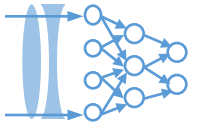
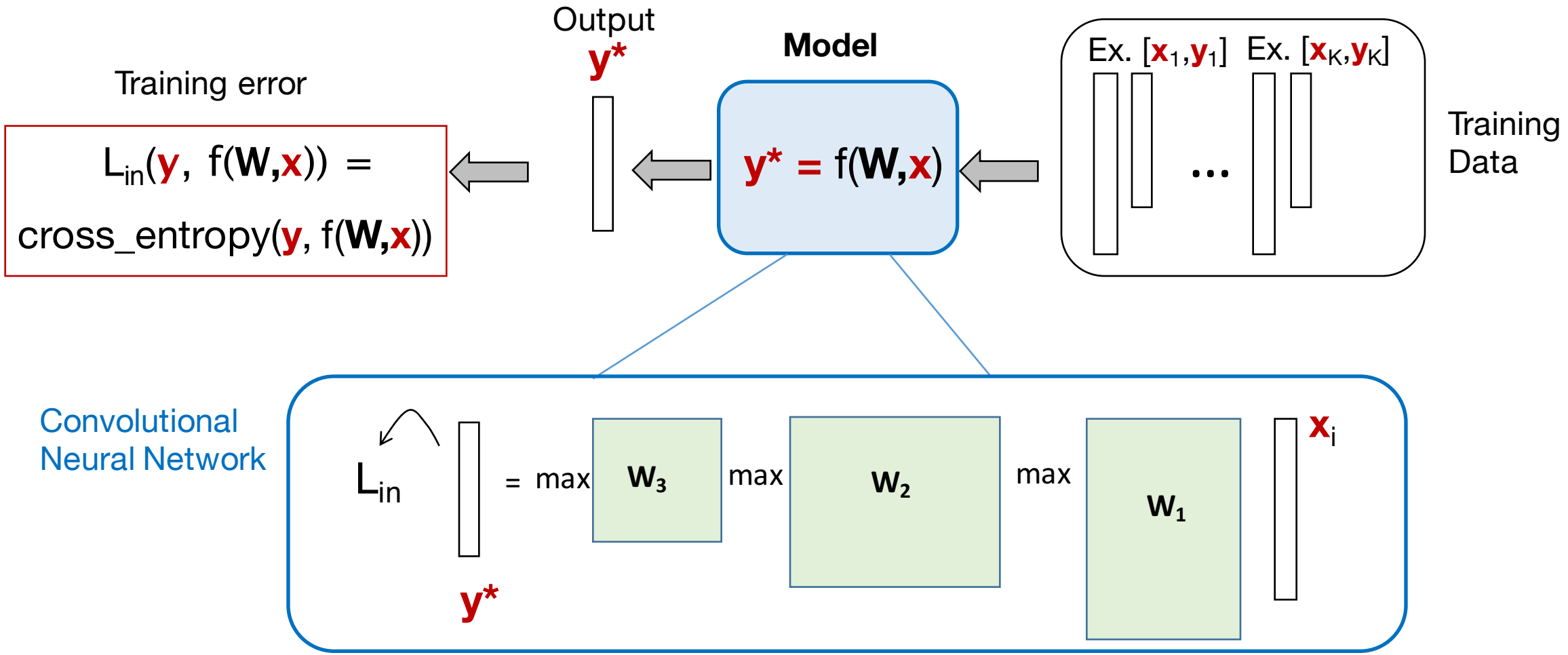


Lecture 12: CNN implementation, visualization and analysis of results

Machine Learning and Imaging

BME 590L
Roarke Horstmeyer

Our very basic convolutional neural network



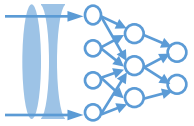
Forward pass: from $\mathbf{x}_i$ and current $\mathbf{W}$'s, find L_{in}

Important components of a CNN

CNN Architecture

Architecture choices

- CONV size, stride, pad, depth
- ReLU & other nonlinearities
- POOL methods
- # of layers, dimensions per layer
- Fully connected layers



Important components of a CNN

CNN Architecture

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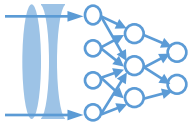
Loss function & optimization

- Type of loss function
- Regularization
- Gradient descent method
- SGD batch and step size

Optimization choices



Important components of a CNN

CNN Architecture

Architecture choices

- CONV size, stride, pad, depth
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Loss function & optimization

- Type of loss function
- Regularization
- Gradient descent method
- SGD batch and step size

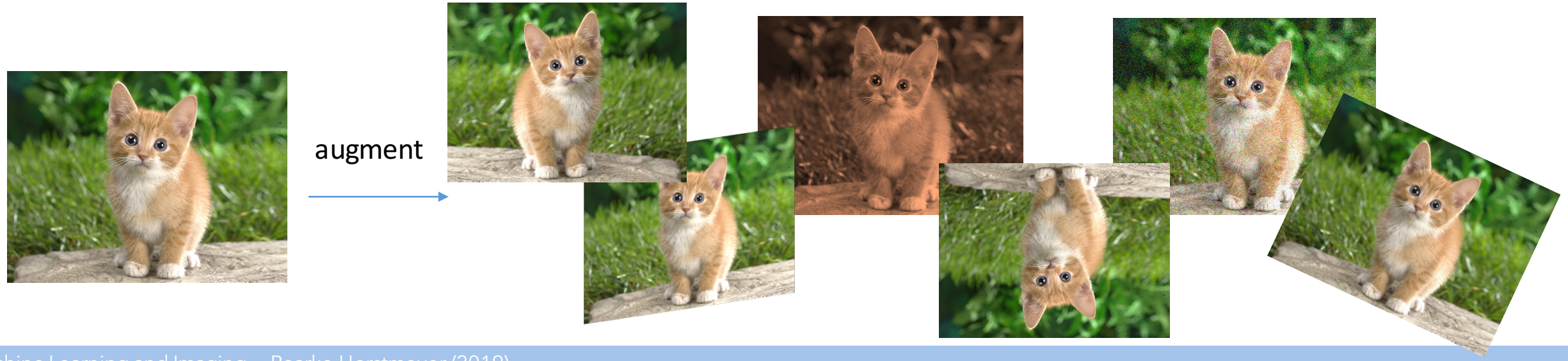
Optimization choices

Other specifics: Initialization, dropout, batch normalization, data normalization & augmentation

Knobs to turn to get things to work…

Data augmentation

- Basic idea: to simulate variation that you might actually see in real life
- It's a form of regularization
- Not an exact science, but try it out – it's free!



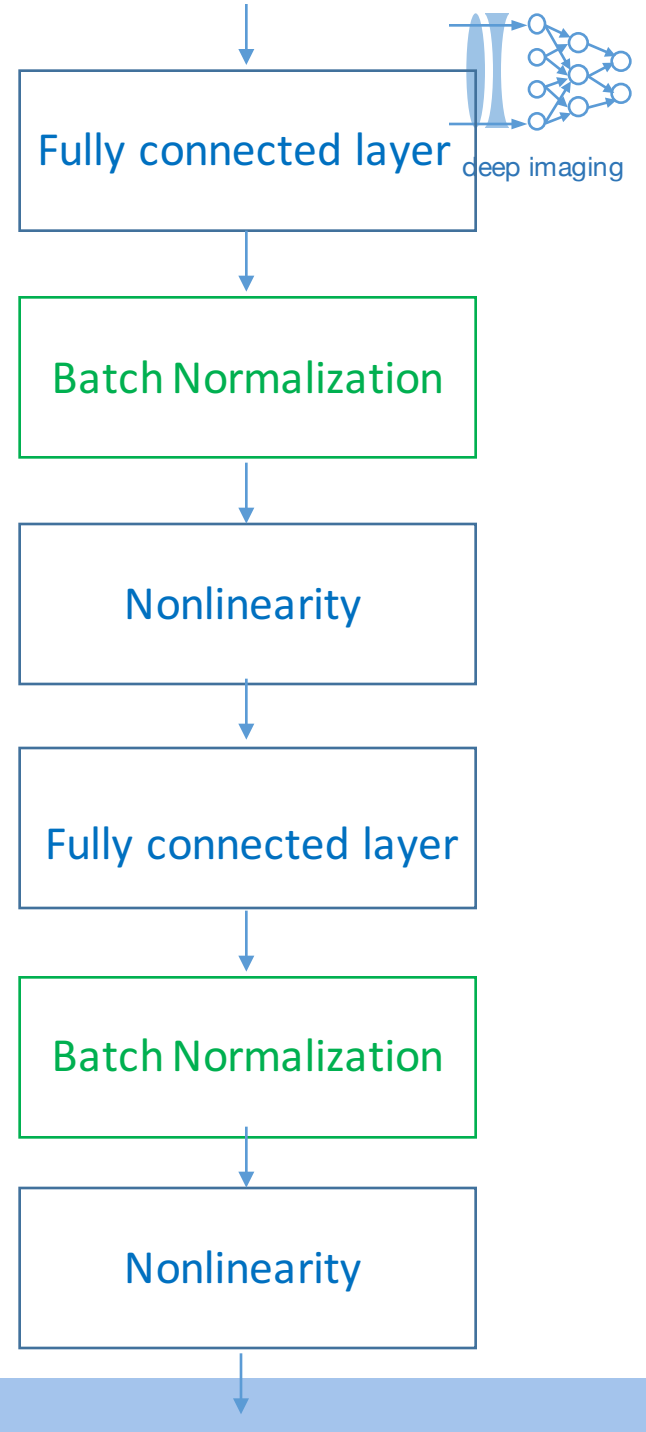
Batch normalization (BN)

