Stochastic Optimization for Deep CCA via Nonlinear Orthogonal Iterations

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Abstract — Deep CCA is a recently proposed deep neural network extension to the traditional canonical correlation analysis (CCA), and has been successful for multi-view representation learning in several domains. However, stochastic optimization of the deep CCA objective is not straightforward, because it does not decouple over training examples. Previous optimizers for deep CCA are either batch-based algorithms or stochastic optimization using large minibatches, which can have high memory consumption. In this paper, we tackle the problem of stochastic optimization for deep CCA with small minibatches, based on an iterative solution to the CCA objective, and show that we can achieve as good performance as previous optimizers and thus alleviate the memory requirement.

I. INTRODUCTION

Stochastic gradient descent (SGD) is a fundamental and popular optimization method for machine learning problems [1], [2], [3], [4], [5]. SGD is particularly well-suited for large-scale machine learning problems because it is extremely simple and easy to implement, it often achieves better generalization (test) performance (which is the focus of machine learning research) than sophisticated batch algorithms, and it usually achieves large error reduction very quickly in a small number of passes over the training set [6]. One intuitive explanation for the empirical success of stochastic gradient descent for large data is that it makes better use of data redundancy, with an extreme example given by [2]: If the training set consists of 10 copies of the same set of examples, then computing an estimate of the gradient over one single copy is 10 times more efficient than computing the full gradient over the entire training set, while achieving the same optimization progress in the following gradient descent step.

At the same time, “multi-view” data are becoming increasingly available, and methods based on canonical correlation analysis (CCA) [7] that use such data to learn representations (features) form an active research area. The views can be multiple measurement modalities, such as simultaneously recorded audio + video [8], [9], audio + articulation [10], images + text [11], [12], [13], or parallel text in two languages [14], [15], [16], [17], [18], but may also be different information extracted from the same source, such as words + context [19] or document text + text of inbound hyperlinks [20]. The presence of multiple information sources presents an opportunity to learn better representations (features) by analyzing multiple views simultaneously.

In the following sections, we briefly introduce deep CCA

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and discuss the difficulties in training it (Section II); motivate and propose our new algorithm (Section III); describe related work (Section IV); and present experimental results comparing different optimizers (Section V).

II. DEEP CCA

Notation In the multi-view feature learning setting, we have access to paired observations from two views, denoted \((x_1, y_1), \ldots, (x_N, y_N)\), where \(N\) is the training set size, \(x_i \in \mathbb{R}^{d_x}\) and \(y_i \in \mathbb{R}^{d_y}\) for \(i = 1, \ldots, N\). We also denote the data matrices for View 1 and View 2 \(X = [x_1, \ldots, x_N]\) and \(Y = [y_1, \ldots, y_N]\), respectively. We use bold-face letters, e.g., \(f\), to denote mappings implemented by DNNs, with a corresponding set of learnable parameters, denoted, e.g., \(W_f\). The dimensionality of the learned features is denoted \(L\).

Deep CCA (DCCA) [21] extends (linear) CCA [7] by extracting \(d_x\) and \(d_y\)-dimensional nonlinear features with two DNNs \(f\) and \(g\) for views 1 and 2 respectively, such that the canonical correlation (measured by CCA) between the DNN outputs is maximized, as illustrated in Fig. 1. The goal of the final CCA is to find \(L \leq \min(d_x, d_y)\) pairs of linear projection vectors \(U \in \mathbb{R}^{d_x \times L}\) and \(V \in \mathbb{R}^{d_y \times L}\) such that the projections of each view (a.k.a. canonical variables, [7]) are maximally correlated with their counterparts in the other view. Formally, the DCCA objective (1) is

\[
\begin{align*}
\max_{W_f, W_g, U, V} & \quad \text{tr} (U^T F G^T V) \\
\text{s.t.} & \quad U^T F F^T U = V^T G G^T V = I,
\end{align*}
\]

where \(F = f(X) = [f(x_1), \ldots, f(x_N)] \in \mathbb{R}^{d_x \times N}\) and \(G = g(Y) = [g(y_1), \ldots, g(y_N)] \in \mathbb{R}^{d_y \times N}\). We assume that \(F\) and \(G\) are centered at the origin for notational simplicity; if they are not, we can center them as a pre-processing operation. Notice that if we use the original input data without further feature extraction, i.e. \(F = X\) and \(G = Y\), then we recover the CCA objective. In DCCA, the final features (projections) are

\[
\begin{align*}
\hat{f}(x) = U^T f(x) & \quad \text{and} \quad \hat{g}(y) = V^T g(y).
\end{align*}
\]

We observe that the last CCA step with linear projection mappings \(U\) and \(V\) can be considered as adding a linear layer on top of the feature extraction networks \(f\) and \(g\) respectively. In the following, we sometimes refer to the concatenated networks \(\hat{f}\) and \(\hat{g}\) as defined in (2), with \(W_f = \{W_f, U\}\) and \(W_g = \{W_g, V\}\).

