Tuned Regularized Estimators for Linear Regression via Covariance Fitting

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Abstract—We consider the problem of finding tuned regularized parameter estimators for linear models. We start by showing that three known optimal linear estimators belong to a wider class of estimators that can be formulated as a solution to a weighted and constrained minimization problem. The optimal weights, however, are typically unknown in many applications. This begs the question, how should we choose the weights using only the data? We propose using the covariance fitting SPICE-methodology to obtain data-adaptive weights and show that the resulting class of estimators yields tuned versions of known regularized estimators—such as ridge regression, LASSO, and regularized least absolute deviation. These theoretical results unify several important estimators under a common umbrella. The resulting tuned estimators are also shown to be practically relevant by means of a number of numerical examples.

I. INTRODUCTION

The linear model

\[ y = \Phi \theta_0 + \epsilon, \]  

(1)

has a wide range of applications in statistics, signal processing and machine learning. Here \( y \) denotes a column vector consisting of \( n \) samples, \( \Phi \) is an \( n \times d \) matrix of regressors, \( \theta_0 \) is an unknown parameter vector and \( \epsilon \) is a vector of zero-mean noise with covariance matrix \( \text{Cov}[\epsilon] = \Sigma_0 \succeq 0 \).

The least-squares (LS) method is the standard approach to estimate \( \theta \). However, in applications with few samples \( n \), high noise levels, or heteroscedastic noise, it can suffer from large errors. Regularized estimators, such as Ridge regression \([1]\), Lasso \([2]\) and regularized LAD \([3]\), alleviate these drawbacks but require separate methods for tuning regularization parameters. In this paper, we are interested in studying a class of tuned regularized estimation methods.

We begin by showing how optimal linear estimators are derived in a class of estimators that is parameterized by positive semi-definite weights. Subsequently, we show that tuning these weight matrices in a data-adaptive manner gives rise to regularized least absolute deviation. These theoretical results are also shown to be practically relevant by means of a number of numerical examples.

II. OPTIMAL LINEAR ESTIMATORS

We being by considering linear estimators, i.e., estimators of the form \( \hat{\theta} = \Phi y \), where \( \Phi \) is a \( d \times n \) matrix that is independent of \( y \). Let the mean-squared error of \( \hat{\theta} \) be denoted as

\[ \text{MSE}(\theta_0) = \mathbb{E} \left[ \| \theta_0 - \hat{\theta} \|^2 \right], \]

where the expectation is taken with respect to the noise \( \epsilon \). We will now show that three different optimal linear estimators belong to a unified class of estimators.

Theorem 1. Consider the following class of estimators,

\[ \hat{\theta}(V) = \arg \min_{\theta} \| y - \Phi \theta \|^2, \]

(2)

s.t. \( y - \Phi \theta \in \mathcal{R}(V) \). The resulting tuned estimators are shown to be practically relevant by means of a number of numerical examples.

Proof. See Appendix A. \( \square \)

Remark 1. Without the constraint, there would be no penalty on parts of the residual \( y - \Phi \theta \) outside the range of \( V \). In the case of \( V = \alpha V_\circ \), the constraint is necessary in order to obtain the optimal unbiased estimator in general. Removing the constraint in (2) yields the optimal estimator if and only if \( V_\circ V_\circ \Phi = \Phi \).

The optimal unbiased estimator can improve \( \text{MSE}(\theta_0) \) over LS in problems with heteroscedastic or correlated noise. But when \( n \) is small, or \( \Phi \) is ill-conditioned, this linear estimator can still suffer from large errors. To cope with such cases we relax the unbiasedness requirement and consider more general linear estimators that minimize \( \text{MSE}(\theta_0) \). Specifically, we consider a class of estimators formed by regularizing the criterion in (2) as follows:

\[ \hat{\theta}(C, V) = \arg \min_{\theta \in \Theta(C, V)} \| y - \Phi \theta \|^2 + \| \theta \|^2, \]

(3)

where \( C \) and \( V \) are positive semi-definite weight matrices. The parameter vector is restricted to the set \( \Theta(C, V) = \{ \theta : y - \Phi \theta \in \mathcal{R}(V) \text{ and } \theta \in \mathcal{R}(C) \} \).
This constraint ensures that it is not possible to hide parts of the residuals or the parameter vector in a subspace that is not penalized when \( V \) or \( C \) are singular.

To study the feasibility of the minimization problem in (3), we introduce the matrix
\[
R(C, V) \triangleq \Phi C \Phi^\top + V \succeq 0.
\]
When there is no risk of confusion we will drop the arguments and just write \( R \).

**Theorem 2.** If \( y \in R(\mathbb{R}) \), then a unique solution to (3) exists and is given by
\[
\hat{\theta}(C, V) = C \Phi^\top R_y \Phi C^\top V,
\]
which is linear in \( y \). If \( y \notin R(\mathbb{R}) \), then \( \Theta(C, V) \) is empty and thus (3) is infeasible.