- Before BN, training very deep networks was hard
  - If using sigmoid activations, large weights could result in saturation
  - Updating earlier layers' weights causes the distribution of weights in later layers to shift – the *internal covariate shift*
- To address this covariate shift, BN "resets" the layer it is applied to by normalizing to 0 mean, 1 variance
  - Mean and variance are computed over the batch at the current iteration

Batch normalization update for inputs x:

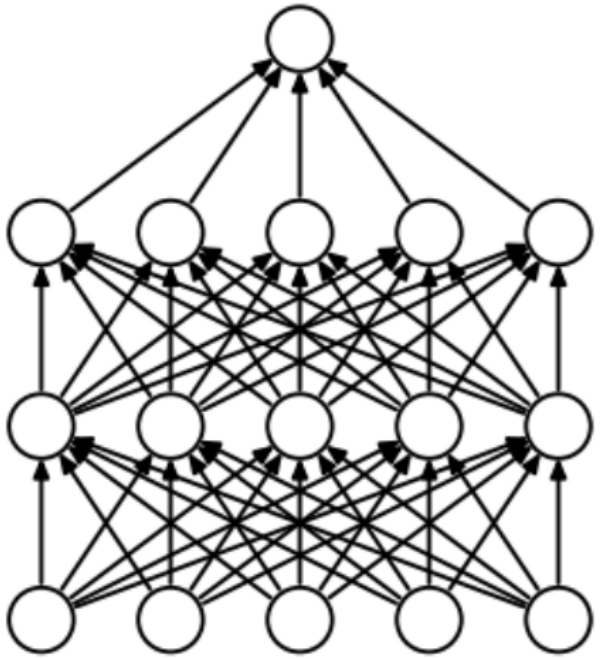
$$x'(i) = (x(i) - E[x(i)]) / STD[x(i)]$$

- Mean subtract
- Normalize by standard deviation

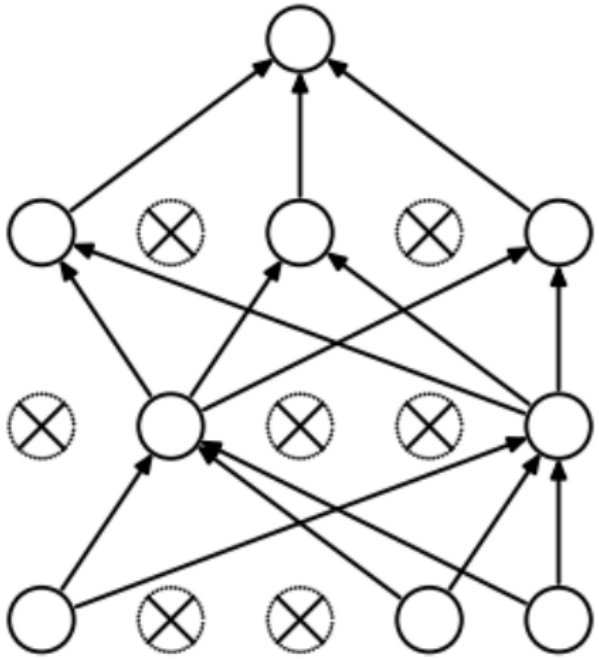


Dropout

- At each train iteration, randomly delete a fraction p of the nodes
- Prevents neurons from being lazy
- A form of model averaging
- (related: DropConnect – drop the connections instead of nodes)



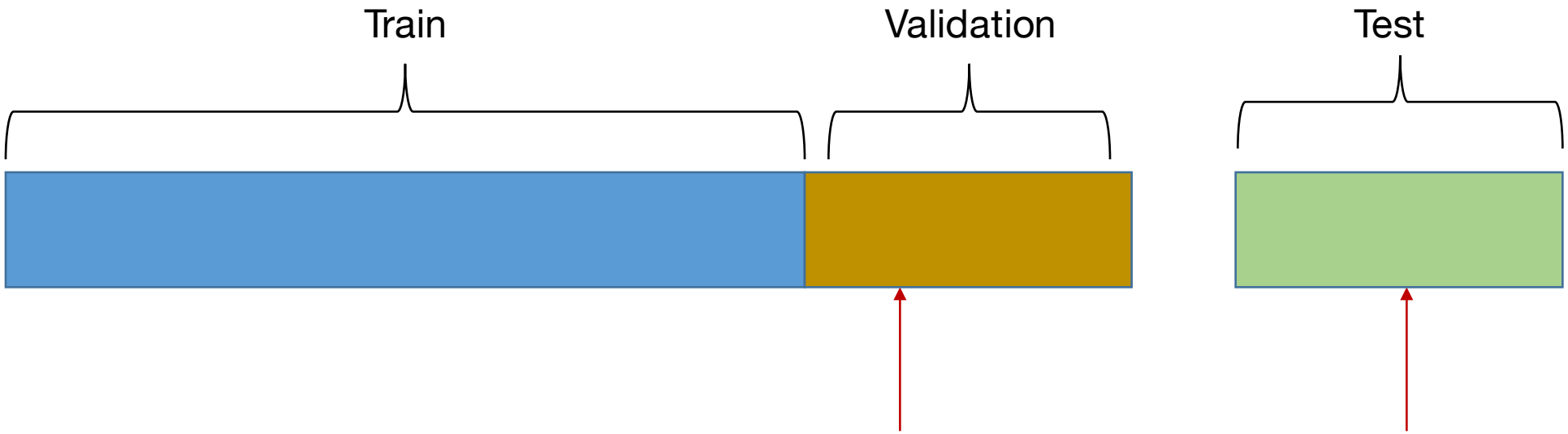
(a) Standard Neural Net



(b) After applying dropout.

https://medium.com/@amarbudhiraja/https-medium-com-amarbudhiraja-learning-less-to-learn-better-dropout-in-deep-machine-learning-74334da4bfc5

As you tune different knobs, take advantage of validation dataset



Use to evaluate while tuning hyperparameters

- effect will creep into model as you continue to use it

Final test set is always separate!
Don't touch until the end!

Regularization: A common pattern

Training: Add some kind of randomness

$$y = f_W(x, z)$$

Testing: Average out randomness (sometimes approximate)

$$y = f(x) = E_z\left[f(x, z)\right] = \int p(z) f(x, z) dz$$

Example: Batch Normalization

Training: Normalize using stats from random minibatches

Testing: Use fixed stats to normalize

Slide from http://cs231n.stanford.edu/

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Example: Batch Normalization

Training: Normalize using stats from random minibatches

Testing: Use fixed stats to normalize

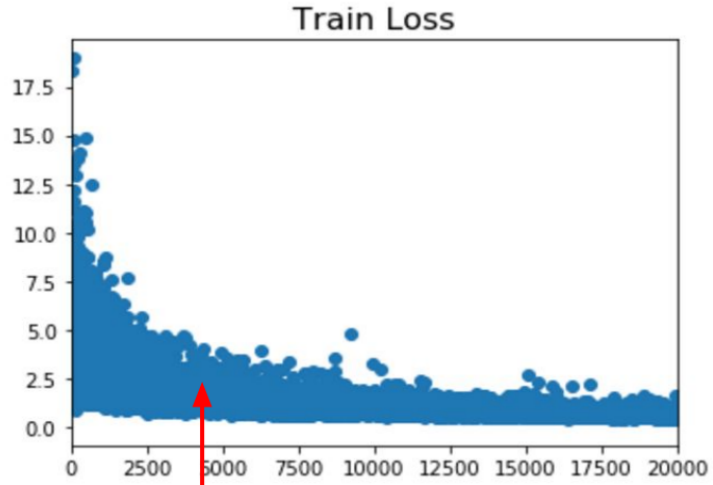
Obvious examples: Dropout, data augmentation

Advanced examples: DropConnect, Fractional Max Pooling, Stochastic Depth

Wan et al, "Regularization of Neural Networks using DropConnect", ICML 2013
Graham, "Fractional Max Pooling", arXiv 2014
Huang et al, "Deep Networks with Stochastic Depth", ECCV 2016

