A GENERALIZED EIGENGAME WITH EXTENSIONS TO DEEP MULTIVIEW REPRESENTATION LEARNING

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ABSTRACT

Generalized Eigenvalue Problems (GEPs) encompass a range of interesting dimensionality reduction methods. Development of efficient stochastic approaches to these problems would allow them to scale to larger datasets. Canonical Correlation Analysis (CCA) is one example of a GEP for dimensionality reduction which has found extensive use in problems with two or more views of the data. Deep learning extensions of CCA require large mini-batch sizes, and therefore large memory consumption, in the stochastic setting to achieve good performance and this has limited its application in practice. Inspired by the Generalized Hebbian Algorithm, we develop an approach to solving stochastic GEPs in which all constraints are softly enforced by Lagrange multipliers. Then by considering the integral of this Lagrangian function, its pseudo-utility, and inspired by recent formulations of Principal Components Analysis and GEPs as games with differentiable utilities, we develop a game-theory inspired approach to solving GEPs. We show that our approaches share much of the theoretical grounding of the previous Hebbian and game theoretic approaches for the linear case but our method permits extension to general function approximators like neural networks for certain GEPs for dimensionality reduction including CCA which means our method can be used for deep multiview representation learning. We demonstrate the effectiveness of our method for solving GEPs in the stochastic setting using canonical multiview datasets and demonstrate state-of-the-art performance for optimizing Deep CCA.

1 INTRODUCTION

A Generalised Eigenvalue Problem (GEP) is defined by two symmetric matrices $A, B \in \mathbb{R}^{d \times d}$. They are usually characterised by the set of solutions to the equation

$$ Aw = \lambda Bw $$

with $\lambda \in \mathbb{R}, w \in \mathbb{R}^d$, called (generalised) eigenvalue and (generalised) eigenvector respectively. Note that by taking $B = I$ we recover the standard eigenvalue problem. We shall only be concerned with the case where $B$ is positive definite to avoid degeneracy; in this case one can find a basis of eigenvectors spanning $\mathbb{R}^d$. Without loss of generality, take $w_1, \ldots, w_d$ such a basis of eigenvectors, with decreasing corresponding eigenvalues $\lambda_1 \geq \cdots \geq \lambda_d$. The following variational characterisation [Stewart & Sun (1990)] provides a useful alternative, iterative definition: $w_k$ solves

$$ \max_{w \in \mathbb{R}^d} w^T Aw \quad \text{subject to} \quad w^T Bw = 1, \ w^T Bw_j = 0 \text{ for } j = 1, \ldots, k - 1. $$

There is also a simpler (non-iterative) variational characterisation for the top-$k$ subspace (that spanned by $\{w_1, \ldots, w_k\}$), namely

$$ \max_{W \in \mathbb{R}^{d \times k}} \text{trace}(W^T AW) \quad \text{subject to} \quad W^T BW = I_k $$

1 or, more generally, Hermitian [Stewart & Sun (1990)]
again see Stewart & Sun (1990), the drawback of this characterisation is it only recovers the subspace and not the individual eigenvectors. We shall see that these two different characterisations lead to different algorithms for the GEP.

Many classical dimensionality reduction methods can be viewed as GEPs including but not limited to Principal Components Analysis (Hotelling, 1933), Partial Least Squares (Haenlein & Kaplan, 2004), Fisher Discriminant Analysis (Mika et al., 1999), and Canonical Correlation Analysis (CCA) (Hotelling, 1992).

Each of the problems above is defined at a population level, using population values of the matrices $A$, $B$, usually functionals of some appropriate covariance matrices. The practical challenge is the sample version: to estimate the population GEP where we only have estimates of $A$, $B$ through some finite number of samples $(z_n)_{n=1}^N$; classically, one just solves the GEP with $A$, $B$ estimated by plugging in the relevant sample covariance matrices.

However for very large datasets, the dimensionality of the associated GEPs makes it memory and compute intensive to compute solutions using existing full-batch algorithms; these are usually variants of the singular value decomposition where successive eigenvalue eigenvector pairs are calculated sequentially by deflation (Mackey, 2008) and so cannot exploit parallelism over the eigenvectors.

This work was motivated in particular by CCA, a classical method for learning representations of data with two or more distinct views: a problem known as multiview (representation) learning. Multiview learning methods are useful for learning representations of data with multiple sets of features, or ‘views’. CCA identifies projections or subspaces in at least two different views that are highly correlated and can be used to generate robust low-dimensional representations for a downstream prediction task, to discover relationships between views, or to generate representations of a view that is missing at test time. CCA has been widely applied across a range of fields such as Neuroimaging (Krishnan et al., 2011), Finance (Cassel et al., 2000), and Imaging Genetics (Hansen et al., 2021).

Deep learning functional forms are often extremely effective for modelling extremely large datasets as they have more expressivity than linear models and scale better than kernel methods. While PCA has found a natural stochastic non-linear extension in the popular autoencoder architecture (Kramer, 1991), applications of Deep CCA (Andrew et al., 2013) have been more limited because estimation of the constraints in the problem outside the full batch setting are more challenging to optimize. In particular, DCCA performs badly when its objective is maximized using stochastic mini-batches. This is unfortunate as DCCA would appear to be well suited to a number of multiview machine learning applications as a number of successful deep multiview machine learning (Suzuki & Matsuo, 2022) and certain self-supervised learning approaches (Zbontar et al., 2021) are designed around similar principals to DCCA; to maximize the consensus between non-linear models of different views (Nguyen & Wang, 2020).

Recently, a number of algorithms have been proposed to approximate GEPs (Arora et al., 2012), and CCA specifically (Bhatia et al., 2018), in the ‘stochastic’ or ‘data-streaming’ setting; these can have big computational savings. Typically, the computational complexity of classical GEP algorithms is $O\left(\left(N+k\right)d^2\right)$; by exploiting parallelism (both between eigenvectors and between samples in a mini-batch), we can reduce this down to $O\left(dk\right)$ (Arora et al., 2016). Stochastic algorithms also introduce a form of regularisation which can be very helpful in these high-dimensional settings.

A key motivation for us was a recent line of work reformulating top-k eigenvalue problems as games (Gemp et al., 2020, 2021), later extended to GEPs in Gemp et al. (2022). We shall refer to these ideas as the ‘Eigengame framework’. Unfortunately, their GEP extension is very complicated, with 3 different hyperparameters; this complication is needed because they constrain their estimates to lie on the unit sphere, which is a natural geometry for the usual eigenvalue problem but not natural for the GEP. By replacing this unit sphere constraint with a Lagrange multiplier penalty, we obtain a much simpler method (GHA-GEP) with only a single hyperparameter; this is a big practical improvement because the convergence of the algorithms is mostly sensitive to step-size (learning rate) parameter (Li & Jordan, 2021), and it allows a practitioner to explore many more learning rates for the same computational budget. We also propose a second class of method ($\delta$-EigenGame) defined

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\[2\text{We need a stronger treatment of this result so give a self contained statement and proof in Proposition C.1 with associated discussion.}\]
via optimising explicit utility functions, rather than being defined via updates, which enjoys the same practical advantages and similar performance. These utilities give unconstrained variational forms for GEPs that we have not seen elsewhere in the literature and may be of independent interest; their key practical advantage is that they only contain linear factors of $A, B$ so we can easily obtain unbiased updates for gradients. The other key advantage of these utility-based methods is that they can easily be extended to use deep learning to solve problems motivated by GEPs. In particular we propose a simple but powerful method for the Deep CCA problem.

1.1 Notation

We have collected here some notational conventions which we think may provide a helpful reference for the reader. We shall always have $A, B \in \mathbb{R}^{d \times d}$. We denote (estimates to or dummy variables for) the $i^{\text{th}}$ generalised eigenvectors by $w_i$; and denote CCA directions $u_i \in \mathbb{R}^p, v_i \in \mathbb{R}^q$. The number of directions we want to estimate will be $k$. For stochastic algorithms, we denote batch-size by $b$. We use $\langle \cdot, \cdot \rangle$ for inner products; implicitly we always take Euclidean inner product over vectors and Frobenius or ‘trace’ inner product for matrices.

2 A Constraint-Free Algorithm for GEPs

Our first proposed method solves the general form of the generalized eigenvalue problem in equation (2) for the top-$k$ eigenvalues and their associated eigenvectors in parallel. We are thus interested in both the top-$k$ subspace problem and the top-$k$ eigenvectors themselves. Our method extends the Generalized Hebbian Algorithm to GEPs, and we thus refer to it as GHA-GEP.

In the full-batch version of our algorithm when $A$ is known to be positive semidefinite, each eigenvector estimate has updates with the form

$$
\Delta_{i}^{\text{GHA-GEP-PSD}} = \text{Reward} \cdot \Delta w_i - \sum_{j \leq i} B \hat{w}_j (\hat{w}_j^T A \hat{w}_i) = \text{Reward} \cdot \Delta w_i - B \hat{w}_i (\hat{w}_i^T A \hat{w}_i) - \sum_{j < i} B \hat{w}_j (\hat{w}_j^T A \hat{w}_i)
$$

$$
= A \hat{w}_i - \sum_{j \leq i} B \hat{w}_j \Gamma_{ij} = A \hat{w}_i - B \hat{w}_i \Gamma_{ii} - \sum_{j < i} B \hat{w}_j \Gamma_{ij}
$$

where $\hat{w}_j$ is our estimator to the eigenvector associated with the $j^{\text{th}}$ largest eigenvalue and in the stochastic setting, we can replace $A$ and $B$ with their unbiased estimates $\hat{A}$ and $\hat{B}$. We will use the notation $\Gamma_{ij} = (\hat{w}_j^T A \hat{w}_i)$ to facilitate comparison with previous work in Appendix [A.3] and recent work in self-supervised learning in Appendix [F].

However, when $A$ has negative eigenvalues, the iteration defined in (4) can ‘blow-up’ from certain initial values. We therefore propose the following modification:

$$
\Delta_{i}^{\text{GHA-GEP}} = A \hat{w}_i - B \hat{w}_i \max(\Gamma_{ii}, 0) - \sum_{j < i} B \hat{w}_j \Gamma_{ij}
$$

Note that this reduces to (4) when $A$ is positive semi-definite. The following proposition, proved in Appendix [B.3] justifies this choice of update.

**Proposition 2.1** (Unique stable stationary point). *Given exact parents and assuming the top-$k$ generalised eigenvalues of $A$ and $B$ are distinct and positive, the only stable stationary point of the iteration defined by (5) is the eigenvector $w_i$ (up to sign).*


2.1 Defining Utilities and Pseudo-Utilities with Lagrangian Functions

Now observe that the updates (4) can be written as the gradients of a Lagrangian pseudo-utility function:

\[
P(U_{i}^{\text{GHA-GEP}}(w_{i}|w_{j<i},\Gamma)) = \frac{1}{2} \hat{w}_{i}^{\top} A \hat{w}_{i} + \frac{1}{2} \Gamma_{ii}(1 - \hat{w}_{i}^{\top} B \hat{w}_{i}) - \sum_{j<i} \Gamma_{ij} \hat{w}_{j}^{\top} B \hat{w}_{i},
\]

(6)

We show how this result is closely related to the pseudo-utility functions in Chen et al. (2019) and suggests an alternative pseudo-utility function for the work in Gemp et al. (2021) in Appendix D.3 which, unlike the original work, does not require stop gradient operators.

If we plug in the relevant \(w_{i}\) and \(w_{j}\) terms into \(\Gamma\), we obtain the following utility function:

\[
U_{i}^{\text{PSD}}(w_{i}; w_{j<i}) = \frac{1}{2} \hat{w}_{i}^{\top} A \hat{w}_{i} + \frac{1}{2} \hat{w}_{i}^{\top} A \hat{w}_{i} (1 - \hat{w}_{i}^{\top} B \hat{w}_{i}) - \sum_{j<i} \hat{w}_{i}^{\top} A \hat{w}_{j} \hat{w}_{j}^{\top} B \hat{w}_{i} = (\hat{w}_{i}^{\top} A \hat{w}_{i}) - \frac{1}{2} ((\hat{w}_{i}^{\top} A \hat{w}_{i})((\hat{w}_{i}^{\top} B \hat{w}_{i}) - \sum_{j<i} ((\hat{w}_{i}^{\top} A \hat{w}_{j})((\hat{w}_{j}^{\top} B \hat{w}_{i})
\]

(7)

Again, we apply a modification to prevent blow-up when \(A\) has negative eigenvalues, giving utility

\[
U_{i}^{\delta}(w_{i}; w_{j<i}) = (\hat{w}_{i}^{\top} A \hat{w}_{i}) - \frac{1}{2} \max(\max(\hat{w}_{i}^{\top} A \hat{w}_{i}), 0) \hat{w}_{i}^{\top} B \hat{w}_{i}) - \sum_{j<i} ((\hat{w}_{i}^{\top} A \hat{w}_{j})((\hat{w}_{j}^{\top} B \hat{w}_{i})
\]

(8)

A remarkable fact is that this utility function actually defines a solution to the GEP problem! We prove the following consistent result in Appendix B.2

**Proposition 2.2** (Unique utility maximiser). Assuming the top-i generalized eigenvalues of the GEP (2) are positive and distinct. Then the unique maximizer of the utility in (8) for exact parents is precisely the \(i\)th eigenvector (up to sign).

This utility function allows us to formalise \(\Delta\)-EigenGame, whose solution corresponds to the top-k solution of equation (4).

**Definition 2.1.** Let \(\Delta\text{-EigenGame}\) be the game with players \(i \in \{1, ..., k\}\), strategy space \(\hat{w}_{i} \in \mathbb{R}^{d}\), where \(d\) is the dimensionality of \(A\) and \(B\), and utilities \(U_{i}^{\delta}\) defined in equation (8).

An immediate corollary of Proposition 2.2 is:

**Corollary 2.1.** The top-k generalized eigenvectors form the unique, strict Nash equilibrium of \(\Delta\)-EigenGame.

Furthermore, the penalty terms in the utility function (6) have a natural interpretation as a projection deflation as shown in appendix D.5

Next note that it is easy to compute the derivative

\[
\Delta^{\delta} = \frac{\partial U_{i}^{\delta}(w_{i}; w_{j<i})}{\partial w_{i}} = 2A \hat{w}_{i} - \{A \hat{w}_{i}((\hat{w}_{i}^{\top} B \hat{w}_{i}) + (\hat{w}_{i}^{\top} A \hat{w}_{i})B \hat{w}_{i})\} - \sum_{j<i} \{A \hat{w}_{j}((\hat{w}_{j}^{\top} B \hat{w}_{i}) + (\hat{w}_{j}^{\top} A \hat{w}_{i})B \hat{w}_{j}\}
\]

(9)

\[
= \Delta_{i}^{\text{GHA-GEP}} + \{A \hat{w}_{i} - \sum_{j<i} A \hat{w}_{j}((\hat{w}_{j}^{\top} B \hat{w}_{i})\}
\]

We can use these gradients as updates step for an alternative algorithm for the GEP which we call \(\delta\)-EigenGame (where, consistent with previous work, we use upper case for the game and lower case for its associated algorithm). We can now discuss stochastic versions of the algorithms introduced above, the setting where our methods excel.

