Sequential Inverse Approximation of a Regularized Sample Covariance Matrix

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Abstract—One of the goals in scaling sequential machine learning methods pertains to dealing with high-dimensional data spaces. A key related challenge is that many methods heavily depend on obtaining the inverse covariance matrix of the data. It is well known that covariance matrix estimation is problematic when the number of observations is relatively small compared to the number of variables. A common way to tackle this problem is through the use of a shrinkage estimator that offers a compromise between the sample covariance matrix and a well-conditioned matrix, with the aim of minimizing the mean-squared error. We derived sequential update rules to approximate the inverse shrinkage estimator of the covariance matrix. The approach paves the way for improved large-scale machine learning methods that involve sequential updates.

I. INTRODUCTION

The covariance matrix of multivariate data is required in many sequential machine learning and neural-networks (NN) based applications [1], including speech recognition [2], deep learning architectures for image processing and computer vision [3], [4], [5], stochastic fuzzy NN’s [6], portfolio optimization problems in financial markets [7], [8], [9], adaptive tracking control problems [10], detection tasks [11], reinforcement learning [12], and many others.

In settings where data arrives sequentially, the covariance matrix is required to be updated in an online manner [13], [14]. Techniques such as cross-validation, which attempt to impose regularization, or model selection are typically not feasible in such settings [15]. Instead, to minimize complexity, it is often assumed that the covariance matrix is known in advance [6] or that it is restricted to a specific simplified structure, such as a diagonal matrix [16], [3]. Moreover, when the number of observations \( n \) is comparable to the number of variables \( p \) the covariance estimation problem becomes far more challenging. In such scenarios, the sample covariance matrix is not well-conditioned nor is it necessarily invertible (despite the fact that those two properties are required for most applications). When \( n \leq p \), the inversion cannot be computed at all [17], [18].

An extensive body of literature concerning improved estimators in such situations exists [19], [20]. However, in the absence of a specific knowledge about the structure of the true covariance matrix, the most successful approach so far has, arguably, been shrinkage estimation [21]. It has been demonstrated in [22] that the largest sample eigenvalues are systematically biased upward, and the smallest ones downward. This bias is corrected by pulling down the largest eigenvalues and pushing up the smallest ones, toward their grand mean.

The optimal solution of the shrinkage estimator is solved analytically, which is a huge advantage for deep learning architectures, since a key factor in realizing such architectures is the resource complexity involved in their training [23]. An example of such deep architecture is the deep spatiotemporal inference network (DeSTIN) [3]. The latter extensively utilizes the quadratic discriminant analysis (QDA) classifier under the simplified assumption that the covariance matrices involved in the process are diagonal. Such assumption is made in order to avoid additional complexity during the training and inference processes. It is well known that for a small ratio of training observations \( n \) to observation dimensionality \( p \), the QDA classifier performs poorly, due to highly variable class conditional sample covariance matrices. In order to improve the classifiers’ performance, regularization is required, with the aim of providing an appropriate compromise between the bias and variance of the solution. It have been demonstrated in [24], [25] that the QDA classifier can be improved tremendously using shrinkage estimators. The sequential approximated inverse of the shrinkage estimator, derived in this paper, allows us to utilize the shrinkage estimator in the DeSTIN architecture with relatively negligible additional complexity to the architecture. In addition, the relatively simple update rules pave the way to implement the inverse shrinkage estimator on analog computational circuits, offering the potential for large improvement in power efficiency [26].

The rest of this paper is organized as follows: Section 2 presents the general idea of the shrinkage estimator. In Section 3, we derived a sequential update for the shrinkage estimator, while in Section 4, the related approximated inverses are derived. In Section 5, we conduct an experimental study and examine the sequential update rules.

