Supervised Dimensionality Reduction for Big Data

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To solve key biomedical problems, experimentalists now routinely measure millions or billions of features (dimensions) per sample, with the hope that data science techniques will be able to build accurate data-driven inferences. Because sample sizes are typically orders of magnitude smaller than the dimensionality of these data, valid inferences require finding a low-dimensional representation that preserves the discriminating information (e.g., whether the individual suffers from a particular disease). There is a lack of interpretable supervised dimensionality reduction methods that scale to millions of dimensions with strong statistical theoretical guarantees. We introduce an approach, XOX, to extending principal components analysis by incorporating class-conditional moment estimates into the low-dimensional projection. The simplest version, “Linear Optimal Low-rank” projection (LOL), incorporates the class-conditional means. We prove, and substantiate with both synthetic and real data benchmarks, that LOL and its generalizations in the XOX framework lead to improved data representations for subsequent classification, while maintaining computational efficiency and scalability. Using multiple brain imaging datasets consisting of \( > 150 \) million features, and several genomics datasets with \( > 500,000 \) features, LOL outperforms other scalable linear dimensionality reduction techniques in terms of accuracy, while only requiring a few minutes on a standard desktop computer.

Supervised learning—the art and science of estimating statistical relationships using labeled training data—has enabled a wide variety of basic and applied findings, ranging from discovering biomarkers in omics data \[72\] to recognizing objects from images \[50\]. A special case of supervised learning is classification, where a classifier predicts the “class” of a novel observation (for example, by predicting sex from an MRI scan). One of the most foundational and important approaches to classification is Fisher’s Linear Discriminant Analysis (LDA) \[35\]. LDA has a number of highly desirable properties for a classifier. First, it is based on simple geometric reasoning: when the data are Gaussian, all the information is in the means and variances, so the optimal classifier uses both the means and the variances. Second, LDA can be applied to multiclass problems. Third, theorems guarantee that when the sample size \( n \) is large and the dimensionality \( p \) is relatively small, LDA converges to the optimal classifier under the Gaussian assumption. Finally, algorithms for implementing it are highly efficient.

Modern scientific datasets, however, present challenges for classification that were not addressed in Fisher’s era. Specifically, the dimensionality of datasets is quickly ballooning. Current raw data can consist of hundreds of millions of features or dimensions; for example, an entire genome or connectome. Yet, the sample sizes have not experienced a concomitant increase. This “large \( p \), small \( n \)” problem is a non-starter for many classical statistical approaches because they were designed with a “small \( p \), large \( n \)” situation in mind. Running LDA when \( p \geq n \) is like trying to fit a line to a point: there are infinitely many equally good fits (all lines that pass through the point), and no way to know which of them is “best”. Therefore, without further constraints these algorithms will overfit, meaning they will choose a classifier based on noise in the data, rather than discarding the noise in favor of the desired signal. We also desire methods that can adapt to the complexity of the data, are robust to outliers, and are computationally efficient. Several complementary strategies have been pursued to address these \( p \geq n \) problems.

First, and perhaps the most widely used method, is Principal Components Analysis (PCA) \[48\]. Accord-
ing to PubMed, PCA has been referenced over 40,000 times, and nearly 4,000 times in 2018 alone. This is in contrast to other methods that receive much more attention in the media, such as deep learning, random forests, and sparse learning, which received $\sim 2,000$, $\sim 1,200$ and $\sim 500$ hits, respectively. This suggests that PCA remains the most popular workhorse for high-dimensional problems. PCA "pre-processes" the data by reducing its dimensionality to those dimensions whose variance is largest in the dataset. While highly successful, PCA is a wholly *unsupervised* dimensionality reduction technique, meaning that PCA does not use the class labels while learning the low-dimensional representation, resulting in sub-optimal performance for subsequent classification. Nonlinear manifold learning techniques generalize PCA [54], but also typically do not incorporate class label information; moreover, they scale poorly. Deep learning provides the most recent version of nonlinear manifold learning, for example, using (supervised) autoencoders, but these methods remain poorly understood, have many parameters to tune, and typically do not provide interpretable results [38]. Further, deep learning tends to suffer in the wide data problem, where the number of samples is far less than the dimensionality.

The second set of strategies regularize or penalize a supervised method, such as regularized LDA [73] or canonical correlation analysis (CCA) [64]. Such approaches can drastically overfit in the $p > n$ setting, tend to lack theoretical support in these contexts, and have multiple “knobs” to tune that are computationally taxing. Partial least squares (PLS) is another popular method in this set that often achieves impressive empirical performance, though it lacks strong theoretical guarantees and a scalable implementation [16, 67]. Sparse methods are the third common strategy to mitigate this “curse of dimensionality” [34, 45, 68]. Unfortunately, exact solutions are computationally intractable, and approximate solutions have theoretical guarantees only under very restrictive assumptions, and are quite fragile to those assumptions [66]. Thus, there is a gap: no existing approach can classify multi-class wide data with millions of features while obtaining strong theoretical guarantees, favorable and interpretable empirical performance, and a flexible, robust, and scalable implementation.

To address these issues, we developed a technique for incorporating class-conditional moment estimates, XOX, the simplest example of which is LOL. The key intuition behind LOL is that we can jointly use the means and variances from each class (like LDA and CCA), but without requiring more dimensions than samples (like PCA), or restrictive sparsity assumptions. Using random matrix theory, we are able to prove that when the data are sampled from a Gaussian, LOL finds a better low-dimensional representation than PCA, LDA, CCA, and other linear methods. Under relatively relaxed assumptions, this is true regardless of the dimensionality of the features, the number of samples, or the number of dimensions in which we project. We then demonstrate the superiority of techniques derived using the XOX approach—including (i) LOL, (ii) a variant of XOX which allows greater flexibility of the class-conditional covariances called QOQ, and (iii) a robust variant of LOL called RLOL—over other methods numerically on a variety of simulated settings including several not following the theoretical assumptions. Finally, we show that on several 500 gigabyte neuroimaging datasets, and several multi-gigabyte genomics datasets, LOL achieves superior accuracy at lower dimensions while requiring only a few minutes of time on a single workstation.

**Supervised Manifold Learning**

A general strategy for supervised manifold learning is schematized in Figure 1, and outlined here. Step (A): Obtain or select $n$ training samples of high-dimensional data. For concreteness, we use one of the most popular benchmark datasets, the MNIST dataset [53]. This dataset consists of images of hand-written digits 0 through 9. Each image is represented by a $28 \times 28$ matrix, which means that the observed dimensionality of the data is $p = 28^2 = 784$. Because we are motivated by the $n \ll p$
Figure 1: Schematic illustrating Linear Optimal Low-rank (LOL) as a supervised manifold learning technique. (A) 300 training samples of the numbers 3, 7, and 8 from the MNIST dataset (100 samples per digit); each sample is a \(28 \times 28 = 784\) dimensional image (boundary colors are for visualization purposes). (B) The first four projection matrices learned by LOL. Each is a linear combination of the sample images. (C) Projecting 500 new (test) samples into the top two learned dimensions; digits color coded as in (A). LOL-projected data from three distinct clusters. (D) Using the low-dimensional data to learn a classifier. The estimated distributions for 3 and 8 of the test samples (after projecting data into two dimensions and using LDA to classify) demonstrate that 3 and 8 are easily separable by linear methods after LOL projections (the color of the line indicates the digit). The filled area is the estimated error rate; the goal of any classification algorithm is to minimize that area. LOL is performing well on this high-dimensional real data example.

Scenario, we subsample the data to select \(n = 300\) examples of the numbers 3, 7, and 8 (100 of each). Step (B): Learn a “projection” that maps the high-dimensional data to a low-dimension representation. One can do so in a way that ignores which images correspond to which digit (the “class labels”), as PCA and most manifold learning techniques do, or try to use the labels, as LDA and sparse methods do. LOL is a supervised linear manifold learning technique that uses the class labels to learn projections that are linear combinations of the original data samples. Step (C): Use the learned projections to map high-dimensional data into the learned lower-dimensional space. This step requires having learned a projection that can be applied to new (test) data samples for which we do not know the true class labels. Nonlinear manifold learning methods typically cannot be applied in this way (though see [12]). LOL, however, can project new samples in such a way as to separate the data into classes. Step (D): Using the low-dimensional representation of the data, learn a classifier. A good classifier correctly identifies as many points as possible with the correct label. For these data, when LDA is used on the low-dimensional data learned by LOL, the data points are mostly linearly separable, yielding a highly accurate classifier.

The Geometric Intuition of LOL

To build intuition for situations when LOL performs well, and when it does not, we consider the simplest high-dimensional classification setting. We observe \(n\) samples \((x_i, y_i)\), where \(x_i\) are \(p\) dimensional feature vectors, and \(y_i\) is the binary class label, that is, \(y_i\) is either 0 or 1. We assume that both classes are distributed according to a multivariate Gaussian distribution, the two classes have the same identity covariance matrix (all features are uncorrelated with unity variance), and data from either class is equally likely, so that the only difference between the classes is their means. In this scenario, the optimal low-dimensional projection is analytically available: it is the dot product of the difference of means and the inverse covariance matrix, commonly referred to as Fisher’s Linear Discriminant Analysis (LDA).
(see Appendix A for derivation). When the distribution of the data is unavailable, as in all real data problems, machine learning methods can be used to estimate the parameters. Unfortunately, when $n < p$, the estimated covariance matrix will not be invertible (because the solution to the underlying mathematical problem is under specified), so some other approach is required. As mentioned above, PCA is commonly used to learn a low-dimensional representation. PCA uses the pooled sample mean and the pooled sample covariance matrix. The PCA projection is composed of the top $d$ eigenvectors of the pooled sample covariance matrix, after subtracting the pooled mean (thereby completely ignoring the class labels).

In contrast, LOL uses the class-conditional means and class-centered covariance. This approach is motivated by Fisher's LDA, which uses the same two terms, and should therefore improve performance over PCA. More specifically, for a two-class problem, LOL is constructed as follows:

1. Compute the sample mean of each class.
2. Estimate the difference between means.
3. Compute the class-centered covariance matrix, that is, compute the covariance matrix after subtracting the class mean from each point.
4. Compute the eigenvectors of this class-conditionally centered covariance.
5. Concatenate the difference of the means with the top $d - 1$ eigenvectors of class-centered covariance.

Note that the sample class-centered covariance matrix estimates the population covariance, whereas the sample pooled covariance matrix is distorted by the difference of the class means. Further, as discussed in Appendix D, the class-centered covariance matrix is equivalent to “Reduced Rank LDA” \cite{42} (rrLDA hereafter, which is simply LDA but truncating the covariance matrix). For the theoretical background on LDA and rrLDA, a formal definition of LOL, and detailed description of the simulation settings that follow, see Appendices A, B, and C, respectively. Figure 2 shows three different examples of 100 data points sampled from a 1,000 dimensional Gaussian to geometrically illustrate the intuition that motivated LOL. In each case, all dimensions are uncorrelated with one another, and all classes are equally likely with the same covariance; the only difference between the classes are their means.

Figure 2A shows “stacked cigars”, in which the difference between the means and the direction of maximum variance are large and aligned with one another. This is an idealized setting for PCA, because PCA finds the direction of maximal variance, which happens to correspond to the direction of maximal separation of the classes. rrLDA performs well here too, for the same reason that PCA does. Because all dimensions are uncorrelated, and one dimension contains most of the information discriminating between the two classes, this is also an ideal scenario for sparse methods. Indeed, ROAD, a sparse classifier designed for precisely this scenario, does an excellent job finding the most useful dimensions \cite{34}. LOL, using both the difference of means and the directions of maximal variance, also does well. To calibrate all of these methods, we also show the performance of the optimal classifier.

Figure 2B shows an example that is worse for PCA. In particular, the variance is getting larger for subsequent dimensions, while the magnitude of the difference between the means is decreasing with dimension. Because PCA operates on the pooled sample covariance matrix, the dimensions with the maximum difference are included in the estimate, and therefore, PCA finds some of them, while also finding some of the dimensions of maximum variance. The result is that PCA performs fairly well in this setting. rrLDA, however, by virtue of subtracting out the difference of the means, is now completely at chance performance. ROAD is not hampered by this problem; it is also able to find the directions of maximal discrimination, rather than those of maximal variance. Again, LOL, by using both the means and the covariance, does extremely well.
Figure 2: LOL achieves near-optimal performance for three different multivariate Gaussian distributions, each with 100 samples in 1000 dimensions. For each approach, we project into the top 3 dimensions, and then use LDA to classify 10,000 new samples. The six rows show (from top to bottom): Row 1: A scatter plot of the first two dimensions of the sampled points, with class 0 and 1 as orange and blue dots, respectively. The next rows each show the estimated posterior for class 0 and class 1, in solid and dashed lines, respectively. The overlap of the distributions—which quantifies the magnitude of the error—is filled. The black vertical line shows the estimated threshold for each method. The techniques include: PCA; reduced rank LDA (rrLDA), a method that projects onto the top $d$ eigenvectors of sample class-conditional covariance; ROAD, a sparse method designed specifically for this model; LOL, our proposed method; and the Bayes optimal classifier. (A) Stacked Cigars The mean difference vector is aligned with the direction of maximal variance, and is mostly concentrated in a single dimension, making it ideal for PCA, rrLDA, and sparse methods. In this setting, the results are similar for all methods, and essentially optimal. (B) Trunk The mean difference vector is orthogonal to the direction of maximal variance; PCA performs worse and rrLDA is at chance, but sparse methods and LOL can still recover the correct dimensions, achieving nearly optimal performance. (C) Rotated Trunk Same as (B), but the data are rotated; in this case, only LOL performs well. Note that LOL is closest to Bayes optimal in all three settings.