**Proof.** See Appendix [B]

**Theorem 3.** Among all linear estimators, the minimum MSE is attained by \( \hat{\theta}(C, V) \) with weight matrices
\[
C = \alpha \theta_o \theta_o^\top \quad \text{and} \quad V = \alpha V_o,
\]
for any \( \alpha > 0 \).

**Proof.** See Appendix [C]

**Remark 2.** It follows that the class of estimators (3) includes the optimal linear estimator, but it is unrealistic since it depends on \( \theta_o \) and \( V_o \), which are typically unknown. Also, by setting \( C = cI \), the estimator \( \hat{\theta}(C, V) \) also includes \( \hat{\theta}(V) \) in (2) when \( c \to \infty \).

Given the practical unrealizability of the optimal linear estimator, a common model-based approach is to consider a prior distribution over \( \theta_o \), with mean and covariance
\[
E[\theta_o] = 0, \quad \text{and} \quad \text{Cov}[\theta_o] = C_o \succeq 0.
\]
Then \( E[\text{MSE}(\theta_o)] \) will denote the mean squared error marginalized over all plausible \( \theta_o \). The parameter \( \theta_o \) is here drawn independently from the measurement noise \( \varepsilon \) in (1).

**Remark 3.** The zero-mean assumption does not incur any loss of generality, since any non-zero mean can be removed from the data \( y \).

**Theorem 4.** Among all linear estimators, the minimum marginalized MSE is attained by \( \hat{\theta}(C, V) \) with weight matrices
\[
C = \alpha C_o \quad \text{and} \quad V = \alpha V_o,
\]
for any \( \alpha > 0 \). This is also known as the ‘linear minimum mean-square estimator’ (LMMSE) \([10, 11]\).

**Proof.** See Appendix [C]

In summary, we see that \( \hat{\theta}(C, V) \) encompasses three different optimal linear estimators depending on the choice of weight matrices \( C \) and \( V \). While the minimizer of the MSE is unrealizable since it depends on \( \theta_o \), the minimizer of the marginal MSE instead defers the problem to the appropriate specification of \( C_o \).

In the following section, we will no longer restrict the discussion to the class of linear estimators and instead consider \( \hat{\theta}(C, V) \) when the weight matrices \( C \) and \( V \) depend on the data \( y \) and \( \Phi \).

### III. DATA-DEPENDENT WEIGHT MATRICES

In the model-based approach, the weight matrices \( C \) and \( V \) in (3) can be viewed as the covariance matrices for \( \theta \) and \( \varepsilon \), respectively. Consequently, \( R(C, V) \) is the (marginal) covariance matrix of \( y \).

A possible way to fit \( C \) and \( V \) to the data is to use the criterion
\[
(C^*, V^*) = \arg \min_{(C, V) \in S} \left\| y y^\top - R \right\|_{R^\top}^2 \quad \text{s.t.} \quad y \in R(\mathbb{R}),
\]
where the constraint \( y \in R(\mathbb{R}) \) ensures that the resulting \( R^* = R(C^*, V^*) \) is indeed a valid covariance matrix for \( y \) even if \( R^* \) is singular. The set
\[
S = \{(C, V) : C \in C, V \in V\}
\]
determines the types of covariance matrices under consideration. We assume that both \( C \) and \( V \) include positive definite matrices. This ensures that for any measurement \( y \) there exist \( (C, V) \in S \) such that \( y \in R(\mathbb{R}) \).

The fitting criterion (4) generalizes the criterion proposed in (4) to handle potentially singular \( R \) and we will also extend the analysis in \([5, 6] \) to consider the cases when the weight matrices are either
- of the form \( \kappa I \) with \( \kappa > 0 \),
- or diagonally structured positive semi-definite matrices,
- or unstructured positive semi-definite matrices.

We will study the resulting estimator \( \hat{\theta}(C^*, V^*) \) in (3), using a fitted \( (C^*, V^*) \) from (4). While Theorem 2 and the constraint in (4) ensures that \( \hat{\theta}(C^*, V^*) \) exist and is unique for any given \( (C^*, V^*) \), there may be multiple solutions to (4) in general. Therefore we define the set of estimates:
\[
\Theta^* = \left\{ \hat{\theta}(C^*, V^*) : (C^*, V^*) \in (4) \right\}
\]

The main results of this paper are to characterize the solution set \( \Theta^* \) as tuned versions of several known regularized estimators thus unifying them under the same umbrella.