2.2 Stochastic/Data-Streaming versions

This paper is motivated by cases where the algorithm only has access to unbiased sample estimates of \(A\) and \(B\). These estimates, denoted \(\hat{A}\) and \(\hat{B}\), are therefore random variables. A nice property of
both our proposed GHA-GEP and $\delta$-EigenGame is that $A$ and $B$ appear as multiplications in both of their updates (as opposed to as divisors). This means that we can simply substitute them for our unbiased estimates at each iteration. For the GHA-GEP algorithm this gives us updates based on stochastic unbiased estimates of the gradient

$$\hat{\Delta}_i^{\text{GHA-GEP}} = \hat{A}\hat{w}_i - \sum_{j \leq i} \hat{B}\hat{w}_j (\hat{w}_j^T \hat{A}\hat{w}_i).$$

(10)

Which we can use to form algorithm 1.

**Algorithm 1** A Sample Based Generalized Hebbian Algorithm for GEP

**Input:** data stream $Z_t$ consisting of $b$ samples from $z_n$. Learning rate $(\eta_t)_t$. Number of time steps $T$. Number of eigenvectors to compute $k$.

**Initialise:** $(\hat{w}_i)_i^{K_i=1}$ with random uniform entries

**for** $t = 1 \text{ to } T$ **do**

**for** $i = 1 \text{ to } k$ **do**

$\hat{w}_i \leftarrow \hat{w}_i + \eta_t \hat{\Delta}_i^{\text{GHA-GEP}}$ \{As defined in (10)\}

end for

end for

Likewise we can form stochastic updates for $\delta$-EigenGame

$$\Delta_i^\delta = 2\hat{A}\hat{w}_i - \{\hat{A}\hat{w}_i(\hat{w}_i^T \hat{B}\hat{w}_i) + (\hat{w}_i^T \hat{A}\hat{w}_i)\hat{B}\hat{w}_i\} - \sum_{j < i} \{\hat{A}\hat{w}_j(\hat{w}_j^T \hat{B}\hat{w}_i) + (\hat{w}_j^T \hat{A}\hat{w}_i)\hat{B}\hat{w}_j\}.$$  

(11)

Which give us algorithm 2.

**Algorithm 2** A Sample Based $\delta$-EigenGame for GEP

**Input:** data stream $Z_t$ consisting of $b$ samples from $z_n$. Learning rate $(\eta_t)_t$. Number of time steps $T$. Number of eigenvectors to compute $k$.

**Initialise:** $(\hat{w}_i)_i^{K_i=1}$ with random uniform entries

**for** $t = 1 \text{ to } T$ **do**

**for** $i = 1 \text{ to } k$ **do**

$\hat{w}_i \leftarrow \hat{w}_i + \eta_t \Delta_i^\delta$ \{As defined in (11)\}

end for

end for

Furthermore, the simplicity of the form of the updates means that, in contrast to previous work, our updates in the stochastic setting require only one hyperparameter - the learning rate.

2.3 Complexity and Implementation

For the GEPs we are motivated by, and in particular for CCA, $\hat{A}$ and $\hat{B}$ are low rank matrices (specifically, they have at most rank $b$ where $b$ is the mini-batch size). This means that, like previous variants of EigenGame, our algorithm has a per-iteration cost of $O(bdk^2)$. We can similarly leverage parallel computing in both the eigenvectors (players) and data to achieve a theoretical complexity of $O(dk)$.

A particular benefit of our proposed form is that we only require one hyperparameter which makes hyperparameter tuning particularly efficient. This is particularly important as prior work has demonstrated that methods related to the stochastic power method are highly sensitive to the choice of learning rate [Li & Jordan (2021)]. Indeed, by using a decaying learning rate the user can in principle run our algorithm just once to a desired accuracy given their computational budget. This is in contrast to recent work proposing an EigenGame solution to stochastic GEPs [Gemp et al., 2022] which requires three hyperparameters.
3 APPLICATION TO CCA AND EXTENSION TO FOR DEEP CCA

Previous EigenGame approaches have not been extended to include deep learning functions. [Gemp et al. (2020)] noted that the objectives of the players in $\alpha$-EigenGame were all generalized inner products which should extend to general function approximators. However, it was unclear how to translate the constraints in previous EigenGame approaches to the neural network setting. In contrast, we have shown that our work is constraint free but can still be written completely as generalized inner products for certain GEPs and, in particular, dimensionality reduction methods like CCA.

3.1 Canonical Correlation Analysis

Suppose we have vector-valued random variables $X, Y \in \mathbb{R}^p, \mathbb{R}^q$ respectively. Then CCA [Hotelling (1992)] defines a sequence of pairs of ‘canonical directions’ $(u_i, v_i) \in \mathbb{R}^{p+q}$ by the iterative maximisations

$$\max_{u \in \mathbb{R}^p, v \in \mathbb{R}^q} \text{Cov}(u^T X, v^T Y) \quad \text{subject to} \quad \text{Cov}(u^T X) = \text{Cov}(v^T Y) = 1,$$

$$\text{Cov}(u^T X, u_j^T X) = \text{Cov}(v^T Y, v_j^T Y) = 0 \quad \text{for} \quad j < i. \quad (12)$$

Now write $\text{Cov}(X) = \Sigma_{XX}, \text{Cov}(Y) = \Sigma_{YY}, \text{Cov}(X, Y) = \Sigma_{XY}$. It is straightforward to show [Borga (1998)] that CCA corresponds to a GEP with

$$A = \begin{pmatrix} 0 & \Sigma_{XY} \\ \Sigma_{YX} & 0 \end{pmatrix}, \quad B = \begin{pmatrix} \Sigma_{XX} & 0 \\ 0 & \Sigma_{YY} \end{pmatrix}, \quad w = \begin{pmatrix} u \\ v \end{pmatrix}, \quad d = p + q. \quad (13)$$

For the sample version of CCA, suppose we have observations $(x_n, y_n)_{n=1}^{N}$, which have been preprocessed to have mean zero. Then the classical CCA estimator solves the GEV above with covariances replaced by sample covariances [Anderson (2003)]. To define our algorithm in the stochastic case, suppose that at time step $t$ we define $A_t, B_t$ by plugging sample covariances of the mini-batch at time $t$.

3.2 $\delta$-EigenGame for CCA

We defined CCA by maximising correlation between linear functionals of the two views of data; we can extend this to DCCA by instead considering non-linear functionals defined by deep neural networks. Consider neural networks $f, g$ which respectively map $X$ and $Y$ to a $d$ dimensional subspace. We will refer to the $k$th dimension of these subspaces using $f_k(X)$ and $g_k(X)$ where $f(X) = [f_1(X), \ldots, f_d(X)]$ and $g(X) = [g_1(X), \ldots, g_d(X)]$. Deep CCA finds $f$ and $g$ which maximize $\text{Corr}(f_i(X), g_i(Y))$ subject to orthogonality constraints.

To motivate an algorithm, note that (8) is just a function of the inner products

$$\langle \hat{w}_i, A \hat{w}_j \rangle = \text{Cov}(u_i^T X, v_j^T Y) + \text{Cov}(v_i^T Y, u_j^T X)$$

$$\langle \hat{w}_i, B \hat{w}_j \rangle = \text{Cov}(u_i^T X, u_j^T X) + \text{Cov}(v_i^T Y, v_j^T Y)$$

So replacing $u_i^T X$ with $f_i(X)$ and $v_i^T Y$ with $g_i(Y)$, and using the short-hand

$$\tilde{A}_{ij} = \text{Cov}(f_i(X), g_j(Y)) + \text{Cov}(g_i(Y), f_j(X)) \quad (14)$$

$$\tilde{B}_{ij} = \text{Cov}(f_i(X), f_j(X)) + \text{Cov}(g_i(Y), g_j(Y)) \quad (15)$$

we obtain the objective

$$U_t^\alpha(f_i, g_i | f_j < i, g_j < i) = 2\tilde{A}_{ii} - \tilde{A}_{ii} \tilde{B}_{ii} - 2 \sum_{j < i} \tilde{A}_{ij} \tilde{B}_{ij} \quad (16)$$
Next observe by symmetry of matrices \( \mathbf{A}, \mathbf{B} \) that if we sum the first \( k \) utilities we obtain

\[
U^\text{sum}_k = \sum_{i=1}^{k} U^g_i = \sum_{i=1}^{k} 2\mathbf{A}_{ii} - \sum_{i,j=1}^{k} \mathbf{A}_{ij}\mathbf{B}_{ij} - 2 \sum_{i=1}^{k} \sum_{i<j}^{k} \mathbf{A}_{ij}\mathbf{B}_{ij}
\]

\[
= 2 \text{trace}(\mathbf{A}) - \sum_{i,j=1}^{k} \mathbf{A}_{ij}\mathbf{B}_{ij}
\]

\[
= 2 \text{trace}(\mathbf{A}) - \text{trace}(\mathbf{A}\mathbf{B}^T) = \text{trace}\left(\mathbf{A}(2I_k - \mathbf{B})\right) \tag{17}
\]

The key strength of this covariance based formulation is that we can obtain a full-batch algorithm by simply plugging in the sample covariance over the full batch; and obtain a mini-batch update by plugging in sample covariances on the mini-batch. We define DCCA-EigenGame in algorithm 3, where we slightly abuse notation: we write mini-batches in matrix form \( X_t \in \mathbb{R}^{b \times p}, Y_t \in \mathbb{R}^{b \times q} \) and use short hand \( f(X_t), f(Y_t) \) to denote applying \( f, g \) to each sample in the mini-batch.

**Algorithm 3 DCCA EigenGame**

**Input:** Stream of data with mini-batch size \( b \) (\( X_t \in \mathbb{R}^{b \times p}, Y_t \in \mathbb{R}^{b \times q} \)), neural networks \( f(X), g(Y) \) parameterized by \( \hat{\theta} \) and \( \hat{\psi} \), learning rate \( \eta \)

**for** \( t = 1 \) to \( T \) **do**

- Construct unbiased estimates \( \hat{\mathbf{A}} \) and \( \hat{\mathbf{B}} \) from \( f(X_t) \) and \( g(Y_t) \)
- \( U \leftarrow \text{trace}\left(\hat{\mathbf{A}}(2I_k - \hat{\mathbf{B}})\right)\)
- \( \nabla_f \leftarrow \frac{\partial U}{\partial f}, \nabla_g \leftarrow \frac{\partial U}{\partial g} \)
- \( \hat{\theta}_{t+1} \leftarrow \hat{\theta}_t + \eta \nabla_f, \hat{\psi}_{t+1} \leftarrow \hat{\psi}_t + \eta \nabla_g \)

**end for**

We have motivated a loss function for SGD by a heuristic argument. We now give a theoretical result justifying the choice. Recall the top-\( k \) variational characterisation of the GEP in (3) was hard to use in practice because of the constraints; we can use this to prove that the form above characterises the GEP.

**Proposition 3.1** (Subspace characterisation). Let \( \mathbf{A} \) be positive semi-definite. Then the top-\( k \) subspace for the GEP (1) can be characterised by

\[
\max_{\mathbf{W} \in \mathbb{R}^{d \times k}} \text{trace}\left(\mathbf{W}^T \mathbf{A} \mathbf{W}(2I_k - \mathbf{W}^T \mathbf{B} \mathbf{W})\right) \tag{18}
\]

We prove this result in Appendix C. We also provide an alternative derivation of the utility of (17) from the paper of Wang et al. (2015c) in Appendix D.1.

## 4 Related Work

In particular we note the contemporaneous work in Gemp et al. (2022), termed \( \gamma \)-EigenGame, which directly addresses the stochastic GEP setting we have described in this work using an EigenGame-inspired approach. Since their method was designed around the Rayleigh quotient form of GEPs, it takes a different and more complicated form and requires additional hyperparameters in order to remove bias from the updates in the stochastic setting due to their proposed utility function containing random variables in denominator terms. It also isn’t clear that their updates are the gradients of a utility function. Meng et al. (2021) developed an algorithm, termed RSG+, for streaming CCA which stochastically approximates the principal components of each view in order to approximate the top-k CCA problem, in effect transforming the data so that \( B = I \) to simplify the problem. Arora et al. (2017) developed a Matrix Stochastic Gradient method for finding the top-k CCA subspace. However, the efficiency of this method depends on mini-batch samples of 1 and scales poorly to larger mini-batch sizes. While there have also been a number of approaches to the top-1 CCA problem (Li & Jordan, 2021; Bhatia et al., 2018), the closest methods in motivation and performance to our work on the linear problem are \( \gamma \)-EigenGame, SGHA, and RSG+. 7
The original DCCA (Andrew et al., 2013) was defined by the objective

\[
\max \text{tracenorm}(\hat{\Sigma}^{-1/2}_X \hat{\Sigma}^{-1/2}_{XY} \hat{\Sigma}^{-1/2}_Y)
\]  

and demonstrated strong performance in multiview learning tasks when optimized with the full batch L-BFGS optimizer (Liu & Nocedal, 1989). However when the objective is evaluated for small mini-batches, the whitening matrices \(\hat{\Sigma}^{-1/2}_X\) and \(\hat{\Sigma}^{-1/2}_Y\) are likely to be ill-conditioned, causing gradient estimation to be biased.

Wang et al. (2015b) observed that despite the biased gradients, the original DCCA objective could still be used in the stochastic setting for large enough mini-batches, a method referred to in the literature as stochastic optimization with large mini-batches (DCCA-STOL). Wang et al. (2015c) developed a method which adaptively approximated the covariance of the embedding for each view in order to whiten the targets of a regression in each view. This mean square error type loss can then be decoupled across samples in a method called non-linear orthogonal iterations (DCCA-NOI). To the best of our knowledge this method is the current state-of-the-art for DCCA optimisation using stochastic mini-batches.

5 EXPERIMENTS

In this section we replicate experiments from recent work on stochastic CCA and Deep CCA in order to demonstrate the accuracy and efficiency of our method.

