#### **Probabilistic Graphical Models**

#### Deep Learning and Graphical Models

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#### **Perceptron and Neural Nets**



#### • From biological neuron to artificial neuron (perceptron)



• From biological neuron network to artificial neuron networks





## A perceptron learning algorithm



• Recall the nice property of sigmoid function

$$\frac{d\sigma}{dt} = \sigma(1 - \sigma)$$

- Consider regression problem f:X $\rightarrow$ Y, for scalar Y:  $y = f(x) + \epsilon$
- We used to maximize the conditional data likelihood

$$\vec{w} = \arg\max_{\vec{w}} \ln\prod_{i} P(y_i|x_i; \vec{w})$$

• Here ...

$$\vec{w} = \arg\min_{\vec{w}} \sum_{i} \frac{1}{2} (y_i - \hat{f}(x_i; \vec{w}))^2$$

x<sub>d</sub> = input t<sub>d</sub> = target output o<sub>d</sub> =observed unit output w<sub>i</sub> =weight i

#### **Gradient Descent**



$$\frac{\partial E[\vec{w}]}{\partial w_j} = \frac{\partial}{\partial w_i} \frac{1}{2} \sum (t_d - o_d)^2$$
$$=$$

Gradient

$$abla E[\vec{w}] \equiv \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \cdots, \frac{\partial E}{\partial w_n}\right]$$

Training rule:

$$\Delta \vec{w} = -\eta \nabla E[\vec{w}]$$

i.e.,

$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

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## The perceptron learning rules

$$\begin{aligned} \frac{\partial E_D[\vec{w}])}{\partial w_j} &= \frac{\partial}{\partial w_i} \frac{1}{2} \sum_d (t_d - o_d)^2 \\ &= \frac{1}{2} \sum_d 2(t_d - o_d) \frac{\partial}{\partial w_i} (t_d - o_d) \\ &= \sum_d (t_d - o_d) \left( -\frac{\partial o_d}{\partial w_i} \right) \\ &= -\sum_d (t_d - o_d) \frac{\partial o_d}{\partial net_i} \frac{\partial net_d}{\partial w_i} \\ &= -\sum_d (t_d - o_d) o_d (1 - o_d) x_d^i \end{aligned}$$

**Batch mode:** 

Do until converge:

**1. compute gradient**  $\nabla E_D[w]$ 

$$\vec{w} = \vec{w} - \eta \nabla E_D[\vec{w}]$$

Incremental mode: Do until converge: • For each training example *d* in *D* 1. compute gradient  $\nabla E_d[w]$ 2.  $\vec{w} = \vec{w} - \eta \nabla E_d[\vec{w}]$ where

$$\nabla E_d[\vec{w}] = -(t_d - o_d)o_d(1 - o_d)\vec{x}_d$$

#### **Neural Network Model**



Inputs



IndependentWeightsHiddenWeightsDependentvariablesLayerVariable

**Prediction** 

#### "Combined logistic models"





IndependentWeightsHiddenWeightsDependevariablesLayerVariable

**Prediction** 







# **Backpropagation Algorithm**

- Initialize all weights to small random numbers
   Until convergence, Do
  - 1. Input the training example to the network and compute the network outputs
  - 1. For each output unit k

$$\delta_k \leftarrow o_k^2 (1 - o_k^2) (t - o_k^2)$$

2. For each hidden unit h

$$\delta_h \leftarrow o_h^1 (1 - o_h^1) \sum_{k \in outputs} w_{h,k} \delta_k$$

3. Undate each network weight  $w_{i,i}$ 

 $w_{i,j} \leftarrow w_{i,j} + \Delta w_{i,j}$  where  $\Delta w_{i,j} = \eta \delta_j x^j$ 



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#### **More on Backpropatation**

- It is doing gradient descent over entire network weight vector
- Easily generalized to arbitrary directed graphs
- Will find a local, not necessarily global error minimum
  - In practice, often works well (can run multiple times)
- Often include weight momentum  $\alpha$

$$\Delta w_{i,j}(t) = \eta \delta_j x_{i,j} + \alpha \Delta w_{i,j}(t-1)$$

- Minimizes error over *training* examples
  - Will it generalize well to subsequent testing examples?
- Training can take thousands of iterations,  $\rightarrow$  very slow!
- Using network after training is very fast

# Learning Hidden Layer Representation

• A network:



• A target function:

Input		Output
10000000	$\rightarrow$	1000000
01000000	$\rightarrow$	01000000
00100000	$\rightarrow$	00100000
00010000	$\rightarrow$	00010000
00001000	$\rightarrow$	00001000
00000100	$\rightarrow$	00000100
00000010	$\rightarrow$	00000010
00000001	$\rightarrow$	0000001

• Can this be learned?

