

STRUCTURED TOTAL MAXIMUM LIKELIHOOD: AN ALTERNATIVE TO STRUCTURED TOTAL LEAST SQUARES*

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Abstract. Linear inverse problems with uncertain measurement matrices appear in many different applications. One of the standard techniques for solving such problems is the total least squares (TLS) method. Recently, an alternative approach has been suggested, based on maximizing an appropriate likelihood function assuming that the measurement matrix consists of random Gaussian variables. We refer to this technique as the total maximum likelihood (TML) method. Here we extend this strategy to the case in which the measurement matrix is structured so that the perturbations are not arbitrary but rather follow a fixed pattern. The resulting estimate is referred to as the structured TML (STML). As we show, the STML can be viewed as a regularized version of the structured TLS (STLS) approach in which the regularization consists of a logarithmic penalty. In contrast to the STLS solution, the STML always exists. Furthermore, its performance in practice tends to be superior to that of the STLS and competitive to other regularized solvers, as we illustrate via several examples. We also consider a few interesting special cases in which the STML can be computed efficiently either by reducing it into a one-dimensional problem regardless of the problem size or by a decomposition via a discrete Fourier transform.

Key words. total least squares, maximum likelihood, nonconvex programming, linear inverse problem, circulant structures

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1. Introduction. The total least squares (TLS) method, introduced first by Golub and van Loan in [23], is a popular approach to deal with approximate linear systems $\mathbf{Ax} \approx \mathbf{b}$ in which both the model matrix \mathbf{A} and the right-hand side vector \mathbf{b} are subject to uncertainties [23, 24, 40]. One of the appealing features of the TLS algorithm is that it coincides with the maximum likelihood (ML) solution when \mathbf{A} and \mathbf{b} are known up to an additive Gaussian distortion. The derivation of TLS as an ML estimate assumes that noisy measurements of \mathbf{A} and \mathbf{b} are given and jointly estimates \mathbf{x} and \mathbf{A} .

Despite its popularity, in practice, the performance of the TLS method can be quite poor. For example, in the case when \mathbf{A} is square and nonsingular, it does not take the uncertainty into account and reduces to the conventional least squares (LS) solution. Furthermore, the TLS estimate can be viewed as a deregularized LS, where the regularization parameter is negative. This deregularization often accounts for the observed poor behavior [40, 43].

Alternative methods have been proposed in the literature in order to deal with the uncertain LS model. In [20, 12] a robust LS strategy is suggested in which the measurement matrix \mathbf{A} lies in a known deterministic set, and the estimate is designed

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to cope with the worst-case \mathbf{A} within the set. A statistical minimax criterion was considered in [17]. Both these techniques require prior knowledge of a set of possible matrices. In contrast, as we noted above, TLS can be viewed as an ML estimate assuming that \mathbf{A} is known up to some Gaussian distortion [3, 19, 15]. Other strategies for improving the TLS performance consist of adding a quadratic constraint [38, 36] or adding a quadratic penalty function that regularizes the solution [21, 5]. However, which penalty function to choose is not obvious.

Recently, a new approach to the solution of linear systems with uncertain \mathbf{A} and \mathbf{b} was introduced [42, 43]. In this strategy, the unknown \mathbf{A} is again assumed to be known up to a Gaussian distortion. However, instead of treating both \mathbf{x} and \mathbf{A} as variables to be estimated, the measurement matrix \mathbf{A} is considered random with a Gaussian distribution, and only \mathbf{x} is estimated. The corresponding ML solution reduces to a regularized TLS estimator, with a regularization parameter that is a solution to a concave-quasiconvex minimax problem. This problem can be solved by a simple line-search over a unimodal¹ function. The resulting estimate can be viewed as a regularized version of the TLS method, with a logarithmic penalty. We refer to this estimate as the *total maximum likelihood* (TML) solution. The TML technique provides statistical reasoning to the regularized TLS method and suggests an inherent logarithmic penalty scheme. Simulations and analysis provided in [43] demonstrate the ability of the TML technique to improve the estimate of \mathbf{x} over TLS method.

