CPSC 340:
Machine Learning and Data Mining

Convolutional Neural Networks

Fall 2020

Admin – Final Lectures

- Exam to appear at 5pm Monday on course website.
  - Roughly the same format as the midterm
  - Due at midnight

- I will finish the "testable content" of the course today.

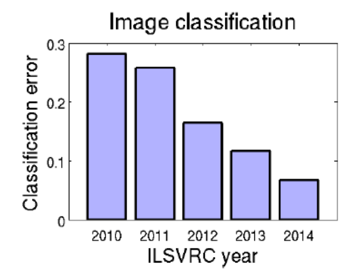
- Monday/Wednesday
  - Automatic differentiation
  - Presentations from project teams

Last Lectures: Deep Learning

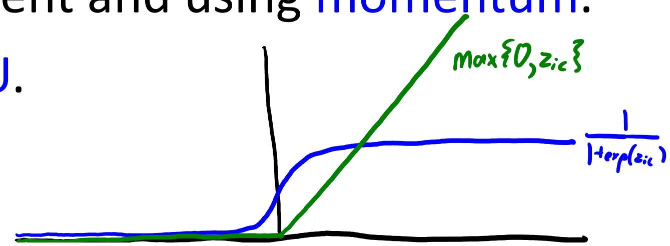
- We've been discussing neural network / deep learning models:

$$\hat{y}_i = v^T h(W^{(m)} h(W^{(m-1)} h(\cdots W^{(2)} h(W^{(1)} x_i)) \cdots))$$

- We discussed unprecedented vision/speech performance.



- We discussed methods to make SGD work better:
  - Parameter initialization and data transformations.
  - Setting the step size(s) in stochastic gradient and using momentum.
  - Alternative non-linear functions like ReLU.



https://arxiv.org/pdf/1409.0575v3.pdf

“Residual” Networks (ResNets)

- Impactful recent idea is residual networks (ResNets):

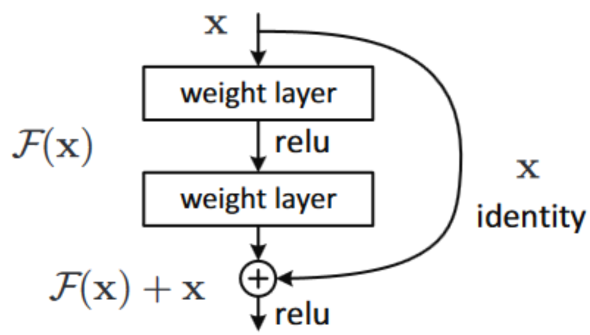


Figure 2. Residual learning: a building block.

  - You can take previous (non-transformed) layer as input to current layer.
    - Also called “skip connections” or “highway networks”.
  - Non-linear part of the network only needs to model residuals.
    - Non-linear parts are just “pushing up or down” a linear model in various places.
  - This was a key idea behind first methods that used 100+ layers.
    - Evidence that biological networks have skip connections like this.

https://en.wikipedia.org/wiki/Residual_neural_network

DenseNet

- More recent variation is “DenseNets”:
  – Each layer can see all the values from many previous layers.
  – Gets rid of vanishing gradients.
  – May get same performance with fewer parameters/layers.

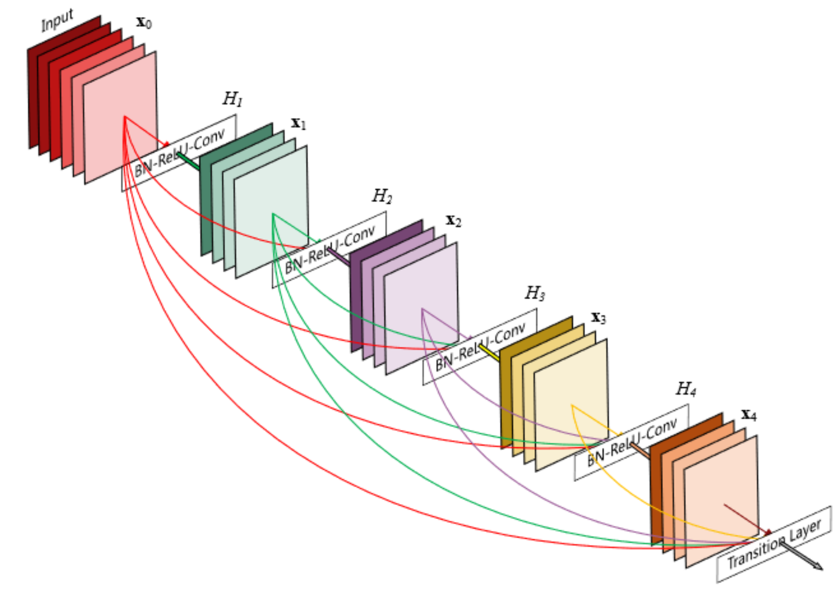


Figure 1: A 5-layer dense block with a growth rate of $k = 4$. Each layer takes all preceding feature-maps as input.

https://arxiv.org/pdf/1512.03385v1.pdf

Deep Learning and the Fundamental Trade-Off

- Neural networks are subject to the fundamental trade-off:
  - With increasing depth, training error of global optima decreases.
  - With increasing depth, training error may poorly approximate test error.

- We want deep networks to model highly non-linear data.
  - But increasing the depth can lead to overfitting.

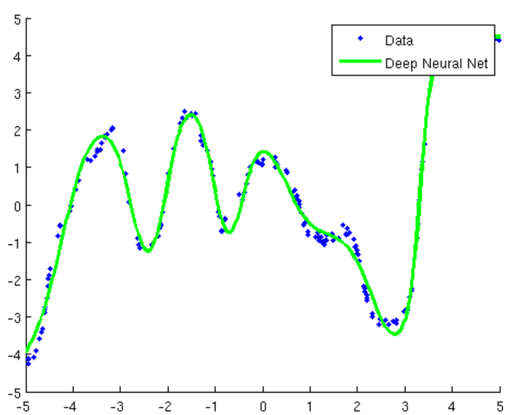
- How could GoogLeNet use 22 layers?
  - Many forms of regularization and keeping model complexity under control.
  - Unlike linear models, typically use multiple types of regularization.

