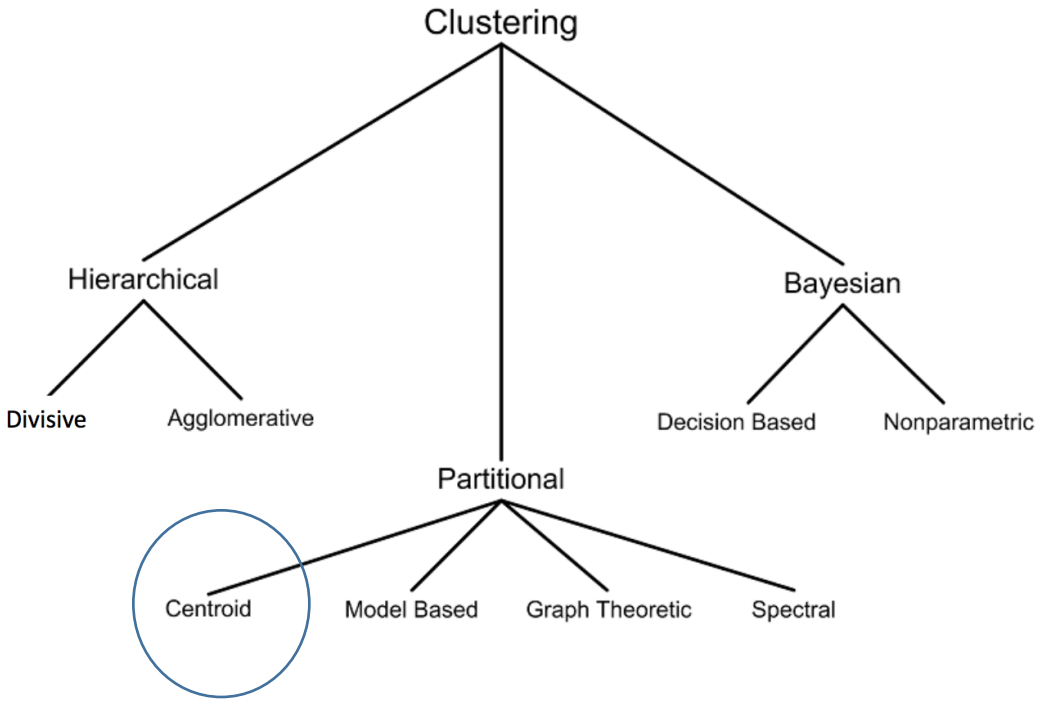
- Eigenvector decomposition
- Principal component analysis
- Singular value decomposition



https://stats.stackexchange.com/questions/183236/what-is-the-relation-between-k-means-clustering-and-pca

Iterative methods for unsupervised learning - Clustering

Clustering techniques



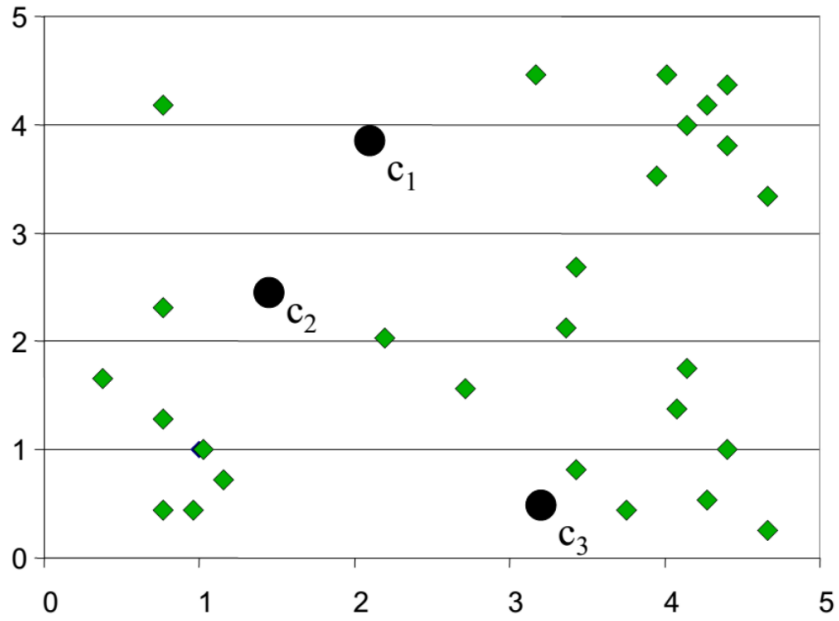
K-Means

- **Hierarchical** algorithms find successive clusters using previously established clusters. These algorithms can be either agglomerative ("*bottom-up*") or divisive ("*top-down*"):
  1. Agglomerative algorithms begin with each element as a separate cluster and merge them into successively larger clusters;
  2. Divisive algorithms begin with the whole set and proceed to divide it into successively smaller clusters.
- **Partitional** algorithms typically determine all clusters at once, but can also be used as divisive algorithms in the hierarchical clustering.
- **Bayesian** algorithms try to generate a *posteriori distribution* over the collection of all partitions of the data.

