CSC421/2516 Lecture 3: Automatic Differentiation & Distributed Representations

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- Lecture 2 covered the algebraic view of backprop.
- This lecture focuses on how to implement an automatic differentiation library:
 - build the computation graph
 - vector-Jacobian products (VJP) for primitive ops
 - the backwards pass
- We'll cover, Autograd, a lightweight autodiff tool. PyTorch's implementation is very similar.
 - You will probably never have to implement autodiff yourself but it is good to know its inner workings.

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- Automatic differentiation (autodiff) refers to a general way of taking a program which computes a value, and automatically constructing a procedure for computing derivatives of that value.
- Backpropagation is the special case of autodiff applied to neural nets
 - But in machine learning, we often use backprop synonymously with autodiff
- Autograd is the name of a particular autodiff library we will cover in this lecture. There are many others, e.g. PyTorch, TensorFlow.

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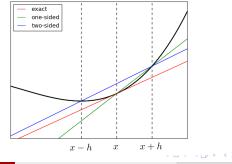
What Autodiff Is Not: Finite Differences

We often use finite differences to check our gradient calculations.
 One-sided version:

$$\frac{\partial}{\partial x_i} f(x_1, \ldots, x_N) \approx \frac{f(x_1, \ldots, x_i + h, \ldots, x_N) - f(x_1, \ldots, x_i, \ldots, x_N)}{h}$$

Two-sided version:

$$\frac{\partial}{\partial x_i}f(x_1,\ldots,x_N)\approx\frac{f(x_1,\ldots,x_i+h,\ldots,x_N)-f(x_1,\ldots,x_i-h,\ldots,x_N)}{2h}$$



What Autodiff Is Not: Finite Differences

- Autodiff is not finite differences.
 - Finite differences are expensive, since you need to do a forward pass for *each* derivative.
 - It also induces huge numerical error.
 - Normally, we only use it for testing.
- Autodiff is both efficient (linear in the cost of computing the value) and numerically stable.

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What Autodiff Is

- An autodiff system will convert the program into a sequence of primitive operations (ops) which have specified routines for computing derivatives.
- In this representation, backprop can be done in a completely mechanical way.

Sequence of primitive operations: $t_{1} = w_{2}$

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Original program:	$\iota_1 = w_{\lambda}$
	$z = t_1 + b$
z = wx + b	$t_3 = -z$
$y = \frac{1}{1 + \exp(-z)}$	$t_4 = \exp(t_3)$
	$t_5 = 1 + t_4$
$\mathcal{L}=rac{1}{2}(y-t)^2$	$y=1/t_5$
-	$t_6 = y - t$
	$t_7 = t_6^2$
	$\mathcal{L}=t_7/2$