Figure 2C is exactly the same as Figure 2B, except the data have been randomly rotated in all 1000 dimensions. This means that none of the original features have much information, but rather, linear combinations of them do. This is evidenced by observing the scatter plot, which shows that the first two dimensions fail to disambiguate the two classes. PCA performs even worse in this scenario than in the previous one. rrLDA is rotationally invariant (see Appendix B.IV for details), so still performs at chance levels. Because there is no small number of features that separate the data well, ROAD fails. LOL performs as well here as it does in the other examples.

When is LOL Better than PCA and Other Supervised Linear Methods?

We desire theoretical confirmation of the above numerical results. To do so, we investigate when LOL is “better” than other linear dimensionality reduction techniques. In the context of supervised dimension-
ality reduction or manifold learning, the goal is to obtain low dimensional representation that maximally separates the two classes, making subsequent classification easier. Chernoff information quantifies the dissimilarity between two distributions. Therefore, we can compute the Chernoff information between distribution of the two classes after embedding to evaluate the quality of a given embedding strategy. As it turns out, Chernoff information is the exponential convergence rate for the Bayes error [23], and therefore, the tightest possible theoretical bound. The use of Chernoff information to theoretically evaluate the performance of an embedding strategy is novel, to our knowledge, and leads to the following main result:

**Main Theoretical Result** LOL is always better than or equal to rrLDA under the Gaussian model when \( p \geq n \), and better than or equal to PCA (and many other linear projection methods) with additional (relatively weak) conditions. This is true for all possible observed dimensionalities of the data, and the number of dimensions into which we project, for sufficiently large sample sizes. Moreover, under relatively weak assumptions, these conditions almost certainly hold as the number of dimensions increases.

Formal statements of the theorems and proofs required to substantiate the above result are provided in Appendix D. The condition for LOL to be better than PCA is essentially that the \( d^{th} \) eigenvector of the pooled sample covariance matrix has less information about classification than the difference of the means vector. The implication of the above theorem is that it is better to incorporate the mean difference vector into the projection matrix, rather than ignoring it, under basically the same assumptions that motivate PCA. The degree of improvement is a function of the dimensionality of the feature set \( p \), the number of samples \( n \), the projection dimension \( d \), and the parameters, but the existence of an improvement—or at least no worse performance—is independent of those factors.

### Flexibility and Accuracy of XOX Framework

We empirically investigate the flexibility and accuracy of XOX using simulations that extend beyond the theoretical claims. For three different scenarios, we sample 100 training samples each with 100 features; therefore, Fisher’s LDA cannot solve the problem (because there are infinitely many ways to overfit). We consider a number of different methods, including PCA, rrLDA, PLS, ROAD, Random Projections (RP), and CCA to project the data onto a low dimensional space. After projecting the data, we train either LDA (for the first two scenarios) or Quadratic Discriminant Analysis (QDA, for the third scenario), which generalizes LDA by allowing each class to have its own covariance matrix [43]. For each scenario, we evaluate the misclassification rate on held-out data.

Figure 3 shows a two-dimensional scatterplot (left) and misclassification rate versus dimensionality (right) for each simulation. The top \( C - 1 \) embedding dimensions for LOL correspond to the performance after projection onto the class-conditional means, and rrLDA corresponds to the performance of projection onto the class-conditional covariance matrix. Figure 3A shows a three class generalization of the Trunk example from Figure 2B. LOL can trivially be extended to more than two classes (see Section B for details), unlike ROAD which only operates in a two-class setting. Figure 3B shows a two-class example with many outliers, as is typical in modern biomedical datasets. A variant of LOL, “Robust LOL” (RLOL), replaces the standard estimators of the mean and covariance with robust variants (the class-conditional medians and robust covariance [27] respectively), thereby dramatically improving performance over LOL (and other techniques) in noisy settings. Hereafter, LOL will refer to the version of LOL with a robust estimate of the first moment, and a truncated estimate of the second moment, as a robust first moment tends to make little difference when a robust estimate was not necessary, and improved performance when a robust estimate was warranted. We do not use a robust estimate of
Figure 3: Three simulations demonstrating the flexibility and accuracy of XOX in settings beyond current theoretical claims. For all cases, training sample size and dimensionality were both 100. The top row depicts the values of the sampled points for two of the 100 dimensions to illustrate the classification task. The bottom row misclassification rate as a function of the number of projected dimensions, for several different embedding approaches. Classification is performed on the embedded data using the LDA classifier for (A) and (B), and using QDA for (C). The simulation settings are: (A) Trunk-3 A variation of Figure 2(B) in which 3 classes are present. (B) Robust Outliers are prominent in the sample while estimating the projection matrix. LOL is robust to the outliers due to the robust estimate of the first moment. (C) Cross The two classes have the same mean but orthogonal covariances. Points are classified using the QDA classifier after projection. QOQ, a variant of LOL where each class' covariance is incorporated into the projection matrix, outperforms other methods, as expected. In essentially all cases and dimensions, LOL, or the appropriate generalization thereof, outperforms other approaches.

the second moment, as typical robust estimates of the second moment available in standard numerical packages require $d < n$, which is unsuitable for wide data. Figure 3C shows an example that does not have an effective linear discriminant boundary because the two classes have orthogonal covariances. Another variant of LOL, Quadratic Optimal QDA (QOQ), computes the eigenvectors separately for each class, concatenates them (sorting them according to their singular values), and then classifies with QDA instead of LOL. For all three scenarios, either LOL—or its extended variants RLOL and QOQ—achieves a misclassification rate comparable to or lower than other methods, for all dimensions. These three results demonstrate how straightforward generalizations of LOL under the XOX framework which incorporate alternate or robust moment estimates can dramatically improve performance over other projection methods. This is in marked contrast to other approaches, for which such flexibility is either not available, or otherwise problematic.

**XOX is Computationally Efficient and Scalable**

When the dimensionality is large (e.g., millions or billions), the main bottleneck is sometimes merely the ability to run anything on the data, rather than its predictive accuracy. We evaluate the computational efficiency and scalability of LOL in the simplest setting: two classes of spherically symmetric Gauss-
sians (see Appendix C for details) with dimensionality varying from 2 million to 128 million, and 1000 samples per class. Because LOL admits a closed form solution, it can leverage highly optimized linear algebra routines rather than the costly iterative programming techniques currently required for sparse or dictionary learning type problems [58]. To demonstrate these computational capabilities, we built FlashLOL, an efficient scalable LOL implementation with R bindings, to complement the R package used for the above figures.

Four properties of LOL enable its scalable implementation. First, LOL is linear in both sample size and dimensionality (Figure 4A, solid red line). Second, LOL is easily parallelizable using recent developments in “semi-external memory” [75–77] (Figure 4A, dashed red line demonstrates that LOL is also linear in the number of cores). Also note that LOL does not incur any meaningful additional computational cost over PCA (orange dashed line). Third, LOL can use randomized approximate algorithms for eigendecompositions to further accelerate its performance [20, 44] (Figure 4A, orange lines). FlashLFL, short for Flash Low-rank Fast Linear embedding, achieves an order of magnitude improvement in speed when using very sparse random projections instead of the eigenvectors. Fourth, hyper-parameter selection for LOL is nested, meaning that once estimating the $d$-dimensional projection, every lower dimensional projection is automatically available. This is in contrast to tuning the weight of a penalty term, which leads to a new optimization problem for each different parameter values. Thus, the computational complexity of LOL is $O(npd/T_c)$, where $n$ is sample size, $p$ is the dimension of the data, $d$ is the dimension of the projection, $T$ is the number of threads, and $c$ is the sparsity of the projection.

![Figure 4](image)

**Figure 4:** Computational efficiency and scalability of LOL using $n = 2000$ samples from spherically symmetric Gaussian data (see Appendix C for details). (A) LOL exhibits optimal (linear) scale up, requiring only 46 minutes to find the projection on a 500 gigabyte dataset, and only 3 minutes using LFL (dashed lines show semi-external memory performance). (B) Error for LFL is the same as LOL in this setting, and both are significantly better than PCA and rrLDA for all choices of projection dimension, regardless of whether a randomized approach is used to compute the projection dimensions.

Finally, note that this simulation setting is ideal for PCA and rrLDA, because the first principal component includes the mean difference vector. Nonetheless, both LOL and LFL achieve near optimal accuracy, whereas rrLDA is at chance, and PCA requires 500 dimensions to even approach the same accuracy that LOL achieves with only one dimension. While PCA would also benefit efficiency wise from a randomized approach, we emphasize that LFL maintains the high performance of LOL in comparison to PCA despite the randomization technique, with the benefit of greater computational efficiency compared to LOL.
Real Data Benchmarks and Applications

Real data often break the theoretical assumptions in more varied ways than the above simulations, and can provide a complementary perspective on the performance properties of different algorithms. We describe two sets of problems, one from brain imaging, and the other from genomics. In both cases we consider a classification problem. To classify participants, researchers typically employ substantive pre-processing pipelines [18] to reduce the dimensionality of the data. Unfortunately, as debates persist about the validity of pre-processing approaches, there is no defacto “standard” for the optimal strategies to pre-process the data. Traditional approaches typically include a deep processing chain, with many steps of parametric modeling and downsampling [39, 40, 49]. We therefore investigate the possibility of directly classifying on the nearly raw, high-dimensional data.

The Consortium for Reliability and Reproducibility (CoRR) [78] has generated anatomical and diffusion magnetic resonance imaging scans from \( n > 800 \) participants from 5 processing sites, each featuring participant-specific annotations for the sex of each individual. At the native resolution, each brain volume is over 150 million dimensions, and each dataset consists of between 42 (60 GB of data) and > 400 samples (600 GB of data).

![Figure 5](image_url)

**Figure 5:** Comparing various dimensionality reduction algorithms on two real datasets: neuroimaging and genomics. (A) Beeswarm plots show the classification performance of each technique with respect to PCA at the optimal number of embedding dimensions, the number of embedding dimensions with the lowest misclassification rate. Performance is measured by the effect size, defined as \( \kappa(LDA \circ PCA) - \kappa(LDA \circ embed) \), where \( \kappa \) is Cohen’s Kappa, and embed is one of the embedding techniques compared to PCA. Each point indicates the performance of PCA relative the other technique on a single dataset, and the sample size-weighted average effect is indicated by the black “x.” LOL always outperforms PCA and all other techniques. (B) Frequency histograms of the relative ranks of each of the embedding techniques on each dataset after classification, where a 1 indicates the best relative classification performance and a 4 indicates the worst relative classification performance, after embedding with the technique indicated. Projecting first with LOL provides a significant improvement over competing strategies (Wilcoxon signed-rank test, \( n = 7, p\text{-value}=.008 \)) on all benchmark problems.
We then also consider a large genomics dataset [31] consisting of 340 individuals: 144 patients with non-metastatic cancer and 196 healthy controls, of which 198 are male and 142 are female. Samples are aligned to >750,000 amplicons distributed throughout the genome to investigate the presence of aneuploidy (abnormal chromosomal counts) in samples from cancer patients (see Appendix E for details). The raw amplicon counts are then used with no further pre-processing. We have two tasks of interest: classification on the basis of either sex or age.

For each of the above described problems, we first compute an embedding matrix to project the training data using LOL, PCA, rrLDA, and RP, and then train LDA to classify the resulting low-dimensional representations. The held-out set is then projected and classified using the embedding matrix and trained classifier respectively, and the average cross-validated error is computed over all folds of the data. For each problem, the optimal dimensionality for each strategy is selected to be the number of embedding dimensions with the lowest average cross-validated error. We compute Cohen’s Kappa κ to compare performance across methods because it normalizes the performance of the classification strategy between zero (the classifier is equivalent to the random chance classifier) and one (the classifier performs perfectly). Finally, for each projection technique, we measure the effect size for each strategy as the difference $\kappa(\text{PCA}) - \kappa(\text{embed})$. See Appendix E for a table detailing the datasets employed.

Our FlashLOL implementations are the only algorithms that could successfully run on these data with a single core on a standard desktop computer. In Figure 5(A), LOL is the only technique to outperform PCA on all problems. Figure 5(B) shows the relative ranks of the average cross-validated misclassification rates for the LDA classifier on each dataset after projection with the specified embedding technique. For all problems, LOL is the technique with the lowest average cross-validated misclassification rate. Further, LOL performs significantly better than all other techniques (Wilcoxon signed-rank statistic, all $p$-values $= 0.008$). The average misclassification rate achieved at the optimal number of embedding dimensions via LOL is between 5% and 15% across all datasets, which is the same performance we and others obtain using extensively processed and downsampled data that is typically required on similar datasets [32, 71]. LOL therefore enables researchers to side-step hotly debated pre-processing issues by hardly pre-processing at all, and instead simply applying LOL to the data in its native dimensionality.

**Discussion**

We have introduced a very simple methodology to improve performance on supervised learning problems with wide data (that is, big data where dimensionality is at least as large as sample size) by using class-conditional moments to estimate a low rank projection under a generalized framework, $\text{XOX}$. In particular, LOL uses both the difference of the means and the class-centered covariance matrices, which enables it to outperform PCA, as well as existing supervised linear classification schemes, in a wide variety of scenarios without incurring any meaningful additional computational cost. Straightforward generalizations enable robust and nonlinear variants by using robust estimators and/or class specific covariance estimators. Our open source implementation optimally scales to terabyte datasets. Moreover, the intuition can be extended for both hypothesis testing and regression (see Appendix F for additional numerical examples in these settings).