In many practical scenarios, the measurement matrix \mathbf{A} has known structure so that its elements cannot be chosen arbitrarily. For example, if \mathbf{A} corresponds to a linear-time invariant channel, then it will have a Toeplitz structure. In the context of image deblurring, blurring with a spatially invariant point spread function corresponds to a value of \mathbf{A} that is block Toeplitz with Toeplitz blocks when zero boundary conditions are assumed and block circulant with circulant blocks (BCCB) in the case of periodic boundary conditions [2]. Intuitively, we should be able to exploit such structures to reduce the number of unknown parameters and improve the performance. The structured TLS (STLS) method extends the TLS design strategy to the structured setting [37, 14, 1, 34, 33, 30]. Similarly to TLS, it can also be developed within an ML framework. In contrast, however, the STLS estimate is a solution to a difficult nonconvex optimization problem. Several algorithms have been proposed for solving the STLS problem. These include the structured total least-norm algorithm [37], which is an implementation of the Gauss–Newton technique, and other general-purpose optimization methods; an excellent review of these results can be found in [31]. For general structures, there is no guarantee that these methods converge to the global minimum of the STLS optimization problem. The few known exceptions in which a global solution can be computed efficiently are the block circulant structure considered in [6] and the restricted and matrix-restricted structures treated in [41] and [4], respectively. We will discuss the matrix-restricted structure in section 4. The performance of STLS, like that of TLS, is often unsatisfactory; in the limiting case in which the lengths of \mathbf{b} and \mathbf{x} are equal and the matrix \mathbf{A} is nonsingular, it is again equal to LS, demonstrating that the structure cannot always properly be accounted for using this objective.

In this paper, we extend the TML approach of [42, 43] to the case in which the measurement matrix is structured. To this end, we assume that our goal is to estimate \mathbf{x} when \mathbf{A} is a random structured matrix whose structure parameters are

¹A function $f : I \rightarrow \mathbb{R}$, $I \subseteq \mathbb{R}$ being a closed interval, is (strictly) unimodal if it has a unique local minimizer on I , is (strictly) decreasing from the left boundary of the interval to this unique minimum, and is (strictly) increasing from the minimum to the right boundary of the interval.

independent and normally distributed. We refer to this new estimate as the *structured TML* (STML) solution. The STML estimate can be viewed as a regularization of the STLS solution with a special choice of a logarithmic-type regularization term. Both STLS and STML have the same order of computational complexity and require the knowledge of the noise variances of the right-hand side vector and of the structure components. A nice feature of the STML estimate is that it always exists, in contrast to the STLS. Furthermore, its performance in practice tends to be much better than STLS, as we illustrate through several examples. When the noise in the measurement matrix is small, our approach is competitive to other regularized solvers such as Tikhonov and LSQR with an appropriate stopping criteria; as the noise increases (relatively to the noise in the right-hand side vector), the performance of our method, which takes uncertainty in \mathbf{A} into account, improves with respect to alternative regularized solvers.

The STML is a solution to a nonconvex optimization problem, and thus finding it is not an easy task. Nevertheless, we show that it can be solved efficiently when the underlying structure is circulant or BCCB and can be reduced into one-dimensional unimodal optimization problems when a matrix-restricted structure is assumed. A common thread to all these cases is that the covariance matrix of the observed vector \mathbf{b} has a special structure which can be exploited in order to derive a simplified method for computing the STML solution.

We note that a similar reduction result for the matrix-restricted scenario was already shown for the STLS estimate in [4]. The circulant structures were not studied in the context of the STLS problem since they correspond to square measurement matrices for which the STLS solution, when it exists, reduces to the conventional LS estimate.

The rest of the paper is organized as follows. In section 2 we begin by reviewing known results regarding TLS and STLS, as well as their interpretations as ML solutions. The STML approach is discussed in section 3. We first show that a solution to the ML problem in this setting always exists and then illustrate via simulations that its performance is superior to STLS. In section 4 we present the class of matrix-restricted structures for which the STML problem can be significantly simplified and in fact be reduced to a one-dimensional problem. Section 5 considers the classes of circulant matrices and BCCB matrices. For both cases we show that a global optimal solution can be obtained by decomposing the objective into one-dimensional unimodal problems. A MATLAB implementation and documentation of the STML estimate can be found in [8].