K-Means Clustering

- Given *k*, the *k-means* algorithm works as follows:
  1. Choose *k* (random) data points (seeds) to be the initial centroids, cluster centers
  2. Assign each data point to the closest centroid
  3. Re-compute the centroids using the current cluster memberships
  4. If a convergence criterion is not met, repeat steps 2 and 3

Randomly initialize seeds



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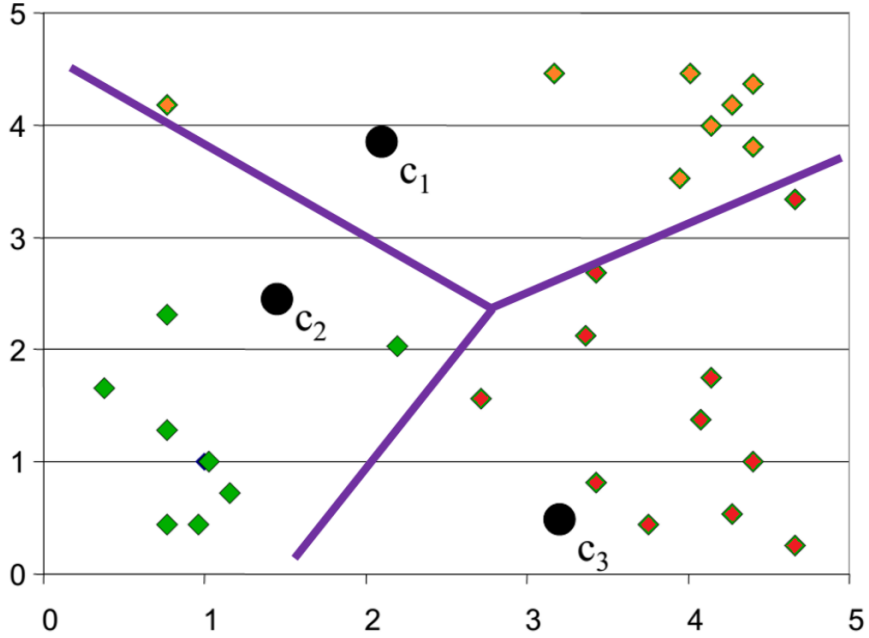
Determine cluster membership for each data point



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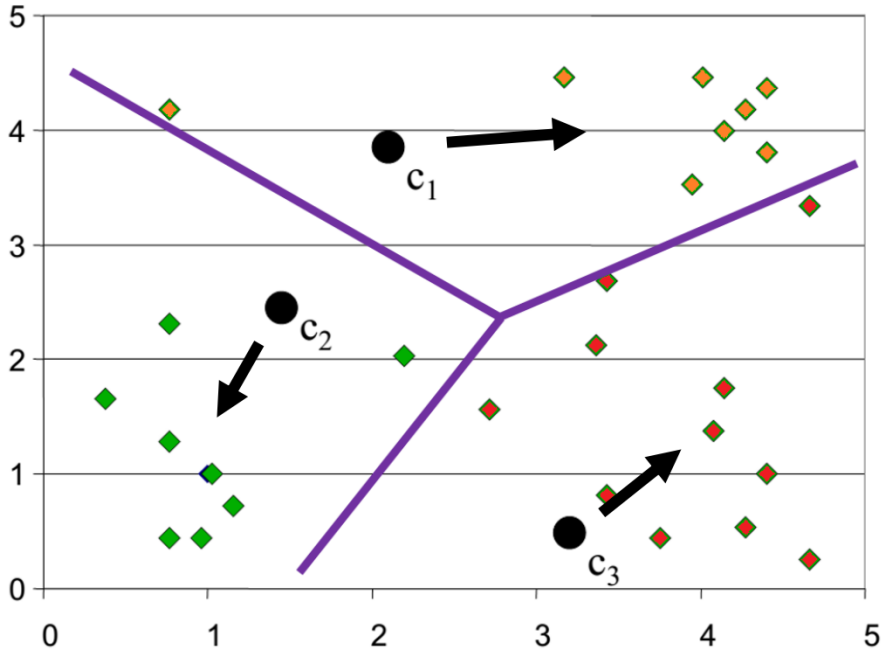
Compute and update new cluster center



