Autoencoding Improves Pre-trained Word Embeddings

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Abstract

Prior work investigating the geometry of pre-trained word embeddings have shown that word embeddings to be distributed in a narrow cone and by centering and projecting using principal component vectors one can increase the accuracy of a given set of pre-trained word embeddings. However, theoretically this post-processing step is equivalent to applying a linear autoencoder to minimise the squared $\ell_2$ reconstruction error. This result contradicts prior work (Mu and Viswanath, 2018) that proposed to remove the top principal components from pre-trained embeddings. We experimentally verify our theoretical claims and show that retaining the top principal components is indeed useful for improving pre-trained word embeddings, without requiring access to additional linguistic resources or labeled data.

1 Introduction

Pre-trained word embeddings have been successfully used as features for representing input texts in many NLP tasks (Dhillon et al., 2015; Mnih and Hinton, 2009; Collobert et al., 2011; Huang et al., 2012; Mikolov et al., 2013; Pennington et al., 2014). Mu and Viswanath (2018) showed that the accuracy of pre-trained word embeddings can be further improved in a post-processing step, without requiring additional training data, by removing the mean of the word embeddings (centering) computed over the set of words (i.e. vocabulary) and projecting onto the directions defined by the principal component vectors, excluding the top principal components. They empirically showed that pre-trained word embeddings are distributed in a narrow cone around the mean embedding vector, and centering and projection help to reinstate isotropy in the embedding space. This post-processing operation has been repeatedly proposed in different contexts such as with distributional (counting-based) word representations (Sahlgren et al., 2016) and sentence embeddings (Arora et al., 2017).

Independently to the above, autoencoders have been widely used for fine-tuning pre-trained word embeddings such as for removing gender bias (Kaneko and Bollegala, 2019), meta-embedding (Bao and Bollegala, 2018), cross-lingual word embedding (Wei and Deng, 2017) and domain adaptation (Chen et al., 2012), to name a few. However, it is unclear whether better performance is obtained simply by applying an autoencoder (a self-supervised task, requiring no labelled data) on pre-trained word embeddings, without performing any task-specific fine-tuning (requires labelled data for the task).

A connection between principal component analysis (PCA) and linear autoencoders was first proved by Baldi and Hornik (1989), extending the analysis by Bourlard and Kamp (1988). We revisit this analysis and theoretically prove that one must retain the largest principal components instead of removing them as proposed by Mu and Viswanath (2018) in order to minimise the squared $\ell_2$ reconstruction loss.

Next, we experimentally show that by applying a non-linear autoencoder we can post-process a given set of pre-trained word embeddings and obtain more accurate word embeddings than by the method proposed by Mu and Viswanath (2018). Although Mu and Viswanath (2018) motivated the removal of largest principal components as a method to improve the isotropy of the word embeddings, our empirical findings show that autoencoding automatically improves isotropy.

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2 Autoencoding as Centering and PCA Projection

Let us consider a set of \( n \)-dimensional pre-trained word embeddings, \( \{x_i\}_{i=1}^N \) for a vocabulary, \( \mathcal{V} \), consisting of \( N \) words. We post-process these pre-trained word embeddings using an autoencoder consisting of a single \( p(< n) \) dimensional hidden layer, an encoder (defined \( W_e \in \mathbb{R}^{n \times p} \) and bias \( b_e \in \mathbb{R}^p \)) and a decoder (defined \( W_d \in \mathbb{R}^{p \times n} \) and bias \( b_d \in \mathbb{R}^n \)). Let \( X \in \mathbb{R}^{n \times N} \) be the embedding matrix. Using matrices \( B \in \mathbb{R}^{p \times N} \), \( H \in \mathbb{R}^{p \times N} \) and \( Y \in \mathbb{R}^{n \times N} \) respectively denoting the activations, hidden states and reconstructed output embeddings, the autoencoder can be specified as follows.

\[
B = W_e X + b_e u^T, \quad H = F(B), \quad Y = W_d H + b_d u^T
\]

Here, \( u \in \mathbb{R}^N \) is a vector consisting of ones and \( F \) is an element-wise activation function. The squared \( \ell_2 \) reconstruction loss, \( J \), for the autoencoder is given by Lemma 1, proved in the appendix.