Let \(\Sigma_{fg} = FG^T\), \(\Sigma_{ff} = FF^T\) and \(\Sigma_{gg} = GG^T\) be the (scaled) cross- and auto-covariance matrices of the feature-mapped data in the two views. It is well-known that, when \(f\) and \(g\) are fixed, the last CCA step in (1) has a closed form solution as follows. Define \(\Sigma_{fg} = \Sigma_{ff}^{1/2} \Sigma_{fg} \Sigma_{gg}^{1/2}\), and let \(\Sigma_{fg} = \hat{U} \Lambda \hat{V}^T\) be its rank-L singular value decomposition (SVD), where \(\Lambda\) contains the singular values \(\sigma_1 \geq \cdots \geq \sigma_L \geq 0\) on its diagonal. Then the optimum of (1) is achieved by \((U, V) = (\Sigma_{ff}^{1/2} U, \Sigma_{gg}^{1/2} V)\), and the optimal objective value (the total canonical correlation) is \(\sum_{j=1}^L \sigma_j\).

By switching \(\max(\cdot)\) with \(\min(-\cdot)\), and adding 1/2 times the constraints, it is straightforward to show that (1) is equivalent to the following:

\[
\begin{align*}
\min_{W_f, W_g, U, V} & \quad \frac{1}{2} \|U^T F - V^T G\|_F^2 \\
\text{s.t.} & \quad (U^T F)(U^T F)^T = (V^T G)(V^T G)^T = I.
\end{align*}
\]

In other words, CCA minimizes the squared difference between the projections of the two views, subject to the whitening constraints. This alternative formulation of CCA will also shed light on our proposed algorithm for DCCA.

The DCCA objective (1) differs from typical DNN regression or classification training objectives. Typically, the objectives are unconstrained and can be written as the expectation (or sum) of error functions (e.g., squared loss or cross entropy) incurred at each training example. This property naturally suggests stochastic gradient descent (SGD) for optimization, where one iteratively generates random unbiased estimates of the gradient based on one or a few training examples (a minibatch) and takes a small step in the opposite direction. However, the objective in (1) cannot be written as an unconstrained sum of errors. The difficulty lies in the fact that the training examples are coupled through the auto-covariance matrices (in the constraints), which can not be reliably estimated with only a small amount of data.

When introducing deep CCA, [21] used the L-BFGS algorithm for optimization. To compute the gradients of the objective with respect to \((W_f, W_g)\), one first computes the gradient \(\hat{f}\) with respect to \((F, G)\) as

\[
\begin{align*}
\frac{\partial \sum_{j=1}^L \sigma_j}{\partial F} = 2 \Delta_{ff} F + \Delta_{fg} G, \\
\text{with} & \quad \Delta_{ff} = -\frac{1}{2} \Sigma_{ff}^{1/2} \hat{U} \hat{A} \hat{U}^T \Sigma_{ff}^{-1/2} \\
& \quad \Delta_{fg} = \Sigma_{gg}^{-1/2} \hat{U} \hat{V}^T \Sigma_{gg}^{-1/2}
\end{align*}
\]

In principle there is no need for the final linear layer; we could define DCCA such that the correlation objective and constraints are imposed on the final nonlinear layer. However, the linearity of the final layer is crucial for algorithmic implementations such as ours.

Technically we are computing subgradients as the “sum of singular values” (trace norm) is not a differentiable function of the matrix.
**Algorithm 1** CCA projections via alternating least squares.

**Input:** Data matrices $F \in \mathbb{R}^{d_x \times N}$, $G \in \mathbb{R}^{d_y \times N}$. Initialization $U_0 \in \mathbb{R}^{d_x \times L}$ s.t. $U_0^T U_0 = I$.

$$A_0 \leftarrow U_0^T \Sigma_{f,g}^{-\frac{1}{2}} F$$

for $t = 1, 2, \ldots, T$

1. $B_t \leftarrow A_{t-1} G^\top (G G^\top)^{-1} G$
2. $A_t \leftarrow (B_t B_t^\top)^{-\frac{1}{2}} B_t$
3. $A_t \leftarrow (A_t A_t^\top)^{-\frac{1}{2}} A_t$

end for

**Output:** $A_T / B_T$ are the CCA projections of view 1/2.

where $\Sigma_{f,g} = \tilde{U} \Lambda \tilde{V}^\top$ is the SVD of $\tilde{\Sigma}_{f,g}$ as in the closed-form solution to CCA, and $\partial \Sigma_{f,g} / \partial G$ has an analogous expression. One can then compute the gradients with respect to $W_f$ and $W_g$ via the standard backpropagation procedure [29]. From the gradient formulas, it is clear that the key to optimizing DCCA is the SVD of $\tilde{\Sigma}_{f,g}$; various nonlinear optimization techniques can be used here once the gradient is computed. In practice, however, batch optimization is undesirable for applications with large training sets or large DNN architectures, as each gradient step computed on the entire training set can be expensive in both memory and time.