5.1 STOCHASTIC SOLUTIONS TO CCA

In this section we compare GHA-GEP and \(\delta\)-EigenGame to previous methods for approximating CCA in the stochastic setting. We optimize for the top-8 eigenvectors for the MediaMill, Split MNIST and Split CIFAR datasets, replicating Gemp et al. (2022); Meng et al. (2021) with double the number of components and mini-batch size 128 and comparing our method to theirs. We use the Scipy (Virtanen et al., 2020) package to solve the population GEPs as a ground truth value and use the proportion of correlation captured (PCC) captured by the learnt subspace as compared to this population ground truth (defined in Appendix G.2).

Figure 1 shows that for all three datasets, both GHA-GEP and \(\delta\)-EigenGame exhibit faster convergence on both a per-iteration basis compared to prior work and likewise in terms of runtime in figure 2. They also demonstrate comparable or higher PCC at convergence. In these experiments \(\delta\)-EigenGame was found to outperform GHA-GEP. These results were broadly consistent across mini-batch sizes from 32 to 128 which we demonstrate in further experiments in Appendix H.1.

The strong performance of GHA-GEP and \(\delta\)-EigenGame is likely to be because their updates adaptively weight the objective and constraints of the problem and are not constrained arbitrarily to the unit sphere. We further explore the shape of the utility function in Appendix D.3.

5.2 STOCHASTIC SOLUTIONS TO DEEP CCA

In this section we compare DCCA-EigenGame and DCCA-SGHA to previous methods for optimizing DCCA in the stochastic setting. We replicated an experiment from Wang et al. (2015c) and compare our proposed methods to DCCA-NOI and DCCA-STOL. Like previous work, we use the total correlation captured (TCC) of the learnt subspace as a metric (defined in Appendix G.1).

In all three datasets, figure 3 shows that DCCA-EigenGame finds higher correlations in the validation data than all methods except DCCA-STOL with \(n = 500\) with typically faster convergence in early iterations compared to DCCA-NOI.

6 CONCLUSION

We have presented two novel algorithms for optimizing stochastic GEPs. The first, GHA-GEP was based on extending the popular GHA and we showed how it could be understood as optimising
Figure 1: CCA with stochastic mini-batches: proportion of correlation captured with respect to Scipy ground truth by GHA-GEP and $\delta$-EigenGame vs prior work. The maximum value is 1.

Figure 2: CCA with stochastic mini-batches: proportion of correlation captured with respect to Scipy ground truth by GHA-GEP and $\delta$-EigenGame vs prior work. The maximum value is 1.

Figure 3: Total correlation captured by the 50 latent dimensions in the validation data. The maximum value is 50. The top row shows results for mini-batch size 20 and the bottom row shows results for mini-batch size 100.
a Lagrangian pseudo-utility function. The second, δ-EigenGame, was developed by swapping the Lagrange multipliers to give a proper utility function which allowed us to define the solution of a GEP with Δ-EigenGame. Our proposed methods have simple and elegant forms and require only one choice of hyperparameter, making them extremely practical and both demonstrated comparable or better runtime and performance as compared to prior work.

We also showed how this approach can also be used to optimize Deep CCA and demonstrated state-of-the-art performance when using stochastic mini-batches. We believe that this will allow researchers to apply DCCA to a much wider range of problems.

In future work, we will apply δ-EigenGame to other practically interesting GEPs like Generalized CCA for more than two views and Fisher Discriminant Analysis. We will also explore the extensions of other GEPs to the deep learning case in order to build principled deep representations.

REFERENCES

T. W. Anderson. An introduction to multivariate statistical analysis. Wiley series in probability and statistics, Wiley-Interscience, Hoboken, N.J, 3rd ed edition, 2003. ISBN 978-0-471-36091-9.

Galen Andrew, Raman Arora, Jeff Bilmes, and Karen Livescu. Deep canonical correlation analysis. In International conference on machine learning, pp. 1247–1255. PMLR, 2013.

Raman Arora, Andrew Cotter, Karen Livescu, and Nathan Srebro. Stochastic optimization for pca and pls. In 2012 50th Annual Allerton Conference on Communication, Control, and Computing (Allerton), pp. 861–868. IEEE, 2012.

Raman Arora, Poorya Mianjy, and Teodor Marinov. Stochastic optimization for multiview representation learning using partial least squares. In International Conference on Machine Learning, pp. 1786–1794. PMLR, 2016.

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

Igor Babuschkin, Kate Baumli, Alison Bell, Surya Bhatpatiraju, Jake Bruce, Peter Buchlovsky, David Budden, Trevor Cai, Aidan Clark, Ivo Danihelka, Claudio Fantacci, Jonathan Godwin, Chris Jones, Tom Hennigan, Matteo Hessel, Steven Kapturowski, Thomas Keck, Iurii Kemaev, Michael King, Lena Martens, Vladimir Mikulik, Tamara Norman, John Quan, George Papanikolas, Roman Ring, Francisco Ruiz, Alvaro Sanchez, Rosalia Schneider, Eren Sezener, Stephen Spencer, Srivatsan Srinivasan, Wojciech Stokowiec, and Fabio Viola. The DeepMind JAX Ecosystem, 2020. URL http://github.com/deepmind.

Randall Balestriero and Yann LeCun. Contrastive and non-contrastive self-supervised learning recover global and local spectral embedding methods. arXiv preprint arXiv:2205.11508, 2022.

Adrien Bardes, Jean Ponce, and Yann LeCun. Vicreg: Variance-invariance-covariance regularization for self-supervised learning. arXiv preprint arXiv:2105.04906, 2021.

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.

Lukas Biewald. Experiment tracking with weights and biases, 2020. URL https://www.wandb.com/ Software available from wandb.com.

Magnus Borga. Learning Multidimensional Signal Processing. PhD thesis, 1998. URL http://urn.kb.se/resolve?urn=urn:nbn:se:liu:diva-54341 Publisher: Linköping University Electronic Press.

Vivek S. Borkar. Stochastic approximation: a dynamical systems viewpoint / Vivek S. Borkar. Cambridge University Press ; Hindustan Book Agency, Cambridge : New Delhi, 2008. ISBN 978-0-521-51592-4.
Marcus Carlsson. von Neumann’s trace inequality for Hilbert–Schmidt operators. *Expositiones Mathematicae*, 39(1):149–157, March 2021. ISSN 0723-0869. doi: 10.1016/j.exmath.2020.05.001. URL https://www.sciencedirect.com/science/article/pii/S0723086920300220.

Claes M Cassel, Peter Hackl, and Anders H Westlund. On measurement of intangible assets: a study of robustness of partial least squares. *Total Quality Management*, 11(7):897–907, 2000.

Zhehui Chen, Xingguo Li, Lin Yang, Jarvis Haupt, and Tuo Zhao. On constrained nonconvex stochastic optimization: A case study for generalized eigenvalue decomposition. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pp. 916–925. PMLR, 2019.

Ian Gemp, Brian McWilliams, Claire Vernade, and Thore Graepel. Eigengame unloaded: When playing games is better than optimizing, 2021.

Ian Gemp, Charlie Chen, and Brian McWilliams. The generalized eigenvalue problem as a nash equilibrium. *arXiv preprint arXiv:2206.04993*, 2022.

Ian M. Gemp, Brian McWilliams, Claire Vernade, and Thore Graepel. Eigengame: PCA as a nash equilibrium. *CoRR*, abs/2010.00554, 2020. URL https://arxiv.org/abs/2010.00554.

Benyamin Ghojogh, Fakhri Karray, and Mark Crowley. Eigenvalue and Generalized Eigenvalue Problems: Tutorial, May 2022. URL http://arxiv.org/abs/1903.11240. arXiv:1903.11240 [cs, stat].

Willem H. Haemers. Interlacing eigenvalues and graphs. *Linear Algebra and its Applications*, 226-228:593–616, September 1995. ISSN 00243795. doi: 10.1016/0024-3795(95)00199-2. URL https://linkinghub.elsevier.com/retrieve/pii/0024379595001992.

Michael Haenlein and Andreas M Kaplan. A beginner’s guide to partial least squares analysis. *Understanding statistics*, 3(4):283–297, 2004.

Justine Hansen, Ross Markello, Jacob Vogel, Jakob Seidlitz, Danilo Bzdok, and Bratislav Misić. Mapping gene transcription and neurocognition across human neocortex. *Nature Human Behaviour*, 5:1–11, 09 2021. doi: 10.1038/s41562-021-01082-z.

Roger A. Horn and Charles R. Johnson. *Matrix Analysis*. Cambridge University Press, Cambridge, 1985. doi: 10.1017/CBO9780511810817. URL https://www.cambridge.org/core/books/matrix-analysis/9CF2CB491C9E97948B15FAD835EF9A3B.

Harold Hotelling. Analysis of a complex of statistical variables into principal components. *Journal of educational psychology*, 24(6):417, 1933.

Harold Hotelling. Relations between two sets of variates. In *Breakthroughs in statistics*, pp. 162–190. Springer, 1992.

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

Mark A Kramer. Nonlinear principal component analysis using autoassociative neural networks. *AIChE journal*, 37(2):233–243, 1991.

Anjali Krishnan, Lynne Williams, Anthony McIntosh, and Hervé Abdi. Partial least squares (pls) methods for neuroimaging: A tutorial and review. *NeuroImage*, 56:455–75, 05 2011. doi: 10.1016/j.neuroimage.2010.07.034.

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

Harold J. Kushner, George Yin, and Harold J. Kushner. *Stochastic approximation and recursive algorithms and applications*. Number 35 in Applications of mathematics. Springer, New York, 2003. ISBN 978-0-387-00894-3.
Yann LeCun, Corinna Cortes, and Chris Burges. Mnist handwritten digit database, 2010.

Chris Junchi Li and Michael I Jordan. Nonconvex stochastic scaled-gradient descent and generalized eigenvector problems. arXiv preprint arXiv:2112.14738, 2021.

Dong C Liu and Jorge Nocedal. On the limited memory bfgs method for large scale optimization. Mathematical programming, 45(1):503–528, 1989.

Lester Mackey. Deflation methods for sparse pca. Advances in neural information processing systems, 21, 2008.

Zihang Meng, Rudrasis Chakraborty, and Vikas Singh. An online riemannian pca for stochastic canonical correlation analysis. Advances in Neural Information Processing Systems, 34:14056–14068, 2021.

Sebastian Mika, Gunnar Ratsch, Jason Weston, Bernhard Scholkopf, and Klaus-Robert Mullers. Fisher discriminant analysis with kernels. In Neural networks for signal processing IX: Proceedings of the 1999 IEEE signal processing society workshop (cat. no. 98th8468), pp. 41–48. Ieee, 1999.

Nam D Nguyen and Daifeng Wang. Multiview learning for understanding functional multiomics. PLoS computational biology, 16(4):e1007677, 2020.

Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, Alban Desmaison, Andreas Kopf, Edward Yang, Zachary DeVito, Martin Raison, Alykhan Tejani, Sasank Chilamkurthy, Benoit Steiner, Lu Fang, Junjie Bai, and Soumith Chintala. Pytorch: An imperative style, high-performance deep learning library. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d’Alché-Buc, E. Fox, and R. Garnett (eds.), Advances in Neural Information Processing Systems 32, pp. 8024–8035. Curran Associates, Inc., 2019.

Ahmed H. Sameh and John A. Wisniewski. A Trace Minimization Algorithm for the Generalized Eigenvalue Problem. SIAM Journal on Numerical Analysis, 19(6):1243–1259, 1982. ISSN 0036-1429. URL https://www.jstor.org/stable/2157207. Publisher: Society for Industrial and Applied Mathematics.

Terence D Sanger. Optimal unsupervised learning in a single-layer linear feedforward neural network. Neural networks, 2(6):459–473, 1989.

Suhail M. Shah. Stochastic Approximation on Riemannian manifolds, November 2017. URL http://arxiv.org/abs/1711.10754 arXiv:1711.10754 [math].

G. W. Stewart and Ji-Guang Sun. Matrix Perturbation Theory. ACADEMIC PressINC, July 1990. ISBN 978-1-4933-0199-7. Google-Books-ID: biYEogEACAAJ.

Masahiro Suzuki and Yutaka Matsuo. A survey of multimodal deep generative models. Advanced Robotics, 36(5-6):261–278, feb 2022. doi: 10.1080/01691864.2022.2035253. URL https://doi.org/10.1080%2F01691864.2022.2035253.

Terry Tao. 254A, Notes 3a: Eigenvalues and sums of Hermitian matrices, January 2010. URL https://terrytao.wordpress.com/2010/01/12/254a-notes-3a-eigenvalues-and-sums-of-hermitian-matrices/.

Pauli Virtanen, Ralf Gommers, Travis E Oliphant, Matt Haberland, Tyler Reddy, David Cournapeau, Evgeni Burovski, Pearu Peterson, Warren Weckesser, Jonathan Bright, et al. Scipy 1.0: fundamental algorithms for scientific computing in python. Nature methods, 17(3):261–272, 2020.

Weiran Wang, Raman Arora, Karen Livescu, and Jeff Bilmes. On deep multi-view representation learning. In International conference on machine learning, pp. 1083–1092. PMLR, 2015a.

Weiran Wang, Raman Arora, Karen Livescu, and Jeff A Bilmes. Unsupervised learning of acoustic features via deep canonical correlation analysis. In 2015 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), pp. 4590–4594. IEEE, 2015b.
Weiran Wang, Raman Arora, Karen Livescu, and Nathan Srebro. Stochastic optimization for deep cca via nonlinear orthogonal iterations. In 2015 53rd Annual Allerton Conference on Communication, Control, and Computing (Allerton), pp. 688–695. IEEE, 2015c.

Svante Wold, Arnold Ruhe, Herman Wold, and WJ Dunn, Iii. The collinearity problem in linear regression. the partial least squares (pls) approach to generalized inverses. SIAM Journal on Scientific and Statistical Computing, 5(3):735–743, 1984.

Jure Zbontar, Li Jing, Ishan Misra, Yann LeCun, and Stéphane Deny. Barlow twins: Self-supervised learning via redundancy reduction. arXiv preprint arXiv:2103.03230, 2021.

A COMPARISON TO PREVIOUS WORK

A.1 GENERALIZED HEBBIAN ALGORITHM

Our update is closely related to the Generalized Hebbian Algorithm (GHA) (Sanger, 1989) for solving the PCA problem with updates:

\[
\Delta_{\text{GHA}}^i = A\hat{w}_i - \sum_{j \leq i} \hat{w}_j (\hat{w}_j^T A\hat{w}_i) = A\hat{w}_i - \sum_{j \leq i} \hat{w}_j \Gamma_{ij}
\]

which was originally designed to be solved sequentially rather than in parallel. Note that for GEPs where \(B = I_d\) like PCA, our proposed method collapses exactly to GHA.

