Embeddings, neural networks and language models

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Chapters 6, 7 and 9 of Jurafsky & Martin, Speech and Language Processing

Outline

- 1. Embeddings: words as euclidean vectors
- 2. Neural networks
- 3. Language models and NNs
- 4. Recursive NNs
- Ultimate objectives?
 - to mathematically encode the relationships between / meaning of words \implies embeddings
 - to train a *language model*, a model that is able to predict the next word in a sentence, given the immediately preceding words ⇒ neural language models

Vector semantics and embeddings

- Meaning of / relationship between words has been conceptualised in many ways (see Sec. 6.1)
- Vector semantics identifies the meaning of a word with its *distribution* in language use:
 - essentially, the relative frequency with which it occurs in proximity to other words
 - i.e. its *co-occurrence* with other words
- *Embeddings* represent the distribution of a word in terms of a vector in Euclidean space
 - 'sparse' embeddings (long vectors with many zeros): tf-idf or PPMI
 - 'dense' embeddings (shorter vectors): word2vec
- Representation is exceedingly useful, because it renders the 'meaning' of a word as a mathematical object
- Encodes words in a manner suitable for input into a language model, neural network, etc.

Vectors and documents

- Suppose we have a corpus of documents, and we want to quantify the similarities / differences between them
- Ultimate objective could be document retrieval: you provide the system with a document, and ask it to retrieve similar documents.
- *Term-document matrix* lists the frequencies with which words appear in each document

	As You Like It	Twelfth Night	Julius Caesar	Henry V
battle	1	0	7	13
good	114	80	62	89
fool	36	58	1	4
wit	20	15	2	3

Figure 6.2 The term-document matrix for four words in four Shakespeare plays. Each cell contains the number of times the (row) word occurs in the (column) document.

• Here the corpus is four works; the vocabulary V consists of four words (|V| = 4)

Vectors and documents

• Column vectors describe ('embed') the documents

	As You Like It	Twelfth Night	Julius Caesar	Henry V	
battle	Π	0	7	13	
good	14	80	62	89	
fool	36	58	1	4	
wit	20	15	2	3	

Figure 6.3 The term-document matrix for four words in four Shakespeare plays. The red boxes show that each document is represented as a column vector of length four.

• How to measure similarity between two documents / vectors, v and w?

- ordinary euclidean distance $\| \mathbf{v} \mathbf{w} \|$ inappropriate, because dependent on magnitudes of entries
- we should first normalise the vectors to have unit length, i.e. v/||v||, etc., then use euclidean distance, or cosine similarity

$$\cos\theta = \frac{\boldsymbol{v}^{\mathsf{T}}\boldsymbol{w}}{\|\boldsymbol{v}\|\|\boldsymbol{w}\|}$$

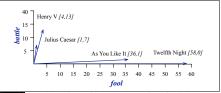


Figure 6.4 A spatial visualization of the document vectors for the four Shakespeare play documents, showing just two of the dimensions, corresponding to the words *battle* and *fool*. The comedies have high values for the *fool* dimension and low values for the *battle* dimension.

Vectors and words

· Row vectors could be used to represent the meaning of words

	As You Like It	Twelfth Night	Julius Caesar	Henry V
battle	1	0	7	13
good fool	114	80	62	89
fool	36	58	1	4
wit	20	15	2	3

Figure 6.5 The term-document matrix for four words in four Shakespeare plays. The red boxes show that each word is represented as a row vector of length four.

• But gives a very coarse-grained measure of meaning (particularly if each document is large!)

Vectors and words

- Better approach is to construct a term-term matrix
 - choose the 'context': a fixed window length, e.g. ± 4 words
 - for each word w in the vocabulary V, record how many times another word v ∈ V appears within w's context, across a corpus
 - yields a |V|-length vector of co-occurrences

	aardvark	 computer	data	result	pie	sugar	
cherry	0	 2	8	9	442	25	
strawberry	0	 0	0	1	60	19	
digital	0	 1670	1683	85	5	4	
information	0	 3325	3982	378	5	13	

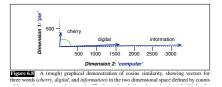
Figure 6.6 Co-occurrence vectors for four words in the Wikipedia corpus, showing six of the dimensions (hand-picked for pedagogical purposes). The vector for *digital* is outlined in red. Note that a real vector would have vastly more dimensions and thus be much sparser.