**Lemma 1.** Let \( X' \) and \( H' \) respectively denote the centred embedding and hidden state matrices. Then, (1) can be expressed using \( X' \) and \( H' \) as

\[
J(W_e, W_d, b_e, b_d) = \|X' - W_d H'\|^2,
\]

where the decoder’s optimal bias vector is given by \( b_d = \frac{1}{N} (X - W_d H) u \).

Lemma 1 holds even for non-linear autoencoders and claims that the centering happens automatically during the minimisation of the reconstruction error. Following Lemma 1, we can assume that the embedding matrix, \( X \), to be already centred and can limit further discussions to this case. Moreover, after centering the input embeddings, the biases can be absorbed into the encoder/decoder matrices by setting an extra dimension that is always equal to 1 in the pre-trained word embeddings. This has the added benefit of simplifying the notations and proofs. Under these conditions, Theorem 2 shows an important connection between linear autoencoders and PCA.

**Theorem 2.** Assume that \( \Sigma_{xx} = XX^\top \) is full-rank with \( n \) distinct eigenvalues \( \lambda_1 > \ldots > \lambda_n \). Let \( I = \{i_1, \ldots, i_p\} \) \( (1 \leq i_1 < \ldots < i_p \leq n) \) be any ordered \( p \)-index set, and \( U_I = [u_{i_1}, \ldots, u_{i_p}] \) denote the matrix formed by the orthogonal eigenvectors of \( \Sigma_{xx} \) associated with the eigenvalues \( \lambda_{i_1}, \ldots, \lambda_{i_p} \). Then, two full-rank matrices \( W_d \) and \( W_e \) define a critical point of (1) for a linear autoencoder if and only if there exists an ordered \( p \)-index set \( I \) and an invertible matrix \( C \in \mathbb{R}^{p \times p} \) such that

\[
\begin{align*}
W_d &= U_I C \\
W_e &= C^{-1} U_I^{-1}
\end{align*}
\]

(2)

Moreover, the reconstruction error, \( J(W_e, W_d) \) can be expressed as

\[
J(W_e, W_d) = \text{tr}(\Sigma_{xx}) - \sum_{i \in I} \lambda_i.
\]

(4)

Proof of Theorem 2 and approximations for non-linear activations are given in the appendix. Because \( \Sigma_{xx} \) is a covariance matrix, it is positive semi-definite. Strict positivity corresponds to it being full-rank and is usually satisfied in practice for pre-trained word embeddings, which are dense and use a small \( n(\ll N) \) independent dimensions for representing the semantics of the words. Moreover, \( W_e, W_d \) are randomly initialised in practice making them full-rank as assumed in Theorem 2.

The connection between linear autoencoders and PCA was first proved by Baldi and Hornik (1989), extending the analysis by Bourlard and Kamp (1988). Reconstructing the principal component vectors from an autoencoder has been discussed by Plaut (2018) without any formal proofs. However, to the best of our knowledge, a theoretical justification for post-processing pre-trained word embeddings by autoencoding has not been provided before.

According to Theorem 2, we can minimise (4) by selecting the largest eigenvalues as \( \lambda_i \). This result contradicts the proposal by Mu and Viswanath (2018) to project the word embeddings away from the
largest principal component vectors, which is motivated as a method to improve isotropy in the word embedding space. They provided experimental evidence to the effect that largest principal component vectors encode word frequency and removal of them is not detrimental to semantic tasks such as semantic similarity measurement and analogy detection. However, the frequency of a word is an important piece of information for tasks that require differentiating stop words and content words such as in information retrieval. Actually, Raunak et al. (2020) demonstrated that removing the top principal components does not necessarily lead to performance improvement. Moreover, contextualised word embeddings such as BERT (Devlin et al., 2019) and Elmo (Peters et al., 2018) have shown to be anisotropic despite their superior performance in a wide-range of NLP tasks (Ethayarajh, 2019). Therefore, it is not readily obvious whether removing the largest principal components to satisfy isotropy is a universally valid strategy. On the other hand, our experimental results show that by autoencoding not only we obtain better embeddings than Mu and Viswanath (2018), but also it improves the isotropy of the pre-trained word embeddings.

3 Experiments

| Parameter     | Value |
|---------------|-------|
| Optimizer     | Adam  |
| Learning rate | 0.0002|
| Dropout rate  | 0.2   |
| Batch size    | 256   |
| Activation function | tanh |

Table 1: Hyperparameter values of the autoencoder.

