SRP: Efficient class-aware embedding learning for large-scale data via supervised random projections

Amir-Hossein Karimi, Alexander Wong, Ali Ghodsi
1 David Cheriton School of Computer Science, University of Waterloo
2 Systems Design Engineering, University of Waterloo
3 Department of Statistics and Actuarial Science, University of Waterloo
{a6karimi, a28wong, aghodsib}@uwaterloo.ca

Abstract

Supervised dimensionality reduction strategies have been of great interest. However, current supervised dimensionality reduction approaches are difficult to scale for situations characterized by large datasets given the high computational complexities associated with such methods. While stochastic approximation strategies have been explored for unsupervised dimensionality reduction to tackle this challenge, such approaches are not well-suited for accelerating computational speed for supervised dimensionality reduction. Motivated to tackle this challenge, in this study we explore a novel direction of directly learning optimal class-aware embeddings in a supervised manner via the notion of supervised random projections (SRP). The key idea behind SRP is that, rather than performing spectral decomposition (or approximations thereof) which are computationally prohibitive for large-scale data, we instead perform a direct decomposition by leveraging kernel approximation theory and the symmetry of the Hilbert-Schmidt Independence Criterion (HSIC) measure of dependence between the embedded data and the labels. Experimental results on five different synthetic and real-world datasets demonstrate that the proposed SRP strategy for class-aware embedding learning can be very promising in producing embeddings that are highly competitive with existing supervised dimensionality reduction methods (e.g., SPCA and KSPCA) while achieving 1-2 orders of magnitude better computational performance. As such, such an efficient approach to learning embeddings for dimensionality reduction can be a powerful tool for large-scale data analysis and visualization.

1 Introduction

Consider the supervised task of predicting a dependent response random variable for an independent high-dimensional explanatory random variable. Conventional classification and regression methods are susceptible to the “curse of dimensionality” where satisfactory results depend on high data dimensionality which in turn requires an exponentially large number of data points. To combat this curse for a dataset, \( X = \{x_1, x_2, \cdots, x_n\} \in \mathbb{R}^{d \times n} \), it is often desirable to find a low-dimensional representation of the dataset to be used for downstream processing. Conventional dimensionality reduction methods such as Principal Component Analysis (PCA) are unsupervised and result in an embedding that preserves directions of maximum variation in the data. However, in many cases, the interesting directions of variation align with the labels, \( Y = \{y_1, y_2, \cdots, y_n\} \in \mathbb{R}^{\ell \times n} \), that accompany the data.

Many methods exist for supervised dimensionality reduction that guide the algorithm toward the modes of variability that are of particular interest. These methods include Fisher’s Discriminant Analysis FDA \([1]\), the large family of methods known as Metric Learning \([2]\ \[3]\), the family of...
The reliance on SVD, however, limits the applicability of SPCA and others on large datasets. Variables can be measured as the cross-correlation between those random variables. On the other hand, nonlinear dependence can be captured by looking at the cross-correlation between all nonlinear explanatory variables, \(X \in \mathbb{R}^{d \times n}\), and \(Y \in \mathbb{R}^{\ell \times n}\) to maximize the dependence of \(U^T X\) on \(Y\). To maximize the dependence of \(Y\) on \(U^T X\), we must consider all forms of dependence, including linear and nonlinear variants. It is commonly known that linear dependence between a pair of random variables can be measured as the cross-correlation between those random variables. On the other hand, nonlinear dependence can be captured by looking at the cross-correlation between all nonlinear transformations of those random variables. Clearly, however, there is a problem with evaluating all nonlinear transformations as there can be infinitely many of them. To overcome this, we turn to the commonly used Hilbert-Schmidt Independence Criterion (HSIC) introduced by Gretton et al. [12]. HSIC essentially projects the random variables from an original space into an abstract Reproducing Kernel Hilbert Space (RKHS), defines cross-correlation in that space, and evaluates dependence in a closed-form manner. Therefore, HSIC is an effective tool for “measuring” (linear and nonlinear) dependence between two random variables. While the exact value of HSIC is measured by computing the cross-covariance between \(F\) and \(G\) (where \(F\) and \(G\) are separable RKHS containing all continuous bounded real-valued functions of \(x\) from \(X\) to \(\mathbb{R}\) and \(y\) from \(Y\) to \(\mathbb{R}\), respectively), empirical approximations to the HSIC value between random variables \(X\) and \(Y\) can simply be calculated by evaluating the following on the observations in the population:

\[
HSIC(S, F, G) = \frac{\text{tr}(KHLH)}{(n - 1)^2}
\]  

(1)
where $H, K, L \in \mathbb{R}^{n \times n}$, $K_{ij} := k(x_i, x_j)$, $L_{ij} := l(y_i, y_j)$, and $H_{ij} := I - ee^T / n$ is the centering matrix. Therefore, to maximize the dependence between $U^T X$ and $Y$, $K$ is set to the kernel of $U^T X$ and therefore we must maximize the following:

$$\text{tr}(KHLH) = \text{tr}(X^T U U^T XHLH) = \text{tr}(U^T XHLHX^T U)$$

where the second line is via properties of trace. This optimization problem, however, is ill-defined as it is unbounded above. To construct the final optimization problem, we add the commonly used condition for orthogonality of the transformation matrix $U$ (incidentally, this condition makes the optimization problem well-defined by bounding the objective function), and we obtain the following:

$$\arg\max_U \text{tr}(U^T XHLHX^T U)$$

subject to $U^T U = I$ (4)

This optimal $U$ that solved Eq. (4) are the eigenvectors corresponding to the top-$k$ eigenvalues of $Q = XHLHX^T$. Because $Q$ is a real, symmetric, and positive semidefinite matrix, the top eigenvectors can be obtained in closed-form via Singular Value Decomposition (SVD).

This approach is called Supervised Principal Component Analysis (SPCA) [7]. Nonlinear extensions of SPCA can be formulated by expressing the transformation matrix $U$ as a linear combination of the projected data points, $U = \Phi(X)\beta$, via representation theory [13]. Plugging $U$ back into Eq. (4), we obtain a new optimization problem:

$$\arg\max_U \text{tr}(\beta^T KHLHK^T \beta)$$

subject to $\beta^T K \beta = I$ (5)

where $K = \Phi(X)^T \Phi(X)$ is the kernel matrix of the data, $X$. The solution, $\beta$, for Kernel Supervised Principal Component Analysis (KSPCA) can be obtained by solving the generalized eigenvector problem above, and obtained by decomposing $Q = HHLKH$ via SVD.

Now that we have established the derivation of SPCA and KSPCA, it is worth restating that computing the eigenvectors corresponding to the top-$k$ eigenvalues of $Q$ ($\in \mathbb{R}^{d \times d}$ for SPCA, and $\in \mathbb{R}^{n \times n}$ for KSPCA) is computationally burdensome for large datasets. See Table 1 for a detailed time analysis.

In the next section, we propose an alternative approach to solving Eq. (4) that allows us to bypass SVD completely. For this, we focus specifically on the symmetrical form of $Q = XHLHX^T$.

### 2.2 Supervised Random Projections

**Claim 1** Let $Z_1 = U^T X$ be the embedding obtained by SPCA and $Z_2 = \Psi H X^T X$, where $X \in \mathbb{R}^{d \times d}$ is the data matrix, $H \in \mathbb{R}^{n \times n}$ is the centering matrix, and $\Psi \in \mathbb{R}^{d \times n}$ is a decomposition of the positive semidefinite matrix such that $L = \Psi^T \Psi$. Suppose further that $U$ and $\Sigma$ are the eigenvectors and eigenvalues of $Q = XHLHX^T$, respectively. It can be shown that $Z_2 = \Sigma^{\frac{1}{2}} Z_1$ up to a rotation.

