THE SYMMETRIC GENERALIZED EIGENVALUE PROBLEM AS A NASH EQUILIBRIUM

Anonymous authors

Paper under double-blind review

ABSTRACT

The symmetric generalized eigenvalue problem (SGEP) is a fundamental concept in numerical linear algebra. It captures the solution of many classical machine learning problems such as canonical correlation analysis, independent components analysis, partial least squares, linear discriminant analysis, principal components and others. Despite this, most general solvers are prohibitively expensive when dealing with *streaming data sets* (i.e., minibatches) and research has instead concentrated on finding efficient solutions to specific problem instances. In this work, we develop a game-theoretic formulation of the top-k SGEP whose Nash equilibrium is the set of generalized eigenvectors. We also present a parallelizable algorithm with guaranteed asymptotic convergence to the Nash. Current state-of-the-art methods require $\mathcal{O}(d^2k)$ runtime complexity per iteration which is prohibitively expensive when the number of dimensions (d) is large. We show how to modify this parallel approach to achieve $\mathcal{O}(dk)$ runtime complexity. Empirically we demonstrate that this resulting algorithm is able to solve a variety of SGEP problem instances including a large-scale analysis of neural network activations.

1 INTRODUCTION

This work considers the symmetric generalized eigenvalue problem (SGEP),

$$Av = \lambda Bv \tag{1}$$

where A is symmetric and B is symmetric, positive definite. While the SGEP is not a common sight in modern machine learning literature, remarkably, it underlies several fundamental problems. Most obviously, when $A = X^\top X$, $B = I$, and X is a data matrix, we recover the ubiquitous SVD/PCA. However, by considering other forms of A and B we recover other well known problems. In general, we assume A and B consist of sums or expectations over outerproducts (e.g., $X^\top Y$ or $\mathbb{E}[xy^\top]$) to enable efficient matrix-vector products. These include, but are not limited to:

Canonical Correlation Analysis (CCA): Given a dataset of *paired* observations (or views) $x \in \mathbb{R}^{d_x}$ and $y \in \mathbb{R}^{d_y}$ (e.g., gene expressions x and medical imaging y corresponding to the same patient), CCA returns the linear projections of x and y that are maximally correlated. CCA is particularly useful for learning multi-modal representations of data and in semi-supervised learning (McWilliams et al., 2013); it is effectively the multi-view generalization of PCA (Guo & Wu, 2019) where A and B contain the cross- and auto-covariances of the two views respectively:

$$A = \begin{bmatrix} \mathbf{0} & \mathbb{E}[xy^\top] \\ \mathbb{E}[yx^\top] & \mathbf{0} \end{bmatrix} \qquad B = \begin{bmatrix} \mathbb{E}[xx^\top] & \mathbf{0} \\ \mathbf{0} & \mathbb{E}[yy^\top] \end{bmatrix}. \tag{2}$$

Independent Component Analysis (ICA): ICA seeks the directions in the data which are most structured, or alternatively, appear least Gaussian (Hyvärinen & Oja, 2000). A common SGEP formulation of ICA uncovers latent variables which maximize the non-Gaussianity of the data as defined by its excess kurtosis. ICA has famously been proposed as a solution to the so-called cocktail party source-separation problem in audio processing and has been used for denoising and more generally, the discovery of explanatory latent factors in data. Here A and B are the excess kurtosis and the covariance of the data respectively (Parra & Sajda, 2003):

$$A = \mathbb{E}[\langle x, x\rangle xx^\top] - tr(B)B - 2B^2 \qquad B = \mathbb{E}[xx^\top]. \tag{3}$$

Normalized Graph Laplacians: The graph Laplacian matrix (L) is central to tasks such as spectral clustering ($A = L$, $B = I$) where its eigenvectors are known to solve a relaxation of min-cut (Von Luxburg, 2007). Alternatives, such as the random walk normalized Laplacian ($A = L$, B is the diagonal node-degree matrix), approximate other min-cut objectives. These normalized variants, in particular, are important to computing representations for learning value functions in reinforcement learning such as successor features (Machado et al., 2017a; Stachenfeld et al., 2014; Machado et al., 2017b), an extension of proto-value functions (Mahadevan, 2005) which uses the un-normalized graph Laplacian ($A = L$, $B = I$).

Partial least squares (PLS) can be formualted similarly to CCA and finds extensive use in chemometrics (Boucher et al., 2015) and medical domains (Altmann et al., 2021). Likewise, linear discriminant analysis (LDA) can be formulated as a SGEP and learns a label-aware projection of the data that separates classes well (Fisher, 1936; Rao, 1948). More examples and uses of the SGEP can be found in (Bie et al., 2005; Borga et al., 1997). We now shift focus to the mathematical properties and challenges of the corresponding SGEP.

In this work, we assume the matrices A and B above can either be defined using expectations under a data distribution (e.g., $\mathbb{E}_{x\sim p(x)}[xx^\top]$) or means over a finite sample dataset (e.g., $\frac{1}{n}X^\top X$ where $X \in \mathbb{R}^{n\times d_x}$). In either case, we typically assume the data has mean zero unless specified otherwise.

Note that the SGEP, $Av = \lambda Bv$, is *similar* to the eigenvalue problem, $B^{-1}Aw = \lambda' w$, in a formal sense (see Proposition 2 in Appx. A). There are two reasons for working with the SGEP instead: 1) inverting B is prohibitively expensive for a large matrix and 2) while A and $B \succ 0$ are symmetric, $B^{-1}A$ is not, which hides useful information about the eigenvalues and eigenvectors (they are necessarily real and B-orthogonal). This also highlights that the SGEP is a fundamentally more challenging problem than SVD and why a direct application of previous game-theoretic approaches such as (Gemp et al., 2021; 2022) is not possible.

The complexity of solving the SGEP is $\mathcal{O}(d^3)$ where d is the dimension of the square matrix A (equiv. B). Several libraries exist for solving the SGEP in-memory (Tzounas et al., 2020). There is also a vast numerics literature we cannot do justice that considers large matrices (Sorensen, 2002).

We specifically focus on the stochastic, streaming data setting which is of particular interest to machine learning methods which learn by iterating over small minibatches of data (e.g., stochastic gradient descent). Under this setting, machine learning research has developed simple approximate solvers for singular value decomposition (SVD) that scale to very large datasets (Allen-Zhu & Li, 2017b). Similarly, in this work, we contribute a simple, elegant solution to the SGEP, including

- A game whose Nash equilibrium is the top-k SGEP solution,
- An easily parallelizable algorithm with $\mathcal{O}(dk)$ per-iteration complexity relying only on matrix-vector products,
- An empirical analysis of neural similarity on activations $1000\times$ larger than prior work.

