Today’s Topics

1. General Ideas in Deep Learning
   - Motivation for Deep Architectures and why is it hard?
   - Main Breakthrough in 2006: Layer-wise Pre-Training

2. Approach 1: Deep Belief Nets [Hinton et al., 2006]
   - Restricted Boltzmann Machines (RBM)
   - Training RBMs with Contrastive Divergence
   - Stacking RBMs to form Deep Belief Nets

3. Approach 2: Stacked Auto-Encoders [Bengio et al., 2006]
   - Auto-Encoders
   - Denoising Auto-Encoders

4. Discussions
   - Why it works, when it works, and the bigger picture
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The Promise of Deep Architectures

very high level representation:

\[
\text{MAN} \quad \text{SITTING} \quad ... \\
\]

\[
... \text{ etc } ... \\
\]

slightly higher level representation

raw input vector representation:

\[ \mathbf{x} = [23, 19, 20, 18] \]

*Understanding in AI requires high-level abstractions, modeled by highly non-linear functions*
The Promise of Deep Architectures

Understanding in AI requires high-level abstractions, modeled by highly non-linear functions. These abstractions must disentangle factors of variation in data (e.g. 3D pose, lighting).

- **Example from [Bengio, 2009]**
The Promise of Deep Architectures

Understanding in AI requires high-level abstractions, modeled by highly non-linear functions. These abstractions must disentangle factors of variation in data (e.g. 3D pose, lighting).

Deep Architecture is one way to achieve this: each intermediate layer is a successively higher level abstraction.

(*Example from [Bengio, 2009]*)
The Promise of Deep Architectures

very high level representation:

\[
\begin{array}{c|c}
\text{MAN} & \text{SITTING} \\
\hline
\end{array}
\]

... etc ...

slightly higher level representation

raw input vector representation:

\[
\mathbf{x} = \begin{bmatrix} 23 & 19 & 20 & \cdots & 18 \end{bmatrix}
\]

\[
\begin{array}{c}
\mathbf{x}_1 \\
\mathbf{x}_2 \\
\mathbf{x}_3 \\
\vdots \\
\mathbf{x}_n
\end{array}
\]
Why are Deep Architectures hard to train?

Vanishing gradient problem in Backpropagation

- $\frac{\partial \text{Loss}}{\partial w_{ij}} = \frac{\partial \text{Loss}}{\partial \text{in}_j} \frac{\partial \text{in}_j}{\partial w_{ij}} = \delta_j x_i$

- $\delta_j = \left[\sum_{j+1} \delta_{j+1} w_{j(j+1)}\right] \sigma'(\text{in}_j)$

- $\delta_j$ may vanish after repeated multiplication
Empirical Results: Poor performance of Backpropagation on Deep Neural Nets [Erhan et al., 2009]

- MNIST digit classification task; 400 trials (random seed)
- Each layer: initialize $w_{ij}$ by uniform $[-1/\sqrt{(\text{FanIn})}, 1/\sqrt{(\text{FanIn})}]$
- Although $L + 1$ layers is more expressive, worse error than $L$ layers

![Graph showing test classification error (perc) vs. number of layers]
Local Optimum Issue in Neural Nets

- For 2-Layer Net and more, the training objective is not convex, so different local optima may be achieved depending on initial point.
- For Deep Architectures, Backpropagation is apparently getting a local optimum that does not generalize well.

*Figure from Chapter 5, [Bishop, 2006]*
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Layer-wise Pre-training [Hinton et al., 2006]

First, train one layer at a time, optimizing data-likelihood objective $P(x)$
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Layer-wise Pre-training [Hinton et al., 2006]

Finally, fine-tune labeled objective $P(y|x)$ by Backpropagation

Adjust weights
Predict $f(x)$
Layer-wise Pre-training [Hinton et al., 2006]

Key Idea:
Focus on modeling the input $P(X)$ better with each successive layer. Worry about optimizing the task $P(Y|X)$ later.