Notations: we denote vectors in lowercase boldface letters and matrices in uppercase boldface. The transpose operator is denoted as \((\cdot)^T\). The trace, the determinant and the Frobenius norm of a matrix are denoted as \(\text{Tr}(\cdot), |\cdot|\) and \(\|\cdot\|_F\), respectively. The identity matrix is denoted as \(I\), while \(e = [1,1,\ldots,1]^T\) is a column vector of all
real matrices $R_1$ and $R_2$, the inner product is defined as $\langle R_1, R_2 \rangle = \text{Tr} (R_1^T R_2)$, where $\langle R_1, R_1 \rangle = \| R_1 \|_F^2$ [17, Sec. 2.20].

II. Shrinkage Estimator for Covariance Matrices

We briefly review a single-target shrinkage estimator by following [22], [27], which is generally applied to high-dimensional estimation problems. Let $\{x_i\}_{i=1}^n$ be a sample of independent identically distributed (i.i.d.) $p$-dimensional vectors drawn from a density with a mean $\mu$ and covariance matrix $\Sigma$. When the number of observations $n$ is large (i.e., $n \gg p$), the most common estimator of $\Sigma$ is the sample covariance matrix

$$S_n = \frac{1}{n-1} \sum_{i=1}^n (x_i - m_n) (x_i - m_n)^T,$$

(1)

where $m_n$ is the sample mean, defined as

$$m_n = \frac{1}{n} \sum_{i=1}^n x_i.$$

(2)

Both $S_n$ and $m_n$ are unbiased estimators of $\Sigma$ and $\mu$, respectively, i.e., $E\{S_n\} = \Sigma$ and $E\{m_n\} = \mu$. The shrinkage estimator $\hat{\Sigma}(\lambda_n)$ is in the form

$$\hat{\Sigma}(\lambda_n) = (1 - \lambda_n)S_n + \lambda_n T_n$$

(3)

where the target $T_n$ is a restricted estimator of $\Sigma$ defined as

$$T_n = \frac{\text{Tr}(S_n)}{p} I.$$

(4)

The work in [22] proposed to find an estimator $\hat{\Sigma}(\lambda_n)$ which minimizes the mean squared error (MSE) with respect to $\lambda_n$, i.e.,

$$\lambda_{On} = \arg \min_{\lambda_n} E\left\{ \left\| \hat{\Sigma}(\lambda_n) - \Sigma \right\|_F^2 \right\}$$

(5)

and can be given by the distribution-free formula

$$\lambda_{On} = \frac{E\left\{ (T_n - S_n, \Sigma - S_n) \right\}}{E\left\{ \|T_n - S_n\|_F^2 \right\}}.$$

(6)

The scalar $\lambda_{On}$ is called the oracle shrinkage coefficient, since its depends on the unknown covariance matrix $\Sigma$. Therefore, $\lambda_{On}$ (6) must be estimated. The latter can be estimated from its sample counterparts as in [27]. We denote this estimator as $\lambda_{On}$.

III. Sequential Update of the Shrinkage Estimator

We want to know what happens to $\hat{\Sigma}(\lambda_n)$ (3) when we add an observation $x_{n+1}$, using only the current knowledge of $S_n$, $m_n$ and $n$. Setting $d_{n+1} = x_{n+1} - m_n$ while using [17, 15.12.(c)], we have the following update rules for $m_n$ (2) and $S_n$ (1) when an observation $x_{n+1}$ is added

$$m_{n+1} = m_n + \frac{1}{n+1} d_{n+1}$$

(7)

$$S_{n+1} = \frac{n-1}{n} S_n + \frac{1}{n+1} d_{n+1} d_{n+1}^T.$$

(8)

Based on $S_{n+1}$ (8), we can write the update rule for the target $T_n$ (4) as

$$T_{n+1} = \frac{n-1}{n} T_n + \frac{1}{(n+1)p} \|d_{n+1}\|_F^2 I$$

(9)

By using $S_{n+1}$ (8) and $T_{n+1}$ (9), the update rule for the shrinkage estimator $\hat{\Sigma}(\lambda_{n+1})$ (3) can be written as

$$\hat{\Sigma}(\lambda_{n+1}) = G_n + F_n$$

(10)

where $G_n$ and $F_n$ defined as

$$G_n = \frac{n-1}{n} \Sigma - (1 - \lambda_{n+1}) \frac{1}{n+1} d_{n+1} d_{n+1}^T$$

(11)

and

$$F_n = \frac{1}{(n+1)p} \lambda_{n+1} \|d_{n+1}\|_F^2 I$$

(12)

respectively. Based on the above update rules, we derive the sequential update rules for the inverse of the shrinkage estimator.

