Dense representation for categorical variables

One drawback that we flagged with One Hot Encoding of a categorical variable

- Tokens that seem to be related in the input domain ("dog", "dogs")
- Become *unrelated* when One Hot Encoded

Because each value is a long vector

- With a single non-zero element
- That is *different* across the two values
- The OHE vectors are *orthogonal*

This means that there is no useful measure of the distance between two tokens

To illustrate the "lack of distance" issue, let rep be a mapping from tokens to their One Hot Encodings.

Using dot product (cosine similarity) as a measure of similarity to the token "dog"

word	**rep(word)**	**Similarity**
dog	[1,0,0,0]	rep(word) · rep(dog) = 1
dogs	[0,1,0,0]	rep(word) · rep(dog) = 0
cat	[0,0,1,0]	rep(word) · rep(dog) = 0
apple	[0,0,0,1]	rep(word) · rep(dog) = 0

All words other than "dog" are equidistant from "dog".

Intuitively, we observe similarity between "dog" and other words

- ("dog", "dogs"): Same root, different Singular/Plural form
- ("dog", "cat"); Same concept: pet

and complete lack of similarity between "dog" and "apple".

Yet all have the same distance measure from "dog": 0.

We can consider an alternate encoding to OHE.

Suppose each dimension of the encoded vector

- Measured the intensity of the token against some concept
    - Singular/Plural
    - Domestic Animal
    - Edible

This type of representation is called *continuous*

- As the strength is a continuous value
- Compared to the *discrete* encoding of OHE as binary 0/1

It is also called a *dense* representation

- Multiple non-zero elements in the vector
- Compared to the single non-zero element in the OHE vector

In a continuous, dense representation two values expressing similar concepts will be "closer" than two values that do not share concepts

- "Cats", "Dogs", "Apples"
    - Share the concept "Plural"
- "Cat", "Dog"
    - Share the concept "Domestic animal"
- "good", "bad"
    - Share the concept "Opposite"

Doing math with words

Let's explore the implication and power of dense vector representation of words.

If each element of the vector

- Expresses a concept
- And the number of concepts is small compared to $||\mathbf{V}||$
- And the concepts are fairly independent
- Then we have found an alternate basis (compared to the $||\mathbf{V}||$ basis vectors of OHE) of smaller dimension
- For representing words

This concept is sometimes called *word embeddings*

Let $\mathbf{v}_w$ denote the dense representation of token w:

$\boldsymbol{w}$	$\mathbf{v}_{\boldsymbol{w}}$
cat	[.7, .5, .01]
cats	[.7, .5, .95]
dog	[.7, .2, .01]
dogs	[.7, .2, .95]
apple	[.1, .4, .01]
apples	[.1, .4, .95]

Notice that "dogs" and "apples"

- Are similar along one dimension (the last, perhaps encoding "Is Plural")
- Are dissimilar along one dimension (the first, perhaps encoding "Is Pet")

Also notice that "dog" and "cat"

- Are similar along the first dimension (reinforcing the notion that this dimension may be "Is Pet")

Taking this a step further: we can perform element-wise math on dense vector representations:

$$\mathbf{v}_{\text{cats}} - \mathbf{v}_{\text{cat}} \approx \mathbf{v}_{\text{dogs}} - \mathbf{v}_{\text{dog}} \approx \mathbf{v}_{\text{apples}} - \mathbf{v}_{\text{apple}}$$

because

- "cats" and "cat" are similar in all concepts *except* "Plural".
- As are "dogs" and "dog"
- As are "apples" and "apple"

If that's the case, we can approximate the vector that expresses the "pure" concept "Is Plural"

- Without expressing any other concept

as $(\mathbf{v}_{\text{cats}} - \mathbf{v}_{\text{cat}})$

Then we can construct the Plural form of "apple"

- By adding the pure vector for Plural to the vector for "apple"

$$\mathbf{v}_{\text{apples}} \approx \mathbf{v}_{\text{apple}} + (\mathbf{v}_{\text{cats}} - \mathbf{v}_{\text{cat}})$$

we can create the Plural form of "apple"

Word analogies

The implications of doing math on words is even more powerful.