"If you want to do computer vision, first learn computer graphics." – Geoff Hinton
Layer-wise Pre-training [Hinton et al., 2006]

Key Idea:
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Extra advantage:
Can exploit large amounts of unlabeled data!
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Recall the problem setup: Learn function $f : x \rightarrow y$
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But rather doing this directly, we first learn hidden features $h$ that model input $x$, i.e. $x \rightarrow h \rightarrow y$
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How do we discover useful latent features $h$ from data $x$?

- Different Deep Learning methods differ by this basic component
- e.g. Deep Belief Nets use Restricted Boltzmann Machines (RBMs)
Restricted Boltzmann Machine (RBM)

- RBM is a simple energy-based model: \( p(x, h) = \frac{1}{Z_\theta} \exp(-E_\theta(x, h)) \)
  - with only \( h \)-\( x \) interactions: \( E_\theta(x, h) = -x^T Wh - b^T x - d^T h \)
  - here, we assume \( h_j \) and \( x_i \) are binary variables
  - normalizer: \( Z_\theta = \sum_{(x, h)} \exp(-E_\theta(x, h)) \) is called partition function
**Restricted Boltzmann Machine (RBM)**

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- Example:
  
  - Let weights \( (h_1, x_1), (h_1, x_3) \) be positive, others be zero, \( b = d = 0 \).
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**Example:**

- Let weights \((h_1, x_1), (h_1, x_3)\) be positive, others be zero, \( b = d = 0 \).
- Then this RBM defines a distribution over \([x_1, x_2, x_3, h_1, h_2, h_3]\) where
  \( p(x_1 = 1, x_2 = 0, x_3 = 1, h_1 = 1, h_2 = 0, h_3 = 0) \) has high probability
Computing Posteriors in RBMs

Computing $p(h|x)$ is easy due to factorization:

$$p(h|x) = \frac{p(x, h)}{\sum_h p(x, h)} = \frac{1/Z_\theta \exp(-E(x, h))}{\sum_h 1/Z_\theta \exp(-E(x, h))}$$

$$= \exp(x^T Wh + b^T x + d^T h) / \sum_h \exp(x^T Wh + b^T x + d^T h)$$

$$= \prod_j \exp(x^T W_j h_j + d_j h_j) \cdot \exp(b^T x) / \sum_{h_1 \in \{0,1\}} \sum_{h_2 \in \{0,1\}} \cdots \sum_h \prod_j \exp(x^T W_j h_j + d_j h_j) \cdot \exp(b^T x)$$

$$= \prod_j \exp(x^T W_j h_j + d_j h_j) / \prod_j \sum_{h_j \in \{0,1\}} \exp(x^T W_j h_j + d_j h_j)$$

$$= \prod_j \frac{\exp(x^T W_j h_j + d_j h_j)}{\sum_{h_j \in \{0,1\}} \exp(x^T W_j h_j + d_j h_j)} = \prod_j p(h_j|x)$$

Note $p(h_j = 1|x) = \exp(x^T W_j + d_j)/Z = \sigma(x^T W_j + d_j)$
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$$= \frac{\exp(x^T W h + b^T x + d^T h)}{\sum_h \exp(x^T W h + b^T x + d^T h)}$$

$$= \prod_j \frac{\exp(x^T W_j h_j + d_j h_j) \cdot \exp(b^T x)}{\sum_{h_1 \in \{0,1\}} \sum_{h_2 \in \{0,1\}} \cdots \sum_{h_j} \prod_j \exp(x^T W_j h_j + d_j h_j) \cdot \exp(b^T x)}$$

$$= \prod_j \frac{\exp(x^T W_j h_j + d_j h_j)}{\prod_j \sum_{h_j \in \{0,1\}} \exp(x^T W_j h_j + d_j h_j)}$$

$$= \prod_j \frac{\exp(x^T W_j h_j + d_j h_j)}{\sum_{h_j \in \{0,1\}} \exp(x^T W_j h_j + d_j h_j)} = \prod_j p(h_j|x)$$

Note $p(h_j = 1|x) = \exp(x^T W_j + d_j)/Z = \sigma(x^T W_j + d_j)$

Similarly, computing $p(x|h) = \prod_i p(x_i|h)$ is easy
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Training RBMs to optimize $P(X)$