The game and accompanying algorithm are developed synergistically to achieve a formulation that is amenable to analysis and naturally leads to an elegant and efficient algorithm.

2 Generalized EigenGame: Players, Strategies, and Utilities

In this work, we take the approach of defining the top-k SGEP as a k-player game. It is an open question how to define a k-player game appropriately such that key properties of the SGEP are captured[1]. As argued in previous work (Gemp et al., 2021; 2022), game formulations make obvious how computation can be distributed over players, leading to high parallelization, which is critical for processing large datasets. They have also clarified geometrical properties of the problem.

Specifically, we are interested in solving the top-k SGEP which means we are interested in finding the (unit-norm) generalized eigenvectors v_i associated with the top-k largest generalized eigenvalues λ_i. Therefore, let there be k **players** denoted $i \in \{1, \ldots, k\}$, and let each select a vector $\hat{v}_i$

[1]The Courant-Fischer min-max principle poses the ith generalized eigenvalue as the solution to a two-player, zero-sum game (Parlett, 1998)—see Appx. A.2 for further discussion.

(**strategy**) from the unit-sphere $\mathcal{S}^{d-1}$ (*strategy space*). We define player i's **utility** function conditioned on its parents (players $j < i$) as follows:

$$u_i(\hat{v}_i|\hat{v}_{j<i}) = \overbrace{\frac{\langle \hat{v}_i, A\hat{v}_i\rangle}{\langle \hat{v}_i, B\hat{v}_i\rangle}}^{\text{generalized Rayleigh Quotient}} - \sum_{j<i} \frac{\langle \hat{v}_j, A\hat{v}_j\rangle \langle \hat{v}_i, B\hat{v}_j\rangle^2}{\langle \hat{v}_j, B\hat{v}_j\rangle^2 \langle \hat{v}_i, B\hat{v}_i\rangle} \tag{4}$$

$$= \underbrace{\hat{\lambda}_i}_{\text{reward}} - \sum_{j<i} \underbrace{\hat{\lambda}_j \langle \hat{y}_i, B\hat{y}_j\rangle^2}_{\text{penalty}} \quad \text{where } \hat{y}_i = \frac{\hat{v}_i}{||\hat{v}_i||_B}, \tag{5}$$

$\hat{\lambda}_i = \frac{\langle \hat{v}_i, A\hat{v}_i\rangle}{\langle \hat{v}_i, B\hat{v}_i\rangle}$, and $||z||_B = \sqrt{\langle z, Bz\rangle}$.

Player i's utility has an intuitive explanation. The first term is recognized as the generalized Rayleigh quotient which can be derived by left multiplying both sides of the SGEP ($v^\top Av = \lambda v^\top Bv$) and solving for λ. Note that the generalized eigenvectors are guaranteed to be B-orthogonal, i.e., $v_i^\top Bv_j = 0$ for all $i \neq j$ (Appx. A Lemma 3). Therefore, the *reward* term incentivizes players to find directions that result in large eigenvalues, but are simultaneously *penalized* for choosing directions that align with their parents (players with index less than i, higher in the hierarchy). Finally, the penalty coefficient $\hat{\lambda}_j$ serves to balance the magnitude of the penalty terms with the reward term such that players have no incentive to "overlap" with parents. In Appx. B Proposition 4, we derive these same utilities via a *deflation* perspective. Next, we formally prove these utilities are well-posed in the sense that, given exact parents, their optima coincide with the top-k SGEP solution.

Lemma 1 (Well-posed Utilities)**.** *Given exact parents and assuming the top-k eigenvalues of $B^{-1}A$ are distinct and positive, the maximizer of player i's utility is the unique generalized eigenvector v_i (up to sign, i.e., $-v_i$ is also valid).*

Note that $\hat{\lambda}_i = \frac{\langle \hat{v}_i, A\hat{v}_i\rangle}{\langle \hat{v}_i, B\hat{v}_i\rangle} = \frac{\langle \hat{v}_i/||\hat{v}_i||_B, A\hat{v}_i/||\hat{v}_i||_B\rangle}{\langle \hat{v}_i/||\hat{v}_i||_B, B\hat{v}_i/||\hat{v}_i||_B\rangle} = \frac{\langle \hat{y}_i, A\hat{y}_i\rangle}{\langle \hat{y}_i, B\hat{y}_i\rangle}$, therefore, the results above still hold for utilities defined using vectors constrained to the unit ellipsoid, $||\hat{y}_i||_B = 1$, rather than the unit-sphere, $||\hat{v}_i||_I = 1$. However, in our setting, B is a massive matrix which can never be explicitly constructed and instead only observed via minibatches. It is then not clear how to handle the constraint $||\hat{y}_i||_B = 1$. We therefore only consider an approach that assumes $||\hat{v}_i||_I = 1$.

Next, we provide intuition for the shape of these utilities. Surprisingly, while non-concave, we prove analytically in Appx. B that they have a simple sinusoidal shape. A numerical illustration is given in Figure 1 to help the reader visualize this property.

Proposition 1 (Utility Shape)**.** *Each player's utility is periodic in the angular deviation (θ) along the sphere. Its shape is sinusoidal, but with its angular axis (θ) smoothly deformed as a function of B. Most importantly, every local maximum is a global maximum.*

Figure 1 illustrates a primary difficulty of solving the SGEP over SVD. Due to the extreme differences in curvature caused by the B matrix, the SGEP should benefit from optimizers employing adaptive per-dimension learning rates. To our knowledge, this 1-d visualization of the difficulty of the SGEP is novel and we exploit this insight in experiments.

Finally, we formally define our proposed game and prove its equilibrium constitutes the top-k SGEP solution. We use the Greek letter ***g**amma* to denote ***g**eneralized*, and we differentiate between the game and the algorithm with upper Γ and lower case γ respectively.