2. Unstructured and STLS.

2.1. TLS methods. We are interested in the problem of estimating an unknown deterministic vector $\mathbf{x} \in \mathbb{R}^n$ from measurements

$$(2.1) \quad \mathbf{b} = \mathbf{A}\mathbf{x} + \mathbf{w},$$

where $\mathbf{A} \in \mathbb{R}^{m \times n}$ is the model matrix and \mathbf{w} is an unknown perturbation vector (or “noise”). In the simplest setting, the matrix \mathbf{A} is assumed to be known. A popular estimation strategy in this case is the LS method in which the estimate $\hat{\mathbf{x}}_{\text{LS}}$ is the solution of [11]:

$$(2.2) \quad (\text{LS}) : \min_{\mathbf{x}, \mathbf{w}} \{\|\mathbf{w}\|^2 : \mathbf{b} = \mathbf{A}\mathbf{x} + \mathbf{w}\}.$$

In other words, we seek a minimal norm perturbation to the clean measurements $\mathbf{A}\mathbf{x}$ such that the system $\mathbf{b} = \mathbf{A}\mathbf{x} + \mathbf{w}$ is consistent. Problem (2.2) can also be written as

the unconstrained minimization:

$$\min_{\mathbf{x}} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2.$$

When \mathbf{A} has full-column rank, the LS solution is explicitly given by

$$\hat{\mathbf{x}}_{\text{LS}} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{b}.$$

The LS estimator coincides with the ML solution when the vector \mathbf{w} consists of independent zero-mean random variables that are normally distributed, with equal variances. It is also known to minimize the mean-squared error (MSE) among all unbiased estimators of \mathbf{x} [29]. Nonetheless, it may be outperformed in terms of MSE by biased methods such as the regularized LS estimator due to Tikhonov and Arsenin [39], the James–Stein method [27], the minimax MSE approach [17, 28, 16], and the blind minimax methods [9].

The LS formulation assumes that the model matrix is known. In many practical applications, the measurement matrix is also subjected to uncertainty. The TLS method is a natural generalization of the LS technique in which the measurements \mathbf{b} are modeled as

$$(2.3) \quad \mathbf{b} = (\mathbf{A} + \mathbf{E})\mathbf{x} + \mathbf{w}.$$

Here $\mathbf{A} \in \mathbb{R}^{m \times n}$ is the nominal (given) measurement matrix, and the matrix $\mathbf{E} \in \mathbb{R}^{m \times n}$ is the unknown perturbation. As in the LS approach, we may seek the values of \mathbf{x} , \mathbf{w} , and \mathbf{E} such that (2.3) is consistent and such that the perturbations \mathbf{w} and \mathbf{E} have minimal norm² [23, 24, 40]:

$$(2.4) \quad (\text{TLS}): \quad \min_{\mathbf{E}, \mathbf{w}, \mathbf{x}} \{\|\mathbf{E}\|^2 + \|\mathbf{w}\|^2 : \mathbf{b} = (\mathbf{A} + \mathbf{E})\mathbf{x} + \mathbf{w}\}.$$

It is well known (see e.g., [24]) that by minimizing with respect to \mathbf{E} and \mathbf{w} , the problem can be cast as the following minimization problem in the variables \mathbf{x} :

$$(2.5) \quad \min_{\mathbf{x}} \frac{\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2}{\|\mathbf{x}\|^2 + 1}.$$

The TLS problem is nonconvex (in either of its two forms (2.4) and (2.5)) and, therefore, seems difficult to solve. Nevertheless, it is known to be tractable and in fact has a simple solution in terms of the singular value decomposition of the augmented matrix (\mathbf{A}, \mathbf{b}) ; see [23, 40] for details. It can also be viewed as a deregularization of the LS solution [40, 43].