Derivative of the Log-Likelihood: $\partial_{wij} \log P_w(x = x^{(m)})$

$$ = \partial_{wij} \log \sum_h P_w(x = x^{(m)}, h) \quad (1)$$

$$ = \partial_{wij} \log \sum_h \frac{1}{Z_w} \exp (- E_w(x^{(m)}, h)) \quad (2)$$

$$ = - \partial_{wij} \log Z_w + \partial_{wij} \log \sum_h \exp (- E_w(x^{(m)}, h)) \quad (3)$$

$$ = \frac{1}{Z_w} \sum_{h,x} e^{-E_w(x,h)} \partial_{wij} E_w(x, h) - \frac{1}{\sum_h e^{-E_w(x^{(m)},h)}} \sum_h e^{-E_w(x^{(m)},h)} \partial_{wij} E_w(x^{(m)}, h)$$

$$ = \sum_{h,x} P_w(x, h)[\partial_{wij} E_w(x, h)] - \sum_h P_w(x^{(m)}, h)[\partial_{wij} E_w(x^{(m)}, h)] \quad (4)$$

$$ = -E_{p(x,h)}[x_i \cdot h_j] + E_{p(h|x=x^{(m)})}[x_i^{(m)} \cdot h_j] \quad (5)$$
Training RBMs to optimize $P(X)$

Derivative of the Log-Likelihood: $\partial_{wij} \log P_w(x = x^{(m)})$

\[
\begin{align*}
\frac{\partial}{\partial w_{ij}} \log P_w(x = x^{(m)}) &= \frac{\partial}{\partial w_{ij}} \log \sum_h P_w(x = x^{(m)}, h) \quad (1) \\
&= \frac{\partial}{\partial w_{ij}} \log \sum_h \frac{1}{Z_w} \exp (-E_w(x^{(m)}, h)) \quad (2) \\
&= -\frac{\partial}{\partial w_{ij}} \log Z_w + \frac{\partial}{\partial w_{ij}} \log \sum_h \exp (-E_w(x^{(m)}, h)) \quad (3) \\
&= \frac{1}{Z_w} \sum_{h,x} e^{-E_w(x,h)} \frac{\partial}{\partial w_{ij}} E_w(x, h) - \frac{1}{\sum_h e^{-E_w(x^{(m)},h)}} \sum_h e^{-E_w(x^{(m)},h)} \frac{\partial}{\partial w_{ij}} E_w(x^{(m)}, h) \\
&= \sum_{h,x} P_w(x, h)[\frac{\partial}{\partial w_{ij}} E_w(x, h)] - \sum_h P_w(x^{(m)}, h)[\frac{\partial}{\partial w_{ij}} E_w(x^{(m)}, h)] \quad (4) \\
&= -E_{p(x|h)}[x_i \cdot h_j] + E_{p(h|x=x^{(m)})}[x_i^{(m)} \cdot h_j] \quad (5)
\end{align*}
\]

Second term (positive phase) increases probability of $x^{(m)}$; First term (negative phase) decreases probability of samples generated by the model.
Contrastive Divergence Algorithm

The negative phase term \( \mathbb{E}_{p(x,h)}[x_i \cdot h_j] \) is expensive because it requires sampling \((x,h)\) from the model.
Contrastive Divergence Algorithm

- The negative phase term ($\mathbb{E}_{p(x,h)}[x_i \cdot h_j]$) is expensive because it requires sampling $(x,h)$ from the model.
- Gibbs Sampling (sample $x$ then $h$ iteratively) works, but waiting for convergence at each gradient step is slow.
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- Gibbs Sampling (sample $x$ then $h$ iteratively) works, but waiting for convergence at each gradient step is slow.
- Contrastive Divergence is a faster but biased method: initialize with training point and wait only a few (usu. 1) sampling steps.
The negative phase term \( \mathbb{E}_{p(x,h)}[x_i \cdot h_j] \) is expensive because it requires sampling \((x,h)\) from the model.

Gibbs Sampling (sample \( x \) then \( h \) iteratively) works, but waiting for convergence at each gradient step is slow.

Contrastive Divergence is a faster but biased method: initialize with training point and wait only a few (usu. 1) sampling steps.

