We introduce primed-PCA (pPCA), an extension of the recently proposed EigenGame algorithm for computing principal components in a large-scale setup. Our algorithm first runs EigenGame to get an approximation of the principal components, and then applies an exact PCA in the subspace they span. Since this subspace is of small dimension in any practical use of EigenGame, this second step is extremely cheap computationally. Nonetheless, it improves accuracy significantly for a given computational budget across datasets. In this setup, the purpose of EigenGame is to narrow down the search space, and prepare the data for the second step, an exact calculation.

We show formally that pPCA improves upon EigenGame under very mild conditions, and we provide experimental validation on both synthetic and real large-scale datasets showing that it systematically translates to improved performance. In our experiments we achieve improvements in convergence speed by factors of 5-25 on the datasets of the original EigenGame paper.

1 Introduction

Principal Component Analysis is a widely used tool both within and outside of computer science. Introduced more than a century ago by [Karl Pearson] [1901], it has been used for compression and feature extraction, and has led to many important works and variants [Turk and Pentland 1991][Schölkopf, Smola, and Müller 1999].

Let $X \in \mathbb{R}^{n \times d}$ be a centered dataset of cardinality $n$ and dimension $d$. Finding the principal components of $X$ amounts to finding the directions in $\mathbb{R}^d$ along which the data has maximal variance. In terms of linear algebra, the principal directions are the eigenvectors of the covariance matrix $X^TX$.

Unfortunately, if $d$ and $n$ are as high as in modern datasets, then traditional approaches, like computing the full-SVD of the covariance matrix gets computationally challenging. Full-SVD has time complexity $O(\min\{n^2d, nd^2\})$ and space complexity $O(nd)$ [Tang 2019].

This has led to several attempts trying to circumvent this problem by using approximate/heuristic alternatives to full-SVD for finding the first few principal components of datasets of larger scale.

Figure 1: The results of an example run of the proposed algorithm on the synthetic data with exponentially decaying spectrum (Section 5). Thin, dotted lines denote the eigenvalues of the covariance matrix. Dashed lines denote the eigenvalue estimates of EigenGame (Section 2.1). Solid lines denote eigenvalue estimates of pPCA (Section 3.1).

The contributions of this paper are:

- We introduce a variant of the EigenGame algorithm that performs a one-time, cheap full-PCA step on the output of EigenGame.
- We analyse this full-PCA step using elementary linear algebra and derive the mild theoretical conditions under which it improves the performance of EigenGame.
- We compare it empirically to EigenGame on several datasets and demonstrate the improvement in accuracy and convergence speed.

Note that the choice of EigenGame is not crucial, the same framework still makes sense with alternative approximate-PCA methods as the first step of the optimisation. We use EigenGame in our experiments because of its impressive performance when compared to other algorithms [Gemp et al. 2020].
2 Related Work
The power method, introduced by Rutishauser (1970), initialises a random vector $x_0 \in \mathbb{R}^d$ of unit norm and iteratively computes

$$x_{i+1} = \frac{Mx_i}{\|Mx_i\|}$$

until the first eigendirection of $M = X^TX$ dominates.

Oja’s learning rule (Oja 1982) considers the output of a single neuron $y = x^Tw = w^Tx$ with update rule

$$\Delta w = \alpha (xy - y^2w) = \alpha (xX^Tw - (w^TX)(x^Tw)w)$$

Averaging over all points $C = \frac{1}{n} \sum x_i x_i^T$, and plugging in the fixed-point condition ($\Delta w = 0$) one gets

$$Cw - \alpha (w^T Cw)w = 0$$

which is an eigenvector-eigenvalue equation for the covariance matrix $C$, i.e. the weights following this dynamics end up as the coordinates of principal directions.

There are also approaches for learning the $k$-dimensional subspace of maximal variance (Ghashami et al. 2015; Feldman, Schmidt, and Sohler 2018), projecting the data onto this lower dimensional subspace and performing full-PCA there.

The EigenGame algorithm (Gemp et al. 2020) parallelises the computation and allows for a multi-device setup, creating the possibility for much larger scale PCA computation. Since our method heavily builds on it, we introduce EigenGame in detail.