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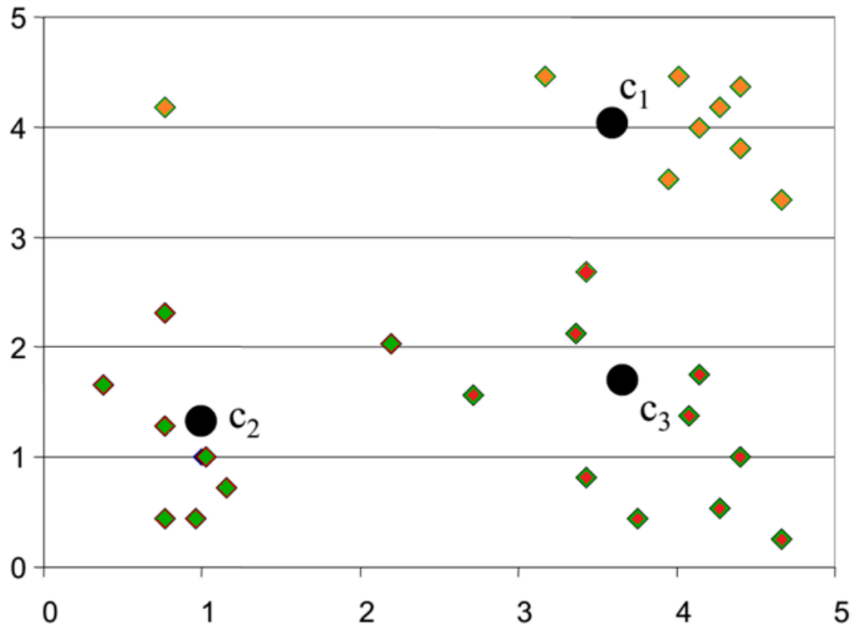
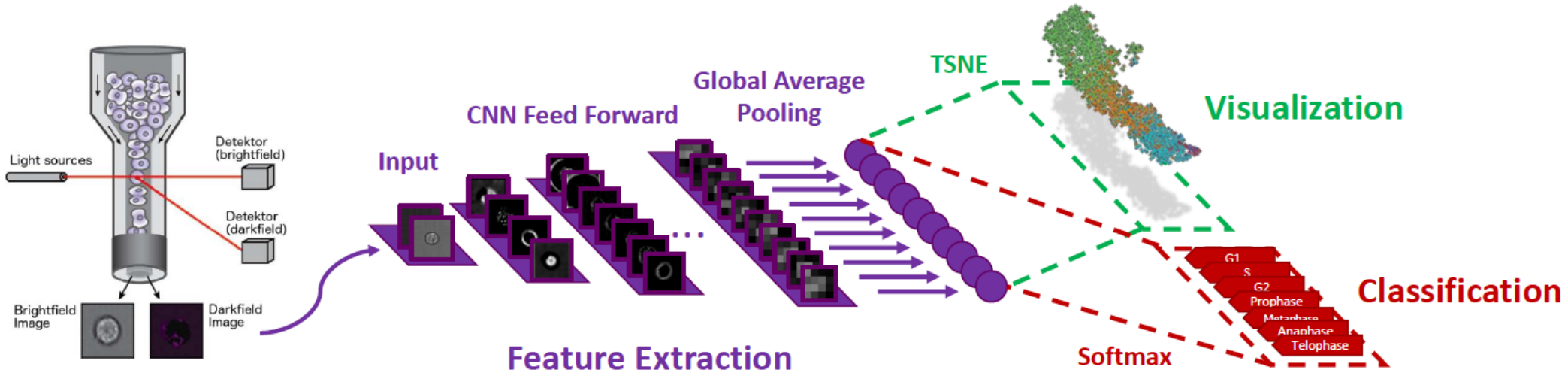
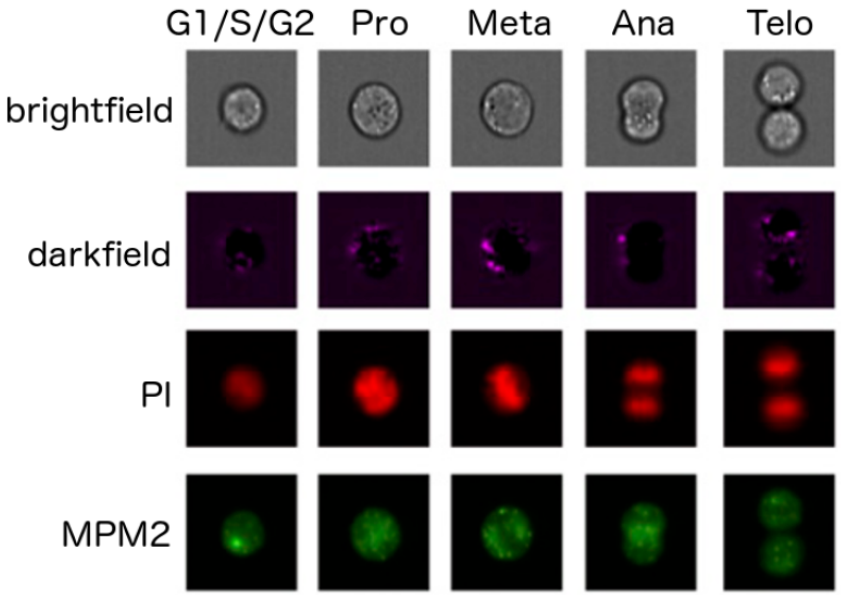
Result of first iteration