Two commonly applied approaches in these settings are partial least squares (PLS) and canonical correlation analysis (CCA). CCA is equivalent to rrLDA whenever $p < n$, which is not of interest here. When $p \geq n$, CCA and rrLDA are not equivalent; however, in such settings, CCA exhibits the “maximal data piling problem” [5] (see Appendix B.VI for details). Specifically, all the points in each class are projected onto the exact same point. This results in severe overfitting of the data, yielding poor empirical
performance in essentially all settings we considered here (the first dimension of CCA is typically worse even than the difference of the means). While PLS does not exhibit these problems, it lacks strong theoretical guarantees and simple geometric intuition. In contrast to XOX, neither CCA nor PLS enable straightforward generalizations, such as when there are outliers or the discriminant boundary is quadratic (see Figure 3). Further, across all simulations, XOX outperforms both of these approaches, sometimes quite dramatically (for example, XOX outperforms CCA on over all of the simulations considered). Finally, no scalable nor parallelized implementations are readily available for these methods (see Figure 4). One could use stochastic gradient descent with penalties to solve these other optimization problems, but they would still need to tune the penalty parameter which would be quite computationally costly. Neither PLS nor CCA could be successfully run on the massive neuroimaging dataset nor the amplicon-level genomics dataset using readily-available tools.

Many previous investigations have addressed similar challenges. The celebrated Fisherfaces paper was the first to compose Fisher’s LDA with PCA (equivalent to PCA in this manuscript) [10]. The authors showed via a sequence of numerical experiments the utility of projecting the data using PCA prior to classifying with LDA. We extend this work by adding a supervised component to the initial projection. Moreover, we provide the geometric intuition for why and when incorporating supervision is advantageous, with numerous examples demonstrating its superiority, and theoretical guarantees formalizing when LOL outperforms PCA. The “sufficient dimensionality reduction” literature has similar insights, but a different construction that typically requires the dimensionality to be smaller than the sample size [25, 36, 37, 55, 69] (although see [26] for some promising work). More recently, communication-inspired classification approaches have yielded theoretical bounds on linear and affine classification performance [62]; they do not, however, explicitly compare different projections, and the bounds we provide are more general and tighter. Moreover, none of the above strategies have implementations that scale to millions or billions of features. Recent big data packages are designed for millions or billions of samples [3, 4]. In biomedical sciences, however, it is far more common to have tens or hundreds of samples, and millions or billions of features (e.g., genomics or connectomics).

Most manifold learning methods, while exhibiting both strong theoretical [6, 29, 33] and empirical performance, are typically fully unsupervised. Thus, in classification problems, they discover a low-dimensional representation of the data, ignoring the labels. This approach can be highly problematic when the discriminant dimensions and the directions of maximal variance in the learned manifold are not aligned (see Figure 1 for some examples). Moreover, nonlinear manifold learning techniques tend to learn a mapping from the original samples to a low-dimensional space, but do not learn a projection, meaning that new samples cannot easily be mapped onto the low-dimensional space, a requirement for supervised learning. Deep learning methods [38] can easily be supervised, but they tend to require huge sample sizes, lack theoretical guarantees, or are opaque “black-boxes” that are insufficient for many biomedical applications. This yields a dearth of “out of the box” supervised scalable dimensionality reduction techniques with strong theoretical guarantees with respect to classification performance bounds designed for wide datasets. Random forests circumvent many of these problems, but implementations that operate on millions of dimensions do not exist [70], and often produce embeddings that perform no better than PCA on wide datasets (Figure 5).

Recently discussed strategies have identified techniques for recovering the loading vectors for PCA from the weights of a single-layer auto-encoder [63]. Similarly, we believe there may be promise in devising a harmony between LOL and supervised auto-encoder strategies to identify the spaces spanned by the first and second moments in unison. Successive techniques, such as unsupervised regularization of supervised autoencoders [2] and supervised dictionary learners [1], may show promise for constructive development of the projection matrix through optimization, rather than estimation, techniques. Unfor-
fortunately, these approaches lack standard numerical packages for direct comparison, evaluation, and implementation. Future work may seek to highlight the similarities, or differences, possible through such techniques.

Other approaches formulate an optimization problem, such as projection pursuit [46] and empirical risk minimization [11]. These methods are limited because they are prone to fall into local minima, require costly iterative algorithms, lack any theoretical guarantees on classification accuracy [11]. Feature selection strategies, such as higher criticism thresholding [30] effectively filter the dimensions, possibly prior to performing PCA on the remaining features [8]. These approaches could be combined with LOL in ultrahigh-dimensional problems. Similarly, another recently proposed supervised PCA variant builds on the elegant Hilbert-Schmidt independence criterion [41] to learn an embedding [9]. Our theory demonstrates that under the Gaussian model, composing this linear projection with the difference of the means will improve subsequent performance under general settings, implying that this will be a fertile avenue to pursue. A natural extension to this work would therefore be to estimate a Gaussian mixture model per class, rather than simply a Gaussian per class, and project onto the subspace spanned by the collection of all Gaussians.

In conclusion, the key XOX idea, appending class-conditional moment estimates to convert unsupervised manifold learning to supervised manifold learning, has many potential applications and extensions. We have presented the first few, including LOL, QOQ, and RLOL, which demonstrated the flexibility of XOX under both theoretical and benchmark settings. Incorporating additional nonlinearities via higher order moments, kernel methods [61], ensemble methods [21] such as random forests [15], and multiscale methods [6] are all of immediate interest.

**Data Availability** Data used within this manuscript are available from [https://neurodata.io/lol/](https://neurodata.io/lol/) and [https://neurodata.io/mri](https://neurodata.io/mri).

**Code Availability** MATLAB, R, and Python code for the experiments performed in this manuscript and a docker container for FlashLOL are available from [https://neurodata.io/lol/](https://neurodata.io/lol/), and an R package is available on the Comprehensive R Archive Network (CRAN) [17].
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A. Theoretical Background

A.I The Classification Problem

Let \((X, Y)\) be a pair of random variables, jointly sampled from \(F := F_{XY} = F_{X|Y}F_Y\), with density denoted \(f_{X,Y}\). Let \(X\) be a multivariate vector-valued random variable, such that its realizations live in \(p\) dimensional Euclidean space, \(x \in \mathbb{R}^p\). Let \(Y\) be a categorical random variable, whose realizations are discrete, \(y \in \{0, \ldots, C - 1\}\). The goal of a classification problem is to find a function \(g(x)\) such that its output tends to be the true class label \(y\):

\[
g^*(x) := \arg\max_{g \in G} \mathbb{P}[g(x) = y].
\]

When the joint distribution of the data is known, then the Bayes optimal solution is:

\[
g^*(x) := \arg\max_y f_y, x = \arg\max_y f_{x|y} f_y = \arg\max_y \{\log f_{x|y} + \log f_y\}
\]

Denote expected misclassification rate of classifier \(g\) for a given joint distribution \(F\),

\[
L^F_g := \mathbb{E}[g(x) \neq y] := \int \mathbb{P}[g(x) \neq y] f_{x,y} dx dy,
\]

where \(\mathbb{E}\) is the expectation, which in this case, is with respect to \(F_{XY}\). For brevity, we often simply write \(L_g\), and we define \(L^* := L_{g^*}\).

A.II Linear Discriminant Analysis (LDA)

Linear Discriminant Analysis (LDA) is an approach to classification that uses a linear function of the first two moments of the distribution of the data. More specifically, let \(\mu_j = \mathbb{E}[F_{X|Y = j}]\) denote the class conditional mean, and let \(\Sigma = \mathbb{E}[F^2_{X}]\) denote the joint covariance matrix, and the class priors are \(\pi_j = \mathbb{P}[Y = j]\). Using this notation, we can define the LDA classifier:

\[
g_{\text{LDA}}(x) := \arg\min_y \left[ \frac{1}{2} (x - \mu_y)^T \Sigma^{-1} (x - \mu_y) - \log \pi_y \right],
\]

Let \(L^F_{\text{LDA}}\) be the expected misclassification rate of the above classifier for distribution \(F\). Assuming equal class prior and centered means, re-arranging a bit, we obtain

\[
g_{\text{LDA}}(x) := \arg\min_y x^T \Sigma^{-1} \mu_y.
\]

In words, the LDA classifier chooses the class that maximizes the magnitude of the projection of an input vector \(x\) onto \(\Sigma^{-1} \mu_y\). When there are only two classes, letting \(\delta = \mu_0 - \mu_1\), the above further simplifies to

\[
g_{2\text{LDA}}(x) := \mathbb{I}\{x^T \Sigma^{-1} \delta > 0\}.
\]

Note that the equal class prior and centered means assumptions merely changes the threshold constant from 0 to some other constant.
A.III LDA Model

A statistical model is a family of distributions indexed by a parameter $\theta \in \Theta$, $\mathcal{F}_\theta = \{ F_\theta : \theta \in \Theta \}$. Consider the special case of the above where $F_{X|Y=y}$ is a multivariate Gaussian distribution, $\mathcal{N}(\mu_y, \Sigma)$, where each class has its own mean, but all classes have the same covariance. We refer to this model as the LDA model. Let $\theta = (\pi, \mu, \Sigma)$, and let $\Theta_{C-LDA} = (\Delta_C, \mathbb{R}^{P \times C}, \mathbb{R}_{>0}^{P \times P})$, where $\mu = (\mu_1, \ldots, \mu_C)$, $\Delta_C$ is the $C$ dimensional simplex, that is $\Delta_C = \{ x : x_i \geq 0 \forall i, \sum_i x_i = 1 \}$, and $\mathbb{R}_{>0}^{P \times P}$ is the set of positive definite $p \times p$ matrices. Denote $\mathcal{F}_{LDA} = \{ F_\theta : \theta \in \Theta_{LDA} \}$. The following lemma is well known [22]:

Lemma 1. $L^F_{LDA} = L^F_\ast$ for any $F \in \mathcal{F}_{LDA}$.

B Formal Definition of LOL and Related Projection Based Classifiers

Let $A \in \mathbb{R}^{d \times p}$ be a “projection matrix”, that is, a matrix that projects $p$-dimensional data into a $d$-dimensional subspace. The question that motivated this work is: what is the best projection matrix that we can estimate, to use to “pre-process” the data prior to classifying the data? Projecting the data $x$ onto a low-dimensional subspace, and then classifying via LDA in that subspace is equivalent to redefining the parameters in the low-dimensional subspace, $\Sigma_A = A \Sigma A^T \in \mathbb{R}^{d \times d}$ and $\delta_A = A \delta \in \mathbb{R}^d$, and then using $g_{LDA}$ in the low-dimensional space. When $C = 2$, $\pi_0 = \pi_1$, and $(\mu_0 + \mu_1)/2 = 0$, this amounts to:

$$g_A^d(x) := \{ (Ax)^T \Sigma_A^{-1} \delta_A > 0 \}, \text{ where } A \in \mathbb{R}^{d \times p}. \quad (2)$$

Let $L_A^d := \int \mathbb{E}[g_A^d(x) = y] f_x(x) dx dy$. Our goal therefore is to be able to choose $A$ for a given parameter setting $\theta = (\pi, \delta, \Sigma)$, such that $L_A$ is as small as possible (note that $L_A$ will never be smaller than $L_\ast$).

In the naive case where $(\Sigma_A, \delta_A)$ are known, we seek to solve the following linear optimization problem:

$$\begin{align*}
\text{minimize} & \quad \mathbb{E}[\{ x^T A^T \Sigma_A^{-1} \delta_A > 0 \} \neq y] \\
\text{subject to} & \quad A \in \mathbb{R}^{d \times p}. \quad (3)
\end{align*}$$

When $(\Sigma_A, \delta_A)$ are not known, however, the optimization problem becomes non-convex. With $\Sigma_A$ and $\delta_A$ as above:

$$\begin{align*}
\text{minimize} & \quad \mathbb{E}[\{ x^T A^T \Sigma_A^{-1} \delta_A > 0 \} \neq y] \\
\text{subject to} & \quad A \in \mathbb{R}^{d \times p}. \quad (4)
\end{align*}$$

While there are numerous approaches to solve related convex optimization problems through various sets of assumptions [34, 57], we do not consider such techniques in this manuscript theoretically. This is because assuming either a structure for $\Sigma_A$ or $\delta_A$ presupposes an understanding of the properties of the feature space for wide data, which is often unsuitable if the dataset is large or has considerable complexity.

Let $A = \{ A : A \in \mathbb{R}^{k \times p}, k \leq p \}$, $A^d = \{ A : A \in \mathbb{R}^{d \times p} \}$, and let $A_* \subset A$ be the set of $A$ that minimizes Eq. (4), and let $A_* \subset A_*$. Let $L_A^* = L_{A_*}$ be the misclassification rate for any $A \in A_*$, that is, $L_A^*$ is the Bayes optimal misclassification rate for the classifier that composes $A$ with LDA.

In our opinion, Eq. (4) is the simplest supervised manifold learning problem there is: a two-class classification problem, where the data are multivariate Gaussians with shared, unknown covariances, the
manifold is linear, and the classification is done via LDA. Nonetheless, solving Eq. (4) is difficult, because we do not know how to evaluate the integral analytically, and we do not know any algorithms that are guaranteed to find the global optimum in finite time. We proceed by studying a few natural choices for \( A \).