Slide from http://cs231n.stanford.edu/

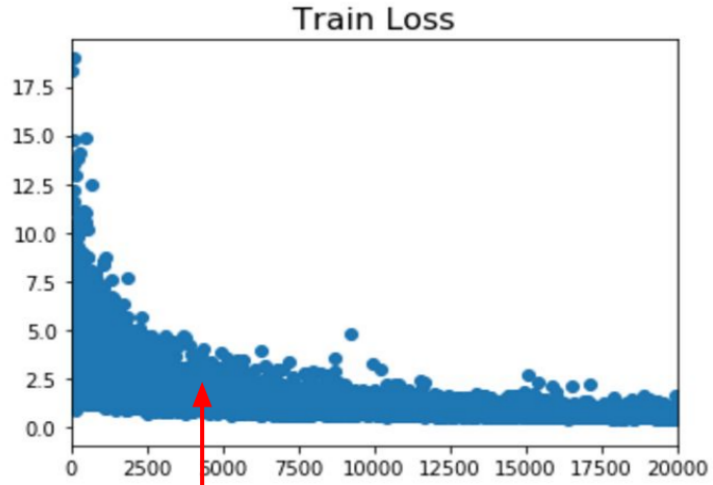
What you'll typically see…



Better optimization algorithms
help reduce training loss

deep imaging

What you'll typically see…

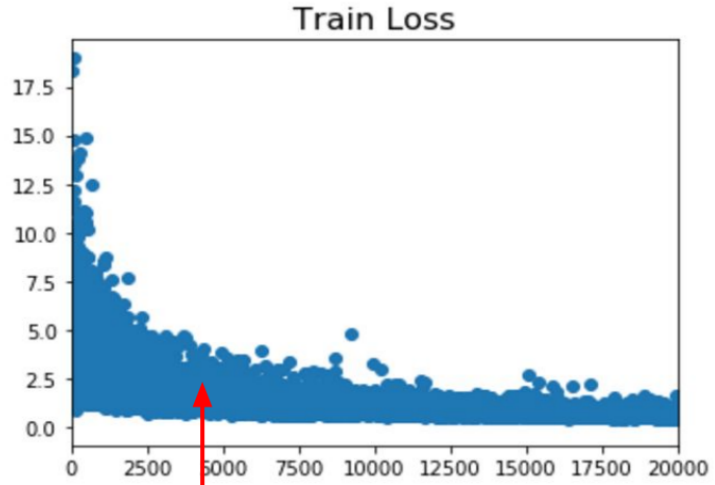


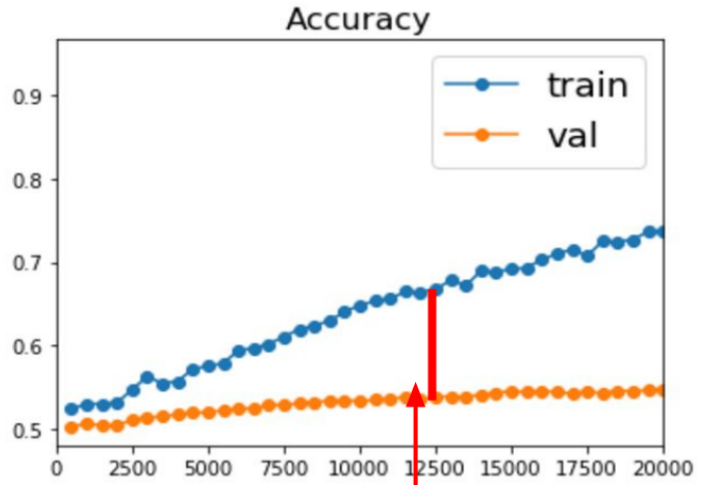
Better optimization algorithms
help reduce training loss

What you can do to help out training error:

- Optimizer choice
- Optimizer step size

What you'll typically see…





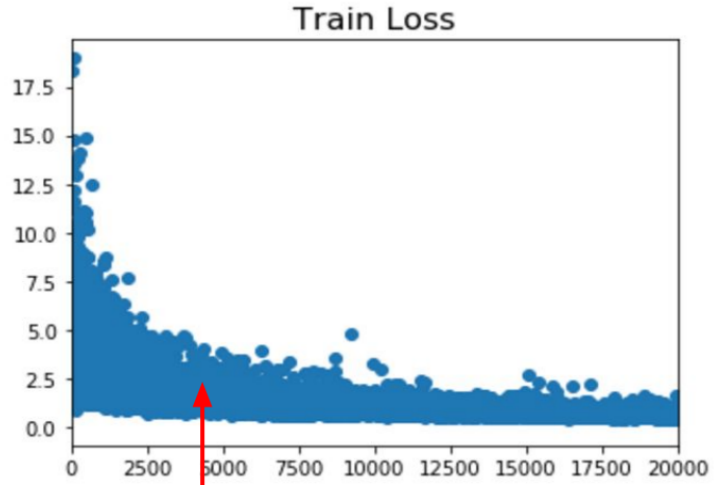
Better optimization algorithms help reduce training loss

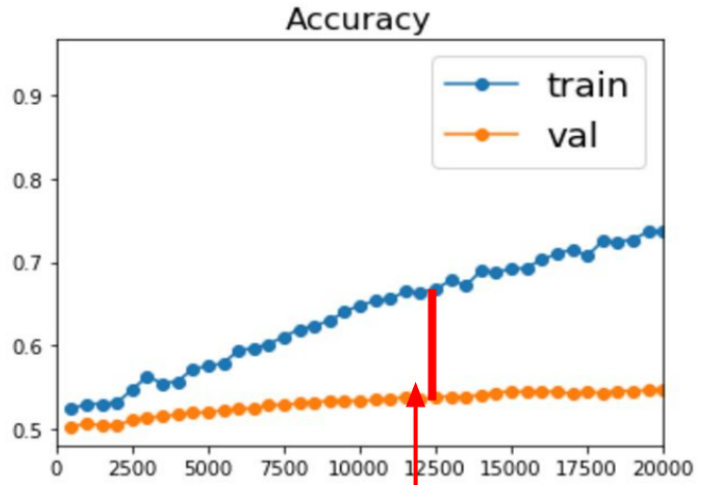
But we really care about error on new data - how to reduce the gap?

What you can do to help out training error:

- Optimizer choice
- Optimizer step size

What you'll typically see…





Better optimization algorithms help reduce training loss

But we really care about error on new data - how to reduce the gap?

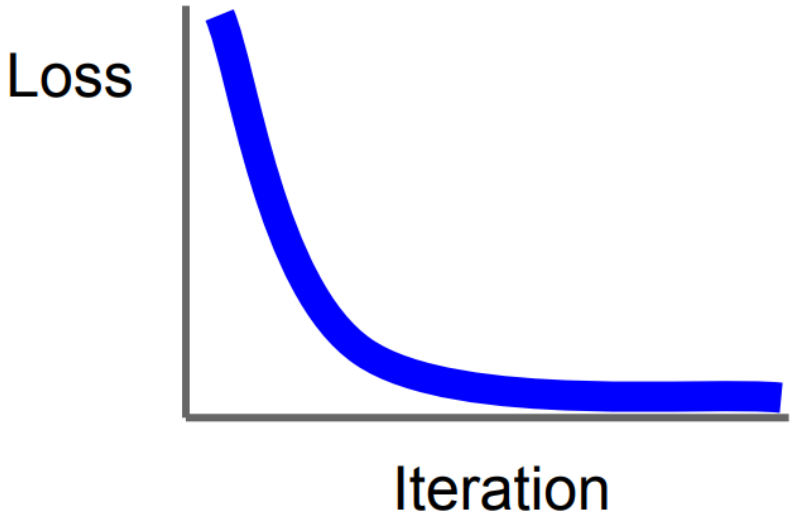
What you can do to help out training error:

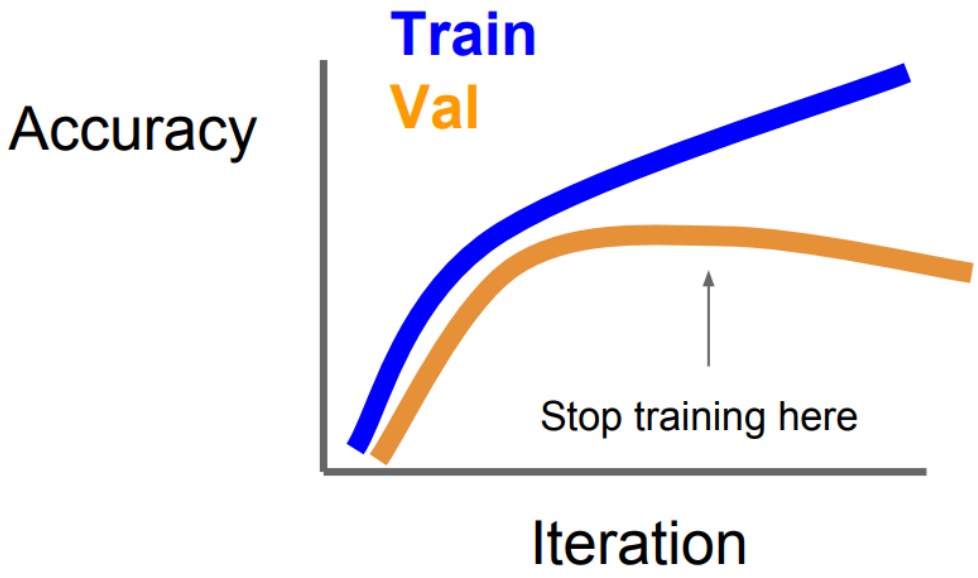
- Optimizer choice
- Optimizer step size

What you can do to help out training error:

- More regularization!
  - Dropout
- Data normalization
- Data augmentation
- A few other tricks..

Trick #1: Early stopping

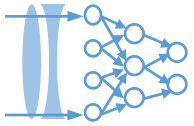




Stop training the model when accuracy on the validation set decreases
Or train for a long time, but always keep track of the model snapshot that worked best on val

Slide from http://cs231n.stanford.edu/

Trick #2: Use Model Ensembles



1. Train multiple independent models
2. At test time average their results
   (Take average of predicted probability distributions, then choose argmax)

Enjoy 2% extra performance

Related concept/term: majority voting

E.g., look at *same* dog image from test data 9X, each w/ uniquely trained model

- Get (let's say) [6, 3] for output classification
- so guess [1,0] = it's a dog
- Will do better than running model once!