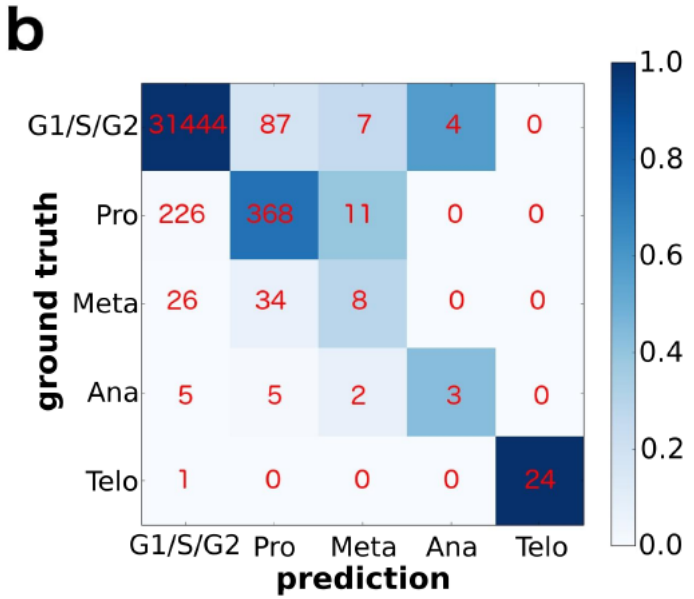


Examples of CNN's for biomedical image classification

P. Eulenberg et al., “Reconstructing cell cycle and disease progression using deep learning”

