Lecture 6: Representation Learning

André Martins, Francisco Melo, Mário Figueiredo

Deep Learning Course, Winter 2022-2023

Announcements

Deadline for Homework 1 is **Friday, December 23, 23:59**

- Please submit your solutions and code in Fenix.
- No late days allowed!!
- Solutions will be posted the day after.

Today's Roadmap

Today's lecture is about:

- Representation learning.
- Principal component analysis (PCA) and auto-encoders.
- Denoising auto-encoders.
- Distributed representations.
- Word embeddings and negative sampling.
- Multilingual and contextual word embeddings.

Outline

Representations

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  - (ii) They may allow transferring representations from one task to another
- We talked about (i) when discussing the multi-layer perceptron
- In this lecture, we'll focus on (ii)

Outline

Hierarchical Compositionality

Key Idea: deep(er) NNs learn **coarse-to-fine** representation layers.

Vision:

- pixels $\rightarrow$ edges $\rightarrow$ textons $\rightarrow$ motifs $\rightarrow$ parts $\rightarrow$ objects $\rightarrow$ scenes

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Text:

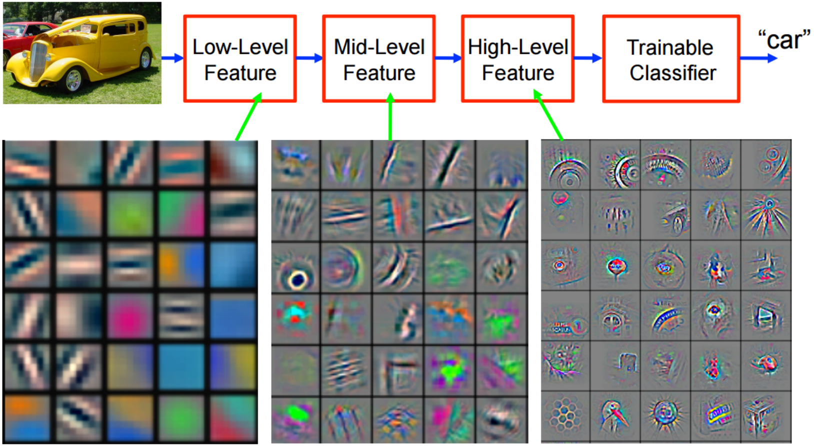
- characters → words → phrases → sentences → stories

(Inspired by Marc'Aurelio Ranzato and Yann LeCun)

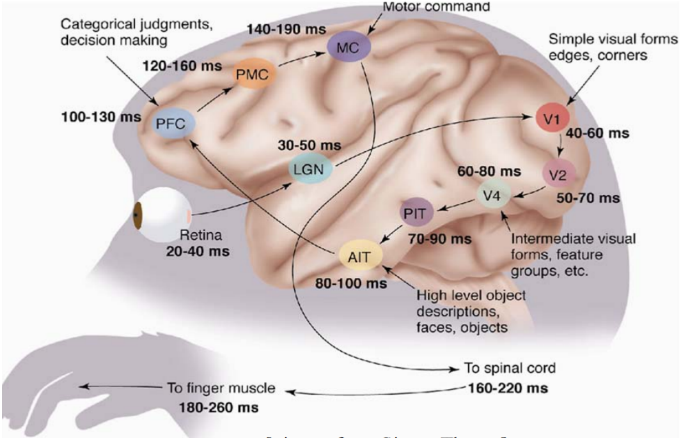
Hierarchical Compositionality

Feature visualization of convolutional NNs trained on ImageNet

(Zeiler and Fergus, 2013)



The Mammalian Visual Cortex is Hierarchical



[picture from Simon Thorpe]

(LGN = lateral geniculate nucleus; PIT = posterior inferotemporal area; AIT = anterior inferotemporal area; PFC = prefrontal cortex; PMC = premotor cortex; MC = motor cortex)

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- Layers farther away from inputs learn more abstract representations (shapes, forms, objects)
- This holds, not only for images, but also text, sounds, ...