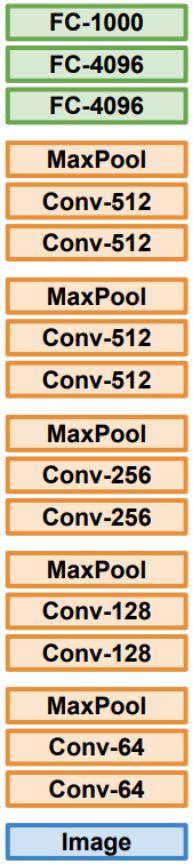
Related technique: Test Time Augmentation

Trick #3: Transfer learning

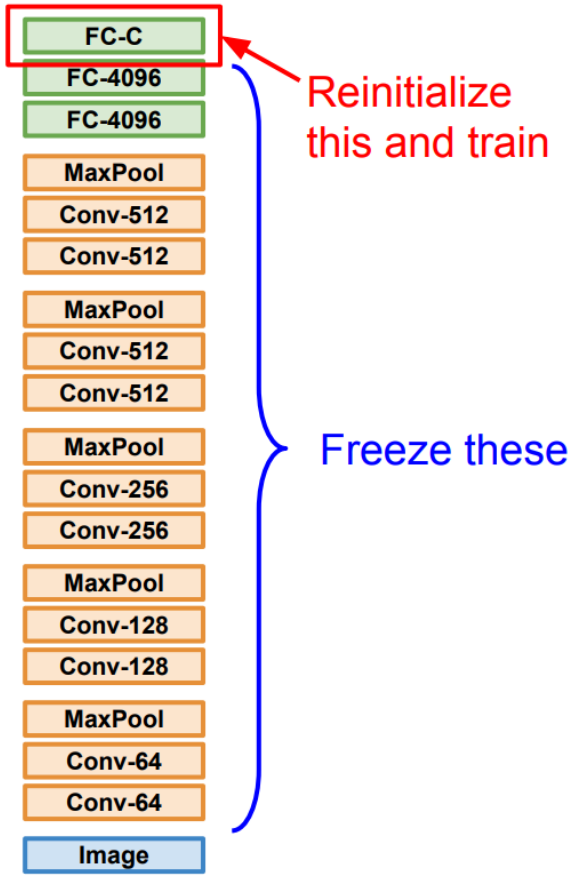
Transfer Learning with CNNs

Donahue et al, "DeCAF: A Deep Convolutional Activation Feature for Generic Visual Recognition", ICML 2014
Razavian et al, "CNN Features Off-the-Shelf: An Astounding Baseline for Recognition", CVPR Workshops 2014

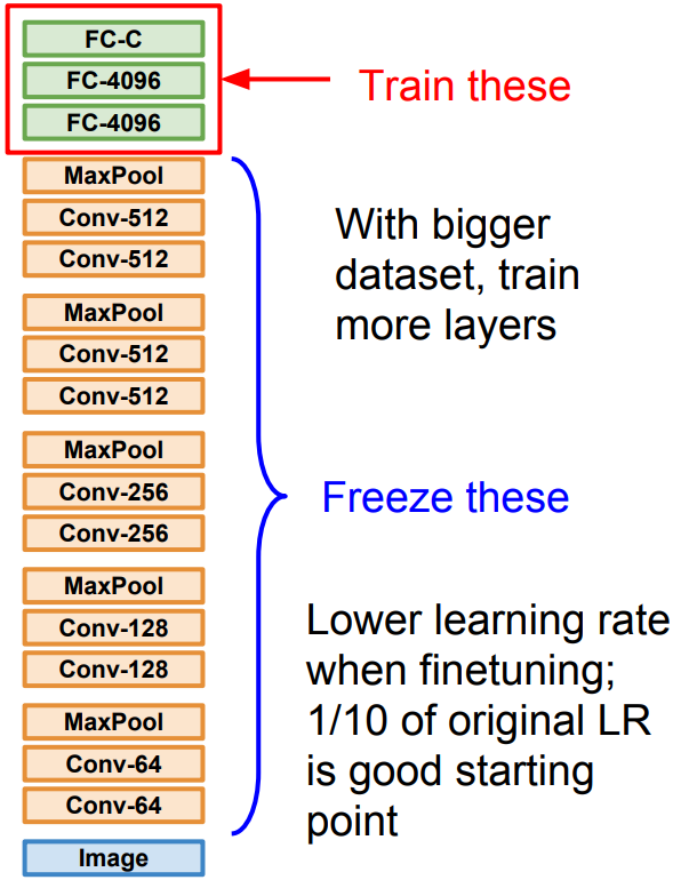
1. Train on Imagenet



2. Small Dataset (C classes)

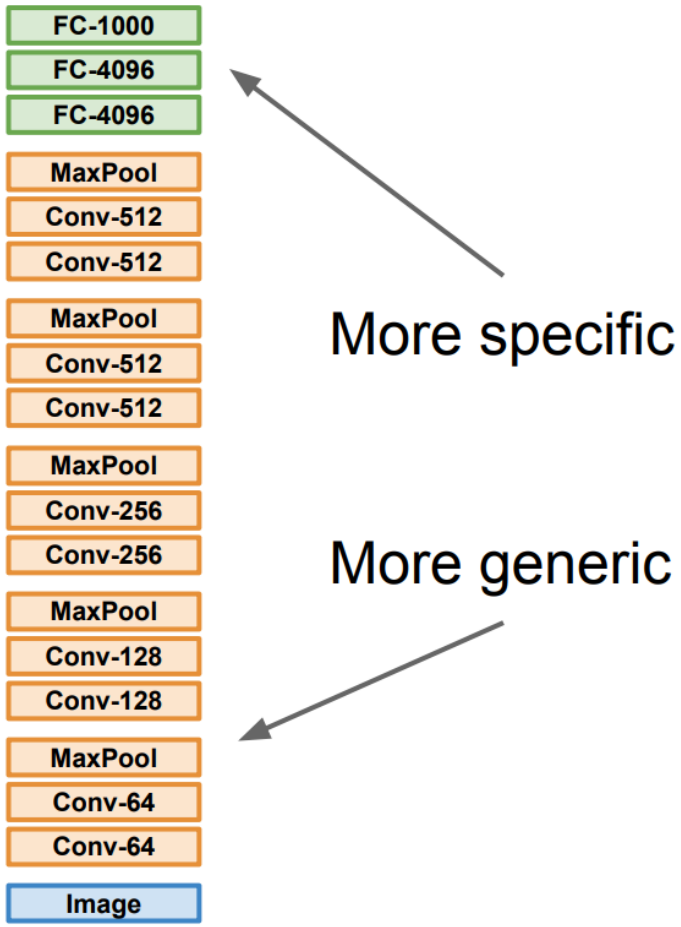


3. Bigger dataset



Slide from http://cs231n.stanford.edu/

Trick #3: Transfer learning

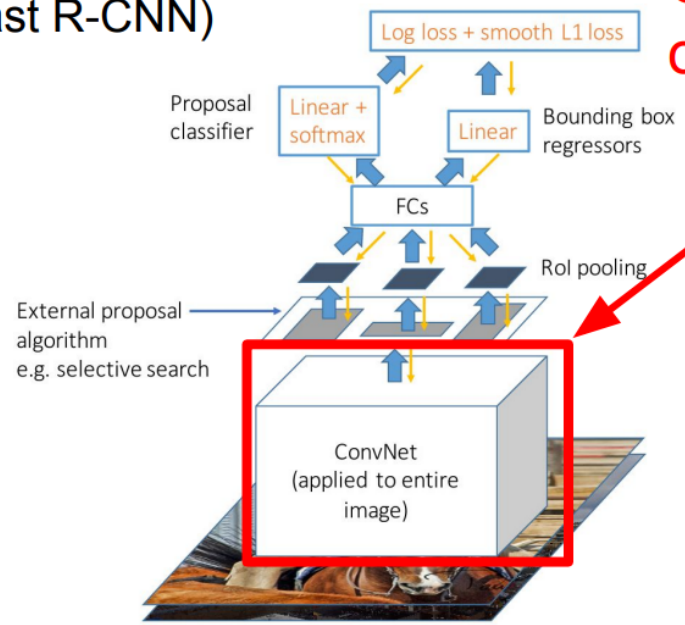


	very similar dataset	very different dataset
very little data	Use Linear Classifier on top layer	You're in trouble… Try linear classifier from different stages
quite a lot of data	Finetune a few layers	Finetune a larger number of layers

Slide from http://cs231n.stanford.edu/

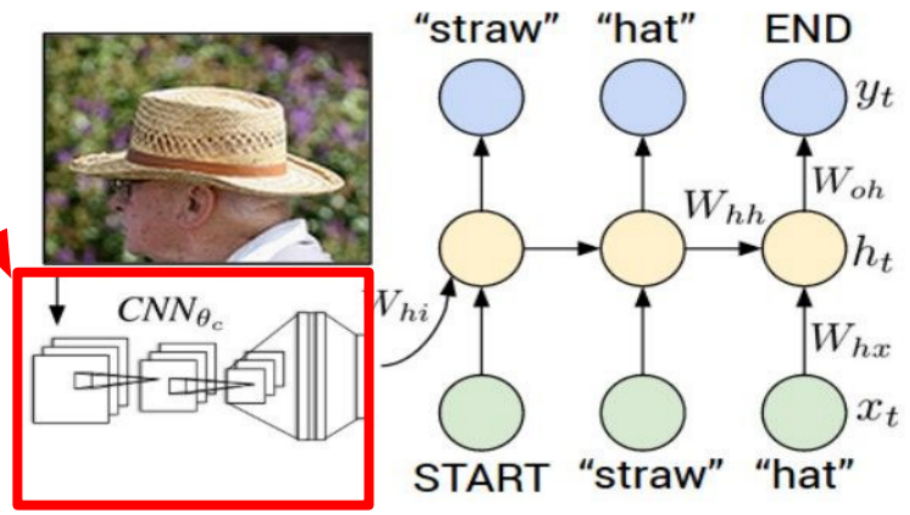
Transfer learning with CNNs is pervasive…
(it's the norm, not an exception)

Object Detection
(Fast R-CNN)



CNN pretrained on ImageNet

Image Captioning: CNN + RNN



Girshick, "Fast R-CNN", ICCV 2015
Figure copyright Ross Girshick, 2015. Reproduced with permission.