Definition 1 (Γ-EigenGame)**.** *Let Γ-EigenGame be the game with players $i \in \{1, \ldots, k\}$, their strategy spaces $\hat{v}_i \in \mathcal{S}^{d-1}$, and their utilities u_i as defined in equation (48).*

Theorem 1 (Nash Property)**.** *Assuming the top-k generalized eigenvalues of the generalized eigenvalue problem $Av = \lambda Bv$ are positive and distinct, their corresponding generalized eigenvectors form the unique, strict Nash equilibrium of Γ-EigenGame.*

Proof. Lemma 1 proves that each generalized eigenvector v_i ($i \in \{1, \ldots, k\}$) is the unique best response to v_{-i}, which implies the entire set constitutes the unique Nash equilibrium. □

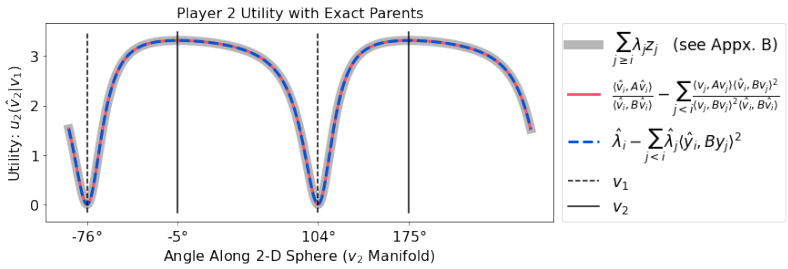

Figure 1: Each player's utility is a sinusoid on the sphere warped tangentially along the axis of angular deviation according to B; values for A and B used in this example are given in Appx. B. Three mathematical representations of the utility are plotted; their equivalence is supported by the overlapping curves. If player 2 aligns with the top eigenvector (dashed vertical), they receive zero utility. If they align with the second eigenvector (solid vertical), they receive λ_2 (optimal) as reward. If $B = I$ as in SVD/PCA, the vertical lines indicating the minima and maxima would be separated by exactly $90°$. In this case, the matrix B redefines what it means for two vectors to be orthogonal ($\langle \hat{v}_i, B\hat{v}_j \rangle = 0$), so that the vectors are $71°$ (equivalently, $180° - 71° = 109°$) from each other.

3 Algorithm: Unbiased Player Updates and Auxiliary Variables

Given that Γ-EigenGame suitably captures the top-k SGEP, we now develop an iterative algorithm to approximate its solution. The basic approach we take is to perform parallel gradient ascent on all player utilities simultaneously. We focus on this approach in particular because it aligns with the predominant machine learning paradigm and hardware. We will first write down the gradient of each player's utility and then introduce several simplifications for the purpose of enabling unbiased estimates in the stochastic setting.

Up to scaling factors, the gradient of player i's utility function with respect to $\hat{v}_i$ is

$$\frac{(\hat{v}_i^\top B\hat{v}_i)A\hat{v}_i - (\hat{v}_i^\top A\hat{v}_i)B\hat{v}_i}{\langle \hat{v}_i, B\hat{v}_i \rangle^2} - \sum_{j<i} \frac{\hat{\lambda}_j}{\langle \hat{v}_j, B\hat{v}_j \rangle} (\hat{v}_i^\top B\hat{v}_j) \frac{\left[\langle \hat{v}_i, B\hat{v}_i \rangle B\hat{v}_j - \langle \hat{v}_i, B\hat{v}_j \rangle B\hat{v}_i\right]}{\langle \hat{v}_i, B\hat{v}_i \rangle^2}. \tag{6}$$

See Lemma 5 in Appx. B for a derivation of the gradient. Recall that B is a matrix that we intend to estimate with samples, i.e., it is a random variable, and it appears several times in the denominator of the gradient. Obtaining unbiased estimates of inverses of random variables is difficult (e.g., the naive approach gives an overestimate; $\mathbb{E}[1/x] \geq 1/\mathbb{E}[x]$ by Jensen's inequality). We can remove the scalar $\langle \hat{v}_i, B\hat{v}_i \rangle^2$ in the denominator because it is common to all terms and will not change the direction of the gradient nor the location of fixed points; this step is critical to the design of our stochastic algorithm which we will explain later. We also use the following two additional relations:

(i) $\hat{\lambda}_j \langle \hat{v}_i, B\hat{v}_j \rangle = \langle \hat{v}_i, A\hat{v}_j \rangle$ if player i's parents match their true solutions, i.e., $\hat{v}_{j<i} = v_{j<i}$,

(ii) $\sqrt{\langle \hat{v}_j, B\hat{v}_j \rangle} = ||\hat{v}_j||_B$ is strictly positive and real-valued because $B \succ 0$,

to arrive at the simplified update direction

$$\tilde{\nabla}_i = \overbrace{(\hat{v}_i^\top B\hat{v}_i)A\hat{v}_i - (\hat{v}_i^\top A\hat{v}_i)B\hat{v}_i}^{\text{reward}} - \sum_{j<i} \overbrace{(\hat{v}_i^\top A\hat{y}_j)\left[\langle \hat{v}_i, B\hat{v}_i \rangle B\hat{y}_j - \langle \hat{v}_i, B\hat{y}_j \rangle B\hat{v}_i\right]}^{\text{penalty}}. \tag{7}$$

Simplifying the gradient using (i) is sound because the hierarchy of players ensures the parents will be learned exactly asymptotically. For instance, player 1's update has no penalty terms and so will converge asymptotically. The argument then proceeds by induction.

Note that B still appears in the denominator via the $\hat{y}_j$ terms (recall equation (48)). We will revisit this issue later, but for now we will show this update converges to the desired solution given exact estimates of expectations (full-batch setting). Lemma 2 is a stepping stone to proving convergence with arbitrary parents in Theorem 2.

Lemma 2. *The direction $\tilde{\nabla}_i$ defined in equation (7) is a steepest ascent direction on utility $u_i(\hat{v}_i|\hat{v}_{j<i})$ given exact parents $\hat{v}_{j<i} = v_{j<i}$.*

Proof. This fact follows from the above argument that removing a positive scalar multiplier does not change the direction of the gradient of u_i w.r.t. $\hat{v}_i$ and applying relation (i). □

We present the deterministic version of γ-EigenGame in Algorithm 1 where k players use $\tilde{\nabla}_i$ in (7) to maximize their utilities in parallel (see **parfor**-loop below). While simultaneous gradient ascent fails to converge to Nash equilibria in games in general, it succeeds in this case because the hierarchy we impose ensures each player has a unique best response (Lemma 1); this type of procedure is known as *iterative strict dominance* in the game theory literature. Theorem 2, proven in Appx. E, guarantees it converges asymptotically to the true solution.