It is easy to see that when \mathbf{A} is square and invertible, $\hat{\mathbf{x}}_{\text{LS}}$ and $\hat{\mathbf{x}}_{\text{TLS}}$ coincide and are equal to the naïve solution $\hat{\mathbf{x}} = \mathbf{A}^{-1}\mathbf{b}$. Indeed, in this case we can choose $\mathbf{w} = \mathbf{0}$ and $\mathbf{E} = \mathbf{0}$ which clearly minimize the norm.

2.2. STLS methods. In many applications \mathbf{A} is known to have some linear structure; that is,

$$(2.6) \quad \mathbf{A} \in \left\{ \sum_{i=1}^p a_i \mathbf{A}_i : a_i \in \mathbb{R}, i = 1, \dots, p \right\},$$

²For a matrix \mathbf{M} , the norm $\|\mathbf{M}\|$ stands for the Frobenius norm of the matrix.

where $\mathbf{A}_1, \dots, \mathbf{A}_p \in \mathbb{R}^{m \times n}$ are the structure matrices and a_1, \dots, a_p are the structure components; typically p is smaller than mn . Instead of allowing \mathbf{E} to be an arbitrary matrix, it is natural to consider only structured perturbations of the form

$$\mathbf{E} = \sum_{i=1}^p e_i \mathbf{A}_i,$$

where e_1, \dots, e_p are the unknown *perturbation structure variables*; we denote by $\mathbf{e} = (e_1, \dots, e_p)^T$ the *perturbation structure vector*.

The measurement model (2.3) now becomes

$$(2.7) \quad \mathbf{b} = \left(\mathbf{A} + \sum_{i=1}^p e_i \mathbf{A}_i \right) \mathbf{x} + \mathbf{w}.$$

The STLS estimate is then the solution to [37, 14, 1, 34, 33, 30]

$$(2.8) \quad (\text{STLS}): \quad \min_{\mathbf{e}, \mathbf{w}, \mathbf{x}} \left\{ \sum_{i=1}^p e_i^2 + \|\mathbf{w}\|^2 : \left(\mathbf{A} + \sum_{i=1}^p e_i \mathbf{A}_i \right) \mathbf{x} = \mathbf{b} + \mathbf{w} \right\}.$$

Note that similarly to the TLS solution, when \mathbf{A} is square and invertible, $\hat{\mathbf{x}}_{\text{STLS}} = \hat{\mathbf{x}}_{\text{LS}}$ and the structure is not accounted for. We also note that the TLS problem is a special case of (2.8), where we choose each value \mathbf{A}_i as a matrix that is all zeros besides one element which is equal to 1. In this case the number of structure variables is equal to mn .

We can formulate the STLS problem as a minimization in the \mathbf{x} variables only. Specifically, by minimizing with respect to e_1, \dots, e_p and \mathbf{w} , (2.8) reduces to

$$(2.9) \quad \min_{\mathbf{x} \in \mathbb{R}^n} \left\{ (\mathbf{A}\mathbf{x} - \mathbf{b})^T \left(\mathbf{I} + \sum_{i=1}^p \mathbf{A}_i \mathbf{x} \mathbf{x}^T \mathbf{A}_i^T \right)^{-1} (\mathbf{A}\mathbf{x} - \mathbf{b}) \right\}.$$

The STLS problem (2.9) is nonconvex, and in contrast to the unstructured TLS problem, finding its global solution is difficult. As noted in the introduction, several algorithms have been proposed to solve (2.9) or, more precisely, to find a stationary point; among these methods we mention efficient implementations of the Gauss–Newton algorithm [37] and BFGS [32].