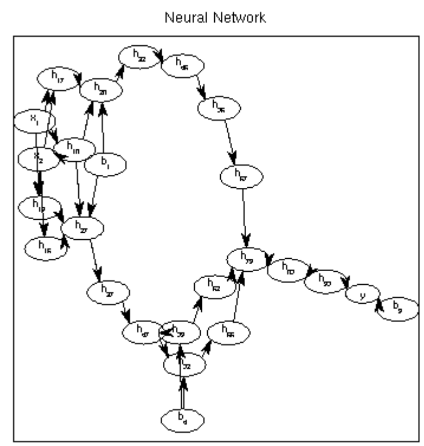
Standard Regularization

- Traditionally, we've added our usual L2-regularizers:

$$f(v, W^{(3)}, W^{(2)}, W^{(1)}) = \frac{1}{2}\sum_{i=1}^{n}\left(v^T h(W^{(3)} h(W^{(2)} h(W^{(1)} x_i))) - y_i\right)^2 + \frac{\lambda_4}{2}\|v\|^2 + \frac{\lambda_3}{2}\|W^{(3)}\|_F^2 + \frac{\lambda}{2}\|W^{(2)}\|_F^2 + \frac{\lambda}{2}\|W^{(1)}\|_F^2$$

- L2-regularization often called "weight decay" in this context.
  - Could also use L1-regularization: gives sparse network.





Standard Regularization

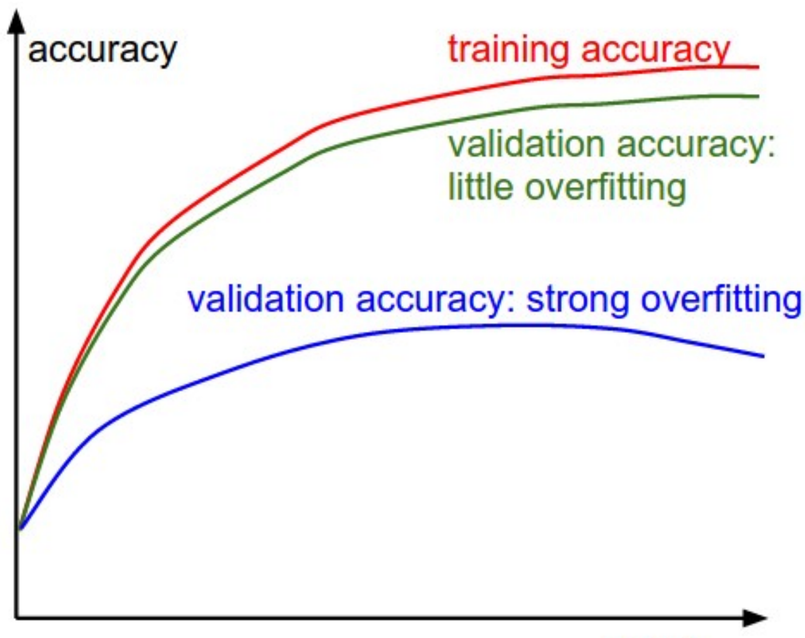
- Traditionally, we've added our usual L2-regularizers:

$$f(v, W^{(3)}, W^{(2)}, W^{(1)}) = \frac{1}{2}\sum_{i=1}^{n}\left(v^T h(W^{(3)}h(W^{(2)}h(W^{(1)}x_i))) - y_i\right)^2 + \frac{\lambda_4}{2}\|v\|^2 + \frac{\lambda_3}{2}\|W^{(3)}\|_F^2 + \frac{\lambda}{2}\|W^{(2)}\|_F^2 + \frac{\lambda}{2}\|W^{(1)}\|_F^2$$

- L2-regularization often called "weight decay" in this context.
  – Could also use L1-regularization: gives sparse network.
- Hyper-parameter optimization gets expensive:
  – Try to optimize validation error in terms of λ_1, λ_2, λ_3, λ_4.
  – In addition to step-size, number of layers, size of layers, initialization.
- Recent result:
  – Adding a regularizer in this way creates bad local optima.

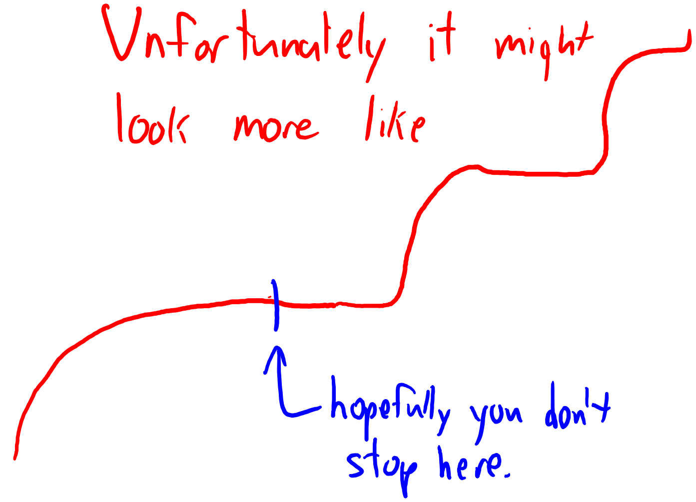
Early Stopping

- Another common type of regularization is "early stopping":
  - Monitor the validation error as we run stochastic gradient.
  - Stop the algorithm if validation error starts increasing.



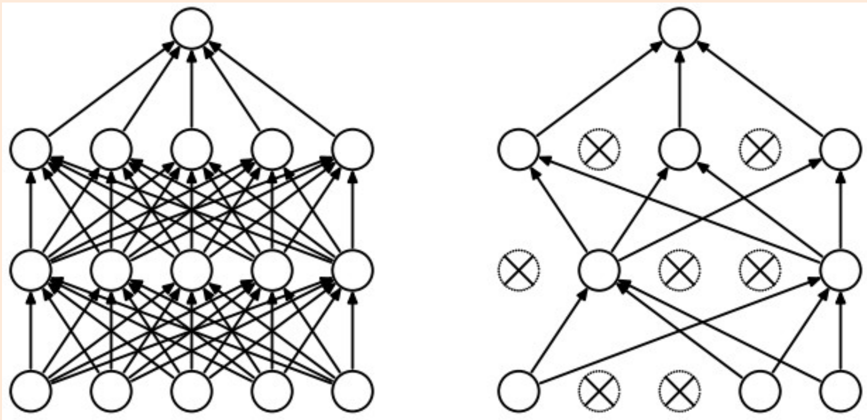
http://cs231n.github.io/neural-networks-3/

Unfortunately it might look more like



Dropout

- Dropout is a more recent form of explicit regularization:
  - On each iteration, randomly set some x_i and z_i to zero (often use 50%).