Later, it was observed by [22] that stochastic optimization still works well even for the DCCA objective, as long as larger minibatches are used to estimate the covariances and $\tilde{\Sigma}_{f,g}$ when computing the gradient with [30]. More precisely, the authors find that learning plateaus at a poor objective value if the minibatch is too small, but fast convergence and better generalization than batch algorithms can be obtained once the minibatch size is larger than some threshold, presumably because a large minibatch contains enough information to estimate the covariances and therefore the gradient accurately enough (the threshold of minibatch size varies for different datasets because they have different levels of data redundancy). Theoretically, the necessity of using large minibatches in this approach can also be established. Let the empirical estimate of $\Sigma_{f,g}$ using a minibatch of $n$ samples be $\Sigma_{f,g}^{(n)}$. It can be shown that the expectation of $\Sigma_{f,g}^{(n)}$ does not equal the true $\Sigma_{f,g}$ computed using the entire dataset, mainly due to the nonlinearities in the matrix inversion and multiplication operations in computing $\Sigma_{f,g}$, and the nonlinearity in the “sum of singular values” (trace norm) of $\Sigma_{f,g}$; moreover, the spectral norm of the error $\left\| \Sigma_{f,g}^{(n)} - \Sigma_{f,g} \right\|$ decays slowly as $\frac{1}{\sqrt{n}}$. Consequently, the gradient estimated on a minibatch using [30] does not equal the true gradient of the objective in expectation, indicating that the stochastic approach of [22] does not qualify as a stochastic gradient descent method for the DCCA objective.

III. Our Algorithm

A. An iterative solution to linear CCA

Our solution to (1) is inspired by the iterative solution for finding the linear CCA projections $(U^\top F, V^\top G)$ for inputs $(F, G)$, as shown in Algorithm 1. This algorithm computes the top-$L$ singular vectors $(U, V)$ of $\Sigma_{f,g}$ via orthogonal iterations [30]. An essentially identical algorithm (named alternating least squares for reasons that will soon become evident) appears in [31, Algorithm 5.2] and according to the authors the idea goes back to J. Von Neumann. A similar algorithm is also recently used by [32, Algorithm 1] for large scale linear CCA with high-dimensional sparse inputs, although their algorithm does not implement the whitening operations $A_t \leftarrow (A_t A_t^\top)^{-\frac{1}{2}} A_t$ and $B_t \leftarrow (B_t B_t^\top)^{-\frac{1}{2}} B_t$ or they use the QR decomposition instead. The convergence of Algorithm 1 is characterized by the following theorem, which parallels [32, Theorem 1].

**Theorem 1:** Let the singular values of $\Sigma_{f,g}$ be

$$\sigma_1 \geq \cdots \geq \sigma_L > \sigma_{L+1} \geq \cdots \geq \sigma_{\min(d_x, d_y)}$$

and suppose $\tilde{U}_0^T \tilde{U}$ is nonsingular. Then the output $(A_T, B_T)$ of Algorithm 1 converges to the CCA projections as $T \to \infty$.

**Proof:** We focus on showing that $A_T$ converges to the view 1 projection; the proof for $B_T$ is similar.

First recall that $\Sigma_{f,g} = U \Lambda V^\top$ is the rank-$L$ SVD of $\Sigma_{f,g}$, and thus $U$ contains the top-$L$ eigenvectors of $\Sigma_{f,g}$, $\tilde{U} = U \Lambda^{\frac{1}{2}} V^\top$.

Since the operation $(A A^\top)^{-\frac{1}{2}} A$ extracts an orthonormal basis of the row space of $A$, at iteration $t$ we can write

$$A_{t-1} G^\top (G G^\top)^{-1} G = P_t B_t$$

$$B_t F^\top (F F^\top)^{-1} F = Q_t A_t$$

where $P_t \in \mathbb{R}^{L \times L}$ and $Q_t \in \mathbb{R}^{L \times L}$ are nonsingular coefficient matrices (as the initialization $\tilde{U}_0$ is nonsingular) for representing the left-hand side matrices in their row space basis. Combining the above two equations gives the following recursion at iteration $t$:

$$A_{t-1} G^\top (G G^\top)^{-1} G = P_t Q_t A_t$$

By induction, it can be shown that by the end of iteration $t$ we have

$$\Sigma_{f,g} = \tilde{U}_t^T \tilde{U}_t$$

where $O_t = P_1 Q_1 \cdots P_t Q_t \in \mathbb{R}^{L \times L}$ is nonsingular. Plugging in the definition of $A_0$, this equation reduces to

$$\tilde{U}_0^T \left( \tilde{\Sigma}_{f,g} \tilde{\Sigma}_{f,g}^\top \right)^{\frac{1}{2}} \Sigma_{f,g} = O_t A_t$$