Algorithm 1 Deterministic / Full-batch γ-EigenGame

Given: $A \in \mathbb{R}^{d\times d}$ and $B \in \mathbb{R}^{d\times d}$, step size sequence η_t, and number of iterations T.
$\hat{v}_i \sim \mathcal{S}^{d-1}$, i.e., $\hat{v}_i \sim \mathcal{N}(\mathbf{0}_d, \mathbf{I}_d)$; $\hat{v}_i \leftarrow \hat{v}_i/||\hat{v}_i|$ for all i
for $t = 1 : T$ **do**
  parfor $i = 1 : k$ **do**
    $\hat{y}_j = \frac{\hat{v}_j}{\sqrt{\langle \hat{v}_j, B\hat{v}_j\rangle}}$
    $\texttt{rewards} \leftarrow (\hat{v}_i^\top B\hat{v}_i)A\hat{v}_i - (\hat{v}_i^\top A\hat{v}_i)B\hat{v}_i$
    $\texttt{penalties} \leftarrow \sum_{j<i}(\hat{v}_i^\top A\hat{y}_j)\big[\langle \hat{v}_i, B\hat{v}_i\rangle B\hat{y}_j - \langle \hat{v}_i, B\hat{y}_j\rangle B\hat{v}_i\big]$
    $\tilde{\nabla}_i \leftarrow \texttt{rewards} - \texttt{penalties}$
    $\hat{v}_i' \leftarrow \hat{v}_i + \eta_t\tilde{\nabla}_i$
    $\hat{v}_i \leftarrow \frac{\hat{v}_i'}{||\hat{v}_i'||}$
  end parfor
end for
return all $\hat{v}_i$

Theorem 2 (Deterministic / Full-batch Global Convergence)**.** *Given a symmetric matrix A and symmetric positive definite matrix B where the top-k eigengaps of $B^{-1}A$ are positive along with a square-summable, not summable step size sequence η_t (e.g., $1/t$), Algorithm 1 converges to the top-k generalized eigenvectors asymptotically ($\lim_{T\to\infty}$) with probability* 1.

In the big data setting, A and B are statistical estimates, i.e., expectations of quantities over large datasets. Precomputing exact estimates is computationally expensive, so we assume a data model that allows drawing small *minibatches* of data at a time. Under such a model, stochastic approximation theory typically guarantees that as long as the update directions are *unbiased*, i.e., equal in expectation to the updates with exact estimates, then an appropriate algorithm will converge to the true solution.

In order to construct an unbiased update direction given access to minibatches of data, we need to draw multiple minibatches independently at random. We can construct an unbiased estimate of products of expectations, e.g., $(\hat{v}_i^\top B\hat{v}_i)A\hat{v}_i$, by drawing an independent batch for each, e.g., one for B and one for A. However, the B that appears in the denominator of $\hat{y}_j$ is problematic; we cannot construct an unbiased estimate of the inverse of a random variable.

These problematic $\hat{y}_j$ terms only appear in the penalties, which are a function of the parents' eigenvector approximations. The first eigenvector has no parents, and so we can easily construct an unbiased estimate for it using multiple minibatches. We can then construct an unbiased estimate for each subsequent player by inductive reasoning. Intuitively, once the parents have been learned, $\hat{v}_j$ should be stable and so it should be possible to estimate $B\hat{v}_j$ from a running average, and in turn, $\hat{y}_j$. This suggests introducing an auxiliary variable, denoted $[B\hat{v}]_j$ to track the running averages of $B\hat{v}_j$ (a similar approach is employed in (Pfau et al., 2018)). This effectively replaces $B\hat{y}_j$ with a non-random variable, avoiding the bias dilemma, at the expense of doubling the number of variables. Note that introducing this auxiliary variable implies the inner product $\langle \hat{v}_j, [B\hat{v}]_j\rangle$ may not be positive definite, therefore, we manually clip the result to be greater than or equal to ρ, the minimum singular value of B.

Algorithm 2 Stochastic γ-EigenGame

Given: paired data streams $X_t \in \mathbb{R}^{b \times d_x}$ and $Y_t \in \mathbb{R}^{b \times d_y}$, number of parallel machines M per player (minibatch size per machine $b' = \frac{b}{M}$), step size sequences η_t and γ_t, scalar ρ lower bounding $\sigma_{min}(B)$, and number of iterations T.
$\hat{v}_i \sim \mathcal{S}^{d-1}$, i.e., $\hat{v}_i \sim \mathcal{N}(\mathbf{0}_d, \mathbf{I}_d)$; $\hat{v}_i \leftarrow \hat{v}_i / ||\hat{v}_i|$ for all i
$[B\hat{v}]_i \leftarrow \hat{v}_i^0$ for all i
for $t = 1 : T$ **do**
  parfor $i = 1 : k$ **do**
    parfor $m = 1 : M$ **do**
      Construct A_{tm} and B_{tm} (*unbiased estimates using independent data batches)
      $\hat{y}_j = \frac{\hat{v}_j}{\sqrt{\max(\langle \hat{v}_j, [B\hat{v}]_j \rangle, \rho)}}$
      $[B\hat{y}]_j = \frac{[B\hat{v}]_j}{\sqrt{\max(\langle \hat{v}_j, [B\hat{v}]_j \rangle, \rho)}}$
      $\texttt{rewards} \leftarrow (\hat{v}_i^\top B_{tm} \hat{v}_i) A_{tm} \hat{v}_i - (\hat{v}_i^\top A_{tm} \hat{v}_i) B_{tm} \hat{v}_i$
      $\texttt{penalties} \leftarrow \sum_{j<i} (\hat{v}_i^\top A_{tm} \hat{y}_j) \big[\langle \hat{v}_i, B_{tm} \hat{v}_i \rangle [B\hat{y}]_j - \langle \hat{v}_i, [B\hat{y}]_j \rangle B_{tm} \hat{v}_i \big]$
      $\tilde{\nabla}_{im} \leftarrow \texttt{rewards} - \texttt{penalties}$
      $\nabla_{im}^{Bv} = (B_{tm} \hat{v}_i - [B\hat{v}]_i)$
    end parfor
    $\tilde{\nabla}_i \leftarrow \frac{1}{M} \sum_m [\tilde{\nabla}_{im}]$
    $\hat{v}_i' \leftarrow \hat{v}_i + \eta_t \tilde{\nabla}_i$
    $\hat{v}_i \leftarrow \frac{\hat{v}_i'}{||\hat{v}_i'||}$
    $\nabla_i^{Bv} \leftarrow \frac{1}{M} \sum_m [\nabla_{im}^{Bv}]$
    $[B\hat{v}]_i \leftarrow [B\hat{v}]_i + \gamma_t \nabla_i^{Bv}$
  end parfor
end for
return all $\hat{v}_i$

Precise pseudocode is given in Algorithm 2. Differences to Algorithm 1 are highlighted in color (auxiliary differences in blue, clipping in red). We point out that introducing an auxiliary variable for player i to track $[B\hat{v}]_i$ is not feasible because unlike player i's parents' variables, $\hat{v}_i$ cannot be assumed non-stationary. This is why removing $\langle \hat{v}_i, B\hat{v}_i \rangle$[2] earlier from the denominator of equation (6) was critical. Lastly, note that these modifications to the update are derived using an understanding of the intended computation and theoretical considerations; put shortly, *autograd* libraries will not uncover this solution. See Appx. E.2 for more discussion and analysis of Algorithm 2.

