CPSC 540: Machine Learning

Deep Structured Models

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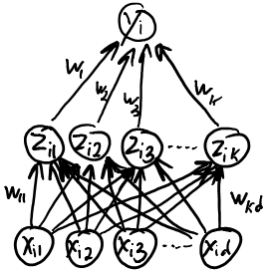
Feedforward Neural Networks

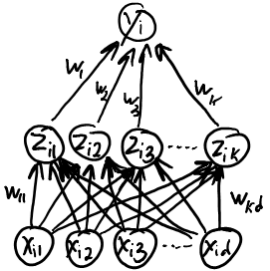
- In 340 we discussed feedforward neural networks for supervised learning.
- With 1 hidden layer the classic model has this structure:



- Motivation:
  - For some problems it's hard to find good features.
  - This learns features z that are good for particular supervised learning problem.

Neural Networks as DAG Models

- It's a DAG model but there is an important difference with our previous models:
  - The latent variables z_c are deterministic functions of the x_j.



- Makes inference given x trivial: if you observe all x_j you also observe all z_c.
  - In this case y is the only random variable.

Neural Network Notation

- We'll continue using our supervised learning notation:

$$X = \begin{bmatrix} \text{---} & (x^1)^T & \text{---} \\ \text{---} & (x^2)^T & \text{---} \\ & \vdots & \\ \text{---} & (x^n)^T & \text{---} \end{bmatrix}, \quad y = \begin{bmatrix} y^1 \\ y^2 \\ \vdots \\ y^n \end{bmatrix},$$

- For the latent features and one hidden layer we'll use

$$Z = \begin{bmatrix} \text{---} & (z^1)^T & \text{---} \\ \text{---} & (z^2)^T & \text{---} \\ & \vdots & \\ \text{---} & (z^n)^T & \text{---} \end{bmatrix}, \quad v = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_k \end{bmatrix}, \quad W = \begin{bmatrix} \text{---} & w_1 & \text{---} \\ \text{---} & w_2 & \text{---} \\ & \vdots & \\ \text{---} & w_k & \text{---} \end{bmatrix},$$

where Z is n by k and W is k by d.

Introducing Non-Linearity

- We discussed how the "linear-linear" model,

$$z^i = Wx^i, \quad \hat{y}^i = v^T z^i,$$

is degenerate since it's still a linear model.

- The classic solution is to introduce a non-linearity,

$$z^i = h(Wx^i), \quad \hat{y}^i = v^T z^i,$$

where a common-choice is applying sigmoid element-wise,

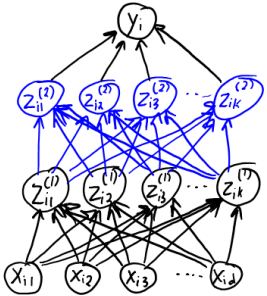
$$z_c^i = \frac{1}{1 + \exp(-w_c^T x^i)},$$

which is said to be the "activation" of neuron c on example i.

  - A universal approximator with k a function of n (also true for $\tanh$, ReLU, etc.)

Deep Neural Networks

- In deep neural networks we add multiple hidden layers,



- Mathematically, with 3 hidden layers the classic model uses

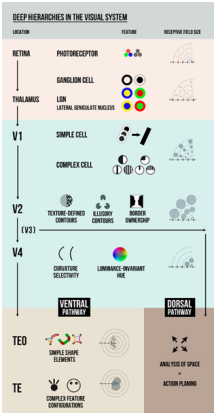
$$\hat{y}^i = v^T\, h(W^3\, h(W^2\, \underbrace{h(W^1 x^i)}_{z^{i1}})) \,.$$

$$\underbrace{\qquad\qquad\qquad\qquad}_{z^{i2}}$$

$$\underbrace{\qquad\qquad\qquad\qquad\qquad\qquad}_{z^{i3}}$$

Biological Motivation

- Deep learning is motivated by theories of deep hierarchies in the brain.



https://en.wikibooks.org/wiki/Sensory_Systems/Visual_Signal_Processing

- But most research is about making models work better, not be more brain-like.