It is then clear that $A_t$ can be written as

$$A_t = \tilde{U}_t^T \tilde{S}_{f,g}^\top F$$

with

$$\tilde{U}_t = \left( \tilde{\Sigma}_{f,g} \tilde{\Sigma}_{f,g}^\top \right)^{\frac{1}{2}} \tilde{U}_0 \tilde{O}_t^{-1} \in \mathbb{R}^{d_x \times L}$$

And since $A_t$ has orthonormal rows, we have

$$I = A_t A_t^\top = \tilde{U}_t^T \tilde{S}_{f,g}^\top F = \tilde{U}_t^T \tilde{U}_t$$

indicating that $\tilde{U}_t$ has orthonormal columns.
As a result, we consider the algorithm as working implicitly in the space of $\{\tilde{U}_T \in \mathbb{R}^{d_t \times L}, t = 0, \ldots, T\}$, and have
\[
(\Sigma f g^\top \Sigma f g)^T \tilde{U}_0 = O_T \tilde{U}_T.
\]
(6)

Following the argument of [30, Theorem 8.2.2]) for orthogonal iterations, under the assumptions of our theorem, the column space of $U_T$ converges to that of $\tilde{U}$, the top-$L$ eigenvectors of $\Sigma f g^2 \Sigma f g^\top$ with a linear convergence rate depending on the ratio $\sigma_{L+1}/\sigma_L$. In view of the relationship between $U_T$ and $\tilde{A}_t$, we conclude that $A_T$ converges to the view 1 CCA projection as $T \to \infty$.

It is interesting to note that, besides the whitening operations $(\tilde{A}_t \tilde{A}_t^\top)^{-\frac{1}{2}} \tilde{A}_t$, the other basic operations in each iteration of Algorithm 1 are of the form
\[
A_t \leftarrow B_t F^\top (F F^\top)^{-1} F
\]
(7)

which is solving a linear least squares (regression) problem with input $F$ and target output $B_t$ satisfying $B_t B_t^\top = I$, i.e.,
\[
\min_{U_t} \|U_t^\top F - B_t\|_F^2.
\]

By setting the gradient of this unconstrained objective to zero, we obtain $U_t = (F F^\top)^{-1} B_t$ and so the optimal projection $U_t^\top F$ coincides with the update (7).

For [32], the advantage of the alternating least squares formulation over the exact solution to CCA is that it does not need to form the high-dimensional (nonsparse) matrix $\Sigma f g^2$ instead it directly operates on the projections, which are much smaller in size, and one can solve the least squares problems using iterative algorithms that require only sparse matrix-vector multiplications.

**B. Extension to DCCA**

Our intuition for adapting Algorithm 1 to DCCA is as follows. During DCCA optimization, the DNN weights $(W_f, W_g)$ are updated frequently and thus the outputs $(f(X), g(Y))$, which are also the inputs to the last CCA step, also change upon each weight update. Therefore, the last CCA step needs to adapt to the fast evolving input data distribution. On the other hand, if we are updating the CCA weights $(U, V)$ based on a small minibatch of data (as happens in stochastic optimization), it is intuitively wasteful to solve $(U, V)$ to optimality rather than to make a simple update based on the minibatch. Moreover, the objective of this “simple update” can be used to derive a gradient estimate for $(W_f, W_g)$.

In view of Algorithm 1, it is a natural choice to embed the optimization of $(f, g)$ into the iterative solution to linear CCA. Instead of solving the regression problem $F \rightarrow B_t$ exactly with $A_t \leftarrow B_t F^\top (F F^\top)^{-1} F$, we try to solve the problem $X \rightarrow B_t$ on a minibatch with a gradient descent step on $(W_f, U)$ jointly (recall $F = f(X)$ is a function of $W_f$). Notice that this regression objective is unconstrained and decouples over training samples, so an unbiased gradient estimate for this problem can be easily derived through standard backpropagation using minibatches (however, this gradient estimate may not be unbiased for the original DCCA objective; see discussion in Section IV).