Karpathy and Fei-Fei, "Deep Visual-Semantic Alignments for Generating Image Descriptions", CVPR 2015
Figure copyright IEEE, 2015. Reproduced for educational purposes.

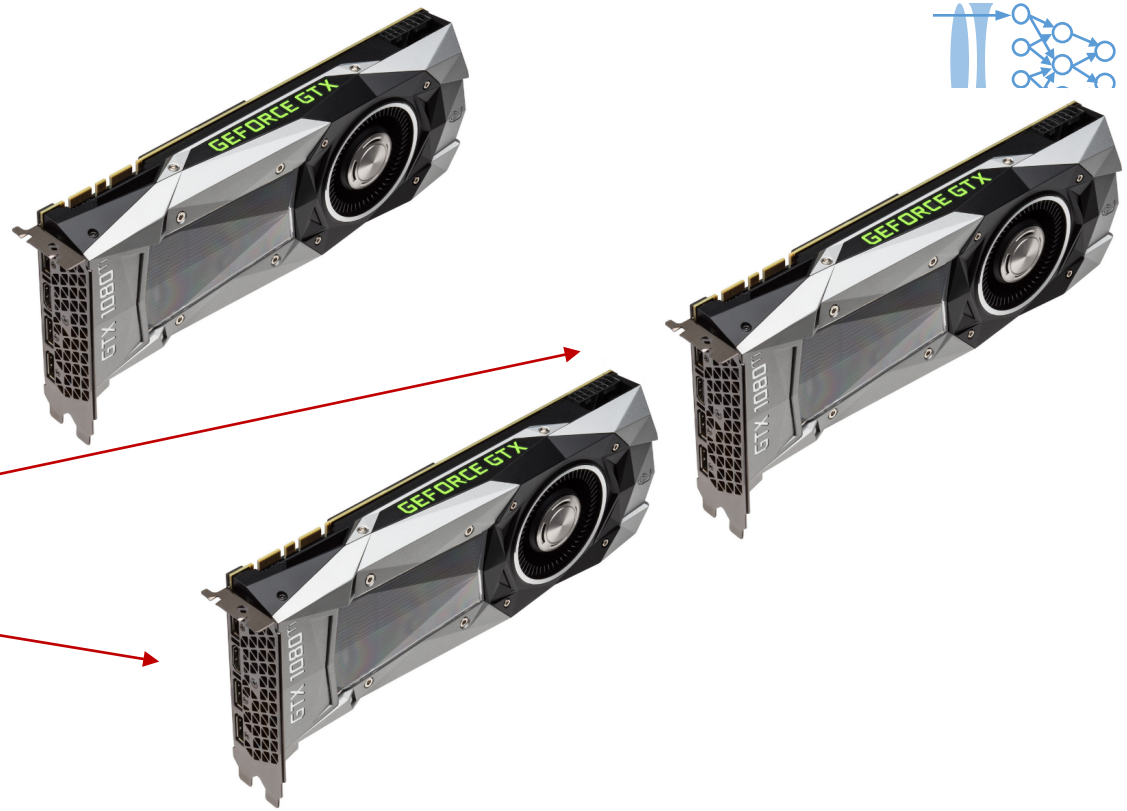
Slide from http://cs231n.stanford.edu/

Trick #4: Hyperparameter optimization

For learning_rate in range(9):

For gradient_scheme in range(5):

⋮



Meta-learning

B. Baker et al., “Designing neural network architectures using reinforcement learning,” arXiv 2017

E. Real, ” Large-Scale Evolution of Image Classifiers,” ICML 2017

Let's identify the following in some example code

- Structure of input/output
- Train/Validation/Test split
- Cost function
- Optimization method, steps (epochs)
- Batch size
- Data augmentation?
- Dropout?

http://deepimaging.github.io/data/basic_tensorflow_eager_example.ipynb

Visualization: a few options at different stages

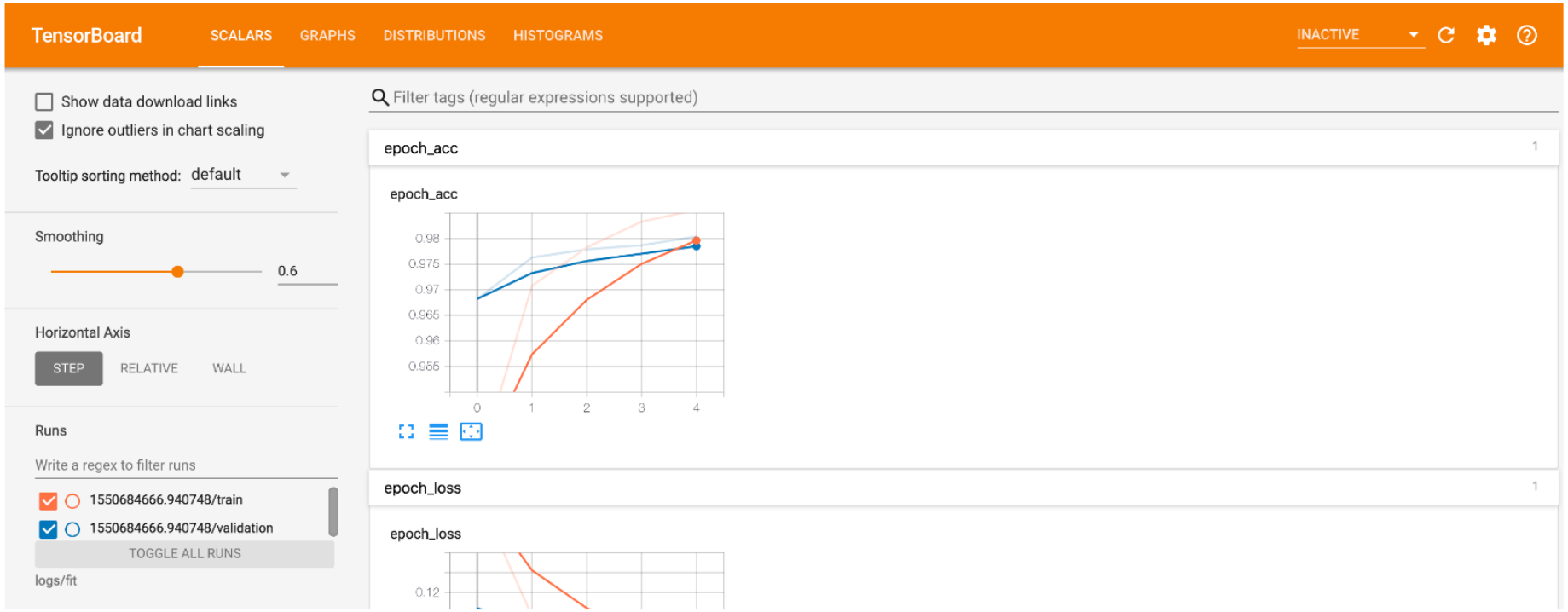
During Training:

- tf.summary()
- Tensorboard
  - Plots of loss/accuracy versus iteration, etc.

After Testing:

- Sliding window
- ROC curve, Precision-Recall
- Confusion matrix
- tSNE visualization

- Beyond classification:
  - image-to-image similarity
  - segmentation overlap

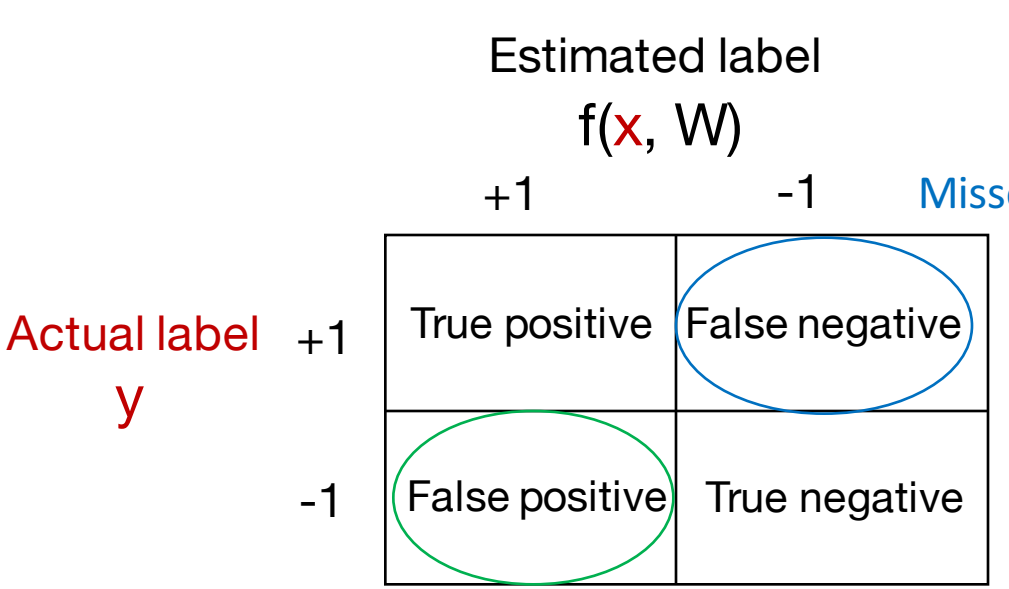



```
model = create_model()
model.compile(optimizer='adam',
              loss='sparse_categorical_crossentropy',
              metrics=['accuracy'])

log_dir="logs/fit/" + datetime.datetime.now().strftime("%Y%m%d-%H%M%S")
tensorboard_callback = tf.keras.callbacks.TensorBoard(log_dir=log_dir, histogram_freq=1)

model.fit(x=x_train,
          y=y_train,
          epochs=5,
          validation_data=(x_test, y_test),
          callbacks=[tensorboard_callback])
```