## Learning Hidden Layer Representation

• A network:



• Learned hidden layer representation:

Input		Hidden				Output
Values						
10000000	$\rightarrow$	.89	.04	.08	$\rightarrow$	10000000
01000000	$\rightarrow$	.01	.11	.88	$\rightarrow$	01000000
00100000	$\rightarrow$	.01	.97	.27	$\rightarrow$	00100000
00010000	$\rightarrow$	.99	.97	.71	$\rightarrow$	00010000
00001000	$\rightarrow$	.03	.05	.02	$\rightarrow$	00001000
00000100	$\rightarrow$	.22	.99	.99	$\rightarrow$	00000100
00000010	$\rightarrow$	.80	.01	.98	$\rightarrow$	00000010
00000001	$\rightarrow$	.60	.94	.01	$\rightarrow$	00000001

### Training



#### **Training**



# Modern ANN topics: "Deep" Learning





#### Non-linear LR vs. ANN



 $Y = a(X_1) + b(X_2) + c(X_3) + d(X_1X_2) + \dots$ 



#### **Computer vision features**





#### **Good Representations are hierarchical**

- In Language: hierarchy in syntax and semantics
  - Words->Parts of Speech->Sentences->Text
  - Objects, Actions, Attributes...-> Phrases -> Statements -> Stories
- In Vision: part-whole hierarchy
  - Pixels->Edges->Textons->Parts->Objects->Scenes

# "Deep" learning: learning hierarchical representations



Extractor

Classifier

• Deep Learning: learning a hierarchy of internal representations

Extractor

- From low-level features to mid-level invariant representations, to object identities
- Representations are increasingly invariant as we go up the layers
- using multiple stages gets around the specificity/invariance dilemma

#### "Deep" models

- Neural Networks: Feed-forward\*
  - You have seen it
- "Deep" Restrictive Boltzmann Machines (RBM)
  - Probabilistic Undirected: MRFs and RBMs\*
- Autoencoders (multilayer NN with output = input)
  - Non-Probabilistic -Directed: PCA, Sparse Coding





**Different loss** 

function designs

#### Example I: The Restrictive Boltzmann Machines, aka., the "Harmonium"





**History:** 

Smolensky ('86), Proposed the architechture.

Freund & Haussler ('92), The "Combination Machine" (binary), learning with projection pursuit. Hinton ('02), The "Restricted Boltzman Machine" (binary), learning with contrastive divergence. Marks & Movellan ('02), Diffusion Networks (Gaussian). Welling, Hinton, Osindero ('02), "Product of Student-T Distributions" (super-Gaussian)

# A Two-layer MRFs





**Boltzmann machines:** 

$$p(x,h \mid \theta) = \exp \left\{ \sum_{i} \theta_{i} \phi_{i}(x_{i}) + \sum_{j} \theta_{j} \phi_{j}(h_{j}) + \sum_{i,j} \theta_{i,j} \phi_{i,j}(x_{i},h_{j}) - A(\theta) \right\}$$

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# A Constructive Definition



#### **A Constructive Definition**





They map to the harmonium random field:

$$p(x,h \mid \theta) = \exp \left\{ \sum_{i} \vec{\theta}_{i} \vec{f}_{i}(x_{i}) + \sum_{j} \vec{\lambda}_{j} \vec{g}_{j}(h_{j}) + \sum_{i,j} \vec{f}_{i}^{T}(x_{i}) \mathbf{W}_{i,j} \vec{g}_{j}(h_{j}) \right\}$$
  
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#### **The Computational Trade-off**

Undirected model: Learning is hard, inference is easy.

**Directed Model**: Learning is "easier", inference is hard.

Example: Document Retrieval.



Retrieval is based on comparing (posterior) topic distributions of documents.

- directed models: inference is slow. Learning is relatively "easy".
- <u>undirected model</u>: inference is fast. Learning is slow but can be done offline.