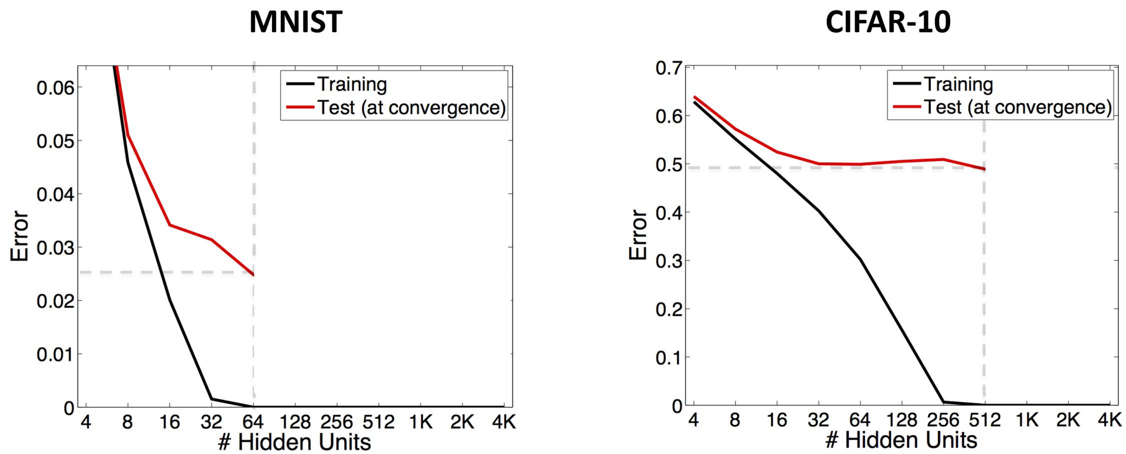
(a) Standard Neural Net (b) After applying dropout.

  - Adds invariance to missing inputs or latent factors
    - Encourages distributed representation rather than relying on specific z_i.
  - Can be interpreted as an ensemble over networks with different parts missing.
  - After a lot of success, dropout may already be going out of fashion.

http://www.cs.toronto.edu/~rsalakhu/papers/srivastava14a.pdf

“Hidden” Regularization in Neural Networks

- Fitting single-layer neural network with SGD and no regularization:



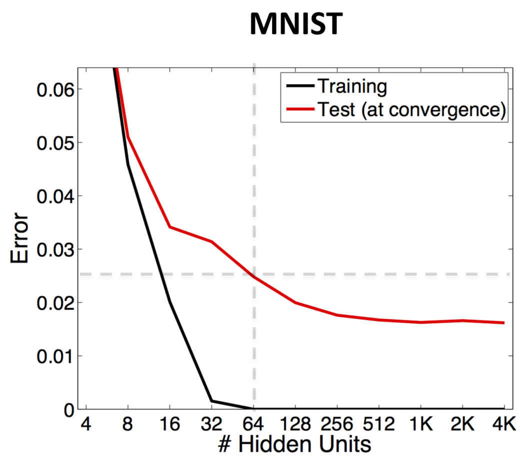
- Training goes to 0 with enough units: we’re finding a global min.

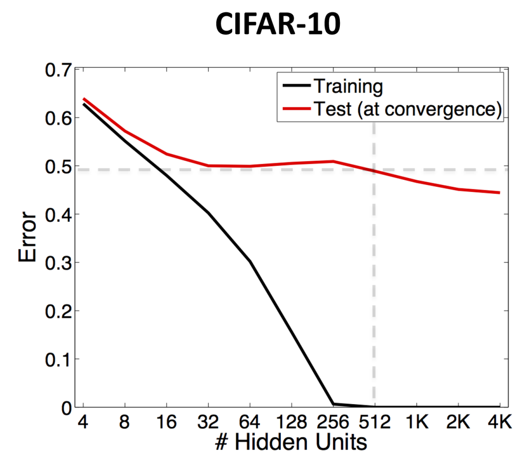
- What should happen to training and test error for larger #hidden?

https://www.neyshabur.net/papers/inductive_bias_poster.pdf

“Hidden” Regularization in Neural Networks

- Fitting single-layer neural network with SGD and no regularization:





- Test error continues to go down!?! Where is fundamental trade-off??
- There exist global mins with large #hidden units have test error = 1.
  - But among the global minima, SGD is somehow converging to “good” ones.

https://www.neyshabur.net/papers/inductive_bias_poster.pdf

Implicit Regularization of SGD

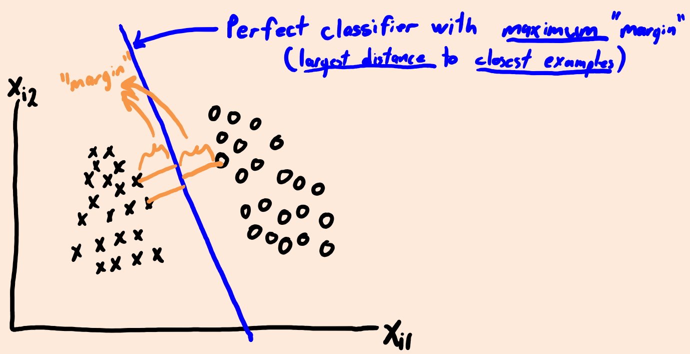
- There is growing evidence that using SGD regularizes parameters.
  - We call this the "implicit regularization" of the optimization algorithm.

- Beyond empirical evidence, we know this happens in simpler cases.

- Example of implicit regularization:
  - Consider a least squares problem where there exists a 'w' where Xw=y.
    - Residuals are all zero, we fit the data exactly.
  - You run [stochastic] gradient descent starting from w=0.
  - Converges to solution Xw=y that has the minimum L2-norm.
    - So using SGD is equivalent to L2-regularization here, but regularization is "implicit".

Implicit Regularization of SGD

- Example of implicit regularization:
  - Consider a logistic regression problem where data is linearly separable.
    - We can fit the data exactly.
  - You run gradient descent from any starting point.
  - Converges to max-margin solution of the problem.
    - So using gradient descent is equivalent to encouraging large margin.



- Similar result known for boosting.

(pause)

Deep Learning "Tricks of the Trade"

- We've discussed heuristics to make deep learning work:
  - Parameter initialization and data transformations.
  - Setting the step size(s) in stochastic gradient and using momentum.
  - RestNets and alternative non-linear functions like ReLU.
  - Different forms of regularization:
    - L2-regularization, early stopping, dropout, implicit regularization from SGD.

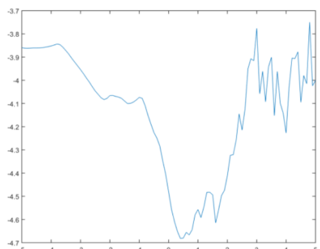
- These are often still not enough to get deep models working.