IV. Sequential Update for the Inverse of the Shrinkage Estimator

In this section, we derived approximated inverses of the shrinkage estimator which are updated sequentially and do not involve any matrix inversion. We start, therefore, from the inverse of the sample covariance matrix $S_{n+1}$ that can be obtained from the current inverse of $S_n$ (1) using the Sherman-Morrison-Woodbury matrix identity [28, Ch. 3] as

$$S_n^{−1} = \frac{n}{n-1} \left( S_n^{−1} - \frac{S_n^{−1} d_{n+1} d_{n+1}^T S_n^{−1}}{\|d_{n+1}\|^2} \right).$$

(13)

The last update rule can be used only if $S_n$ is invertible. It will not be invertible for $n \leq p$. Since the shrinkage estimator $\hat{\Sigma}(\lambda_n)$ (3) is a regularized version of $S_n$ (1), an inverse exists for any $n$. This inverse of $\hat{\Sigma}(\lambda_n)$ (3) involves two main steps. The first one is to update the inverse of $G_n$ (11) from an inverse of $\hat{\Sigma}(\lambda_n)$ (3). The second is to update the next step inverse of $\hat{\Sigma}(\lambda_n)$ from $F_n$ (12) and the inverse of $G_n$ (11) calculated in the first step. Suppose, for example, that the exact inverse of $\hat{\Sigma}(\lambda_n)$ (3), denoted as $\hat{\Sigma}^{−1}(\lambda_n)$, is known. In the same manner as in $S_{n+1}^{-1}$ (13), the inverse for $G_n$ (11) can be calculated from $\hat{\Sigma}^{−1}(\lambda_n)$ as

$$\frac{n}{n+1} \left( \hat{\Sigma}^{−1}(\lambda_n) - \frac{\hat{\Sigma}^{−1}(\lambda_n) d_{n+1} d_{n+1}^T \hat{\Sigma}^{−1}(\lambda_n)}{\|d_{n+1}\|^2} \right).$$

(14)

Using [17, 15.11.(b)], the exact inverse of $\hat{\Sigma}(\lambda_{n+1})$ can be calculated from $G_n^{-1}$ (14) and $F_n$ (12) with $p$ iterations

$$\left( G_n^{(p+1)} \right)^{-1} = \left( G_n^{(p)} + f_i e_i^T \right)^{-1}.$$
where $f_i$ and $e_i$ are the $i$ columns of $F_n$ (12) and the identity matrix $I$, respectively. The inverse of $\Sigma_1^{-1}(\lambda_{n+1})$ (10) is equal to the output of the last iteration, i.e.,

$$\Sigma_1^{-1}(\lambda_{n+1}) = (G_n^{(p+1)})^{-1}.$$  

In order to avoid the calculation of $p$ iterations, we can use approximations for $\Sigma_1^{-1}(\lambda_{n+1})$ (16). The inverse approximations of the shrinkage estimator are discussed in the following section.