To evaluate the proposed post-processing method, we use the following pre-trained word embeddings: Word2Vec[1] (300-dimensional embeddings for ca. 3M words learnt from the Google News corpus), GloVe[2] (300-dimensional word embeddings for ca. 2.1M words learnt from the Common Crawl), and fastText[3] (300-dimensional embeddings for ca. 2M words learnt from the Common Crawl).

We use the following benchmarks datasets: for semantic similarity WS-353: Agirre et al. (2009), SIMLEX-999: Hill et al. (2015), RG-65: Rubenstein and Goodenough (1965), MTurk-287: Radinsky et al. (2011), MTurk-771: Halawi et al. (2012) and MEN: Bruni et al. (2014), for analogy Google, MSR (Mikolov et al., 2013), and SemEval: Jurgens et al. (2012)) and for concept categorisation BLESS: Baroni and Lenci (2011) and ESSLI: Baroni et al. (2008)) to evaluate word embeddings.

Table 1 lists the hyperparameters and their values for the autoencoder-based post-processing method used in the experiments. We used the syntactic analogies in the MSR: Mikolov et al. (2013) dataset for setting the hyperparameters. We input each set of embeddings separately to an autoencoder with one hidden layer and minimise the squared $\ell_2$ error using Adam as the optimiser. The pre-trained embeddings are then sent through the trained autoencoder and its hidden layer outputs are used as the post-processed word embeddings. We train an autoencoder (denoted as AE) with a 300-dimensional hidden layer and a tanh activation. Moreover, to study the effect of nonlinearities we train the a linear autoencoder (LAE) without using any nonlinear activation functions in its 300-dimensional hidden layer. Due to space limitations, we show results for autoencoders with different hidden layer sizes in the appendix. We compare the embeddings post-processed using ABTT (stands for all-but-the-top) (Mu and Viswanath, 2018), which removes the top principal components from the pre-trained embeddings.

Table 2 compares the performance of the Original embeddings against the embeddings post-processed using ABTT, LAE and AE. For the semantic similarity task, a high degree of Spearman correlation between human similarity ratings and the cosine similarity scores computed using the word embeddings is considered as better. From Table 2, we see that AE improves word embeddings and outperforms ABTT in almost all semantic similarity datasets. For the word analogy task, we use the PairDiff method (Levy and Goldberg, 2014) to predict the fourth word needed to complete a proportional analogy and the accuracy of the prediction is reported. For the word analogy task, we see that for the GloVe embeddings AE reports the best performance but ABTT performs better for fastText. Overall, the improvements due to

[1] https://code.google.com/archive/p/word2vec/
[2] https://github.com/stanfordnlp/GloVe
[3] https://fasttext.cc/docs/en/english-vectors.html
Table 2: Results are shown for the original embeddings and their post-processed versions by ABTT, linear autoencoder (LAE) and nonlinear autoencoder (AE) for pre-trained Word2Vec, GloVe and fastText embeddings.

**Table 3:** The measure of isotropy of original embeddings and after post-processed using ABTT and AE.

Following the definition given by Mu and Viswanath (2018), we empirically estimate the isotropy of a set of embeddings as $\gamma = \frac{\min_{c \in C} Z(c)}{\max_{c \in C} Z(c)}$, where $C$ is the set of principal component vectors computed for the given set of pre-trained word embeddings and $Z(c) = \sum_{x \in V} \exp(c^\top x)$ is the normalisation coefficient in the partition function defined by Arora et al. (2016). $\gamma$ values close to one indicate a high level of isotropy in the embedding space. From Table 3 we see that compared to the original embeddings ABTT, LAE and AE all improve isotropy.

An alternative approach to verify isotropy is to check whether $Z(c)$ is a constant independent of $c$, which is also known as the self-normalisation property (Andreas and Klein, 2015). Figure 1 shows the histogram of $Z(c)$ of the original pre-trained embeddings, post-processed embeddings using ABTT and AE for pre-trained (a) Word2Vec, (b) GloVe and (c) fastText embeddings for a set of randomly chosen 1000 words $c$ with unit $\ell_2$ norm. Horizontal axes are normalized by the mean of the values. From Figure 1 we see that the original word embeddings in all Word2Vec, GloVe and fastText are far from being
isotropic. On the other hand, AE word embeddings are isotropic, similar to ABTT word embeddings, in all Word2Vec, GloVe and fastText. This result shows that isotropy materialises automatically during autoencoding and does not require special processing such as removing the top principal components as done by ABTT.