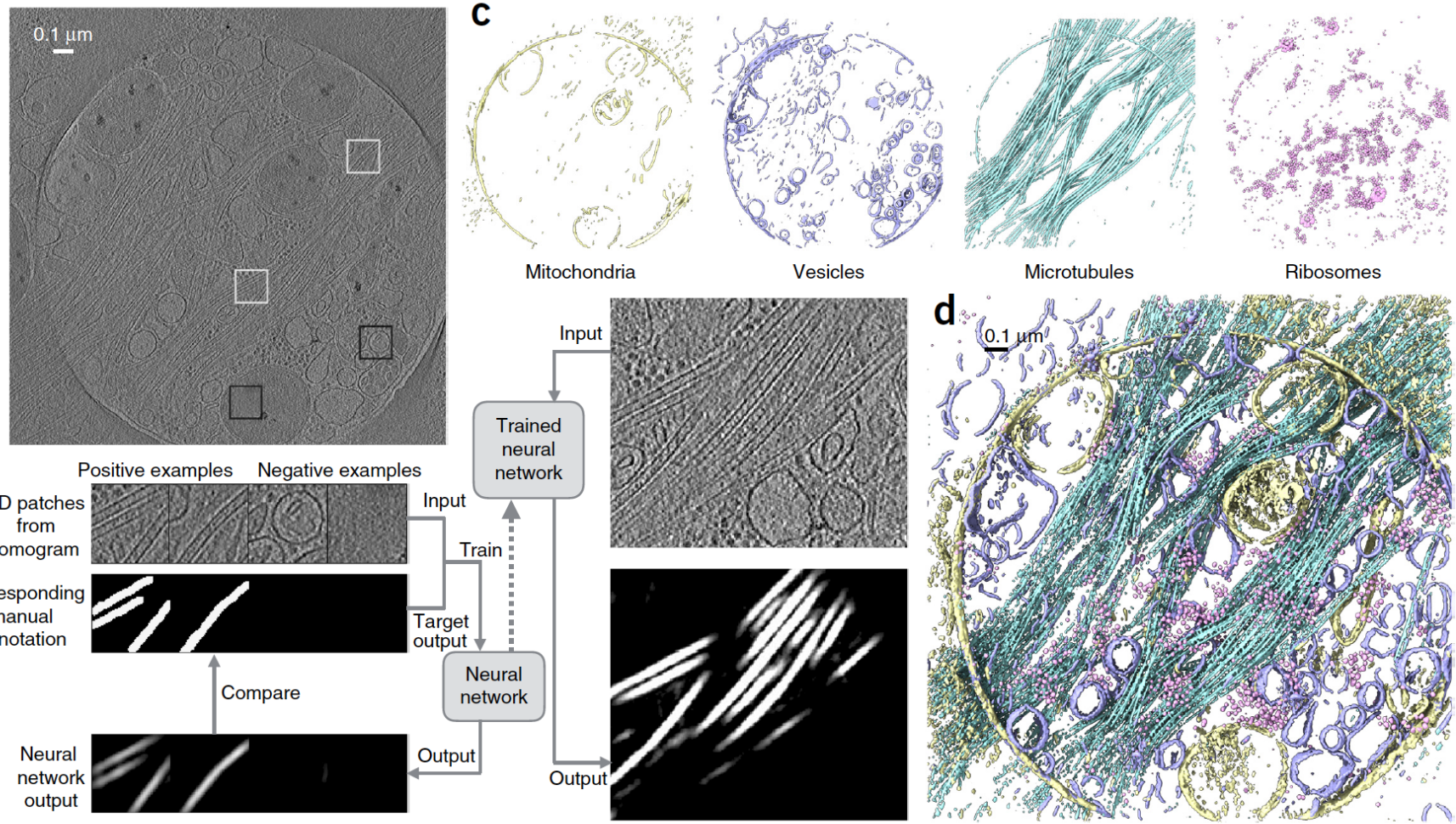






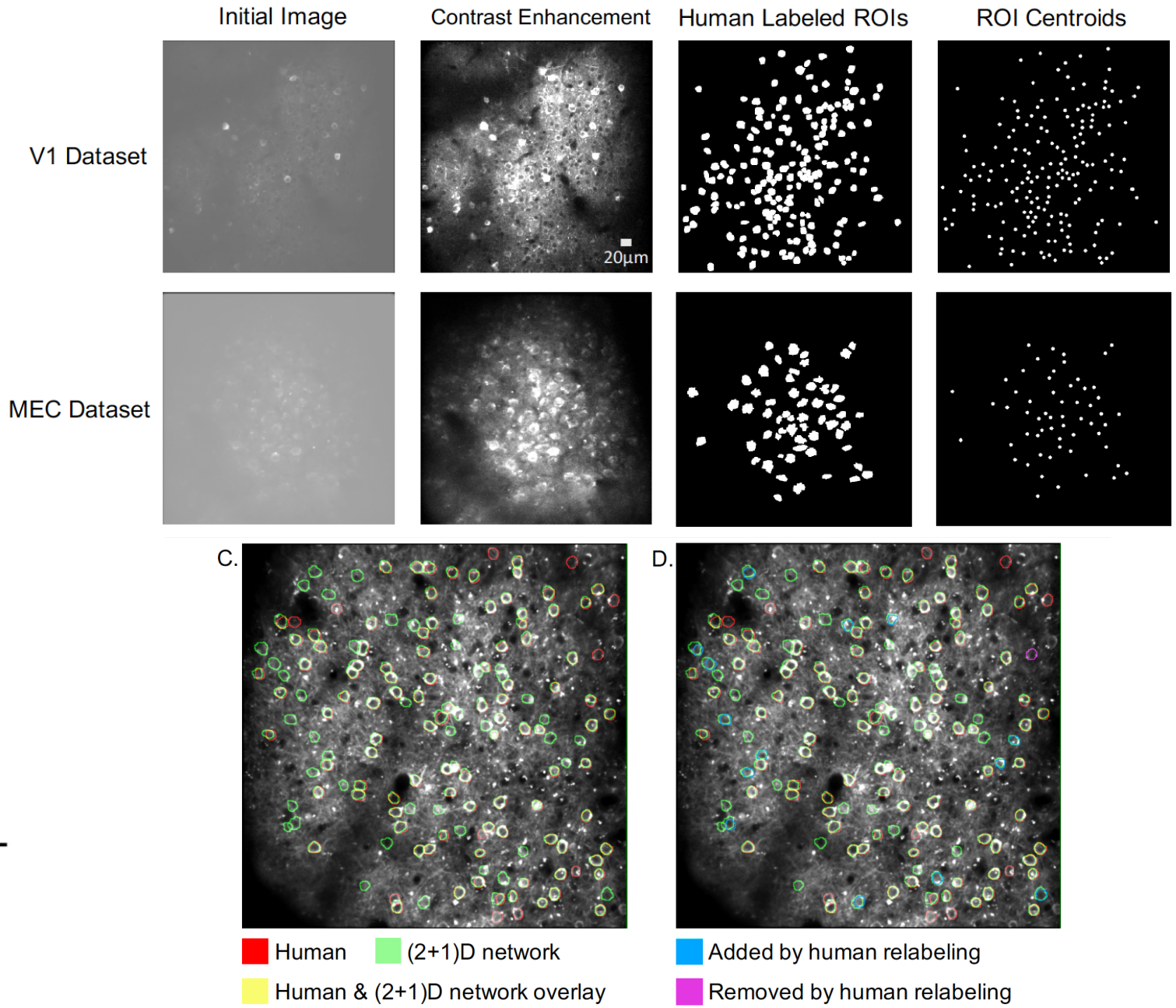
Convolutional neural networks for automated annotation of cellular cryo-electron tomograms