Deep Neural Network History

- Popularity of deep learning has come in waves over the years.
  - Currently, it is one of the hottest topics in science.
- Recent popularity is due to unprecedented performance on some difficult tasks:
  - Speech recognition.
  - Computer vision.
  - Machine translation.
- These are mainly due to big datasets, deep models, and tons of computation.
  - Plus tweaks to classic models and focus on structured networks (CNNs, LSTMs).
- For a NY Times article discussing some of the history/successes/issues, see:

https://mobile.nytimes.com/2016/12/14/magazine/the-great-ai-awakening.html

Training Deep Neural Networks

- If we're training a 3-layer network with squared error, our objective is

$$f(v, W^1, W^2, W^3) = \frac{1}{2}\sum_{i=1}^{n}(\underbrace{v^T h(W^3 h(W^2 h(W^1 x^i)))}_{\hat{y}^i} - y^i)^2.$$

- Usual training procedure is stochastic gradient.
  - But we're discovering sets of tricks to make things easier to tune.
- Highly non-convex and notoriously difficult to tune.
- Recent empirical/theoretical work indicates non-convexity may not be an issue:
  - All local minima may be good for "large enough" networks.

Training Deep Neural Networks

- Some common data/optimization tricks we discussed in 340:
  - Data transformations.
    - For images, translate/rotate/scale/crop each x^i to make more data.
  - Data standardization: centering and whitening.
  - Adding bias variables.
  - Parameter initialization: "small but different", standardizing within layers.
  - Step-size selection: "babysitting", Bottou trick, Adam.
  - Momentum: heavy-ball and Nesterov-style modifications.
  - Batch normalization: adaptive standardizing within layers.
  - ReLU: replacing sigmoid with $\max\{0, w_c^T x^i\}$.
    - Avoids gradients extremely-close to zero.

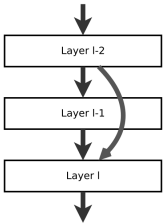
Training Deep Neural Networks

- Common forms tricks to fight overfitting:
  - Standard L2-regularization or L1-regularization "weight decay".
    - Sometimes with different λ for each layer.
    - Recent work shows this introduces bad local optima.
  - Early stopping of the optimization based on validation accuracy.
  - Dropout randomly zeroes z values to discourage dependence.
  - Implicit regularization from using SGD.
  - Hyper-parameter optimization to choose various tuning parameters.
  - Special architectures like convolutional neural networks:
    - Yields W^m that are very sparse and have many tied parameters.

"Residual" Networks (ResNets)

- Suppose we fit a deep neural network to a linearly-separable dataset.
  - Original features x are sufficient to perfectly classify training data.
  - For a deep neural network to work, each layer needs to preserve information in x.
    - You might be "wasting" parameters just re-representing data from previous layers.

- Consider residual networks:



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

- Take a previous (non-transformed) layer as input to current layer.
  - Also called "skip connections" or "highway networks".

"Residual" Networks (ResNets)

- ResNets seemingly make learning easier:
  - You can "default" to just copying the previous layer.
  - The non-linear transform is only learning how to modify the input.
    - "Fitting the residual".
- This was a key idea behind first methods that used 100+ layers.
  - Easy for information about x to reach y through huge number of layers.
  - Won all tasks in ImageNet 2015 competition.
  - Evidence that biological networks have skip connections like this.
- Dense networks (DenseNets): connect to many previous layers.
  - Basically gets rid of vanishing gradient issue.

