[70240413 Statistical Machine Learning, Spring, 2015]

Deep Learning

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Why going deep?

Data are often high-dimensional.

- There is a huge amount of structure in the data, but the structure is too complicated to be represented by a simple model.
- Insufficient depth can require more computational elements than architectures whose depth matches the task.
- Deep nets provide simpler but more descriptive models of many problems.



Microsoft's speech recognition system

http://v.youku.com/v_show/id_XNDc0MDY4ODI0.html





Human-Level Control via Deep RL

Deep Q-network with human-level performance on A



Minjie will talk more in next lecture

[Mnih et al., Nature 518, 529–533, 2015]



MIT 10 Breakthrough Tech 2013



Introduction The 10 Technologies Past Years

Deep Learning

With massive amounts of computational power, machines can now recognize objects and translate speech in real time. Artificial intelligence is finally getting smart.

6



http://www.technologyreview.com/featuredstory/513696/deep-learning/



Deep Learning in industry



Driverless car



Face identification



Speech recognition



Web search





Deep Learning Models



How brains seem to do computing?



The business end of this is made of lots of these joined in networks like this

Much of our own "computations" are performed in/by this network

Learning occurs by changing the effectiveness of the synapses so that the influence of one neuron on another changes



History of neural networks





History of neural networks



Smolensky



Hinton





Harmoniums (Restricted Boltzmann Machine)



Contrastive Divergence



Deep Belief Networks



Model of a neuron





Activation function

Threshold function & piecewise linear function:





Activation function with negative values

Threshold function & piecewise linear function:

$$\operatorname{sgn}(x) = \begin{cases} 1 & \text{if } x \ge 0\\ -1 & \text{if } x < 0 \end{cases}$$

Hyperbolic tangent function





McCulloch & Pitts's Artificial Neuron

The first model of artificial neurons in 1943

Activation function: a threshold function





Network Architecture

Feedforward networks



Recurrent networks







Learning Paradigms

Unsupervised learning (learning without a teacher)
Example: clustering





Learning Paradigms

Supervised Learning (learning with a teacher)
For example, classification: learns a separation plane





Learning Rules

- Error-correction learning
- Competitive learning
- Hebbian learning
- Soltzmann learning
- Memory-base learning
 - Nearest neighbor, radial-basis function network



Error-correction learning

The generic paradigm:



• Error signal:

$$e_j = y_j - d_j$$

• Learning objective:

$$\min_{\mathbf{w}} R(\mathbf{w}; \mathbf{x}) := \frac{1}{2} \sum_{j} e_{j}^{2}$$



Example: Perceptron

One-layer feedforward network based on error-correction learning (no hidden layer):



• Current output (at iteration t):

$$d_j = (\mathbf{w}_t^j)^\top \mathbf{x}$$

Update rule (exercise?):

$$\mathbf{w}_{t+1}^j = \mathbf{w}_t^j + \eta (y_j - d_j) \mathbf{x}$$



Perceptron for classification

Consider a single output neuron

Sinary labels:

$$y\in\{+1,-1\}$$

Output function:

$$d = \operatorname{sgn}\left(\mathbf{w}_t^{\top}\mathbf{x}\right)$$

Apply the error-correction learning rule, we get ... (next slide)



Perceptron for Classification

- Set w₁ = 0 and t=1; scale all examples to have length 1 (doesn't affect which side of the plane they are on)
- Given example x, predict positive iff

 $\mathbf{w}_t^\top \mathbf{x} > 0$

♦ If a mistake, update as follows
■ Mistake on positive: w_{t+1} ← w_t + η_tx
■ Mistake on negative: w_{t+1} ← w_t - η_tx
t ← t + 1





Convergence Theorem

For linearly separable case, the perceptron algorithm will converge in a finite number of steps



Mistake Bound

Theorem:

- Let S be a sequence of labeled examples consistent with a linear threshold function $\mathbf{w}_*^\top \mathbf{x} > 0$, where \mathbf{w}_* is a unit-length vector.
- The number of mistakes made by the online Perceptron algorithm is at most $(1/\gamma)^2$, where

$$\gamma = \min_{\mathbf{x} \in \mathcal{S}} \frac{|\mathbf{w}_*^\top \mathbf{x}|}{\|\mathbf{x}\|}$$