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# An RMB for text/image





EFH or DWH (welling et al 2005, Xing et al 2005):



 $h_i = 3$ : topic j has strength 3  $h_j \in \mathbf{R}, \qquad \langle h_i \rangle = \sum_i \vec{W}_{i,j} \bullet \vec{x}_i$  $x_{i,n} = 1$ : word *i* has count *n*  $\vec{x}_i = [x_{i,1}, x_{i,2}, ..., x_{i,N_{max}}], x_{i,n} \in \{0,1\}, \Sigma_n x_{i,n} = 1$ 

words counts

 $p(\mathbf{h} | \mathbf{x}) = \prod_{i} \text{Normal}_{h_i} \left[ \sum_{i} \vec{W}_{ij} \vec{x}_i, 1 \right]$  $p(\mathbf{x} | \mathbf{h}) = \prod_{i} \text{ Softmax }_{\vec{x}_{i}} \left[ \vec{\alpha}_{i} + \sum_{i} \vec{W}_{ij} h_{j} \right]$ Softmax  $_{\vec{x}_i}[\vec{\alpha}_i + \sum_j \vec{W}_{ij}h_j] \propto \exp\{(\vec{\alpha}_i + \sum_j \vec{W}_{ij}h_j)^T \vec{x}_i\}$ , note parameterization cost! (  $\vec{W}_{ii} = [w_{i,i}^1, ..., w_{i,i}^{N_{\max}}], \forall i, j$ In practice, only 1-0 counting is used!!! © Eric Xing @ CMU, 2015 28

## Recall Properties of Directed Networks





- Semantic naturalness:
  - intuitive causal structural, easy to design, comprehend and manipulate
- Bayesian extensions:
  - straightforward to set up, conjugate ..., but hyper-para fitting is non-trivial
- Computational properties:

#### **Properties of Directed Networks**

- Factors are marginally *independent.*
- Factors are conditionally *dependent* given observations on the visible nodes.

 $P(\ell \mid \mathbf{w}) = \frac{P(\mathbf{w} \mid \ell)P(\ell)}{P(\mathbf{w})}$ 

• Easy ancestral sampling.

• Learning with (variational) EM

 $p_{\theta}(h)$ 

 $h \sim p(h)$ 

 $\bigcirc x \sim p(x \mid h)$ 

 $\max Q(\theta_t \mid \theta_{t-1})$ 

#### **Properties of RBMs**

- Factors are marginally dependent.
- Factors are conditionally *independent* given observations on the visible nodes.

 $P(\ell \mid \mathbf{w}) = \prod_{i} P(\ell_{i} \mid \mathbf{w})$ 

• Iterative Gibbs sampling.





#### **Deep RBMs**





# Example II: Convolutional Networks



#### Hierarchical Architecture

Representations are more global, more invariant, and more abstract as we go up the layers

#### Alternated Layers of Filtering and Spatial Pooling

- Filtering detects conjunctions of features
- Pooling computes local disjunctions of features

#### Fully Trainable

All the layers are trainable

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#### Filtering + NonLinearity + Pooling = 1 stage of a Convolutional Net



- [Hubel & Wiesel 1962]:
  - simple cells detect local features
  - complex cells "pool" the outputs of simple cells within a retinotopic neighborhood. "Simple cells"



# **Convolutional Net Architecture** for Hand-writing recognition



• Convolutional net for handwriting recognition (400,000 synapses)

- Convolutional layers (simple cells): all units in a feature plane share the same weights
- Pooling/subsampling layers (complex cells): for invariance to small distortions.
- Supervised gradient-descent learning using back-propagation
- The entire network is trained end-to-end. All the layers are trained simultaneously.
- [LeCun et al. Proc IEEE, 1998]

#### How to train?

To compute all the derivatives, we use a backward sweep called the **back-propagation** algorithm that uses the recurrence equation for  $\frac{\partial E}{\partial X_i}$ 



#### But this is very slow !!!



















features

input









features

input





#### Even more abstract features

#### More abstract features

features

input





#### **Feature learning**

• Successful learning of intermediate representations [Lee et al ICML 2009, Lee et al NIPS 2009]



#### **Deep Learning is Amazing!!!**

 Tasks for Which Deep Convolutional Nets are the Best
 Y LeCun

 MA Ranzato

Handwriting recognition MNIST (many), Arabic HWX (IDSIA) OCR in the V ild 2011]: StreetView House Numbers (NYU and others) conit n [2011] GTSRB competition (IDSIA, NYU) Traffic sign Pedestrian [ t o [2013]: INRIA datasets and others (NYU) Volumetric b a n ge gmentation [2009] connectomics (IDSIA, MIT) Human Actio e hif n 2 11 Holly bod II data et (Stanford) io 2C 2] n ge et or petition Object Recog 20 ] ftf bw, Barce bi a  $\mathcal{O}(YJ)$ Scene Parsin tant rob ( Scene parsing from lep vi age [. 13] NYU RGB-L dat set (NYU) Speech Recognition [20] Acou tic hod ling (IBM and Google) Breast cancer cell mitosis detection [2011] MITOS (IDSIA)

The list of perceptual tasks for which ConvNets hold the record is growing.
 Most of these tasks (but not all) use purely supervised convnets.