DenseNets

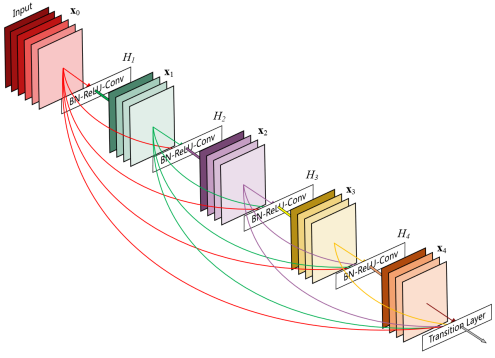


Figure 1: A 5-layer dense block with a growth rate of $k = 4$. Each layer takes all preceding feature-maps as input.

https://arxiv.org/pdf/1608.06993.pdf

Backpropagation as Message-Passing

- Computing the gradient in neural networks is called backpropagation.
  - Derived from the chain rule and memoization of repeated quantities.
- We're going to view backpropagation as a message-passing algorithm.
- Key advantages of this view:
  - It's easy to handle different graph structures.
  - It's easy to handle different non-linear transformations.
  - It's easy to handle multiple outputs (as in structured prediction).
  - It's easy to add non-deterministic parts and combine with other graphical models.

Outline

Backpropagation Forward Pass

- Consider computing the output of a neural network for an example i,

$$\begin{aligned} y^i &= v^T h(W^3 h(W^2 h(W^1 x^i))) \\ &= \sum_{c=1}^{k} v_c h\left(\sum_{c'=1}^{k} W^3_{c'c} h\left(\sum_{c''=1}^{k} W^2_{c''c'} h\left(\sum_{j=1}^{d} W^1_{c''j} x^i_j\right)\right)\right). \end{aligned}$$

  where we've assume that all hidden layers have k values.
  - In the second line, the h functions are single-input single-output.

- The nested sum structure is similar to our message-passing structures.

- However, it's easier because it's deterministic: no random variables to sum over.
  - The messages will be scalars rather than functions.

Backpropagation Forward Pass

- Forward propagation through neural network as message passing:

$$
\begin{aligned}
y^i &= \sum_{c=1}^{k} v_c h\left(\sum_{c'=1}^{k} W^3_{c'c} h\left(\sum_{c''=1}^{k} W^2_{c''c'} h\left(\sum_{j=1}^{d} W^1_{c''j} x^i_j\right)\right)\right) \\
&= \sum_{c=1}^{k} v_c h\left(\sum_{c'=1}^{k} W^3_{c'c} h\left(\sum_{c''=1}^{k} W^2_{c''c'} h(M_{c''})\right)\right) \\
&= \sum_{c=1}^{k} v_c h\left(\sum_{c'=1}^{k} W^3_{c'c} h(M_{c'})\right) \\
&= \sum_{c=1}^{k} v_c h(M_c) \\
&= M_y,
\end{aligned}
$$

where intermediate messages are the z values.

Backpropagation Backward Pass

- The backpropagation backward pass computes the partial derivatives.
  - For a loss f, the partial derivatives in the last layer have the form

$$\frac{\partial f}{\partial v_c} = z_c^{i3} f'(v^T h(W^3 h(W^2 h(W^1 x^i)))),$$

where

$$z_{c'}^{i3} = h\left(\sum_{c'=1}^{k} W_{c'c}^3 h\left(\sum_{c''=1}^{k} W_{c''c'}^2 h\left(\sum_{j=1}^{d} W_{c''j}^1 x_j^i\right)\right)\right).$$

  - Written in terms of messages it simplifies to

$$\frac{\partial f}{\partial v_c} = h(M_c) f'(M_y).$$

Backpropagation Backward Pass

- In terms of forward messages, the partial derivatives have the forms:

$$\frac{\partial f}{\partial v_c} = h(M_c) f'(M_y),$$

$$\frac{\partial f}{\partial W^3_{c'c}} = h(M_{c'}) h'(M_c) w_c f'(M_y),$$

$$\frac{\partial f}{\partial W^2_{c''c'}} = h(M_{c''}) h'(M_{c'}) \sum_{c=1}^{k} W^3_{c'c} h'(M_c) w_c f'(M_y),$$

$$\frac{\partial f}{\partial W^1_{jc''}} = h(M_j) h'(M_{c''}) \sum_{c'=1}^{k} W^2_{c''c'} h'(M_{c'}) \sum_{c=1}^{k} W^3_{c'c} h'(M_c) w_c f'(M_y),$$

which are ugly but notice all the repeated calculations.