### B.I Bayes Optimal Projection

**Lemma 2.** \( \delta^T \Sigma^{-1} \in \mathcal{A}_* \)

**Proof.** Let \( B = (\Sigma^{-1} \delta)^T = \delta^T (\Sigma^{-1})^T = \delta^T \Sigma^{-1} \), so that \( B^T = \Sigma^{-1} \delta \), and plugging this in to Eq. (2). By the above, and noting the symmetry and invertibility of \( \Sigma \):

\[
\Sigma_B = B \Sigma B^T = \delta^T \Sigma^{-1} \Sigma \delta \Sigma^{-1} \delta^T \delta \Sigma^{-1} \delta = \delta^T \Sigma^{-1} \delta
\]

\[
\Rightarrow \Sigma_B^{-1} = \delta^{-1} \Sigma \delta^{-1}
\]

\[
\delta_B = B \delta = \delta^T \Sigma^{-1} \delta
\]

We obtain:

\[
g_B(x) = \mathbb{I}\{ x^T B^T \Sigma_B^{-1} \delta_B > 0 \}
\]

\[
= \mathbb{I}\{ x^T (\Sigma^{-1} \delta) (\Sigma^{-1} \delta_B) > 0 \}
\]

\[
= \mathbb{I}\{ x^T (\Sigma^{-1} \delta) (\delta^{-1} \Sigma \delta^{-1} \delta^T \Sigma^{-1} \delta) > 0 \}
\]

\[
= \mathbb{I}\{ x^T \Sigma^{-1} \delta > 0 \}
\]

In other words, letting \( B \) be the Bayes optimal projection recovers the Bayes classifier, as it should. Or, more formally, for any \( F \in \mathcal{F}_\text{LDA} \), \( L_B^T \Sigma^{-1} = L_* \).

### B.II Principle Components Analysis (PCA) Projection

Principle Components Analysis (PCA) finds the directions of maximal variance in a dataset. PCA is closely related to eigendecompositions and singular value decompositions (SVD). In particular, the top left singular vector of a matrix \( X \in \mathbb{R}^{p \times n} \), whose columns are centered, is the eigenvector with the largest eigenvalue of the centered covariance matrix \( XX^T \). SVD enables one to estimate this eigenvector without ever forming the outer product matrix, because SVD factorizes a matrix \( X \) into \( USV^T \), where \( U \) and \( V \) are orthonormal \( p \times n \) matrices, and \( S \) is a diagonal matrix, whose diagonal values are decreasing, \( s_1 \geq s_2 \geq \cdots \geq s_n \). Defining \( U = [u_1, u_2, \ldots, u_n] \), where each \( u_i \in \mathbb{R}^p \), then \( u_i \) is the \( i^{th} \) eigenvector, and \( s_i \) is the square root of the \( i^{th} \) eigenvalue of \( XX^T \). Let \( A_{d\times p}^{\text{PCA}} = [u_1, \ldots, u_d] \) be the truncated PCA orthonormal matrix, and let \( I_{d \times p} \) denote a \( d \times p \) dimensional identity matrix.

The PCA matrix is perhaps the most obvious choice of an orthonormal matrix for several reasons. First, truncated PCA minimizes the squared error loss between the original data matrix and all possible rank \( d \) representations:

\[
\arg\min_{A \in \mathbb{R}^{d \times p}} \left\| X - A^T A \right\|_F^2.
\]
Second, the ubiquity of PCA has led to a large number of highly optimized numerical libraries for computing PCA (for example, LAPACK [7]).

In this supervised setting, we consider two different variants of PCA, each based on centering the data differently. For the first one, which we refer to as “pooled PCA” (or just PCA for brevity), we center the data by subtracting the “pooled mean” from each sample, that is, we let \( \tilde{x}_i = x - \mu \), where \( \mu = \mathbb{E}[x] \).

For the second, which we refer to as “class conditional PCA”, we center the data by subtracting the “class-conditional mean” from each sample, that is, we let \( \tilde{x}_i = x - \mu_y \), where \( \mu_y = \mathbb{E}[x|Y = y] \).

Notationally, let \( U_d = [u_1, \ldots, u_d] \in \mathbb{R}^{p \times d} \), and note that \( U_d^T U_d = I_d \times d \) and \( U_d^T U_d = I_p \times p \). Similarly, let \( USU^T = \Sigma \), and \( US^{-1}U^T = \Sigma^{-1} \). Let \( S_d \) be the matrix whose diagonal entries are the eigenvalues, up to the \( d \)th one, that is \( S_d(i,j) = s_i \) for \( i = j \leq d \) and zero otherwise. Similarly, \( \Sigma_d = US_dU^T = U_dS_dU_d^T \).

Reduced-rank LDA (rrLDA) is a regularized LDA algorithm. Specifically, rather than using the full rank covariance matrix, it uses a rank-\( d \) approximation. Formally, let \( g_{\text{LDA}} := \mathbb{I}\{x^T \Sigma^{-1} \delta > 0\} \) be the LDA classifier, and let \( g^d_{\text{LDA}} := \mathbb{I}\{x^T \Sigma^{-1} \delta > 0\} \) be the regularized LDA classifier, that is, the LDA classifier where the the bottom \( p - d \) eigenvalues of the covariance matrix are set to zero.

**Lemma 3.** Using class-conditional PCA to pre-process the data, then using LDA on the projected data, is equivalent to rrLDA.

**Proof.** Plugging \( U_d \) into Eq. (2) for \( A \), and considering only the left side of the operand, we have

\[
(Ax)^T \Sigma_{A}^{-1} \delta_A = x^T A^T A \Sigma^{-1} A^T A \delta,
\]

\[
= x^T U_d U_d^T \Sigma^{-1} U_d U_d^T \delta,
\]

\[
= x^T U_d U_d^T U S^{-1} U^T U_d U_d^T \delta,
\]

\[
= x^T U_d I_d \times p S^{-1} I_p \times p U_d^T \delta,
\]

\[
= x^T U_d S_d^{-1} U_d^T \delta,
\]

\[
= x^T \Sigma_d^{-1} \delta.
\]

The implication of this lemma is that if one desires to implement rrLDA, rather than first learning the eigenvectors and then learning LDA, one can instead directly implement regularized LDA by setting the bottom \( p - d \) eigenvalues to zero. This latter approach removes the requirement to run SVD twice, therefore reducing the computational burden as well as the possibility of numerical instability issues. We therefore refer to the projection composed of \( d \) eigenvectors of the class-conditionally centered covariance matrices, \( A^d_{\text{LDA}} \).

**B.III Linear Optimal Low-Rank (LOL) Projection**

The basic idea of LOL is to use both \( \delta \) and the top \( d \) eigenvectors of the class-conditionally centered covariance. When there are only two classes, \( \delta = \mu_0 - \mu_1 \). When there are \( C > 2 \) classes, there are \( \binom{C}{2} \) pairwise combinations, \( \delta_{ij} = \mu_i - \mu_j \) for all \( i \neq j \). However, since \( \binom{C}{2} \) is nearly \( C^2 \), when \( C \) is large, this would mean incorporating many mean difference vectors. Note that \( [\delta_{1,2}, \delta_{1,3}, \ldots, \delta_{C-1,C}] \) is in fact a rank \( C - 1 \) matrix, because it is a linear function of the \( C \) different means. Therefore, we only need \( C - 1 \) differences to span the space of all pairwise differences. To
mitigate numerical instability issues, we adopt the following convention. For each class, estimate the expected mean and the number of samples per class, \( \mu_c \) and \( \pi_c \). Sort the means in order of decreasing \( \pi_c \), so that \( \pi_1 > \pi_2 > \cdots > \pi_C \). Then, subtract \( \mu_i \) from all other means: \( \delta_i = \mu_1 - \mu_i \), for \( i = 2, \ldots, C \). Finally, \( \delta = [\delta_2, \ldots, \delta_C] \).

Given \( \delta \) and \( A_{\text{LDA}}^{d-1} \), to obtain LOL naively, we could simply concatenate the two, \( A_{\text{LOL, naive}} = [\delta, A_{\text{LDA}}^{d-1}] \). Recall that eigenvectors are orthonormal. To maintain orthonormality between the eigenvectors and vectors of \( \delta \), we could easily apply Gram-Schmidt, \( A_{\text{LOL, naive}} = \text{Orth}(\delta, A_{\text{LDA}}^{d-1}) \). In practice, this orthogonalization step does not matter much, so we ignore it hereafter. To ensure that \( \delta \) and \( \Sigma \) are balanced appropriately, we normalize each vector in \( \delta \) to have norm unity. Formally, let \( \tilde{\delta} = \frac{\delta_j}{\|\delta_j\|} \), where \( \delta_j \) is the \( j \)th difference of the mean vector and let \( A_{\text{LOL}} = [\tilde{\delta}, A_{\text{LDA}}^{d-(C-1)}] \).

When the distribution of the data is not provided, each of the above terms must be estimated from the data. We use the maximum likelihood estimators for each, specifically:

\[
\begin{align*}
n_c &= \sum_{i=1}^{n} \mathbb{I}\{y_i = c\}, \quad (5) \\
\hat{\pi}_c &= \frac{n_c}{n}, \quad (6) \\
\hat{\mu} &= \frac{1}{n} \sum_{i=1}^{n} x_i, \quad (7) \\
\hat{\mu}_c &= \frac{1}{n_c} \sum_{i=1}^{n} x_i \mathbb{I}\{y_i = c\}. \quad (8)
\end{align*}
\]

For completeness, below we provide pseudocode for learning the sample version of LOL. The population version does not require the estimation of the parameters.

**B.IV  \( \text{rrLDA} \) is rotationally invariant**

For certain classification tasks, the observed dimensions (or features) have intrinsic value, e.g. when simple interpretability is desired. However, in many other contexts, interpretability is less important [14]. When the exploitation task at hand is invariant to rotations, then we have no reason to restrict our search space to be sparse in the observed dimensions. For example, we can consider sparsity in the eigenvector basis. Let \( W \) be a rotation matrix, that is \( W \in W = \{W : W^T = W^{-1} \text{ and } \det(W) = 1\} \). Moreover, let \( W \circ F \) denote the distribution \( F \) after transformation by an operator \( W \). For example, if \( F = \mathcal{N}(\mu, \Sigma) \) then \( W \circ F = \mathcal{N}(W\mu, W\Sigma W^T) \).

**Definition 1.** A rotationally invariant classifier has the following property:

\[
L^F_g = L^{W_0 F}_g, \quad F \in \mathcal{F} \text{ and } W \in W.
\]

In words, the Bayes risk of using classifier \( g \) on distribution \( F \) is unchanged if \( F \) is first rotated.

Now, we can state the main lemma of this subsection: \( \text{rrLDA} \) is rotationally invariant.

**Lemma 4.** \( L^F_{\text{LDA}} = L^{W_0 F}_{\text{LDA}}, \text{ for any } F \in \mathcal{F} \).

**Proof.** \( \text{rrLDA} \) is in fact simply thresholding \( x^T \Sigma^{-1} \delta \) whenever its value is larger than some constant. Thus, we can demonstrate rotational invariance by demonstrating that \( x^T \Sigma^{-1} \delta \) is rotationally invariant.
\[(Wx)^T (W \Sigma W^T)^{-1} W \delta = x^T W^T (WUSU^T W^T)^{-1} W \delta\] 
\[= x^T W^T (\tilde{U} S \tilde{U}^T)^{-1} W \delta\] 
\[= x^T W^T \tilde{U} S^{-1} \tilde{U}^T W \delta\] 
\[= x^T W^T WUS^{-1} U^T W W^T \delta\] 
\[= x^T US^{-1} U^T \delta\] 
\[= x^T \Sigma^{-1} \delta\] 

by substituting \(USU^T\) for \(\Sigma\)

by letting \(\tilde{U} = WU\)

by the laws of matrix inverse

by un-substituting \(WU = \tilde{U}\)

by un-substituting \(US^{-1} U^T = \Sigma\)

One implication of this lemma is that we can reparameterize without loss of generality. Specifically, defining \(W := U^T\) yields a change of variables: \(\Sigma \mapsto S\) and \(\delta \mapsto U^T \delta := \delta''\), where \(S\) is a diagonal covariance matrix. Moreover, let \(d = (\sigma_1, \ldots, \sigma_D)^T\) be the vector of eigenvalues, then \(S^{-1} \delta' = d^{-1} \odot \delta\), where \(\odot\) is the Hadamard (entrywise) product. The LDA classifier may therefore be encoded by a unit vector, \(\tilde{d} := \frac{1}{m} d^{-1} \odot \tilde{\delta}'\), and its magnitude, \(m := \left\|d^{-1} \odot \tilde{\delta}\right\|\). This will be useful later.

### B.V Rotation of Projection Based Linear Classifiers

By a similar argument as above, one can easily show that:

\[(AWx)^T (AW \Sigma W^T A^T)^{-1} AW \delta = x^T (W^T A^T)(AW) \Sigma^{-1} (W^T A^T)(AW) \delta\] 
\[= x^T Y^T Y \Sigma^{-1} Y^T Y \delta\] 
\[= x^T Z \Sigma^{-1} Z^T \delta\] 
\[= x^T (Z \Sigma Z^T)^{-1} \delta = x^T \tilde{\Sigma}^{-1} \delta,\]

where \(Y = AW \in \mathbb{R}^{d \times p}\) so that \(Z = Y^T Y\) is a symmetric \(p \times p\) matrix of rank \(d\). In other words, rotating and then projecting is equivalent to a change of basis. The implications of the above is:

**Lemma 5.** \(g_A\) is rotationally invariant if and only if \(\text{span}(A) = \text{span}(\Sigma_d)\). In other words, \(rrLDA\) is the only rotationally invariant projection.