### IV. MAIN RESULTS

In this section, we show that the estimators with data-dependent weight matrices in (6) correspond to several known tuned regularized estimators. The derivations are deferred to Section [VI]. For notational simplicity, we let \( \Sigma = \frac{1}{n} \Phi^\top \Phi \succeq 0 \) denote the sample covariance matrix of the regressor vectors and also let
\[
\text{MSD}(\theta) = \frac{1}{n} \| y - \Phi \theta \|_2^2 \quad \text{and} \quad \text{MAD}(\theta) = \frac{1}{n} \| y - \Phi \theta \|_1
\]
denote the (empirical) mean squared/absolute deviation. Recall that the least-squares and least absolute deviation estimators are the minimizers of \( \text{MSD}(\theta) \) and \( \text{MAD}(\theta) \), respectively.
A. Diagonally structured weight matrices

In this section, we consider cases when both weight matrices $C$ and $V$ have diagonal structures. We will show that $\hat{\theta}(C^*, V^*)$ in (6) above is then a minimizer of one of the following criteria:

1. Criteria using MAD$(\theta)$ (i.e., (8) and (10)) are known to be better suited for problems with noise outliers than those based on MSD$(\theta)$ (i.e., (7) and (9)).

2. The weighted regularization term in (9) and (10) corresponds to standardizing the regression variables by their (empirical) standard deviations. This $\ell_1$-regularization term is suited for problems with sparse parameter vectors.

3. The minimizer for a criterion containing the square-root fitting term $\sqrt{\text{MSD}(\theta)}$ is also the minimizer of a criterion with MSD$(\theta)$, but with a different $\lambda$. That is, for (7) there is a corresponding ridge regression criterion, and for (9) there is a corresponding LASSO-criterion.

Our main result is that $\hat{\theta}(C^*, V^*)$ in (6) yields tuned regularized estimators according to Table I. The structure of $V$ determines the data-fitting term of the criterion, while the structure of $C$ determines the regularization term and the parameter $\lambda$. Choosing between nonuniform and uniform diagonal structures of $V$ thus depends on whether the measurement $y$ is subject to noise outliers or not, while choosing between nonuniform and uniform diagonal structures of $C$ depends on whether the unknown $\theta_o$ is sparse or not. This result unifies and extends the connections between the covariance fitting and regularized estimation developed in [5]–[7].

B. Unstructured weight matrices

The derivations of the results above, to be presented in Section VI, also cover the case of unstructured weight matrices. The cases with unstructured $V$ can readily be dismissed as uninteresting: When this matrix can be any positive semi-definite matrix, then the output in (4) can be explained completely by the noise, setting $V^* = y y^T$ and $C^* = 0$. This gives $\hat{\theta}(C^*, V^*) = 0$, an uninteresting estimator.

Let us therefore consider cases when $C$ is unstructured:

1. If $V = v I$, then

   $\hat{\theta}(C^*, V^*) \in \arg \min_{\theta} \frac{\sqrt{\text{MSD}(\theta)}}{\text{tr} (V^*)} \{ \theta \} \in \frac{1}{\sqrt{n}} \text{tr} (V^*)$

   where

   $\hat{\theta}(C^*, V^*) \in \arg \min_{\theta} \text{MAD}(\theta) + \frac{1}{\sqrt{n}} \| \theta \|_2^2$.

   It can be noted that setting $V = v I$ yields the posterior mean of $\theta_o$ using a g-prior and a Gaussian data model [15]. The parameter $q$ can intuitively be seen as an estimate of an inverse signal-to-noise ratio, so the criterion shrinks the least squares solution towards zero if the estimated signal-to-noise ratio is low.

   While these cases are of theoretical interest, their practical relevance is limited since the resulting estimators usually are not sufficiently regularized. For example, if there exist $\theta$ such that $y = \Phi \theta$, then all $\hat{\theta}(C^*, V^*)$ will be ordinary least squares solutions, as shown in Appendix D. Since this typically happens when $n < d$, the method offers no regularization in this important scenario.

   For these reasons we believe that unstructured weight matrices have less practical importance.

V. NUMERICAL EXPERIMENTS

In this section we will evaluate the tuned methods in three different settings where regularization can improve over the standard Ls method. In each setting we use a fixed $\Phi$ with elements drawn from an i.i.d. zero mean Gaussian distribution, and generate $y$ as

$y = \Phi \theta_o + \varepsilon, \quad \theta_o \sim N(0, C_o), \quad \varepsilon \sim N(0, V_o)$,

or equivalently $y \sim N(0, R(C_o, V_o))$. The following three cases will be considered:

1. $V_o = v I$ and $C_o = I$.

2. $V_o = v I$ and $C_o$ is a diagonal matrix with only 10 non-zero elements. This means that $\theta_o$ is sparse, with only 10 non-zero elements.

3. $C_o$ is diagonal with only 10 non-zero elements. $V_o$ is first set equal to $v I$. Then two elements are changed to 500. This means that $\theta_o$ is sparse, and there are two outliers in the data.

In all cases $n = d = 100$ and $v$ is chosen so that the signal-to-noise ratio is

$\text{SNR} = \frac{\text{tr} \{ \Phi C_o \Phi^T \}}{\text{tr} \{ V_o \}} = 10$.