In addition to the theoretical and empirical advantages of autoencoding as a post-processing method, it is also practically attractive. For example, unlike PCA, which must be computed using the embeddings for all the words in the vocabulary, autoencoders could be run in an online fashion using only a small mini-batch of words at a time. Moreover, non-linear transformations and regularisation (e.g. in the from of dropout) can be easily incorporated into autoencoders, which can also be stacked for further post-processing. Although online [Warmuth and Kuzmin, 2007; Feng et al., 2013a; Feng et al., 2013b] and non-linear [Scholz et al., 2005] variants of PCA have been proposed, they have not been popular among practitioners due to their computational complexity, scalability and the lack of availability in deep learning frameworks.

4 Conclusion

We showed that autoencoding improves pre-trained word embeddings and outperforms the prior proposal for removing top principal components. Unlike PCA, which must be computed using the embeddings for all the words in the vocabulary, autoencoders could be run in an online fashion using only a small mini-batch of words at a time. Moreover, non-linear transformations and regularisation (e.g. in the from of dropout) can be easily incorporated into autoencoders, which can also be stacked for further post-processing. Although online [Warmuth and Kuzmin, 2007; Feng et al., 2013a; Feng et al., 2013b] and non-linear [Scholz et al., 2005] variants of PCA have been proposed, they are less attractive due to computational complexity, scalability and the lack of availability in deep learning frameworks.

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A Theoretical Proofs

The connection between linear autoencoders and principal component analysis (PCA) was first proved by (Baldi and Hornik, 1989), which provides the basis for Theorem 2. The vast applications of autoencoders such as in language (Socher et al., 2011; Silberer and Lapata, 2014), speech (Gosztolya et al., 2019) and vision (Pu et al., 2016) domains suggest that non-linear autoencoders can indeed learn better representations than PCA.

In this section, we first show that centering of pre-trained word embeddings happens automatically during the optimisation of an autoencoder. This result is stated as Lemma 1 in the paper and holds true irrespectively of the activation function used in the autoencoder, including non-linear activation functions. Next, for linear autoencoders, we recite and prove the connection between linear autoencoders and PCA in the form of Theorem 2. Finally, we discuss the approximations of the Theorem 2 for non-linear autoencoders.

Recall that we defined the autoencoder as follows:

\[
B = W_e X + b_e u^\top
\]

\[
H = F(B)
\]

\[
Y = W_d H + b_d u^\top
\]

Here, \(u \in \mathbb{R}^N\) is a vector consisting of ones and \(F\) is an element-wise activation function. The squared \(\ell_2\) reconstruction loss, \(J\), for the autoencoder is given by (8).

\[
J(W_e, W_d, b_e, b_d) = \left\| W_d F(W_e X + b_e u^\top) + b_d u^\top \right\|^2
\]

For such an autoencoder, Lemma 1 holds.

**Lemma 1.** Let \(X'\) and \(H'\) respectively denote the centred embedding and hidden state matrices. Then, (8) can be expressed using \(X'\) and \(H'\) as \(J(W_e, W_d, b_d, \hat{b}_d) = \|X' - W_d H'\|^2\), where the optimal decoder bias is \(\hat{b}_d = \frac{1}{N} (X - W_d H) u\).

**Proof.** Note that the squared \(\ell_2\) reconstruction error can be written as in (9).

\[
J(W_e, W_d, b_e, b_d) = \|X - Y\|^2
\]

Substituting for \(Y\) from (7) in (9) we have

\[
J(W_e, W_d, b_e, b_d) = \|X - W_d H - b_d u^\top\|^2
\]

\[
= tr \left( (X - W_d H - b_d u^\top) (X - W_d H - b_d u^\top)\right)
\]

From the definition, \(u \in \mathbb{R}^N\) is a vector with all elements set to 1, where \(N\) is the total number of words in the vocabulary \(V\) for which we are given pre-trained embeddings, arranged as columns in \(X \in \mathbb{R}^{n \times N}\). The minimiser of \(J\), w.r.t. \(b_d, \hat{b}_d\) satisfies \(\frac{\partial J}{\partial b_d} = 0\), and is given by (13).

\[
\left( X - W_d H - b_d u^\top \right) u = 0
\]

\[
\hat{b}_d = \frac{1}{N} (X - W_d H) u
\]
In (13) we used $u^\top u = N$. Substituting this minimiser $\hat{b}_d$ back in (10) we obtain the following.