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1. Representation Learning
   - Hierarchical Compositionality
   - Distributed Representations
   - Auto-Encoders
   - Word Embeddings

2. Conclusions

Distributed Representations (Hinton, 1984)

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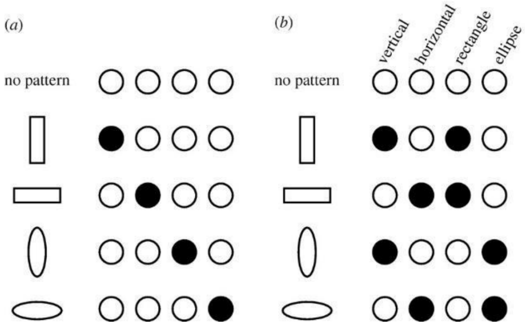
- What is each hidden unit actually representing?
- How can a NN generalize to objects that is has not seen before?

Local vs Distributed Representations

Consider two alternative representations:

- Local (one-hot) representations (one dimension per object)
- Distributed representations (one dimension per property)



(Inspired by Moontae Lee and Dhruv Batra)

Distributed Representations

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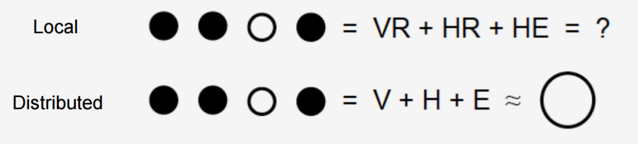
cf. the grandmother cell

The Power of Distributed Representations

- Distributed representations are more compact (there can be $O(\exp N)$ objects combining N properties)
- They are also more powerful, as they can generalize to unseen objects in a meaningful way:



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Next: how to learn useful object representations from raw inputs (no labels)?

Example: Unsupervised Pre-Training

- Training deep NNs (with many hidden layers) can be challenging
- This has been a major difficulty with NNs for a long time
- Initialize hidden layers using unsupervised learning (Erhan et al., 2010):
  - Force network to represent latent structure of input distribution
  - Encourage hidden layers to encode that structure
  - This can be done with an auto-encoder!

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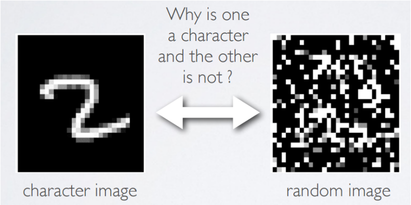
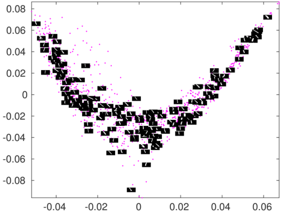
Data Manifold

Key idea: learn the manifold where the input objects live





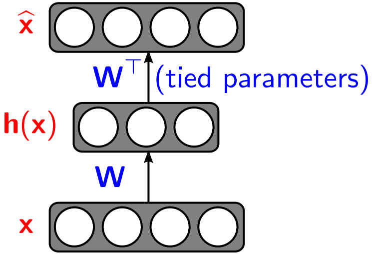
(Image credit: Hugo Larochelle)

Learn representations that encode well points in that manifold

Auto-Encoders

Auto-encoder: feed-forward NN trained to reproduce its input at the output

- Encoder: $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{g}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$



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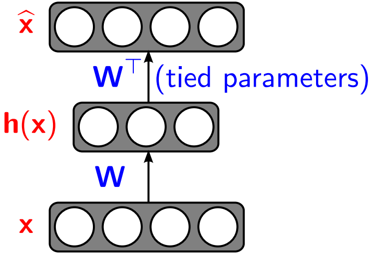

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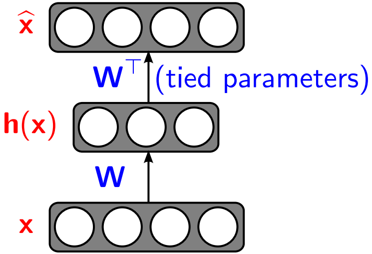