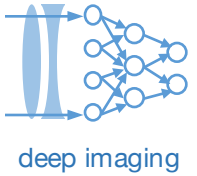
```
%tensorboard --logdir logs/fit
```

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



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

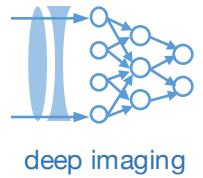
Estimated label
f(x, W)

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



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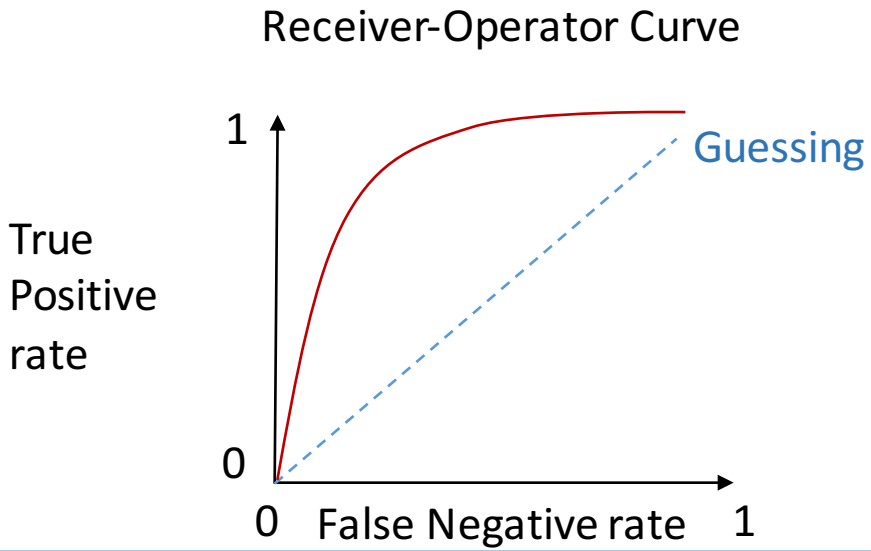
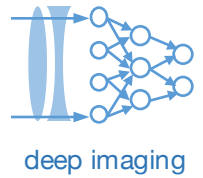


ROC curve and confusion matrix



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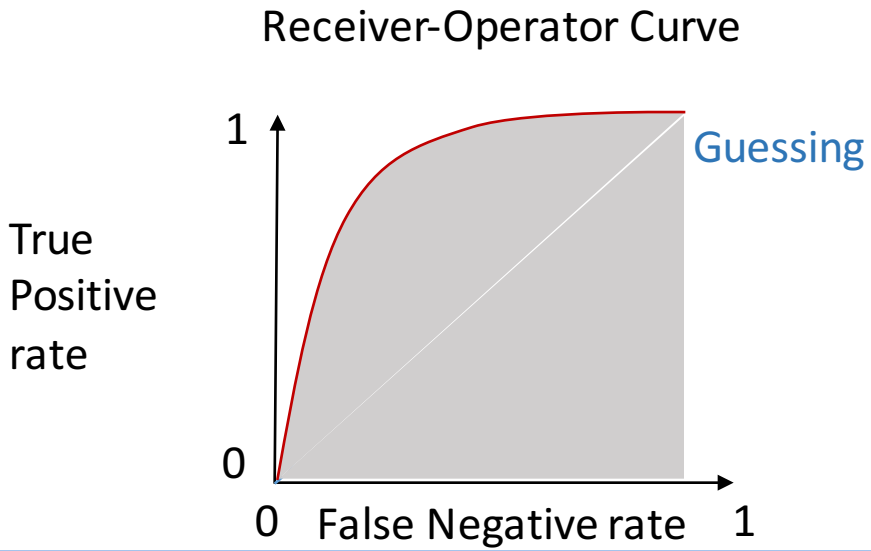
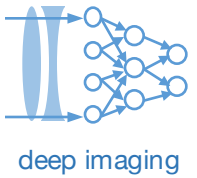


Area under the curve (AUC): Integral of ROC curve

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

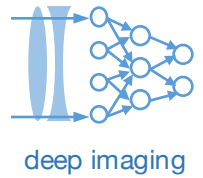
Missed an event

Predict event when there isn't one

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

- 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



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

Estimated label
f(x, W)

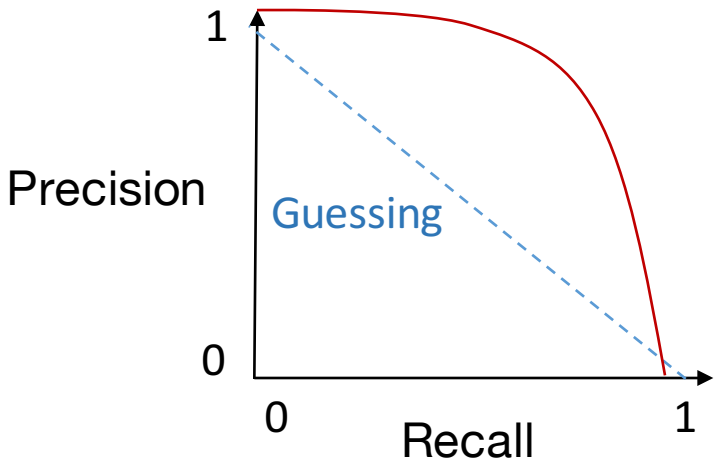
Actual label y	+1	-1
+1	True positive	False negative
-1	False positive	True negative

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

deep imaging

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 %

Other performance metrics

deep imaging

- Overlap between segmented areas: Jaccard similarity coefficient

  J = |R1 ∩ R2| / |R1 U R2|

- MSE, PSNR

- Structural Similarity (SSIM)

$$\mathrm{SSIM}(x,y) = \frac{(2\mu_x\mu_y + c_1)(2\sigma_{xy} + c_2)}{(\mu_x^2 + \mu_y^2 + c_1)(\sigma_x^2 + \sigma_y^2 + c_2)}$$

with:

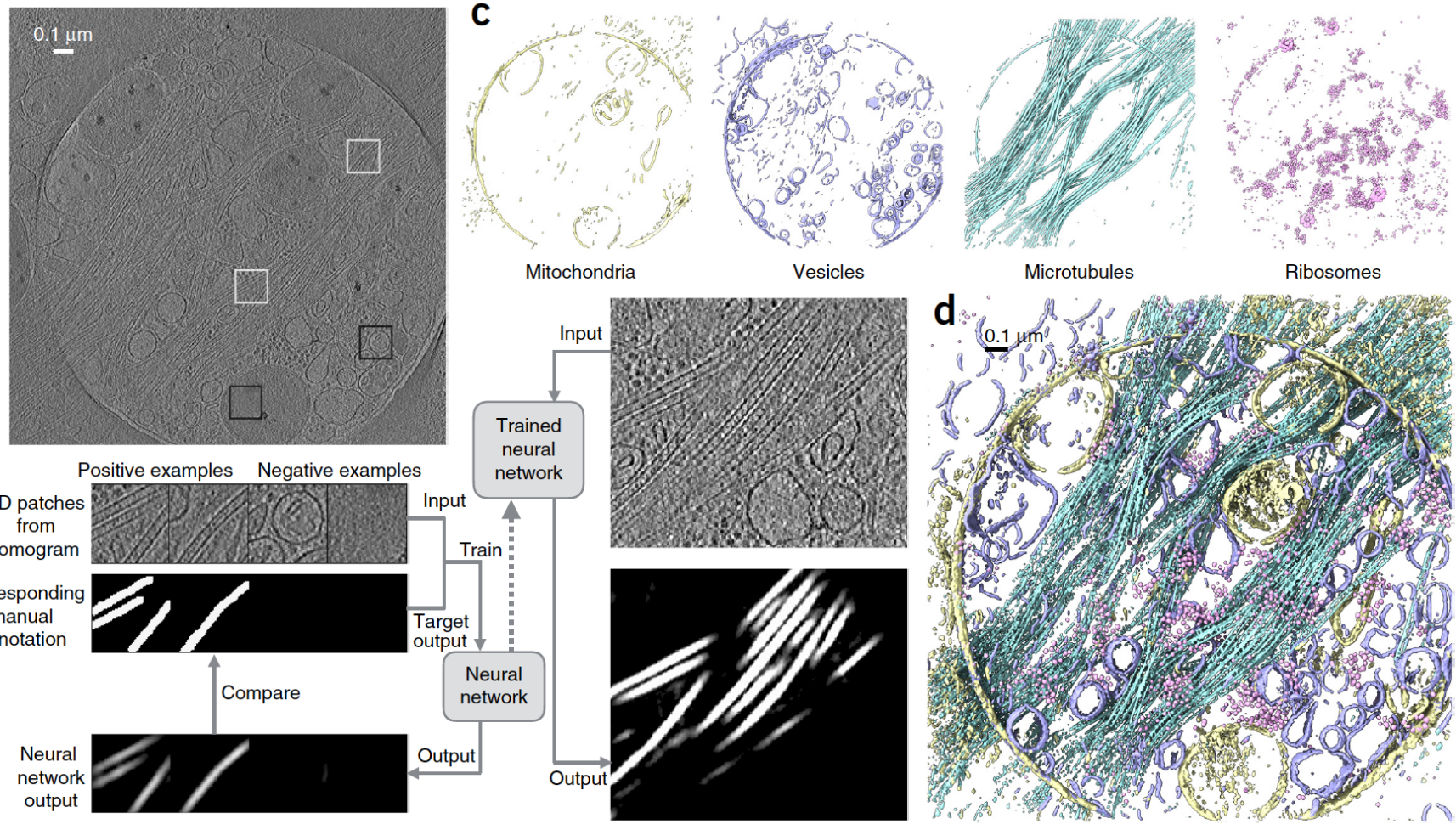
- μ_x the average of x;
- μ_y the average of y;
- σ_x^2 the variance of x;
- σ_y^2 the variance of y;
- σ_{xy} the covariance of x and y;
- $c_1=(k_1 L)^2$, $c_2=(k_2 L)^2$ two variables to stabilize the division with weak denominator;
- L the dynamic range of the pixel-values (typically this is $2^{\#bits\ per\ pixel}-1$);
- $k_1=0.01$ and $k_2=0.03$ by default.