**Proof:** Starting with the SVD of real, symmetric, and positive semidefinite matrix, $Q$, we have:

$$Q = U\Sigma U^T$$

$$= U\Sigma^{\frac{1}{2}} R^T R \Sigma^{\frac{1}{2}} U^T$$

$$Q = XHLHX^T$$

$$= XH\Psi^T \Psi H X^T$$

where $R$ is an orthonormal rotation matrix. Therefore, we can conclude $R \Sigma^{\frac{1}{2}} U^T = \Psi H X^T$, and:

$$\implies Z_2 = \Psi H X^T X$$

$$= R \Sigma^{\frac{1}{2}} U^T X$$

$$= R \Sigma^{\frac{1}{2}} Z_1$$

Interestingly, we can obtain a $\Psi$ to approximate $L = \Psi^T \Psi$ simply through the use of kernel approximations (Section 2.3). The method presented in this section will henceforth be referred to as Supervised Random Projections (SRP). In order to embed the data into $k$ dimensions, SPCA constructed a matrix, $U$, whose columns were the eigenvectors corresponding to the top-$k$ eigenvalues
Kernel methods are successful techniques used broadly in many machine learning problems [14]. Despite the success of these methods, kernel methods have limited applicability in large-scale problems due to poor scaling in the face of increasing number of training samples. This problem, commonly known as the curse of support, presents itself when storing the Kernel matrix, and more importantly at test time when the Kernel matrix is used to evaluate a decision function for a new test sample. In their seminal work, Rahimi and Recht [15] suggested that by mapping the data (both train and test) into a relatively low-dimensional randomized feature space, one can operate on an explicit lower-dimensional space satisfying:

\[ k(x, y) = \langle \phi(x), \phi(y) \rangle \approx \psi(x)^T \psi(y) \]  

where the parameters of \( \psi \) are random bases sampled independently from the inverse Fourier transform of the desired shift-invariant kernel (see Bochner’s theorem). Incidentally, this covers a wide class of kernel functions including Gaussian RBF, Laplace, Matern, etc. Thus, instead of evaluating the entries of the kernel matrix individually, the entire kernel matrix \( K \) can be approximated via a fixed set of random bases drawn from the above distribution applied to the data samples. This

\[ Q = XHLHX^T \]

\[ = XH1HX^T \]

\[ = (XH)(XH)^T \]

\[ = (X - \mu_x)(X - \mu_x)^T \]

\[ = \text{Cov}(X) \]

Table 1: Comparing time complexities of SPCA, KSPCA, SRP, and KSRP. Reminder: \( X^{d \times n}, Y^{t \times n}, K^{n \times n}, L^{n \times n}, H^{n \times n}, \Psi_X^{k_x \times n}, \Psi_Y^{k_y \times n} \) where \( n \) is the number of training samples, \( d \) is the original data dimensionality, \( t \) is the label dimensionality, and \( k_x \) and \( k_y \) are the explicit embedding space dimensionality or the number of random bases used to approximate \( K = \Psi_X^T \Psi_X \) and \( L = \Psi_Y^T \Psi_Y \), respectively. Because \( k_y \) determines the dimension of the embedding space (see text), we have \( k_y < d \). We set \( k_x = 1000 \) to well-approximate the data kernel \( K \); this value does not effect the dimensionality of the embedding space. Finally, it is assumed we have more data than dimensions: \( d < n \).

| Method               | Matrix Mult | Kernel Computation (L, \( \Psi_Y \)) | SVD (top-k) exact approx |
|----------------------|-------------|-------------------------------------|--------------------------|
| \( \hat{U}_{SPCA} = e_{1g}(XHLHX^T) \) | \( O(n^3) \) | \( O(n^2t) \) -                     | \( O(d^2k) \) \( O(d^2 \log(k)) \) |
| \( \hat{U}_{KSPCA} = e_{1g}(HLHK) \)       | \( O(n^3) \) | \( O(n^2t) \) \( O(dn^3) \)       | \( O(n^2k) \) \( O(n^2 \log(k)) \) |
| \( \hat{U}_{SRP} = XH\Psi_Y^T \)            | \( O(k_y n^2) \) | \( O(k_y dn) \) -                  | -                        |
| \( \hat{U}_{KSRP} = \Psi_X H\Psi_Y^T \)     | \( O(k_x n^2) \) | \( O(k_y dn) \) \( O(k_x dn) \)   | -                        |