Backpropagation Backward Pass

- It's again simpler using appropriate messages

$$\frac{\partial f}{\partial v_c} = h(M_c) f'(M_y),$$

$$\frac{\partial f}{\partial W^3_{c'c}} = h(M_{c'}) h'(M_c) w_c V_y,$$

$$\frac{\partial f}{\partial W^2_{c''c'}} = h(M_{c''}) h'(M_{c'}) \sum_{c=1}^{k} W^3_{c'c} V_c,$$

$$\frac{\partial f}{\partial W^1_{jc''}} = h(M_j) h'(M_{c''}) \sum_{c'=1}^{k} W^2_{c''c'} V_{c'},$$

where $M_j = x_j$.

Backpropagation as Message-Passing

- The general forward message for child c with parents p and weights W is

$$M_c = \sum_p W_{cp} h(M_p),$$

  which computes weighted combination of non-linearly transformed parents.
  - In the first layer we don't apply h to x.
- The general backward message from child c to *all* its parents is

$$V_c = h'(M_c) \sum_{c'} W_{cc'} V_{c'},$$

  which weights the "grandchildren's gradients".
  - In the last layer we use f instead of h.
- The gradient of W_{cp} is $h(M_c)V_p$, which works for general graphs.

Automatic Differentiation

- Automatic differentiation:
  - Input is a function.
  - Output is one or more derivatives of the function.
- Forward-mode automatic differentiation:
  - Computes a directional derivative for cost of evaluating function.
    - So computing gradient would be d-times more expensive than function.
  - Low memory requirements.
  - Most useful for evaluating Hessian-vector products, $\nabla^2 f(w)d$.
- Reverse-mode automatic differentiation:
  - Computes gradient for cost of evaluating function.
  - But high memory requirements: need to store intermediate calculations.
    - Backpropagation is (essentially) a special case.
- Reverse-mode is replacing "gradient by hand" (less time-consuming/bug-prone).

Combining Neural Networks and CRFs

- Last time we saw conditional random fields like

$$p(y \mid x) \propto \exp\left(\sum_{c=1}^{k} y_c v^T x_c + \sum_{(c,c') \in E} y_c y_{c'} w\right),$$

which can use logistic regression at each location c and Ising dependence on y_c.

- Instead of logistic regression, you could put a neural network in there:

$$p(y \mid x) \propto \exp\left(\sum_{c=1}^{k} y_c v^T h(W^3 h(W^2(W^1 x_c))) + \sum_{(c,c') \in E} y_c y_{c'} w\right).$$

- Sometimes called a conditional neural field or deep structured model.
- Backprop generalizes:
  1. Forward pass through neural network to get $\hat{y}_c$ predictions.
  2. Belief propagation to get marginals of y_c (or Gibbs sampling if high treewidth).
  3. Backwards pass through neural network to get all gradients.

Automatic Differentiation (AD) vs. Inference

- If you use exact inference methods, automatic differentiation will give gradient.
  - You write message-passing code to compute Z.
  - AD modifies your code to compute expectations in gradient.
- With approximate inference, AD may or may not work:
  - AD will work for iterative variational inference methods (which we'll cover late).
  - AD will not tend to work for Monte Carlo methods.
    - Can't AD through sampling (but there exist tricks like "common random numbers").
- Recent trend: run iterative variational method for a fixed number of iterations.
  - AD can give gradient of result after this fixed number of iterations.
  - "Train the inference you will use at test time".

Motivation: Gesture Recognition

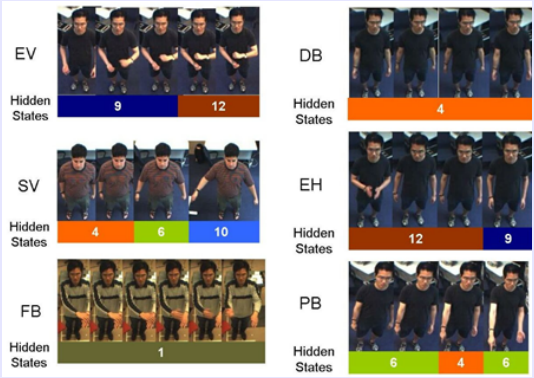
- Want to recognize gestures from video:

http://groups.csail.mit.edu/vision/vip/papers/wang06cvpr.pdf

- A gesture is composed of a sequence of parts:
  - And some parts appear in different gestures.