Examples of CNN's for biomedical image classification

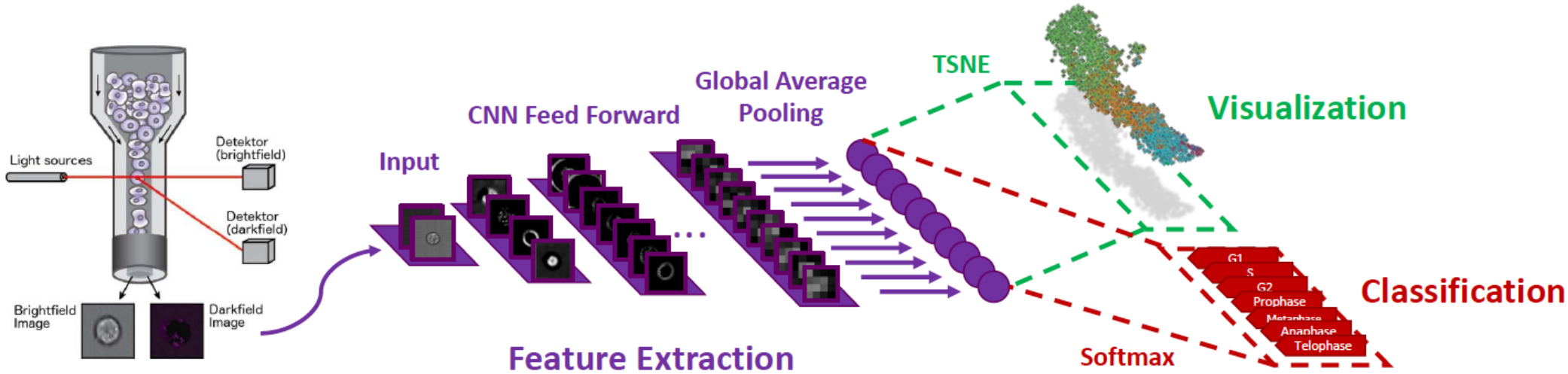
Convolutional neural networks for automated annotation of cellular cryo-electron tomograms

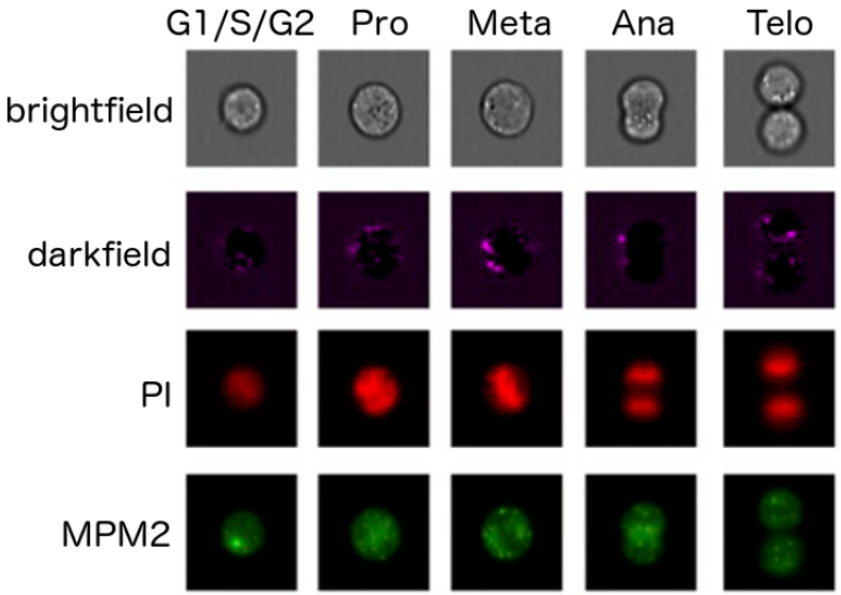
Muyuan Chen[1,2], Wei Dai[2,4], Stella Y Sun[2], Darius Jonasch[2], Cynthia Y He[3], Michael F Schmid[2], Wah Chiu[2] & Steven J Ludtke[2]