- i.e.: if we scale examples to have length 1, then γ is the minimum distance of any example to the plane $\mathbf{w}_*^\top \mathbf{x} = 0$
- γ is often called the "margin" of \mathbf{W}_* ; the quantity $\frac{\mathbf{W}_*^\top \mathbf{X}}{\|\mathbf{X}\|}$ is the cosine of the angle between \mathbf{X} and \mathbf{W}_*



Deep Nets

- Multi-layer Perceptron
- CNN
- Auto-encoder
- RBM
- Deep belief nets
- Deep recurrent nets



XOR Problem



Single-layer perceptron can't solve the problem



XOR Problem

♦ A network with 1-layer of 2 neurons works for XOR:

threshold activation function



• Many alternative networks exist (not layered)





Multilayer Perceptrons

- Computational limitations of single-layer Perceptron by Minsky & Papert (1969)
- Multilayer Perceptrons:
 - Multilayer feedforward networks with an error-correction learning algorithm, known as error *back-propagation*

• A generalization of single-layer percetron to allow nonlinearity



Backpropagation

Learning as loss minimization

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \frac{1}{2} \sum_j e_j^2(\mathbf{x})$$
$$e_j = y_j - d_j$$



Learning with gradient descent

 $\mathbf{w}_{t+1} = \mathbf{w}_t - \lambda_t \nabla R(\mathbf{w}; \mathcal{D})$



Backpropagation

- Step function in perceptrons is non-differentiable
- Differentiable activation functions are needed to calculate gradients, e.g., sigmoid:

$$\psi_{\alpha}(v) = \frac{1}{1 + \exp(-\alpha v)}$$





Backpropagation

 \blacklozenge Derivative of a sigmoid function ($\alpha=1$)

$$\nabla_v \psi(v) = \frac{e^{-v}}{(1+e^{-v})^2} = \psi(v)(1-\psi(v))$$

- Notice about the small scale of the gradient
- Gradient vanishing issue
- Many other activation functions examined



Gradient computation at output layer

Output neurons are separate:





 ∂R

 ∂v_i

Gradient computation at output layer

Signal flow:



 $\nabla_{w_{ji}}R = \frac{\partial R_j}{\partial e_j}\frac{\partial e_j}{\partial d_j}\frac{\partial d_j}{\partial v_j}\frac{\partial v_j}{\partial w_{ji}}$

 $= -e_j \psi'(v_j) f_i(\mathbf{x})$

 $= e_j \cdot (-1) \cdot \psi'(v_j) \cdot f_i(\mathbf{x})$

Local gradient: $\delta_j =$

$$R_j = \frac{1}{2}e_j^2$$

$$R = \frac{1}{2} \sum_{j} e_j^2$$



Gradient computation at hidden layer

Output neurons are NOT separate:









Back-propagation formula

The update rule of local gradients:
for hidden neuron *i*:

$$\delta_i = \psi'(v_i) \sum_j \delta_j w_{ji}$$

Only depends on the activation function at hidden neuron i

Flow of error signal:




Back-propagation formula

The update rule of weights:

• Output neuron:

$$\Delta w_{ji} = \lambda \cdot \delta_j \cdot f_i(\mathbf{x})$$

• Hidden neuron:

$$\Delta w_{ik}' = \lambda \cdot \delta_i \cdot g_k(\mathbf{x})$$

$$\begin{pmatrix} Weight \\ correction \\ \Delta w_{ji} \end{pmatrix} = \begin{pmatrix} learning \\ rate \\ \lambda \end{pmatrix} \cdot \begin{pmatrix} local \\ gradient \\ \delta_j \end{pmatrix} \cdot \begin{pmatrix} input \ signal \\ of \ neuron \ j \\ v_i \end{pmatrix}$$



Two Passes of Computation

Forward pass

- Weights fixed
- Start at the first hidden layer
- Compute the output of each neuron
- End at output layer

Backward pass

- Start at the output layer
- Pass error signal backward through the network
- Compute local gradients



Stopping Criterion

No general rules

Some reasonable heuristics:

• The norm of gradient is small enough

- The number of iterations is larger than a threshold
- The training error is stable
- ••••



Improve Backpropagation

Many methods exist to improve backpropagation
E.g., backpropagation with momentum

$$\Delta w_{ij}^t = -\lambda \frac{\partial R}{\partial w_{ij}} + \alpha \Delta w_{ij}^{t-1}$$





Neurons as Feature Extractor

- Compute the similarity of a pattern to the ideal pattern of a neuron
- Threshold is the minimal similarity required for a pattern
- Reversely, it visualizes the connections of a neuron





weights

1	1	1	1	1
-1	-1	1	-1	-1
-1	-1	1	-1	-1
-1	-1	1	-1	-1
-1	-1	1	-1	-1



Vanishing gradient problem

The gradient can decrease exponentially during back-prop

Solutions:

- Pre-training + fine tuning
- Rectifier neurons (sparse gradients)

Ref:

 Gradient flow in recurrent nets: the difficulty of learning longterm dependencies. Hochreiter, Bengio, & Frasconi, 2001



Deep Rectifier Nets

Sparse representations without gradient vanishing



- Non-linearity comes from the path selection
 - Only a subset of neurons are active for a given input
- Can been seen as a model with an exponential number of linear models that share weights

[Deep sparse rectifier neural networks. Glorot, Bordes, & Bengio, 2011]



CNN

- Hubel and Wiesel's study on annimal's visual cortex:
 - Cells that are sensitive to small sub-regions of the visual field, called a *receptive field*
 - Simple cells respond maximally to specific edge-like patterns within their receptive field. Complex cells have larger receptive fields and are locally invariant to the exact position of the pattern.



Convolutional Neural Networks

Sparse local connections (spatially contiguous receptive fields)



Shared weights: each filter is replicated across the entire visual field, forming a feature map





CNN

Each layer has multiple feature maps







• *Max-pooling*, a form of non-linear down-sampling.

 Max-pooling partitions the input image into a set of non-overlapping rectangles and, for each such sub-region, outputs the maximum value.



Example: CNN for image classification



- Network dimension: 150,528(input)-253,440–186,624–64,896– 64,896–43,264–4096–4096–1000(output)
 - In total: 60 million parameters

IM GENET

- Task: classify 1.2 million high-resolution images in the ImageNet LSVRC-2010 contest into the 1000 different classes
- Results: state-of-the-art accuracy on ImageNet

14,197,122 images, 21841 synsets indexed

Explore Download ChallengeNew People Publication About



Issues with CNN

- Computing the activations of a single convolutional filter is much more expensive than with traditional MLPs
- Many tuning parameters
 - # of filters:
 - Model complexity issue (overfitting vs underfitting)
 - Filter shape:
 - the right level of "granularity" in order to create abstractions at the proper scale, given a particular dataset
 - Usually 5x5 for MNIST at 1st layer
 - Max-pooling shape:
 - typical: 2x2; maybe 4x4 for large images



Auto-Encoder

Encoder: (a distributed code)

$$\mathbf{y} = s(\mathbf{W}\mathbf{x} + \mathbf{b})$$

Decoder:

$$\mathbf{z} = s(\mathbf{W}'\mathbf{y} + \mathbf{b}')$$

Minimize reconstruction error

Connection to PCA

- PCA is linear projection, which Auto-Encoder is nonlinear
- Stacking PCA with nonlinear processing may perform as well (MaYi's work)
- Denoising Auto-Encoder
 - A stochastic version with corrupted noise to discover more robust features
 - E.g., randomly set some inputs to zero



Left: no noise; right: 30 percent noise



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Deep Generative Models



Stochastic Binary Units

- Each unit has a state of 0 or 1
- The probability of turning on is determined by





Generative Models

 Directed acyclic graph with stochastic binary units is termed Sigmoid Belief Net (Radford Neal, 1992)

 Undirected graph with stochastic binary units is termed Boltzmann Machine (Hinton & Sejnowski, 1983)







Learning Deep Belief Nets

- Easy to generate an unbiased example at the leaf nodes
- Hard to infer the posterior distribution over all possible configurations of hidden causes – explain away effect!
 Hard to even get a sample from the posterior





Learning Boltzmann Machine

- Hard to generate an unbiased example for the visible units
- Hard to infer the posterior distribution over all possible configurations of hidden causes
 - Hard to even get a sample from the posterior





Restricted Boltzmann Machines

An energy-based model with hidden units

$$P(x) = \sum_{h} P(x,h) = \sum_{h} \frac{e^{-E(x,h)}}{Z}$$

Graphical structure:

$$E(v,h) = -b'v - c'h - h'Wv$$



hidden

visible

Restrict the connectivity to make learning easier.