Computational Complexity and Parallelization. The naive, per-iteration runtime and work costs of this update are $\mathcal{O}(bdk^2)$ with batch size b, but due to the simplicty of the update (i.e., purely matrix-vector products), there are several opportunities for both model and data parallelism to reduce runtime cost to $\mathcal{O}(dk)$ (see Appx. I for steps). Note that low aggregate batch sizes can induce high gradient variance, slowing convergence (Durmus et al., 2021), making data parallelism desireable.

To give a concrete example, if each player (model) parallelizes over $M = b$ machines (data) as indicated by the two **parfor**-loops, the complexity reduces to $\mathcal{O}(dk)$. This is easy to implement with modern libraries, e.g., `pmap` using Jax, and as in prior work (Gemp et al., 2021), the communication of parents $v_{j<i}$ between machines is efficient in systems with fast interconnects (e.g., TPUs) although this presents a bottleneck we hope to alleviate in future work. Alternative parallel implementations are discussed in Appx. F. Lastly, the update consists purely of inexpensive elementwise operations and matrix-vector products that can be computed quickly on deep learning hardware (e.g., GPUs and TPUs); unlike previous state-of-the-art in (Meng et al., 2021), no calls to CPU-bound linear algebra subroutines are necessary.

4 Related Work

[2]Run with `logcosh` approximation to negentropy (see (Hyvärinen & Oja, 2000) for explanation).

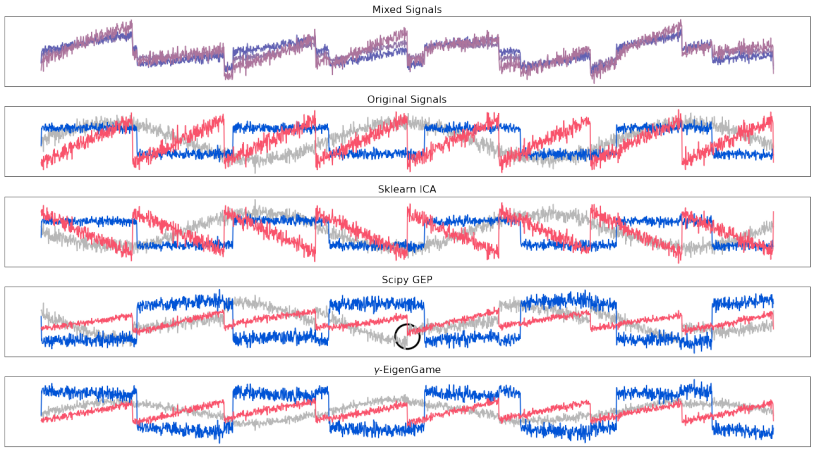

Figure 2: Blind Source Separation. Algorithm 2 (γ-EigenGame) run for 1000 epochs with mini-batches of size $\frac{n}{4}$ subsampled i.i.d. from the dataset recovers the three original signals from the linearly mixed signals. Scikit-learn's FastICA[2] also recovers the signals by maximizing an alternative measure of non-Gaussianity. Directly solving the SGEP using `scipy.linalg.eigh(A, B)` fails to cleanly recover the gray sinusoid (black circle highlights a discontinuity) due to overfitting to the sample dataset. We confirm this by training γ-EigenGame for many more iterations and show it exhibits similar artifacts in Appx. G.

The SGEP is a fundamental problem in numerical linear algebra with numerous applications in machine learning and statistics. There is a long history in numerical computing of solving large SGEP problems (Sorensen, 2002; Knyazev & Skorokhodov, 1994; Golub & Ye, 2002; Aliaga et al., 2012; Klinvex et al., 2013). Many methods iterate with what can be viewed as "gradient-like" updates (D'yakonov & Knyazev, 1982; D'yakonov & Knyazev, 1992), however, they are not immediately applicable in the stochastic, streaming data setting. To our knowledge, efficient approaches for the SGEP or specific sub-problems (e.g., CCA) scale at best $\mathcal{O}(d^2k)$ in the streaming data setting.

Ge et al. (2016) give an algorithm for top-k SGEP that makes repeated use of a linear system solver to approximate the subspace of the true generalized eigenvectors, but may return an arbitrary rotation of the solution. While their method is theoretically efficient, it requires precomputing A and B which prohibits its use in a streaming data setting. The sequential least squares CCA algorithm proposed by Wang et al. (2016) similarly requires access to the full dataset up front, however, in their case, it is to ensure the generalized eigenvectors are exactly unit-norm relative to the matrix B. Allen-Zhu & Li (2017a) develop a SGEP algorithm that is theoretically linear in the size of the input (nd) and k, however, they assume access to the entire dataset (non-streaming). LOBPCG (Knyazev, 2017) is a non-streaming, Rayleigh maximizing technique with line-search and a preconditioned gradient.

Arora et al. (2017) propose a convex relaxation of the CCA problem along with a streaming algorithm with convergence guarantees. However, instead of learning $V_x \in \mathbb{R}^{d_x}$ and $V_y \in \mathbb{R}^{d_y}$ directly, it learns $M = V_x V_y^\top \in \mathbb{R}^{d_x \times d_y}$ which is prohibitively expensive to store in memory for high-dimensional problems. Moreover, the complexity of this algorithm is $\mathcal{O}(d^3)$ due to an expensive projection step requiring an SVD of M. They propose an alternative version *without* guarantees that reduces the cost per iteration to $\mathcal{O}(dk^2)$.

Gao et al. (2019) also consider the streaming setting, but instead focuse on top-1 CCA and like (Wang et al., 2016) and (Allen-Zhu & Li, 2017a), use shift-invert preconditioning to accelerate convergence. Bhatia et al. (2018) solves top-1 SGEP in the streaming setting.

Most recently, Meng et al. (2021) proposed a method to estimate top-k CCA in a streaming setting. Their algorithm requires several expensive Riemmanian optimization subroutines, giving a per iteration complexity of $\mathcal{O}(d^2k)$. Their convergence guarantee is in terms of subspace error, so as mentioned above, the projection matrices V_x and V_y may be rotations of their ordered (by correlation) counterparts. Their approach is the current state-of-the-art when considering CCA in the streaming setting for large datasets.