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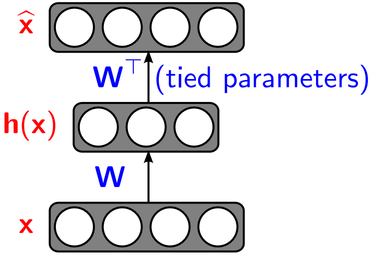
- Objective (dropping the biases):

$$\widehat{\boldsymbol{W}} = \arg\min_{\boldsymbol{W}} \sum_i \|\boldsymbol{W}^\top \boldsymbol{g}(\boldsymbol{W}\boldsymbol{x}_i) - \boldsymbol{x}_i\|^2$$



The Simplest Auto-Encoder: Linear

What happens if the activation function $\boldsymbol{g}$ is linear?

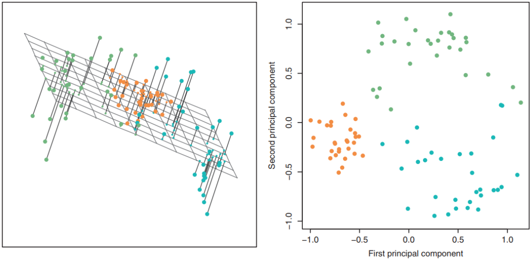


FIGURE 10.2. *Ninety observations simulated in three dimensions.* Left: *the first two principal component directions span the plane that best fits the data. It minimizes the sum of squared distances from each point to the plane.* Right: *the first two principal component score vectors give the coordinates of the projection of the 90 observations onto the plane. The variance in the plane is maximized.*

(From "An Introduction to Statistical Learning" by James, Witten, Hastie, Tibshirani)

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- Orthonormality of $\boldsymbol{U}$ and $\boldsymbol{V}$: $\boldsymbol{U}^T\boldsymbol{U} = \boldsymbol{I}$ and $\boldsymbol{V}^T\boldsymbol{V} = \boldsymbol{I}$.

Singular Value Decomposition (SVD)

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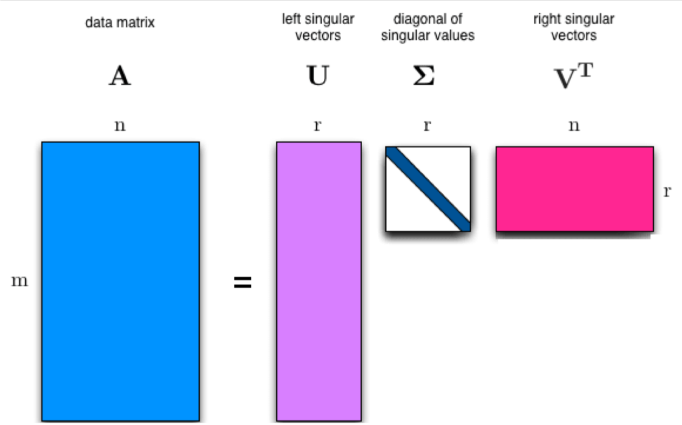

Picture credits: Mukesh Mithrakumar

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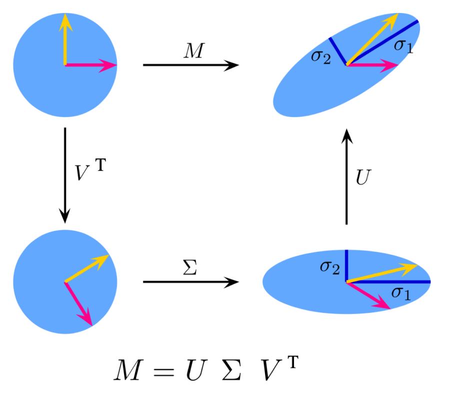