Now consider an estimator $\hat{\theta}$ which minimizes any given regularized criterion (7)-(10) with a parameter $\lambda$. We evaluate
its performance using the marginalized and normalized mean square error,

\[
NMSE(\lambda) = \frac{\mathbb{E}[\|\theta_\theta - \hat{\theta}_\lambda\|^2]}{\text{tr}(C_\theta)},
\]

that is approximated using 1000 Monte-Carlo simulations. Note that NMSE(0) is the performance of an unregularized estimator and as \( \lambda \to \infty \) we have that NMSE(\( \lambda \)) \( \to 1 \) since \( \hat{\theta}_\lambda \to 0 \). We also show the NMSE of the oracle estimator \( \hat{\theta}(C_\theta, V_\theta) \), which is a lower bound on the error.

Figure 4 displays NMSE(\( \lambda \)) as a function of \( \lambda \) using the four regularized estimators in the three cases above. In each case we show the lower bound as well as the tuned \( \lambda \) that follows from using the fitted weight matrices (see Table 1). Note that in all cases, regularization can reduce the error below NMSE(0).

Case 1) with uniform noise power and a dense parameter vector: We see that the lower bound can be attained by an L2-L2 estimator (as expected). We also see that using a nonuniform diagonal matrix \( V \) leads to slightly worse performance, while assuming a nonuniform \( C \) does not hurt the performance in a noticeable way.

Case 2) with uniform noise power and a sparse parameter vector: Here we see that using a nonuniform diagonal matrix \( C \) clearly outperforms the alternative, and the tuned L2-WL1 is close to the lower bound. Again, using a nonuniform diagonal \( V \) gives slightly worse performance.

Case 3) with nonuniform noise power and a sparse parameter vector: When a nonuniform diagonal matrix \( V \) is used, the performance is about the same as in Case 2 with no outliers. However, when a uniform diagonal matrix \( V \) is used, the outliers impair the performance of the resulting estimators.

In summary, when we let \( C \) and \( V \) in (4) have the same structure as the true covariance matrices of the data generating process, then the corresponding regularized minimization problems in (7)-(10) can be tuned to yield estimators whose performance is quite close to the optimal oracle estimator. In such cases, furthermore, we observe that corresponding tuned versions in Table 1 are close to the optimal tuning. Finally, assuming a more general structure for \( C \) and \( V \) than necessary does not hurt the performance much. These observations suggest using a nonuniform diagonal structures for both \( C \) and \( V \)—i.e., the L1-WL1 estimator—if there is no prior knowledge about the data generating process.

VI. DERIVATION

In this section we will show that the tuned regularized estimators presented in Section IV indeed give the estimates \( \hat{\theta}(C^*, V^*) \) in (6).

Define the cost function

\[
J(\theta; C, V) \triangleq \|y - \Phi \theta\|_V^2 + \|\theta\|^2_C + \frac{1}{\|y\|_2^2} \text{tr} \{R\}
\]

where

\[
f(x, D; W) \triangleq \|x\|^2_D + \frac{1}{\|y\|_2^2} \text{tr} \{WD\}.
\]

Note that this is the criterion in (3) with a weighted trace of \( R \) added. To see the connection between \( J \) and the criterion in (4), let

\[
F(C, V) \triangleq \min_{\theta \in \Phi(C, V)} J(\theta; C, V). \tag{12}
\]

Theorem 5. For \((C, V) \in S\) such that \( y \in \mathcal{R}(R(C, V))\),

\[
F(C, V) = J(\hat{\theta}(C, V); C, V) = \frac{1}{\|y\|_2^2} \|yy^\top - R\|_R^2 + 2,
\]

where \( \hat{\theta}(C, V) = C\Phi^\top R^\dagger y \).

Proof. See Appendix E.

From this it can be seen that the minimization of \( F(C, V) \) is equivalent to minimization of (4). We will now switch the order of minimization. Let

\[
G(\theta) \triangleq \inf_{(C, V) \in S} J(\theta; C, V) \tag{13}
\]

subject to \( \theta \in \mathcal{R}(C, V) \).

It will be seen below that in most cases the infimum in (13) will be attained by some \((C, V)\) for all \( \theta \). However, when \( C \) contains all positive semi-definite matrices and \( \Phi^\top \Phi \) is singular, there is a special (but uninteresting) case where this is not true. So for generality we use \( \inf \) instead of \( \min \) here. The following theorem shows that as long as all \( \theta_G \in \arg \min_{\theta} G(\theta) \) are such that the infimum is attained, then

\[
\Theta^* = \arg \min_{\theta \in \mathbb{R}^d} G(\theta).
\]

Theorem 6. The set \( \Theta^* \) in (6) satisfy

\[
\Theta^* \subseteq \arg \min_{\theta \in \mathbb{R}^d} G(\theta).
\]

Furthermore, for all \( \theta_G \in \arg \min_{\theta \in \mathbb{R}^d} G(\theta) \) for which the infimum in (13) is attained, \( \theta_G \in \Theta^* \).

Proof. See Appendix F.