Under the assumption that e_1, \dots, e_p and the components of \mathbf{w} are independent normal random variables with equal variances, the STLS solution is an ML estimate. This was first shown by Aoki and Yue [3]. Since the TLS solution is a special case, it is also ML optimal. To develop the ML interpretation, we can rewrite the linear model (2.7) equivalently as follows:

$$(2.10) \quad \begin{aligned} \mathbf{b} &= \left(\sum_{i=1}^p g_i \mathbf{A}_i \right) \mathbf{x} + \mathbf{w}, \\ \mathbf{a} &= \mathbf{g} - \mathbf{e}, \end{aligned}$$

where \mathbf{a} is the observed structure variables vector and \mathbf{g} is the “true” unknown structure variables vector. We then view both \mathbf{g} and \mathbf{x} as unknown deterministic parameters which we seek to estimate from the measurements \mathbf{b} and \mathbf{a} . Assuming that the components of \mathbf{e} and \mathbf{w} are independently normally distributed with

zero-mean and variances σ_e^2 and σ_w^2 , respectively, the ML estimate for \mathbf{x} and \mathbf{g} is the solution to

$$(2.11) \quad \min_{\mathbf{x}, \mathbf{g}} \frac{1}{\sigma_w^2} \left\| \left(\sum_{i=1}^p g_i \mathbf{A}_i \right) \mathbf{x} - \mathbf{b} \right\|^2 + \frac{1}{\sigma_e^2} \|\mathbf{g} - \mathbf{a}\|^2.$$

When $\sigma_e = \sigma_w$, (2.11) is equivalent to the STLS problem (2.8).

3. The STML estimate. The behavior of the TLS solution is often unsatisfactory. In [42, 43] a different approach was advocated in order to treat the model (2.3). The motivation for this new method comes from the ML formulation. For the TLS setting, the ML strategy of (2.11) treats both \mathbf{x} and the perturbation matrix \mathbf{E} as unknown variables to be estimated. However, in many applications, we are not really interested in the nuisance parameter matrix \mathbf{E} but rather only in the vector \mathbf{x} . We may therefore formulate an alternative ML approach in which only \mathbf{x} is estimated, under the same statistical model.

To derive the TML estimate, we assume, as before, that $\mathbf{b} = (\mathbf{A} + \mathbf{E})\mathbf{x} + \mathbf{w}$, where \mathbf{E} is a matrix comprised of independent normal random variables with zero-mean and variance σ_e^2 . In this case, \mathbf{b} is a Gaussian random vector with mean $\mathbf{A}\mathbf{x}$ and variance $\sigma_e^2 \|\mathbf{x}\|^2 + \sigma_w^2$. Therefore, computing the ML estimate of \mathbf{x} reduces to solving [42, 43]

$$(3.1) \quad \min_{\mathbf{x}} \left\{ \frac{\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2}{\sigma_e^2 \|\mathbf{x}\|^2 + \sigma_w^2} + m \log(\sigma_e^2 \|\mathbf{x}\|^2 + \sigma_w^2) \right\},$$

where σ_w^2 is the variance of the components of the noise vector \mathbf{w} . It was shown in [42, 43] that problem (3.1) can be solved efficiently by transforming it into a single-variable minimization of a unimodal function.

The objective in (3.1) can be viewed as a regularization of the TLS problem (2.5). Therefore, this technique provides statistical reasoning to regularized TLS and suggests an inherent logarithmic penalty scheme. Statistical analysis carried out in [43], as well as numerical simulations, demonstrates the superiority of the TML approach over TLS. It is therefore our goal to extend this approach to the structured model (2.7).

3.1. The STML estimate and its existence. To derive the STML estimate, suppose that the components of \mathbf{e} and \mathbf{w} are independent zero-mean normal random variables with variances σ_e^2 and σ_w^2 , respectively. The observation \mathbf{b} then follows a normal distribution,

$$(3.2) \quad \mathbf{b} \sim N \left(\mathbf{A}\mathbf{x}, \sigma_e^2 \sum_{i=1}^p \mathbf{A}_i \mathbf{x} \mathbf{x}^T \mathbf{A}_i^T + \sigma_w^2 \mathbf{I} \right),$$

so that the log likelihood is

$$\log f(\mathbf{b}; \mathbf{x}) = -\frac{m}{2} \log(2\pi) - \frac{1}{2} \log \det \boldsymbol{\Sigma}_{\mathbf{x}} - \frac{1}{2} (\mathbf{A}\mathbf{x} - \mathbf{b})^T \boldsymbol{\Sigma}_{\mathbf{x}}^{-1} (\mathbf{A}\mathbf{x} - \mathbf{b}),$$

where

$$(3.3) \quad \boldsymbol{\Sigma}_{\mathbf{x}} = \sigma_e^2 \sum_{i=1}^p \mathbf{A}_i \mathbf{x} \mathbf{x}^T \mathbf{A}_i^T + \sigma_w^2 \mathbf{I}.$$