Consider solving the analogy problem

king:man :: ?:woman

That is: what is the female analog of "king" ?

Suppose the concepts ("dimensions") of the dense represenation were

- Gender (man or woman)
- Regal (Royal or commoner)

Then

$$\mathbf{v}_{\text{king}} - \mathbf{v}_{\text{man}} + \mathbf{v}_{\text{woman}} \approx \mathbf{v}_{\text{queen}}$$

because

$$\begin{aligned}
\mathbf{v}_{\text{king}} &= (\text{Man, Royal}) && \text{vector representatio} \\
\mathbf{v}_{\text{king}} - (\text{Man}, 0) &= (0, \text{Royal}) && \text{subtract vector for ''} \\
\mathbf{v}_{\text{king}} - (Man, 0) + (\text{Woman}, 0) &= (\text{Woman, Royal}) && \text{add vector for ''pure} \\
&= \text{Queen} && \text{the word having con}
\end{aligned}$$

We can use math on dense vectors to compute analogies!

Let's formalize the "math" of word vectors

For tokens w, w' with dense vectors $\mathbf{v}_w, \mathbf{v}_{w'}$

- Define a metric $d(\mathbf{v}_w, \mathbf{v}_{w'})$ of the distance between the words
- For example:

$$d(\mathbf{v}_w, \mathbf{v}_{w'}) = 1 - \text{cosine similarity}(\mathbf{v}_w, \mathbf{v}_{w'})$$

Define the set of tokens $N_{n',d}(w)$ in vocabulary $\mathbf{V}$

- That are among the n' "closest" to a token w
- According to distance metric d

$$\begin{array}{lll} \text{wv}_{n',d}(w) & = & \{ \mathbf{v}_{w'} \,|\, \text{rank}_V(d(\mathbf{v}_w, \mathbf{v}_{w'})) \le n' \} \quad \text{the dense vectors of the } n' \text{ t} \\ N_{n',d}(w) & = & \{ w' \,|\, \mathbf{v}_{w'} \in \text{wv}_{n',d}(w) \} \end{array}$$

This is the "neighborhood" of token w as defined by the distance metric.

Token w' is defined to be *approximately equal to* token w

- Denoted as $w \approx_{n',d} w'$
- If w' is in the neighborhood of w

$$w \approx_{n',d} w' \quad \text{if } \mathbf{w}' \in N_{n',d}(w)$$

Thus, the analogy

a:*b* :: *c*:*d*

implies

$$\mathbf{v}_a - \mathbf{v}_b \approx_{n',d} \mathbf{v}_c - \mathbf{v}_d$$

So to solve the word analogy for c:

$$\mathbf{v}_c \approx_{n',d} \mathbf{v}_a - \mathbf{v}_b + \mathbf{v}_d$$

GloVe: Pre-trained embeddings

Fortunately, you don't have to create your own word-embeddings from scratch.

There are a number of pre-computed embeddings freely available.

GloVe is a family of word embeddings that have been trained on large corpra

- GloVe6b
    - Trained on 6 Billion tokens
    - 400K words
    - Corpus: Wikipedia (2014) + GigaWord5 (version 5, news wires 1994-2010)
    - Many different dense vector lengths to choose from
        - 50, 100, 200, 300

We will illustrate the power of word embeddings using GloVe6b vectors of length 100.

$$\begin{aligned}
\text{king- man} + \text{woman} &\approx_{n',d} \text{queen} \\
\text{man - boy} + \text{girl} &\approx_{n',d} \text{woman} \\
\text{Paris - France} + \text{Germany} &\approx_{n',d} \text{Berlin} \\
\text{Einstein - science} + \text{art} &\approx_{n',d} \text{Picasso}
\end{aligned}$$

You can see that the dense vectors seem to encode "concepts", that we can manipulate mathematically.

You may discover some unintended bias

$$\begin{aligned} \text{doctor - man} + \text{woman} &\approx_{n',d} \text{nurse} \\ \text{mechanic - man} + \text{woman} &\approx_{n',d} \text{teacher} \end{aligned}$$

Domain specific embeddings

Do we speak Wikipedia English in this room ?