### B.VI Low-Rank Canonical Correlation Analysis

We now contrast LOL and low-rank CCA. For discriminant analysis, low-rank CCA corresponds to finding the eigenvectors of \(S_X^T S_B\) where

\[S_X = \sum_i (X_i - \bar{X})(X_i - \bar{X})^T; \quad \bar{X} = \sum_i X_i\]

is the sample covariance matrix of the \(X_i\), \(S_X^\dagger\) is the inverse of \(S_X\) (or Moore-Penrose pseudo-inverse of \(S_X\) if \(S_X\) is not invertible), and

\[S_B = \frac{n_0}{n} (\bar{X}_0 - \bar{X})(\bar{X}_0 - \bar{X})^T + \frac{n_1}{n} (\bar{X}_1 - \bar{X})(\bar{X}_1 - \bar{X})^T; \quad \bar{X}_j = \sum_{i: Y_i = j} X_i\text{ for } j \in \{0, 1\}\]

is the sample covariance matrix of the \(Y\) and their means, respectively.
is the between class covariance matrix \([64]\). It is widely known (see section 11.5 of \([59]\)) that if \(S_X\) is invertible then the above formulation reduces to that of Fisher L, namely that of finding \(\hat{v}\) satisfying

\[
\hat{v} = \arg\max_{v \neq 0} \frac{v^\top S_B v}{v^\top S_W v}
\]

\[
S_W = \sum_{i : Y_i = 0} (X_i - \bar{X}_0)(X_i - \bar{X}_0)^\top + \sum_{i : Y_i = 1} (X_i - \bar{X}_1)(X_i - \bar{X}_1)^\top;
\]

where \(S_W\) is the pooled within-sample covariance matrix and \(S_X = S_W + S_B\). In the context of our current paper where \(X\) is assumed to be high-dimensional, it is well-known that \(S_X\) is not a good estimator of the population covariance matrix \(\Sigma_X = \mathbb{E}[(X - \mu)(X - \mu)^\top]\) and thus computing \(S_X^{-1}\) is suboptimal for subsequent inference unless some form of regularization is employed. Our consideration of low-rank linear transformations \(AX\) provides one principled approach to regularizations of high-dimensional \(S_X\). In contrasts, the above (unregularized) formulation of low-rank CCA frequently yields discrimination direction vectors corresponding to “maximum data piling” (MDP) directions \([5, 64]\) in high-dimensional settings (and always yield maximum data piling directions when \(p \geq n\)). These MDP directions lead to perfect discrimination of the training data, but can suffer from poor generalization performance, as the examples in \([5, 64]\) indicate.

Naïvely computing the low-rank CCA projection requires storing and inverting a \(p \times p\) matrix. However, we devised an implementation for low-rank CCA that does not require ever materializing this matrix. Modern eigensolvers computes eigenvalues by performing a sequence of matrix vector multiplication. For example, to compute eigenvalues of \(S_X\), an eigensolver performs \(S_X v\) multiple times until the algorithm converges. Assume that the number of iteration is \(i\), the computation complexity of the eigensolver is \(O(n \times p \times i)\). Performing pseudo-inverse of \(S_X\) computes truncated SVD on \(S_X\), resulting in \(S_X v = \sum_i (X_i - \bar{X})(X_i - \bar{X})^\top v_i\). Here we never physically generate \(S_X\). Instead, we always compute \(v' = (X_i - \bar{X})^\top v\) and then \(v'' = (X_i - \bar{X}) v'\) to compute \(S_X v\). Assume \(k\) classes, \(S_X v\) has the computation complexity of \(O(n \times p \times k)\) and the space complexity of \(O(n \times p \times k)\). \(S_X\) can be decomposed into \(U \Sigma V\), where \(U\) is a \(n \times n\) matrix and \(V\) is a \(n \times p\) matrix.

\[
S_X = U \Sigma V^\top
\]

\[
S_X = U \Sigma^{-1} V (\frac{m_0}{n} (\bar{X}_0 - \bar{X})(\bar{X}_0 - \bar{X})^\top + \frac{m_1}{n} (\bar{X}_1 - \bar{X})(\bar{X}_1 - \bar{X})^\top).
\]

Computing eigenvalues of \(S_X^\top S_B\) requires

\[
S_X^\top S_B v = U \Sigma^{-1} V (\frac{m_0}{n} (\bar{X}_0 - \bar{X})(\bar{X}_0 - \bar{X})^\top v + \frac{m_1}{n} (\bar{X}_1 - \bar{X})(\bar{X}_1 - \bar{X})^\top v)).
\]

Similar to \(S_X v\), we never physically generate \(S_X^\top v\) or \(S_B\). Instead, we always multiply the terms on the right with \(v\) first, which results in the computation complexity of \(O(n \times p)\) and the space complexity of \(O(n \times p)\). To our knowledge, this algorithm is novel, and the implementation is also of course novel.

### C Simulations

Let \(f_{x|y}\) denote the conditional distribution of \(X\) given \(Y\), and let \(f_y\) denote the prior probability of \(Y\). For simplicity, assume that realizations of the random variable \(X\) are \(p\)-dimensional vectors, \(x \in \mathbb{R}^p\), and realizations of the random variable \(Y\) are binary, \(y \in \{0, 1\}\). For most simulation settings, each class is Gaussian: \(f_{x|y} = \mathcal{N}(\mu_y, \Sigma_y)\), where \(\mu_y\) is the class-conditional mean and \(\Sigma_y\) is the class-conditional covariance. Moreover, we assume \(f_y\) is a Bernoulli distribution with probability \(\pi\) that \(y = 1\), \(f_y = \mathcal{B}(\pi)\). We typically assume that both classes are equally likely, \(\pi = 0.5\), and the covariance matrices are the same, \(\Sigma_0 = \Sigma_1 = \Sigma\). Under such assumptions, we merely specify \(\theta = \{\mu_0, \mu_1, \Sigma\}\). We consider the following simulation settings:
Stacked Cigars

• $\mu_0 = 0$,
• $\mu_1 = (a, b, a, \ldots, a)$,
• $\Sigma$ is a diagonal matrix, with diagonal vector, $d = (1, b, 1 \ldots, 1)$,

where $a = 0.15$ and $b = 4$.

Trunk

• $\mu_0 = \frac{b}{\sqrt{(1, 3, 5, \ldots, 2p)}}$,
• $\mu_1 = -\mu_0$,
• $\Sigma$ is a diagonal matrix, with diagonal vector, $d = 100/\sqrt{(p, p - 1, p - 2, \ldots, 1)}$,

where $b = 4$.

Rotated Trunk  Same as Trunk, but the data are randomly rotated, that is, we sample $Q$ uniformly from the set of $p$-dimensional rotation matrices, and then set:

• $\mu_0 \leftarrow Q\mu_0$,
• $\mu_1 \leftarrow Q\mu_1$,
• $\Sigma \leftarrow Q\Sigma Q^T$.

3 Classes  Same as Trunk, but with a third mean equal to the zero vector, $\mu_2 = 0$.

• $\mu_0 = \frac{b}{\sqrt{(1, 3, 5, \ldots, 2p)}}$,
• $\mu_1 = -\mu_0$,
• $\mu_2 = 0$,
• $\Sigma$ is a diagonal matrix, with diagonal vector, $d = 100/\sqrt{(p, p - 1, p - 2, \ldots, 1)}$,

where $b = 4$.

Robust  An experiment in which outliers are present for estimation of the projection matrix, but removed for training and testing of the classifier. This is due to the strong amount of noise present in the robust experiment will lead to poor generalizability of the estimated LDA classifier. Parameters indexed by $i$ correspond to the generative model for the inliers, and those with $o$ correspond to the outliers.

• $\mu_0^{(i)} = \frac{b}{\sqrt{(1, 3, 5, \ldots, p)}}$ for the first $p/2$ dimensions and 0 otherwise,
• $\mu_1^{(i)} = -\mu_0$,
• $\Sigma^{(i)} = b^3/\sqrt{(1, 2, \ldots, p)}$,
• $\mu^{(o)} = 0$,
• $\Sigma^{(o)} = b^6/\sqrt{(1, 2, \ldots, p)}$,
• $\pi^{(i)} = 0.7$,
• $\pi^{(o)} = 0.3$,

and outliers are randomly assigned class 0 or class 1 with equal probability.

Cross  An experiment in which the two classes have identical means but different covariance matrices, meaning the optimal discriminant boundary is quadratic.

• $\mu_0 = \mu_1 = 0$, 

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• $\Sigma_0$ is a diagonal matrix, with diagonal $(a, \ldots, a, b, \ldots, b)$ where the first $d_3$ elements are $a$, and the rest are $b$.
• $\Sigma_1$ is a diagonal matrix, with diagonal $(b, \ldots, b, a, \ldots, a, b, \ldots, b)$ where the middle $d_3$ elements are $a$, and the others are $b$.
and we let $a = 1$, and $b = \frac{1}{4}$.

**Hump-$K$** An experiment with $K$ classes, in which the class means display an alternating series of humps, and the class covariance is a scalar multiple of the identity.

• $\pi_k = \frac{1}{K}$
• $x_{l,k} = \left\lfloor -\frac{K}{2} \right\rfloor$ the left endpoint of the hump
• $x_{r,k} = d - x_{l,K-k+1}$ the right endpoint of the hump
• $x_{m,k} = \left(\frac{x_{l,k} + x_{r,k}}{2}\right)$ the midpoint of the hump
• Let $a_k, b_k, c_k$ be the unique coefficients such that $c_k + b_k x + a_k x^2$ passes through $x_{l,k}$ at $y = 0$, passes through $x_{r,k}$ at $y = b$, and passes through $x_{m,k}$ at $y = 0$.
• Let $\alpha_k = \begin{cases} 1 & k \text{ is odd} \\ -1 & k \text{ is even} \end{cases}$
• for $j = 1, \ldots, d$, let $\mu_{k,j} = \begin{cases} 0 & j \notin [x_{l,k}, x_{r,k}] \\ c_k + b_k j + a_k j^2 & j \in [x_{l,k}, x_{r,k}] \end{cases}$
• $\Sigma$ is a diagonal matrix, with diagonal vector $(\sigma, \ldots, \sigma)$.

where $b = 4$ and $\sigma = \frac{100}{K}$.

**Computational Efficiency Experiments** These experiments used the Trunk setting, increasing the observed dimensionality.

**Hypothesis Testing Experiments** We considered two related joint distributions here. The first joint (Diagonal) is described by:

• $\mu_0 = 0$,
• $\mu_1 \sim \mathcal{N}(0, I)$, $\mu_1 = \overline{\mu}_1 / \|\overline{\mu}_1\|$, 
• $\Sigma$ is the same Toeplitz matrix (where the top row is $\rho(0,1,2,\ldots,p-1)$), and the matrix is rescaled to have a Frobenius norm of 50.

The second (Dense) is the same except that the eigenvectors are uniformly random sampled orthonormal matrices, rather than the identity matrix.

**Regression Experiments** In this experiment we used a distribution similar to the Toeplitz distribution as described above, but $y$ was a linear function of $x$, that is, $y = Ax$, where $x \sim \mathcal{N}(0, \Sigma)$, where $\Sigma$ is the above described Toeplitz matrix, and $A$ is a diagonal matrix whose first two diagonal elements are non-zero, and the rest are zero.

**D Theorems and Proofs of Main Result**
D.I Chernoff information

We now introduce the notion of the Chernoff information, which serves as our surrogate measure for the Bayes error of any classification procedure given the projected data. Our discussion of the Chernoff information is under the context of decision rules for hypothesis testing, nevertheless, as evidenced by the fact that the maximum a posteriori decision rule—equivalently the Bayes classifier—achieves the Chernoff information rate, this distinction between hypothesis testing and classification is mainly for ease of exposition.

Let $F_0$ and $F_1$ be two absolutely continuous multivariate distributions in $\Omega \subset \mathbb{R}^d$ with density functions $f_0$ and $f_1$, respectively. Suppose that $X_1, X_2, \ldots, X_m$ are independent and identically distributed random variables, with $X_i$ distributed either $F_0$ or $F_1$. We are interested in testing the simple null hypothesis $H_0: F = F_0$ against the simple alternative hypothesis $H_1: F = F_1$. A test $T$ is a sequence of mapping $T_m: \Omega^m \mapsto \{0, 1\}$ such that given $X_1 = x_1, X_2 = x_2, \ldots, X_m = x_m$, the test rejects $H_0$ in favor of $H_1$ if $T_m(x_1, x_2, \ldots, x_m) = 1$; similarly, the test decides $H_1$ instead of $H_0$ if $T_m(x_1, x_2, \ldots, x_m) = 0$. The Neyman-Pearson lemma states that, given $X_1, X_2, \ldots, X_m$ are independent and identically distributed random variables $X_1, X_2, \ldots, X_m$. A classical result of Chernoff states that the Bayes risk is intrinsically linked to a quantity known as the Chernoff information. More specifically, let $C(F_0, F_1)$ be the quantity

$$C(F_0, F_1) = - \log \left[ \inf_{t \in (0, 1)} \int_{\mathbb{R}^d} f_0^t(x)f_1^{1-t}(x)dx \right]$$

Moreover, the likelihood ratio test is the most powerful test at significance level $\alpha_m = \alpha(\eta_m)$, i.e., the likelihood ratio test minimizes the type II error $\beta_m$ subject to the constraint that the type I error is at most $\alpha_m$.