• Vectors are *sparse*: if V = 50,000, most words will *never* appear in the neighbourhood of most others

Vectors and words

· As with documents, we can use cosine to gauge similarity between words

	pie	data	computer
cherry	442	8	2
digital	5	1683	1670
information	5	3982	3325



- Raw frequencies overly skewed by high co-occurrences with words that are uninformative about meaning, e.g. *the*, *it*, *they*, etc.
- Whereas words that occur very infrequently may be *highly* informative about the meaning of neighbouring words
- Weighting schemes (td-idf) or the PPMI algorithm provide an alternative way of producing (sparse) vectors, that are less affected by these problems (Sec. 6.5–6.7)

Dense embeddings

- However, a better approach in practice appears to be to use dense embedding vectors (of length around 300 rather than 30,000)
- Appear better able e.g. to capture synonymy between words, which is lost by a sparse vector that treats very similar words (e.g. *car* and *automobile*) as entirely separate entries of the vocabulary
- Leading example is the word2vec algorithm, which is based on a classification / prediction problem

- Suppose we take the *context* of a word w to a ± 2 word window, as e.g.
 - ... lemon, a [tablespoon of apricot jam, a] pinch ... c1 c2 w c3 c4
- Given the word w, what is the probability P(+ | w, c) that some other word c ∈ V appears in w's context?
- Let w and c denote (dense) \mathbb{R}^d -valued embeddings for these words. Then

$$\mathbb{P}(+ \mid w, c) = \frac{1}{1 + \exp(-\boldsymbol{c}^{\mathsf{T}}\boldsymbol{w})} = \sigma(\boldsymbol{c}^{\mathsf{T}}\boldsymbol{w})$$

so the probability is highest for words that are 'similar' in the sense that $\bm{c}^{\mathsf{T}}\bm{w}$ is large and positive

- Ultimately, the collection of w's and c's, stacked (columnwise) in the matrices W and C, will provide our embeddings for the words in V
- The problem then is to estimate W and C, i.e. to 'train the classifier' on a corpus of text

- ... lemon, a [tablespoon of apricot jam, a] pinch ... c1 c2 w c3 c4
- Want to construct a quasi-likelihood / loss function to estimate the model. What do we learn when observe the above?
- 1. $c_1, \ldots, c_L \in V$ appear in the context of w; if we assume (heroically!) that context words appear independently of each other

$$\mathbb{P}(+ \mid w, c_1, \ldots, c_L) = \prod_{i=1}^L \mathbb{P}(+ \mid w, c_i) = \prod_{i=1}^L \sigma(\boldsymbol{c}_i^{\mathsf{T}} \boldsymbol{w})$$

2. $c \in V \setminus \{c_1, \ldots, c_L\}$ did *not* appear in the context for *w*; for a *single* word *c*, this occurs with probability

$$\mathbb{P}(-\mid \boldsymbol{w}, \boldsymbol{c}) = 1 - \sigma(\boldsymbol{c}^{\mathsf{T}}\boldsymbol{w});$$

 Assuming independence, the log quasi-likelihood of observing w in the context of (c₁,..., c_L) would be

$$\sum_{i=1}^{L} \log \sigma(\boldsymbol{c}_{i}^{\mathsf{T}} \boldsymbol{w}) + \sum_{\boldsymbol{c} \in \boldsymbol{V} \setminus \{\boldsymbol{c}_{1}, \dots, \boldsymbol{c}_{L}\}} \log[1 - \sigma(\boldsymbol{c}^{\mathsf{T}} \boldsymbol{w})]$$

$$\sum_{i=1}^{L} \log \sigma(\boldsymbol{c}_{i}^{\mathsf{T}} \boldsymbol{w}) + \sum_{\boldsymbol{c} \in V \setminus \{\boldsymbol{c}_{1}, \dots, \boldsymbol{c}_{L}\}} \log[1 - \sigma(\boldsymbol{c}^{\mathsf{T}} \boldsymbol{w})]$$

• Problem: objective is overwhelmed by the second term

nositivo ovomplos

• So instead, replace the by a random selection of k 'noise' words, chosen in proportion to some weighted frequency measure, e.g.