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# A Few Thoughts on How We May Want to Further Study DNN



#### What makes it work? Why?





#### An MLer's View of the World



#### Loss functions (likelihood, reconstruction, margin, ...)

#### Structures

(Graphical, group, chain, tree, iid, ...)

**Constraints** (normality, sparsity, label, prior, KL, sum,

Algorithms MC (MCMC, Importance), Opt (gradient, IP),

**Stopping criteria** Change in objective, change in update ...

**Empirical Performances?** 

	DL	<b>♦ ?</b> ML (e.g., GM)
Empirical goa	al: e.g., classification, learning	, feature variable inference
Structure:	Graphical	Graphical
Objective:	Something aggreg local functions	gated from Something aggregated from local functions
Vocabulary:	Neuron, activation	/gate function Variables, potential function
Algorithm:	A single, unchaller inference algorithm	nged, m BP A major focus of open research, many algorithms, and more to come
Evaluation:	On a black-box sco performance	ore end On almost every intermediate quantity
Implementati	on: Many untold-tricks	More or less standardized
Experiments	Massive, real data unknown)	(GT Modest, often simulated data (GT known)



# A slippery slope to mythology?

- How to conclusively determine what an improve in performance could come from:
  - Better model (architecture, activation, loss, size)?
  - Better algorithm (more accurate, faster convergence)?
  - Better training data?
- Current research in DL seem to get everything above mixed by evaluating on a black-box "performance score" that is not directly reflecting
  - Correctness of inference
  - Achievability/usefulness of model
  - Variance due to stochasticity



#### **Inference quality**

- Training error is the old concept of a classifier with no hidden states, no <u>inference</u> is involved, and thus inference accuracy is not an issue
- But a DNN is not just a classifier, some DNNs are not even fully supervised, there are MANY hidden states, why their inference quality is not taken seriously?
- In DNN, inference accuracy = visualizing features
  - Study of inference accuracy is badly discouraged
  - Loss/accuracy is not monitored

# Inference/Learning Algorithm, and their evaluation

# Learning a GM with Hidden Variables – the thought process



• In fully observed iid settings, the log likelihood decomposes into a sum of local terms (at least for directed models).

 $\ell_{c}(\theta; D) = \log p(x, z \mid \theta) = \log p(z \mid \theta_{z}) + \log p(x \mid z, \theta_{x})$ 

• With latent variables, all the parameters become coupled together via marginalization



# Gradient Learning for mixture models



• We can learn mixture densities using gradient descent on the log likelihood. The gradients are quite interesting:

$$l(\theta) = \log p(\mathbf{x} \mid \theta) = \log \sum_{k} \pi_{k} p_{k}(\mathbf{x} \mid \theta_{k})$$
$$\frac{\partial l}{\partial \theta_{k}} = \frac{1}{p(\mathbf{x} \mid \theta)} \sum_{k} \pi_{k} \frac{\partial p_{k}(\mathbf{x} \mid \theta_{k})}{\partial \theta_{k}}$$
$$= \sum_{k} \frac{\pi_{k}}{p(\mathbf{x} \mid \theta)} p_{k}(\mathbf{x} \mid \theta_{k}) \frac{\partial \log p_{k}(\mathbf{x} \mid \theta_{k})}{\partial \theta_{k}}$$
$$= \sum_{k} \pi_{k} \frac{p_{k}(\mathbf{x} \mid \theta_{k})}{p(\mathbf{x} \mid \theta)} \frac{\partial \log p_{k}(\mathbf{x} \mid \theta_{k})}{\partial \theta_{k}} = \sum_{k} r_{k} \frac{\partial p_{k}(\mathbf{x} \mid \theta_{k})}{\partial \theta_{k}}$$

- In other words, the gradient is aggregated from many other intermediate states
  - Implication: costly iteration, heavy coupling between parameters
- Other issues: imposing constraints, identifiability ...