2.1 EigenGame
EigenGame interprets PCA in a game-theoretical framework, where vectors on the unit sphere $S^{d-1} \subset \mathbb{R}^d$ correspond to strategies of players, playing the following multiplayer game. Let $v_1, \ldots, v_k \in \mathbb{R}^d (k < d)$ denote the players. The utility function of the first player is

$$U_1(v_1) = v_1^T(X^T X)v_1$$

i.e. player 1 is trying to tune the vector $v_1 \in S^{d-1}$ in a way that captures the maximum variance of the data. By definition, $v_1$’s goal is to find the first principal component of $X$. To make $v_2$ find the second principal component, the authors set the utility function of $v_2$ to

$$U_2(v_2) = v_2^T(X^T X)v_2 - \frac{(v_2^T(X^T X)v_1)^2}{v_1^T(X^T X)v_1}$$

where the first term rewards if $v_2$ finds a direction of high variance and the second one penalises if this direction is not orthogonal to $v_1$. Similarly, the utility function of $v_j (1 < j \leq k)$ is

$$U_j(v_j) = v_j^T(X^T X)v_j - \sum_{1 \leq i < j} \frac{(v_j^T(X^T X)v_i)^2}{v_i^T(X^T X)v_i}$$

Finding the Nash-equilibrium of the game defined by the utility functions $U_1, \ldots, U_k$ is equivalent to finding the principal components of $X$.

This Gram-Schmidt-like setup defines a hierarchy between the players. Intuitively, $v_1$ aims to maximise it’s variance without having to care about the other players, while all other players are also trying to maximise their variance, but have the additional constraint to stay orthogonal to the players with lower indices.

3 Priming PCA
During the training process of EigenGame, it can happen that the exact principal directions $e_1, \ldots, e_k$ are not yet properly captured by the corresponding players $v_1, \ldots, v_k$, but they already lie (up to some error term) in $\text{span}(v_1, \ldots, v_k)$.

3.1 PCA as post-processing

**Question 1** Are $v_1, \ldots, v_k$ the best approximations of $e_1, \ldots, e_k$ in $\text{span}(v_1, \ldots, v_k)$?

Whenever the answer to this question is not affirmative, it makes sense to further optimize $v_1, \ldots, v_k$ within $\text{span}(v_1, \ldots, v_k)$. Since usually $k \ll d$, full-PCA is feasible after projecting the data to this $k$-dimensional subspace. This paper proposes to do exactly this.

We expect that this step will ease numerical issues and inaccuracies related to stochastic gradient descent and speed up convergence. In this paper we investigate how full-PCA improves the accuracy and speeds up the EigenGame algorithm.

3.2 Extra components
Knowing that after running EigenGame, we will post-process the output and not accept it as the final prediction of the principal components, allows us to modify the EigenGame algorithm in a way that makes the job of full-PCA step easier.

For instance, if we are interested in the first $k$ principal components of $X$, we could run EigenGame with $k + l$ components, project onto the $(k + l)$-dimensional $\text{span}(v_1, \ldots, v_k, v_{k+l})$ and do full-PCA to extract the first $k$ components. Since EigenGame scales quadratically in the number of players, $l$ has to be small. The question, of course, is whether or not the performance gained from a few additional components compensates for increased computational costs needed to run EigenGame with more players. In the rest of the paper, we refer to pPCA with $l$ additional players as pPCA$_l$.

**Algorithm 1: Primed PCA (pPCA$_l$)**

**Input:** Dataset of dimension $d$, $\{x_i\}_{i=1}^n$

**Parameter:** $k > 0$, $l > 0$

**Output:** First $k$ principal components

1. $v_1, \ldots, v_k, v_{k+l} \leftarrow \text{EigenGame} (\{x_i\}_{i=1}^n, k + l)$
2. $V \leftarrow \text{span}(v_1, \ldots, v_k, v_{k+l})$
3. $x_i \leftarrow \text{proj}_V(x_i)$
4. $e_1, \ldots, e_k \leftarrow \text{full-PCA} (\{x_i\}_{i=1}^n, k)$
5. return $e_1, \ldots, e_k$
Figure 2: Plots showing the effect of the full-PCA step and the extra components on the small-scale experiments for $V = \pi/8$. Shaded regions denote $\pm$ standard error of the mean.