What Autodiff Is

```
import autograd.numpy as np 
from autograd import grad
                                    verv sneakv!
def sigmoid(x):
    return 0.5*(np.tanh(x) + 1)
def logistic_predictions(weights, inputs):
    # Outputs probability of a label being true according to logistic model.
    return sigmoid(np.dot(inputs. weights))
def training_loss(weights):
    # Training loss is the negative log-likelihood of the training labels.
    preds = logistic_predictions(weights, inputs)
    label_probabilities = preds * targets + (1 - preds) * (1 - targets)
    return -np.sum(np.log(label probabilities))
                        ... (load the data) ...
# Define a function that returns gradients of training loss using Autograd.
training_gradient_fun = grad(training_loss)

    Autograd constructs a

# Optimize weights using gradient descent.
                                             function for computing derivatives
weights = np.array([0.0, 0.0, 0.0])
print "Initial loss:", training_loss(weights)
for i in xrange(100):
    weights -= training gradient fun(weights) * 0.01
print "Trained loss:", training_loss(weights)
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```

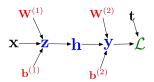
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Autograd

- The rest of this lecture covers how Autograd is implemented.
- Source code for the original Autograd package:
 - https://github.com/HIPS/autograd
- Autodidact, a pedagogical implementation of Autograd you are encouraged to read the code.
 - https://github.com/mattjj/autodidact
 - Thanks to Matt Johnson for providing this!

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Building the Computation Graph

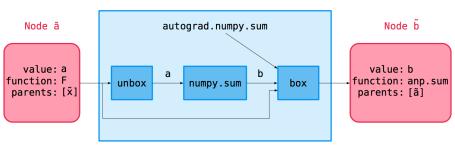


- Most autodiff systems, including Autograd, explicitly construct the computation graph.
 - Some frameworks like TensorFlow provide mini-languages for building computation graphs directly. Disadvantage: need to learn a totally new API.
 - Autograd instead builds them by tracing the forward pass computation, allowing for an interface nearly indistinguishable from NumPy.
- The Node class (defined in tracer.py) represents a node of the computation graph. It has attributes:
 - value, the actual value computed on a particular set of inputs
 - fun, the primitive operation defining the node
 - args and kwargs, the arguments the op was called with
 - parents, the parent Nodes

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Building the Computation Graph

- Autograd's fake NumPy module provides primitive ops which look and feel like NumPy functions, but secretly build the computation graph.
- They wrap around NumPy functions:



primitive

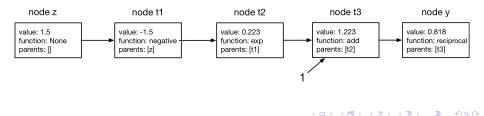
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Building the Computation Graph

Example:

```
def logistic(z):
    return 1. / (1. + np.exp(-z))
# that is eauivalent to:
def logistic2(z):
    return np.reciprocal(np.add(1, np.exp(np.negative(z))))
```

```
z = 1.5
y = logistic(z)
```



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Recap: Vector-Jacobian Products

• Recall: the Jacobian is the matrix of partial derivatives:

$$\mathbf{J} = \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_n} \end{pmatrix}$$

 The backprop equation (single child node) can be written as a vector-Jacobian product (VJP):

$$\overline{x_j} = \sum_i \overline{y_i} \frac{\partial y_i}{\partial x_j} \qquad \overline{\mathbf{x}} = \overline{\mathbf{y}}^\top \mathbf{J}$$

That gives a row vector. We can treat it as a column vector by taking

$$\overline{\mathbf{x}} = \mathbf{J}^{\top}\overline{\mathbf{y}}$$

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Recap: Vector-Jacobian Products

Examples

Matrix-vector product

$$z = Wx$$
 $J = W$ $\overline{x} = W^{\top}\overline{z}$

Elementwise operations

$$\mathbf{y} = \exp(\mathbf{z})$$
 $\mathbf{J} = \begin{pmatrix} \exp(z_1) & 0 \\ & \ddots & \\ 0 & \exp(z_D) \end{pmatrix}$ $\overline{\mathbf{z}} = \exp(\mathbf{z}) \circ \overline{\mathbf{y}}$

• Note: we never explicitly construct the Jacobian. It's usually simpler and more efficient to compute the VJP directly.

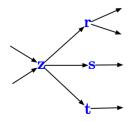
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Vector-Jacobian Products

- For each primitive operation, we must specify VJPs for *each* of its arguments. Consider $y = \exp(x)$.
- This is a function which takes in the output gradient (i.e. y), the answer (y), and the arguments (x), and returns the input gradient (x)
- defvjp (defined in core.py) is a convenience routine for registering VJPs. It just adds them to a dict.
- Examples from numpy/numpy_vjps.py

21 2 1 2	lambda g, lambda g, lambda g,	ans, x:	ans * g)
defvjp(add,	lambda	g, ans,	х, у : g,
	lambda	g, ans,	x, y : g)
<pre>defvjp(multiply,</pre>			x, y : y * g,
	lambda	g, ans,	x, y : x * g)
<pre>defvjp(subtract,</pre>	lambda	g, ans,	х, у: g,
	lambda	g, ans,	x, y : -g)

Backprop as Message Passing



 Consider a naïve backprop implementation where the z module needs to compute z using the formula:

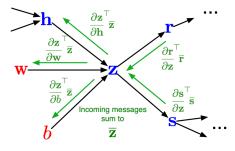
$$\overline{\mathbf{z}} = \frac{\partial \mathbf{r}}{\partial \mathbf{z}}\overline{\mathbf{r}} + \frac{\partial \mathbf{s}}{\partial \mathbf{z}}\overline{\mathbf{s}} + \frac{\partial \mathbf{t}}{\partial \mathbf{z}}\overline{\mathbf{t}}$$

• This breaks modularity, since **z** needs to know how it's used in the network in order to compute partial derivatives of **r**, **s**, and **t**.

Backprop as Message Passing

Backprop as message passing:

• Each node receives a bunch of messages from its children, which it aggregates to get its error signal. It then passes messages to its parents.



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- Each of these messages is a VJP.
- This formulation provides modularity: each node needs to know how to compute its outgoing messages, i.e. the VJPs corresponding to each of its parents (arguments to the function).

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• The implementation of z doesn't need to know where \overline{z} came from.

Backward Pass

- The backwards pass is defined in core.py.
- The argument g is the error signal for the end node; for us this is always $\overline{\mathcal{L}} = 1$.