A.2 STOCHASTIC GENERALIZED HEBBIAN ALGORITHM

To understand how our method extends GHA to generalized eigenvalue problems we consider the Stochastic Generalized Hebbian Algorithm (SGHA) (Chen et al., 2019). SGHA is derived from the min-max Lagrangian form of (3):

\[
\begin{align*}
\min_{W \in \mathbb{R}^{d \times k}} \max_{\Gamma \in \mathbb{R}^{k \times k}} & \quad \mathcal{L}(W, \Gamma) = -\text{tr} (W^T AW) + \langle \Gamma, W^T BW - I_k \rangle \\
\end{align*}
\]

Where \(W\) is a matrix that captures the top-k subspace (but not necessarily the top-k eigenvectors) and \(\Gamma\) is a Lagrange multiplier that enforces the constraint in (2) along with the \(B\)-orthogonality of each eigenvector. By solving for the KKT conditions of equation (21), we have \(\Gamma = (W^T AW)\) and the authors propose to combine the primal and dual updates into a single step to give symmetrical updates for each eigenvector:

\[
\Delta_{\text{SGHA}}^i = A\hat{w}_i - \sum_{j} B\hat{w}_j (\hat{w}_j^T A\hat{w}_i) = A\hat{w}_i - \sum_{j} B\hat{w}_j \Gamma_{ij}
\]

Where we highlight in red the key difference between our method and SGHA: that there is no hierarchy imposed on eigenvectors, so method can only recover top-k subspace; this is in contrast to our proposal, all eigengame methods, and indeed the original GHA method. As noted by Gemp et al. (2020), imposing a hierarchy often appears to improve the stability of the algorithm in experiments and has the additional benefit of returning ordered eigenvectors.

A.3 \(\mu\)-EIGENGAME

Finally, our method is closely related to \(\mu\)-EigenGame (Gemp et al., 2021) - though this is only defined for the \(B = I_d\) case. Their method restricts estimates to lie on the unit sphere, using

\[\text{Though the authors called this SGHA, it is rather different to the original proposal, because it is a subspace method rather than an iterative one}\]
Riemannian optimization tools to update in directions defined by
\[
\Delta_i^\mu = A\hat{w}_i - \sum_{j<i} \hat{w}_j (\hat{w}_j^T A\hat{w}_i) = A\hat{w}_i - \sum_{j<i} \hat{w}_j \Gamma_{ij}
\] (23)
where we again highlight in red the difference compared to our proposal: \(\mu\)-EigenGame however does not have the \(j = i\) term in its penalty (and therefore does not use the \(\Gamma_{ii}\) Lagrange multipliers associated with the unit variance constraint \(\hat{w}_i^T \hat{w}_i = 1\)).

B PROOFS AND FURTHER ANALYSIS FOR SEQUENTIAL ALGORITHMS

B.1 NEW NOTATION

For the rest of this section we will find it convenient to introduce some new notation. Firstly, we change notation from the main text and index the normalised solutions to the GEV with superscripts:
\[
\langle w^{(i)}, Bw^{(i)} \rangle = 1, \quad \langle w^{(i)}, Aw^{(i)} \rangle = \lambda^{(i)} \forall i,
\]
while we continue to index our estimates with subscripts. We can write our estimates in this basis to define the coefficients \(\hat{w}_i = \sum_p \nu_i^{(p)} w^{(p)}\). First note this gives
\[
\langle \hat{w}_i, Aw^{(j)} \rangle = \lambda^{(j)} \nu_i^{(j)} \quad \langle \hat{w}_i, Bw^{(j)} \rangle = \nu_i^{(j)}
\]
It is also convenient to write the matrix \(\Lambda = \text{diag}(\lambda^{(p)})\) and the vector \(\nu_i = (\nu_i^{(p)})_{p=1}^d\). We then get the following nice identities:
\[
\langle \hat{w}_i, A\hat{w}_j \rangle = \sum_p \lambda^{(p)} \nu_i^{(p)} \nu_j^{(p)} = \nu_i^T \Lambda \nu_j
\]
\[
\langle \hat{w}_i, B\hat{w}_j \rangle = \sum_p \nu_i^{(p)} \nu_j^{(p)} = \nu_i^T \nu_j
\]
Next define
\[
m_i = ||\nu_i||^2_2 = \sum_p (\nu_i^{(p)})^2
\]
\[
z_i^{(j)} = (\nu_i^{(j)})^2 / m_i = (\nu_i^{(j)})^2 / \sum_p (\nu_i^{(p)})^2
\]
\[
\bar{\lambda}_i = \sum_j z_i^{(j)} \lambda^{(j)} = \nu_i^T \Lambda \nu_i / m_i
\]
so that the vector \(z_i = (z_i^{(j)})_j\) takes values in the simplex. We can think of \(m_i\) as a magnitude, \(z_i\) as a direction, and \(\bar{\lambda}_i\) as an appropriate ‘average’ value of \(\lambda\). We will see that the utility functions and dynamics analysed below often decompose nicely as functions of these quantities.

B.2 \(\Delta\)-EIGENGAME THEORY

We recall proposition 2.2.

**Proposition 2.2 (Unique utility maximiser).** Assuming the top-\(i\) generalized eigenvalues of the GEP (2) are positive and distinct. Then the unique maximizer of the utility in (8) for exact parents is precisely the \(i^{th}\) eigenvector (up to sign).

**Proof of special case, where A is positive semi-definite.** Since A is positive semi-definite, (7) reduces to (8).
First note that using the notation in Section B.1
\[
\langle \hat{w}_i, A\hat{w}_i \rangle = m_i \bar{\lambda}_i = m_i \sum_j z_i^{(j)} \lambda^{(j)}
\]
\[
\langle \hat{w}_i, B\hat{w}_i \rangle = \nu_i^T \nu_i = m_i
\]
while with exact parents \( \hat{w}_j = w^{(j)} \) for \( j < i \) we get
\[
\langle \hat{w}_i, B\hat{w}_j \rangle \langle \hat{w}_j, A\hat{w}_i \rangle = \lambda^{(j)} (\nu_i^j)^2 = m_i \lambda^{(j)} z_i^{(j)}
\]
Thus we can simplify the utility function for player \( i \) to:
\[
u_i (\hat{w}_i | \hat{w}_{j<i}) = 2 \langle \hat{w}_i, A\hat{w}_i \rangle - 2 \sum_{j<i} \langle \hat{w}_i, B\hat{w}_j \rangle \langle \hat{w}_j, A\hat{w}_i \rangle - \langle \hat{w}_i, B\hat{w}_i \rangle \langle \hat{w}_i, A\hat{w}_i \rangle
\]
\[
= 2 \sum_j m_i \lambda^{(j)} z_i^{(j)} - 2 \sum_{j<i} m_i \lambda^{(j)} z_i^{(j)} - m_i \left( \sum_j m_i \lambda^{(j)} z_i^{(j)} \right)
\]
\[
= 2 \sum_{j \geq i} m_i \lambda^{(j)} z_i^{(j)} - \sum_j m_i^2 \lambda^{(j)} z_i^{(j)}
\]
\[
= (2m_i - m_i^2) \sum_{j \geq i} \lambda^{(j)} z_i^{(j)} - m_i^2 \sum_{j<i} \lambda^{(j)} z_i^{(j)}
\]
We claim this is maximized precisely when \( m_i = 1 \) \( z_i^{(j)} = \delta_{ij} \); this corresponds to \( \nu_i^{(i)} = \pm 1 \) and \( \nu_i^{(j)} = 0 \) for \( j \neq i \) and so indeed \( \hat{w}_i = \pm w^{(i)} \). To prove the claim we have to consider two cases:

- \( m_i \in [0, 2] \) case: then \( 2m_i - m_i^2 > 0 \). The objective is just a linear function of \( z_i \), with maximal coefficient \( (2m_i - m_i^2) \lambda^{(i)} > 0 \), so is maximised by taking \( z_i^{(j)} = \delta_{ij} \). The utility then reduces to \( (2m_i - m_i^2) \lambda^{(i)} \) so is maximised by taking \( m_i = 1 \), giving maximal value of \( \lambda^{(i)} \) (assumed strictly positive). Note that this argument still holds even if some of the later \( \lambda^{(j)} \)'s are negative (recall the first \( i \) eigenvalues were assumed positive).

- \( m_i > 2 \) case: now \( 2m_i - m_i^2 < 0 \) so the coefficients of \( z_i^{(j)} \) are all negative. The utility is therefore also negative.

So the maximum is attained in the case \( m_i \in [0, 2] \), as required. \( \square \)

**Proof of general case, where \( A \) may have negative eigenvalues.** Instead of (24) we now have
\[
u_i (\hat{w}_i | \hat{w}_{j<i}) = 2 \sum_{j \geq i} m_i \lambda^{(j)} z_i^{(j)} - m_i \max \left( \sum_j m_i \lambda^{(j)} z_i^{(j)}, 0 \right)
\]
Note the term inside the maximum function is just \( \bar{\lambda}_i m_i \), so has the same sign as \( \bar{\lambda}_i \). When this is positive, we just recover the previous expression for utility. We can therefore write
\[
u_i (\hat{w}_i | \hat{w}_{j<i}) = \mathbb{1}_{\{\bar{\lambda}_i > 0\}} \left[ (2m_i - m_i^2) \sum_{j \geq i} \lambda^{(j)} z_i^{(j)} - m_i^2 \sum_{j<i} \lambda^{(j)} z_i^{(j)} \right] + \mathbb{1}_{\{\bar{\lambda}_i \leq 0\}} \left[ 2m_i \sum_{j \geq i} \lambda^{(j)} z_i^{(j)} \right]
\]
So to handle negative eigenvalues, we require this further split of our optimisation region (now by the values of \( z_i \), which determine \( \bar{\lambda}_i \), rather than of \( m_i \)).

- \( \bar{\lambda}_i > 0 \) case: the objective reduces to the objective of the previous case. Our analysis of the case \( m_i \in [0, 2] \) goes through unchanged (by previous remark) and the previous maximiser \( m_i = 1, z_i^{(j)} = \delta_{ij} \) does satisfy \( \bar{\lambda}_i = \lambda^{(i)} > 0 \).
In the case where \( m_i > 2 \), more care is needed. The key observation is that \(-m_i^2 < 2m_i - m_i^2\). Hence we again have
\[
u_i(\hat{w}_i | \hat{w}_{j < i}) = (2m_i - m_i^2) \sum_{j \geq i} \lambda^{(j)} z_i^{(j)} - m_i^2 \sum_{j < i} \lambda^{(j)} z_i^{(j)}
\]
\[
\leq (2m_i - m_i^2) \sum_{j} \lambda^{(j)} z_i^{(j)}
\]
\[
= (2m_i - m_i^2) \bar{\lambda}_i \leq 0
\]
so we see the maximiser in this combined case is as claimed.

• \( \bar{\lambda}_i \leq 0 \) case: again we show the utility is negative in this regime. Again we use \( \bar{\lambda}_i = \sum_{j} \lambda^{(j)} z_i^{(j)} \). Now, because we assumed the first \( i \) eigenvalues were positive, we see
\[
\sum_{j \geq i} \lambda^{(j)} z_i^{(j)} = \bar{\lambda}_i - \sum_{j < i} \lambda^{(j)} z_i^{(j)} \leq \bar{\lambda}_i \leq 0
\]
so the utility \( 2m_i \sum_{j \geq i} \lambda^{(j)} z_i^{(j)} \leq 0 \) also.

Again, combining the cases we see the maximum value is \( \lambda^{(i)} \), and is attained precisely when \( m_i = 1 \) \( z_i^{(j)} = \delta_{ij} \).

\[\Box\]

Note that in the previous lemma, the utility function took a simple form when we chose the true generalised eigenvectors as a basis; indeed, when using coefficients with respect to the basis, the utility only depended on the generalised eigenvalues and not the basis itself. This simple form shows how our utility interacts naturally with the geometry of the GEV problem. We will now analyse the corresponding simple form of the update steps.

### B.3 GHA-GEP Theory

We recall proposition 2.1

**Proposition 2.1** (Unique stable stationary point). Given exact parents and assuming the top-\( k \) generalised eigenvalues of \( A \) and \( B \) are distinct and positive, the only stable stationary point of the iteration defined by (5) is the eigenvector \( w_i \) (up to sign).

**Proof in the special case where \( A \) is positive definite.** Again we use the notation of Section B.1. By positive definiteness the update (5) reduces to (4). So we get
\[
\Delta_i = A \hat{w}_i - B \hat{w}_i (\hat{w}_i^T A \hat{w}_i) - \sum_{j < i} B \hat{w}_j (\hat{w}_j^T A \hat{w}_i)
\]
\[
= A \hat{w}_i - \sum_{j \leq i} B \hat{w}_j (\hat{w}_j^T A \hat{w}_i)
\]
\[
= \sum_p \lambda^{(p)} \nu_i^{(p)} B w^{(p)} - \sum_{j \leq i} \left( \sum_p \nu_j^{(p)} B w^{(p)} \right) (\nu_i^T A \nu_j)
\]
\[
= \sum_p B w^{(p)} \left\{ \lambda^{(p)} \nu_i^{(p)} - \sum_{j \leq i} \nu_j^{(p)} (\nu_i^T A \nu_j) \right\}
\]

Now by orthonormality of the \( w^{(p)} \), we can equate coefficients and combine to vector form to obtain the update step for the coefficient vectors, which we shall notate by
\[
\Delta(\nu)_i = A \nu_i - \sum_{j \leq i} \nu_j (\nu_j^T A \nu_i)
\]
\[
= \left( I - \sum_{j < i} \nu_j \nu_j^T \right) A \nu_i - \nu_i (\nu_i^T A \nu_i)
\]
\[\Box\]
Only now do we consider the assumption of exact parents. This corresponds to the coefficient vectors \( \nu_j = e_j \forall j < i \) where \( e_j \) is the \( j \)th unit vector (\( (e_j)_k = \delta_{jk} \)). Then

\[
(I - \sum_{j < i} \nu_j \nu_j^T) = \begin{pmatrix} 0_{(i-1) \times (i-1)} & 0_{(i-1) \times (i-1)} \\ 0_{(d-i+1) \times (i-1)} & I_{(d-i+1) \times (d-i+1)} \end{pmatrix}
\]

So writing \( \nu_i^T \Lambda \nu_i = m_i \bar{\lambda}_i \) as before, the update equations for our coefficients become:

\[
\Delta(\nu_i^{(p)}) = -m_i \bar{\lambda}_i \nu_i^{(p)} \quad \text{for} \quad p < i \tag{27}
\]

\[
\Delta(\nu_i^{(p)}) = (\lambda^{(p)} - m_i \bar{\lambda}_i) \nu_i^{(p)} \quad \text{for} \quad p \geq i \tag{28}
\]

So if we observe the qualitative behaviour:

- For \( p < i \) the coefficients are shrunk towards zero (for sufficiently small step sizes).
- For \( p \geq i \) the coefficients grow/decay depending on their generalised eigenvalue. The larger the eigenvalue, the more the components grow / the less they shrink. So over time only the \( i \)th component will be selected.
- The overall magnitude of the solution shrinks faster when \( \bar{\lambda}_i \) is large.