Assume that $\pi \in (0, 1)$ is a prior probability of $H_0$ being true. Then, for a given $\alpha_m^* \in (0, 1)$, let $\beta_m^* = \beta_m^*(\alpha_m^*)$ be the type II error associated with the likelihood ratio test when the type I error is at most $\alpha_m^*$. The quantity $\inf_{m \in (0, 1)} \pi \alpha_m^* + (1 - \pi) \beta_m^*$ is then the Bayes risk in deciding between $H_0$ and $H_1$ given the $m$ independent random variables $X_1, X_2, \ldots, X_m$. A classical result of Chernoff states that the Bayes risk is intrinsically linked to a quantity known as the Chernoff information. More specifically, let $C(F_0, F_1)$ be the quantity

$$C(F_0, F_1) = - \log \left[ \inf_{t \in (0, 1)} \int_{\mathbb{R}^d} f_0^t(x)f_1^{1-t}(x)dx \right]$$

Then we have

$$\lim_{m \to \infty} \frac{1}{m} \inf_{\alpha_m^* \in (0, 1)} \log (\pi \alpha_m^* + (1 - \pi) \beta_m^*) = - C(F_0, F_1).$$

Thus $C(F_0, F_1)$ is the exponential rate at which the Bayes error $\inf_{m \in (0, 1)} \pi \alpha_m^* + (1 - \pi) \beta_m^*$ decreases as $m \to \infty$; we also note that the $C(F_0, F_1)$ is independent of $\pi$. We also define, for a given $t \in (0, 1)$ the Chernoff divergence $C_t(F_0, F_1)$ between $F_0$ and $F_1$ by

$$C_t(F_0, F_1) = - \log \int_{\mathbb{R}^d} f_0^t(x)f_1^{1-t}(x)dx.$$
The result of Eq. (10) can be extended to $K + 1 \geq 2$ hypothesis, with the exponential rate being the minimum of the Chernoff information between any pair of hypothesis. More specifically, let $F_0, F_1, \ldots, F_K$ be distributions on $\mathbb{R}^d$ and let $X_1, X_2, \ldots, X_m$ be independent and identically distributed random variables with distribution $F \in \{F_0, F_1, \ldots, F_K\}$. Our inference task is in determining the distribution of the $X_i$ among the $K + 1$ hypothesis $H_0: F = F_0, \ldots, H_K: F = F_K$. Suppose also that hypothesis $H_k$ has a priori probability $\pi_k$. For any decision rule $g$, the risk of $g$ is $r(g) = \sum_k \pi_k \sum_{l \neq k} \alpha_{lk}(g)$ where $\alpha_{lk}(g)$ is the probability of accepting hypothesis $H_l$ when hypothesis $H_k$ is true. Then we have [52]

$$\inf_{g} \lim_{m \to \infty} \frac{r(g)}{m} = -\min_{k \neq l} C(F_k, F_l), \quad (11)$$

where the infimum is over all decision rules $g$, i.e., for any $g$, $r(g)$ decreases to 0 as $m \to \infty$ at a rate no faster than $\exp(-m \min_{k \neq l} C(F_k, F_l))$.

When the distributions $F_0$ and $F_1$ are multivariate normal, that is, $F_0 = \mathcal{N}(\mu_0, \Sigma_0)$ and $F_1 = \mathcal{N}(\mu_1, \Sigma_1)$; then, denoting by $\Sigma_t = t\Sigma_0 + (1 - t)\Sigma_1$, we have

$$C(F_0, F_1) = \sup_{t \in (0, 1)} \left(\frac{(1 - t)}{2} (\mu_1 - \mu_2)\top \Sigma_t^{-1} (\mu_1 - \mu_2) + \frac{1}{2} \log \frac{\|\Sigma_t\|_{\Sigma_0}^{-1} \Sigma_1^{-1} t - (1 - t)}{\|\Sigma_0\|_{\Sigma_1}^{-1} t - (1 - t)}\right).$$

D.II Projecting data and Chernoff information

We now discuss how the Chernoff information characterizes the effect a linear transformation $A$ of the data has on classification accuracy. We start with the following simple result whose proof follows directly from Eq. (11).

**Lemma 6.** Let $F_0 = \mathcal{N}(\mu_0, \Sigma)$ and $F_1 = \mathcal{N}(\mu_1, \Sigma)$ be two multivariate normals with equal covariance matrices. For any linear transformation $A$, let $F_0^{(A)}$ and $F_1^{(A)}$ denote the distribution of $AX$ when $X \sim F_0$ and $X \sim F_1$, respectively. We then have

$$C(F_0^{(A)}, F_1^{(A)}) = \frac{1}{8} (\mu_1 - \mu_0)\top A\top (A\Sigma A\top)^{-1} A(\mu_1 - \mu_0)$$

$$= \frac{1}{8} (\mu_1 - \mu_0)\top \Sigma^{-1/2} \Sigma^{1/2} A\top (A\Sigma A\top)^{-1} A \Sigma^{1/2} \Sigma^{-1/2} (\mu_1 - \mu_0) \quad (12)$$

where $P_Z = Z(Z\top Z)^{-1} Z\top$ denotes the matrix corresponding to the orthogonal projection onto the columns of $Z$.

Thus for a classification problem where $X|Y = 0$ and $X|Y = 1$ are distributed multivariate normals with mean $\mu_0$ and $\mu_1$ and the same covariance matrix $\Sigma$, Lemma 6 then states that for any two linear transformations $A$ and $B$, the transformed data $AX$ is to be preferred over the transformed data $BX$ if

$$(\mu_1 - \mu_0)\top A\top (A\Sigma A\top)^{-1} A(\mu_1 - \mu_0) > (\mu_1 - \mu_0)\top B\top (B\Sigma B\top)^{-1} B(\mu_1 - \mu_0).$$

In particular, using Lemma 6, we obtain the following result showing the dominance of LOL over reduced-rank LDA (or simply rLDA for brevity) when the class conditional distributions are multivariate normal with a common variance.
Theorem 1. Let $F_0 = N(\mu_0, \Sigma)$ and $F_1 \sim N(\mu_1, \Sigma)$ be multivariate normal distributions in $\mathbb{R}^p$. Let $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_p$ be the eigenvalues of $\Sigma$ and $u_1, u_2, \ldots, u_p$ the corresponding eigenvectors. For $d \leq p$, let $U_d = \begin{bmatrix} u_1 & u_2 & \cdots & u_d \end{bmatrix} \in \mathbb{R}^{p \times d}$ be the matrix whose columns are the eigenvectors $u_1, u_2, \ldots, u_d$. Let $A = [\delta \mid U_{d-1}]$ and $B = U_d$ be the LDA and rLDA linear transformations into $\mathbb{R}^d$, respectively. Then

$$C(F_0^{(A)}, F_1^{(A)}) - C(F_0^{(B)}, F_1^{(B)}) = \frac{\delta^T (I - U_{d-1}U_d^T) \delta}{\delta^T (\Sigma - \Sigma_{d-1}) \delta} - \delta^T (\Sigma_d^\dagger - \Sigma_{d-1}^\dagger) \delta \geq \frac{1}{\lambda_d} \delta^T (I - U_{d-1}U_d^T) \delta - \frac{1}{\lambda_d} \delta^T (U_dU_d^T - U_{d-1}U_{d-1}^T) \delta \geq 0$$

(13)

and the inequality is strict whenever $\delta^T (I - U_dU_d^T) \delta > 0$.

Proof. We first note that

$$A\Sigma A^\top = \begin{bmatrix} \delta | U_{d-1} \end{bmatrix}^\top \Sigma \begin{bmatrix} \delta | U_{d-1} \end{bmatrix} = \begin{bmatrix} \delta^\top \Sigma \delta & \delta^\top \Sigma U_{d-1} \\ U_{d-1}^\top \Sigma \delta & U_{d-1}^\top \Sigma U_{d-1} \end{bmatrix} = \begin{bmatrix} \delta^\top \Sigma \delta & \delta^\top \Sigma U_{d-1} \\ U_{d-1}^\top \Sigma \delta & \Lambda_{d-1} \end{bmatrix}$$

where $\Lambda_{d-1} = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_{d-1})$ is the $(d-1) \times (d-1)$ diagonal matrix formed by the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_{d-1}$. Therefore, letting $\gamma = \delta^\top \Sigma \delta - \delta^\top \Sigma U_{d-1} \Lambda_{d-1}^{-1} U_{d-1}^\top \Sigma \delta$, we have

$$(A\Sigma A^\top)^{-1} = \begin{bmatrix} \delta^\top \Sigma \delta & \delta^\top \Sigma U_{d-1} \\ U_{d-1}^\top \Sigma \delta & U_{d-1}^\top \Sigma U_{d-1} \end{bmatrix}^{-1} = \begin{bmatrix} \gamma^{-1} & -\delta^\top \Sigma U_{d-1} \Lambda_{d-1}^{-1} \gamma^{-1} \\ -\Lambda_{d-1}^{-1} U_{d-1}^\top \Sigma \delta \gamma^{-1} & (\Lambda_{d-1} - \frac{U_{d-1}^\top \Sigma \delta \gamma^{-1}}{\delta^\top \Sigma \delta})^{-1} \end{bmatrix}.$$
Therefore,
\[
\delta^\top A^\top (A\Sigma A^\top)^{-1}A\delta = \delta^\top \delta | U_{d-1} \left[ -\gamma^{-1}U_{d-1}^\top \delta \Lambda_{d-1}^{-1} + \gamma^{-1}U_{d-1}^\top \delta^\top U_{d-1} \right] \delta | U_{d-1} \right. \\
= \left[ \delta^\top \delta | \delta^\top U_{d-1} \right. \\
-\gamma^{-1}U_{d-1}^\top \delta \Lambda_{d-1}^{-1} + \gamma^{-1}U_{d-1}^\top \delta^\top U_{d-1} \right]\left[ \delta_U \right.
= (\delta^\top \delta)^2 - 2\gamma^{-1}\delta^\top U_{d-1} U_{d-1}^\top \delta + \delta^\top U_{d-1} \Lambda_{d-1}^{-1} U_{d-1}^\top \delta
= (\delta^\top \delta)^2 + \delta^\top U_{d-1} \Lambda_{d-1}^{-1} U_{d-1}^\top \delta
= \gamma^{-1}(\delta^\top (I - U_{d-1}^\top U_{d-1})^\top \delta)^2 + \delta^\top U_{d-1} \Lambda_{d-1}^{-1} U_{d-1}^\top \delta
\]

where $\Sigma_{d-1}$ is the Moore-Penrose pseudo-inverse of $\Sigma_{d-1}$. The LDA projection matrix into $\mathbb{R}^d$ is given by $B = U_d^\top$ and hence
\[
\delta^\top B^\top (B\Sigma B^\top)^{-1}B\delta = \delta^\top U_d \Lambda_d^{-1} U_d^\top \delta = \delta^\top \Sigma_d \delta. \tag{14}
\]

We thus have
\[
C(F_0^{(A)}, F_1^{(A)}) - C(F_0^{(B)}, F_1^{(B)}) = \gamma^{-1}(\delta^\top (I - U_{d-1}^\top U_{d-1})^\top \delta)^2 - \delta^\top (\Sigma_{d} - \Sigma_{d-1}^\top) \delta
= \frac{(\delta^\top (I - U_{d-1}^\top U_{d-1})^\top \delta)^2}{\delta^\top (\Sigma - \Sigma_{d-1}) \delta} - \delta^\top (\Sigma_d^\top - \Sigma_{d-1}^\top) \delta
\geq \frac{(\delta^\top (I - U_{d-1}^\top U_{d-1})^\top \delta)^2}{\lambda_\delta^\top (I - U_{d-1}^\top U_{d-1})^\top \delta} - \frac{1}{\lambda_\delta^\top} \delta^\top u_d u_d^\top \delta
= \frac{1}{\lambda_\delta^\top} \delta^\top (I - U_{d-1}^\top U_{d-1})^\top \delta - \frac{1}{\lambda_\delta^\top} \delta^\top (U_d U_d^\top - U_{d-1}^\top U_{d-1}) \delta \geq 0
\]

where we recall that $u_d$ is the $d$-th column of $U_d$. Thus $C(F_0^{(A)}, F_1^{(A)}) \geq C(F_0^{(B)}, F_1^{(B)})$ always, and the inequality is strict whenever $\delta^\top (I - U_d U_d^\top) \delta > 0$.

\begin{remark}
Theorem 1 can be extended to the case wherein the linear transformations are $A = [\delta | U_{d-1}]$ and $B = U_d$, respectively, such that $U_d$ is an arbitrary $p \times d$ matrix with $U_d^\top U_d = I$, and $U_{d-1}$ is the first $d - 1$ columns of $U_d$. A similar derivation to that in the proof of Theorem 1 then yields
\[
C(F_0^{(A)}, F_1^{(A)}) = \frac{(\delta^\top \Sigma_{d-1}^{-1/2}(I - V_{d-1}^\top V_{d-1}) \Sigma_{d-1}^{1/2} \delta)^2}{\delta^\top \Sigma_{d-1}^{1/2}(I - V_{d-1}^\top V_{d-1}) \Sigma_{d-1}^{1/2} \delta} + \delta^\top (V_{d-1}^\top V_{d-1})^{1/2} \Sigma_{d-1}^{-1/2} \delta \tag{15}
\]
\[
C(F_0^{(B)}, F_1^{(B)}) = \delta^\top \Sigma_{d-1}^{1/2} V_d^\top V_d \Sigma_{d-1}^{1/2} \delta \tag{16}
\]
where $V_d V_{d-1} = \Sigma_{d-1}^{1/2} U_d (U_d^\top U_d)^{-1} U_{d-1}^\top \Sigma_{d-1}^{1/2}$ is the orthogonal projection onto the column space of $\Sigma_{d-1}^{1/2} U_d$. Hence $C(F_0^{(A)}, F_1^{(A)}) \geq C(F_0^{(B)}, F_1^{(B)})$ if and only if
\[
\frac{(\delta^\top \Sigma_{d-1}^{-1/2}(I - V_{d-1}^\top V_{d-1}) \Sigma_{d-1}^{1/2} \delta)^2}{\delta^\top \Sigma_{d-1}^{1/2}(I - V_{d-1}^\top V_{d-1}) \Sigma_{d-1}^{1/2} \delta} > \delta^\top \Sigma_{d-1}^{-1/2}(V_d V_d^\top - V_{d-1}^\top V_{d-1}) \Sigma_{d-1}^{-1/2} \delta. \tag{17}
\]

We recover Eq. 13 by letting $U_d$ be the matrix whose columns are the eigenvectors corresponding to the $d$ largest eigenvalue of $\Sigma$.
\end{remark}

We next present a result relating the Chernoff information for LOL and rRLDA.
Theorem 2. Assume the setting of Theorem 1. Let \( C = \bar{U}^T_d \) where \( \bar{U}_d \) is the \( p \times d \) matrix whose columns are the \( d \) largest eigenvectors of the pooled covariance matrix \( \bar{\Sigma} = \mathbb{E}[ (X - \mu_0 - \mu_1) (X - \mu_0 - \mu_1)^T ] \). Then \( C \) is the linear transformation for PCA and
\[
C(F_0^{(C)}, F_1^{(C)}) - C(F_0^{(A)}, F_1^{(A)}) = \frac{(\delta^T (I - U_d^{-1}U_d^T) \delta)^2}{\delta^T (\Sigma - \Sigma_{d-1}) \delta} + \delta^T \Sigma_{d-1} \delta - \frac{(\delta^T \bar{\Sigma} \delta)^2}{4 - \delta^T \bar{\Sigma} \delta}
\]
(18)
where \( \bar{\Sigma}_d = \bar{U}_d \bar{S}_d \bar{U}_d^T \) is the best rank \( d \) approximation to \( \Sigma = \Sigma + \frac{1}{4} \delta \delta^T \).