A. Inverse Approximations for the Shrinkage Estimator

We consider two approximations for $\Sigma_1^{-1}(\lambda_{n+1})$ (16). The first approximation is defined as

$$\tilde{\Sigma}_1^{-1}(\lambda_{n+1}) = \tilde{G}_n^{-1} - \alpha_n \tilde{G}_n^{-1} F_n \tilde{G}_n^{-1}$$  

(17)

where

$$\tilde{G}_n^{-1} = \frac{n}{n-1} \left( \tilde{\Sigma}_1^{-1}(\lambda_n) - \tilde{\Sigma}_1^{-1}(\lambda_n) \frac{d_{n+1} d_{n+1}^T \tilde{\Sigma}_1^{-1}(\lambda_n) \tilde{G}_n^{-1}}{n^2 - 1} \right).$$  

(18)

The matrix $\tilde{G}_n^{-1}$ (18) differs from $G_n^{-1}$ (14) in the fact that it relies on the approximated inverse $\tilde{\Sigma}_1^{-1}(\lambda_n)$ (17), instead of the exact inverse $\Sigma_1^{-1}(\lambda_n)$ (16). A possible motivation to justify the update rule (17) stems from the mean value theorem as explained in [29]. Another motivation arises from the Neumann series [17, Sec.19.15] where $\Sigma_1^{-1}(\lambda_{n+1})$ (16) is approximately equal to $\tilde{\Sigma}_1^{-1}(\lambda_{n+1})$ (17) for $\alpha = 1$ and relatively small $F_n$. We define $\alpha_n$ as the value that minimizes the reconstruction squared error, i.e.,

$$\alpha_n = \arg \min_\alpha \left\| \tilde{G}_n^{-1} - \alpha \tilde{G}_n^{-1} F_n \tilde{G}_n^{-1} \right\|_F^2$$  

(19)

and is equal to

$$\alpha_n = \frac{\text{Tr} \left( \tilde{G}_n^{-1} F_n \tilde{G}_n^{-1} \Sigma(\lambda_{n+1}) \left( \tilde{G}_n^{-1} \Sigma(\lambda_{n+1}) - I \right) \right)}{\left\| \tilde{G}_n^{-1} F_n \tilde{G}_n^{-1} \Sigma(\lambda_{n+1}) \right\|_F^2}$$  

(20)

Additional simplification can be taken by looking at the last term in $F_n$ (12). Under the assumption that the difference $\lambda_n - \lambda_{n+1}$ is relatively small, we can write an approximation for $F_n$ (12) by neglecting its last term, i.e.,

$$F_n = \frac{1}{n+1} \lambda_{n+1} \left\| d_{n+1} \right\|_F \mathbf{1}$$  

(21)

This will lead to the second approximation for $\Sigma_1^{-1}(\lambda_{n+1})$ (16), denoted as

$$\tilde{\Sigma}_2^{-1}(\lambda_{n+1}) = \tilde{G}_n^{-1} - \alpha'_n \tilde{G}_n^{-1} F_n \tilde{G}_n^{-1}$$  

(22)

where

$$\alpha'_n = \frac{n}{n+1} \left( \tilde{\Sigma}_2^{-1}(\lambda_n) - \frac{\tilde{\Sigma}_2^{-1}(\lambda_n) d_{n+1} d_{n+1}^T \tilde{\Sigma}_2^{-1}(\lambda_n) \tilde{G}_n^{-1}}{n^2 - 1} \right)$$  

(23)

and $\alpha'_n$ is calculated by

$$\alpha'_n = \left( \frac{n+1}{p} \text{Tr} \left( \tilde{G}_n^{-2} \Sigma(\lambda_{n+1}) \left( \tilde{G}_n^{-1} \Sigma(\lambda_{n+1}) - I \right) \right) \right)$$

$$\lambda_{n+1} \left\| d_{n+1} \right\|_F \left\| \tilde{G}_n^{-2} \Sigma(\lambda_{n+1}) \right\|_F^2$$  

(24)

We examine these two approximations in the following section.

V. EXPERIMENTS

In this section we implement and evaluate the sequential update of the inverse shrinkage estimator. As in [30], we assume that the observations are i.i.d Gaussian vectors. In order to study the estimators performance, an autoregressive covariance matrix $\Sigma$ is used. We let $\Sigma$ be the covariance matrix of a Gaussian AR(1) process [31], denoted by

$$\Sigma_{AR} = \{ \sigma_{ij} = e^{\lambda_{ij}} \}.$$  

(25)

As in [19], [30], we use $r = 0.5$. In all simulations, we set $p = 50$ and let $n$ range from 1 to 30. Each simulation is repeated 200 times and the average values are plotted as a function of $n$. The experimental results are summarized in box plots. On each box, the central mark is the median, the edges of the box are the 25th and 75th percentiles, and the whiskers correspond to approximately +/- 2.7σ or 99.3 coverage if the data are normally distributed. The outliers are plotted individually.

