The rest of the semester

- **HWs get shorter**
  - Start them after Wed lecture; finish in a week; Keep up!

- **Start thinking about final project**
  - 3 person Teams (+/- 1)
  - Real data set
    - with enough complexity to be interesting
    - Kaggle = minimal
    - But not too much data cleaning!
  - Details and rubric Nov 3

- **No class next Friday**
  - extra 90 min worksheet instead
Unsupervised Neural Nets: Autoencoders and ICA

ICA vs. PCA
Autoencoder types
denoising
variational

Lyle Ungar
with figures from
Quoc Le, Socher & Manning
Unsupervised Neural Nets

- **Auto-encoders generalize PCA**
  - Take same image as input and output
  - Learn weights to minimize the reconstruction error
  - Avoid perfect fitting
    - Pass through a “bottleneck” or impose sparsity
    - Or add noise to the input
      - *Denoising auto-encoder*

http://ufldl.stanford.edu/wiki/index.php/Autoencoders_and_Sparsity
Denoising Auto-encoder

- Image reconstruction (in CNN)
  - $X =$ image with noise added
  - $Y =$ original image
- Intermediate neural outputs are an embedding
Transformer

- Masking in NLP (in LSTM)
  - $X =$ sentence with words removed
  - $Y =$ the words that were removed
- Intermediate neural outputs are an embedding
Variational Auto-Encoder (VAE)

- Minimize reconstruction error and maximize independence of "components"
  - Reminiscent of a mixture model

- Intermediate neural outputs (components) are an embedding
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
    - whiten: make unit covariance
    - whiten: $X (X^TX)^{-1/2}$

- Very similar to PCA
  - But the loss function is not quadratic
  - So optimization cannot be done by SVD

Trendy deep learning generalization: “disentanglement”
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
  ● $x \sim \sum_j s_j w_j^*$

◆ 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 \( S = XW \)

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

\[
H(y) = -\int p(y) \log p(y) dy
\]

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

\[ \text{MI}(y_1, y_2, \ldots, y_m) = \text{KL}(p(y_1, y_2, \ldots, y_m) \parallel p(y_1)p(y_2) \cdots p(y_m)) \]

How well do the independent distributions approximate the joint distribution?
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)
- Used for semi-supervised learning

Unsupervised deep learning

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

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

Linear manifold

LSA example:
$x$ = (normalized) 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
- Gives embeddings

from Socher and Manning
Tera-scale deep learning

Quoc V. Le
Stanford University and Google

Now at google
Joint work with

Kai Chen  Greg Corrado  Jeff Dean  Matthieu Devin

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.**  $WW^T = I$

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**Reconstruction ICA:**

$$\min_{W} \frac{\lambda}{m} \sum_{i=1}^{m} \left\| W^T W x^{(i)} - x^{(i)} \right\|_2^2 + \sum_{j} \sum_{i} h_j(W; x^{(i)})$$

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

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**Lemma 3.2** The column orthonormality cost $\lambda \left\| W^T W - I_n \right\|_F^2$ is equivalent to the row orthonormality cost $\lambda \left\| W W^T - I_k \right\|_F^2$ 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**

**Le, et al., ICA with Reconstruction Cost for Efficient Overcomplete Feature Learning.** NIPS 2011
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
Most are local features
The face neuron

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

Top stimuli from the test set

Optimal stimulus by numerical optimization

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

◆ ICA
  ● Like PCA but does *disentanglement* as well as reconstruction

◆ Unsupervised neural nets (auto-encoders)
  ● Generalize PCA or ICA
  ● Denoising or variational
  ● Often trained recursively
  ● Often learn an “overcomplete basis”
  ● Used in semi-supervised learning

◆ Transformers use masking