\[
J(W_e, W_d, b_e, \hat{b}_d) = \left\| X - W_dH - \frac{1}{N} (X - W_dH) uu^\top \right\|^2
\]

(14)

\[
= \left\| \left( X - \frac{1}{N}Xuu^\top \right) - W_d \left( H - \frac{1}{N}Hu u^\top \right) \right\|^2
\]

(15)

\[
= \left\| \left( X - \mu_X u^\top \right) - W_d \left( H - \mu_H u^\top \right) \right\|^2
\]

(16)

\[
= \left\| X' - W_dH' \right\|^2
\]

(17)

In (16) we use the mean vectors of embeddings, $\mu_X$, and hidden states $\mu_H$ given respectively by (18) and (19).

\[
\mu_X = \frac{1}{N}Xu
\]

(18)

\[
\mu_H = \frac{1}{N}Hu
\]

(19)

Moreover, we defined the mean-subtracted (i.e. centred) versions of $X$ and $H$ in (17) respectively by $X'$ and $H'$ defined as follows.

\[
X' = X - \mu_X u^\top
\]

(20)

\[
H' = H - \mu_H u^\top
\]

(21)

Using Lemma 1, we can replace the embedding matrix, $X$, by its pre-centred version and further drop the biases as they can be absorbed into the encoder/decoder weight matrices by introducing a dimension set to 1 in the input and output embeddings. Theorem 2 holds under these transformations.

**Theorem 2.** Assume that $\Sigma_{xx}$ is full-rank with $n$ distinct eigenvalues $\lambda_1 > \ldots > \lambda_n$. Let $I = \{i_1, \ldots, i_p\}$ $(1 \leq i_1 < \ldots < i_p \leq n)$ is any ordered $p$-index set, and $U_I = [u_{i_1}, \ldots, u_{i_p}]$ denote the matrix formed by the orthogonal eigenvectors of $\Sigma_{xx}$ associated with the eigenvalues $\lambda_{i_1}, \ldots, \lambda_{i_p}$. Then two full-rank matrices $W_d$ and $W_e$ define a critical point of (8) for a linear autoencoder if and only if there exists an ordered $p$-index set $I$ and an invertible matrix $C \in \mathbb{R}^{p \times p}$ such that

\[
W_d = U_I C,
\]

(22)

\[
W_e = C^{-1}U_I^{-1}.
\]

(23)

Moreover, the reconstruction error, $J(W_e, W_d)$ can be expressed as

\[
J(W_e, W_d) = \text{tr}(\Sigma_{xx}) - \sum_{i \in I} \lambda_i.
\]

(24)

**Proof.** The squared $\ell_2$ reconstruction error can be written by dropping the bias terms and using the centred word embedding matrix $X$ as in (26).

\[
J(W_e, W_d) = \text{tr} \left( (X - W_dW_eX)^\top (X - W_dW_eX) \right)
\]

(25)

\[
= \text{tr}(XX^\top) - 2\text{tr}(XX^\top W_dW_e) + \text{tr}(X^\top W_e^\top W_d^\top W_dW_eX)
\]

(26)
When $W_e$ and $W_d$ are critical points, by setting $\frac{\partial J}{\partial W} = 0$ we obtain
\begin{align*}
-2W_d^TXX^T + 2W_d^TW_dW_eXX^T &= 0 \\
(W_d^T - W_d^TW_d)XX^T &= 0
\end{align*}
(27)

Because the covariance matrix for the pre-trained embeddings, $\Sigma_{xx} = XX^T$ is full-rank and is thus invertible, $W_e$ is given by (23).

\begin{align*}
W_e &= (W_d^T W_d)^{-1} W_d^T \\
\Sigma_{xx} W_e^T (W_e \Sigma_{xx} W_e^T)^{-1} &= W_d
\end{align*}
(29)

Likewise, from $\frac{\partial J}{\partial W_d} = 0$ we obtain
\begin{align*}
0 &= -2XX^TW_e^T + 2W_d(W_eX)(W_eX)^T \\
W_d &= XX^TW_e^T(W_eXX^TW_e^T)^{-1} \\
W_d &= \Sigma_{xx} W_e^T (W_e \Sigma_{xx} W_e^T)^{-1}
\end{align*}
(30)

We will first show that (22) and (23) satisfy respectively (32) and (29), thereby proving the necessary condition. Specifically, from (29) and (22) we have the following.

\begin{align*}
(W_d^T W_d)^{-1} W_d^T &= (U_I C)^T (U_I C)^{-1} (U_I C)^T \\
&= (C^T U_I^T U_I C)^{-1} C^T U_I^T \\
&= C^{-1} (C^T)^{-1} C^T U_I^T \\
&= C^{-1} U_I = W_e
\end{align*}
(33)

In (34), from the orthogonality of $U_I$, we used $U_I^T U_I = I$, where $I \in \mathbb{R}^{p \times p}$ is the identity matrix.