```
def backward_pass(g, end_node):
    outgrads = {end_node: g}
    for node in toposort(end_node):
        outgrad = outgrads.pop(node)
        fun, value, args, kwargs, argnums = node.recipe
        for argnum, parent in zip(argnums, node.parents):
            vjp = primitive_vjps[fun][argnum]
            parent_grad = vjp(outgrad, value, *args, **kwargs)
            outgrads[parent] = add_outgrads(outgrads.get(parent), parent_grad)
    return outgrad
```

```
def add_outgrads(prev_g, g):
    if prev_g is None:
        return g
    return prev_g + g
```

Backward Pass

- grad (in differential_operators.py) is just a wrapper around make_vjp (in core.py) which builds the computation graph and feeds it to backward_pass.
- grad itself is viewed as a VJP, if we treat $\overline{\mathcal{L}}$ as the 1×1 matrix with entry 1.

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \frac{\partial \mathcal{L}}{\partial \mathbf{w}} \overline{\mathcal{L}}$$

```
def make_vjp(fun, x):
    """Trace the computation to build the computation graph, and return
    a function which implements the backward pass."""
    start_node = Node.new_root()
    end_value, end_noade = trace(start_node, fun, x)
    def vjp(g):
        return backward_pass(g, end_node)
    return vjp, end_value