- Deep computer vision models are all convolutional neural networks:
  - The $W^{(m)}$ are very sparse and have repeated parameters ("tied weights").
  - Drastically reduces number of parameters (speeds training, reduces overfitting).

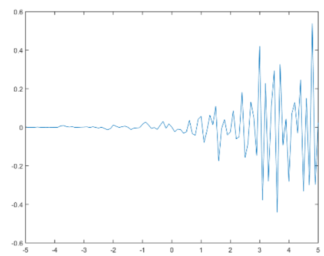
1D Convolution as Matrix Multiplication

- 1D convolution:
  - Takes signal ‘x’ and filter ‘w’ to produces vector ‘z’:

$$x \ast w = z$$



$$[-1 \quad 2 \quad -1]$$



  - Can be written as a matrix multiplication:

$$W_x = \begin{bmatrix} 1 & -2 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ & & & \vdots & & & & & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & -2 & 1 \end{bmatrix} x = z$$

1D Convolution as Matrix Multiplication

- Each element of a convolution is an inner product:

$$z_i = \sum_{j=-m}^{m} w_j x_{i+j}$$

$$= w^T x_{(i-m:i+m)}$$

$$= \tilde{w}^T x \quad \text{where } \tilde{w} = [\,0 \;\; 0 \;\; 0 \;\; \overbrace{\text{—— } w \text{ ——}}^{\text{positions } i-m \text{ through } i+m} \;\; 0 \;\; 0\,]$$

- So convolution is a matrix multiplication (I'm ignoring boundaries):

$$z = \tilde{W}x \quad \text{where } \tilde{W} = \begin{bmatrix} \text{—— } w \text{ ——} & 0 & 0 & 0 \\ 0 & \text{—— } w \text{ ——} & 0 & 0 \\ 0 & 0 & \text{—— } w \text{ ——} & 0 \\ 0 & 0 & 0 & \text{—— } w \text{ ——} \end{bmatrix}$$

matrix can be very sparse and only has $2m+1$ variables.

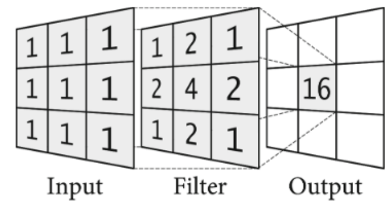
- The shorter 'w' is, the more sparse the matrix is.

2D Convolution as Matrix Multiplication

- 2D convolution:
  - Signal ‘x’, filter ‘w’, and output ‘z’ are now all images/matrices:

$$x \quad * \quad w \quad = \quad z$$

$$\begin{bmatrix} -2 & -1 & 0 \\ -1 & 0 & 1 \\ 0 & 1 & 2 \end{bmatrix}$$



  - Vectorized ‘z’ can be written as a matrix multiplication with vectorized ‘x’:

$$W = \left[\begin{array}{ccccccccc|ccccccccc|ccccccccc|ccc}
-2 & -1 & 0 & 0 & 0 & 0 & \cdots & 0 & & -1 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & & 0 & 1 & 2 & 0 & 0 & 0 & \cdots & 0 & & 0 & 0 & \cdots \\
0 & -2 & -1 & 0 & 0 & 0 & \cdots & 0 & & 0 & -1 & 0 & 1 & 0 & 0 & \cdots & 0 & & 0 & 0 & 1 & 2 & 0 & 0 & \cdots & 0 & & 0 & 0 & \cdots \\
 & & & \cdots & & & 2 & -1 & 0 & 0 & 0 & 0 & \cdots & & & -1 & 0 & 1 & 0 & 0 & 0 & \cdots & & & 0 & 1 & 2 & 0 & 0 & \cdots \\
0 & 0 & 0 & \cdots & & & & & & & & & & & & & & & & & & & & & & & & & & \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & & 2 & -1 & 0 & 0 & 0 & 0 & \cdots & 0 & & -1 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & & 0 & 1 & 2 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & & 0 & 2 & -1 & 0 & 0 & 0 & \cdots & 0 & & 0 & -1 & 0 & 1 & 0 & 0 & \cdots & 0 & & 0 & 0 & 1 \\
 & & \vdots & & & & & & & & & & \vdots & & & & & & & & & & \vdots & & & & & & & &
\end{array}\right]$$

Motivation for Convolutional Neural Networks

- Consider training neural networks on 256 by 256 images.
  - This is 256 by 256 by 3 ≈ 200,000 inputs.
- If first layer has k=10,000, then it has about 2 billion parameters.
  - We want to avoid this huge number (due to storage and overfitting).

- Key idea: make Wx_i act like several convolutions (to make it sparse):
  1. Each row of W only applies to part of x_i.
  2. Use the same parameters between rows.

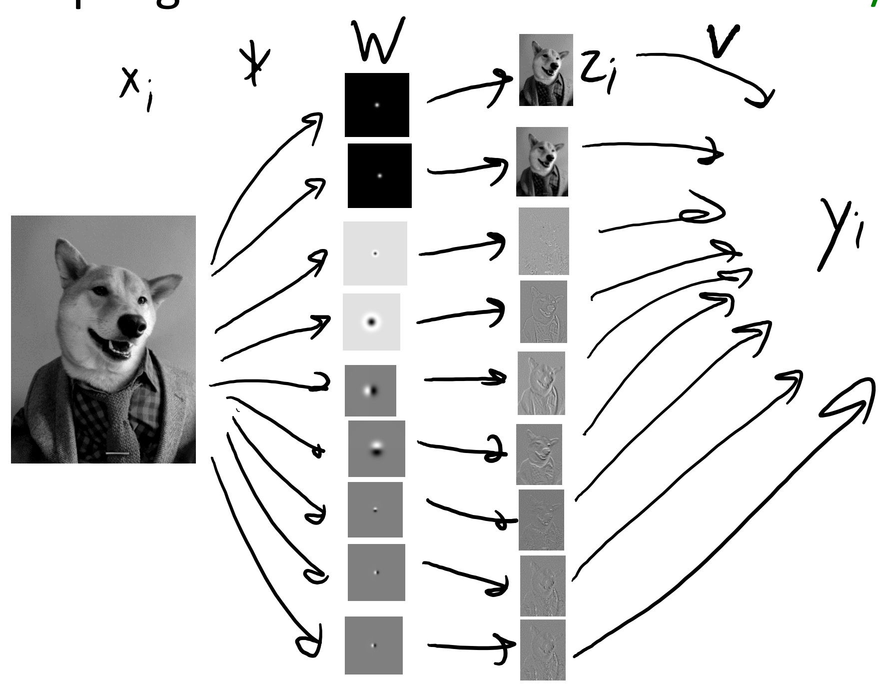
$$w_1 = [0 \quad 0 \quad 0 \ —— \ w \ —— \ 0 \quad 0 \quad 0]$$

$$w_2 = [0 \ —— \ w \ —— \ 0 \quad 0 \quad 0 \quad 0 \quad 0]$$

- Forces most weights to be zero, reduces number of parameters.