Likewise, from (32) and (23) we have the following.

\begin{align*}
\Sigma_{xx} W_e^T (W_e \Sigma_{xx} W_e^T)^{-1} &= \Sigma_{xx} (C^{-1} U_I^{-1})^T (C^{-1} U_I^{-1} \Sigma_{xx} (U_I^{-1})^T (C^{-1})^T)^{-1} \\
&= \Sigma_{xx} (U_I^T)^{-1} (C^T)^{-1} C^T U_I^T \Sigma_{xx} U_I C \\
&= U_I C = W_d
\end{align*}
(37)

This completes the proof for the necessary condition.

Next, let us look at the sufficient condition. For this purpose, we define for a matrix $M \in \mathbb{R}^{n \times p}$ ($p \ll n$) the orthogonal projection onto the subspace spanned by the columns of $M$ by $P_M$ given by (40).

\begin{align*}
P_M &\triangleq M(M^T M)^{-1} M^T
\end{align*}
(40)

Therefore, for an orthogonal matrix $U$, we can evaluate $P_{U^T W_d}$ as follows.

\begin{align*}
P_{U^T W_d} &= U^T W_d \left( (U^T W_d)^T (U^T W_d) \right)^{-1} (U^T W_d)^T \\
&= U^T W_d \left( W_d^T U U^T W_d \right)^{-1} W_d^T U \\
&= U^T W_d \left( W_d^T W_d \right)^{-1} W_d^T U \\
&= U^T P_{W_d} U
\end{align*}
(41)
In (44), from the definition in (40) we used \( P_{d} = W_d (W_d^T W_d)^{-1} W_d^T \). From (44) we can write \( P_{d} \) as given in (45).

\[
P_{d} = UP_{U^T d} U^T
\]  

(45)

On the other hand, from (32) we have

\[
W_d = \Sigma_{xx} W_e^T (W_e \Sigma_{xx} W_e^T)^{-1},
\]  

(46)

\[
W_d (W_e \Sigma_{xx} W_e^T) = \Sigma_{xx} W_e^T.
\]  

(47)

Right multiplying both sides in (47) by \( W_d^T \) we arrive at

\[
W_d W_e \Sigma_{xx} W_e^T W_d^T = \Sigma_{xx} (W_d W_e)^T.
\]  

(48)

However, by left multiplying (29) by \( W_d \) we get

\[
W_d W_e = W_d (W_d^T W_d)^{-1} W_d^T = P_{W_d}.
\]  

(49)

Substituting for \( W_d W_e \) from (49) back in (48) we obtain

\[
P_{W_d} \Sigma_{xx} P_{W_d}^T = \Sigma_{xx} P_{W_d}^T.
\]  

(50)

Note that by the definition in (40), \( P_{W_d} \) is symmetric (i.e. \( P_{W_d}^T = P_{W_d} \)). Therefore, (50) can be further simplified as given by (51).

\[
P_{W_d} \Sigma_{xx} P_{W_d} = \Sigma_{xx} P_{W_d}
\]  

(51)

Taking the transpose of both sides in (51) we can further show that

\[
(P_{W_d} \Sigma_{xx} P_{W_d})^T = (\Sigma_{xx} P_{W_d})^T
\]  

(52)

\[
P_{W_d} \Sigma_{xx} P_{W_d} = \Sigma_{xx}
\]  

(53)

From (51) and (53) we can deduce that

\[
P_{W_d} \Sigma_{xx} = \Sigma_{xx} P_{W_d} = P_{W_d} \Sigma_{xx} P_{W_d}
\]  

(54)

Because \( \Sigma_{xx} \) is real and symmetric, it can be diagonalised using an orthogonal matrix \( \mathbf{U} \), containing the eigenvectors \( u_1, \ldots, u_n \) of \( \Sigma_{xx} \) in columns, corresponding to the eigenvalues \( \lambda_1, \ldots, \lambda_n \). Specifically, we can write this as in (55).

\[
\Sigma_{xx} = \mathbf{U} \Lambda \mathbf{U}^T
\]  

(55)

Here, \( \Lambda \) is a diagonal matrix with non-increasing eigenvalues \( \lambda_1, \ldots, \lambda_n \).