Finally, we will explore how the choice of \( C \) and \( V \) determines \( G(\theta) \). Note that

\[
G(\theta) = h(y - \Phi \theta, I; V) + h(\theta, \Phi^\top \Phi; C)
\]

where

\[
h(x, W; D) = \inf_{D \in \mathcal{D}} f(x, D; W) \tag{14}
\]

subject to \( x \in \mathcal{R}(D) \).

The following lemmas explore how different choices of the set \( \mathcal{D} \) will affect the functional form of \( h \).

Lemma 7. If \( \mathcal{D} = \{D : D = \kappa I \text{ with } 0 \leq \kappa < \infty\} \), then

\[
h(x; W, D) = \frac{2}{\|y\|_2^2} \|x\|_2 \sqrt{\text{tr}(W)},
\]

and the minimum in (14) is attained by

\[
\hat{D} = \frac{\|y\|_2 \|x\|_2}{\sqrt{\text{tr}(W)}} I.
\]
Fig. 1. The normalized mean-squared error $\text{NMSE}(\lambda)$ as a function of the regularization parameter $\lambda$ (blue curves) in three different cases. The horizontal lines indicate the lower bound set by an oracle estimator. We consider four different estimators \((7)-(10)\) that are obtained using the data-adaptive weight matrices in \((3)\), see Table \(\|$ and the corresponding red dots on the curves.

**Proof.** For $x \not= 0$, just insert $D = \kappa I$ in \((14)\), and set the derivative with respect to $\kappa$ to zero. If $x = 0$, then $\kappa = 0$ gives $h = 0$, which clearly is the minimum. \(\square\)

**Lemma 8.** If $D = \{D : D = \text{diag}(a_1, \ldots, a_d), 0 \leq a_i < \infty\}$, then

$$h(x; W, D) = \frac{2}{\|y\|_2} \left\| \sqrt{D} \odot W x \right\|_1,$$

and the minimum in \((14)\) is attained by

$$\hat{D} = \|y\|_2 \text{diag} \left( \frac{|x_1|}{\sqrt{w_{1,1}}}, \ldots, \frac{|x_d|}{\sqrt{w_{d,d}}} \right),$$

where $w_{i,i}$ is the $i$th diagonal elements of $W$.

**Proof.** See Appendix \(\|$.

**Lemma 9.** If $D = \{D : D \succeq 0\}$ then

$$h(x; W, D) = \frac{2}{\|y\|_2} \|x\|_W.$$

The minimum in \((14)\) is attained if $x = 0$ or $W x \neq 0$, and is then given by

$$\hat{D} = \begin{cases} \frac{\|y\|_2}{\|x\|_W} x x^T & \text{if } W x \neq 0 \\ 0 & \text{if } x = 0 \end{cases}.$$

**Remark 4.** In the case that $x \not= 0$ but $W x = 0$, the infimum in \((14)\) is zero but it is not attained by any finite $D$. This can only occur in the term related to $C$, if $W = \Phi \times \Phi$ is singular. It will only be a problem if $G(\theta)$ is minimized by $\hat{\theta} \neq 0$ such that $\Phi \hat{\theta} = 0$. In this case $\hat{\theta} \not\in \Theta^*$. However, then $G(\theta)$ is also minimized by $\theta = 0 \in \Theta^*$.

With these lemmas we can take different combinations of $C$ and $V$ and find the corresponding $G(\theta)$ to see that minimization of $G(\theta)$ is equivalent to the results in Section \(\|$.

**VII. Conclusion**

We began by showing that a weighted and constrained minimization problem spans a class of estimators that encompass three known optimal linear estimators. The constrained form ensures that singular covariance matrices can be handled, while the weight matrices determine the resulting estimator.

However, the optimal weight matrices depend on the unknown parameters, or their prior covariance matrix, as well as the noise covariance. Since these properties are typically unknown, how should the weight matrices be chosen based only on the data? The proposed method in this paper was to use the covariance-fitting SPICE-methodology to find data-adaptive weight matrices. Interestingly, while the class of estimators is an $\ell_2$-regularized form of weighted least-squares, using the data-adaptive weights yielded several different known tuned regularized estimators – ridge regression, LASSO, and regularized least absolute deviation – depending on the assumed structure of the unknown covariances matrices. In this way the paper connects several important estimators, and also extends the analysis of the SPICE-methodology to singular covariance matrices.

Finally a numerical experiment was performed. It was seen that when the covariance matrices of the data-generating process corresponded to the structure assumed in the SPICE-criterion, the resulting estimator is not far from the optimal one. Furthermore, assuming a more general structure than necessary does not incur any significant loss to performance. These observations suggest that it is sensible to assume nonuniform diagonal structure for the covariance matrices when no prior knowledge about the data-generating process is available, and thus use an L1-WL1 estimator.
A. Proof of Theorem 1

It can be seen that the optimization is feasible if and only if 
\( y \in \mathcal{R}(\Phi \Phi^\dagger + V) \), cf. Appendix A. Also note that this is 
satisfied for any \( y \) generated according to (1) if \( V = \alpha V_0 \).