Restricted Boltzmann Machines

Factorized conditional distribution over hidden units

$$p(\boldsymbol{h} \mid \boldsymbol{v}) = \frac{1}{p(\boldsymbol{v})} \frac{1}{Z} \exp\left\{\boldsymbol{b}^{\top} \boldsymbol{v} + \boldsymbol{c}^{\top} \boldsymbol{h} + \boldsymbol{v}^{\top} \boldsymbol{W} \boldsymbol{h}\right\}$$
$$= \frac{1}{Z'} \exp\left\{\boldsymbol{c}^{\top} \boldsymbol{h} + \boldsymbol{v}^{\top} \boldsymbol{W} \boldsymbol{h}\right\}$$
$$= \frac{1}{Z'} \exp\left\{\sum_{j=1}^{n} c_{j} h_{j} + \sum_{j=1}^{n} \boldsymbol{v}^{\top} \boldsymbol{W}_{:,j} \boldsymbol{h}_{j}\right\}$$
$$= \frac{1}{Z'} \prod_{j=1}^{n} \exp\left\{c_{j} h_{j} + \boldsymbol{v}^{\top} \boldsymbol{W}_{:,j} \boldsymbol{h}_{j}\right\}$$



Restricted Boltzmann Machines

- For Gibbs sampling
 - Hidden units:

$$\begin{split} P(h_j = 1 \mid \boldsymbol{v}) &= \frac{\tilde{P}(h_j = 1 \mid \boldsymbol{v})}{\tilde{P}(h_j = 0 \mid \boldsymbol{v}) + \tilde{P}(h_j = 1 \mid \boldsymbol{v})} \\ &= \frac{\exp\left\{c_j + \boldsymbol{v}^\top \boldsymbol{W}_{:,j}\right\}}{\exp\left\{0\right\} + \exp\left\{c_j + \boldsymbol{v}^\top \boldsymbol{W}_{:,j}\right\}} \\ &= \operatorname{sigmoid}\left(c_j + \boldsymbol{v}^\top \boldsymbol{W}_{:,j}\right). \end{split}$$

• Observed units:

$$P(\boldsymbol{v} \mid \boldsymbol{h}) = \prod_{i=1}^{d} \text{sigmoid} (b_i + \boldsymbol{W}_{i,:} \boldsymbol{h})$$



MLE

Log-likelihood $\ell(\boldsymbol{W}, \boldsymbol{b}, \boldsymbol{c}) = \sum_{t=1}^{n} \log P(\boldsymbol{v}^{(t)})$ $= \sum_{t=1}^{n} \log \sum_{\boldsymbol{h}} \exp\left\{-E(\boldsymbol{v}^{(t)}, \boldsymbol{h})\right\} - n \log Z$