1. Let \( x^{(m)} \) be training point, \( \mathcal{W} = [w_{ij}] \) be current model weights.
2. Sample \( \hat{h}_j \in \{0,1\} \) from \( p(h_j|x = x^{(m)}) = \sigma(\sum_i w_{ij}x_i^{(m)} + d_j) \ \forall j \).
3. Sample \( \tilde{x}_i \in \{0,1\} \) from \( p(x_i|h = \hat{h}) = \sigma(\sum_j w_{ij}\hat{h}_j + b_i) \ \forall i \).
4. Sample \( \tilde{h}_j \in \{0,1\} \) from \( p(h_j|x = \tilde{x}) = \sigma(\sum_i w_{ij}\tilde{x}_i + d_j) \ \forall j \).
5. \( w_{ij} \leftarrow w_{ij} + \gamma(x_i^{(m)} \cdot \hat{h}_j - \tilde{x}_i \cdot \tilde{h}_j) \)
Goal: Make RBM $p(x, h)$ have high probability on training samples.

To do so, we’ll ”steal” probability mass from nearby samples that incorrectly preferred by the model.

For detailed analysis, see [Carreira-Perpinan and Hinton, 2005]
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Deep Belief Nets (DBN) = Stacked RBM

Layer1 RBM
Layer2 RBM
Layer3 RBM

DBN defines a probabilistic generative model $p(x) = \sum_{h, h', h''} p(x|h)p(h|h')p(h', h'')$ (top 2 layers is interpreted as a RBM; lower layers are directed sigmoids)
Deep Belief Nets (DBN) = Stacked RBM

- DBN defines a probabilistic generative model $p(x) = \sum_{h,h',h''} p(x|h)p(h|h')p(h',h'')$ (top 2 layers is interpreted as a RBM; lower layers are directed sigmoids)
- Stacked RBMs can also be used to initialize a Deep Neural Network (DNN)
After training on 20k images, the generative model of [Salakhutdinov and Hinton, 2009]* can generate random images (dimension=8976) that are amazingly realistic!

This model is a Deep Boltzmann Machine (DBM), different from Deep Belief Nets (DBN) but also built by stacking RBMs.
Summary: Things to remember about DBNs

1. Layer-wise pre-training is the innovation that rekindled interest in deep architectures.
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3. Why RBM? \( p(h|x) \) is tractable, so it’s easy to stack.
4. RBM training can be expensive. Solution: contrastive divergence.
5. DBN formed by stacking RBMs is a probabilistic generative model.
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Auto-Encoders: simpler alternatives to RBMs

Encoder: $h = \sigma(Wx + b)$

Decoder: $x' = \sigma(W'h + d)$

Encourage $h$ to give small reconstruction error: 

$$\text{Loss} = \sum_{m} ||x(m) - \text{DECODER(ENCODER(x(m)))}||^2$$

Reconstruction: $x' = \sigma(W'\sigma(Wx + b) + d)$
Auto-Encoders: simpler alternatives to RBMs

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- Reconstruction: $x' = \sigma(W'\sigma(Wx + b) + d)$
- This can be trained with the same Backpropagation algorithm for 2-layer nets, with $x^{(m)}$ as both input and output
Stacked Auto-Encoders (SAE)

- The encoder/decoder gives same form $p(h|x)$, $p(x|h)$ as RBMs, so can be stacked in the same way to form Deep Architectures
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- Unlike RBMs, Auto-encoders are deterministic.
  - \( h = \sigma(Wx + b) \), not \( p(h = \{0,1\}) = \sigma(Wx + b) \)

![Diagram of stacked auto-encoders](image-url)
Stacked Auto-Encoders (SAE)

- The encoder/decoder gives same form $p(h|x)$, $p(x|h)$ as RBMs, so can be stacked in the same way to form Deep Architectures

- Unlike RBMs, Auto-encoders are deterministic.
  - $h = \sigma(Wx + b)$, not $p(h = \{0, 1\}) = \sigma(Wx + b)$
  - Disadvantage: Can’t form deep generative model
  - Advantage: Fast to train, and useful still for Deep Neural Nets
Many Variants of Auto-Encoders