The less trivial part of Algorithm 1 to implement in DCCA is the whitening operation $(\tilde{A}_t \tilde{A}_t^\top)^{-\frac{1}{2}} \tilde{A}_t$, which needs $\tilde{A}_t \in \mathbb{R}^{L \times N}$, the projections of all training samples. We would like to avoid the exact computation of $\tilde{A}_t$ as it requires feeding forward the entire training set $X$ with the updated $W_f$, and the computational cost of this operation is as high as (half of) the cost of evaluating the batch gradient (the latter requires both the forward and backward passes).

We bypass this difficulty by noting that the only portion of $\tilde{A}_t$ needed is the updated projection of the minibatch used in the subsequent view 2 regression problem $X \rightarrow A_t$ (corresponding to the step $B_{t+1} \leftarrow A_t G^\top (G G^\top)^{-1} G$ in Algorithm 1). Therefore, if we have an estimate of the covariance $\Sigma_{ff} := \tilde{A}_t \tilde{A}_t^\top$ without feeding forward the entire training set, we can estimate the updated projection for this minibatch only. Specifically, we estimate this quantity by
\[
\Sigma_{ff}^t \leftarrow \rho \Sigma_{ff}^{t-1} + (1 - \rho) \frac{N}{|b|} \tilde{f}(X_b) \tilde{f}(X_b)^\top,
\]
(8)

where $\rho \in [0, 1]$, $X_b$ denotes a minibatch of data with index set $b$, and $|b|$ denotes the size (number of samples) of this minibatch. The time constant $\rho$ controls how much the previous covariance estimate is kept in the update; a larger $\rho$ indicates forgetting the “memory” more slowly. Assuming that the parameters do not change much from time $t - 1$ to $t$, then $\Sigma_{ff}^{t-1}$ will be close to $\Sigma_{ff}^t$, and incorporating it helps to reduce the variance from the term $\tilde{f}(X_b) \tilde{f}(X_b)^\top$ when $|b| \ll N$. The update in (8) has a form similar to that of the widely used momentum technique in the optimization [33] and neural network literature [34], [35], and is also used by [36], [37], [38] for online subspace tracking and anomaly detection. We note that the memory cost of $\Sigma_{ff}^t \in \mathbb{R}^{L \times L}$ is small as we look for low-dimensional projections (small $L$) in practice. These advantages validate our choice of whitening operations over the more commonly used QR decomposition used by [32].

We give the resulting nonlinear orthogonal iterations procedure (NOI) for DCCA in Algorithm 2. Now adaptively whitening is used to obtain suitable target outputs of the regression problems for computing derivatives $(\partial W_f, \partial W_g)$, and we no longer maintain the whitened projections of the entire training set at each iteration. Therefore, by the end of the algorithm, $(\tilde{f}(X), \tilde{g}(Y))$ may not satisfy the whitening constraints of 1. One may use an additional CCA step on $(\tilde{f}(X), \tilde{g}(Y))$ to obtain a feasible solution of the original problem if desired, and this amounts to linear transforms in $\mathbb{R}^L$, which do not change the canonical correlations between the projections for both the training and test sets. In practice, we adaptively estimate the mean of $(\tilde{f}(X), \tilde{g}(Y))$ with an update formula similar to that of (8) and center the samples accordingly before estimating the covariances and computing the target outputs. We also use momentum in

\footnote{We add a small value $\epsilon > 0$ to the diagonal of the covariance estimates in our implementation for numerical stability.}
### Algorithm 2: Nonlinear orthogonal iterations (NOI) for DCCA.

**Input:** Data matrix $\mathbf{X} \in \mathbb{R}^{d_x \times N}$, $\mathbf{Y} \in \mathbb{R}^{d_y \times N}$. Initialization $(\mathbf{W}_f, \mathbf{W}_g)$, time constant $\rho$, learning rate $\eta$.

Randomly choose a minibatch $(\mathbf{X}_{b_0}, \mathbf{Y}_{b_0})$

$$
\Sigma_{ff} \leftarrow \frac{1}{|b_0|} \sum_{i \in b_0} \mathbf{f}(\mathbf{x}_i)^\top \mathbf{f}(\mathbf{x}_i),
\Sigma_{gg} \leftarrow \frac{1}{|b_0|} \sum_{i \in b_0} \mathbf{g}(\mathbf{y}_i)^\top \mathbf{g}(\mathbf{y}_i)^\top
$$

for $t = 1, 2, \ldots, T$ do

Randomly choose a minibatch $(\mathbf{X}_{b_t}, \mathbf{Y}_{b_t})$

$$
\Sigma_{ff} \leftarrow \rho \Sigma_{ff} + (1 - \rho) \frac{1}{|b_t|} \sum_{i \in b_t} \mathbf{f}(\mathbf{x}_i)^\top \mathbf{f}(\mathbf{x}_i)^\top,
\Sigma_{gg} \leftarrow \rho \Sigma_{gg} + (1 - \rho) \frac{1}{|b_t|} \sum_{i \in b_t} \mathbf{g}(\mathbf{y}_i)^\top \mathbf{g}(\mathbf{y}_i)^\top
$$