lemon,	a [tablespoon	of	apricot	jam,	a] pinch
	c1	c2	W	c3	c4

positive examples +		negative examples -						
W	$c_{\rm pos}$	w	cneg	W	cneg			
apricot	tablespoon	apricot	aardvark	apricot	seven			
apricot	of	apricot	my	apricot	forever			
apricot	jam	apricot	where	apricot	dear			
apricot	a	apricot	coaxial	apricot	if			

• Leads to, for $c_{*,i}$ drawn randomly from $V \setminus \{c_1, \ldots, c_L\}$:

$$\sum_{i=1}^{L} \log \sigma(\boldsymbol{c}_{i}^{\mathsf{T}} \boldsymbol{w}) + \sum_{i=1}^{kL} \log[1 - \sigma(\boldsymbol{c}_{*,i}^{\mathsf{T}} \boldsymbol{w})]$$

$$\sum_{i=1}^{L} \log \sigma(\boldsymbol{c}_{i}^{\mathsf{T}} \boldsymbol{w}) + \sum_{i=1}^{kL} \log[1 - \sigma(\boldsymbol{c}_{*,i}^{\mathsf{T}} \boldsymbol{w})]$$

- We then sum this over all word w and context (c_1, \ldots, c_L) pairs, and maximise with the aid of stochastic gradient ascent.
- Yields a collection of word *w_i* and context *c_i* parameter vectors / embeddings of length *d*; for each word *w_i* ∈ *V*
- We may take \boldsymbol{w}_i or e.g. $\boldsymbol{w}_i + \boldsymbol{c}_i$ to be the word2vec embedding
- [How should we choose d? Cross-validation / information criteria?]
- For some of the 'nice' semantic properties of these embeddings, see Sec. 6.10

Next step: language models

- Now we have a way to (usefully) represent words as vectors
- We can start to mathematically model the dependence between words in sentences
- But this dependence may be very complicated ...

Neural networks: motivation

• The mapping from context to (the distribution of the next) word

$$\underbrace{I \text{ have to make sure the cat gets}}_{\text{context}} \begin{cases} \text{fed} \\ \text{spayed} \\ ??? \end{cases}$$

- is potentially highly nonlinear with unknown functional forms
- we have a potentially enormous large corpus of text from which to estimate it
- but little a priori theoretical guidance as to what class a 'good' model might come from
- A nonparametric estimation problem?
 - we need a flexible class of models capable of approximating a wide range of functions
 - neural networks provide a nonlinear universal approximator

Computational units

• Simple NNs are composed of (layers of) units of the form

$$\boldsymbol{g} = \boldsymbol{g}(\boldsymbol{w}^{\mathsf{T}}\boldsymbol{x}) = \boldsymbol{g}\left(\sum_{i=1}^{n} w_i x_i\right)$$

• $\mathbf{x} = (x_1, \dots, x_n)$ is a vector of *n* inputs (includes a constant input)

- *a* is the real-valued output
- g is monotone, typically either:
 - sigmoid: $\sigma(z) = 1/(1 + e^{-z})$, maps to [0, 1]
 - $tanh(z) = (e^{z} e^{-z})/(e^{z} + e^{-z})$, maps to [-1, 1]
 - 'rectified linear': $\operatorname{ReLU}(z) = \max\{z, 0\}$, maps to $[0, \infty)$.

Computational units

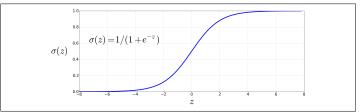
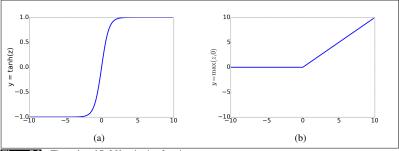


Figure 7.1 The sigmoid function takes a real value and maps it to the range (0,1). It is nearly linear around 0 but outlier values get squashed toward 0 or 1.