Figure 3: Figure (a) shows the estimates of the eigenvalues by pPCA and EigenGame on the Exponential Synthetic dataset with $k = 5$ (as in Figure 1). Figure (b) is obtained by normalizing the curves of (a) by the average value of their respective final 5 datapoints.

Figure 4: Plots showing the effect of the full-PCA on the large-scale experiments. Figures (a) and (c) show the estimates of the eigenvalues by pPCA and EigenGame. Figures (b) and (d) are obtained by normalizing the curves of (a) and (c).
4 Theoretical analysis

It is intuitive to expect that the extra full-PCA step on the projected data should improve (or at least not hurt) the accuracy of the predicted principal directions. In this section, we analyse under what conditions this intuitive expectation holds up.

4.1 A counterexample

Consider the following 3-dimensional, centered dataset of 6 elements

$$X = \{ \pm 3(1, 0, 0), \pm 2(0, 1, 0), \pm (0, 0, 1) \}$$

Suppose we are interested in finding the first 2 principal components using the process described above. The covariance matrix of the projected data is then

$$\frac{1}{n} X^T X = \frac{1}{3} \begin{pmatrix} 9 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and the first two principal components are

$$e_1 = (1, 0, 0) \quad e_2 = (0, 1, 0)$$

Now let us suppose that EigenGame (or any other algorithm that approximates the principal directions) results in the vectors

$$e_1^{EG} = (\epsilon, 0, \sqrt{1 - \epsilon^2}) \quad e_2^{EG} = (0, 1, 0)$$

for some small $\epsilon \ll 1$. That is, the second player is doing a perfect job. On the other hand, the first player is, for some reason, a linear combination of the first and third principal directions almost having no contribution from the first one.

Now, projecting the data onto $\text{span}(e_1^{EG}, e_2^{EG})$ gives us

$$\tilde{X} = \{ \pm \epsilon (1, 0, 0), \pm 2(0, 1, 0), \pm \sqrt{1 - \epsilon^2}(1, 0, 0) \}$$

Or, in the basis of $\{ e_1^{EG}, e_2^{EG} \}$,

$$\tilde{X} = \{ \pm \epsilon (1, 0, 0), \pm 2(0, 1, 0), \pm \sqrt{1 - \epsilon^2}(1, 0, 0) \}$$

The covariance matrix of the projected data is then

$$\frac{1}{n} \tilde{X}^T \tilde{X} = \frac{1}{3} \begin{pmatrix} 9\epsilon^2 + 2(1 - \epsilon^2) & 0 \\ 0 & 4 \end{pmatrix}$$

If $\epsilon$ is small enough, the full-PCA after the projection will predict the principal directions to be

$$e_1^{PCA} = e_2^{EG} \quad e_2^{PCA} = e_1^{EG}$$

i.e it changes the ordering of the principal directions. Unfortunately,

$$\langle e_1^{EG}, e_1 \rangle^2 = \langle (\epsilon, 0, \sqrt{1 - \epsilon^2}), (1, 0, 0) \rangle^2 = \epsilon^2$$

$$\langle e_1^{PCA}, e_1 \rangle^2 = \langle (0, 1, 0), (1, 0, 0) \rangle^2 = 0$$

In other words, we had a better approximation of the first principal direction before doing the full-PCA step.

It is important to note, however, the absurdity of this example. The starting assumption that $e_1^{EG} = (\epsilon, 0, \sqrt{1 - \epsilon^2})$ would mean that EigenGame almost completely ignored the first two principal components and aligned itself with the third, smallest one. This, of course, can happen but it is not the expected behavior from an algorithm that is designed to find the principal components. A more realistic scenario would be that EigenGame finds $e_1$ up to some small error, and the remaining variance is picked up by the other players with lower indices. This is the case where the final full-PCA step will be useful.

Non-theorem The full-PCA step cannot decrease the accuracy of predicted principal components.