A stationary point of the iteration therefore requires \( \nu_i^{(p)} = 0 \) for \( p < i \). Then for each \( p \geq i \) we must have either \( m_i \bar{\lambda}_i = \lambda^{(p)} \) or \( \nu_i^{(p)} = 0 \). Furthermore, \( \nu_i^{(i)} \) grows at a faster rate than any of the other components, so provided this was non-zero at initialisation, it will be extracted uniquely. Finally, if \( \nu_i^{(p)} = 0 \forall p \neq i \) but \( \nu_i^{(i)} \neq 0 \) then by definition of \( \bar{\lambda}_i \) we must have \( \bar{\lambda}_i = \lambda^{(i)} \) but then zeroing \((28)\) requires \( m_i \bar{\lambda}_i = \lambda^{(i)} \); so combining we get \( m_i = 1 \) and so \( \nu_i^{(i)} = \pm 1 \), as required.

**Proof in the general case, where \( A \) may have negative eigenvalues.** The steps above go through verbatim if we replace the \( \nu_i^T \Lambda \nu_i \) terms with \( \max(\nu_i^T \Lambda \nu_i, 0) \), and correspondingly replace \( \bar{\lambda}_i \) terms with \( \max(\bar{\lambda}_i, 0) \).}

**B.3.1 Discussion of continuous dynamics**

In particular note that in the continuous time case above with exact parents, we can write the solutions to \( \frac{d}{dt} \nu_i(t) = \Delta(\nu_i) \) with \( \Delta(\nu_i) \) as in \((27)\) \((28)\) as

\[
\nu_i^{(p)}(t) = \nu_i^{(p)}(0) \exp\left( \mathbb{1}_{\{p \geq i\}} \lambda^{(p)} t - \int_{s=0}^{t} m_i(s) \max\left(\bar{\lambda}_i(s), 0\right) ds \right)
\]

So when \( z_i^{(i)}(0) \neq 0 \) (hopefully this is almost sure), the trajectories on the simplex satisfy

\[
\frac{z_i^{(j)}(t)}{z_i^{(j)}(0)} = \frac{z_i^{(j)}(0)}{z_i^{(j)}(0)} \exp\left( 2 \mathbb{1}_{\{p \geq i\}} \lambda^{(p)} - \lambda^{(i)} t \right) \to 0 \quad \text{as} \quad t \to \infty
\]

and we do indeed select the correct coefficient vector at an exponential rate. Note that in particular this equation for trajectory on the simplex is decoupled from the trajectory of the norm \( m_i \) of the coefficients.

Of course, we are really interested in the case of in-exact parents. We can provide a heuristic argument similar to one of [Gemp et al., 2021]. Note that the updates for \( w_i \) only depend on it’s parents \( w_{j<i} \), and one can show that an \( \mathcal{O}(\epsilon) \) error in the parents propagates to an \( \mathcal{O}(\epsilon) \) direction in the child gradient. We know \( w_1 \) will converge very fast to an arbitrary accuracy; then the gradient for \( w_2 \) will be very close to that corresponding to exact parents, so will quickly converge to that a similar order of accuracy; then the gradient of \( w_3 \) will be close to that for exact parents and so on.
B.3.2 EXTENDING TO STOCHASTIC CASE

The real case of interest is the discrete time case with mini-batches. Gemp et al. (2021) claim that their algorithm converges almost surely provided the step-size sequence $\eta_t$ satisfies

$$\sum_{t=1}^{\infty} \eta_t = \infty, \quad \sum_{t=1}^{\infty} \eta_t^2 < \infty$$

Their key tool is a result on Stochastic Approximation (SA) on Riemannian manifolds Shah (2017). This result extends the now-classical ODE method for analysis of SA schemes to Riemannian manifolds, mostly drawing on the presentation of Borkar (2008). One key difficulty of applying the literature on SA schemes is obtaining stability bounds (saying that the estimates never get too big); this becomes trivial when considering updates on compact manifolds like the unit sphere, which is why Gemp et al. (2021) are able to apply their SA tool ‘out-of-the-box’. In our case, because we do not restrict to the unit sphere, we are able to apply more classical results on SA, for example Kushner et al. (2003), however, we would need to prove the corresponding stability estimates. These should hold intuitively because the variance penalty term should keep estimates small, but they are technically difficult. We note that obtaining such stability estimates has attracted a lot of theoretical attention, but in practice they are often unnecessary because only a bounded subset of the parameter space is physically sensible. This applies to our GEP: it only makes sense to consider vectors $w$ with $w^T B w \leq 1$; and though $B$ is unknown in general, we may well be able to lower bound its eigenvalues, giving a bounded parameter space of interest. We could modify our algorithm to project onto this bounded subset of parameter space. The theory of Kushner et al. (2003) can be applied to such a case of projected SA; indeed this theory has the added advantage of requiring weaker conditions on the step-sizes, namely only that

$$\sum_{t=1}^{\infty} \eta_t = \infty, \quad \eta_t \to 0$$

Note such step-size schedules with slower decay is sometimes observed to give better empirical results in other SA problems Kushner et al. (2003).

We now point out what we understand to be a technical oversight in the proof of almost sure convergence in Gemp et al. (2021). They proof that $w_i$ converges a.s. to true value given fixed exact parents $w_j < i$ appears valid; as does the conclusion that $w_i$ converges a.s. to a corresponding optimum given fixed inexact parents; and also does their statement that if parents are close to correct then the corresponding optimum is close to correct. However, this does not say anything about convergence of $w_i$ when the parents are inexact and varying; in particular the arguments of Shah (2017) do not apply in this case. We believe that it would be possible to fix this oversight by considering a suitable coupling of solution paths starting from an $\epsilon$-covering of a neighbourhood of the true solution. Alternatively, it may be possible to apply the result of Shah (2017) to the combined estimates $(w_1, \ldots, w_k)$. Similar analysis will be needed for GEP-GHA because we also propose parallel updates for computational speed.

We next note that this SA literature also applies to our $\delta$-eigengame algorithm, whose updates are unbiased estimates to the gradient of the utilities $U_i^\delta$. In this case, analysis may be more straightforward because we can also apply other existing literature on stochastic gradient descent.

We have not yet had time to make the discussion above more rigorous; we plan to do so in future work. Our algorithms fit very naturally into the well-studied SA framework, and we expect this literature to contain useful intuition and suggestions for implementation, as well as theoretical guarantees.

C PROOF OF SUBSPACE CHARACTERISATIONS

Our main objective in this section is to prove proposition 3.1 restated below.

**Proposition 3.1 (Subspace characterisation).** Let $A$ be positive semi-definite. Then the top-$k$ subspace for the GEP (1) can be characterised by

$$\max_{W \in \mathbb{R}^{d \times k}} \text{trace} \left( W^T A W (2 I_k - W^T B W) \right)$$

(18)
We previously claimed that top-$k$ subspaces to a GEP $(A, B)$ can be characterised by
\[
\max_{W \in \mathbb{R}^{d \times k}} \text{trace}(W^T AW) \quad \text{subject to} \quad W^T BW = I_k
\]

(30)

It is accepted in the Machine Learning community that this is maximised precisely when $W$ is a top-$k$ subspace (Ghojogh et al. (2022), Sameh & Wisniewski (1982)); however, we were unable to find a proof of this. In the matrix analysis literature, it is only usually established that
\[
\max_{W \in \mathbb{R}^{d \times k}, W^T BW = I_k} \text{trace}(W^T AW) \leq \sum_{i=1}^{k} \lambda_i = \text{trace}(W^* AW^*)
\]

(31)

but there is no detail given for the equality case; for example see Stewart & Sun (1990), Horn & Johnson (1985), Tao (2010); to remedy this, we provide a self-contained proof to the result, which we state formally in Proposition C.1 below. First, we explicitly define terms introduced in the main text.

**Definition C.1** (Top-$k$ subspace). Let the GEP $(A, B)$ on $\mathbb{R}^d$ have eigenvalues $\lambda_1 \geq \cdots \geq \lambda_d$. Then a top-$k$ subspace is that spanned by some $w_1, \ldots, w_k$, where $w_i$ is a $\lambda_i$-eigenvector of $(A, B)$ for $i = 1, \ldots, k$.

**Definition C.2** (B-orthonormality). Let $B \in S_{++}^d$ and $W \in \mathbb{R}^{d \times k}$. Then we say $W$ has B-orthonormal columns if $W^T BW = I_k$.

**Proposition C.1** (Constrained characterisation). Let $B \in S_{++}^d$ and let $A \in \mathbb{R}^{d \times d}$ be symmetric with an orthonormal set of (generalised) eigenvectors $u_1, \ldots, u_d$ with (generalised) eigenvalues $\lambda_1 \geq \cdots \lambda_d$. Consider $W \in \mathbb{R}^{d \times k}$ such that $W^T BW = I_k$. Then
\[
\text{trace}(W^T AW) \leq \sum_{i=1}^{k} \lambda_i
\]

(32)

with equality if and only if $W$ defines a top-$k$ subspace for $(A, B)$.

We can now write proposition 3.1 more explicitly as

**Proposition C.2** (Unconstrained characterisation). Let $B \in S_{++}^d$ and now let $A \in S_{++}^d$ be positive semi-definite. Then
\[
\max_{W \in \mathbb{R}^{d \times k}} \text{trace} \left( W^T AW \left(2I_k - W^T BW \right) \right) = \sum_{i=1}^{k} \lambda_i
\]

(33)

For any maximiser $W$, the columns of $W$ span a top-$k$ subspace for $(A, B)$. Moreover, if the top-$k$ eigenvalues are positive (i.e. $\lambda_k > 0$), then $W$ is a maximiser if and only if it has B-orthonormal columns spanning a top-$k$ subspace for $(A, B)$.

First a quick remark. When $W$ is B-orthonormal, the left hand side of (33) reduces to that of (32). Moreover, if the columns of $W$ are some (ordered) top-$k$ eigenvectors then $W^T AW = \text{diag}(\lambda_1, \ldots, \lambda_k)$ and so the maximum is certainly attained. The hard part is to characterise which $W$ achieve this maximum.

The rest of this section is as follows. In Section C.2 we show it is sufficient to prove Propositions C.1 and C.2 for the case where $B = I$. In Section C.3 we give a self contained proof of Proposition C.1. In Section C.4 we use this to give a self contained proof of Proposition C.2. Finally in Section C.5 we give an alternative (and shorter) proof of Proposition C.2 which we believe gives complementary intuition; this uses a powerful (but little known) trace inequality originally due to von Neumann.
C.2 Reduction to $B = I$ cases

In this section we show it is sufficient to prove Propositions C.1 and C.2 for the case where $B = I$. To start, consider an arbitrary $W \in \mathbb{R}^{d \times k}$. Then write $\tilde{W} = B^{-1/2}W$ and $\tilde{A} = B^{-1/2}AB^{-1/2}$. Note the map $W \mapsto \tilde{W}$ is bijective because $B \in S_+^{d \times d}$. We will see a correspondence between the variational characterisations over $W$ for $(A, B)$ with those over $\tilde{W}$ for $(\tilde{A}, I)$.

Firstly, there is a correspondence of eigenvectors: it is well known that $\tilde{w}_i$ is a $\lambda_i$-eigenvector of $\tilde{A}$ precisely when $w_i := B^{-1/2}\tilde{w}_i$ is a $\lambda_i$-generalised eigenvector of $(A, B)$; indeed, if $\tilde{w}_i$ is a $\lambda_i$-eigenvector of $\tilde{A}$ then

$$A(B^{-1/2}\tilde{w}_i) = B^{1/2}B^{-1/2}AB^{-1/2}B^{-1/2}\tilde{w}_i = B^{1/2}(\tilde{A}\tilde{w}_i) = B^{1/2}(\lambda_i \tilde{w}_i) = \lambda_i B(B^{-1/2}\tilde{w}_i)$$

so $w_i := B^{-1/2}\tilde{w}_i$ is a $\lambda_i$-generalised eigenvector of $(A, B)$. The reverse implication is similar. Therefore we see $\tilde{W}$ is a top-$k$ subspace for $\tilde{A}$ if and only if $W$ is a top-$k$ subspace for $(A, B)$.

We also see correspondence of the objective and orthogonality conditions via

$$W^T B W = \tilde{W}^T B^{-1/2} B B^{-1/2} \tilde{W} = \tilde{W}^T \tilde{W}$$
$$W^T A W = \tilde{W}^T B^{-1/2} AB^{-1/2} \tilde{W} = \tilde{W}^T \tilde{A} \tilde{W}$$

Finally note that $A$ is positive semi-definite if and only if $\tilde{A}$ is positive semi-definite.

It is now easy to check that all conditions and results in Propositions C.1 and C.2 precisely map from statements about $W$ for the GEP $(A, B)$ to statements about $\tilde{W}$ for eigenvalue problem $(\tilde{A}, I)$. In the remaining proofs we will drop the tilde’s for readability.

C.3 Proof of constrained characterisation

We shall work via a series of Lemmas. These build up to Lemma C.3, the inequality case here corresponds to (31) and is well known (Stewart & Sun (1990), Horn & Johnson (1985), Tao (2010)); however, to analyse the equality case we needed a small extra argument; the key is Lemma C.2 which is a special case of Theorem 2.1 from Haemers (1995); the corresponding proof makes extensive use of Raleigh’s principle, Lemma C.1. We adapt results to our notation and present all proofs here for completeness. Note that there is no restriction on the eigenvalues of $A$ to be non-negative in this sub-section.

C.3.1 Results from Haemers (1995)

Lemma C.1 (Rayleigh’s principle). Let $A \in \mathbb{R}^{d \times d}$ be symmetric with an orthonormal set of eigenvectors $u_1, \ldots, u_d$ with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_d$. Then

$$\frac{u^T A u}{u^T u} \geq \lambda_i \text{ if } u \in \langle u_1, \ldots, u_i \rangle \text{ and } \frac{u^T A u}{u^T u} \leq \lambda_i \text{ if } u \in \langle u_1, \ldots, u_{i-1} \rangle \perp$$

In either case, equality implies that $u$ is a $\lambda_i$ eigenvector of $A$.