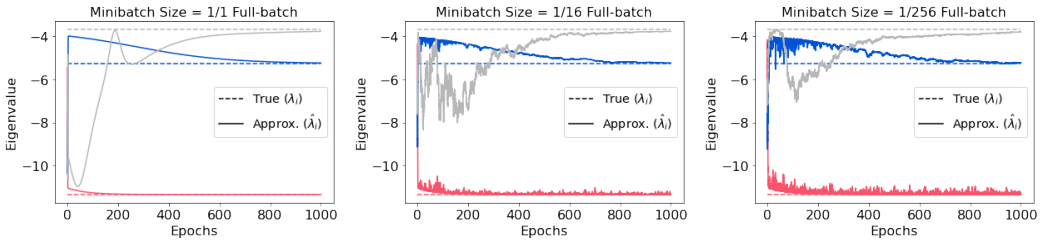

Figure 3: γ-EigenGame converges to the true SGEP solution regardless of minibatch size in support of the unbiased nature of the derived update scheme (Algorithm 2). See Appx. G.2 for additional experiments showing learning in sequence performs worse than its parallel counterpart above.

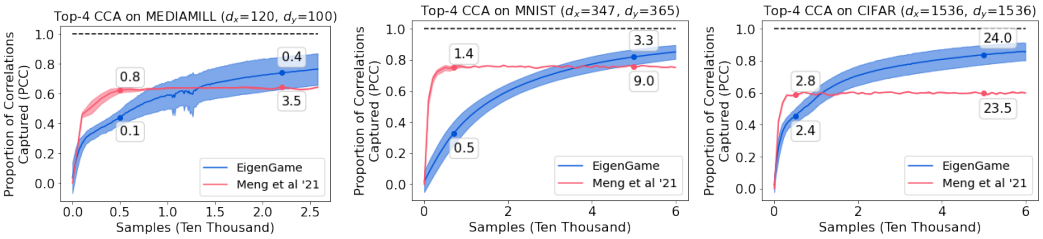

Figure 4: γ-EigenGame compared to (Meng et al., 2021) on *proportion of correlations captured*—$\sum_i^k \hat{\lambda}_i / \sum_i^k \lambda_i$. Shading indicates ± 1 stdev. Markers indicate runtime in seconds.

5 Experiments

We demonstrate our proposed stochastic approach, Algorithm 2, on solving ICA and CCA via their SGEP formulations, and provide empirical support for its veracity. We plan to open source this approach in Jax. Scipy's `linalg.eigh(A, B)` (Virtanen et al., 2020) is treated as ground truth when the data size permits. Hyperparameters are listed in Appx. H.

5.1 ICA

As mentioned in the introduction, ICA can be used to disentangle mixed signals such as in the cocktail party problem. Here, we use the SGEP formulation to unmix three linearly mixed signals. Note that because the SGEP learns a linear unmixing of the data, the magnitude (and sign) of the original signals cannot be learned. Any change in the magnitude of a signal extracted by the SGEP can be offset by adjusting the magnitude and sign of a mixing weight.

We replicate a synthetic experiment from `scikit-learn`(Pedregosa et al., 2011) and compare Algorithm 2 to several approaches. Figure 2 shows our stochastic approach (γ-EigenGame) is able to recover the shapes of the original signals (length $n = 2000$ time series).

Implicit Regularization via Fixed Step Size Updates. Note that if we run Algorithm 2 for $100\times$ more iterations with $1/10$th the step size, we converge to the exact SGEP solution (as found by `scipy`) and see similar artifacts in the extracted signals due to overfitting. Recently, Durmus et al. (2021) proved that fixed step size Riemannian approximation schemes converge to a stationary distribution around their solutions, which suggests γ-EigenGame enjoys a natural regularization property and explains its high performance on this the unmixing task. In Appx. G, we show that it is difficult to achieve similar results with `scipy` by regularizing A or B directly (e.g., $A + \epsilon I$) prior to calling `scipy.linalg.eigh`.

Unbiased Updates. Here, we empirically support our claim that the fixed point of Algorithm 2 is unbiased regardless of minibatch size.[3] Not only does γ-EigenGame recover the same general-

[3]The gray line converges last because we chose to minimize rather than maximize kurtosis.

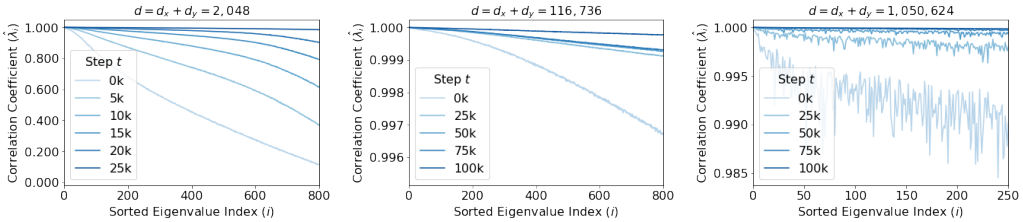

Figure 5: γ-EigenGame compares the representation (activations) of a deep network trained on CIFAR-10 for t steps to that of its final learned representation ($25k$ or $100k$ steps). Curves with higher correlation coefficients indicate more similar representations.

ized eigenvalues, but the plots also suggests that the algorithm takes a similar trajectory for each minibatch size.

5.2 CCA

Here, we use γ-EigenGame to linearly project multimodal datasets into lower-dimensional spaces such that they are maximally correlated. As discussed in related work, several approaches have been developed to extend CCA to streaming, high-dimensional datasets. Recall that our approach has per-iteration complexity $\mathcal{O}(bdk)$ with the previous state-of-the-art in the streaming setting having $\mathcal{O}(d^2k)$ (Meng et al., 2021). We replicate the experiments of (Meng et al., 2021) and compare against their approach on three datasets.

Figure 4 shows our approach is competitive with (Meng et al., 2021). We also point out that while the previous approach by Meng et al. (2021) enjoys theoretical convergence guarantees with rates, it appears to slow in progress near a biased solution. These datasets are low dimensional ($d \leq 3072$), so we are able to obtain ground truth eigenvectors efficiently using `scipy`. Our next set of experiments considers much higher dimensional where a naive call to `scipy` fails.

5.2.1 Large-scale Neural Network Analysis

Recently, CCA has been used to aid in interpreting the representations of deep neural networks (Raghu et al., 2017; Morcos et al., 2018; Kornblith et al., 2019). These approaches are restricted to layer-wise comparisons of representations, reduced-dimensionality views of representations (via PCA), or small dataset sizes to accomodate current limits of CCA approaches. We replicate one of their analyses (specifically Fig. 1a of (Morcos et al., 2018)) on the activations of an entire network (not just a layer), unblocking this type of analysis for larger deep learning models.