Compute the gradient $\partial f_{\mathbf{W}_f}$ of the objective

$$
\min_{\mathbf{W}_f} \frac{1}{|b_t|} \sum_{i \in b_t} \left\| \mathbf{f}(\mathbf{x}_i) - \Sigma_{gg}^{-\frac{1}{2}} \mathbf{g}(\mathbf{y}_i) \right\|^2
$$

Compute the gradient $\partial g_{\mathbf{W}_g}$ of the objective

$$
\min_{\mathbf{W}_g} \frac{1}{|b_t|} \sum_{i \in b_t} \left\| \mathbf{g}(\mathbf{y}_i) - \Sigma_{ff}^{-\frac{1}{2}} \mathbf{f}(\mathbf{x}_i) \right\|^2
$$

$\mathbf{W}_f \leftarrow \mathbf{W}_f - \eta \partial f_{\mathbf{W}_f}$, $\mathbf{W}_g \leftarrow \mathbf{W}_g - \eta \partial g_{\mathbf{W}_g}$.

end for

Output: The updated $(\mathbf{W}_f, \mathbf{W}_g)$.

### Algorithm 3: CCA via gradient descent over least squares.

**Input:** Data matrix $\mathbf{F} \in \mathbb{R}^{d_x \times N}$, $\mathbf{G} \in \mathbb{R}^{d_y \times N}$. Initialization $\mathbf{u}_0 \in \mathbb{R}^{d_x}$, $\mathbf{v}_0 \in \mathbb{R}^{d_y}$. Learning rate $\eta$.

for $t = 1, 2, \ldots, T$ do

$$
\mathbf{u}_t \leftarrow \mathbf{u}_{t-1} - \eta \mathbf{F}^\top \mathbf{u}_{t-1} - \frac{1}{\parallel \mathbf{v}_{t-1} \parallel^2} \mathbf{G}^\top \mathbf{v}_{t-1},
\mathbf{v}_t \leftarrow \mathbf{v}_{t-1} - \eta \mathbf{G}^\top \mathbf{v}_{t-1} - \frac{1}{\parallel \mathbf{u}_{t-1} \parallel^2} \mathbf{F}^\top \mathbf{u}_{t-1}
$$

end for

Output: $\mathbf{u}/\mathbf{v}$ are the CCA directions of view 1/2.

(For a one-dimensional projection, to be consistent with the notation of [47]) in Algorithm 3 where we take a batch gradient descent step over the least squares objectives in each iteration. This algorithm is equivalent to Algorithm 3 of [47]. Although intuitively very simple, the analysis of this algorithm is challenging. In [47] it is shown that the solution to the CCA objective is a fixed point of this algorithm, but no global convergence property is given. We also notice that the gradients used in this algorithm are derived from the alternating least squares problems

$$
\min_{\mathbf{u}} \parallel \mathbf{u}^\top \mathbf{F} - \frac{\mathbf{v}^\top \mathbf{G}}{\parallel \mathbf{v}^\top \mathbf{G} \parallel_F} \parallel^2_F \text{ and } \min_{\mathbf{v}} \parallel \mathbf{v}^\top \mathbf{G} - \frac{\mathbf{u}^\top \mathbf{F}}{\parallel \mathbf{u}^\top \mathbf{F} \parallel_F} \parallel^2_F,
$$

while the true CCA objective can be written as

$$
\min_{\mathbf{u}, \mathbf{v}} \parallel \mathbf{u}^\top \mathbf{F} - \mathbf{v}^\top \mathbf{G} \parallel^2_F.
$$

This shows that Algorithm 3 is not implementing gradient descent over the CCA objective.

When extending Algorithm 3 to stochastic optimization, we observe the key differences between their algorithm and ours as follows. Due to the evolving $(\mathbf{W}_f, \mathbf{W}_g)$, the last CCA step in the DCCA model is dealing with different $(\mathbf{f}(\mathbf{X}), \mathbf{g}(\mathbf{Y}))$ and covariance structures in different iterates, even though the original inputs $(\mathbf{X}, \mathbf{Y})$ are the same; this motivates the adaptive estimate of covariances in (8). In the whitening steps of [47], however, the covariances are estimated using only the current minibatch at each iterate, without consideration of the remaining training samples or previous estimates, which corresponds to $\rho \rightarrow 0$ in our estimate. [47] also suggests using a minibatch size of the order $O(L)$, the dimensionality of the covariance matrices to be estimated, in order to obtain a high-accuracy estimate for whitening. As we will show in the experiments, in both CCA and DCCA, it is important to incorporate the previous covariance estimates ($\rho \rightarrow 1$) at each step to reduce the variance, especially when small minibatches are used. Based on the above analysis for batch gradient descent, solving the least squares problem with stochastic gradient descent is
not implementing stochastic gradient descent over the CCA objective. Nonetheless, as shown in the experiments, this stochastic approach works remarkably well and can match the performance of batch optimization, for both linear and nonlinear CCA, and is thus worth careful analysis.