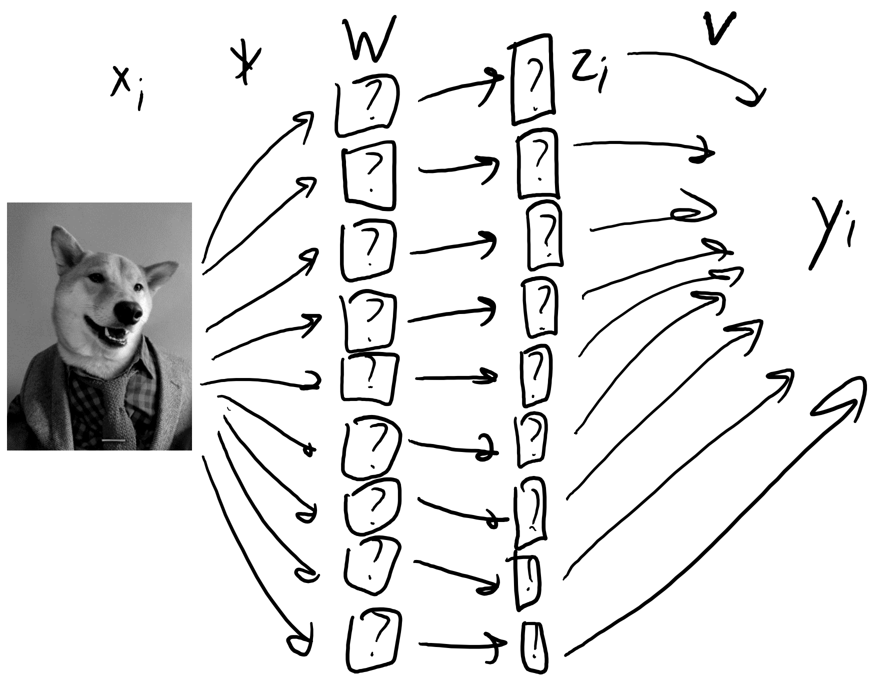
Motivation for Convolutional Neural Networks

- Classic vision methods uses fixed convolutions as features:
  - Usually have different types/variances/orientations.
  - Can do subsampling or take maxes across locations/orientations/scales.



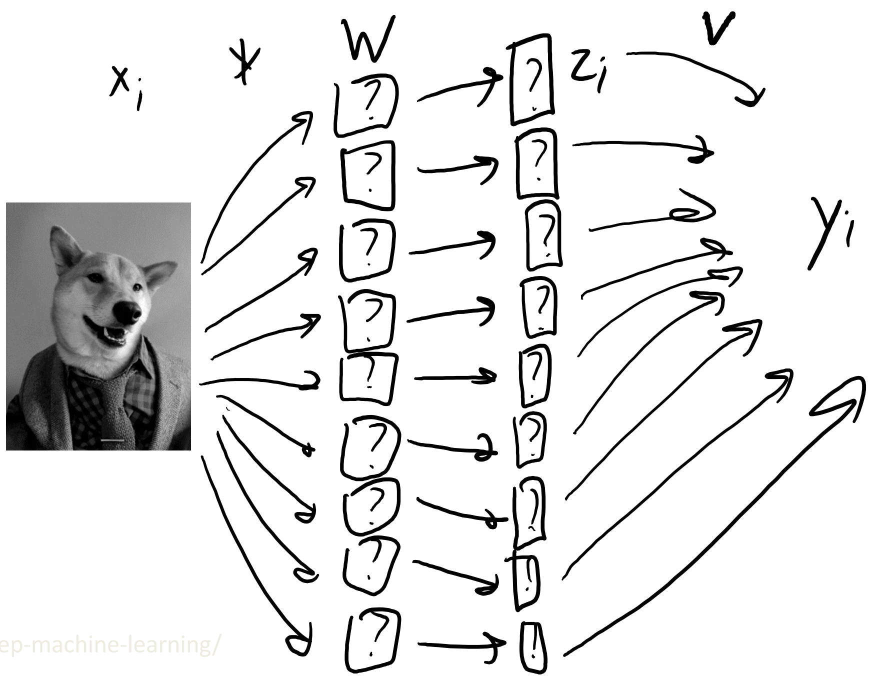
Motivation for Convolutional Neural Networks

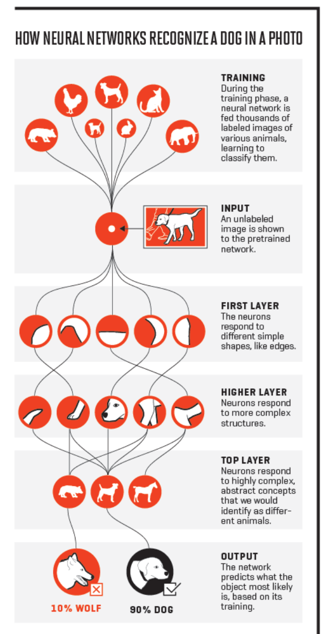
- Convolutional neural networks learn the convolutions:
  - Learning ‘W’ and ‘v’ automatically chooses types/variances/orientations.
  - Don’t pick from fixed convolutions, but learn the elements of the filters.



Motivation for Convolutional Neural Networks

- Convolutional neural networks learn the convolutions:
  - Learning 'W' and 'v' automatically chooses types/variances/orientations.
  - Can do multiple layers of convolution to get deep hierarchical features.





http://fortune.com/ai-artificial-intelligence-deep-machine-learning/

Convolutional Neural Networks

- Convolutional Neural Networks classically have 3 layer “types”:
  - Fully connected layer: usual neural network layer with unrestricted W.

$$W^{(m)} = \begin{bmatrix} \text{---} & w_1^{(m)} & \text{---} \\ \text{---} & w_2^{(m)} & \text{---} \\ & \vdots & \\ \text{---} & w_k^{(m)} & \text{---} \end{bmatrix}$$

Convolutional Neural Networks

- Convolutional Neural Networks classically have 3 layer "types":
  – Fully connected layer: usual neural network layer with unrestricted W.
  – Convolutional layer: restrict W to act like several convolutions.