Let us substitute for \( P_{W_d} \) from (45) and for \( \Sigma_{xx} \) from (55) in (54).

\[
P_{W_d} \Sigma_{xx} = \Sigma_{xx} P_{W_d} = P_{W_d} \Sigma_{xx} P_{W_d}
\]  

(56)

\[
UP_{U^T d} \mathbf{U}^T \mathbf{U} \Lambda \mathbf{U}^T = \mathbf{U} \Lambda \mathbf{U}^T UP_{U^T d} \mathbf{U}^T
\]  

(57)

\[
UP_{U^T d} \mathbf{U} \Lambda = \mathbf{U} \Lambda P_{U^T d} \mathbf{U}^T
\]  

(58)

\[
P_{U^T d} = \mathbf{I}_d
\]  

(59)

Because \( \lambda_1 > \ldots > \lambda_n \), \( P_{U^T d} \) must be a diagonal matrix to satisfy (59). Specifically, \( P_{U^T d} \) contains 1 as an eigenvalue (\( p \) times) and 0 (\( n - p \) times), and can be written using a diagonal matrix \( \mathbf{I}_d \) as follows.

\[
P_{U^T d} = \mathbf{I}_d
\]  

(60)
where the \((i, i)\) diagonal element of \(I_I\) is given by \((61)\).

\[
(I_I)_{(i, i)} = \begin{cases} 
1 & \text{if } i \in \mathcal{I} \\
0 & \text{otherwise}
\end{cases} \quad (61)
\]

Therefore, there exists a unique index set \(\mathcal{I} = \{i_1, \ldots, i_p\}\) with \(1 \leq i_1 < \ldots < i_p \leq n\) such that \(P_{U^TW_d}\) is a diagonal matrix as given by \((60)\).

From \((45)\) and \((49)\) we can write,

\[
P_{W_d} = UP_{U^TW_d}U^T = UI_{I}U^T = W_dW_e, \quad (62)
\]

where \(U_{I} = [u_{i_1}, \ldots, u_{i_p}]\). Therefore, \(P_{W_d}\) is the orthogonal projection onto the subspace spanned by the columns of \(U_{I}\). Since the column space of \(W_d\) coincides with the column space of \(U_{I}\), there exists an invertible \(C \in \mathbb{R}^{p \times p}\) matrix such that

\[
W_d = U_{I}C, \quad \text{and} \quad W_e = C^{-1}U_{I}^{-1}. \quad (63), (64)
\]

Therefore, the parameters (i.e. encoder and decoder matrices) of the autoencoder is uniquely determined only up to the scaling matrix \(C\).

Next, we will consider the reconstruction loss. First, let us substitute \(\Sigma_{xx}\) in \((26)\) and rearrange the terms inside the traces as follows.

\[
J(W_e, W_d) = \text{tr}(\Sigma_{xx}) - 2\text{tr}(\Sigma_{xx}W_dW_e) + \text{tr}(\Sigma_{xx}W_e^TW_dW_dW_e) \quad (65)
\]

In \((65)\), we used \(\text{tr}(ABC) = \text{tr}(CAB) = \text{tr}(BCA)\) when the product of the three matrices \(A, B, C\) are suitably defined.

Substituting for the product \(W_dW_e\) from \((62)\) in \((65)\) we obtain,

\[
J(W_e, W_d) = \text{tr}(\Sigma_{xx}) - 2\text{tr}(\Sigma_{xx}P_{W_d}) + \text{tr}(\Sigma_{xx}P_{W_d}^TP_{W_d}). \quad (66)
\]

From the definition in \((40)\), we see that \(P_{W_d}\) is symmetric (hence, \(P_{W_d}^T = P_{W_d}\)) and moreover that \(P_{W_d}P_{W_d} = P_{W_d}\). Using this fact in \((66)\) we can rewrite,

\[
J(W_e, W_d) = \text{tr}(\Sigma_{xx}) - \text{tr}(\Sigma_{xx}P_{W_d}). \quad (67)
\]