- Enforce compression to get latent factors (lower dimensional $h$)
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- Linear encoder/decoder with squared reconstruction error learns same subspace of PCA [Bourlard and Kamp, 1988]

- Enforce sparsity and over-complete representations (high dimensional $h$) [Ranzato et al., 2006]
- Enforce binary hidden layers to build hash codes [Salakhutdinov and Hinton, 2007]
- Incorporate domain knowledge, e.g. denoising auto-encoders [Vincent et al., 2010]
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Denoising Auto-Encoders

Encoder: \[ h = \sigma(W\tilde{x} + b) \]

Decoder: \[ x' = \sigma(W'h + d) \]

1. Perturb input data \( x \) to \( \tilde{x} \) using invariance from domain knowledge.
2. Train weights to reduce reconstruction error with respect to original input: \[ ||x - x'|| \]
Denoising Auto-Encoders

- Example: Randomly shift, rotate, and scale input image; add Gaussian or salt-and-pepper noise.
- A "2" is a "2" no matter how you add noise, so the auto-encoder will be forced to cancel the variations that are not important.
Summary: things to remember about SAE

1. Auto-Encoders are cheaper alternatives to RBMs.
   ▶ Not probabilistic, but fast to train using Backpropagation or SGD
Auto-Encoders are cheaper alternatives to RBMs.
- Not probabilistic, but fast to train using Backpropagation or SGD

Auto-Encoders learn to "compress" and "re-construct" input data. Again, the focus is on modeling $p(x)$ first.
Summary: things to remember about SAE

1. Auto-Encoders are cheaper alternatives to RBMs.
   - Not probabilistic, but fast to train using Backpropagation or SGD

2. Auto-Encoders learn to ”compress” and ”re-construct” input data. Again, the focus is on modeling $p(x)$ first.

3. Many variants, some provide ways to incorporate domain knowledge.
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   - Restricted Boltzmann Machines (RBM)
   - Training RBMs with Contrastive Divergence
   - Stacking RBMs to form Deep Belief Nets

3. Approach 2: Stacked Auto-Encoders [Bengio et al., 2006]
   - Auto-Encoders
   - Denoising Auto-Encoders

4. Discussions
   - Why it works, when it works, and the bigger picture
Why does Layer-wise Pre-Training work?

One Hypothesis [Bengio, 2009, Erhan et al., 2010]:
- A deep net can fit the training data in many ways (non-convex):
  1. By optimizing upper-layers really hard
  2. By optimizing lower-layers really hard

- Even if lower-layers are random weights, upper-layer may still fit well.
  But this might not generalize to new data.

- Pre-training with objective on $P(x)$ learns more generalizable features

Pre-training seems to help put weights at a better local optimum.
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Is Layer-wise Pre-Training always necessary?

Answer in 2006: Yes!
Answer in 2014: No!

1. If initialization is done well by design (e.g., sparse connections and convolutional nets), maybe won't have vanishing gradient problem.
2. If you have an extremely large dataset, maybe won't overfit. (But maybe that also means you want an ever deeper net.)
3. New architectures are emerging:
   - Stacked SVM's with random projections [Vinyals et al., 2012]
   - Sum-Product Networks [Poon and Domingos, 2011]
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  $$p(x) = \sum_h p(h)p(x|h),$$ but much more compact
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- Philosophical connections to:
  - Semi-supervised Learning: exploit both labeled and unlabeled data
  - Curriculum Learning: start on easy task, gradually level-up
  - Multi-task Learning: learn and share sub-tasks
Early days of AI. Invention of artificial neuron [McCulloch and Pitts, 1943] & perceptron [Rosenblatt, 1958]
**History**

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Why does unsupervised pre-training help deep learning?

The difficulty of training deep architectures and the effect of unsupervised pre-training.
In *AISTATS*.

A fast learning algorithm for deep belief nets.
References IV

Le, Q. V., Ranzato, M., Monga, R., Devin, M., Chen, K., Corrado, G. S., Dean, J., and Ng, A. Y. (2012). Building high-level features using large scale unsupervised learning. In ICML.