1D example

distance between centers of convolution is called "stride"

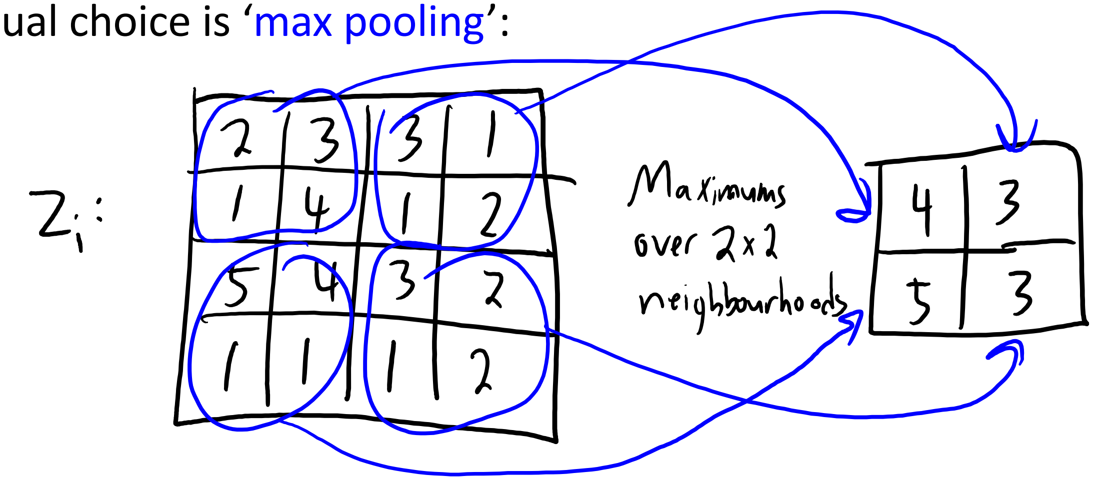
$$W^{(m)} = \begin{bmatrix} \text{———} & w_1^{(m)} & \text{———} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \text{———} & w_1^{(m)} & \text{———} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \text{———} & w_1^{(m)} & \text{———} \\ \text{———} & w_2^{(m)} & \text{———} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \text{———} & w_2^{(m)} & \text{———} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \text{———} & w_2^{(m)} & \text{———} \end{bmatrix}$$

Same $w_1^{(m)}$ used across multiple rows.