# Then Alternative Approaches Were Proposed



- The EM algorithm
  - M: a convex problem
  - E: approximate constrained optimization
    - Mean field
    - BP/LBP
    - Marginal polytope



- Spectrum algorithm:
  - redefine intermediate states, convexify the original problem

Θ

## Learning a DNN

To compute all the derivatives, we use a backward sweep called the **back-propagation** algorithm that uses the recurrence equation for  $\frac{\partial E}{\partial X_i}$ 



#### Learning a DNN



• In a nutshell, sequentially, and recursively apply:

$$w_{j,i}^{t+1} = w_{j,i}^t - \eta_t \delta_j z_i$$

$$\delta_i = h'(a_i) \sum_j \delta_j w_{j,i}$$

• Things can getting hairy when locally defined losses are introduced, e.g., auto-encoder, which breaks a loss-driven global optimization formulation



- Depending on starting point, BP converge or diverge with probability 1
  - A serious problem in Large-Scale DNN

## Some new ideas to speed up



#### • Approximate Inference

- Undirected connections for all layers (Markov net) [Related work: Salakhutdinov and Hinton, 2009]
- Block Gibbs sampling or mean-field
- Hierarchical probabilistic inference
- Layer-wise Unsupervised Learning

#### **Backprop in Practice**

- Use ReLU non-linearities (tanh and logistic are falling out of favor)
- Use cross-entropy loss for classification
- Use Stochastic Gradient Descent on minibatches
- Shuffle the training samples
- Normalize the input variables (zero mean, unit variance)
- Schedule to decrease the learning rate
- Use a bit of L1 or L2 regularization on the weights (or a combination)
  But it's best to turn it on after a couple of epochs
- Use "dropout" for regularization
  - Hinton et al 2012 http://arxiv.org/abs/1207.0580
- Lots more in [LeCun et al. "Efficient Backprop" 1998]
- Lots, lots more in "Neural Networks, Tricks of the Trade" (2012 edition) edited by G. Montavon, G. B. Orr, and K-R Müller (Springer)



#### DL

#### GM

#### Utility of the network

- A vehicle to conceptually synthesize complex decision hypothesis
  - stage-wise projection and aggregation
- A vehicle for organizing computing operations
  - stage-wise update of latent states
- A vehicle for designing processing steps/computing modules
  - Layer-wise parallization
- No obvious utility in evaluating DL algorithms

#### **Utility of the Loss Function**

• Global loss? Well it is non-convex anyway, why bother ?

- A vehicle for synthesizing a global loss function from local structure
  - potential function, feature function
- A vehicle for designing sound and efficient inference algorithms
  - Sum-product, mean-field
- A vehicle to inspire approximation and penalization
  - Structured MF, Tree-approx
- A vehicle for monitoring theoretical and empirical behavior and accuracy of inference
- A major measure of quality of algorithm and model

#### An Old Study of DL as GM Learning [Xing, Russell, Jordan, UAI 2003]



#### A sigmoid belief network at a GM, and mean-field partitions



#### Study focused on only inference/learning accuracy, speed, and partition



Now we can ask, with a correctly learned DN, is it doing will on the desired task?

#### Why A Graphical Model formulation of DL might be fruitful?



- Modular design: easy to incorporate knowledge and interpret, easy to integrate feature learning with high level tasks, easy to built on existing (partial) solutions
- Defines an explicit and natural objective
- Guilds strategies for **systematic study** of inference, parallelization, evaluation, and theoretical analysis
- A clear path to further **upgrade**:
  - structured prediction
  - Integration of multiple data modality
  - Modeling complex: time series, missing data, online data ...
- Big DL on **distributed architectures**, where things can get messy everywhere due to incorrect parallel computations

#### Easy to incorporate knowledge and interpret





# Easy to integrate feature learning with high level tasks



Hidden Markov Model + Gaussian Mixture Model

**1** Jointly trained, but shallow





Hidden Markov Model + Deep Graphical Models



#### Conclusion

- In GM: lots of efforts are directed to improving inference accuracy and convergence speed
  - An advanced tutorial would survey dozen's of inference algorithms/theories, but few use cases on empirical tasks
- In DL: most effort is directed to comparing different architectures and gate functions (based on empirical performance on a downstream task)
  - An advanced tutorial typically consist of a list of all designs of nets, many use cases, but a single name of algorithm: back prop of SGD
- The two fields are similar at the beginning (energy, structure, etc.), and soon diverge to their own signature pipelines
- A convergence might be necessary and fruitful