"In such a case, the \( L \) kernel is set equal to the identity matrix, i.e., a kernel which only captures the similarity between a point and itself. Therefore, (from [11]), \( Q \) becomes the covariance matrix of mean-subtracted samples \( X \), and decomposing the covariance matrix is the same as decomposing \( Q \) and consequently the same as maximizing \( \text{tr}(U^T QU) \). In other words, setting \( L = I \) means that we retain the maximal diversity between observations, and therefore PCA is a special case of SPCA."
method came to be known as Random Fourier Features and was later extended and referred to as Random Kitchen Sinks [15].

To summarize, we set out to find $U^T X$, a transformation of the data $X$ that had maximum dependence with the labels $Y$. This problem was formulated as on optimization problem \( \ref{eq:opt} \), subject to simple constraints, the solution for which was initially obtained via SVD, but now has a direct formulation using random kernel approximations.

## 3 Experiments

In this section we study the effectiveness of the proposed Supervised Random Projections (SRP) and Kernel Supervised Random Projections (KSRP) methods in comparison with Supervised Principal Component Analysis (SPCA) and Kernel Supervised Principal Component Analysis (KSPCA). These methods are compared on a number of visualization and classification problems, assessing their embedding performance using metrics such 1-Nearest Neighbor classification performance (common for evaluating embedding quality; see [16]), and wall-clock duration measurements.

In all of the following experiments, the input features are first normalized to the range $[0, 1]$. Wherever a data kernel was used in the methods above, $K$ was an RBF kernel with variance $\sigma_X$ obtained using 10-fold cross-validation. For the labels kernel, we apply a delta kernel \( L(p, q) = \delta(p, q) \) to compute $L$. This choice of kernel results in embeddings where instances of the same class are grouped together, as desired. In order to apply kernel approximation techniques for the delta kernel, we simply approximate $L$ using an RBF kernel with a very small variance. In our experiments, we use $\sigma_Y = 10^{-10}$.

A critical element of SRP and KSRP is the number of random bases used to approximate the kernels $K = \Psi^T_X \Psi_X$ and $L = \Psi^T_Y \Psi_Y$. Because $k_y$ determines the dimension of the embedding space (see Section 2.2), we set $k_y = k$, the desired dimensionality; therefore, $k_y < d$. We set $k_x = 1000$ to well-approximate the data kernel $K$; this value does not affect the dimensionality of the embedding space. Refer to Table 1 for detailed analysis of the effect of these parameters on time complexity. In fact, for KSRP, we can use the actual kernel $K$ instead of an approximate, but an approximate is more efficient computationally.

### 3.1 Visualization

First, the applicability of the proposed method on a data visualization task is examined. We compare performances on two synthetic datasets as well as a real-world dataset. The first synthetic dataset used was Binary XOR, which comprised of 2 classes distributed in fours clusters that are pair-wise positioned across from one another in 2 dimensions. The second synthetic dataset was Spirals, with each of the two arms corresponding to a separate class. For each synthetic datasets, we appended 8 dimensions of random noise to all samples, which yielded 500 samples in 10-dimensions. Due to the relative positioning of the classes in the original space, these datasets are highly nonlinear and therefore we expect superior performance from KSPCA and KSRP compared to SPCA and SRP. The real-world data used here was UCI-Sonar from the UCI machine learning repository [17], comprising 2 classes with 208 samples in 60 dimensions. For all datasets we performed 70%/30% train/test split.