def grad(fun, argnum=0):
    def gradfun(*args, **kwargs):
        unary_fun = lambda x: fun(*subval(args, argnum, x), **kwargs)
        vjp, ons = make_vjp(unary_fun, args[argnum])
        return vjp(np.ones_like(ans))
    return gradfun
```

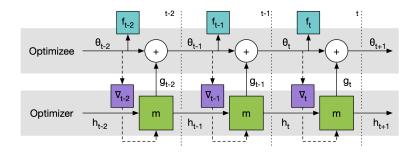
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- We saw three main parts to the code:
 - tracing the forward pass to build the computation graph
 - vector-Jacobian products for primitive ops
 - the backwards pass
- Building the computation graph requires fancy NumPy gymnastics, but other two items are basically what I showed you.
- You're encouraged to read the full code (< 200 lines!) at:

https://github.com/mattjj/autodidact/tree/master/autograd

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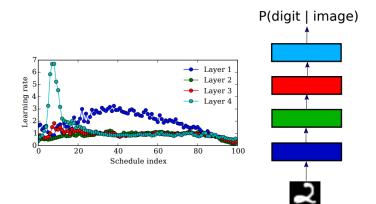
Learning to learning by gradient descent by gradient descent



https://arxiv.org/pdf/1606.04474.pdf

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Gradient-Based Hyperparameter Optimization



https://arxiv.org/abs/1502.03492

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After the break

After the break: Distributed Representations

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Overview

- Let's now take a break from backpropagation and see a real example of a neural net to learn feature representations of words.
 - We'll see a lot more neural net architectures later in the course.
- We'll also introduce the models used in Programming Assignment 1.

Review: Probability and Bayes' Rule

Suppose we want to build a speech recognition system.

We'd like to be able to infer a likely sentence s given the observed speech signal a. The generative approach is to build two components:

- An observation model, represented as $p(\mathbf{a} | \mathbf{s})$, which tells us how likely the sentence \mathbf{s} is to lead to the acoustic signal \mathbf{a} .
- A prior, represented as p(s), which tells us how likely a given sentence **s** is. E.g., it should know that "recognize speech" is more likely that "wreck a nice beach."

Review: Probability and Bayes' Rule

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Given these components, we can use Bayes' Rule to infer a posterior distribution over sentences given the speech signal:

$$p(\mathbf{s} \mid \mathbf{a}) = \frac{p(\mathbf{s})p(\mathbf{a} \mid \mathbf{s})}{\sum_{\mathbf{s}'} p(\mathbf{s}')p(\mathbf{a} \mid \mathbf{s}')}.$$

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From here on, we will focus on learning a good distribution $p(\mathbf{s})$ of sentences. This problem is known as language modeling.

Assume we have a corpus of sentences $\mathbf{s}^{(1)}, \ldots, \mathbf{s}^{(N)}$. The maximum likelihood criterion says we want our model to maximize the probability our model assigns to the observed sentences. We assume the sentences are independent, so that their probabilities multiply.

$$\max\prod_{i=1}^N p(\mathbf{s}^{(i)}).$$

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In maximum likelihood training, we want to maximize $\prod_{i=1}^{N} p(\mathbf{s}^{(i)})$.

- The probability of generating the whole training corpus is vanishingly small like monkeys typing all of Shakespeare.
 - The log probability is something we can work with more easily. It also conveniently decomposes as a sum:

$$\log \prod_{i=1}^{N} p(\mathbf{s}^{(i)}) = \sum_{i=1}^{N} \log p(\mathbf{s}^{(i)}).$$

• This is equivalent to the cross-entropy loss.

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Language Modeling

• Probability of a sentence? What does that even mean?

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Language Modeling

- Probability of a sentence? What does that even mean?
 - A sentence is a sequence of words w_1, w_2, \ldots, w_T . Using the chain rule of conditional probability, we can decompose the probability as

 $p(\mathbf{s}) = p(w_1, \ldots, w_T) = p(w_1)p(w_2 | w_1) \cdots p(w_T | w_1, \ldots, w_{T-1}).$

- Therefore, the language modeling problem is equivalent to being able to predict the next word!