Proof. For the first case, suppose $u = \sum_{j=1}^i \nu_j u_j$ for some coefficients $\nu_j \in \mathbb{R}$. Then the Raleigh quotient

$$\frac{u^T A u}{u^T u} = \frac{\sum_{j=1}^i \lambda_j \nu_j^2}{\sum_{j=1}^i \nu_j^2} \geq \frac{\lambda_i \sum_{j=1}^i \nu_j^2}{\sum_{j=1}^i \nu_j^2} = \lambda_i$$

with equality if and only if $\nu_j = 0$ whenever $\lambda_j > \lambda_i$; so indeed

$$A u = \sum_{j=1}^i \lambda_j \nu_j u_j = \lambda_i \sum_{j=1}^i \nu_j u_j = \lambda_i u$$

Similarly, for the second case, we have $u = \sum_{j=i+1}^d \nu_j u_j$ so

$$\frac{u^T A u}{u^T u} = \frac{\sum_{j=i+1}^d \lambda_j \nu_j^2}{\sum_{j=i}^d \nu_j^2} \leq \frac{\lambda_i \sum_{j=i+1}^d \nu_j^2}{\sum_{j=i}^d \nu_j^2} = \lambda_i$$
with equality if and only if \( \nu_j = 0 \) whenever \( \lambda_j < \lambda_i \); so indeed

\[
Au = \sum_{j=i}^{d} \lambda_j \nu_j u_j = \lambda_i \sum_{j=i}^{d} \nu_j u_j = \lambda_i u
\]

\[\square\]

**Lemma C.2.** Let \( S \in \mathbb{R}^{d \times k} \) such that \( S^T S = I \) and let \( A \in \mathbb{R}^{d \times d} \) be symmetric with an orthonormal set of eigenvectors \( u_1, \ldots, u_d \) with eigenvalues \( \lambda_1 \geq \ldots \lambda_d \). Define \( C = S^T AS \), and let \( C \) have eigenvalues \( \mu_1 \geq \ldots \geq \mu_k \) with respective eigenvectors \( v_1 \ldots v_k \).

Then

- \( \mu_i \leq \lambda_i \) for \( i = 1, \ldots, k \).
- if \( \mu_i = \lambda_i \) for some \( i \) then \( C \) has a \( \mu_i \)-eigenvector \( v \) such that \( Sv \) is a \( \mu_i \)-eigenvector of \( A \).
- if \( \mu_i = \lambda_i \) for \( i = 1, \ldots, k \) then \( Sv_i \) is a \( \mu_i \)-eigenvector of \( A \) for \( i = 1, \ldots, k \).

**Proof.** With \( u_1, \ldots, u_d \) as above, for each \( i \in [1, k] \), take a non-zero \( s_i \) in

\[
\langle v_1, \ldots, v_i \rangle \cap \langle S^T u_1, \ldots, S^T u_{i-1} \rangle^\perp
\]

Then \( S s_i \in \langle u_1, \ldots, u_{i-1} \rangle^\perp \), so by Raleigh’s principle

\[
\lambda_i \geq \frac{(S s_i)^T A (S s_i)}{(S s_i)^T (S s_i)} = \frac{s_i^T C s_i}{s_i^T s_i} \geq \mu_i.
\]

The second bullet then follows from the equality case of Raleigh’s principle: if \( \lambda_i = \mu_i \) then \( s_i \) and \( S s_i \) are \( \lambda_i \)-eigenvectors of \( C \) and \( A \) respectively.

For the final bullet we use induction on \( l \): suppose \( Sv_i = u_i \) for \( i = 1, \ldots, l-1 \). Then we may take \( s_l = v_l \) in (34), but by the preceding argument, we saw \( Sv_l = S s_l \) is a \( \lambda_l \)-eigenvector of \( A \).

The following lemma is now straightforward to prove.

**Lemma C.3.** Under the notation of Lemma C.2 we have

\[
\text{trace}(S^T AS) \leq \sum_{i=1}^{k} \lambda_i
\]

with equality if and only if \( S \) defines a top-\( k \) subspace for \( A \).

**Proof.** By Lemma C.2 letting \( \mu_1 \geq \ldots \geq \mu_k \) be the eigenvalues of \( C = S^T AS \), we have

\[
\text{trace}(S^T AS) = \sum_{i=1}^{k} \mu_i \geq \lambda_1 + \sum_{i=2}^{k} \mu_i \geq \sum_{i=1}^{k} \lambda_i
\]

with equality if and only if all the inequalities above are equalities, i.e. \( \mu_i = \lambda_i \) for \( i = 1, \ldots, k \). But then by Lemma C.2 we have that \( Sv_i \) is a \( \mu_i \)-eigenvector of \( A \).

In particular, note that \( V = (v_1, \ldots, v_k) \) is orthogonal and \( SV = (S v_1, \ldots, S v_k) \) is a matrix whose columns are a choice of top-\( k \) eigenvectors for \( A \).

From this Lemma we can immediately deduce Proposition C.1 by the arguments of Section C.2. We state this again now for reference.

**Proposition C.1** (Constrained characterisation). Let \( B \in \mathbb{S}_+^{d \times d} \) and let \( A \in \mathbb{R}^{d \times d} \) be symmetric with an orthonormal set of (generalised) eigenvectors \( u_1, \ldots, u_d \) with (generalised) eigenvalues \( \lambda_1 \geq \ldots \lambda_d \). Consider \( W \in \mathbb{R}^{d \times k} \) such that \( W^T BW = I_k \). Then

\[
\text{trace}(W^T AW) \leq \sum_{i=1}^{k} \lambda_i
\]

with equality if and only if \( W \) defines a top-\( k \) subspace for \( (A, B) \).
C.4 PROOF OF UNCONSTRAINED CHARACTERISATION

For this section we introduce the notation
\[ h(W; A, B) := \text{trace} \left( W^T AW \left( 2I - W^T BW \right) \right) \]  \hspace{1cm} (35)

Again, by the arguments of Section C.2, it would be sufficient to consider the case \( B = I \); however, this does not save much work in this section, so we often leave the \( B \) terms in to help intuition. The key idea here is that for any \( W \) we can find a matrix with the same column space as \( W \) and \((B-) orthonormal columns which improves \( h \); this then reduces the result to the constrained characterisation C.1. We again work via a sequence of lemmas, progressively analysing \( h \) under more general conditions. The hardest part is arguably the compactness argument in Lemma C.4 which crucially requires \( A \) to have strictly positive eigenvalues. Zero eigenvalues lead to some degeneracy and are dealt with carefully in Lemma C.5. We first consider square \( M \) for any \( B \) this does not save much work in this section, so we often leave the \( B \) terms in to help intuition.

**Lemma C.4 (Matrix perspective).** Let \( A \in \mathbb{R}^{p \times p} \) be diagonal with strictly positive entries. Then for any \( M \in S^d_+ \) we have
\[ I_1(M) := \text{trace} \left( \Lambda M (2I - M) \right) \leq \text{trace}(\Lambda) \]
with equality if and only if \( M = I_p \).

**Proof.** For an arbitrary \( M \in S^d_+ \), we can write \( M = \sum_{i=1}^p \mu_i v_i v_i^T \) for some \( \mu_1 \geq \cdots \geq \mu_p \geq 0 \) and orthonormal sets of vectors \((v_i)_{i=1}^p \). Now suppose that \( |\mu_1 - 1| > 0 \). Then
\[
I_1(M) := \text{trace} \left( \Lambda M (2I - M) \right) \\
= \text{trace} \left( \Lambda \sum_{i=1}^p (\mu_i - 1) v_i v_i^T \right) \\
= \sum_{i=1}^p (\mu_i - 1) \text{trace} \left( \Lambda v_i v_i^T \right) \\
\leq \lambda_{\min} \left( 1 - (\mu_1 - 1)^2 + (p-1)\lambda_{\max} \right)
\]
So in particular, if we have \( |\mu_1| \geq 1 + \sqrt{1 + \frac{(p-1)\lambda_{\max}}{\lambda_{\min}}} =: R^* \) then \( (\mu_i - 1)^2 \geq 1 + \frac{(p-1)\lambda_{\min}}{\lambda_{\max}} \) and so \( I_1(M) \leq 0 \).

However, we have \( I(I_p) = \text{trace}(\Lambda) > 0 \). So it is sufficient to show that \( I_p \) is the unique maximiser on the compact set \( S = \{ M \succ 0 : \|M\|_{op} \leq R^* \} \).

Now note that \( I_1 \) is a continuous function of \( M \), so the maximum on \( S \) is attained (by compactness); yet this maximum cannot be on the boundary, because \( I_1(M) \leq 0 \) for such \( M \). So any maximiser must be on the interior of \( S \). Moreover, \( I_1 \) is differentiable, and so the derivative at such a maximiser must be zero.

Indeed, we can explicitly compute the derivative. Consider a symmetric perturbation \( H \). Note that \( \text{trace}(\Lambda M H) = \text{trace}(H^T M^T \Lambda^T) = \text{trace}(\Lambda H M) \) by transpose and cyclic invariance of trace. So we can write:
\[
I_1(M + H) - I_1(M) = \text{trace} \left( \Lambda (M + H)(2I - M - H) \right) - \text{trace} \left( \Lambda M (2I - M) \right) \\
= \text{trace} \left( \Lambda (H(2I - M) - MH - H^2) \right) \\
= \text{trace} \left( \Lambda (2H - HM - MH) \right) + o(H) \\
= 2 \text{trace} \left( H^T \Lambda (I - M) \right) + o(H)
\]
from which we conclude that \( M = I \) is the only stationary point. Therefore, it must be the unique maximiser. \( \square \)
**Lemma C.5** (Diagonal case). Let $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_p, 0, \ldots, 0) \in \mathbb{R}^{k \times k}$ be diagonal with $\lambda_i > 0$ for $i = 1, \ldots, p$. Let $\Phi = \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} \in \mathbb{R}^{k \times k}$ with $\Phi_1 \in \mathbb{R}^{p \times k}, \Phi_2 \in \mathbb{R}^{(k-p) \times k}$. Then

$$h(\Phi; \Lambda, I_k) \leq \sum_{i=1}^{p} \lambda_i = \text{trace} (\Lambda)$$

with equality if and only if $\Phi_1 \Phi_2^T = I$ and $\Phi_1 \Phi_2^T = 0$.

**Proof.** Write $\Lambda_1 = \text{diag}(\lambda_1, \ldots, \lambda_p) \in \mathbb{R}^{p \times p}$. Then

$$h(\Phi; \Lambda, I) = \text{trace} \left( \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}^T \begin{pmatrix} \Lambda_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 2I - \Phi_1^T \Phi_1 - \Phi_2^T \Phi_2 \end{pmatrix} \right)$$

$$= \text{trace} \left( \Phi_1^T \Lambda_1 \Phi_1 (2I - \Phi_1^T \Phi_1 - \Phi_2^T \Phi_2) \right)$$

$$= \text{trace} \left( \Phi_1^T \Lambda_1 \Phi_1 (2I - \Phi_1^T \Phi_1) \right) - \text{trace} \left( \Phi_1^T \Lambda_1 \Phi_2^T \Phi_2 \right)$$

$$= \text{trace} \left( \Phi_1^T \Lambda_1 \Phi_1 (2I - \Phi_1^T \Phi_1) \right) - \text{trace} \left( \Phi_2^T \Lambda_1 \Phi_1 \Phi_2 \right)^T \text{trace} \left( \Lambda_1 \Phi_1 \Phi_2 \right)$$

$$\leq \text{trace} \left( \Phi_1^T \Lambda_1 \Phi_1 (2I - \Phi_1^T \Phi_1) \right)$$

$$= h\left( \begin{pmatrix} \Phi_1 \\ 0 \end{pmatrix}; \Lambda, I \right)$$

With equality if and only if $\Phi_1 \Phi_2^T = 0$ (because $\Lambda_1$ is strictly positive definite); i.e. the rows of $\Phi_1$ are orthogonal to the rows of $\Phi_2$.

Now we show we can further improve $h$ by picking a $\tilde{\Phi}$ with orthogonal rows. We have by cyclicity of trace and rearranging the brackets that

$$h\left( \begin{pmatrix} \Phi_1 \\ 0 \end{pmatrix}; \Lambda, I \right) = \text{trace} \left( \Phi_1^T \Lambda_1 \Phi_1 (2I - \Phi_1^T \Phi_1) \right)$$

$$= \text{trace} \left( \Lambda_1 \Phi_1 \Phi_1^T (2I - \Phi_1^T \Phi_1) \right)$$

$$\leq \text{trace} (\Lambda_1)$$

$$= \text{trace} (\Lambda)$$

with equality if and only if $\Phi_1 \Phi_1^T = I$ by Lemma C.4

Combining the two results we conclude the claim: $h(\Phi; \Lambda, I) \leq \text{trace}(\Lambda)$ with equality if and only if $\Phi_1 \Phi_1^T = I$ and $\Phi_1 \Phi_2^T = 0$.

In addition, we note that the choice $\Phi = I$ attains the maximum, but there may be some extra flexibility corresponding to zero eigenvalues of $\Lambda$. \hfill $\square$

**Lemma C.6** (Square case). Let $A \in \mathbb{S}^k_+$, $B \in \mathbb{S}^k_+$, and $W \in \mathbb{R}^{k \times k}$. Then for any $B$-orthogonal matrix $W \in \mathbb{R}^{k \times k}$

$$h(W; A, B) \leq h(W; A, B) = \sum_{i=1}^{k} \lambda_i$$

**Proof.** Let $W^*$ be a matrix whose columns are successive generalised eigenvectors of the GEP $(A, B)$. Then $W^T B W^* = I_k$ and $(W^*)^T A W^* = \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_k)$ by construction. Therefore $W^*$ is invertible and we can write $W = W^* \Phi$ for some $\Phi \in \mathbb{R}^{k \times k}$, Then

$$h(W; A, B) = \text{trace} \left( \Phi^T (W^*)^T A W^* \Phi (2I - \Phi^T (W^*)^T B W^* \Phi) \right)$$

$$= \text{trace} \left( \Phi^T \Lambda \Phi (2I - \Phi^T \Phi) \right)$$

$$= h(\Phi; \Lambda, I)$$

$$\leq \text{trace}(\Lambda)$$

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where the inequality is from Lemma C.5. Moreover, \( W \) is \( B \)-orthogonal precisely when \( \Phi \) is orthogonal, and so we have equality from Lemma C.5 in this case.

**Lemma C.7** (General case). Let \( A \in \mathbb{S}_+^d \), \( B \in \mathbb{S}_+^{d+d} \) and \( W \in \mathbb{R}^{d \times k} \). Then there exists some \( \bar{W} \in \mathbb{R}^{d \times k} \) with the same column space as \( W \) such that \( \bar{W}^T B \bar{W} = I_k \) and

\[
h(W; A, B) \leq h(\bar{W}; A, B)
\]

**Proof.** We have

\[
h(W; A, B) = h(I_k; W^T A W, W^T B W) \\
\leq h(\Gamma; W^T A W, W^T B W) \\
= h(\bar{W}; A, B)
\]

by Lemma C.6 where \( \Gamma \) is some \( W^T B W \)-orthogonal matrix, and \( \bar{W} = \Gamma \). Then \( \bar{W}^T B \bar{W} = \Gamma^T (W^T B W) \Gamma = I_k \) as required.