Muyuan Chen[1,2], Wei Dai[2,4], Stella Y Sun[2], Darius Jonasch[2], Cynthia Y He[3], Michael F Schmid[2], Wah Chiu[2] & Steven J Ludtke[2]



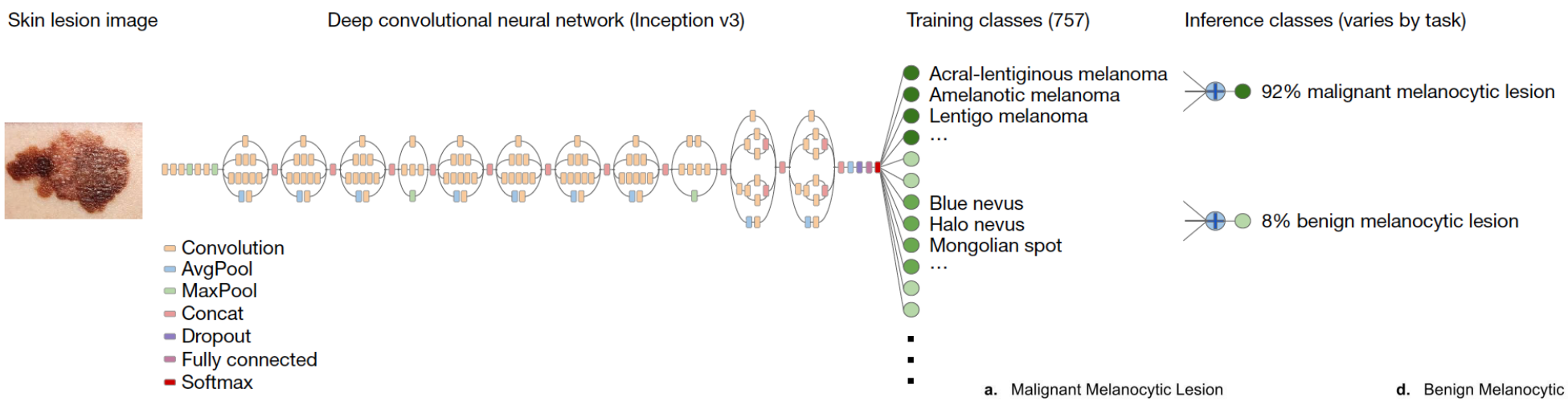
Automatic Neuron Detection in Calcium Imaging Data Using Convolutional Networks