The constraint \( y - \Phi \theta \in \mathcal{R}(V) \) can be written as 
\[ V^\dagger (y - \Phi \theta) = y - \Phi \theta \]
and with some slight rearrangement we get
\[ (I - V^\dagger V) \Phi \theta = (I - V^\dagger V)y. \]
If \( \hat{\theta} \) is an optimal solution if \( y - \Phi \hat{\theta} \in \mathcal{R}(V) \) and there exist \( \lambda \) such that
\[ -\Phi^\dagger V^\dagger (y - \Phi \hat{\theta}) + \Phi^\dagger (I - V^\dagger V)\lambda = 0. \]

This solution is unique if \( \Phi \) has full column rank, since the 
constrained problem is strictly convex in this case.

In order to find a solution, we assume that \( y \in \mathcal{R}(\Phi \Phi^\dagger + V) \) so the problem is feasible. Hence we can write
\[ y = (\Phi \Phi^\dagger + V)x \]
for some \( x \). We will now show that the optimality conditions are satisfied by
\[ \hat{\theta}(V) = \Phi^\dagger [I - VM(MVM)^\dagger M]y, \]
where \( M = I - \Phi \Phi^\dagger \). Note that \( M \Phi = 0 \) and \( \Phi^\dagger M = 0 \). 
Hence \( My = MVx \), and
\[ MVM(MVM)^\dagger My = MVM(MVM)^\dagger MVx = MVx, \]
where the last equality can be seen by setting \( V = LL^\dagger \) and then make use of the pseudo-inverse identity 
\( XX^\dagger (XX^\dagger)^\dagger X = X \). This can be used to see that
\[ y - \Phi \theta = y - (I - M)(I - VM(MVM)^\dagger M)y = VM(MVM)^\dagger My \in \mathcal{R}(V). \]

Hence, setting
\[ \lambda = -M(MVM)^\dagger My \]
in (15) shows that (16) is indeed the optimal solution.

The theorem then follows by noting that (16) gives the 
BLUE when \( \Phi \) has full rank, see e.g. [10].

B. Proof of Theorem 2

We first show that \( \Theta(C, V) \) is non-empty if and only if 
\( y \in \mathcal{R}(R) \). First assume that \( \Theta(C, V) \) is non-empty and that 
\( \theta \in \Theta(C, V) \). Hence \( y - \Phi \theta \in \mathcal{R}(V) \) so \( y - \Phi \theta = Vx \) for 
some \( x \), and
\[ y = \Phi \theta + Vx. \]
Clearly \( Vx \in \mathcal{R}(V) \subseteq \mathcal{R}(R) \). Furthermore \( \theta \in \mathcal{R}(C) \) 
\( = \mathcal{R}(C^{1/2}) \), so
\[ \Phi \theta \in \mathcal{R}(\Phi C^{1/2}) = \mathcal{R}(\Phi C \Phi^\dagger) \subseteq \mathcal{R}(R). \]

With this we can conclude that \( y \in \mathcal{R}(R) \).

In the other direction, assume that \( y \in \mathcal{R}(R) \). We can clearly see that 
\( \hat{\theta} = C \Phi^\dagger R^\dagger y \in \mathcal{R}(C) \). Furthermore 
\( y \in \mathcal{R}(R) \) implies that \( y = RR^\dagger y \), so
\[ y - \Phi \theta = RR^\dagger y - \Phi C \Phi^\dagger R^\dagger y = VR^\dagger y \in \mathcal{R}(V). \]
Hence it can be concluded that \( \hat{\theta} \in \Theta(C, V) \).

To show that there is a unique solution when \( y \in \mathcal{R}(R) \), 
we note that \( ||\theta||_2^2 \) is strictly convex on \( \Theta(C, V) \). Hence, the 
full problem is strictly convex, so it has a unique solution if 
it is feasible.

The constraint \( \theta \in \Theta(C, V) \) can be written as
\[ \left[ \begin{array}{c} (I - V^\dagger V) \Phi \\ I - C^\dagger C \end{array} \right] \theta = \left[ \begin{array}{c} (I - V^\dagger V)y \\ 0 \end{array} \right]. \]

Hence \( \hat{\theta} \) is optimal if \( \hat{\theta} \in \Theta(C, V) \) and there exists \( \lambda \) such that
\[ -\Phi^\dagger V^\dagger (y - \Phi \hat{\theta}) + C^\dagger \hat{\theta} + [\Phi^\dagger (I - V^\dagger V) - I - C^\dagger C] \lambda = 0. \]

Above we have seen that \( \hat{\theta} = C \Phi^\dagger R^\dagger y \in \Theta(C, V) \) if \( y \in \mathcal{R}(R) \). Furthermore, by using (17), it can be seen that the 
optimality equation is satisfied with
\[ \lambda = \left[ \begin{array}{c} -R^\dagger y \\ \Phi^\dagger y \end{array} \right], \]
so \( \hat{\theta} = C \Phi^\dagger R^\dagger y \) is indeed the unique optimal solution if 
\( y \in \mathcal{R}(R) \).