The reason why the above example fails is that the subspace spanned by the vectors $e_i^{EC}$ is almost orthogonal to the first principal direction. Projecting the data onto this subspace “forgets” that the original data has had high variance along $e_1$ and $e_1$ becomes impossible to recover because the lower principal components dominate the projected data.

4.2 When does the full-PCA step help?

Let now $V$ be the subspace of $\mathbb{R}^d$ spanned by the vectors learnt by EigenGame. The full-PCA step on the projected data searches for the principal directions $e_i$ within $V$. The best approximation of $e_i$ within $V$ is its projection $\hat{e}_i = \pi_V(e_i)$ onto $V$. full-PCA helps if this $\hat{e}_i$ is also the $i$-th principal component of the projected data $\tilde{X}$.

In other words, full-PCA helps if and only if $V$ is such that the following diagram commutes.

$$\begin{array}{ccc}
X & \xrightarrow{\text{PCA}} & \{e_1, \ldots, e_k\} \\
\pi_V & & \pi_V \\
\tilde{X} & \xrightarrow{\text{PCA}} & \{\hat{e}_1, \ldots, \hat{e}_k\}
\end{array}$$

The variance of the projected data The variance of the data $X$ in a direction $v \in S^{d-1}$ is

$$\text{Var}_v(X) = v^T (X^T X) v$$

Let now $\tilde{X}$ be the projection of the data onto the subspace $V = \text{span}(e_1^{EG}, \ldots, e_k^{EG})$, i.e. $\tilde{X} = XP_V$, where $P_V$ is the projection matrix from $\mathbb{R}^d$ onto $V$. The variance of $\tilde{X}$ in a given direction $v \in V \cap S^{d-1}$ is then

$$\text{Var}_v(\tilde{X}) = v^T (\tilde{X}^T \tilde{X}) v = v^T (P_V^T X^T X P_V) v = (P_V v)^T (X^T X) (P_V v) = v^T (X^T X) v$$

$^1$By best approximation of $e_i$ in $V$ we mean the unit vector $v^* \in V \cap S^{d-1}$ such that the angle between $e_i$ and $v^*$ is minimal
i.e. the quadratic form of the variance of $\tilde{X}$ is just that of $X$ after restricting its domain to $V$.

$$\text{Var}_{\ominus} (\tilde{X}) = \text{Var}_{\ominus} (X) \big|_V$$

The **first principal component** If $\pi_V (e_1)$ maximises $\text{Var}_{\ominus} (X)$ on $V$, then the full-PCA step on $V$ returns $\pi_V (e_1)$ as the first principal component. If EigenGame already output $\pi_V (e_1)$ as the first principal component, then this has no effect on the accuracy, in all other cases, accuracy is improved. We can summarise in

**Proposition 1** If $\pi_V (e_1)$ maximises $\text{Var}_{\ominus} (X)$ on $V$, then the full-PCA step on $V$ cannot decrease the accuracy of the predicted first principal component.

In essence, the only thing that can go wrong for the first principal component is that $V = \text{span} (e_1^{\text{EG}}, \ldots, e_k^{\text{EG}})$ is such that the variance of $\tilde{X}$ in the direction of $\pi_V (e_1)$ is smaller than in the direction of, say, $\pi_V (e_2)$.

The **other principal components** Suppose now that the conditions of Proposition 1 are satisfied and let us consider the second principal direction. Since the eigenvectors of the covariance matrix are orthogonal, we can play the same game but now over the orthogonal complement of $\pi_V (e_1)$ in $V$, and we have

**Proposition 2** If $\pi_V (e_1)$ maximises $\text{Var}_{\ominus} (X)$ on $V$, and $\pi_V (e_2)$ maximises $\text{Var}_{\ominus} (X)$ on $\pi_V (e_1)^{\perp}$, then the full-PCA step on $V$ cannot decrease the accuracy of the predicted first and second principal components.