- We typically make a Markov assumption, i.e. that the distribution over the next word only depends on the preceding few words. I.e., if we use a context of length 3,

$$p(w_t | w_1, \ldots, w_{t-1}) = p(w_t | w_{t-3}, w_{t-2}, w_{t-1}).$$

- Such a model is called memoryless.
- Now it's basically a supervised prediction problem. We need to predict the conditional distribution of each word given the previous *K*.
- When we decompose it into separate prediction problems this way, it's called an autoregressive model.

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• One sort of Markov model we can learn uses a conditional probability table, i.e.

	cat	and	city	• • •
the fat	0.21	0.003	0.01	
four score	0.0001	0.55	0.0001	
New York	0.002	0.0001	0.48	
:		:		

• Maybe the simplest way to estimate the probabilities is from the empirical distribution:

$$egin{aligned} p(w_3 = \operatorname{cat} \mid w_1 = \operatorname{the}, w_2 = \operatorname{fat}) &= rac{p(w_1 = \operatorname{the}, w_2 = \operatorname{fat}, w_3 = \operatorname{cat})}{p(w_1 = \operatorname{the}, w_2 = \operatorname{fat})} \ &pprox rac{\operatorname{count}(\operatorname{the} \operatorname{fat} \operatorname{cat})}{\operatorname{count}(\operatorname{the} \operatorname{fat})} \end{aligned}$$

- The phrases we're counting are called n-grams (where n is the length), so this is an n-gram language model.
 - Note: the above example is considered a 3-gram model, not a 2-gram are

Shakespeare:

1 gram	 -To him swallowed confess hear both. Which. Of save on trail for are ay device and rote life have -Hill he late speaks; or! a more to leg less first you enter
2 gram	-Why dost stand forth thy canopy, forsooth; he is this palpable hit the King Henry. Live king. Follow.-What means, sir. I confess she? then all sorts, he is trim, captain.
3 gram	-Fly, and will rid me these news of price. Therefore the sadness of parting, as they say, 'tis done.-This shall forbid it should be branded, if renown made it empty.
4 _{gram}	-King Henry. What! I will go seek the traitor Gloucester. Exeunt some of the watch. A great banquet serv'd in; -It cannot be but so.

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Wall Street Journal:

1 gram	Months the my and issue of year foreign new exchange's september were recession exchange new endorsed a acquire to six executives
2 gram	Last December through the way to preserve the Hudson corporation N. B. E. C. Taylor would seem to complete the major central planners one point five percent of U. S. E. has already old M. X. corporation of living on information such as more frequently fishing to keep her
3 gram	They also point to ninety nine point six billion dollars from two hundred four oh six three percent of the rates of interest stores as Mexico and Brazil on market conditions

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• Problems with n-gram language models

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- Problems with n-gram language models
 - The number of entries in the conditional probability table is exponential in the context length.
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- Problems with n-gram language models
 - The number of entries in the conditional probability table is exponential in the context length.
 - Data sparsity: most n-grams never appear in the corpus, even if they are possible.
- Traditional ways to deal with data sparsity
 - Use a short context (but this means the model is less powerful)
 - Smooth the probabilities, e.g. by adding imaginary counts
 - Make predictions using an ensemble of n-gram models with different n

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Distributed Representations

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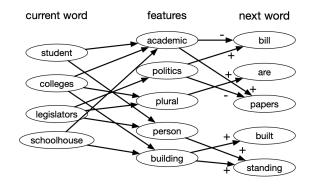
- Conditional probability tables are a kind of localist representation: all the information about a particular word is stored in one place, i.e. a column of the table.
- But different words are related, so we ought to be able to share information between them. For instance, consider this matrix of word attributes:

	academic	politics	plural	person	building
students	1	0	1	1	0
colleges	1	0	1	0	1
legislators	0	1	1	1	0
schoolhouse	1	0	0	0	1

• And this matrix of how each attribute influences the next word:



 Imagine these matrices are layers in an MLP. (One-hot representations of words, softmax over next word.)



- Here, the information about a given word is distributed throughout the representation. We call this a distributed representation.
- In general, when we train an MLP with backprop, the hidden units won't have intuitive meanings like in this cartoon. But this is a useful intuition pump for what MLPs can represent.

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Distributed Representations

- We would like to be able to share information between related words.
 E.g., suppose we've seen the sentence
 The cat got squashed in the garden on Friday.
- This should help us predict the words in the sentence *The dog got flattened in the yard on Monday.*
- An n-gram model can't generalize this way, but a distributed representation might let us do so.

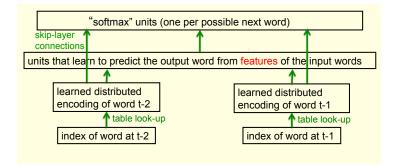
- Predicting the distribution of the next word given the previous K is just a multiway classification problem.
- Inputs: previous K words
- Target: next word
- Loss: cross-entropy. Recall that this is equivalent to maximum likelihood:

$$egin{aligned} &-\log p(\mathbf{s}) = -\log \prod_{t=1}^T p(w_t \mid w_1, \dots, w_{t-1}) \ &= -\sum_{t=1}^T \log p(w_t \mid w_1, \dots, w_{t-1}) \ &= -\sum_{t=1}^T \sum_{v=1}^V t_{tv} \log y_{tv}, \end{aligned}$$

where t_{iv} is the one-hot encoding for the *i*th word and y_{iv} is the predicted probability for the *i*th word being index v.

Bengio's Neural Language Model

• Here is a classic neural probabilistic language model, or just neural language model:

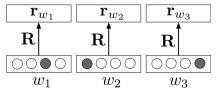


http://www.jmlr.org/papers/volume3/bengio03a/bengio03a.pdf

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• If we use a 1-of-K encoding for the words, the first layer can be thought of as a linear layer with tied weights.



- The weight matrix basically acts like a lookup table. Each column is the representation of a word, also called an embedding, feature vector, or encoding.
 - "Embedding" emphasizes that it's a location in a high-dimensonal space; words that are closer together are more semantically similar
 - "Feature vector" emphasizes that it's a vector that can be used for making predictions, just like other feature mappigns we've looked at (e.g. polynomials)

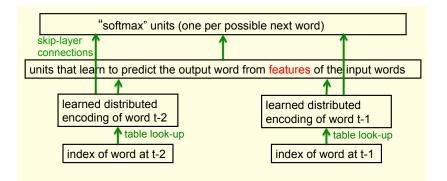
- We can measure the similarity or dissimilarity of two words using
 - the dot product $\mathbf{r}_1^\top \mathbf{r}_2$
 - Euclidean distance $\|\mathbf{r}_1 \mathbf{r}_2\|$
- If the vectors have unit norm, the two are equivalent:

$$\|\mathbf{r}_1 - \mathbf{r}_2\|^2 = (\mathbf{r}_1 - \mathbf{r}_2)^\top (\mathbf{r}_1 - \mathbf{r}_2)$$
$$= \mathbf{r}_1^\top \mathbf{r}_1 - 2\mathbf{r}_1^\top \mathbf{r}_2 + \mathbf{r}_2^\top \mathbf{r}_2$$
$$= 2 - 2\mathbf{r}_1^\top \mathbf{r}_2$$

• In this case, the dot product is called cosine similarity.

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• This model is very compact: the number of parameters is *linear* in the context size, compared with exponential for n-gram models.



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- What do these word embeddings look like?
- It's hard to visualize an *n*-dimensional space, but there are algorithms for mapping the embeddings to two dimensions.
- The following 2-D embeddings are done with an algorithm called tSNE which tries to make distnaces in the 2-D embedding match the original 30-D distances as closely as possible.
- Note: the visualizations are from a slightly different model.

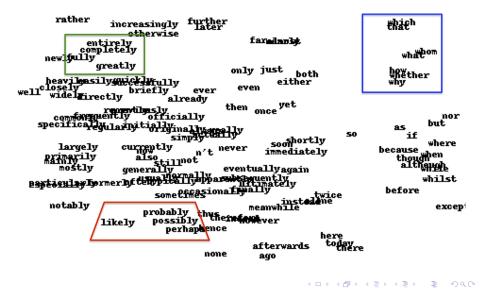
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- Thinking about high-dimensional embeddings
 - Most vectors are nearly orthogonal (i.e. dot product is close to 0)
 - Most points are far away from each other