Motivation: Gesture Recognition

- We may not know the set of "parts" that make up gestures.

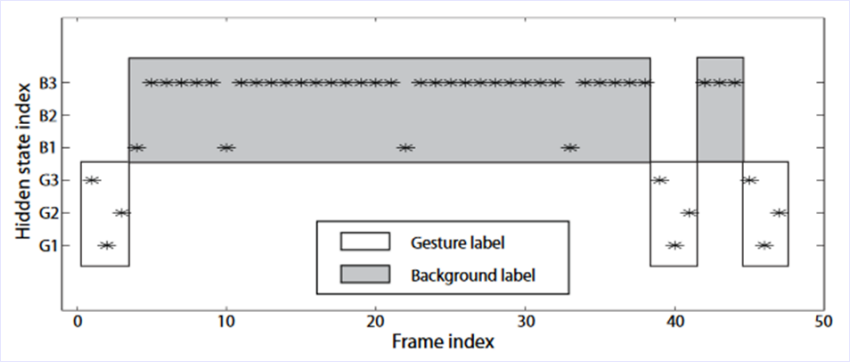


http://groups.csail.mit.edu/vision/vip/papers/wang06cvpr.pdf

- We can consider learn the "parts" and their latent dynamics (transitions).

Motivation: Gesture Recognition

- We're given a labeled video sequence, but don't observe "parts":

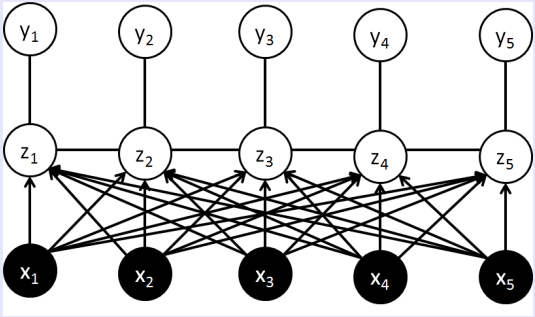


http://www.lsi.upc.edu/~aquattoni/AllMyPapers/cvpr_07_L.pdf

- Our videos are labeled with "gesture" and "background" frames,
  - But we don't know the parts (G1, G2, G3, B1, B2, B3) that define the labels.

Latent-Dynamic Conditional Random Field

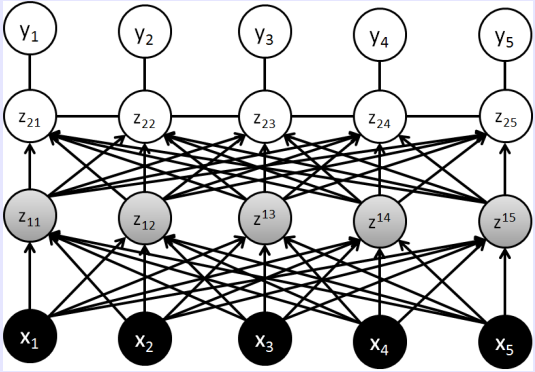
- Here we could use a latent-dynamic conditional random field



- Observed variable x_j is the image at time j (in this case x_j is a video frame).
- The gesture y is defined by sequence of parts z_j.
  - We're learning what the parts should be.
  - We're learning "latent dynamics": how the hidden parts change over time.
- Notice in the above case that the conditional UGM is a tree.

Neural Networks with Latent-Dynamics

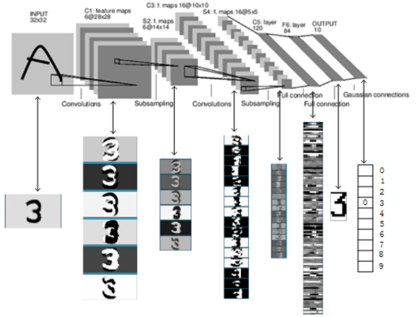
- Neural networks with latent dynamics:



- Combines deep learning, mixture models, and graphical models.
  - Achieved among state of the art in several applications.