Feedforward neural networks

- One unit cannot approximate much on its own: [see their XOR example]
 - it is merely a transformed linear (affine) function
 - the extent of the possible nonlinearity is extremely circumscribed
- We can do much better by 'nesting' multiple units within each other
 - hierarchy of units: taking inputs from previous 'layers', providing output to subsequent 'layers' of units
 - basis for feedforward neural networks (NNs): multiple layers, but no cycles
- Nonlinearity is important: multiple nested layers of *linear* units are equivalent to a single linear function

Feedforward neural networks

- 2-layer example: one 'hidden' and one 'output' layer
- n_0 inputs given by $\boldsymbol{x} = (x_1, \dots, x_{n_0})$
- n₁ units in the hidden layer, of the form

$$\boldsymbol{h} = \begin{bmatrix} h_1 \\ \vdots \\ h_{n_1} \end{bmatrix} = \begin{bmatrix} g(\boldsymbol{w}_1^{\mathsf{T}} \boldsymbol{x}) \\ \vdots \\ g(\boldsymbol{w}_{n_1}^{\mathsf{T}} \boldsymbol{x}) \end{bmatrix} = \boldsymbol{g}(\boldsymbol{W} \boldsymbol{x}), \qquad \boldsymbol{W} = \begin{bmatrix} \boldsymbol{w}_1^{\mathsf{T}} \\ \vdots \\ \boldsymbol{w}_{n_1}^{\mathsf{T}} \end{bmatrix}$$

- produces a representation of the input
- output layer:
 - takes linear combinations z = Uh of the outputs of the hidden layer
 - produces a Rⁿ²-valued output, where n2 (and the transformation of z used to get it) depends on the problem
 - e.g. if we want to produce a probability distribution over the next word, use

$$[\operatorname{softmax}(\boldsymbol{z})]_i = \frac{\exp(z_i)}{\sum_{j=1}^d \exp(z_j)}$$

for $\boldsymbol{z} = (z_1, \dots, z_d) \in \mathbb{R}^d$; the softmax function [the multinomial logit pmf]

Feedforward neural networks

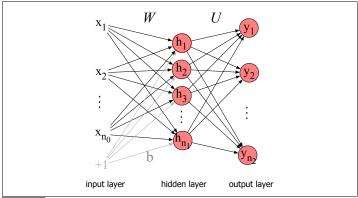


Figure 7.8 A simple 2-layer feedforward network, with one hidden layer, one output layer, and one input layer (the input layer is usually not counted when enumerating layers).

hidden:
$$\boldsymbol{h} = \boldsymbol{g}(\boldsymbol{W}\boldsymbol{x})$$

output: $\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{U}\boldsymbol{h})$

Training [estimation]

- Data: suppose we observe pairs of the form (y, x)
 - y is a K-vector of all zeros, except for one element equal to unity
 - nonzero element indicates which of the K outcomes actually 'happened'
 - 'self supervised' learning, because the data automatically contains the correct outcomes
- NN yields a ('probabilistic') prediction $\hat{y} = \hat{y}(x)$ of y
- 'Loss function': cross entropy loss; for a single observation

$$egin{aligned} &L_{ ext{CE}}(oldsymbol{W},oldsymbol{U};oldsymbol{y},oldsymbol{x}) &= -\sum_{k=1}^{K} y_k \log \hat{y}_k(oldsymbol{x};oldsymbol{W},oldsymbol{U}) \ &= -\sum_{k=1}^{K} 1\{y_k=1\} \log \hat{y}_k(oldsymbol{x};oldsymbol{W},oldsymbol{U}) \end{aligned}$$

- equals conditional probability assigned by the model to the *actual* outcome
- just the negative of the (quasi-)loglikelihood, for a model in which y has MNL distribution with probabilities given by $\hat{y} = \hat{y}(x)$, conditional on x

Training [estimation]

$$L_{\rm CE}(\boldsymbol{W}, \boldsymbol{U}; \boldsymbol{y}, \boldsymbol{x}) = -\sum_{k=1}^{K} y_k \log \hat{y}_k(\boldsymbol{x}; \boldsymbol{W}, \boldsymbol{U})$$

- Want to minimise the loss / maximise the quasi-likelihood
- Can we use (stochastic) gradient descent?
 - ŷ_k(x; W, U) is a potentially complicated nonlinear function of W and U: multiple units in multiple layers
 - but all the constituent units involve only smooth transformations, so derivatives always exist
- Calculation of the gradient:
 - can be broken down into manageable pieces via 'backwards differentiation'
 - basically, compute gradient at each layer, and then combine as per the chain rule
- Non-convex objective, so potentially highly sensitive to starting values

Language models and NNs

- Language models:
 - aim to predict the next next word in a sentence, based on the preceding words, the *context*

I have to make sure the cat gets ???