C.4.1 COMBINING

We now combine the results of the previous sections to prove our original proposition.

**Proposition C.2** (Unconstrained characterisation). Let \( B \in \mathbb{S}_+^d \) and now let \( A \in \mathbb{S}_+^d \) be positive semi-definite. Then

\[
\max_{W \in \mathbb{R}^{d \times k}} \text{trace} \left( W^T A W \left( 2 I_k - W^T B W \right) \right) = \sum_{i=1}^k \lambda_i
\]

(33)

For any maximiser \( W \), the columns of \( W \) span a top-\( k \) subspace for \((A, B)\). Moreover, if the top-\( k \) eigenvalues are positive (i.e. \( \lambda_k > 0 \)), then \( W \) is a maximiser if and only if it has \( B \)-orthonormal columns spanning a top-\( k \) subspace for \((A, B)\).

**Proof. of Proposition C.2**. Let \( W \in \mathbb{R}^{d \times k} \). Then by Lemma C.7, there exists some \( B \)-orthogonal \( \bar{W} \) with the same column space as \( W \) and \( h(W; A, B) \leq h(\bar{W}; A, B) \). So combining with Proposition C.1 we see

\[
h(W; A, B) \leq h(\bar{W}; A, B) = \text{trace} \left( \bar{W}^T A \bar{W} \right) \leq \sum_{i=1}^k \lambda_i
\]

(36)

where the second inequality is an equality if and only if \( \bar{W} \) defines a top-\( k \) subspace. This proves the first two claims.

For the final claim, note \( W \) is a maximiser if and only if both inequalities in (36) are equalities. In this case, we can write \( \bar{W} = W^* \Phi \) for some \( W^* \in \mathbb{R}^{d \times k} \) whose columns are some top-\( k \) eigenvectors and \( \Phi \in \mathbb{R}^{k \times k} \) (because \( \bar{W} \) has the same column space as \( W \) and defines a top-\( k \) subspace). Then

\[
\sum_{i=1}^k \lambda_i = h(W; A, B) = h(\Phi; \Lambda_k, I_k)
\]

where \( \Lambda_k = \text{diag}(\lambda_1, \ldots, \lambda_k) \). If \( \lambda_k > 0 \) then \( \Lambda_k > 0 \) so by the equality case of Lemma C.5, \( \Phi \) must be orthogonal. So indeed \( W \) has \( B \)-orthonormal columns spanning a top-\( k \) subspace.

Note that in the case where some of the top-\( k \) eigenvalues are zero, the equality case of Lemma C.5 still gives some sort of orthogonality in the subspace of positive eigenvectors but allows degeneracy in the zero eigenspace (both arbitrary magnitudes and non-orthogonal directions).
C.5 Alternative proof using von Neumann’s trace inequality

C.5.1 Trace inequality and other background

Here we give a cleaner proof of Proposition C.2 using the following result originally due to von Neumann; a simple proof (which also extends the result to infinite dimensional Hilbert spaces) and recent discussion is given in [Carlsson (2021)], we shall only state the matrix case for readability. First however, we need a new definition.

**Definition C.3** (Sharing singular vectors). Let \( a, b \in \mathbb{N} \) and \( q = \min(a, b) \). We say two matrices \( X, Y \in \mathbb{R}^{a \times b} \) share singular vectors if there exist some (orthonormal sets) \( \{u_j\}_{j=1}^q \) and \( \{v_j\}_{j=1}^q \) such that

\[
X = \sum_{j=1}^q \sigma_j(X) u_j v_j^T, \quad Y = \sum_{j=1}^q \sigma_j(Y) u_j v_j^T
\]

**Theorem C.1** (von Neumann’s trace inequality). Let \( a, b \in \mathbb{N} \) and \( q = \min(a, b) \). Let \( X, Y \in \mathbb{R}^{a \times b} \). Then

\[
\langle X, Y \rangle \leq \sum_{j=1}^q \sigma_j(X) \sigma_j(Y)
\]

with equality if and only if \( X \) and \( Y \) share singular vectors (in the sense of Definition C.3).

We stress that ‘sharing singular vectors’ does not just say that \( X, Y \) have the same singular vectors, but these are in the same order. Why do we need this non-standard definition of ‘sharing singular vectors’? This is just a convenient way to deal with the degeneracy associated to repeated singular values; indeed it is often more natural to think in terms of partial isometries and polar decompositions when proving such results; see [Carlsson (2021)] for further discussion.

Next we give a corollary which is adapted to our case of interest. First this requires a simple lemma relating SVD to eigendecomposition. This is well known but we give a quick proof for completeness. It is necessary to assume \( A \) is **positive semi-definite**, the result is false for general \( A \).

**Lemma C.8.** Let \( A \in \mathbb{S}^d_+ \) have some SVD \( A = \sum_{i=1}^q \lambda_i u_i v_i^T \) with \( \lambda_i > 0 \) for \( i = 1, \ldots, q \). Then this in fact gives an eigendecomposition, i.e. \( u_i = u_i \) is a \( \lambda_i \)-eigenvector of \( A \) for each \( i = 1, \ldots, d \).

**Proof.** If \( v \) is an eigenvector of \( A \) then it is also an eigenvector of \( A^2 \). Further, the eigenvectors of \( A \) span \( \mathbb{R}^d \) so these provide an eigenbasis for \( A^2 \). Hence any eigenvector of \( A^2 \) is in fact an eigenvector of \( A \). Next, by symmetry of \( A \)

\[
A^2 v_k = A^T A v_k = \sum_{j=1}^d \sum_{i=1}^d \lambda_i \lambda_j v_j u_j^T v_i u_i^T v_k = \sum_{i,j=1}^d \lambda_i \lambda_j v_j u_j^T v_i u_i^T v_k = \lambda_k^2 v_k
\]

So by the observation above, \( v_k \) must be a \( \lambda_k \)-eigenvector of \( A \). But then

\[
\lambda_k v_k = A v_k = \sum_{j=1}^d \lambda_j v_j u_j^T v_k = \lambda_k u_k
\]

so cancelling the \( \lambda_k \)'s gives \( u_k = v_k \) as required. \( \square \)

To state the corollary we need a new definition analogous to Definition C.3. We stress again that the eigenvectors share the same ordering - so this is stronger than saying the matrices are simultaneously diagonalisable. The final conclusion of the corollary is very weak and just provides a clean consequence of the notion of sharing eigenvectors to our previous notion of top-\( k \) subspaces.

**Definition C.4** (Sharing eigenvectors). Let symmetric matrices \( A, M \in \mathbb{R}^{d \times d} \) have eigenvalues \( \lambda_1 \geq \cdots \geq \lambda_d, \mu_1 \geq \cdots \geq \mu_d \) respectively. We say \( A, M \) share eigenvectors if there exist (an orthonormal set) \( \{w_j\}_{j=1}^d \) such that

\[
A = \sum_{j=1}^d \lambda_j w_j w_j^T, \quad M = \sum_{j=1}^d \mu_j w_j w_j^T
\]
Corollary C.1 (Positive-definite von Neumann). Let $A \in S^d_+$ and $M \in \mathbb{R}^{d \times d}$ be symmetric with eigenvalues $(\lambda_i)_{i=1}^d$, $(\mu_i)_{i=1}^d$ respectively. Then

$$\langle A, M \rangle \leq \sum_{i=1}^{d} \lambda_i \mu_i$$

(38)

with equality if and only if $A$ and $M$ share eigenvectors. Equality therefore implies that any unique top-$k$ subspace for $A$ is a top-$k$ subspace for $M$ and vice versa.

**Proof.** Write $M^+ = M - \mu_d I_d$. Then $M^+ \in S^d_+$. Note that for positive semidefinite matrices, their eigendecomposition provides a valid singular value decomposition; therefore (by uniqueness of SVD) the singular values of $A, M^+$ respectively are precisely $(\lambda_i)_{i=1}^d$, $(\mu_i - \mu_d)_{i=1}^d$. Applying von Neumann’s inequality to $A, M^+$ gives

$$\langle A, M \rangle = \langle A, M^+ \rangle + \mu_d \langle A, I_d \rangle \leq \left( \sum_{i=1}^{d} \lambda_i (\mu_i - \mu_d) \right) + \mu_d \sum_{i=1}^{d} \lambda_i = \sum_{i=1}^{d} \lambda_i \mu_i$$

and so there exists some shared set of singular vectors $((u_i, v_i))_{i=1}^d$ for $(A, M^+)$. Now applying Lemma C.8 we conclude that in fact the $((u_i))_{i=1}^d$ give a shared eigenvector basis for $(A, M^+)$, and therefore also for $(A, M)$.

For the final conclusion, let the shared eigenvectors be $((u_i))_{i=1}^{d-1}$. Then $\text{span}(u_1, \ldots, u_k)$ is a top-$k$ subspace for $A$, so the unique such subspace must be this, which is also a top-$k$ subspace for $M$ (by definition). 

C.5.2 PROOF OF VARIATIONAL CHARACTERISATION

We can now use this to prove Proposition C.2.

**Proof of Proposition C.2** Following the discussion in Section C.2 we may assume that $B = I$. then by cyclicity of trace

$$\text{trace}\left(W^T AW (2 I_k - W^T W)\right) = \text{trace}\left(A \left\{ WW^T (2 I_d - WW^T) \right\} \right)_{:=M}$$

Note that $M$ defined above is of rank at most $k$ with eigenvalues $\leq 1$. Indeed, if we have the singular value decomposition $W = UDV^T$ then $WW^T = UD^2V^T VDU^T = UD^2U^T$ and so

$$M = UD^2U^T (2 I_k - UD^2U^T) = U(2D^2 - D^4)U^T$$

so if $D$ has diagonal elements $(d_i)_{i=1}^k$ then the eigenvalues of $M$ are just

$$\mu_i := 2d_i^2 - d_i^4 = 1 - (1 - d_i^2)^2 \leq 1$$

for $i = 1, \ldots, k$ (the remaining $d - k$ eigenvalues are zeros, corresponding to the null space $U^\perp$). Without loss of generality, suppose we have ordered these elements such that $\mu_1 \geq \cdots \geq \mu_k$. Then

$$h(W; A, I) = \text{trace}(AM) \leq \sum_{i=1}^{d} \lambda_i \mu_i = \sum_{i=1}^{k} \lambda_i \mu_i \leq \sum_{i=1}^{k} \lambda_i$$

(39)

where the first inequality is our positive definite version of von Neumann trace inequality (Corollary C.1), the central equality uses $\mu_{k+1} = \cdots = \mu_d = 0$, and the final inequality uses $\mu_i \leq 1$.

We now move on to examine the case of equality.

- If $\lambda_k > 0$ then equality holds for the final inequality if and only if $\mu_i = 1$ for $i = 1, \ldots, k$. But then the equality case of Corollary C.1 tells us that this unique top-$k$ subspace for $M$ must be some top-$k$ subspace for $A$. Next note $\mu_i = 1 \implies d_i^2 = 1$ for all $i = 1, \ldots, k$ so $D^2 = I$ (and $D$ is orthogonal). Thus $W^T W = VDU^T UD^2V^T = VD^2V^T = VV^T = I$ so $W$ has orthonormal columns.
• The case where $\lambda_k = 0$ requires more care. Suppose $A$ has $q < k$ nonzero eigenvalues (i.e. $\lambda_q > 0, \lambda_{q+1} < 0$). Then replacing the end of (39) with

$$\sum_{i=1}^{k} \lambda_i \mu_i = \sum_{i=1}^{q} \lambda_i \mu_i \leq \sum_{i=1}^{q} \lambda_i = \sum_{i=1}^{k} \lambda_i$$

we see that equality holds if and only if $\mu_i = 1$ for $i = 1, \ldots, q$ (note the remaining $\mu_i$'s are no longer constrained). Now consider the (unique) top-$q$ subspace of $A$ corresponding to non-zero eigenvalues. This must also be a top-$q$ subspace of $M$ (by Corollary C.1) and so all must be eigenvectors of $M$ with eigenvalue 1. In particular this top-$q$ subspace must be contained within the subspace spanned by the columns of $U$ corresponding to diagonal elements $d_i \in \{+1, -1\}$, so is certainly also contained within the column space of $W$. But since all the remaining eigenvalues are precisely zero, we see the column space of $W$ is indeed a top-$k$ subspace for $A$.

\[\square\]

C.6 DISCUSSION

We now offer some intuition: a key strength of this unconstrained formulation is that it is straightforward to transform with respect to arbitrary changes of basis; therefore one can do analysis in the basis of generalised eigenvectors. By contrast, the orthogonality constraint in (3) only permits orthogonal changes of basis. This may give intuition to why $\mu$-eigengame only works in the $B = I$ case but our approach is effective for general GEPs.