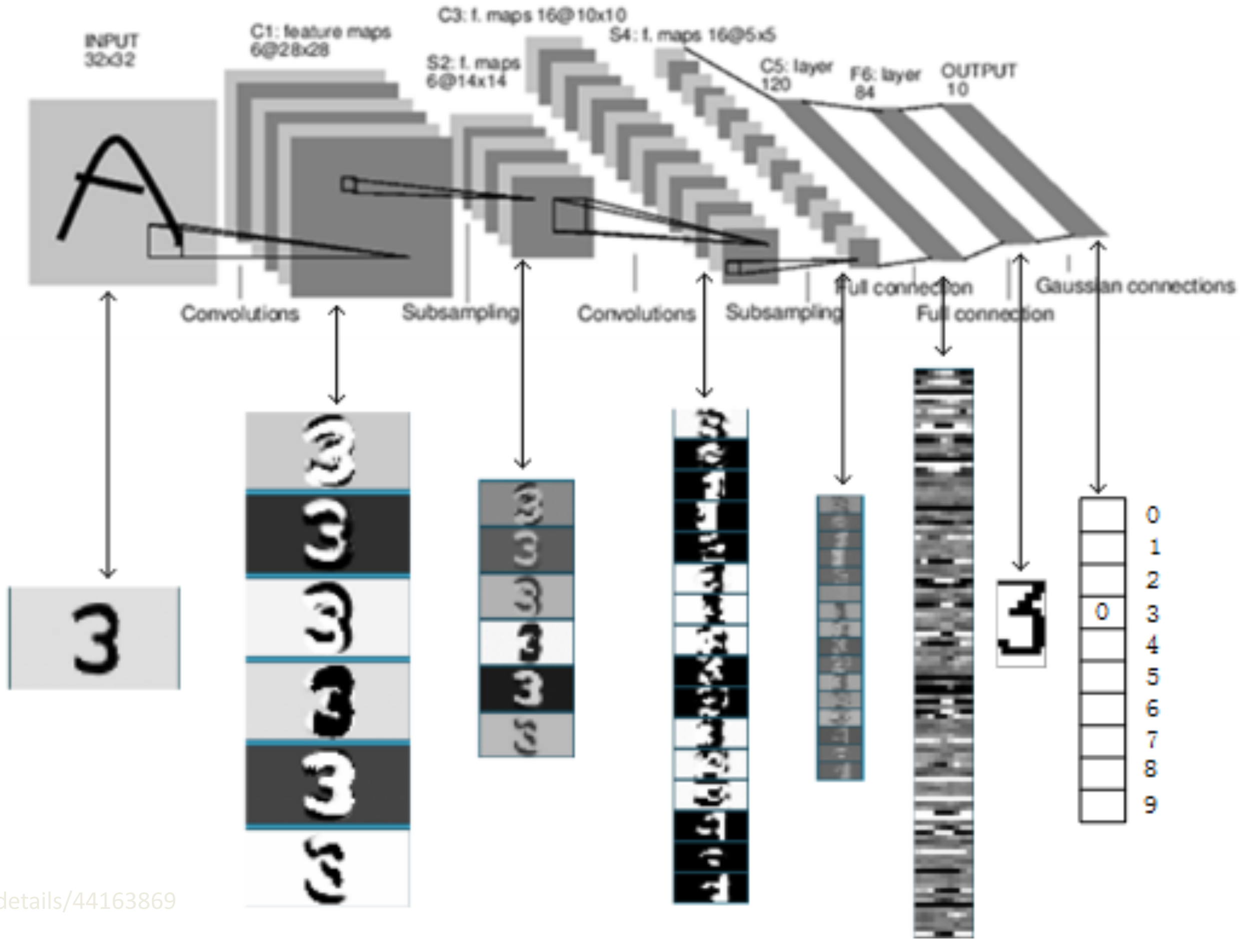
Sparse and small number of parameters

Convolutional Neural Networks

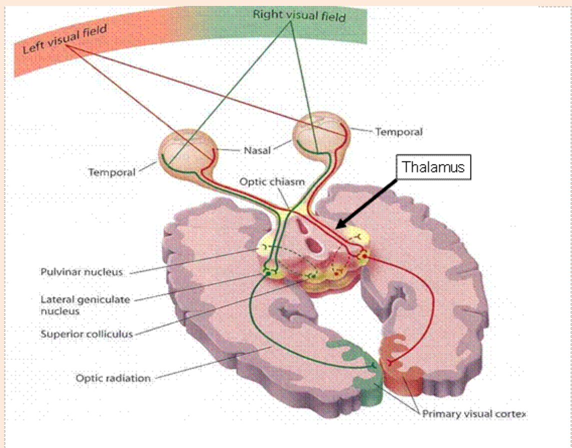
- Convolutional Neural Networks classically have 3 layer "types":
  - Fully connected layer: usual neural network layer with unrestricted W.
  - Convolutional layer: restrict W to act like several convolutions.
  - Pooling layer: combine results of convolutions.
    - Can add some invariance or just make the number of parameters smaller.
    - Usual choice is 'max pooling':

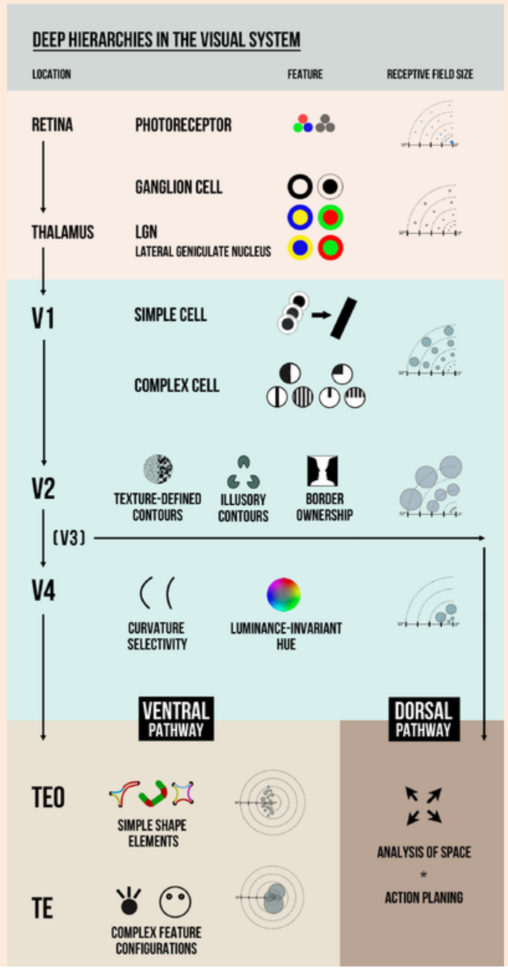


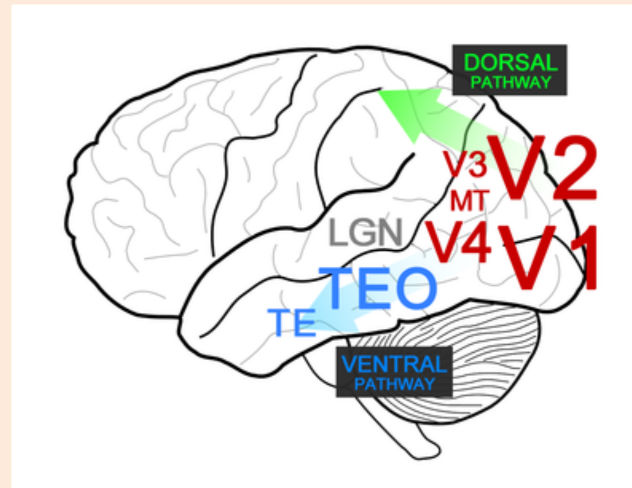
LeNet for Optical Character Recognition



Deep Hierarchies in the Visual System

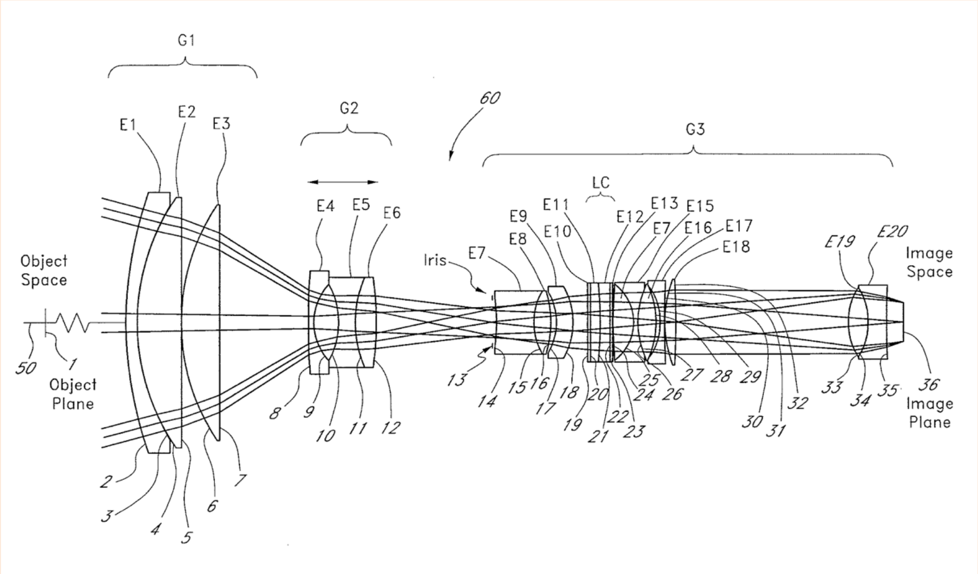


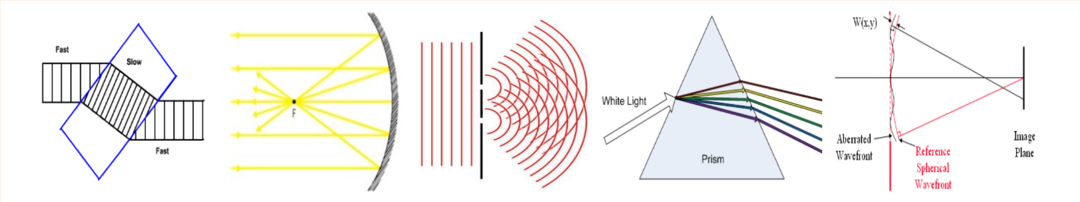




http://www.strokenetwork.org/newsletter/articles/vision.htm
https://en.wikibooks.org/wiki/Sensory_Systems/Visual_Signal_Processing