Substituting \((55)\) and \((45)\) in \((67)\) we obtain,

\[
J(W_e, W_d) = \text{tr}(\Sigma_{xx}) - \text{tr}(UAU^TP_{U^TW_d}U^T) \quad (68)
\]

\[
= \text{tr}(\Sigma_{xx}) - \text{tr}(UAP_{U^TW_d}U^T) \quad (69)
\]

\[
= \text{tr}(\Sigma_{xx}) - \text{tr}(AP_{U^TW_d}U^TU) \quad (70)
\]

\[
= \text{tr}(\Sigma_{xx}) - \text{tr}(AP_{U^TW_d}) \quad (71)
\]

\[
= \text{tr}(\Sigma_{xx}) - \text{tr}(AI_{I}) \quad (72)
\]

\[
= \text{tr}(\Sigma_{xx}) - \sum_{t \in \mathcal{I}} \lambda_t \quad (73)
\]

In \((72)\) above we used \((60)\). For a given set of word embeddings, \(\Sigma_{xx}\) is fixed. Therefore, to minimise \(J(W_e, W_d)\) we must select the largest eigenvalues as \(\lambda_t\) (and their corresponding eigenvectors). This completes the proof of \textbf{Theorem 2}.

\[\square\]
Table 4: The autoencoder results using 150, 300 and 600 dimensions for the hidden layer in contrast to original word embeddings.

A.1 Linear approximations to non-linear activation functions

The autoencoder considered in [Theorem 2] is linear in the sense that the elementwise activation function is assumed to be $H = F(B) = B$. However, in practice autoencoders are used with nonlinear activation units such as rectified linear units ReLU; Nair and Hinton (2007), hyperbolic tangent ($\tanh$) and sigmoid ($\sigma$) functions (LeCun et al., 2012). Exact analysis of [Theorem 2] in the general case is complicated due to the non-linearity of the activation functions. Therefore, instead, we consider first-order linear approximations for the above-mentioned non-linear activation functions.

ReLU is a piece-wise linear function as given by (74).

$$F_{\text{relu}}(x) = \begin{cases} x & x > 0 \\ 0 & \text{otherwise} \end{cases}$$

(74)

Therefore, when ReLU is in its active region, it can be seen as a linear unit.

For $\tanh$ and $\sigma$, when $x$ is small, we use the first-order Taylor expansion to obtain linear approximations as follows.

$$F_{\text{tanh}}(x) = \frac{1}{1 + \exp(-x)} \approx \frac{1}{2} + \frac{1}{4}x$$

(75)

$$F_{\sigma}(x) = \frac{\exp(x) - \exp(-x)}{\exp(x) + \exp(-x)} \approx 0 + x$$

(76)

Therefore, in their linear regions close to zero, both $\tanh$ and $\sigma$ behave like linear functions.

As empirically investigated in the main paper, the performance difference in the word embeddings post-processed using linear vs. non-linear autoencoders is statistically insignificant. Considering the theoretical equivalence between PCA and linear autoencoders, this result shows that it is more important to perform centering and apply PCA rather than using a non-linear activation in the hidden layer of the autoencoder.

B Experimental Settings and Additional Results

We use semantic similarity (WS-353; Agirre et al. (2009), SIMLEX-999; Hill et al. (2015), RG-65: Rubenstein and Goodenough (1965), MTurk-287; Radinsky et al. (2011), MTurk-771; Halawi et al. (2012) and MEN; Bruni et al. (2014), analogy (Google, MSR (Mikolov et al., 2013), and SemEval; Jurgens et al. (2012)) and concept categorisation BLESS; Baroni and Lenci (2011) and ESSLI; Baroni et al. (2008) benchmark datasets that were already mentioned in the main article for additional experiments. Experiments are conducted using the same 300 dimensional pre-trained embedding learnt using Word2Vec, GloVe and fastText as described in the main body of the paper.
To evaluate the effect of the dimensionality of the hidden layer in the autoencoder on the performance of the post-processed embeddings, in Table 4 we train autoencoders with hidden layer dimensionalities of 150, 300 and 600 and compare the performance against the original (non-post-processed) word embeddings. For the pre-trained embeddings using Word2Vec and fastText, we see that setting the hidden layer’s dimensionality to 300, which is equal to the dimensionality of the input word embeddings, produces better results than with 150 or 600 dimensions in the majority of the datasets. On the other hand, for pre-trained GloVe embeddings we see that overall the performance increases with the dimensionality of the hidden layer, and the best performance is reported with a 600 dimensional hidden layer in the majority of the datasets.