Unsupervised Neural Nets (and ICA)

Learning objectives
- Semi-supervised intuition
- ICA reconstruction
- Autoencoder architecture

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with contributions from
Quoc Le, Socher & Manning
Semi-Supervised Learning

• Hypothesis: $P(c|x)$ can be more accurately computed using shared structure with $P(x)$

from Socher and Manning
Semi-Supervised Learning

- Hypothesis: $P(c|x)$ can be more accurately computed using shared structure with $P(x)$

from Socher and Manning
Unsupervised Neural Nets

◆ Autoencoders
  ● Take same image as input and output
  ● Learn weights to minimize the reconstruction error
  ● Avoid perfect fitting
    ■ Pass through a “bottleneck” or
    ■ Impose sparsity
      ✗ Dropout
    ■ Add noise to the input
      ✗ denoising auto-encoder

◆ Generalize PCA or ICA

http://ufldl.stanford.edu/wiki/index.php/Autoencoders_and_Sparsity
Independent Components Analysis (ICA)

- Given observations $X$, find $W$ such that components $s_j$ of $S = XW$ are “as independent of each other as possible”
  - E.g. have maximum KL-divergence or low mutual information
  - Alternatively, find directions in $X$ that are most skewed
    - farthest from Gaussian
  - Usually mean center and “whiten” the data (make unit covariance) first
    - whiten: $X (X^TX)^{-1/2}$

- Very similar to PCA
  - But the loss function is not quadratic
  - So optimization cannot be done by SVD
Independent Components Analysis (ICA)

- Given observations $X$, find $W$ and $S$ such that components $s_j$ of $S = XW$ are “as independent of each other as possible”
  - $S_k$ = “sources” should be independent
- Reconstruct $X \sim (XW)W^+ = SW^+$
  - $S$ like *principal component scores*
  - $W^+$ like *loadings*
  - $x \sim \Sigma_j s_j w_j^+$
- **Auto-encoder** – nonlinear generalization that “encodes” $X$ as $S$ and then “decodes” it
Reconstruction ICA (RICA)

- **Reconstruction ICA**: find $W$ to minimize
  - Reconstruction error
    - $||X - SW^+||_2 = ||X - (XW)W^+||_2$

And minimize
- Mutual information between sources $S = XW$

$$I(s_1, s_2, ..., s_k) = \sum_{i-1}^{k} H(s_i) - H(s)$$

$$H(y) = -\int p(y) \log p(y) dy$$

Difference between the entropy of each “source” $s_i$ and the entropy of all of them together

Note: this is a bit more complex than it looks, as we have real numbers, not distributions

Mutual information

\[ I(y_1, y_2, \ldots, y_m) = KL(p(y_1, y_2, \ldots, y_m) \parallel p(y_1)p(y_2) \ldots p(y_m)) \]

Or the difference between the sum of the entropies of the individual distributions and the joint distribution
Unsupervised Neural Nets

Auto-encoders

- Take same image as input and output
  - often adding noise to the input
    (denoising auto-encoder)
- Learn weights to minimize the reconstruction error
- This can be done repeatedly (reconstructing features)
- Use for semi-supervised learning

from Socher and Manning
PCA = Linear Manifold = Linear Auto-encoder

input $x$, 0-mean
features = code $= h(x) = W x$
reconstruction $= W^T h(x) = W^T W x$
$W = \text{principal eigen-basis of } \text{Cov}(X)$

LSA example:
$x = (\text{normalized}) \text{ distribution of co-occurrence frequencies}$
from Socher and Manning
The Manifold Learning Hypothesis

- Examples concentrate near a lower dimensional “manifold” (region of high density where small changes are only allowed in certain directions).
Auto-Encoders are like nonlinear PCA

Minimizing reconstruction error forces latent representation of “similar inputs” to stay on manifold

from Socher and Manning
Stacking for deep learning

from Socher and Manning
Stacking for deep learning

Now learn to reconstruct the features (using more abstract ones)

from Socher and Manning
Stacking for deep learning

- Recurse – many layers deep
- Can be used to initialize supervised learning

from Socher and Manning
Tera-scale deep learning

Quoc V. Le
Stanford University and Google

Now at google
Joint work with

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Rajat Monga  Andrew Ng  Marc’Aurelio Ranzato  Paul Tucker  Ke Yang

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Warning: this x and W are the transpose of what we use

TICA:

\[ \min_W \sum_j \sum_i h_j(W; x^{(i)}) \]

s.t. \[ WW^T = I \]

Reconstruction ICA:

\[ \min_W \frac{\lambda}{m} \sum_{i=1}^m \| W^T W x^{(i)} - x^{(i)} \|_2^2 + \sum_j \sum_i h_j(W; x^{(i)}) \]

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**Lemma 3.1** When the input data \( \{x^{(i)}\}_{i=1}^m \) is whitened, the reconstruction cost \( \frac{\lambda}{m} \sum_{i=1}^m \| W^T W x^{(i)} - x^{(i)} \|_2^2 \) is equivalent to the orthonormality cost \( \lambda \| W^T W - I \|_F^2 \).

**Lemma 3.2** The column orthonormality cost \( \lambda \| W^T W - I_n \|_F^2 \) is equivalent to the row orthonormality cost \( \lambda \| W W^T - I_k \|_F^2 \) up to an additive constant.

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Equivalence between Sparse Coding, Autoencoders, RBMs and ICA

Build deep architecture by treating the output of one layer as input to another layer

Visualization of features learned

Most are local features
Challenges with 1000s of machines
Asynchronous Parallel SGDs

Le, et al., *Building high-level features using large-scale unsupervised learning*. ICML 2012
Local receptive field networks

Le, et al., *Tiled Convolutional Neural Networks*. NIPS 2010
10 million 200x200 images
1 billion parameters
Training

Dataset: 10 million 200x200 unlabeled images from YouTube/Web

Train on 2000 machines (16000 cores) for 1 week

1.15 billion parameters
- 100x larger than previously reported
- Small compared to visual cortex

Le, et al., *Building high-level features using large-scale unsupervised learning*. ICML 2012
The face neuron

Le, et al., *Building high-level features using large-scale unsupervised learning*. ICML 2012
The cat neuron

Le, et al., *Building high-level features using large-scale unsupervised learning*. ICML 2012
What you should know

◆ **Supervised neural nets**
  - Generalize *logistic regression or other MLE*
  - Often have built-in structure
    - local receptive fields, max pooling
  - Usually solved by minibatch stochastic gradient descent

◆ **Unsupervised neural nets**
  - Generalize PCA or ICA
  - Generally learn an “overcomplete basis”
  - Often trained recursively as nonlinear auto-encoders
  - Used in semi-supervised learning