C. Proof of Theorem 3 and Theorem 4

We here prove the theorems for the case that \( \alpha = 1 \), but 
note that scaling \( C \) and \( V \) with the same constant will not 
change \( \hat{\theta} \). Consider any linear estimator
\[ \hat{\theta} = My. \]
The MSE is then given by
\[ \text{MSE}(\Theta_0) = \text{tr} \left( I - M \Phi \theta_0 \theta_0^\dagger (I - M \Phi)^\dagger + MV_0 M \right). \]
To show Theorem 3 we set \( C = \theta_0 \theta_0^\dagger \) and \( V = V_0 \). In 
Theorem 4 we take the expectation over the MSE and thus 
instead use \( C = C_0 \) where \( C_0 = \mathbb{E}[\theta_0 \theta_0^\dagger] \). It follows that in 
both cases we want to find the \( M \) that minimize the trace of
\[ X(M) = (I - M \Phi) C (I - M \Phi)^\dagger + MV \]
\[ = C + MRM^\dagger - M \Phi C - C \Phi^\dagger M^\dagger, \]
where \( R = \Phi C \Phi^\dagger + V \). From Theorem 2 we know that 
minimizing (3) corresponds to
\[ M^* = C \Phi^\dagger R^\dagger. \]
Using the identity \( R^\dagger RR^\dagger = R^\dagger \) it follows that
\[ X(M^*) = C - C \Phi^\dagger R^\dagger \Phi C. \]
Using this we can see that for any \( M \)
\[ X(M) - X(M^*) = (M - C \Phi^\dagger R^\dagger) R (M - C \Phi^\dagger R^\dagger)^\dagger \geq 0. \]
To see that this equality holds, just expand the right-hand side 
and use the fact that \( R^\dagger R \Phi C = RR^\dagger \Phi C = \Phi C \) since 
\( \mathcal{R}(\Phi C) \subseteq \mathcal{R}(R) \). This shows that \( \text{tr}(X(M)) \geq \text{tr}(X(M^*)) \) 
so the two theorems follow.
D. General C

In this section we will show that (4) with general positive semi-definite C do not result in any regularization compared to least squares if there exist a $\theta$ such that $y = \Phi \theta$. In this case any least squares solution $\hat{\theta}_{LS}$ satisfies $y = \Phi \hat{\theta}_{LS}$.

Hence, we can minimize (4) by setting $V^* = 0$ and $C^* = \hat{\theta}_{LS} \hat{\theta}_{LS}^\top$, since this gives $R = yy^\top$. Using Theorem 2 we thus get

$$\hat{\theta}(C^*, V^*) = C^* \Phi^\top R^\dagger y = \hat{\theta}_{LS} y^\top (yy^\top)^\dagger y = \hat{\theta}_{LS}.$$

E. Proof of Theorem 5

Consider $(C, V) \in S$ such that $y \in \mathcal{R}(R)$. From Theorem 2 it follows that

$$F(C, V) = J(\hat{\theta}(C, V); C, V).$$

Using (17) we see that $y - \Phi \hat{\theta} = VR^\dagger y$, so

$$F(C, V) = \|VR^\dagger y\|^2_R + \|C \Phi^\top R^\dagger y\|^2_C + \frac{1}{2} \text{tr}\{R\} = \|yy^\top - R\|^2_R + \frac{1}{2} \text{tr}\{R\} - 2\|y\|^2_R.$$

Also note that, since $y \in \mathcal{R}(R)$, it follows that $y = RR^\dagger y = R^\dagger R y$ and thus the criterion in (4) can be rewritten as

$$\|yy^\top - R\|^2_R = \|y\|^2_R \|y\|^2_R + \text{tr}\{R\} - 2\|y\|^2_R.$$

The theorem follows by combining these two expressions.

F. Proof of Theorem 6

Let $\Theta^* \in \Theta^*$. By definition of $\Theta^*$ there exist a pair $(C^*, V^*) \in S$ that minimize (4) such that $\theta^* = \theta(C^*, V^*)$ defined in (3).

It follows from Theorem 5 that

$$\min \theta G(\theta) = \inf_{(C, V) \in S} J(\theta; C, V) = \inf_{(C, V) \in S} F(C, V) = F(C^*, V^*).$$

Next note that

$$G(\theta^*) = \inf_{(C, V) \in S} J(\theta^*; C, V) \leq J(\theta^*; C^*, V^*) = F(C^*, V^*) = \min \theta G(\theta)$$

This implies that

$$\min \theta G(\theta) = G(\theta^*) = F(C^*, V^*),$$

and thus $\theta^*$ is a minimizer of $G(\theta)$. Hence $\Theta^* \subseteq \arg \min \theta G(\theta)$.