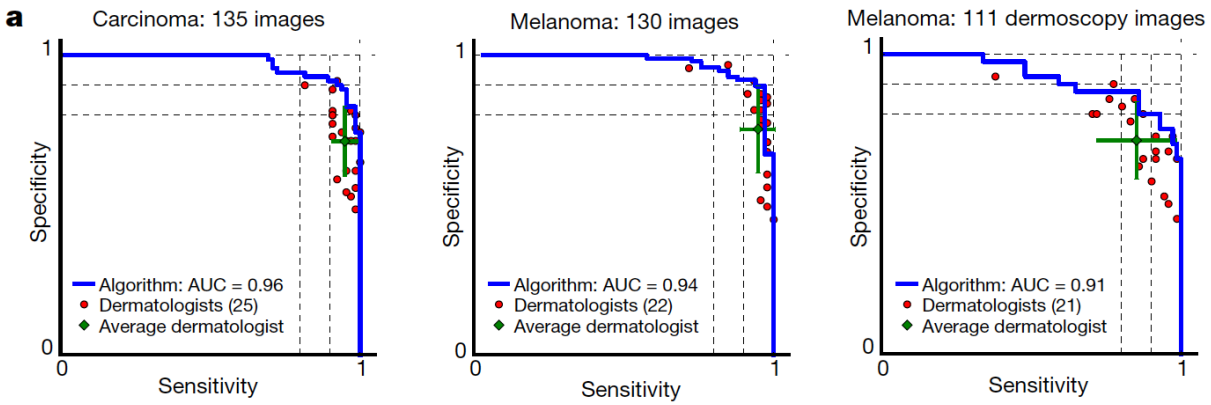
Noah J. Apthorpe[1*] Alexander J. Riordan[2*] Rob E. Aguilar[1] Jan Homann[2]
Yi Gu[2] David W. Tank[2] H. Sebastian Seung[12]
[1]Computer Science Department [2]Princeton Neuroscience Institute
Princeton University

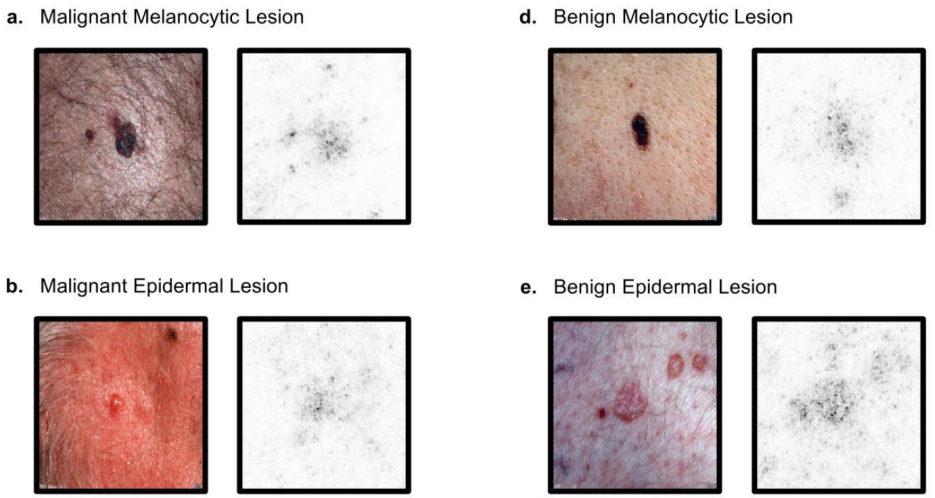


Dermatologist-level classification of skin cancer with deep neural networks

Andre Esteva[1]*, Brett Kuprel[1]*, Roberto A. Novoa[2,3], Justin Ko[2], Susan M. Swetter[2,4], Helen M. Blau[5] & Sebastian Thrun[6]