Here are the neighborhoods of some financial terms, according to GloVe:

$$
\begin{aligned}
N(\text{bull}) &= [\text{cow, elephant, dog, wolf, pit, bear, rider, lion, horse}] \\
N(\text{short}) &= [\text{rather, instead, making, time, though, well, longer, shorter, lo} \\
N(\text{strike}) &= [\text{workers, struck, action, blow, striking, protest, stoppage, wal} \\
N(\text{FX}) &= [\text{showtime, cnbc, ff, nickelodeon, hbo, wb, cw, vh1}]
\end{aligned}
$$

It may be desirable to create word embeddings on a narrow (domain specific) corpus.

This is not difficult provided you have enough data.

Obtaining Dense Vectors: Transfer Learning

How do we obtain Dense Vector representations that seem to have these wonderful properties ?

- Through Machine Learning !
- As a by-product of solving a specific Source task
- Once we have the embeddings, we can re-use them in many other Target tasks.

This is exactly what we called Transfer Learning

- We train a Source Task
- The layers and associated weights learned in training the Source Task
- Are re-used for a different Target Task

The layer and associated weights that implement the dense vector encoding are re-used

- Called an *Embedding Layer*

We will show code that trains an Embedding Layer shortly.

Word prediction problems: high-level

The Source Task we will use to create word embeddings is from a class of *Word Prediction* tasks

- Given a set of tokens (the "context")
- Predict a related token

For example

- Given prefix $\mathbf{w}_{(1)} \dots \mathbf{w}_{(t-1)}$ of a sequence of tokens $\mathbf{w}$
- Predict the next token $\mathbf{w}_{(t)}$.

"Machine Learning is $\langle ??? \rangle$"

Or a similar problem

- Predict token $\mathbf{w}_{(t)}$
- From surrounding tokens $\mathbf{w}_{(t-o)}, \ldots, \mathbf{w}_{(t-1)}, \langle ??? \rangle, \mathbf{w}_{(t+1)} \ldots, \mathbf{w}_{(t+o)}$

"Machine $\langle ??? \rangle$ is easy"

The inspiration behind using a Word Prediction task to learn embeddings

- Is that meaning of a word can be inferred by context
- "You are known by the company that you keep"

For example

- "I ate an apple"
- "I ate a blueberry"
- "I ate a pie"

"apple", "blueberry", "pie" concept: things that you eat

The Word Prediction task is thus a form of Classification.

We need a large number of training examples as this is a Supervised Learning problem.

One reason that Word Prediction is used is that it is fairly easy to obtain training examples

- From any source of raw text
- Just reformat
- That is: the target/label for an example is just an adjacent token

Since targets can be derived from examples, this is sometimes called *Semi-Supervised Learning*

Let $\mathbf{w}$ be the sequence of $n_{\mathbf{w}}$ words

A *word prediction* is a mapping

- from input $\mathbf{w}$
- to a probability distribution $\hat{\mathbf{y}}$ over all words in vocabulary $\mathbf{V}$
  - $\hat{\mathbf{y}}_j = p(V_j)$
  - That is: it assigns a probability to each word in the vocabulary

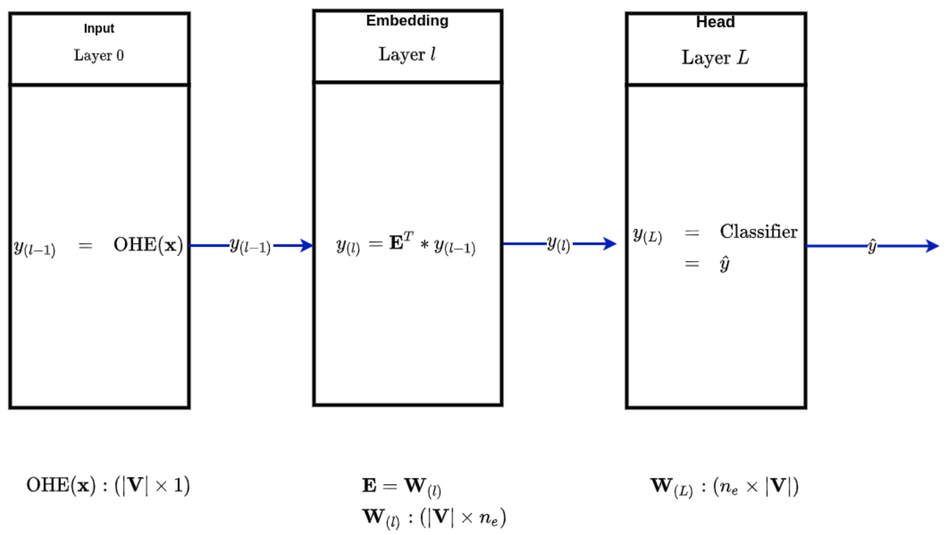
Here are some simple word prediction problems:

$$\begin{array}{lll}
\text{predict next word from context} & p(\mathbf{w}_{(t)}| & \mathbf{w}_{(t-o)} \ldots, \mathbf{w}_{(t-1)}) \\
\text{predict a surrounding word} & p(\mathbf{w}_{(t')}| & \mathbf{w}_{(t)}) \\
 & & t' = \{t-o, \ldots, t+o\} - \{t\} \\
\text{predict center word from context} & p(\mathbf{w}_{(t)}| & [\mathbf{w}_{(t-o)} \ldots \mathbf{w}_{(t-1)} \mathbf{w}_{(t+1)} \ldots \mathbf{w}_{(t+o)}]
\end{array}$$

Here is the Neural Network we construct for the Source Task that will learn embeddings

- Ignoring for the moment the issue of converting variable length sequences to a fixed length

Embedding Layer


Input
Layer 0
$y_{(l-1)} = \mathrm{OHE}(\mathbf{x})$
$y_{(l-1)}$
Embedding
Layer l
$y_{(l)} = \mathbf{E}^T * y_{(l-1)}$
$y_{(l)}$
Head
Layer L
$y_{(L)} = \text{Classifier} = \hat{y}$
$\hat{y}$
$\mathrm{OHE}(\mathbf{x}) : (|\mathbf{V}| \times 1)$
$\mathbf{E} = \mathbf{W}_{(l)}$
$\mathbf{W}_{(l)} : (|\mathbf{V}| \times n_e)$
$\mathbf{W}_{(L)} : (n_e \times |\mathbf{V}|)$

Layers:

- One Hot Encoded token
- Embedding: converts sparse encoding to dense encoding
- Classifier: operating on dense encodings

The only "new" layer type is the Embedding layer

- This is nothing more than Matrix Multiplication
- The mapping can be implemented an $(|\mathbf{V}| \times n_e)$ matrix $\mathbf{E}$
- Where n_e is the length chosen for the dense vector

That is because

- The OHE vector for the j^{th} word $\mathbf{V}_j$ in vocabulary $\mathbf{V}$
- Is the $(|\mathbf{V}| \times 1)$ vector of all 0's except at index j
$$V^{(j)} = 1$$
- $\mathbf{E}^T * \text{OHE}(\mathbf{V}_j)$
- Selects row j of $\mathbf{E}$, which is the is the $(n_e \times 1)$ *dense vector* encoding of $\mathbf{V}_j$

Matrix $\mathbf{E}$ are *weights to be learned* by training

- Along with the weights of the Classifier layer

In other words

- We train the Neural Network
- To create an embedding
- That makes it easy for a Classifier
- To solve the Source Task

Conclusion

Categorical variables (such as tokens/words) are easily represented as One Hot Encoded values.

This is perfectly adequate when there is no relationship between tokens.

Word embeddings/Dense representations create a representation

- Not just of a token is isolation
- But a token with multiple dimensions of meaning
- Which enable inter-token relationships

We showed how to create dense representation of words as a by-product of solving a Source Task.

The Source Task we used was Word Prediction, but other tasks may work as well.

The embeddings learned for the Source Task may be useful in other tasks

- This is Transfer Learning in the real world

```
In [ ]: print("Done")
```