The largest dimensions handled in (Raghu et al., 2017) are $\mathcal{O}(10^3)$. Figure 5 demonstrates our approach (parallelized over 8 TPU chips) on $\mathcal{O}(10^3)$ dimensions (left), $\mathcal{O}(10^5)$ dimensions (middle), and $\mathcal{O}(10^6)$ dimensions (right). Note that in these experiments, we are loading minibatches of CIFAR-10 images, running them through a deep convolutional network, harvesting the activations, and then passing them to our distributed γ-EigenGame solver. As mentioned in Section 2, our understanding of the geometry of the utilities suggests replacing the standard gradient ascent on $\hat{v}_i$ with Adam (Kingma & Ba, 2014); Adam exhibits behavior that implicitly improves stability around equilibria (Gemp & McWilliams, 2019). For the smaller $\mathcal{O}(10^3)$ setting, where we can exactly compute ground truth using `scipy`, we confirm that our approach converges to the top-1024 (out of 2048 possible) eigenvectors with a subspace error of 0.002 (see Appx. A).

6 Conclusion

We presented Γ-EigenGame, a game-theoretic formulation of the generalized eigenvalue problem (SGEP). Our formulation enabled the development of a novel algorithm that scales to massive streaming datasets. The SGEP underlies many classical data processing tools across the sciences, and we believe our proposed approach unblocks its use on the ever-growing size of modern datasets in the streaming setting. In particular, it achieves this by parallelizing computation using modern AI-centric distributed compute infrastructure such as GPUs and TPUs.

REFERENCES

Jose I Aliaga, Paolo Bientinesi, Davor Davidović, Edoardo Di Napoli, Francisco D Igual, and Enrique S Quintana-Orti. Solving dense generalized eigenproblems on multi-threaded architectures. *Applied mathematics and computation*, 218(22):11279–11289, 2012.

Zeyuan Allen-Zhu and Yuanzhi Li. Doubly accelerated methods for faster cca and generalized eigendecomposition. In *International Conference on Machine Learning*, pp. 98–106. PMLR, 2017a.

Zeyuan Allen-Zhu and Yuanzhi Li. First efficient convergence for streaming k-PCA: a global, gap-free, and near-optimal rate. In *2017 IEEE 58th Annual Symposium on Foundations of Computer Science (FOCS)*, pp. 487–492. IEEE, 2017b.

Andre Altmann, Neda Jahanshad, Paul M Thompson, and Marco Lorenzi. Partial least squares provides a whole-genome whole-brain imaging genetics approach. 2021.

Raman Arora, Teodor Vanislavov Marinov, Poorya Mianjy, and Nati Srebro. Stochastic approximation for canonical correlation analysis. *Advances in Neural Information Processing Systems*, 30, 2017.

Haim Avron. A generalized courant-fischer minimax theorem. 2008.

Kush Bhatia, Aldo Pacchiano, Nicolas Flammarion, Peter L Bartlett, and Michael I Jordan. Genoja: Simple & efficient algorithm for streaming generalized eigenvector computation. *Advances in neural information processing systems*, 31, 2018.

Tijl De Bie, Nello Cristianini, and Roman Rosipal. Eigenproblems in pattern recognition. In *Handbook of geometric computing*, pp. 129–167. Springer, 2005.

Magnus Borga, Tomas Landelius, and Hans Knutsson. *A unified approach to PCA, PLS, MLR and CCA*. Linköping University, Department of Electrical Engineering, 1997.

Thomas F Boucher, Marie V Ozanne, Marco L Carmosino, M Darby Dyar, Sridhar Mahadevan, Elly A Breves, Kate H Lepore, and Samuel M Clegg. A study of machine learning regression methods for major elemental analysis of rocks using laser-induced breakdown spectroscopy. *Spectrochimica Acta Part B: Atomic Spectroscopy*, 107:1–10, 2015.

Li Deng. The mnist database of handwritten digit images for machine learning research. *IEEE Signal Processing Magazine*, 29(6):141–142, 2012.

Alain Durmus, Pablo Jiménez, Éric Moulines, and SAID Salem. On riemannian stochastic approximation schemes with fixed step-size. In *International Conference on Artificial Intelligence and Statistics*, pp. 1018–1026. PMLR, 2021.

EG D'yakonov and AV Knyazev. Group iterative method for finding lower-order eigenvalues. *Moscow University Computational Mathematics and Cybernetics*, 15:32–40, 1982.

EG D'yakonov and AV Knyazev. On an iterative method for finding lovver eigenvalues. *Russian Journal of Numerical Analysis and Mathematical Modeling*, 1992.

Ronald A Fisher. The use of multiple measurements in taxonomic problems. *Annals of eugenics*, 7 (2):179–188, 1936.

Chao Gao, Dan Garber, Nathan Srebro, Jialei Wang, and Weiran Wang. Stochastic canonical correlation analysis. *J. Mach. Learn. Res.*, 20:167–1, 2019.

Rong Ge, Chi Jin, Sham M. Kakade, Praneeth Netrapalli, and Aaron Sidford. Efficient algorithms for large-scale generalized eigenvector computation and canonical correlation analysis. In *International Conference on Machine Learning*, pp. 2741–2750. PMLR, 2016.

Ian Gemp and Brian McWilliams. The unreasonable effectiveness of adam on cycles. In *NeurIPS Workshop on Bridging Game Theory and Deep Learning*, 2019.

Ian Gemp, Brian McWilliams, Claire Vernade, and Thore Graepel. Eigengame: PCA as a Nash equilibrium. In *International Conference for Learning Representations*, 2021.

Ian Gemp, Brian McWilliams, Claire Vernade, and Thore Graepel. Eigengame unloaded: When playing games is better than optimizing. *International Conference for Learning Representations*, 2022.

Gene H Golub and Qiang Ye. An inverse free preconditioned krylov subspace method for symmetric generalized eigenvalue problems. *SIAM Journal on Scientific Computing*, 24(1):312–334, 2002.

Navin Goyal and Abhishek Shetty. Sampling and optimization on convex sets in riemannian manifolds of non-negative curvature. In *Conference on Learning Theory*, pp. 1519–1561. PMLR, 2019.

Chenfeng Guo and Dongrui Wu. Canonical correlation analysis (CCA) based multi-view learning: An overview. *arXiv preprint arXiv:1907.01693*, 2019.

Charles R. Harris, K. Jarrod Millman, Stéfan J. van der Walt, Ralf Gommers, Pauli Virtanen, David Cournapeau, Eric Wieser, Julian Taylor, Sebastian Berg, Nathaniel J. Smith, Robert Kern, Matti Picus, Stephan Hoyer, Marten H. van Kerkwijk, Matthew Brett, Allan Haldane, Jaime Fernández del Río, Mark Wiebe, Pearu Peterson, Pierre Gérard-Marchant, Kevin Sheppard, Tyler Reddy, Warren Weckesser, Hameer Abbasi, Christoph Gohlke, and Travis E. Oliphant. Array programming with NumPy. *Nature*, 585(7825):357–362, September 2020. doi: 10.1038/s41586-020-2649-2. URL https://doi.org/10.1038/s41586-020-2649-2.