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We want to minimize

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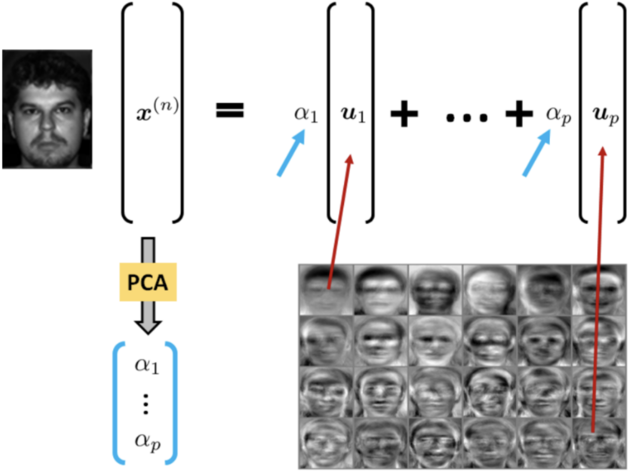
This is called principle component analysis (PCA)

PCA: EigenFaces



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We need some sort of regularization to:

- encourage a smooth representation (small perturbations of the input will lead to similar representations)
- avoid overfitting to the training data

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- **Variational auto-encoders:** a generative probabilistic model that minimizes a variational bound (this will be covered in another lecture!)

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- One exception are sparse auto-encoders:
  - Sparse auto-encoders incorporate a sparsity penalty $\Omega(\boldsymbol{h})$ on the code layer, e.g., $\Omega(\boldsymbol{h}) = \lambda\|\boldsymbol{h}\|_1$
  - Typically the number of hidden units is large, e.g., larger than the input dimension
  - The sparsity penalty encourages sparse codes, where most hidden units are inactive.

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- In this case, the encoder and decoder are not deterministic functions, but involve some noise/randomness
- Uses distribution $p_{\text{encoder}}(\boldsymbol{h} \mid \boldsymbol{x})$ for the encoder and a distribution $p_{\text{decoder}}(\boldsymbol{x} \mid \boldsymbol{h})$ for the decoder

Stochastic Auto-Encoders

- In this case, the encoder and decoder are not deterministic functions, but involve some noise/randomness
- Uses distribution $p_{\text{encoder}}(\boldsymbol{h} \mid \boldsymbol{x})$ for the encoder and a distribution $p_{\text{decoder}}(\boldsymbol{x} \mid \boldsymbol{h})$ for the decoder
- The auto-encoder can be trained to minimize

$$-\log p_{\text{decoder}}(\boldsymbol{x} \mid \boldsymbol{h}).$$

Denoising Auto-Encoders

- Use a perturbed version of the input, $\tilde{\boldsymbol{x}} = \boldsymbol{x} + \boldsymbol{n}$, where $\boldsymbol{n}$ is random noise (e.g. Gaussian noise $\boldsymbol{n} \sim \mathcal{N}(0, \sigma^2 \boldsymbol{I})$)

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- This is a form of implicit regularization that ensures smoothness: it forces the system to represent well not only the data points, but also their perturbations

Denoising Auto-Encoders

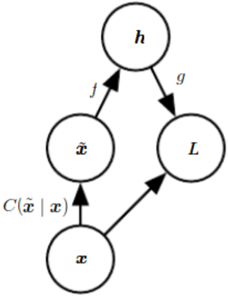

Figure 14.3: The computational graph of the cost function for a denoising autoencoder, which is trained to reconstruct the clean data point $\boldsymbol{x}$ from its corrupted version $\tilde{\boldsymbol{x}}$. This is accomplished by minimizing the loss $L = -\log p_{\text{decoder}}(\boldsymbol{x} \mid \boldsymbol{h} = f(\tilde{\boldsymbol{x}}))$, where $\tilde{\boldsymbol{x}}$ is a corrupted version of the data example $\boldsymbol{x}$, obtained through a given corruption process $C(\tilde{\boldsymbol{x}} \mid \boldsymbol{x})$. Typically the distribution p_{decoder} is a factorial distribution whose mean parameters are emitted by a feedforward network g.

(From Goodfellow et al.'s book.)