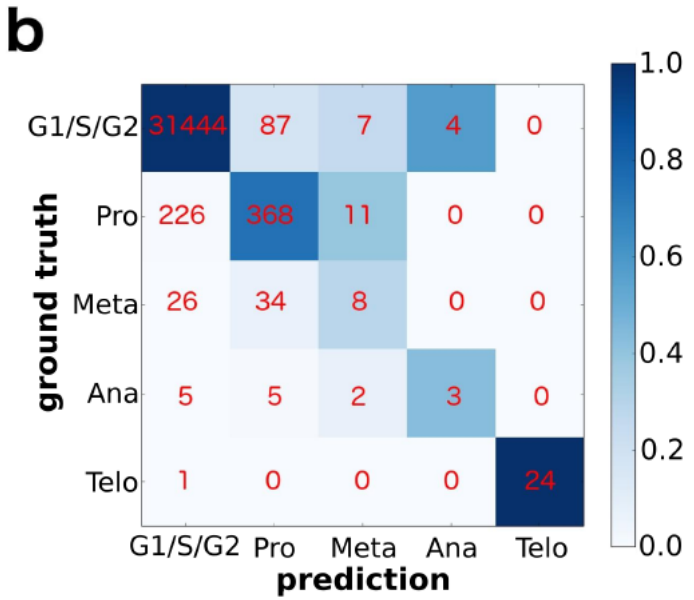
deep imaging



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

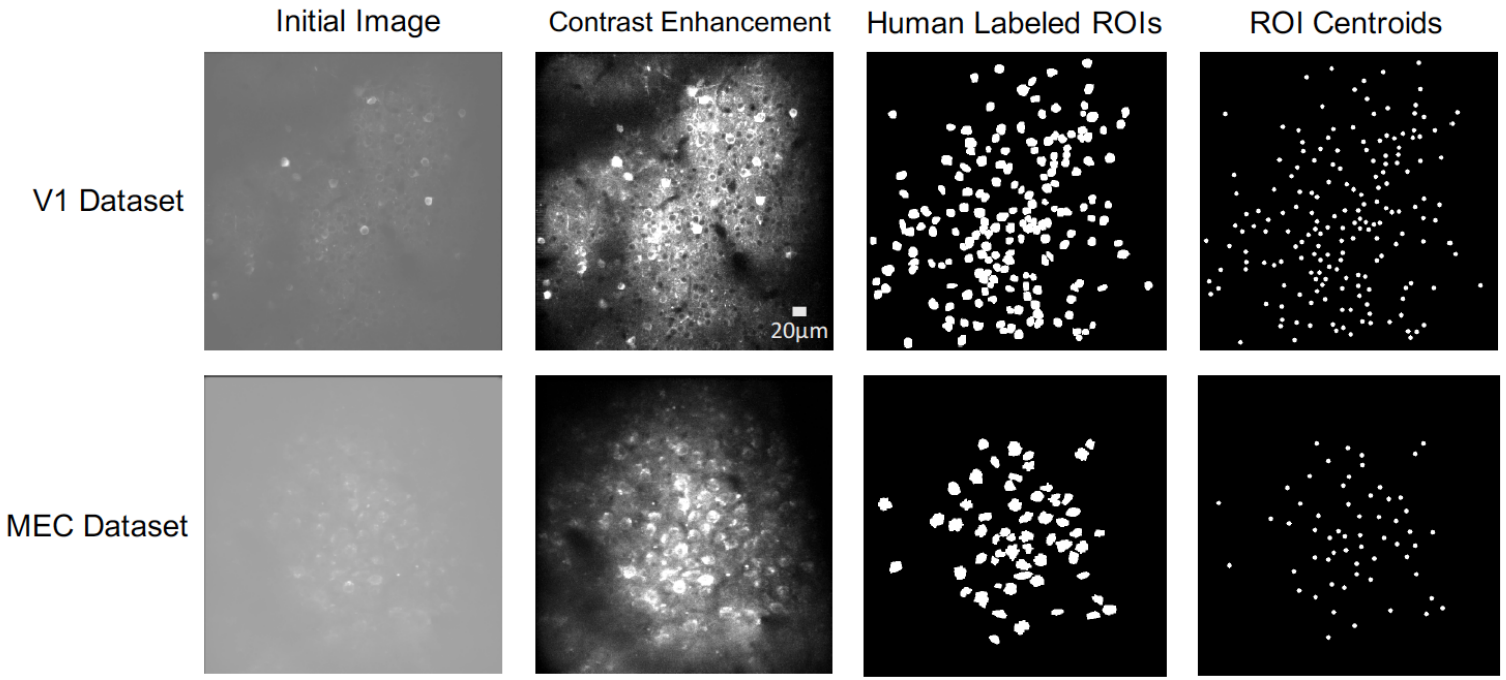


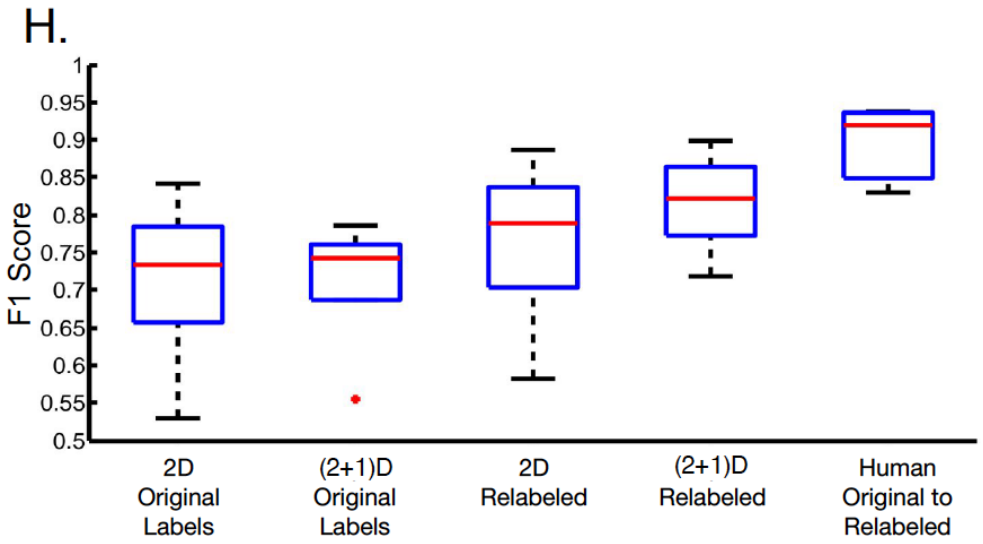


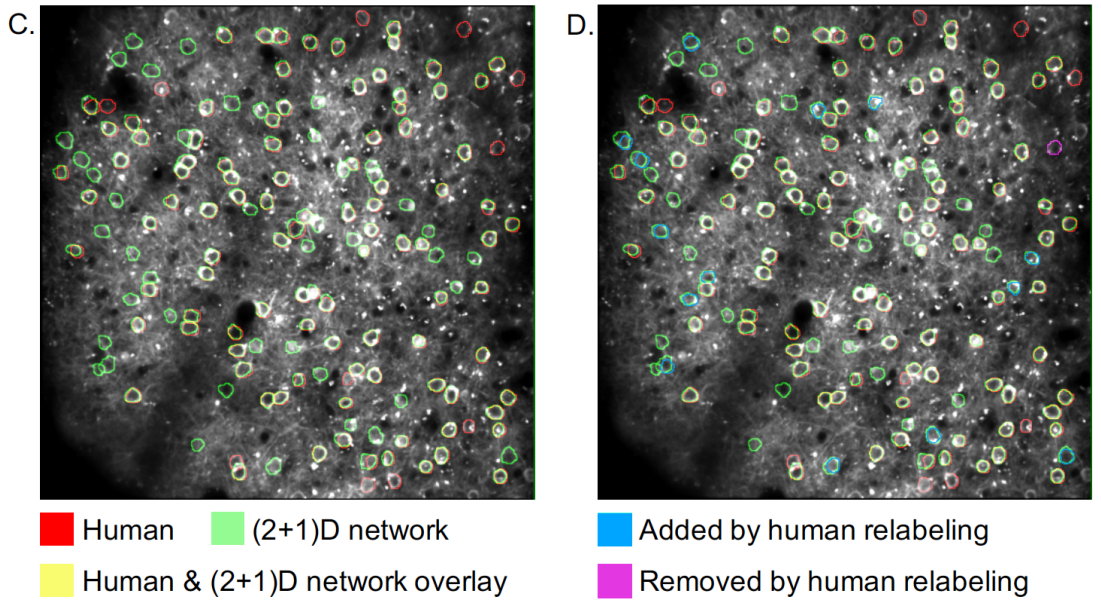


Automatic Neuron Detection in Calcium Imaging Data Using Convolutional Networks

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

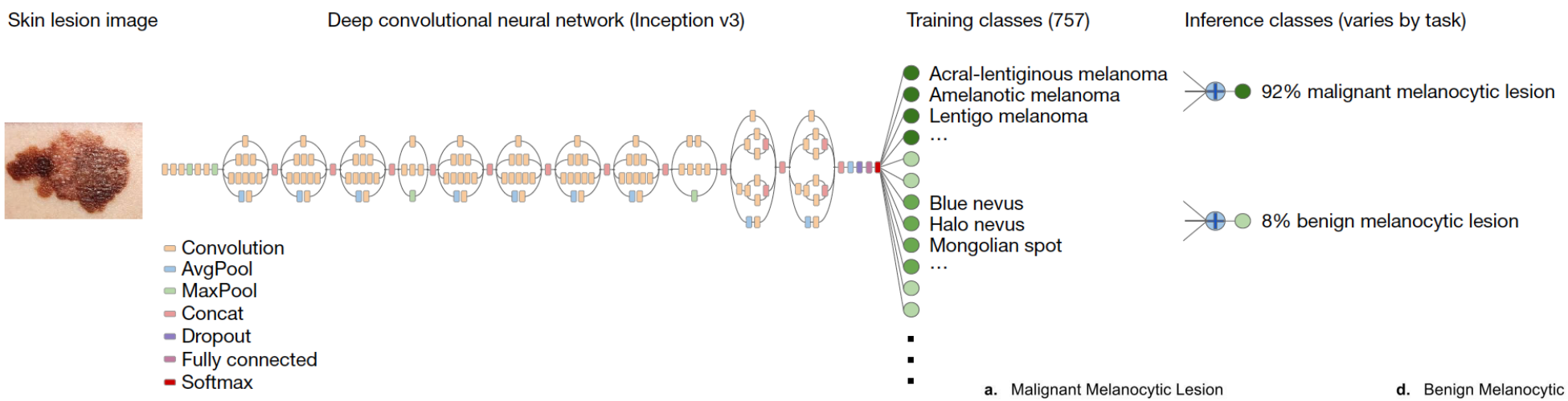


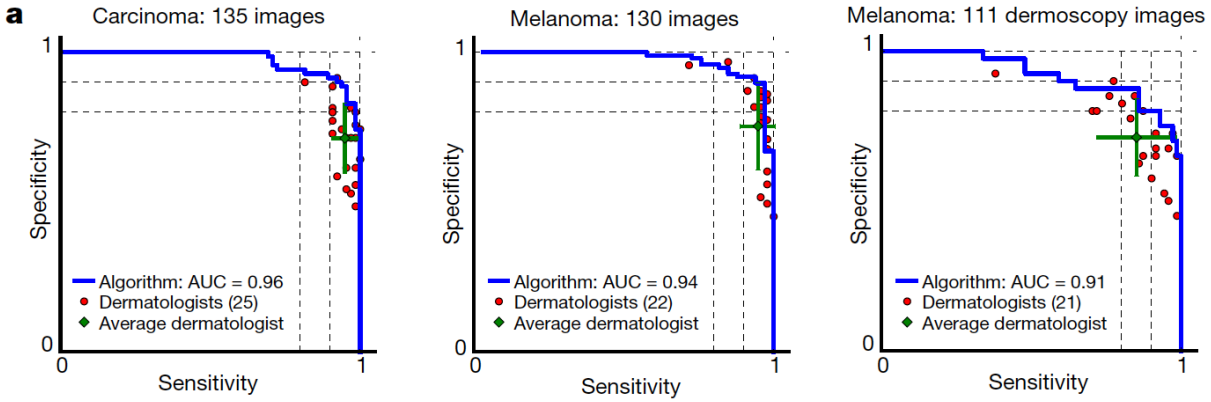


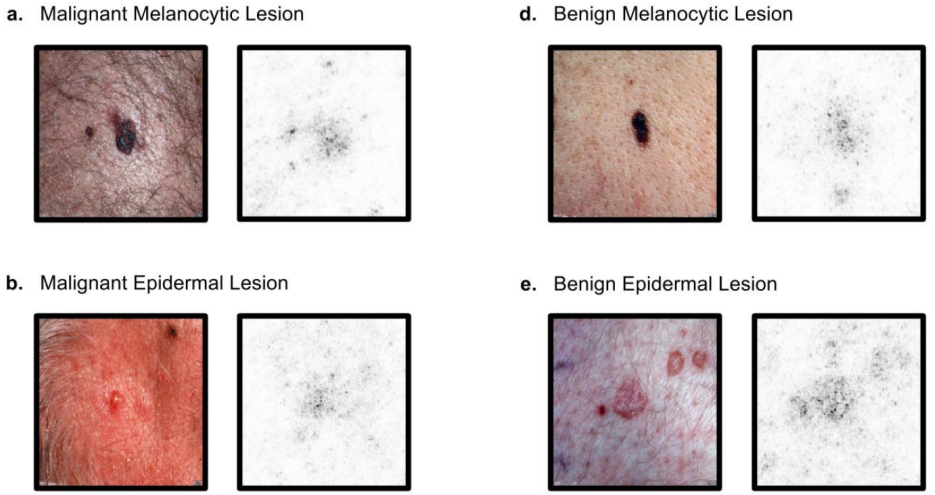


Dermatologist-level classification of skin cancer with deep neural networks

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]