 - "In a 30-dimensional grocery store, anchovies can be next to fish and next to pizza toppings." – Geoff Hinton
- The 2-D embeddings might be fairly misleading, since they can't preserve the distance relationships from a higher-dimensional embedding. (I.e., unrelated words might be close together in 2-D, but far apart in 30-D.)

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• Fitting language models is really hard:

- It's really important to make good predictions about relative probabilities of rare words.
- Computing the predictive distribution requires a large softmax.
- Maybe this is overkill if all you want is word representations.
- Global Vector (GloVe) embeddings are a simpler and faster approach based on a matrix factorization similar to principal component analysis (PCA).
 - First fit the distributed word representations using GloVe, then plug them into a neural net that does some other task (e.g. language modeling, translation).

- Distributional hypothesis: words with similar distributions have similar meanings ("judge a word by the company it keeps")
- Consider a co-occurrence matrix **X**, which counts the number of times two words appear nearby (say, less than 5 positions apart)
- This is a $V \times V$ matrix, where V is the vocabulary size (very large)
- Intuition pump: suppose we fit a rank-K approximation X ≈ RR^T, where R and R are V × K matrices.
 - Each row \mathbf{r}_i of \mathbf{R} is the K-dimensional representation of a word
 - Each entry is approximated as $x_{ij} \approx \mathbf{r}_i^\top \tilde{\mathbf{r}}_j$
 - Hence, more similar words are more likely to co-occur
 - Minimizing the squared Frobenius norm

$$\|\mathbf{X} - \mathbf{R}\widetilde{\mathbf{R}}^{\top}\|_{F}^{2} = \sum_{i,j} (x_{ij} - \mathbf{r}_{i}^{\top}\widetilde{\mathbf{r}}_{j})^{2}$$
 is basically PCA.

• **Problem 1: X** is extremely large, so fitting the above factorization uisng least squares is infeasible.

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- Global Vector (GloVe) embedding cost function:

$$\begin{split} \mathcal{J}(\mathbf{R}) &= \sum_{i,j} f(x_{ij}) (\mathbf{r}_i^\top \tilde{\mathbf{r}}_j + b_i + \tilde{b}_j - \log x_{ij})^2 \\ f(x_{ij}) &= \begin{cases} \left(\frac{x_{ij}}{100}\right)^{3/4} & \text{if } x_{ij} < 100 \\ 1 & \text{if } x_{ij} \ge 100 \end{cases} \end{split}$$

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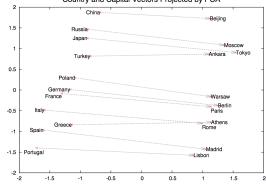
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- b_i and \tilde{b}_j are bias parameters.
- We can avoid computing $\log 0$ since f(0) = 0.
- We only need to consider the nonzero entries of **X**. This gives a big computational savings since **X** is extremely sparse!

Word Analogies

- Here's a linear projection of word representations for cities and capitals into 2 dimensions.
- The mapping city \rightarrow capital corresponds roughly to a single direction in the vector space: Country and Capital Vectors Projected by PCA



• Note: this figure actually comes from skip-grams, a predecessor to GloVe.

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Word Analogies

- In other words,
 vector(Paris) vector(France) ≈ vector(London) vector(England)
- This means we can analogies by doing arithmetic on word vectors:
 - e.g. "Paris is to France as London is to _____'
 - Find the word whose vector is closest to vector(France) - vector(Paris) + vector(London)
- Example analogies:

Relationship	Example 1	Example 2	Example 3	
France - Paris	Italy: Rome	Japan: Tokyo	Florida: Tallahassee	
big - bigger	small: larger	cold: colder	quick: quicker	
Miami - Florida	Baltimore: Maryland	Dallas: Texas	Kona: Hawaii	
Einstein - scientist	Messi: midfielder	Mozart: violinist	Picasso: painter	
Sarkozy - France	Berlusconi: Italy	Merkel: Germany	Koizumi: Japan	
copper - Cu	zinc: Zn	gold: Au	uranium: plutonium	
Berlusconi - Silvio	Sarkozy: Nicolas	Putin: Medvedev	Obama: Barack	
Microsoft - Windows	Google: Android	IBM: Linux	Apple: iPhone	
Microsoft - Ballmer	Google: Yahoo	IBM: McNealy	Apple: Jobs	
Japan - sushi	Germany: bratwurst	France: tapas	USA: pizza	