Gradient

$$\frac{\partial}{\partial \theta} \ell(\theta) = \frac{\partial}{\partial \theta} \sum_{t=1}^{n} \log \sum_{h} \exp\left\{-E(\boldsymbol{v}^{(t)}, \boldsymbol{h})\right\} - n\frac{\partial}{\partial \theta} \log \sum_{\boldsymbol{v}, \boldsymbol{h}} \exp\left\{-E(\boldsymbol{v}, \boldsymbol{h})\right\}$$
$$= \sum_{t=1}^{n} \frac{\sum_{h} \exp\left\{-E(\boldsymbol{v}^{(t)}, \boldsymbol{h})\right\} \frac{\partial}{\partial \theta} - E(\boldsymbol{v}^{(t)}, \boldsymbol{h})}{\sum_{h} \exp\left\{-E(\boldsymbol{v}^{(t)}, \boldsymbol{h})\right\}}$$
$$- n\frac{\sum_{\boldsymbol{v}, \boldsymbol{h}} \exp\left\{-E(\boldsymbol{v}, \boldsymbol{h})\right\} \frac{\partial}{\partial \theta} - E(\boldsymbol{v}, \boldsymbol{h})}{\sum_{\boldsymbol{v}, \boldsymbol{h}} \exp\left\{-E(\boldsymbol{v}, \boldsymbol{h})\right\}}$$
$$= \sum_{t=1}^{n} \mathbb{E}_{P(\boldsymbol{h} \mid \boldsymbol{v}^{(t)})} \left[\frac{\partial}{\partial \theta} - E(\boldsymbol{v}^{(t)}, \boldsymbol{h})\right] - n\mathbb{E}_{P(\boldsymbol{v}, \boldsymbol{h})} \left[\frac{\partial}{\partial \theta} - E(\boldsymbol{v}, \boldsymbol{h})\right]$$



Contrastive Divergence (CD)

- Gibbs sampling for negative phase
 - □ Random initialization: v'->h'-
 - $> \ldots \rightarrow v \rightarrow h$
 - Slow because of long burn-in period
- Intuition of CD
 - Start from a data closed to the model samples
- CD-k for negative phase
 - Start from empirical data and ran k-steps
 - □ Typically, k=1: v1->h1->v2->h2



RBM







Samples (RBM is a generative model)





Issues with RBM

- Log-partition function is intractable
- No direct metric for choosing hyper-parameters
- (one hidden layer) Much too simple for modeling highdimensional and richly structured sensory data





Neural Evidence?

Our visual systems contain multilayer generative models

- Top-down connections:
 - Generate low-level features of images from high-level representations
 - Visual imagery, dreaming?
- Sottom-up connections:
 - Infer the high-level representations that would have generated an observed set of low-level features

[Hinton, Trends in Cognitive Science, 11(10), 2007]



Recent Advances on DGMs

Models:

- Deep belief networks (Salakhutdinov & Hinton, 2009)
- Autoregressive models (Larochelle & Murray, 2011; Gregor et al., 2014)
- Stochastic variations of neural networks (Bengio et al., 2014)

• ...

- Applications:
 - □ Image recognition (Ranzato et al., 2011)
 - □ Inference of hidden object parts (Lee et al., 2009)
 - Semi-supervised learning (Kingma et al., 2014)
 - Multimodal learning (Srivastava & Salakhutdinov, 2014; Karpathy et al., 2014)
 - ••••
- Learning algorithms
 - Stochastic variational inference (Kingma & Welling, 2014; Rezende et al., 2014)
 - ...



Learning with a Recognition Model



♦ For example:

$$q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x},y) = \mathcal{N}(\boldsymbol{\mu}(\mathbf{x},y;\boldsymbol{\phi}),\boldsymbol{\sigma}^2(\mathbf{x},y;\boldsymbol{\phi}))$$

 where both mean and variance are nonlinear function of data by a DNN



Long Short-Term Memory

♦ A RNN architecture without gradient vanishing issue

A RNN with LSTM blocks

 Each block is a "smart" network, determing when to remember, when to continue to remember or forget, and when to output



[Graves et al., 2009. A Novel Connectionist System for Improved Unconstrained Handwriting Recognition]



Issues

The sharpness of Gates' activation functions maters!

$$f(x) = \frac{1}{1 + e^{-\alpha * x}}$$



[Lv & Zhu, 2014. Revisit Long Short-Term Memory: an Optimization Perspective]



Discussions



Challenges of DL

- Learning
 - Backpropagation is slow and prone to gradient vanishing
 - Issues with non-convex optimization in high-dimensions

Overfitting

Big models are lacking of statistical information to fit

\bullet Interpretation

 Deep nets are often used as black-box tools for learning and inference



Expensive to train "Big Model + Big Data + Big/Super Cluster"



9 layers sparse autoencoder with:

- -local receptive fields to scale up;
- local L2 pooling and local contrast normalization for invariant features
 - 1B parameters (connections)
 - 10M 200x200 images
 - train with 1K machines (16K cores) for 3 days

-able to build high-level concepts, e.g., cat faces and human bodies

-15.8% accuracy in recognizing 22K objects (70% relative improvements)


Local Optima vs Saddle Points

Statistic Physics provide analytical tools

High-dimensional optimization problem
Most critical points are saddle points
The likelihood grows exponentially!