Denoising Auto-Encoders

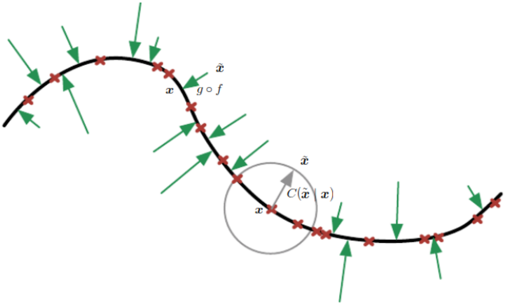

Figure 14.4: A denoising autoencoder is trained to map a corrupted data point $\tilde{\boldsymbol{x}}$ back to the original data point $\boldsymbol{x}$. We illustrate training examples $\boldsymbol{x}$ as red crosses lying near a low-dimensional manifold, illustrated with the bold black line. We illustrate the corruption process $C(\tilde{\boldsymbol{x}} \mid \boldsymbol{x})$ with a gray circle of equiprobable corruptions. A gray arrow demonstrates how one training example is transformed into one sample from this corruption process. When the denoising autoencoder is trained to minimize the average of squared errors $||g(f(\tilde{\boldsymbol{x}})) - \boldsymbol{x}||^2$, the reconstruction $g(f(\tilde{\boldsymbol{x}}))$ estimates $\mathbb{E}_{\mathbf{x}, \tilde{\mathbf{x}} \sim p_{\text{data}}(\mathbf{x}) C(\tilde{\mathbf{x}} \mid \mathbf{x})}[\mathbf{x} \mid \tilde{\mathbf{x}}]$. The vector $g(f(\tilde{\boldsymbol{x}})) - \tilde{\boldsymbol{x}}$ points approximately toward the nearest point on the manifold, since $g(f(\tilde{\boldsymbol{x}}))$ estimates the center of mass of the clean points $\boldsymbol{x}$ that could have given rise to $\tilde{\boldsymbol{x}}$. The autoencoder thus learns a vector field $g(f(\boldsymbol{x})) - \boldsymbol{x}$ indicated by the green arrows. This vector field estimates the score $\nabla_{\boldsymbol{x}} \log p_{\text{data}}(\boldsymbol{x})$ up to a multiplicative factor that is the average root mean square reconstruction error.

Why Do We Use Auto-Encoders?

Historically, training deep neural networks was hard

One of the initial successful uses of auto-encoders was for unsupervised pre-training (Erhan et al., 2010).

Unsupervised Pre-Training

A greedy, layer-wise procedure:

- train one layer at a time, from first to last, with unsupervised criterion (e.g. an auto-encoder)

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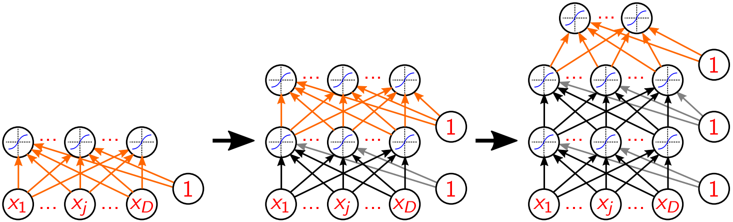

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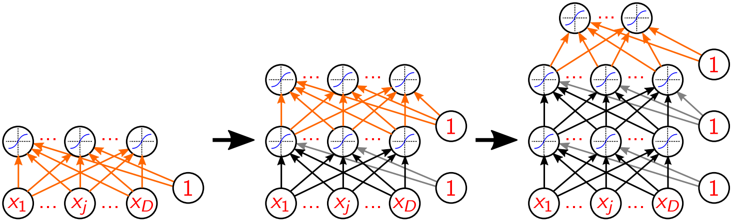

Pre-training initializes the parameters in a region such that the near local optima overfit less the data.

Fine-Tuning

Once all layers are pre-trained:

- add output layer
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Supervised learning is performed as in a regular feed-forward network:

- forward propagation, backpropagation, and update
- all parameters are "tuned" for the supervised task at hand
- representation is adjusted to be more discriminative

Other Applications of Auto-Encoders

- Dimensionality reduction
- Information retrieval and semantic hashing (via binarizing the codes)
- Conversion of discrete inputs to low-dimensional continuous space

Outline

1. Representation Learning

   Hierarchical Compositionality

   Distributed Representations

   Auto-Encoders

   Word Embeddings

2. Conclusions

Word Representations

- Learning representations of words in natural language;
- Also called word embeddings;
- An extremely successful application of representation learning;
- Still an active area of research.