- mathematically, model the conditional distribution of the *t*th word w_t given w_{t-1}, w_{t-2}, \ldots
- N-gram language models: [Ch. 3]
 - suppose this dependence is Markovian, for some window length N

$$p(w_t \mid w_{t-1}, w_{t-2}, \ldots) = p(w_t \mid w_{t-1}, \ldots, w_{t-N+1}) = p(w_t \mid c_{t-1})$$

- estimate p(w_t | c_{t-1}) 'nonparametrically' using observed relative frequencies (or modifications thereof)
- Weaknesses of *N*-gram models:
 - we may see very few occurrences of the exact (w_t, c_{t-1}) even in huge datasets
 - no way of exploiting similarities between meanings of words to learn about p(w_t | c_{t-1}) from 'similar' (w'_t, c'_{t-1}) [e.g. '... dog gets fed' above]

Language models and NNs

- Neural language models:
 - may make the same Markovian assumption as N-gram models
 - but work with word embeddings, which encode approximate similarities between word meanings
 - embeddings encoded in a matrix $\boldsymbol{E} \in \mathbb{R}^{d \times |V|}$, where d is the dimension of the embedding, and |V| the length of the vocabulary
- Structure otherwise that of a generic neural network

input:
$$\boldsymbol{e} = [\boldsymbol{E}\boldsymbol{x}_{t-N+1}; \dots; \boldsymbol{E}\boldsymbol{x}_{t-1}]$$

hidden: $\boldsymbol{h} = \boldsymbol{g}(\boldsymbol{W}\boldsymbol{e})$
output: $\boldsymbol{y} = \operatorname{softmax}(\boldsymbol{U}\boldsymbol{h})$

where $x_{it} = 1$ if observed word w_t = the *i*th entry in the vocabulary *V*, and 0 otherwise

- output = conditional probability distribution over w_t , given $w_{t-1}, \ldots, w_{t-N+1}$
- Parameters to be estimated: W, U (as before), and (possibly) also E

Language models and NNs

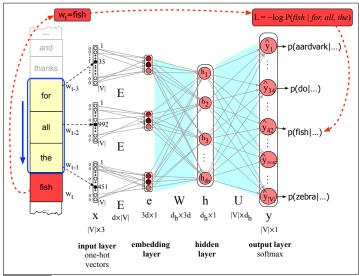


Figure 7.18 Learning all the way back to embeddings. Again, the embedding matrix E is shared among the 3 context words.

Recursive NNs: background

- How can we improve on the preceding?
- Feedforward neural language models impose *finite dependence* of w_t on the context $c_{t-1} = (w_{t-1}, \dots, w_{t-N+1})$
 - only the previous N words matter, e.g. if N = 3

I have to make sure the cat gets ???

anything prior to 'the' is entirely forgotten

• a consequence of the Markov assumption, recall

 $p(w_t \mid w_{t-1}, w_{t-2}, \ldots) = p(w_t \mid w_{t-1}, \ldots, w_{t-N+1}) = p(w_t \mid c_{t-1})$

- but this isn't how any language works!
- How can we build a model with potentially longer-lived dependence? We need to relax the Markov assumption!

Aside: linear state-space models

• The linear counterpart of a feedforward NN is an AR(N) model

$$w_t = \theta_1 w_{t-1} + \theta_2 w_{t-2} + \dots + \theta_N w_{t-N+1} + u_t$$
$$= \theta w_{t-1} + u_t$$

taking N = 1 for simplicity; here u_t is (say) i.i.d.