Proof. Assume, without loss of generality, that \( \mu_1 = -\mu_0 = \mu \). We then have
\[
\bar{\Sigma} = \mathbb{E}[XX^T] = \pi \Sigma + \pi \mu_0 \mu_0^T + (1 - \pi) \Sigma + (1 - \pi) \mu_1 \mu_1^T = \Sigma + \mu \mu^T = \Sigma + \frac{1}{4} \delta \delta^T.
\]
Therefore
\[
(C \Sigma C^T)^{-1} = (\bar{U}_d^T \Sigma \bar{U}_d)^{-1} = (\bar{U}_d^T (\Sigma - \frac{1}{4} \delta \delta^T) \bar{U}_d)^{-1} = (\bar{S}_d - \frac{1}{4} \bar{U}_d \delta \delta^T \bar{U}_d)^{-1} = \bar{S}_d^{-1} + \frac{\bar{S}_d^{-1} \bar{U}_d \delta \delta^T \bar{U}_d \bar{S}_d^{-1}}{4 - \delta^T \bar{U}_d \bar{S}_d^{-1} \bar{U}_d^T} \delta
\]
where \( \bar{S}_d \) is the diagonal matrix containing the \( d \) largest eigenvalues of \( \bar{\Sigma} \). Hence
\[
C(F_0^{(C)}, F_1^{(C)}) = \delta^T C^T (C \Sigma C^T)^{-1} C \delta = \delta^T \bar{U}_d \left( \bar{S}_d^{-1} + \frac{\bar{S}_d^{-1} \bar{U}_d \delta \delta^T \bar{U}_d \bar{S}_d^{-1}}{4 - \delta^T \bar{U}_d \bar{S}_d^{-1} \bar{U}_d^T} \delta \right) \bar{U}_d^T \delta
\]
\[
= \delta^T \bar{U}_d \bar{S}_d^{-1} \bar{U}_d^T \delta + \frac{(\delta^T \bar{U}_d \bar{S}_d^{-1} \bar{U}_d^T \delta)^2}{4 - \delta^T \bar{U}_d \bar{S}_d^{-1} \bar{U}_d^T \delta}
\]
(19)
\[
= \delta^T \Sigma_{d-1} \delta + \frac{(\delta^T \bar{\Sigma} \delta)^2}{4 - \delta^T \bar{\Sigma} \delta}
\]
as desired. \( \square \)

Remark 2. We recall that the LOL projection \( A = [ \delta \mid U_{d-1} ]^T \) yields
\[
C(F_0^{(A)}, F_1^{(A)}) = \frac{(\delta^T (I - U_{d-1}U_{d-1}^T) \delta)^2}{\delta^T (\Sigma - \Sigma_{d-1}) \delta} + \delta^T \Sigma_{d-1} \delta.
\]
To illustrate the difference between the LOL projection and that based on the eigenvectors of the pooled covariance matrix, consider the following simple example. Let \( \Sigma = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_p) \) be a diagonal matrix with \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \). Also let \( \delta = (0, 0, \ldots, 0, s) \). Suppose furthermore that \( \lambda_p + s^2/4 \leq \lambda_d \). Then we have \( \bar{S}_d = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_d, 0, 0, \ldots, 0) \). Thus \( \bar{\Sigma}_d = \text{diag}(1/\lambda_1, 1/\lambda_2, \ldots, 1/\lambda_d, 0, 0, \ldots, 0) \) and \( \delta^T \bar{\Sigma} \delta = 0 \). Therefore, \( C(F_0^{(B)}, F_1^{(B)}) = 0 \).

On the other hand, we have
\[
C(F_0^{(A)}, F_1^{(A)}) = \frac{(\delta^T (I - U_{d-1}U_{d-1}^T) \delta)^2}{\delta^T (\Sigma - \Sigma_{d-1}) \delta} + \delta^T \Sigma_{d-1} \delta = \frac{s^4}{s^2 \lambda_p} + 0 = s^2/\lambda_p.
\]
A more general form of the previous observation is the following result which shows that LOL is preferable over PCA when the dimension \( p \) is sufficiently large.
Proposition 1. Let $\Sigma$ be a $p \times p$ covariance matrix of the form

$$\Sigma = \begin{bmatrix} \Sigma_d & 0 \\ 0 & \Sigma_d^\dagger \end{bmatrix}$$

where $\Sigma_d$ is a $d \times d$ matrix. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d$ be the eigenvalues of $\Sigma$, with $\lambda_1, \lambda_2, \ldots, \lambda_d$ being the eigenvalues of $\Sigma_d$. Suppose that the entries of $\delta$ are i.i.d. with the following properties.

1. $\delta_i \sim Y_i \sim N(\tau, \sigma^2)$ where $Y_1, Y_2, \ldots, Y_p$ i.i.d. Bernoulli$(1-\epsilon)$.
2. $p(1-\epsilon) \rightarrow \theta$ as $p \rightarrow \infty$ for some constant $\theta$.

Then there exists a constant $C > 0$ such that if $\lambda_d - \lambda_{d+1} \geq C\theta \tau^2 \log p$, then, with probability at least $\epsilon^d$

$$C(F_0^{(A)}, F_1^{(A)}) > C(F_0^{(B)}, F_1^{(B)}) = 0$$

Proof. The above construction of $\Sigma$ and $\delta$ implies, with probability at least $\epsilon^d$, that the covariance matrix for $\tilde{\Sigma}$ is of the form

$$\tilde{\Sigma} = \begin{bmatrix} \Sigma_d & 0 \\ 0 & \Sigma_d^\dagger + \frac{1}{4}(\tilde{\delta}\tilde{\delta}^\top) \end{bmatrix}$$

where $\tilde{\delta} \in \mathbb{R}^{p-d}$ is formed by excluding the first $d$ elements of $\delta$. Now, if $\lambda_{d+1} + \frac{1}{4}\|\tilde{\delta}\|^2 < \lambda_d$, then the $d$ largest eigenvalues of $\tilde{\Sigma}$ are still $\lambda_1, \lambda_2, \ldots, \lambda_d$, and thus the eigenvectors corresponding to the $d$ largest eigenvalues of $\tilde{\Sigma}$ are the same as those for the $d$ largest eigenvalues of $\Sigma$. That is to say,

$$\lambda_{d+1} + \frac{1}{4}\|\tilde{\delta}\|^2 < \lambda_d \Rightarrow \Sigma_d^\dagger \Rightarrow \delta^\top \Sigma_d^\dagger \delta = 0 \Rightarrow C(F_0^{(B)}, F_1^{(B)}) = 0.$$

We now compute the probability that $\lambda_{d+1} + \frac{1}{4}\|\tilde{\delta}\|^2 < \lambda_d$. Suppose for now that $\epsilon > 0$ is fixed and does not vary with $p$. We then have

$$\frac{\sum_{i=d+1}^{d} \delta_i^2 - (p - d)(1 - \epsilon)^2}{\sqrt{(p - d)(2(1 - \epsilon)(2\tau^2\sigma^2 + \sigma^4) + \epsilon(1 - \epsilon)(\tau^4 + 2\tau^2\sigma^2 + \sigma^4))}} \xrightarrow{d} N(0, 1).$$

Thus, as $p \rightarrow \infty$, the probability that $\lambda_{d+1} + \frac{1}{4}\|\tilde{\delta}\|^2 < \lambda_d$ converges to that of

$$\Phi\left(\frac{4(\lambda_d - \lambda_{d+1}) - (p - d)(1 - \epsilon)^2}{\sqrt{(p - d)(2(1 - \epsilon)(2\tau^2\sigma^2 + \sigma^4) + \epsilon(1 - \epsilon)(\tau^4 + 2\tau^2\sigma^2 + \sigma^4))}}\right).$$

This probability can be made arbitrarily close to 1 provided that $\lambda_d - \lambda_{d+1} \geq C\theta \tau^2$ for all sufficiently large $p$ and for some constant $C > 1/4$. Since the probability that $\delta_1 = \delta_2 = \cdots = \delta_d$ is at least $\epsilon^d$, we thus conclude that for sufficiently large $p$, with probability at least $\epsilon^d$,

$$C(F_0^{(B)}, F_1^{(B)}) = 0 < C(F_0^{(A)}, F_1^{(A)}).$$

In the case where $\epsilon = o(p)$, we may take $p(1 - \epsilon) \rightarrow \theta$ for some constant $\theta$, then the probability that $\lambda_{d+1} + \frac{1}{4}\|\tilde{\delta}\|^2 < \lambda_d$ converges to the probability that

$$\frac{1}{4} \sum_{i=1}^{K} \sigma_i^2 \chi_1^2(\tau) \geq \lambda_d - \lambda_{d+1}$$

where $K$ is Poisson distributed with mean $\theta$ and $\chi_1^2(\tau)$ is the non-central chi-square distribution with one degree of freedom and non-centrality parameter $\tau$. Thus if $\lambda_d - \lambda_{d+1} \geq C\theta \tau^2 \log p$ for sufficiently large $p$ and for some constant $C$, then this probability can also be made arbitrarily close to 1. \qed
Remark 3. The previous comparisons are done for the case of \( C = 2 \) classes. Extending these comparisons to the case of \( C > 2 \) classes is, however, non-trivial. More precisely, suppose we have \( Y \in \{1, 2, \ldots, C\} \) and that, conditional on \( Y = c \), \( X \sim \mathcal{N}(\mu_c, \Sigma) \) is multivariate normal with mean \( \mu_c \) and common covariance matrix \( \Sigma \). Then, given \( X = x \), the Bayes optimal classifier for \( Y \) is still

\[
g_{\text{LDA}}(x) = \arg\min_{y \in \{1, 2, \ldots, C\}} \left[ \frac{1}{2} (x - \mu_y)^\top \Sigma^{-1} (x - \mu_y) - \log \pi_y \right] = \arg\min_{y \in \{1, 2, \ldots, C\}} \left[ -x^\top \Sigma^{-1} \mu_y + \frac{1}{2} \mu_y^\top \Sigma^{-1} \mu_y - \log \pi_y \right]
\]

Taking \( \frac{1}{2} \mu_y^\top \Sigma^{-1} \mu_y - \log \pi_y \) as either a given constant or as an intercept term to be learned or estimated, the reduced-rank LDA for \( C > 2 \) classes still corresponds to looking at the top \( d \) eigenvectors of \( \Sigma \). That is to say, we transform the predictor variables via \( x \mapsto U_d x \) followed by performing LDA on the transformed data. Similarly, the PCA transformation corresponds to using the top \( d \) eigenvectors of the pooled covariance matrix \( \hat{\Sigma} = \mathbb{E}[(X - \sum_c \pi_c \mu_c)(X - \sum_c \pi_c \mu_c)^\top] \) followed by performing LDA. Suppose we now compare LOL, rrLDA, and PCA in this multi-class setting. Let \( A : X \mapsto AX \) be a linear transformation. Then by Eq. (11) and Eq. (12), the Chernoff information for the transformed data in this multi-class setting is

\[
\min_{c \neq c'} \frac{1}{8} (\mu_c - \mu_{c'})^\top A^\top (A \Sigma A^\top)^{-1} A (\mu_c - \mu_{c'}) .
\]

We now see that, in the case of rrLDA and PCA the linear transformation \( A \) depends only on the covariance matrix \( \Sigma \) and \( \hat{\Sigma} \), respectively. That is to say, the linear transformation \( A \) does not depend on the choice of \( c \) and \( c' \). In contrast, currently for LOL the linear transformation \( A \) depends on both \( \Sigma \) as well as \( \mu_c - \mu_{c'} \). In other words, there is no single choice for \( A \) but rather that \( A \) changes as \( c, c' \) changes. Direct comparison, in the multi-classes setting, between LOL and either of rrLDA or PCA is thus an open problem that we leave for future work. Finally we note that if we allow the linear transformation for LOL to vary with the classes \( c \) and \( c' \), i.e., taking a one-vs-one approach to multi-classes classification, then the resulted presented in this paper are valid for all pairs \( c, c' \).

D.III Finite Sample Performance

We now consider the finite sample performance of LOL and PCA-based classifiers in the high-dimensional setting with small or moderate sample sizes, e.g., when \( p \) is comparable to \( n \) or when \( n \ll p \). Once again we assume that \( X \mid Y = i \sim \mathcal{N}(\mu_i, \Sigma) \) for \( i = 0, 1 \). Furthermore, we also assume that \( \Sigma \) belongs to the class \( \Theta(p, r, k, \tau, \lambda) \) as defined below.