D FURTHER CONNECTIONS TO PREVIOUS WORK

D.1 RELATIONSHIP TO PREVIOUS DCCA FORMULATIONS

In Wang et al. (2015c), DCCA is formalised as

$$\max_{f, g, U \in \mathbb{R}^{d_x \times k}, V \in \mathbb{R}^{d_y \times k}} \text{trace}(U^T F G^T V) \quad \text{subject to} \quad U^T F F^T U = V^T G G^T V = I_k$$

where $F = (f(x_1), \ldots, f(x_N)), G = (g(y_1), \ldots, g(y_n))$ are matrices whose columns are images of the training data under functions $f, g$ defined by neural networks in some class of functions $\mathcal{F}, \mathcal{G}$ with input and output dimensions $(p, d_x), (q, d_y)$ respectively. Observe that this optimisation is really targeting the population problem

$$\max_{f \in \mathcal{F}, g \in \mathcal{G}, U \in \mathbb{R}^{d_x \times k}, V \in \mathbb{R}^{d_y \times k}} \text{trace}(U^T \Sigma_{fg} V) \quad \text{subject to} \quad U^T \Sigma_{ff} U = V^T \Sigma_{gg} V = I_k$$

Where $\Sigma_{ff} = \text{Var}(f(X)), \Sigma_{fg} = \text{Cov}(f(X), g(Y)), \Sigma_{gg} = \text{Var}(g(Y))$. We now abuse notation to write $R_k(f(X), g(Y))$ to correspond to the sum of the first $k$ canonical correlations of the pair of random variables $f(X), g(Y)$. It is well known that if we fix $f, g$ in the above then the optimisation problem defines the top-$k$ subspace for CCA. So we can write the optimisation as

$$\max_{f \in \mathcal{F}, g \in \mathcal{G}} R_k(f(X), g(X))$$

But then using proposition [3.1] this optimisation is also equivalent to

$$\max_{f \in \mathcal{F}, g \in \mathcal{G}, W \in \mathbb{R}^{(d_x + d_y) \times k}} \text{trace} \left( W^T A_{fg} W (2I_k - W^T B_{fg} W) \right)$$

where we define

$$A_{fg} = \begin{pmatrix} 0 & \Sigma_{fg} \\ \Sigma_{gf} & 0 \end{pmatrix}, \quad B_{fg} = \begin{pmatrix} \Sigma_{ff} & 0 \\ 0 & \Sigma_{gg} \end{pmatrix}, \quad d = p + q.$$  

We have now almost recovered the form of (17), the only difference is that there is an optimisation over $W$ in the above. To finish the derivation we follow Wang et al. (2015c) and define the augmented function classes:

$$\tilde{\mathcal{F}} = \{ \tilde{f} = U^T f : f \in \mathcal{F}, U \in \mathbb{R}^{d_x \times k} \}, \quad \tilde{\mathcal{G}} = \{ \tilde{g} = V^T g : g \in \mathcal{G}, V \in \mathbb{R}^{d_y \times k} \}$$
For any $W \in \mathbb{R}^{(d_x+d_y) \times k}$ there exist unique $U \in \mathbb{R}^{d_x \times k}, V \in \mathbb{R}^{d_y \times k}$ with $W^T = (U^T, V^T)$. Also for $\tilde{f} = U^T f, \tilde{g} = V^T g$ it follows from definition of covariance that

$$U^T \Sigma_{ff} U = \Sigma_{\tilde{f}\tilde{f}}, \quad U^T \Sigma_{fg} U = \Sigma_{\tilde{f}\tilde{g}}, \quad V^T \Sigma_{gg} V = \Sigma_{\tilde{g}\tilde{g}}$$

so indeed we can write (40) as

$$\max_{f \in \tilde{F}, g \in \tilde{G}} \text{trace} \left( A \tilde{f} \tilde{g} (2 I - B \tilde{f} \tilde{g}) \right)$$

(41)

which precisely matches our objective in (17).

We now comment on this analysis: the definition from Wang et al. (2015c) proposes DCCA to find a pair of low-dimensional feature maps under which the two sets of data are highly correlated. Intuitively, this analysis says that if we take a sufficiently expressive class of neural networks, we only need to consider a $k$ dimensional latent space to recover the top-$k$ subspace of ‘deep canonical directions’. Note also that one only needs to apply a $k$-dimensional classical CCA to recover the top-$k$ directions from this subspace. Finally, we warn that in general these directions may be highly non-unique, and that many of the nice properties of CCA are dependent on the structure of Euclidean space and do not hold for DCCA.

D.2 Derivation of SGHA algorithm from Chen et al. (2019)

The Lagrangian function in Chen et al. (2019) corresponding to (3) is given as:

$$L(W, \Gamma) = \text{tr} \left( W^T A W \right) - \langle \Gamma, W^T B W - I \rangle$$

(42)

Differentiating with respect to $W$ gives

$$2AW - 2BW \Gamma = 0$$

Left multiplying by $W^T$ and using the constraint $W^T BW = I_k$ shows that at any stationary point we have

$$\Gamma = W^T AW$$

(43)

They then plug this value of $\Gamma$ into a gradient descent step for $W$ to obtain an update direction:

$$\Delta_{\text{SGHA}}(W) = -AW - BW(W^T AW)$$

(where we follow their exposition and drop the factor of 2 at this point). Note that this technique of plugging in the optimal dual variable is non-standard to our knowledge. The algorithm needs their theoretical results for more concrete justification.

D.3 Pseudo-Utilities in Previous Work

Recall we defined the pseudo-utility of GHA-GEP to be

$$\mathcal{P}U_i^{\text{GHA-GEP}}(w_i|w_j < i, \Gamma) = \hat{w}_i^T A \hat{w}_i + \Gamma_{ii}(1 - \hat{w}_i^T B \hat{w}_i) - 2 \sum_{j < i} \Gamma_{ij} \hat{w}_j^T B \hat{w}_i$$

(44)

is closely related to expressions in previous work. Consider first SGHA. The Lagrangian function in Chen et al. (2019) is given above in (42).

Considering a single ‘player’ this utility can be written:

$$\mathcal{P}U_i^{\text{SGHA}}(w_i, \Gamma) = \hat{w}_i^T A \hat{w}_i + \Gamma_{ii}(1 - \hat{w}_i^T B \hat{w}_i) - \sum_j \Gamma_{ij} \hat{w}_j^T B \hat{w}_i$$

(45)

We can also write the updates of $\mu$-EigenGame (Gemp et al., 2021) as a Lagrangian pseudo-utility. Note that this is a slightly different expression to that given by the authors.

$$\mathcal{P}U_i^{\mu}(w_i|w_j < i, \Gamma) = \hat{w}_i^T A \hat{w}_i - \sum_{j < i} \Gamma_{ij} \hat{w}_j^T \hat{w}_i$$

(46)
D.4 Utility Shape

Lemma D.1. Let $\hat{w}_i = m(\cos(\theta_i) w_i + \sin(\theta_i) \Delta_i)$ where $\hat{w}_i^T B \hat{w}_i = m$, then:

$$U_i(\hat{w}_i, w_{j<i}) = U_i(mw_i, w_{j<i}) - \sin^2(\theta_i)(U_i(mw_i, w_{j<i}) - U_i(m\Delta_i, w_{j<i}))$$  \hspace{1cm} (47)

We will show that this result follows from similar logic to [Gemp et al., 2020] once the scaling factor $m$ is accounted for.

Proof. Let $\Delta_i = \sum_{l=1}^d p_l w_l, \|p\| = 1$. Decomposing the utility function for player $i$ we have:

$$U_i(\hat{w}_i, w_{j<i}) = 2(\hat{w}_i, A\hat{w}_i) - (\hat{w}_i, B\hat{w}_i)(\hat{w}_i, A\hat{w}_i) - 2\sum_{j<i}(\hat{w}_i, Bw^{(j)})(w^{(j)}, A\hat{w}_i)$$  \hspace{1cm} (48)

$$= (2m - m^2)(\cos^2(\theta_i)\lambda_{ii} + \sin^2(\theta_i)(\Delta_i, \lambda\Delta_i))$$

$$- 2m\sum_{j<i}(\cos(\theta_i) w_i + \sin(\theta_i) \Delta_i, Aw_j)(\cos(\theta_i) w_i + \sin(\theta_i) \Delta_i, Bw_j)$$  \hspace{1cm} (49)

$$= (2m - m^2)(\cos^2(\theta_i)\lambda_{ii} + \sin^2(\theta_i)(\Delta_i, \lambda\Delta_i))$$

$$- 2m\sum_{j<i}\sin^2(\theta_i)(\Delta_i, Aw_j)(\Delta_i, Bw_j)$$  \hspace{1cm} (50)

$$= (2m - m^2)\lambda_{ii}$$

$$- (2m - m^2)\sin^2(\theta_i)\lambda_{ii} + \sin^2(\theta_i)((2m - m^2)(\Delta_i, A\Delta_i)$$

$$- 2m\sum_{j<i}(\Delta_i, Aw_j)(\Delta_i, Bw_j)$$  \hspace{1cm} (51)

$$= (2m - m^2)\lambda_{ii}$$

$$- \sin^2(\theta_i)((2m - m^2)\lambda_{ii} + (2m - m^2)(\Delta_i, A\Delta_i) - 2m\sum_{j<i}(\Delta_i, Aw_j)(\Delta_i, Bw_j))$$  \hspace{1cm} (52)

$$= u_i(mw_i, w_{j<i}) - \sin^2(\theta_i)(U_i(mw_i, w_{j<i}) - U_i(m\Delta_i, w_{j<i}))$$  \hspace{1cm} (53)

\[
\]

D.5 Utility as a Projection Deflation

$$U^\delta_i = 2\hat{w}_i^T[I - \sum_{j<i}B\hat{w}_j\hat{w}_j^T]A\hat{w}_i - \hat{w}_i^T B\hat{w}_i \hat{w}_i^T A\hat{w}_i$$  \hspace{1cm} (54)

Analogously to the previous work in $\alpha$-EigenGame [Gemp et al., 2020], the matrix $[I - \sum_{j\leq i}B\hat{w}_j\hat{w}_j^T]$ has a natural interpretation as a projection deflation.
E

VECTORIZED $\delta$-EIGENGAME

Algorithm 4 Vectorized $\delta$-EigenGame

Input: data stream $Z_t$ consisting of $b$ samples from $z_n$, learning rate $\eta$

for $t = 1$ to $T$ do
  Construct independent unbiased estimates $\hat{A}$ and $\hat{B}$ from $Z_t$
  Rewards ← $2\hat{A}\hat{W}$
  Penalties ← $B\hat{W}$ triu($\hat{W}^T\hat{A}\hat{W}$)
  $\nabla ←$ Rewards - Penalties
  $\hat{W}' ← \hat{W} + \eta t \nabla$
end for

Where triu returns a matrix with the entries below the main diagonal set to zero.

F

A CONNECTION TO SELF-SUPERVISED LEARNING METHODS

Reorganizing our update equation (5), we find that the intuition of our method can also be understood as three terms encouraging variance in $A$, penalizing variance in $B$, and discouraging covariance.

$$\Delta_i^\delta = \text{Reward} - \text{Variance Penalty} - \text{Orthogonality Penalty}$$

The motivation is similar to that in recent work in self-supervised learning (Zbontar et al., 2021) and in particular the VICReg method in Bardes et al. (2021). Recent work has shown links between several self-supervised learning approaches and classical spectral embedding methods (Balestriero & LeCun, 2022), some of which could be represented by GEPs. Like CCA, many self-supervised learning approaches are based on finding a function which is invariant to an image and its augmented version i.e. the learnt representations of both are correlated.

G

EXPERIMENT DETAILS

G.1 TOTAL CORRELATION CAPTURED (TCC)

This is the sum of the canonical correlations of the learnt representation (i.e. the sum of the top-k canonical correlations of $X$ and $Y$).

G.2 PROPORTION OF CORRELATION CAPTURED (PCC)

This is the sum of the canonical correlations of the learnt representation as a proportion of the sum of the canonical correlations of the learnt representation using the population ground truth (i.e. the sum of the top-k canonical correlations of $X$ and $Y$).

G.3 STOCHASTIC CCA

The latter two datasets are formed from left and right halves of the canonical datasets (LeCun et al., 2010; Krizhevsky et al., 2009). With the same initialization for all methods, we trained for 10 epochs on each dataset with a mini-batch size of 128 and illustrate the models with the best performance in the validation set.

G.4 STOCHASTIC CCA HYPERPARAMETERS

Learning rate was tuned from $\eta = (10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5})$ and $\gamma$-EigenGame parameter $\gamma$ was tuned from the same range. We used Jax (Babuschkin et al., 2020) to optimize the linear CCA
models using the Jaxline framework. We used WandB (Biewald 2020) for experiment tracking to develop insights for this paper.

G.5 DEEP CCA

We use two variants of paired MNIST datasets. The first is identical to the split MNIST dataset in the previous section. The second harder problem is closely related to an experiment by Wang et al. (2015a). Their ‘noisy’ paired MNIST data takes two different digits with the same class. The first is rotated randomly while the second has additive gaussian noise. Finally, we use the X-Ray Microbeam (XRMB) dataset from Arora et al. (2016). For all of the datasets, we use two encoders with 50 latent dimensions and two hidden layers with size 800 and leaky ReLu activation functions, a similar architecture to that used in Wang et al. (2015c). We compare our proposed method to DCCA-NOI at mini-batch sizes of 20 and 100 and DCCA-STOL with mini-batch size 100 and 500 (DCCA-STOL cannot be used for mini-batch sizes less than the number of latent dimensions).

G.6 DCCA HYPERPARAMETERS

We trained for 30 epochs on each dataset with mini-batch sizes of 20 and 100. Learning rate was tuned from $\eta = \left(10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}\right)$ and the DCCA-NOI parameter $\rho$ was tuned between 0 and 1. We use PyTorch (Paszke et al. 2019) with the Adam optimizer (Kingma & Ba, 2014).

H ADDITIONAL EXPERIMENTS

H.1 STOCHASTIC CCA WITH SMALLER MINI-BATCH SIZES

In this section we repeat the experiments described in the main text with smaller mini-batch sizes (64 and 32).

Results for mini-batch sizes 32 and 64 are broadly similar to those in the main text for mini-batch size 128. In the MNIST data we can see again that there is a tradeoff between speed of convergence in early iterations and the quality of the solution.

Figure 4: CCA with stochastic mini-batches of size 64 (top) and 32 (bottom): proportion of correlation captured with respect to Scipy ground truth by $\delta$-EigenGame vs prior work. The maximum value is 1.
H.2 Partial Least Squares

The Partial Least Squares (PLS) [Wold et al. (1984)] problem can also be formulated as a similar GEP but with $B$ replaced by the identity matrix. PLS is equivalent to finding the singular value decomposition (SVD) of the covariance matrix $X^\top Y$. It has an interpretation as a (infinitely) ridge regularised CCA where the covariance matrices $\Sigma_{XX}$ and $\Sigma_{YY}$ are replaced by identity matrices; this corresponds to assuming no collinearity between variables.

H.2.1 PLS with stochastic mini-batches

In this experiment we compare our method to the Stochastic Power method [Arora et al. (2016)], $\gamma$-EigenGame, and SGHA for the stochastic PLS problem.

For these experiments we use the Proportion of Variance captured (PV). This is the sum of the singular values of the learnt representation using each stochastic optimisation method as a proportion of the sum of the singular values of the learnt representation using the population ground truth (i.e. the sum of the top-k singular values of the covariance matrix $X^\top Y$).

Figure 5 shows that all of the methods perform similarly in terms of variance captured across the datasets. While the stochastic power method is very fast to converge in the MNIST and CIFAR data, its solutions can be suboptimal. The performance of $\delta$-EigenGame is arguably more surprising for the PLS problem because both the Stochastic Power method and $\gamma$-EigenGame explicitly enforce the constraints at each iteration whereas $\delta$-EigenGame only enforces the constraint via penalty terms.

Figure 5: PLS with stochastic mini-batches: proportion of variance captured with respect to Scipy ground truth by $\delta$-EigenGame vs prior work. The maximum value is 1.
Figure 6: PLS with stochastic mini-batches of size 64 (top) and 32 (bottom): proportion of variance captured with respect to Scipy ground truth by $\delta$-EigenGame vs prior work. The maximum value is 1.