- given w_{t-1} , the conditional distribution of w_t does not depend on w_{t-s} for any $s \geq 2$
- Compare with the state-space model

$$w_{t+1} = \beta h_t + u_{t+1}$$
$$h_t = \phi h_{t-1} + w_t$$

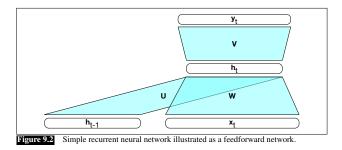
 $\{w_t\}$ is the observed process, h_t the unobserved state

• if $h_0 = 0$, can be 'unrolled' back to period t = 0 as

$$w_{t+1} = \beta h_t + u_{t+1} = \beta \sum_{i=0}^{t-1} \phi^i w_{t-i} + u_{t+1}$$

- now the conditional distribution of w_t depends on every past w_{t-i} (which decreases if |φ| < 1)
- Recursive NN: extend this idea to neural network models, by introducing (a vector of) latent hidden autoregressive states

Recursive NNs



Basic structure:

hidden:
$$\boldsymbol{h}_t = \boldsymbol{g}(\boldsymbol{U}\boldsymbol{h}_{t-1} + \boldsymbol{W}\boldsymbol{x}_t)$$

output: $\boldsymbol{y}_{t+1} = \boldsymbol{f}(\boldsymbol{V}\boldsymbol{h}_t)$

- if $\boldsymbol{U} = 0$, this reduces to a feedforward NN
- e.g. f = softmax
- May have multiple layers, e.g. we may build 'stacked RNNs'
- Can be 'unrolled' in the same way as a linear state-space model

Recursive NNs: unrolling

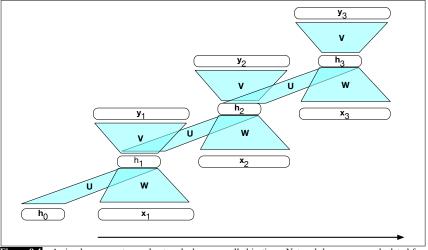


Figure 9.4 A simple recurrent neural network shown unrolled in time. Network layers are recalculated for each time step, while the weights U, V and W are shared across all time steps.

Language models and RNNs

· As with a feedforward neural LM, inputs are vector embeddings of words

input:
$$\boldsymbol{e}_t = \boldsymbol{E} \boldsymbol{x}_t$$

hidden: $\boldsymbol{h}_t = \boldsymbol{g}(\boldsymbol{U}\boldsymbol{h}_{t-1} + \boldsymbol{W}\boldsymbol{e}_t)$
output: $\boldsymbol{y}_{t+1} = \text{softmax}(\boldsymbol{V}\boldsymbol{h}_t)$

• or $e = [Ex_{t-N+1}; ...; Ex_{t-1}]$, etc.; each x_t selects a column from E

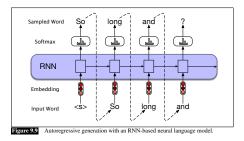
- by construction, \boldsymbol{h}_t depends on *all* previous inputs $\boldsymbol{x}_t, \boldsymbol{x}_{t-1}, \dots$
- 'Forward inference' / prediction is straightforward: requires some initialisation for h_0 , e.g. $h_0 = 0$
- Training / estimation proceeds as for a feedforward NN, using cross-entropy loss

$$L_{\text{CE}}(\boldsymbol{W}, \boldsymbol{U}, \boldsymbol{V}) = -\sum_{k=1}^{K} y_k \log \hat{y}_k(\boldsymbol{x}; \boldsymbol{W}, \boldsymbol{U}, \boldsymbol{V})$$

- 'Weight tying':
 - **V** is a $|V| \times d_h$ matrix that 'scores' the relative conditional probability of the next word, given its context
 - rows provide embeddings for each word in the vocabulary
 - performs the same role as *E* (= dim of *E*^T); we may force *V* = *E*^T to reduce number of model parameters

Generative AI

- Usage as 'generative AI': use the model to recursively predict, until the end of a sentence is reached
- 1. Initialise by setting x_0 to the symbol <s> (or some more task-appropriate context) for the beginning of a sentence; e_0 the corresponding embedding
- 2. At the *t*th step, take x_{t+1} to indicate the element of the vocabulary for which the corresponding element of $y_{t+1} = \operatorname{softmax}(Vh_t)$ is highest
- 3. The next input, $\boldsymbol{e}_{t+1} = \boldsymbol{E} \boldsymbol{x}_{t+1}$ is the embedding corresponding to \boldsymbol{x}_{t+1}



• Continue until the end of sentence marker </s> is output.