Sample embeddings in 2 dimensions are depicted in Figure 1. Firstly, we observe that the embeddings for all datasets generalize to unseen test samples. For the highly nonlinear Binary XOR and Spirals datasets we can see that nonlinear approaches (i.e., KSPCA, KSRP) perform better by creating embeddings which congregates samples of the same class. Finally, for the UCI-Sonar dataset we can see that a KSPCA and KSRP can embed a real-world dataset from 60 dimensions to 2 while keeping the classes well-separated. We additionally compare these embeddings with those obtained from label-agnostic PCA and KPCA, showing that the supervised approaches that leverage label information result in meaningful embeddings. In the next section, we present detailed time comparison for these methods, while quantitatively assessing embedding performance using 1-NN classification accuracy.

### 3.2 Classification

In this section we focus on classification problems and study the behavior of SRP and KSRP in comparison to SPCA and KSPCA. In [17], SPCA and KSPCA were compared against other
representative methods of supervised dimensionality reduction, and superior performance of these methods was demonstrated. Therefore, in this section, we suffice to only compare the proposed methods with SPCA and KSPCA. To do so, we run experiments on the synthetic Binary XOR dataset described above, MNIST [18] dataset, as well as UCI-Ionosphere from the UCI machine learning repository [17]. The former contains 60,000 training samples and 10,000 testing samples in 784 dimensions, and the latter contains 351 samples in 34 dimensions where we randomly perform a 70%/30% train/test split.

The results presented in Figure 2 compare 1-NN and time performance on the three datasets, averaged over 30 runs. We make a number of interesting observations. Firstly, we note that increasing the number of random bases / projected dimension (i.e., $k$) results in better 1-NN performance. This is expected because with higher $k$s, we are retaining more information about the dataset in the embedding space. Assuming the test data is sampled from the same distribution as the training data (which may include the same noise distribution), higher $k$ should result in better performance 1-NN on the test set in the embedding space.

When comparing the time performances of various methods, we immediately notice the burdensome compute time required for KSPCA compared to that of KSRP and linear SPCA and SRP. We should keep in mind that, as mentioned in Section 2.3 there are kernel approximation schemes that are much faster than Random Kitchen Sinks which was used in our setup. This suggests that the efficiency gains observed here can be even more dramatic if we employ a kernel approximation method such as FastFood [19].

Bearing in mind the time complexities from Table 1 and considering that the number of samples in many datasets is typically larger than the dimensionality of the samples (i.e., $n > d$), this shows that while KSPCA has a total complexity of $O(n^3)$, SPCA and SRP have a complexity of $O(dn^2)$ and KSRP has a time complexity of $O(\max\{k_xn^2, k_yn^2\})$. This aligns perfectly with the observed time duration results of Figure 2.

Figure 1: Visualization results for Binary XOR (top-left), Spirals (top-right), and UCI-Sonar (bottom) datasets in 2 dimensions.
Figure 2: Classification results for Binary XOR (top-left), UCI-Ionosphere (top-right), and MNIST (bottom) datasets in 2 dimensions.

For the synthetic XOR plots (i.e., bottom row) of Figure 2, it agrees with our intuition that KSPCA and KSRP outperform their linear counterparts in lower dimensions. For MNIST, we omit the results for KSPCA because we ran out of memory on a 64GB machine when computing the data kernel matrix. We also noticed that linear approaches (SPCA, SRP) outperformed KSRP and therefore omitted these results in the figure for better illustration between SPCA and SRP. Across all plots, we see that randomized approaches have 1-NN performance very close to their exact counterpart (i.e., SPCA-SRP and KSPCA-KSRP pairs), while providing $5 - 20 \times$ speed up in terms of wall-clock time.

4 Conclusion

In this work, we propose a novel approach for efficiently finding an embedding of a large-scale dataset in the context of supervised dimensionality reduction. To achieve this, we were inspired by Supervised Principal Component Analysis (SPCA) and Kernel Supervised Principal Component Analysis (KSPCA) where an optimization function is solved in closed-form yielding an embedding that is maximally dependent on the labels. This work builds on the theory of SPCA and that of kernel approximation to construct Supervised Random Projections (SRP) and Kernel Supervised Random Projections (KSRP). We evaluated and compared these methods on five different datasets for visualization and classification, concluding that SRP and KSRP perform very competitively with SPCA and KSPCA: yielding a small drop in 1-NN classification performance while providing orders of magnitude better time performance.
References

[1] R. A. Fisher, “The use of multiple measurements in taxonomic problems,” *Annals of human genetics*, vol. 7, no. 2, pp. 179–188, 1936.