Distributional Similarity

Key idea: represent a word by means of its neighbors

- *"You shall know a word by the company it keeps"* (J. R. Firth, 1957)
- One of the most successful ideas of modern statistical NLP!

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For example:

- Adjectives are normally surrounded by nouns
- Words like *book, newspaper, article*, are commonly surrounded by *reading, read, writes*, but not by *flying, eating, sleeping*

Word Embeddings

- Obtain (lower dimensional) vector representations of words.

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- Two possible methods:

  ✓ Factorization of a co-occurrence word/context matrix (latent semantic analysis, etc.)

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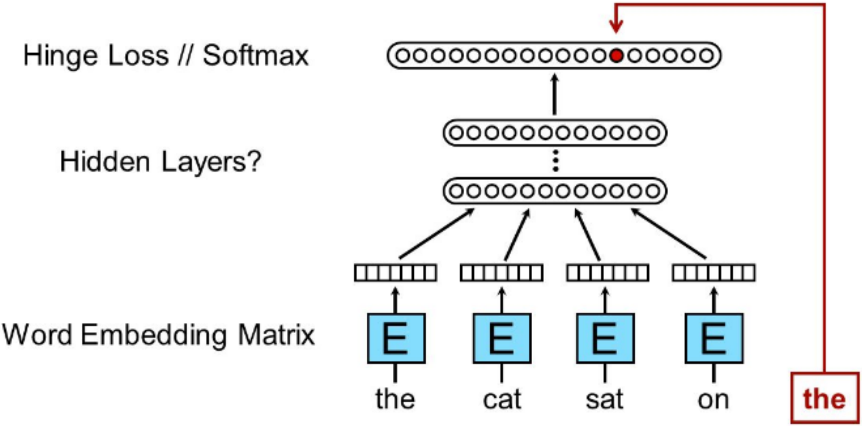
  ✓ Directly learn low-dimensional vectors by training a network to *predict* the context of a given word

- We focus on the latter, namely word2vec (Mikolov et al., 2013), which follows previous ideas (Bengio et al., 2003; Collobert et al., 2011).

Neural Language Model (Bengio et al., 2003)



(Image credits: Quoc Le)

Neural Language Model (Bengio et al., 2003)

Embedding matrix: assigns a vector to every word in the vocabulary.

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Variants of this model outperform smoothed K-th order Markov models

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  - ✓ We don't need to predict the probability of every word, just make sure that the true word is more likely than a random one
- These insights underlie the word2vec model of Mikolov et al. (2013).

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  ✓ **continuous bag-of-words** (CBOW): predict the central word from the context

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- Word2vec comes with two variants:
  - ✓ **skip-gram**: predict surrounding context words in a window of length m of every word
  - ✓ **continuous bag-of-words** (CBOW): predict the central word from the context
- We focus on the skip-gram model (more widely used).

Skip-Gram

- **Objective:** maximize the log probability of any context word given the central word:

$$J(\Theta) = \frac{1}{T} \sum_{t=1}^{T} \sum_{-m \leq j \leq m,\ j \neq 0} \log p_{\Theta}(x_{t+j} \mid x_t)$$

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  - ✓ Embeddings $\boldsymbol{u}_o$ for each word o appearing as the center word
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- In the end, we use the $\boldsymbol{u}$ as the word embeddings, discarding $\boldsymbol{v}$

The Large Vocabulary Problem

- Recall that

$$p_\Theta(x_{t+j} = c \mid x_t = o) = \frac{\exp(\boldsymbol{u_o}^T \boldsymbol{v}_c)}{\sum_{c'} \exp(\boldsymbol{u_o}^T \boldsymbol{v}_{c'})}$$

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  - ✓ Negative sampling
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- We focus on negative sampling.