Continuing this line of reasoning, always requiring the projection of the next principal component to maximise the variance on the orthogonal complement of the previous eigenvectors, we arrive at

**Theorem 1** If

- $\pi_V (e_1)$ maximises $\text{Var}_{\ominus} (X)$ on $V$
- $\pi_V (e_2)$ maximises $\text{Var}_{\ominus} (X)$ on $\pi_V (e_1)^{\perp}$
- 
- $\pi_V (e_1)$ maximises $\text{Var}_{\ominus} (X)$ on the orthogonal complement of $\text{span} \{ \pi_V (e_1), \ldots, \pi_V (e_i) \}$

then the full-PCA step on $V$ cannot decrease the accuracy of the predicted 1st, 2nd, ..., $i$th principal components.

It is important to note that even though these conditions appear to be cumbersome, they are almost always satisfied as we will see in the next section. A variant of the
5 Experiments and results

We test the proposed algorithm on several datasets of varying size. Here we present in order of increasing complexity. Doing full-PCA in the original data space is doable for the small-scale datasets (synthetic, MNIST, CIFAR10 and “NIPS bag of words”), but infeasible for the Large Lobster Image Dataset and ResNet activations.

5.1 Small-scale Datasets

We run EigenGame for each of the datasets 10 times with learning rates $\{10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}\}$. We then choose the learning rate with the smallest angular error when summing over runs, timesteps and principal components. The other methods (pPCA, pPCA2, pPCA4) are then executed also 10 times with the learning rate that best fitted EigenGame. In all these experiments, we are interested in finding the first 16 principal components.

**Synthetic data** We generate synthetic datasets along the lines of the synthetic experiments of the EigenGame paper (Gemp et al., 2020). The data consists of 5000 points in 50 dimensions with a spectrum that decays exponentially (resp. linearly) over 3 orders of magnitudes, from 1000 to 1. We train with a batch size of 1000 for 200 (resp. 600) epochs.

**MNIST and CIFAR10** We flatten the training images of MNIST (LeCun and Cortes, 2010) and CIFAR10 (He et al., 2015) that results in a dataset of cardinality 60,000 (resp. 50,000) and dimensionality 784 (resp. 3092). We use a batch size of 1000 and train for 50 (resp. 80) epochs.

**NIPS bag of words** This dataset contains the frequency of 11,463 words in 5812 NIPS papers published between 1987 and 2015 (Perrone et al., 2016). Each entry in the 11,463-by-5812 matrix holds the number of occurrences of a given word in the corresponding paper. We train with a batch size of 1000 for 200 epochs.

5.2 Large-scale Datasets

**Large Lobster Image Dataset** The Large Lobster Image Dataset (Vo et al., 2020) contains 6654 images of 238 southern rock lobsters taken at a lobster processor in Tasmania over the course of 6 days. The images have a resolution of $1944 \times 2592$ and 3 color channels. After flattening, we end up with a $15.6M$ dimensional vectors. We use a batch size of 1024 and train for 300 training steps ($\sim 43$ epochs) with a learning rate of $10^{-4}$ to find the first 8 principal components.

**ResNet activations** Following the original EigenGame paper, we build a dataset from the activation patterns of a pretrained ResNet-152 (He et al., 2015) evaluated on the validation set of ImageNet (Deng et al., 2009). Each datapoint is constructed from the outputs of all residual blocks of the ResNet-152. This results in a dataset of dimension $d \sim 13.1M$ and cardinality $n = 50000$. We use a batch size of 1024 and train for 600 training steps ($\sim 12$ epochs) with a learning rate of $10^{-9}$ to find the first 8 principal components. The time-cost of the full-PCA step (in particular, of the projection) is comparable to the time cost of 1 training epoch. In this experiment, we only train for 12 epochs, therefore the the cost of full-PCA is not negligible in this setting. Circumventing this issue, we only project 10% of the data for computing full-PCA, reducing the overhead for full-PCA from $\sim 95$ to $\sim 9.5$ minutes.

5.3 Training details

We train with SGD using Nesterov momentum with a factor of 0.9 (Nesterov, 1983). Everything is implemented in Pytorch, the experiments on the small-scale datasets are executed on a NVIDIA RTX 3090 while the experiments on the large-scale datasets are executed on an NVIDIA A100.