[2] E. P. Xing, M. I. Jordan, S. J. Russell, and A. Y. Ng, “Distance metric learning with application to clustering with side-information,” in *Advances in neural information processing systems*, 2003, pp. 521–528.

[3] K. Q. Weinberger, J. Blitzer, and L. K. Saul, “Distance metric learning for large margin nearest neighbor classification,” in *Advances in neural information processing systems*, 2006, pp. 1473–1480.

[4] K. Fukumizu, F. R. Bach, and M. I. Jordan, “Dimensionality reduction for supervised learning with reproducing kernel hilbert spaces,” *Journal of Machine Learning Research*, vol. 5, no. Jan, pp. 73–99, 2004.

[5] K.-C. Li, “Sliced inverse regression for dimension reduction,” *Journal of the American Statistical Association*, vol. 86, no. 414, pp. 316–327, 1991.

[6] E. Bair, T. Hastie, D. Paul, and R. Tibshirani, “Prediction by supervised principal components,” *Journal of the American Statistical Association*, vol. 101, no. 473, pp. 119–137, 2006.

[7] E. Barshan, A. Ghodsi, Z. Azimifar, and M. Z. Tahrimi, “Supervised principal component analysis; Visualization, classification and regression on subspaces and submanifolds,” *Pattern Recognition*, vol. 44, no. 7, pp. 1357–1371, 2011.

[8] G. Stewart, “The decompositional approach to matrix computation,” *Computing in Science & Engineering*, vol. 2, no. 1, pp. 50–59, 2000.

[9] M. Holmes, A. Gray, and C. Isbell, “Fast svd for large-scale matrices,” in *Workshop on Efficient Machine Learning at NIPS*, vol. 58, 2007, pp. 249–252.

[10] N. Halko, P.-G. Martinsson, and J. A. Tropp, “Finding structure with randomness: Probabilistic algorithms for constructing approximate matrix decompositions,” *SIAM review*, vol. 53, no. 2, pp. 217–288, 2011.

[11] Y. Rokhlin, A. Szlam, and M. Tygert, “A randomized algorithm for principal component analysis,” *SIAM Journal on Matrix Analysis and Applications*, vol. 31, no. 3, pp. 1100–1124, 2009.

[12] A. Gretton, O. Bousquet, A. Smola, and B. Schölkopf, “Measuring statistical dependence with hilbert-schmidt norms,” in *International conference on algorithmic learning theory*. Springer, 2005, pp. 63–77.

[13] J. L. Alperin, *Local representation theory: Modular representations as an introduction to the local representation theory of finite groups*. Cambridge University Press, 1993, vol. 11.

[14] B. Schölkopf and A. J. Smola, *Learning with kernels: support vector machines, regularization, optimization, and beyond*. MIT press, 2002.

[15] A. Rahimi and B. Recht, “Random features for large-scale kernel machines,” in *Advances in Neural Information Processing Systems (NIPS)*, 2007.

[16] L. Van Der Maaten, E. Postma, and J. Van den Herik, “Dimensionality reduction: a comparative review,” *J Mach Learn Res*, vol. 10, pp. 66–71, 2009.

[17] A. Asuncion and D. Newman, “Uci machine learning repository,” 2007.

[18] Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner, “Gradient-based learning applied to document recognition,” *Proceedings of the IEEE*, vol. 86, no. 11, pp. 2278–2324, 1998.

[19] Q. Le, T. Sarlós, and A. Smola, “Fastfood - computing hilbert space expansions in loglinear time,” *The Journal of Machine Learning Research*, vol. 28, pp. 244–252, 2013.