Finally, we remark that other possible approaches for solving (1) exist. Since the difficulty lies in the whitening constraints, one can relax the constraints and solve the Lagrangian formulation repeatedly with updated Lagrangian multipliers, as done by [25]; or one can introduce auxiliary variables and apply the quadratic penalty method [48], as done by [49]. The advantage of such approaches is that there exists no coupling of all training samples when optimizing the primal variables (the DNN weight parameters) and thus one can easily apply SGD there, but one also needs to deal with the Lagrange multipliers or to set a schedule for the quadratic penalty parameter (which is non-trivial) and alternately optimize over two sets of variables repeatedly in order to obtain a solution of the original constrained problem.

V. EXPERIMENTS

A. Experimental setup

We now demonstrate the NOI algorithm on the two real-world datasets used by [21] when introducing DCCA. The first dataset is a subset of the University of Wisconsin X-Ray Microbeam corpus [50], which consists of simultaneously recorded acoustic and articulatory measurements during speech. Following [21], [22], the acoustic view inputs are 39D Mel-frequency cepstral coefficients and the articulatory view inputs are horizontal/vertical displacement of 8 pellets attached to different parts of the vocal tract, each then concatenated over a 7-frame context window, for speaker ‘JW11’. The second dataset consists of left/right halves of the images in the MNIST dataset [51], and so the input of each view consists of $28 \times 14$ grayscale images. We do not tune neural network architectures as it is out of the scope of this paper. Instead, we use DNN architectures similar to those used by [21] with ReLU activations [52], and we achieve better generalization performance with these architectures mainly due to better optimization. The statistics of each dataset and the chosen DNN architectures (widths of input layer-hidden layers-output layer) are given in Table I. The projection dimensionality $L$ is set to 112/50 for JW11/MNIST respectively as in [21]; these are also the maximum possible total canonical correlations for the two datasets.

We compare three optimization approaches: full batch optimization by L-BFGS [21], using the implementation of [53] which includes a good line-search procedure; stochastic optimization with large minibatches [22], denoted STOL; and our algorithm, denoted NOI. We create training/tuning/test splits for each dataset and measure the total canonical correlations on the test sets (measured by linear CCA on the projections) for different optimization methods. Hyperparameters of each algorithm, including $\rho$ for NOI, minibatch size $n = |b_1| = |b_2|, \ldots$, learning rate $\eta$ and momentum $\mu$ for both STOL and NOI, are chosen by grid search on the tuning set. All methods use the same random initialization for DNN weight parameters. We set the maximum number of iterations to 300 for L-BFGS and number of epochs (one pass over the training set) to 50 for STOL and NOI.

B. Effect of minibatch size

In the first set of experiments, we vary the minibatch size $n$ of NOI over \{10, 20, 50, 100\}, while tuning $\rho$, $\eta$ and $\mu$. Learning curves (objective value vs. number of epochs) on the tuning set for each $n$ with the corresponding optimal hyperparameters are shown in Fig. 2. For comparison, we also show the learning curves of STOL with $n = 100$ and $n = 500$, while $\eta$ and $\mu$ are also tuned by grid search. We observe that STOL performs very well at $n = 500$ (with the performance on MNIST being somewhat better due to higher data redundancy), but it cannot achieve much progress in the objective over the random initialization with $n = 100$, for the reasons described earlier. In contrast, NOI achieves very competitive performance with various small minibatch sizes, with fast improvement in objective during the first few iterations, although larger $n$ tends to achieve slightly higher correlation on tuning/test sets eventually. Total canonical correlations on the test sets are given in Table II showing that we achieve better results than [21] with similar DNN architectures.