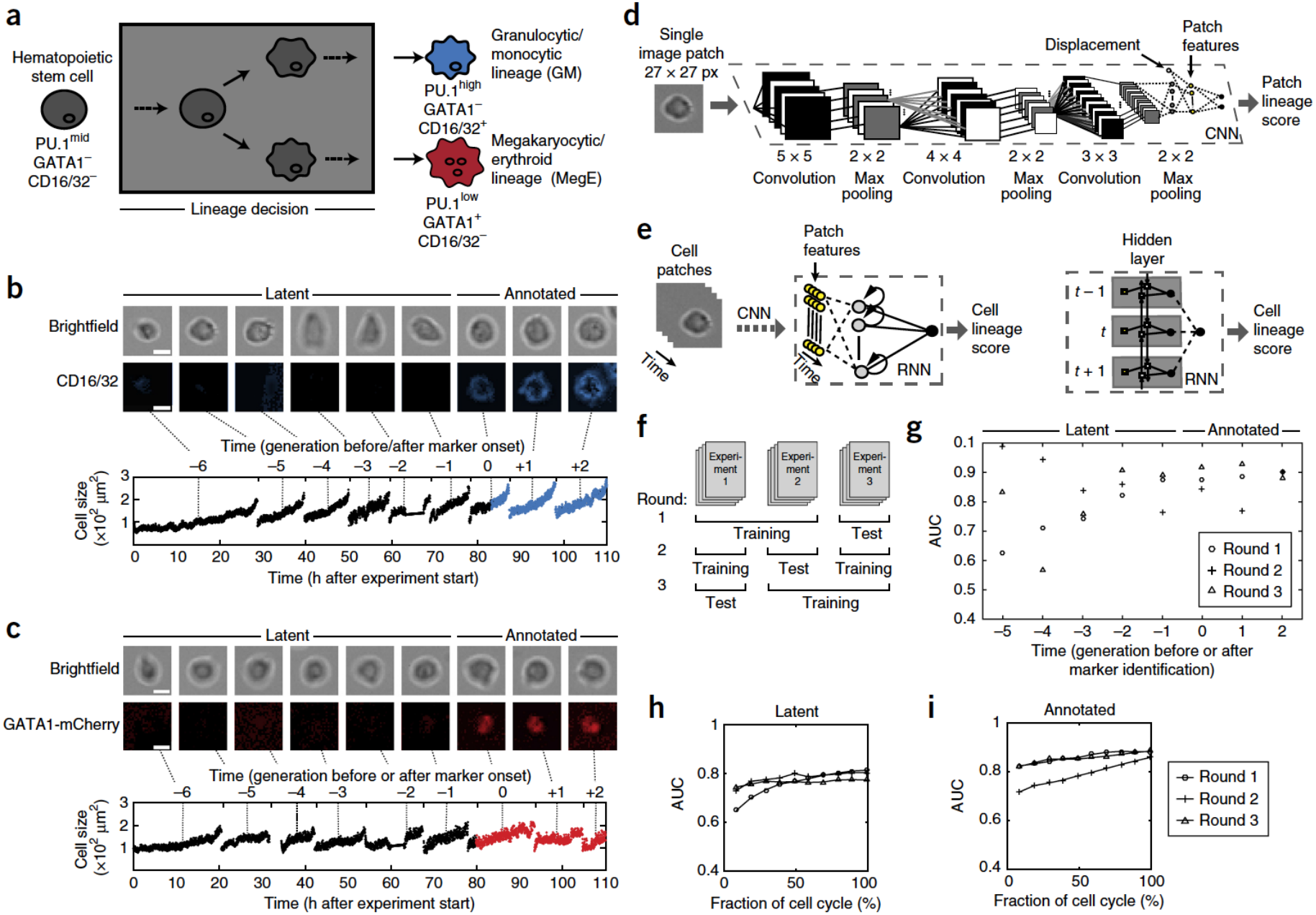






Prospective identification of hematopoietic lineage choice by deep learning

Felix Buggenthin[1,6], Florian Buettner[1,2,6], Philipp S Hoppe[3,4], Max Endele[3], Manuel Kroiss[1,5], Michael Strasser[1], Michael Schwarzfischer[1], Dirk Loeffler[3,4], Konstantinos D Kokkaliaris[3,4], Oliver Hilsenbeck[3,4], Timm Schroeder[3,4], Fabian J Theis[1,5] & Carsten Marr[1]



A good time to talk about the class project!

- Select a “base” dataset
- Simulate parameters of a physical (imaging) system with base dataset
- Train deep neural net with simulated dataset
- Report results

What you’ll need to submit:
1) The project’s source code

2) A short research-style paper (3 pages minimum, 5 pages maximum) that includes an introduction, results, a discussion section, references and at least 2 figures

3) A completed web template containing the main results from the research paper

4) An 8-minute presentation that each student will deliver to the class

Example project topics:

Can we design a new lens/transducer/antenna shape to improve classification of X?

What is the tradeoff between image resolution and classification accuracy for X?

Can we determine an optimal set of colors to improve fluorophore distinguishability?

If we capture 2 images that are overlapped on one sensor, what is the best way to pre-blur them to then be able to tell them apart? Or to be able to classify them together?

If we just had a few sensors, how should be arrange them e.g. a mask to be able to predict the position of X?

Is there some optimal shift-variant blur that we can to use for a particular task?

Or, given a shift-variant PSF image, can we establish a good deconvolution using locally connected layers?

What is the optimal way to layout filters on a sensor to capture a color image for classification? Or an HDR image?

HDR image generation with filters over pixels – what is optimal design?

What if we could make a sensor with different sized pixels – how should they be laid out to achieve the best X?