Aapo Hyvärinen and Erkki Oja. Independent component analysis: algorithms and applications. *Neural networks*, 13(4-5):411–430, 2000.

Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.

A Klinvex, Faisal Saied, and A Sameh. Parallel implementations of the trace minimization scheme tracemin for the sparse symmetric eigenvalue problem. *Computers & Mathematics with Applications*, 65(3):460–468, 2013.

Andrew Knyazev. Recent implementations, applications, and extensions of the locally optimal block preconditioned conjugate gradient method (LOBPCG). *arXiv preprint arXiv:1708.08354*, 2017.

Andrew V Knyazev and Alexander L Skorokhodov. Preconditioned gradient-type iterative methods in a subspace for partial generalized symmetric eigenvalue problems. *SIAM journal on numerical analysis*, 31(4):1226–1239, 1994.

Simon Kornblith, Mohammad Norouzi, Honglak Lee, and Geoffrey Hinton. Similarity of neural network representations revisited. In *International Conference on Machine Learning*, pp. 3519–3529. PMLR, 2019.

Alex Krizhevsky, Geoffrey Hinton, et al. Learning multiple layers of features from tiny images. 2009.

Yuanyuan Liu, Fanhua Shang, James Cheng, Hong Cheng, and Licheng Jiao. Accelerated first-order methods for geodesically convex optimization on Riemannian manifolds. In *Advances in Neural Information Processing Systems*, pp. 4868–4877, 2017.

Marlos C Machado, Marc G Bellemare, and Michael Bowling. A laplacian framework for option discovery in reinforcement learning. In *International Conference on Machine Learning*, pp. 2295–2304. PMLR, 2017a.

Marlos C Machado, Clemens Rosenbaum, Xiaoxiao Guo, Miao Liu, Gerald Tesauro, and Murray Campbell. Eigenoption discovery through the deep successor representation. *arXiv preprint arXiv:1710.11089*, 2017b.

Sridhar Mahadevan. Proto-value functions: developmental reinforcement learning. In *Proceedings of the International Conference on Machine learning*, pp. 553–560, 2005.

MATLAB. *9.7.0.1190202 (R2019b)*. The MathWorks Inc., Natick, Massachusetts, 2018.

Brian McWilliams, David Balduzzi, and Joachim M Buhmann. Correlated random features for fast semi-supervised learning. In *Advances in Neural Information Processing Systems*, pp. 440–448, 2013.

Zihang Meng, Rudrasis Chakraborty, and Vikas Singh. An online riemannian pca for stochastic canonical correlation analysis. *Advances in Neural Information Processing Systems*, 34, 2021.

Ari Morcos, Maithra Raghu, and Samy Bengio. Insights on representational similarity in neural networks with canonical correlation. *Advances in Neural Information Processing Systems*, 31, 2018.

Beresford N Parlett. *The symmetric eigenvalue problem*. SIAM, 1998.

Lucas Parra and Paul Sajda. Blind source separation via generalized eigenvalue decomposition. *The Journal of Machine Learning Research*, 4:1261–1269, 2003.

F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and E. Duchesnay. Scikit-learn: Machine learning in Python. *Journal of Machine Learning Research*, 12:2825–2830, 2011.

David Pfau, Stig Petersen, Ashish Agarwal, David GT Barrett, and Kimberly L Stachenfeld. Spectral inference networks: Unifying deep and spectral learning. In *International Conference on Learning Representations*, 2018.

Maithra Raghu, Justin Gilmer, Jason Yosinski, and Jascha Sohl-Dickstein. SVCCA: Singular vector canonical correlation analysis for deep learning dynamics and interpretability. In *Advances in Neural Information Processing Systems*, pp. 6076–6085, 2017.

C Radhakrishna Rao. The utilization of multiple measurements in problems of biological classification. *Journal of the Royal Statistical Society. Series B (Methodological)*, 10(2):159–203, 1948.

Suhail M Shah. Stochastic approximation on Riemannian manifolds. *Applied Mathematics & Optimization*, pp. 1–29, 2019.

Cees GM Snoek, Marcel Worring, Jan C Van Gemert, Jan-Mark Geusebroek, and Arnold WM Smeulders. The challenge problem for automated detection of 101 semantic concepts in multimedia. In *Proceedings of the 14th ACM international conference on Multimedia*, pp. 421–430, 2006.

Danny C Sorensen. Numerical methods for large eigenvalue problems. *Acta Numerica*, 11:519–584, 2002.

Kimberly L Stachenfeld, Matthew Botvinick, and Samuel J Gershman. Design principles of the hippocampal cognitive map. *Advances in neural information processing systems*, 27, 2014.

Vincent Tan, Nick Firoozye, and Stefan Zohren. Canonical portfolios: Optimal asset and signal combination. *arXiv preprint arXiv:2202.10817*, 2022.

Cheng Tang. Exponentially convergent stochastic k-PCA without variance reduction. In *Advances in Neural Information Processing Systems*, pp. 12393–12404, 2019.

Georgios Tzounas, Ioannis Dassios, Muyang Liu, and Federico Milano. Comparison of numerical methods and open-source libraries for eigenvalue analysis of large-scale power systems. *Applied Sciences*, 10(21):7592, 2020.

Pauli Virtanen, Ralf Gommers, Travis E. Oliphant, Matt Haberland, Tyler Reddy, David Cournapeau, Evgeni Burovski, Pearu Peterson, Warren Weckesser, Jonathan Bright, Stéfan J. van der Walt, Matthew Brett, Joshua Wilson, K. Jarrod Millman, Nikolay Mayorov, Andrew R. J. Nelson, Eric Jones, Robert Kern, Eric Larson, C J Carey, İlhan Polat, Yu Feng, Eric W. Moore, Jake VanderPlas, Denis Laxalde, Josef Perktold, Robert Cimrman, Ian Henriksen, E. A. Quintero, Charles R. Harris, Anne M. Archibald, Antônio H. Ribeiro, Fabian Pedregosa, Paul van Mulbregt, and SciPy 1.0 Contributors. SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python. *Nature Methods*, 17:261–272, 2020. doi: 10.1038/s41592-019-0686-2.

Ulrike Von Luxburg. A tutorial on spectral clustering. *Statistics and Computing*, 17(4):395–416, 2007.

Weiran Wang, Jialei Wang, Dan Garber, and Nati Srebro. Efficient globally convergent stochastic optimization for canonical correlation analysis. *Advances in Neural Information Processing Systems*, 29, 2016.