Negative Sampling

Key idea:

- Replace the huge softmax by binary logistic regressions for a true pair (center word and word in its context window) and k of random pairs (center word, random word):

$$J_t(\Theta) = \log \sigma(\boldsymbol{u}_o^\top \boldsymbol{v}_c) + \sum_{i=1}^{k} \log \sigma(-\boldsymbol{u}_o^\top \boldsymbol{v}_{j_i}), \qquad j_i \sim P(x)$$

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- Negative sampling is a simple form of unsupervised pre-training.

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$$\boldsymbol{x}_{\text{apple}} - \boldsymbol{x}_{\text{apples}} \approx \boldsymbol{x}_{\text{car}} - \boldsymbol{x}_{\text{cars}} \approx \boldsymbol{x}_{\text{family}} - \boldsymbol{x}_{\text{families}}$$

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- Semantically:

$$\begin{aligned} \boldsymbol{x}_{\text{shirt}} - \boldsymbol{x}_{\text{clothing}} &\approx \boldsymbol{x}_{\text{chair}} - \boldsymbol{x}_{\text{furniture}} \\ \boldsymbol{x}_{\text{king}} - \boldsymbol{x}_{\text{man}} &\approx \boldsymbol{x}_{\text{queen}} - \boldsymbol{x}_{\text{woman}} \end{aligned}$$

Visualization

- Typical embedding dimensions are in the hundreds (e.g. 300)
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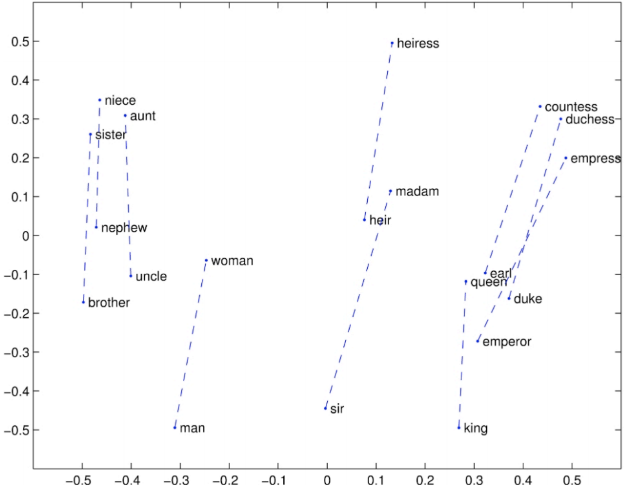
- Simple way: project them in 2D with something like PCA
- Most used: t-SNE (t-distributed stochastic neighbor embedding (Maaten and Hinton, 2008)))
  `https://lvdmaaten.github.io/tsne`

Word Analogies (Mikolov et al., 2013)



(Slide credit to Richard Socher)

Other Methods for Obtaining Word Embeddings

GloVe: Global Vectors for Word Representation (Pennington et al., 2014)

- `https://nlp.stanford.edu/projects/glove`
- Training is performed on aggregated global word-word co-occurrence statistics from a corpus

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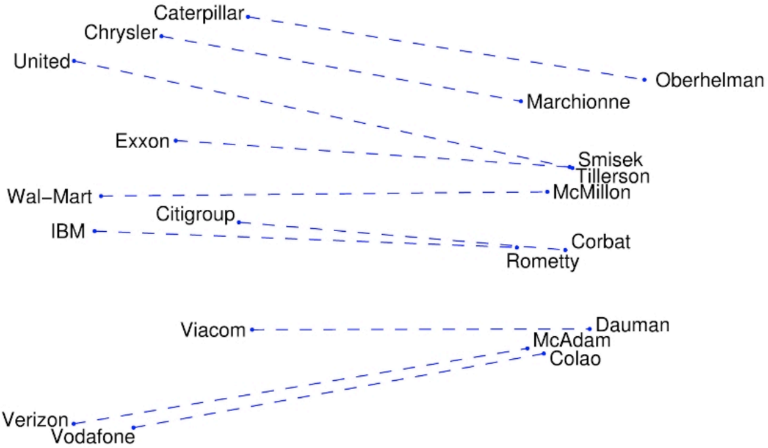
FastText (Bojanowski et al., 2016): embeds also character *n*-grams for generating embeddings for out-of-vocabulary words