Deep Hierarchies in Optics

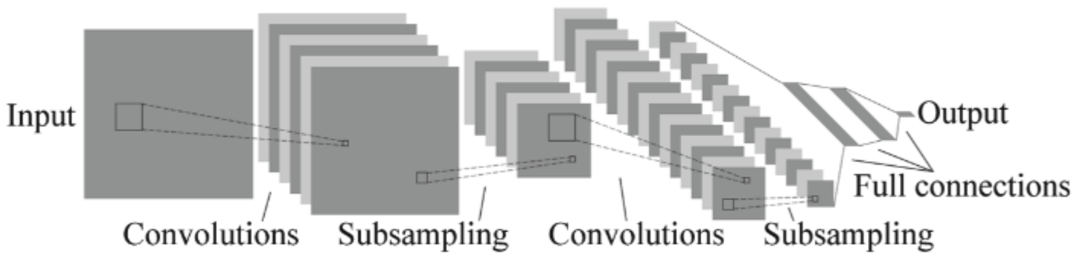




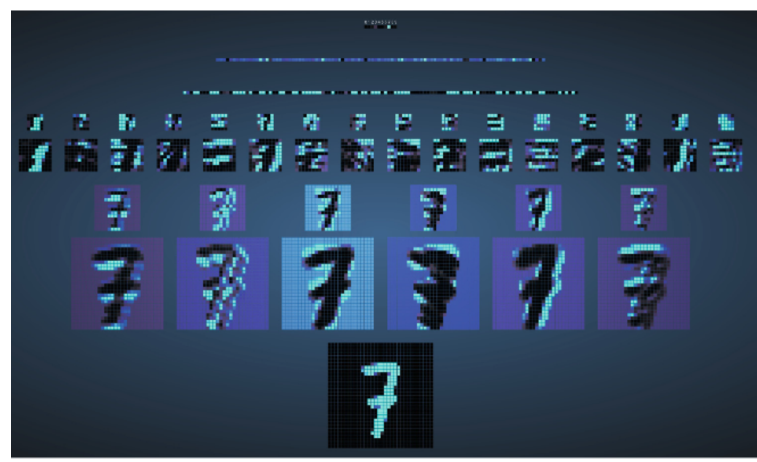
http://www.argmin.net/2018/01/25/optics/

Convolutional Neural Networks

- Classic convolutional neural network (LeNet):



- Visualizing the "activations" of the layers:
  - http://scs.ryerson.ca/~aharley/vis/conv
  - http://cs231n.stanford.edu



softmax
2 "fully-connected"
max pooling
3D convolutions
max pooling
2D convolutions

http://scs.ryerson.ca/~aharley/vis/harley_vis_isvc15.pdf

Summary

- ResNets include untransformed previous layers.
  - Network focuses non-linearity on residual, allows huge number of layers.
- Regularization is crucial to neural net performance:
  - L2-regularization, early stopping, dropout, implicit regularization of SGD.
- Convolutional neural networks:
  - Restrict $W^{(m)}$ matrices to represent sets of convolutions.
  - Often combined with max (pooling).

- Next time: automatic differentiation

(End of testable content for final exam)

CPSC 340: Overview

1. Intro to supervised learning (using counting and distances).
   - Training vs. testing, parametric vs. non-parametric, ensemble methods.
   - Fundamental trade-off, no free lunch, universal consistency.
2. Intro to unsupervised learning (using counting and distances).
   - Clustering, outlier detection, finding similar items.
3. Linear models and gradient descent (for supervised learning)
   - Loss functions, change of basis, regularization, feature selection.
   - Gradient descent and stochastic gradient.
4. Latent-factor models (for unsupervised learning)
   - Typically using linear models and gradient descent.
5. Neural networks (for supervised and multi-layer latent-factor models).

Topics from Previous Years

- Slides for other topics that were covered in previous years:
  – Ranking: finding "highest ranked" training examples (Google PageRank).
  – Semi-supervised: using unlabeled data to help supervised learning.
  – Sequence mining: approximate matching of patterns in large sequences.

- In previous years we did a course review on the last day:
  – Overview of topics covered in 340, and topics coming in 540.
  – Slides here: this could help with studying for the final.

CPSC 330 vs. 340

- CPSC 330 : “Applied Machine Learning”.
  - Not intended as a sequel to 340 (or even a prequel).

- There is some overlap in content, but focus is different:
  - More emphasis on the other steps of the data processing pipeline:
    - Data cleaning, feature extraction, reproducible workflows, communicating results.
  - More emphasis of “how to use packages”, less on “how stuff works”.

- If you found 340 too hard to keep up with, 330 might make sense.
  - In this situation, tell your friends about 330.

CPSC 330 vs. 440

- CPSC 440.
  - Intended as a direct sequel to 340.
  - We're basically starting with CNNs and going from there.
- Main focuses:
  - What if y_i is a sentence or an image or a protein?
  - Giving you the background to understand the latest advances.
- Prerequisites:
  - Expect you to know everything in this course and CPSC 320.
- This course is now listed as CPSC 440.
  - I removed topics related to optimization research from the course.

CPSC 540 Topics

- Review of machine learning fundamentals.
- Differentiable programming and end-to-end learning.
- Density estimation and the exponential family.
- Conditional independence and Bayesian statistics.
- Markov and hidden-Markov models.
- Graphical models and deep structured models.
- Monte Carlo approximation and Markov chain Monte Carlo.
- Non-conjugate and hierarchical Bayesian models.
- Mixture models and expectation maximization.
- Variational inference.
- Empirical Bayes and advanced Monte Carlo methods.
- Non-parametric Bayes and deep generative models.

Other ML-Related Courses

- CPSC 406:
  - Numerical optimization algorithms (like gradient descent).
- CPSC 422:
  - Includes topics like time series and reinforcement learning.
- CPSC 440:
  - Probabilistic machine learning (a follow-on to this course).
- CPSC 532R/533R:
  - Deep learning for vision, sound, and language.
- CPSC 532W:
  - Probabilistic programming.
- CPSC 533V:
  - Deep learning for computer graphics.
- CPSC 540:
  - Graduate-level machine learning (usually with a focus on optimization theory)
- EECE 592:
  - Deep learning and reinforcement learning.
- STAT 406:
  - Similar/complementary topics.
- STAT 460/461:
  - Advanced statistical issues (what happens when 'n' goes to ∞?)

Final Slide

- Good luck with finals/projects and the next steps!