Convolutional Neural Networks

- In 340 we discussed convolutional neural networks (CNNs):

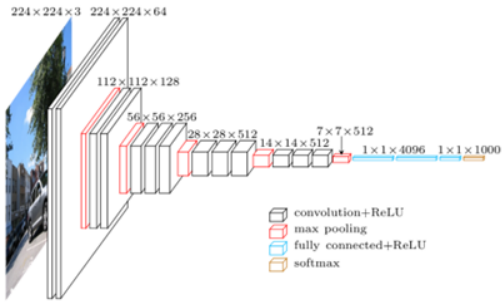


http://blog.csdn.net/strint/article/details/44163869

- Convolutional layers where W acts like a convolution (sparse with tied parameters).
- Pooling layers that usually take maximum among a small spatial neighbourhood.
- Fully-connected layers that use an unrestricted W.

Motivation: Beyond Classification

- Convolutional structure simplifies the learning task:
  - Parameter tieing means we have more data to estimate each parameter.
  - Sparsity drastically reduces number of parameters.

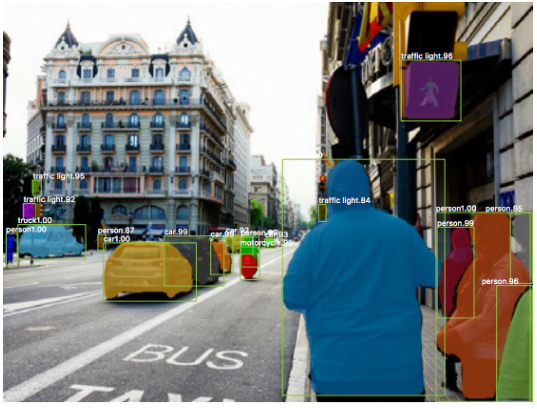


https://www.cs.toronto.edu/~frossard/post/vgg16

- We discussed CNNs for image classification: "is this an image of a cat?".
  - But many vision tasks are not image classification tasks.

Object Localization

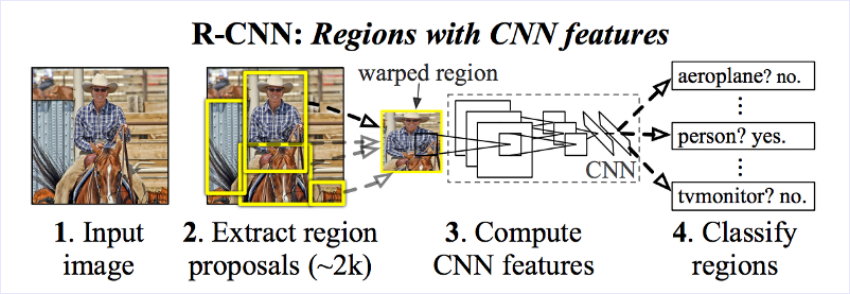
- Object localization is task of finding locations of objects:
  - Need to find *where* in the image the object is.
  - May need to recognize *more than one* object.



https://blog.athelas.com/a-brief-history-of-cnns-in-image-segmentation-from-r-cnn-to-mask-r-cnn-34ea83205de4

Region Convolutional Neural Networks: "Pipeline" Approach

- Early approach (region CNN):
  1. Propose a bunch of potential boxes.
  2. Compute features of box using a CNN.
  3. Classify each box based on an SVM.
  4. Refine each box using linear regression.



https://blog.athelas.com/a-brief-history-of-cnns-in-image-segmentation-from-r-cnn-to-mask-r-cnn-34ea83205de4

- Improved on state of the art, but not very elegant with its 4 steps.

Summary

- Neural networks learn features for supervised learning.
  - For structured prediction, may reduce the need to rely on inference.
- Backpropagation can be viewed as a message passing algorithm.
- Combining CRFs with deep learning.
  - You can learn the features and the label dependency at the same time.
- Next time: "end-to-end" learning