For the other direction, consider $\theta_G \in \arg \min \theta G(\theta)$, and assume that the infimum in (13) is attained for $\theta_G$. That is, we assume that there are $(C_G, V_G) \in S$ such that $\theta_G \in \Theta(C_G, V_G)$ and

$$G(\theta_G) = \min \theta G(\theta) = J(\theta_G; C_G, V_G).$$

Note that

$$J(\theta_G; C_G, V_G) \geq \min_{\theta \in \Theta(C_G, V_G)} J(\theta; C_G, V_G) = J(\theta_G; C_G, V_G).$$

However, since $\min_{\theta} G(\theta) = F(C^*, V^*) \leq F(C_G, V_G)$, the above inequality must actually be an equality. That is, $(C_G, V_G)$ is a solution to (4) and

$$J(\theta_G; C_G, V_G) = \min_{\theta \in \Theta(C_G, V_G)} J(\theta; C_G, V_G).$$

Finally note that it follows by Theorem 2 that the right-hand side has a unique minimizer, so $\theta_G = \theta(C_G, V_G) \in \Theta^*$.

G. Proof of Lemma 9

With $D = \text{diag}(a_1, \ldots, a_d)$ we get

$$f(x, D, W) = \|x\|^2_D + \frac{1}{\|y\|^2} \text{tr}\{WD\} = \sum_{i=1}^d \left( a_i^2 x_i^2 + \frac{1}{\|y\|^2} a_i w_{i,i} \right)$$

where $w_{i,i}$ are the diagonal elements of $W$ and

$$a_i = \begin{cases} 1/a_i & \text{if } a_i \neq 0 \\ 0 & \text{if } a_i = 0 \end{cases}$$

Note that setting $a_i = 0$ will make the corresponding term in the sum equal to zero. However, to satisfy the constraint $x \in \mathcal{R}(D)$, we must have $a_i > 0$ if $x_i \neq 0$. So if $x_i \neq 0$, then $a_i = 1/a_i$, and we can find the optimal $a_i$ by taking the derivative and setting it equal to zero. This gives

$$a_i = \frac{\|y\|^2 \|x_i\|}{\sqrt{w_{i,i}}}.$$

We note that this formula also works for the case that $x_i = 0$. Inserting this back into the sum we get

$$h(x, W; D) = \frac{2}{\|y\|^2} \sum_{i=1}^d \sqrt{w_{i,i}} |x_i| = \frac{2}{\|y\|^2} \| \sqrt{\mathcal{C}} \circ WBx \|_1.$$
If we let \( a_i = |u_i^\top x|/\sqrt{x} \) and \( b_i = \sqrt{x}/\|u_i\| \), then each term in the sum can be written as
\[
a_i^2 + b_i^2 \geq 2ab = \frac{2}{\|y\|_2} |u_i^\top x| \sqrt{u_i^\top W u_i},
\]
Hence,
\[
f(x, D; W) \geq \frac{2}{\|y\|_2} \sum_{i=1}^m |u_i^\top x| \sqrt{u_i^\top W u_i},
\]
\[
= \frac{2}{\|y\|_2} \sum_{i=1}^m |u_i u_i^\top x|_W
\]
\[
\geq \frac{2}{\|y\|_2} \left( \sum_{i=1}^m u_i u_i^\top x \right)_W = \frac{2}{\|y\|_2} \|x\|_W
\]  \hspace{1cm} (18)
where the second inequality follows from the triangle inequality, and the last equality follows from
\[
\sum_{i=1}^m u_i u_i^\top x = U U^\top x = U U^\top x = x
\]
since \( x \in \mathcal{R}(D) = \mathcal{R}(U) \).
Assuming that \( Wx \neq 0 \), we can achieve this lower bound by using
\[
\tilde{D} = \frac{\|y\|_2}{\|x\|_W} xx^\top,
\]
which clearly satisfy \( x \in \mathcal{R}(\tilde{D}) \). To see this, note that for \( x \neq 0 \) and \( \alpha \neq 0 \)
\[
(\alpha xx^\top)^\dagger = \frac{xx^\top}{\alpha \|x\|^2_2}
\]
If \( Wx = 0 \) then the lower bound just states \( f(x, D, W) \geq 0 \). For \( x = 0 \) this lower bound can be achieved by setting \( D = 0 \).
However, if \( x \neq 0 \), then the constraint \( x \in \mathcal{R}(D) \) ensures that
\[
\|x\|^2_\mathcal{R}(D) > 0
\]
But by choosing \( \tilde{D}(\lambda) = \lambda xx^\top \), we get
\[
f(x, \tilde{D}(\lambda), W) = \frac{1}{\lambda} \rightarrow 0
\]
as \( \lambda \rightarrow \infty \). Hence the lower bound can be reached in the limit also for these \( x \), so for all \( x \),
\[
h(x; W; D) = \frac{2}{\|y\|_2} \|x\|_W
\]
But in the special case that \( Wx = 0 \) but \( x \neq 0 \), the infimum in (13) cannot be attained.

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