- `https://fasttext.cc` (from FAIR)
- open-source, free, lightweight library that allows users to learn text representations and text classifiers
- contains multi-lingual word vectors for 157 different languages

GloVe Visualizations: Company → CEO



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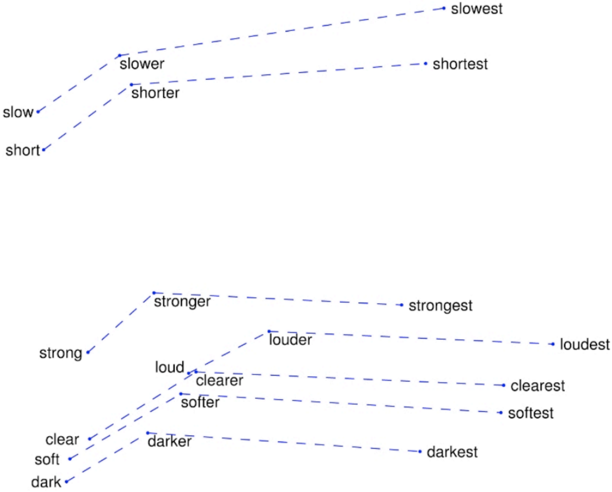
GloVe Visualizations: Superlatives



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Word Embeddings: Some Open Problems

- Can we have word embeddings for multiple languages in the same space?
- How to capture polysemy?
- These word embeddings are static, can we compute embeddings on-the-fly depending on the context?

Cross-Lingual Word Embeddings

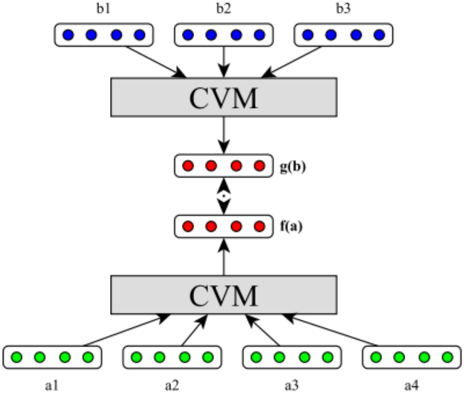

Figure 1: Model with parallel input sentences a and b. The model minimises the distance between the sentence level encoding of the bitext. Any composition functions (CVM) can be used to generate the compositional sentence level representations.

(From Hermann and Blunsom (2014).)

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- Use a corpus of parallel sentences in two languages

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Cross-Lingual Word Embeddings

Other approaches:

- Define a bilingual dictionary and apply canonical correlation analysis (Faruqui and Dyer, 2014)

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This is a very active area of research!

Contextual Embeddings

Words can have different meanings, depending on the context

In 2018, a model called ELMo learned context-dependent embeddings and achieved impressive results on 6 NLP downstream tasks (Peters et al., 2018)

Key idea:

- Pre-train a BILSTM language model on a large dataset (we'll see in a later class what this is)
- Save all the encoder parameters at all layers, not only the embeddings
- Then, for your downstream task, tune a scalar parameter for each layer, and pass the entire sentence through this encoder.

BERT, GPT, etc.

Some time later, a Transformer-based model (BERT) achieved even better performance:

BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding

Jacob Devlin Ming-Wei Chang Kenton Lee Kristina Toutanova
Google AI Language
{jacobdevlin,mingweichang,kentonl,kristout}@google.com

Huge improvements in multiple NLP tasks!

(Trained on 64 TPU chips!!)

Other related models include GPT-2, GPT-3, etc.

This will be covered in a later lecture!

Outline

Conclusions

- Neural nets learn internal representations that can be transferred across tasks
- Distributed representations are exponentially more compact and allow generalizing to unseen objects
- Deeper neural nets exhibit hierarchical compositionality: upper level layers learn more abstract/semantic representations than bottom level layers
- Auto-encoders are an effective means for learning representations
- Word embeddings are continuous representations of words that are extremely useful in NLP

Thank you!

Questions?

References I

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