The reconstruction errors of the approximated inverses $\tilde{\Sigma}_1^{-1}(\lambda_n)$ (17) and $\tilde{\Sigma}_2^{-1}(\lambda_n)$ (22) are defined by

$$e_1(n) = \frac{1}{p} \left\| \tilde{\Sigma}_1^{-1}(\lambda_n) \Sigma(\lambda_n) - I \right\|_F^2,$$  

(26)

and

$$e_2(n) = \frac{1}{p} \left\| \tilde{\Sigma}_2^{-1}(\lambda_n) \Sigma(\lambda_n) - I \right\|_F^2,$$  

(27)

respectively. These reconstruction errors are normalized with $p$ since it is the squared Frobenius norm of the identity matrix $I$. We examine the approximated inverse $\tilde{\Sigma}_1^{-1}(\lambda_n)$ (17) and $\tilde{\Sigma}_2^{-1}(\lambda_n)$ (22) where $\lambda_n$ is equal to $\tilde{\lambda}_{On}$ [27]. The experimental results for the reconstruction errors $e_1(n)$ (26) and $e_2(n)$ (27) are summarized in Fig. 1 and Fig. 2, respectively. The values of $e_1(n)$ (26) converge on average to zero as the number of observations $n$ increase. In several simulations, however, the update rule accumulates error and diverges.

The related reconstruction error $e_2(n)$ (27) is depicted in Fig. 2. The reconstruction error $e_2(n)$ (27) does not converge to zero due to its relative simplification involving the use of $F_n$ (21) instead of $F_n$ (12). However, the use of $F_n$ (21) renders $\tilde{\Sigma}_2^{-1}(\lambda_n)$ (22) much more robust to outliers in comparison to
Section 5 clearly demonstrates that the reconstruction errors of sequential update rules that approximate the inverse conditioned matrix. The optimal shrinkage coefficient, in the sense of mean-squared error, is analytically obtained, which is a notable advantage since a key factor in realizing large-scale architectures is the resource complexity involved. In Section 4, sequential update rules that approximate the inverse shrinkage estimator are derived. The experimental results in Section 5 clearly demonstrate that the reconstruction errors of the approximated inverses are relatively small. The sequential update rules that approximate the inverse of the shrinkage estimator provide a general result that can be utilized in a wide range of sequential machine learning applications. Therefore, the approach paves the way for improved large-scale machine learning methods that involve sequential updates in high-dimensional data spaces.

VI. CONCLUSIONS

A key challenge in many large-scale sequential machine learning methods stems from the need to obtain the covariance matrix of the data, which is unknown in practice and should be estimated. In order to avoid additional complexity during the modeling process, it is commonly assumed that the covariance matrix is known in advanced or, alternatively, that simplified estimators are employed. In Section 3, we derived a sequential update rule for the shrinkage estimator that offers a compromise between the sample covariance matrix and a well-conditioned matrix. The optimal shrinkage coefficient, in the sense of mean-squared error, is analytically obtained, which is a notable advantage since a key factor in realizing large-scale architectures is the resource complexity involved. In Section 4, sequential update rules that approximate the inverse shrinkage estimator are derived. The experimental results in Section 5 clearly demonstrate that the reconstruction errors of the approximated inverses are relatively small. The sequential update rules that approximate the inverse of the shrinkage estimator provide a general result that can be utilized in a wide range of sequential machine learning applications. Therefore, the approach paves the way for improved large-scale machine learning methods that involve sequential updates in high-dimensional data spaces.

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