**Definition** Let \( \lambda > 0, \tau \geq 1 \) and \( k \leq p \) be given. Denote by \( \Theta(p, r, k, \tau, \lambda, \sigma^2) \) the collection of matrices \( \Sigma \) such that

\[
\Sigma = V \Lambda V^\top + \sigma^2 I
\]

where \( V \) is a \( p \times r \) matrix with orthonormal columns and \( \Lambda \) is a \( r \times r \) diagonal matrix whose diagonal entries \( \lambda_1, \lambda_2, \ldots, \lambda_r \) satisfy \( \lambda \geq \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r \geq \lambda / \tau \). In addition, assume also that \( |\text{supp}(V)| \leq k \) where \( \text{supp}(V) \) denote the non-zero rows of \( V \), i.e., \( \text{supp}(V) \) is the subset of \( \{1, 2, \ldots, p\} \) such that \( V_j \neq 0 \) if and only if \( j \in \text{supp}(V) \).

We note that in general \( r \leq k \ll p \) and \( \lambda / \tau \gg \sigma^2 \). We then have the following result.

**Theorem 3 ([19]).** Suppose there exist constants \( M_0 \) and \( M_1 \) such that \( M_1 \log p \geq \log n \geq M_0 \log \lambda \). Then there exists a constant \( c_0 = c_0(M_0, M_1) \) depending on \( M_0 \) and \( M_1 \) such that for all \( n \) and \( p \) for...
there exists an estimate \( \hat{V} \) of \( V \) such that

\[
\sup_{\Sigma \in \Theta(p, r, k, \tau, \lambda, \sigma^2)} \mathbb{E} \| \hat{V} \hat{V}^T - VV^T \|^2 \leq \frac{Ck(\sigma \lambda + \sigma^2)}{n\lambda^2} \log \frac{ep}{k}
\]

(20)

where \( C \) is a universal constant not depending on \( p, r, k, \tau, \lambda \) and \( \sigma^2 \).

**Theorem 3** then implies the following result for comparing the Chernoff information of the sample version of LOL against that for PCA.

**Corollary 4.** Let \( \Sigma \in \Theta(p, r, k, \tau, \lambda) \) as defined above. Suppose that \( C(F_0^{(A)}, F_1^{(A)}) > C(F_0^{(B)}, F_1^{(B)}) \) where \( A \) and \( B \) denote the LOL and PCA projection matrices based on the eigenvectors of \( \Sigma \) associated with the \( d \leq r \) largest eigenvalues, i.e., \( A = \delta [V_{1:d-1}] \) and \( B = V_{1:d} \). Then there exists constants \( M \) and \( c \) such that if \( \log n \geq M \log \lambda + \frac{\tau k}{n} \log \frac{ep}{k} \leq c \), then there exists an estimate \( \hat{V} \) of \( V \) such that, with \( A = \delta [V_{1:d-1}] \) and \( B = [V_{1:d}] \), we have

\[
\mathbb{E}[C(F_0^{(A)}, F_1^{(A)})] > \mathbb{E}[C(F_0^{(B)}, F_1^{(B)})]
\]

The above corollary states that for \( \Sigma \in \Theta(p, r, k, \tau, \lambda) \), then provided that the Chernoff information of the population version of LOL is larger than the Chernoff information of the population version of PCA, we can choose \( n \) sufficiently large (as compared to \( \lambda \) and \( \tau \) and \( k \)) such that the expected Chernoff information for the sample version of LOL is also larger than the expected Chernoff information of the sample version of PCA. We emphasize that it is necessary that the LOL and the PCA version are both projected into the top \( d \leq r \) dimension of the sample covariance matrices. The constants \( M \) and \( c \) in the statement of the above corollary are chosen so that \( M \) (which depends on \( M_0 \) and \( M_1 \) in the statement of **Theorem 3**) is sufficiently large and \( c \) (which depends on \( c_0 \)) is sufficiently small to ensure that the bound in Eq. (20) is sufficiently small. If \( C(F_0^{(A)}, F_1^{(A)}) > C(F_0^{(B)}, F_1^{(B)}) \) and \( \| \hat{V} \hat{V}^T - VV^T \| \) is sufficiently small, then \( \mathbb{E}[C(F_0^{(A)}, F_1^{(A)})] > \mathbb{E}[C(F_0^{(B)}, F_1^{(B)})] \) as desired.

**E  Real-Data Performance Analysis**

PCA, the industry-standard dimensionality reduction technique for high-dimensional problems, is compared to LOL, RP, and rRLDA in terms of cross-validated classification error.

In the experiments, we used \( k \) fold cross-validation. Testing sets were rotated across all folds, with the training sets comprising the remaining \( k-1 \) folds. A low-dimensional projection matrix \( A \) is first learned through the training set, and the low-dimensional training points are then used to train an LDA classifier \( C \). The testing points are embedded via \( A \), and classification error is determined using the trained classifier \( C \).

Performance is assessed using Cohen’s kappa [24], which normalizes the classification error typically between 0 (the classifier performs no better than the classifier which guesses the most-likely class from the training set, the chance classifier) and 1 (the trained classifier performs perfectly). Negative scores can be achieved if the trained classifier performs worse than the chance classifier. The effect size is measured as the difference between Cohen’s kappa for the trained classifier after embedding
with $\text{PCA}(\kappa)$ and the trained classifier after embedding with technique $\varepsilon$, $\kappa(\varepsilon)$. Table 1 provides details about each neuroimaging dataset.

| Problem         | Sample Size ($n$) | Training Size* | # Features ($p$) | Classes ($K$) | Source               |
|-----------------|-------------------|----------------|-----------------|--------------|----------------------|
| Templeton114    | 111               | 100            | $> 1.5 \times 10^8$ | 2            | MRN                  |
| BNU1            | 110               | 100            | $> 1.5 \times 10^8$ | 2            | CoRR [78]            |
| BNU3            | 47                | 43             | $> 1.5 \times 10^8$ | 2            | CoRR [78]            |
| SWU4            | 453               | 407            | $> 1.5 \times 10^8$ | 2            | CoRR [78]            |
| KKI2009         | 42                | 38             | $> 1.5 \times 10^8$ | 2            | KKI [51]             |
| Genomics        | 340               | 306            | 745,184         | 2            | Douville et al. [31] |

Table 1: Table of datasets used in this study. The top 5 datasets (neuroimaging) are pre-processing by only registering the brains to the MNI152 template[47, 60, 65, 74]. The neuroimaging dataset comprises a total of 5 classification problems (5 datasets across a single sex classification task). The bottom dataset (genomics) is pre-processed by aligning sequencing data to 745,184 amplicons on the human genome. The genomics dataset comprises two benchmark classification problems (sex or age).

F Extensions to Other Supervised Learning Problems

F.I Large numbers of classes

Here, we explore an experiment in which the number of classes increases for a given simulation. We look at the multiclass hump-$K$ problem, described in Section C. In this simulation, while the space spanned by the differences of means conveys more information than the directions of maximal variance, we expect that the shift in the means for a given class at a given dimension should also increase the variance fractionally in that direction as well. Figure 6A shows the simulation setup, for $K = 10$. Figure 6B indicates the misclassification rate as a function of Cohen’s Kappa. We use Cohen’s Kappa instead of the misclassification rate for direct evaluation since $K$ varies widely across these simulations at a fixed number of total samples $n = 128$, making the difficulty of the problem as $K$ increases two-fold: not only are there more classes, but there are also fewer examples of each class per simulation setting. In all cases, the best random classifier would be the classifier that continually guesses a single class continuously, which has expected accuracy of $\frac{1}{K}$. On all simulations, we see that both PLS and LOL rapidly approach a higher Kappa statistic (better performance relative the random classifier) as they learn the space spanned by the differences of means. PLS rapidly declines in performance as successive dimensions are added, and LOL sees a small performance decline, as successive dimensions should convey no information regarding the class. PCA is able to ultimately identify the space spanned by the differences of the means, but takes far more embedding dimensions to do so, and yields a lower Kappa statistic than either of the other two strategies.

F.II Hypothesis Testing

The utility of incorporating the mean difference vector into supervised machine learning extends beyond classification. In particular, hypothesis testing can be considered as a special case of classification, with a particular loss function. We therefore apply the same idea to a hypothesis testing scenario. The multivariate generalization of the t-test, called Hotelling’s Test, suffers from the same problem as does the classification problem; namely, it requires inverting an estimate of the covariance matrix,
Figure 6: The Multiclass Hump Simulation. We show the results of the multiclass trunk problem, as the number of classes increases from 2 to 10, with the number of dimensions and the number of samples fixed. Effect size is measured with Cohen’s Kappa. LOL and PLS provide better performance over competing techniques including PCA, and this gap widens as the number of classes increases.

which would result in a matrix that is low-rank and therefore singular in the high-dimensional setting. To mitigate this issue in the hypothesis testing scenario, prior work applied similar tricks as they have done in the classification setting. One particularly nice and related example is that of Lopes et al. [56], who addresses this dilemma by using random projections to obtain a low-dimensional representation, following by applying Hotelling’s Test in the lower-dimensional subspace. Figure 7A and B show the power of their test (labeled RP) alongside the power of PCA, LOL, and LFL for two different conditions. In each case we use the different approaches to project to low dimensions, followed by using Hotelling’s test on the projected data. In the first example the true covariance matrix is diagonal, and in the second, the true covariance matrix is dense. The horizontal axis on both panels characterizes the decay rate of the eigenvalues, so larger numbers imply the data is closer to low-rank (see Methods for details). The results indicate that the LOL test has higher power for essentially all scenarios. Moreover, it is not merely replacing random projections with PCA (solid magenta line), nor simply incorporating the mean difference vector (dashed green line), but rather, it appears that LOL for testing uses both modifications to improve performance.

F.III Regression

High-dimensional regression is another supervised learning method that can use the LOL idea. Linear regression, like classification and Hotelling’s Test, requires inverting a matrix as well. By projecting the data onto a lower-dimensional subspace first, followed by linear regression on the low-dimensional data, we can mitigate the curse of high-dimensions. To choose the projection matrix, we partition the data into $K$ partitions (we select $K = 10$ arbitrarily), based on the percentile of the target variable, we obtain a K-class classification problem. Then, we can apply LOL to learn the projection. Figure 7C shows an example of this approach, contrasted with Lasso and partial least squares, in a sparse simulation setting (see Methods for details). LOL is able to find a better low-dimensional projection than Lasso, and performs significantly better than partial least squares, for essentially all choices of number of dimensions to project into.
Figure 7: The intuition of including the mean difference vector is equally useful for other supervised manifold
learning problems, including testing and regression. (A) and (B) show two different high-dimensional testing
settings, as described in Methods. Power is plotted against the decay rate of the spectrum, which approximates
the effective number of dimensions. LOL composed with Hotelling’s test outperforms the random projections
variants described in [56], as well as several other variants. (C) A sparse high-dimensional regression setting,
as described in Methods, designed for sparse methods to perform well. Log_{10} mean squared error is plotted
against the number of projected dimensions. LOL composed with linear regression outperforms \textit{Lasso} (cyan),
the classic sparse regression method, as well as partial least squares (PLS; black). These three simulation
settings therefore demonstrate the generality of this technique.

G The R implementation of LOL

Figure 8 shows the R implementation of LOL for binary classification using FlashMatrix [77]. The
implementation takes a $D \times I$ matrix, where each column is a training instance and each instance has
$D$ features, and outputs a $D \times k$ projection matrix.

LOL <- function(m, labels, k) {
  counts <- fm.table(labels)
  num.labels <- length(counts$val)
  num.features <- dim(m)[1]
  nv <- k - (num.labels - 1)
  gr.sum <- fm.groupby(m, 1, fm.as.factor(labels, 2), fm.bo.add)
  gr.mean <- fm.mapply.row(gr.sum, counts$Freq, fm.bo.div, FALSE)
  diff <- fm.get.cols(gr.mean, 1) - fm.get.cols(gr.mean, 2)
  svd <- fm.svd(m, nv=0, nu=nv)
  fm.cbind(diff, svd$u)
}

Figure 8: The R implementation of LOL.
Pseudocode 1 Simple pseudocode for two class LOL on sample data.

Input: \( X \) a \( p \times n \) matrix \( (n \ll p) \), where columns are observations; rows are features. An \( n \) length vector of observation labels, \( y \). An integer \( k \) to specify desired output dimension.

Output: \( A \in \mathbb{R}^{p \times k} \)

1: function \( \text{LOL\_TRAIN}(X, Y, k) \)
2:   for all \( j \in J \) do
3:     \( n_j = \sum_{i=1}^{n} I(y_i = j) \) \hspace{1cm} \( \triangleright \) sample size per class
4:     \( \hat{\mu}_j = \frac{1}{n_j} \sum_{i=1}^{n} x_i I(y_i = j) \) \hspace{1cm} \( \triangleright \) class means
5:   end for
6:   \( \hat{\delta} = \hat{\mu}_1 - \hat{\mu}_2 \) \hspace{1cm} \( \triangleright \) difference of means
7:   \( \hat{\delta} = \hat{\delta} / \| \hat{\delta} \| \) \hspace{1cm} \( \triangleright \) unit normalize difference of means
8:   for all \( i \in [n] \) do
9:     \( \tilde{x}_i = x_i - \hat{\mu}_{y_i} \) \hspace{1cm} \( \triangleright \) class centered data
10: end for
11: \( [\hat{u}, \hat{d}, \hat{v}] = \text{svds}(\tilde{x}, k - 1) \) \hspace{1cm} \( \triangleright \) compute top \( k \) singular vectors
12: \( A = [\hat{\delta}, \hat{u}] \) \hspace{1cm} \( \triangleright \) concatenate difference of the means and the top \( k \) right singular vectors
13: end function