Dynamics of Various Opt. Techniques

♦ SGD:

• Gradient is accurate, but may suffer from slow steps

- Newton method:
 - Wrong directions when negative curvatures present
 - Saddle points become attractors! (can't escape)
- Saddle-free method:
 - A generalization of Newton's method to escape saddle points (more rapidly than SGD)





Some Empirical Results





Overfitting in Big Data

Predictive information grows slower than the amount of Shannon entropy (Bialek et al., 2001)





Overfitting in Big Data

Predictive information grows slower than the amount of Shannon entropy (Bialek et al., 2001)



Model capacity grows faster than the amount of predictive information!



Overfitting in DL

Increasing research attention, e.g., dropout training (Hinton, 2012)



More theoretical understanding and extensions

MCF (van der Maaten et al., 2013); Logistic-loss (Wager et al., 2013); Dropout SVM (Chen, Zhu et al., 2014)



Model Complexity

- What do we mean by structure learning in deep GMs?
 - # of layers
 - # of hidden units at each layer
 - The type of each hidden unit (discrete or continuous?)
 - The connection structures (i.e., edges) between hidden units
- Adams et al. presented a structure learning method using nonparametric Bayesian techniques – a cascading IBP (CIBP) process [Admas, Wallach & Ghahramani, 2010]

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Multi-Layer Belief Networks

A sequence of binary matrices => deep BNs





The Cascading IBP (CIBP)

- A stochastic process which results in an infinite sequence of infinite binary matrices
 - Each matrix is exchangeable in both rows and columns
- How do we know the CIBP converges?
 - The number of dishes in one layer depends only on the number of customers in the previous layer
 - Can prove that this Markov chain reaches an absorbing state in finite time with probability one



Samples from CIBP Prior





Some counter-intuitive properties

- Stability w.r.t small perturbations to inputs
 - Imperceptible non-random perturbation can arbitrarily change the prediction (adversarial examples exist!)







[Szegedy et al., Intriguing properties of neural nets, 2013]



Criticisms of DL

Just a buzzword, or largely a rebranding of neural networks

Lack of theory

- gradient descent has been understood for a while
- DL is often used as black-box
- DL is only part of the larger challenge of building intelligent machines, still lacking of:
 - causal relationships
 - logic inferences
 - integrating abstract knowledge



How can neural science help?

- The current DL models:
 - loosely inspired by the densely interconnected neurons of the brain
 - mimic human learning by changing weights based on experience

How to improve?

- Transparent architecture?
 - Attention mechanism?
- Cheap learning?
 - (partially) replace back-propagation?
- Others?



Will DL make other ML methods obsolete?

Quora 2014/12/23

Yes (2 post, 113 upvotes)

- best predictive power when data sufficient
- DL is far from saturated
- Google et al invests on DL, it is the "richest" AI topic

No (10 posts, 284 upvotes)

• simpler algorithms are just fine in many cases

- methods with domain knowledge works better
- DL is feature learning, needs other methods to work

• DL is not that well developed, a lot of work to be done using more traditional methods

• No free lunch

• a lot like how ANN was viewed in the late 80s





What are people saying?

Yann LeCun:

 "AI has gone from failure to failure, with bits of progress. This could be another leapfrog"

Jitendra Malik:

- in the long term, deep learning may not win the day; ... "Over time people will decide what works best in different domains."
- "Neural nets were always a delicate art to manage. There is some black magic involved"

Andrew Ng:

- "Deep learning happens to have the property that if you feed it more data it gets better and better,"
- "Deep-learning algorithms aren't the only ones like that, but they're arguably the best certainly the easiest. That's why it has huge promise for the future."

[Nature 505, 146–148 (09 January 2014)]



What are people saying?

Oren Etzioni:

"It's like when we invented flight" (not using the brain for inspiration)

Alternatives:

Logic, knowledge base, grammars?

• Quantum AI/ML?

[Nature 505, 146–148 (09 January 2014)]



Thank You!