C. Effect of time constant $\rho$

In the second set of experiments, we demonstrate the importance of $\rho$ in NOI for different minibatch sizes. The total canonical correlations achieved by NOI on the tuning set for $\rho = \{0, 0.2, 0.4, 0.6, 0.8, 0.9, 0.99, 0.999, 0.9999\}$ are shown in Fig. 3 while other hyper-parameters are set to their optimal values. We confirm that for relatively large $n$, NOI works reasonably well with $\rho = 0$ (so we are using the same covariance estimate/whitening as [47]). But also as expected, when $n$ is small, it is beneficial to incorporate the

| dataset | training/tuning/test | $L$ | DNN architectures |
|---------|----------------------|-----|------------------|
| JW11    | 30K/11K/9K           | 112 | 273-180-180-112  |
|         |                      |     | 112-1200-1200-112 |
| MNIST   | 50K/10K/10K          | 50  | 392-800-800-50   |
|         |                      |     | 392-800-800-50   |

Fig. 2. Learning curves of different algorithms on tuning sets with different minibatch size $n$.
TABLE II
TOTAL TEST SET CANONICAL CORRELATION OBTAINED BY DIFFERENT ALGORITHMS.

| dataset | L-BFGS | STOL | NOI |
|---------|--------|------|-----|
| JW11    | 78.7   | 33.0 | 86.7|
| MNIST   | 47.0   | 26.1 | 46.4|

Fig. 3. Total correlation achieved by NOI on tuning sets with different $\rho$.

Fig. 4. Pure stochastic optimization of linear CCA using NOI. We show total correlation achieved by NOI with $n = 1$ on the MNIST training sets at different $\rho$, by the random initialization used by NOI, by the exact solution, and by STOL with $n = 500$.  

previous estimate of the covariance because the covariance information contained in each small minibatch is noisy. Also, as $\rho$ becomes too close to 1, the covariance estimates are not adapted to the DNN outputs and the performance of NOI degrades. Moreover, we observe that the optimal $\rho$ value seems different for each $n$.

D. Pure stochastic optimization for CCA

Finally, we carry out pure stochastic optimization ($n = 1$) for linear CCA on the MNIST dataset. Notice that linear CCA is a special case of DCCA with $(f, \hat{g})$ both being single-layer linear networks (although we have used small weight-decay terms for the weights, leading to a slightly different objective than that of CCA). Total canonical correlations achieved by STOL with $n = 500$ and by NOI (50 training epochs) on the training set with different $\rho$ values are shown in Fig. 4. The objective of the random initialization and the closed-form solution (by SVD) are also shown for comparison. NOI could not improve over the random initialization without memory ($\rho = 0$, corresponding to the algorithm of [47]), but gets very close to the optimal solution and matches the objective obtained by the previous large minibatch approach when $\rho \to 1$. This result demonstrates the importance of our adaptive estimate (8) also for CCA.

VI. CONCLUSIONS

In this paper, we have proposed a stochastic optimization algorithm NOI for training DCCA which updates the DNN weights based on small minibatches and performs competitively to previous optimizers.

One direction for future work is to better understand the convergence properties of NOI, which presents several difficulties. First, we note that convergence of the alternating least squares formulation of CCA (Algorithm 1) or rather orthogonal iterations) is usually stated as the angle between the estimated subspace and the ground-truth subspace converging to zero. In the stochastic optimization setting, we need to relate this measure of progress (or some other measure) to the nonlinear least squares problems we are trying to solve in the NOI iterations. As discussed in Section IV even the convergence of the linear CCA version of NOI with batch gradient descent is not well understood [47]. Second, the use of memory in estimating covariances (8) complicates the analysis and ideally we would like to come up with ways of determining the time constant $\rho$.

We have also tried using the same form of adaptive covariance estimates in both views for the STOL approach for computing the gradients (4), but its performance with small minibatches is much worse than that of NOI. Presumably this is because the gradient computation of STOL suffers from noise in both views which are further combined through various nonlinear operations, whereas the noise in the gradient computation of NOI only comes from the output target (due to inexact whitening), and as a result NOI is more tolerant to the noise resulting from using small minibatches. This deserves further analysis as well.

REFERENCES

[1] L. Bottou, “Stochastic gradient learning in neural networks,” in Proc. Neurontimes, 1991.
[2] Y. LeCun, L. Bottou, G. B. Orr, and K.-R. Müller, “Efficient backprop,” in Neural Networks: Tricks of the Trade, ser. Lecture Notes in Computer Science, vol. 1524, 1998, pp. 9–50.
[3] L. Bottou, “Stochastic learning,” in Advanced Lectures on Machine Learning, ser. Lecture Notes in Artificial Intelligence 3176, 2004, pp. 146–168.
[4] T. Zhang, “Solving large scale linear prediction problems using stochastic gradient descent algorithms,” in Proc. of the 21st Int. Conf. Machine Learning (ICML’04), 2004, pp. 919–926.
[5] D. P. Bertsekas, “Incremental gradient, subgradient, and proximal methods for convex optimization: A survey,” in Optimization for Machine Learning, S. Sra, S. Nowozin, and S. J. Wright, Eds. MIT Press, 2011.