5.4 Evaluating the experiments

**Small-scale** To evaluate the small-scale experiments we use the “Longest Correct Eigenvector Streak” metric proposed in the EigenGame paper by Gemp et al. (2020) to evaluate performance. Given the ground truth principal directions $\{e_1, \ldots, e_k\}$, the approximate directions coming from the learning algorithm $\{v_1, \ldots, v_k\}$ and a threshold value $0 < V < \pi/2$, we compute if the angle between $v_i$ and $e_i$ is smaller than $V$ for all $i \in \{1, \ldots, k\}$. Then, the number of consecutive pairs from index 1 that are within angle $V$ of each other is by definition the Longest Correct Eigenvector Streak. For instance, if for a given $V$ the angles are $[V/2, V/3, 2V, V/2, \ldots]$, then the Longest Correct Eigenvector Streak for this $V$ is 2. In our experiments, we evaluate all runs with $V \in \{\pi/8, \pi/16, \ldots, \pi/1024\}$. 
Large-scale  The remaining 2 experiments (Lobsters and ResNet activations) need to evaluated differently, since the real principal directions are not available. This means that we can only evaluate performance indirectly. We plot the variance captured by the result of EigenGame and pPCA. When the algorithm converges to the actual principal directions of the data, the variance will converge to the corresponding eigenvalue of the covariance matrix. Convergence of the variance is therefore a hint (but not evidence!) of convergence of the corresponding eigenvalues/principal directions.

5.5 Results
Small-scale Figure 2 shows the plots of the Longest Correct Eigenvector Streak for the small-scale experiments described above. We reuse the threshold from the EigenGame paper (Gemp et al., 2020) and set it to $V = \pi/8$ for the plots of Figure 2. In the Appendix, plots are available for all threshold values $V \in \{\pi/8, \pi/16, ..., \pi/1024\}$. A qualitative comparison is also available in Table 1. In all these experiments, we compare EigenGame, pPCA, pPCA$_2$ and pPCA$_3$.

Large-scale Figure 4 displays the results for the large-scale experiments. Figure 6 in the Appendix shows the eigenvectors found by both methods after 30 and 300 training steps of the Large Scale Lobster Experiment. After 300 training steps the methods converge to vectors that are indistinguishable by the human eye. Looking at the results after 30 training steps, we can also conclude the pPCA already found the first 4 components, while EigenGame only the first 2. Note that this is exactly what Figure 4 suggests.

6 Conclusion
We introduced primed PCA, a method for computing the first $k$ principal directions by combining the EigenGame algorithm introduced by Gemp et al. and a centralized, cheap, post-processing full-PCA step. We have demonstrated on several datasets that pPCA greatly improves upon EigenGame in terms of convergence speed and worked out the algebraic condition that guarantees that in most cases this is expected to happen. We have also demonstrated on small-scale datasets that using extra components in EigenGame improves performance further.

Future Work As discussed in Subsection 3.2 the fact that after running EigenGame we will post-process the results allows for modifications of the original EigenGame algorithm. Since EigenGame was not designed to be followed by a post-processing step, it is possible that EigenGame in its current form is not the optimal preprocessing step for the full-PCA, although they seem to be very efficient together. It could also be investigated how the optimal value of additional EigenGame players, $l$, changes as the parameters of the dataset, $d$ and $n$, or the number of principal components of interest, $k$, vary.

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Figure 6: Each of the subplots show the first 8 principal components of the Large Lobster Image Dataset organised into 8 columns found by the respective algorithms. The two lines show the positive and negative parts of the vectors. After 30 training steps pPCA already finds the first 4 vectors, while EigenGame only predicts the first 2 correctly. After 300 training steps, the methods have the same output for all 8 principal directions.
Figure 7: The best learning for EigenGame on the Synthetic data with exponential spectrum was $10^{-5}$. 
Figure 8: The best learning for EigenGame on the Synthetic data with linear spectrum was $10^{-6}$. 
Figure 9: The best learning for EigenGame on MNIST was $10^{-3}$.
Figure 10: The best learning for EigenGame on CIFAR10 was $10^{-5}$. 
Figure 11: The best learning for EigenGame on the NIPS bag of words dataset was $10^{-5}$.