The ML estimate of \mathbf{x} is the solution to

$$(3.4) \quad (\text{STML}) : \min_{\mathbf{x}} \{(\mathbf{Ax} - \mathbf{b})^T \Sigma_{\mathbf{x}}^{-1} (\mathbf{Ax} - \mathbf{b}) + \log \det \Sigma_{\mathbf{x}}\}.$$

When $\sigma_e = \sigma_w$, the first term $(\mathbf{Ax} - \mathbf{b})^T \Sigma_{\mathbf{x}}^{-1} (\mathbf{Ax} - \mathbf{b})$ is a scalar times the STLS objective function (2.9). The second term, $\log \det \Sigma_{\mathbf{x}}$, can be considered as a regularization function and serves to stabilize the solution. One evidence of this property is the next theorem which shows that the solution of the STML problem—as opposed to the STLS solution—is always attained.

THEOREM 3.1. *The optimal solution of the STML problem (3.4) is attained.*

Proof. See Appendix A. \square

We emphasize that attainment is not guaranteed for the STLS problem. Consider, for example, the simple problem in \mathbb{R} with $A = 0$, $b = 1$, and $A_1 = 1$. In this setting, (2.9) becomes

$$\min_x \frac{1}{1 + x^2},$$

which, of course, does not have a global solution.

3.2. Numerical examples. The STML objective (3.4) is nonconvex, and thus general optimization procedures are not guaranteed to obtain its global optimal solution. This is true also for the STLS problem. In special cases, a globally optimal point can be found by exploiting the problem structure. We discuss two such settings in section 5. In section 4 we analyze a class of problems which can be reduced to a single-variable minimization. For the general case we will use the BFGS method implemented by the MATLAB function `fminunc`. In order to invoke such a method, computation of the gradient is necessary. An explicit expression for the gradient is given in the following lemma, whose very simple and technical proof is omitted.

LEMMA 3.2. *Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be the function given by*

$$(3.5) \quad f(\mathbf{x}) = \log \det \Sigma_{\mathbf{x}} + (\mathbf{Ax} - \mathbf{b})^T \Sigma_{\mathbf{x}}^{-1} (\mathbf{Ax} - \mathbf{b}),$$

where $\mathbf{A}, \mathbf{A}_1, \dots, \mathbf{A}_p \in \mathbb{R}^{m \times n}$, $\mathbf{b} \in \mathbb{R}^m$, and $\Sigma_{\mathbf{x}}$ is defined in (3.3). Then

$$\begin{aligned} \nabla f(\mathbf{x}) &= 2\sigma_e^2 \sum_{i=1}^p \mathbf{A}_i^T \Sigma_{\mathbf{x}}^{-1} \mathbf{A}_i \mathbf{x} + 2\mathbf{A}^T \Sigma_{\mathbf{x}}^{-1} (\mathbf{Ax} - \mathbf{b}) \\ &\quad - 2\sigma_e^2 \sum_{i=1}^p \mathbf{A}_i^T \Sigma_{\mathbf{x}}^{-1} (\mathbf{Ax} - \mathbf{b}) \mathbf{x}^T \mathbf{A}_i^T \Sigma_{\mathbf{x}}^{-1} (\mathbf{Ax} - \mathbf{b}). \end{aligned}$$

We now illustrate the performance of STML and STLS by a simple numerical example. Consider an exact linear system

$$\mathbf{b}_t = \mathbf{A}_t \mathbf{x}_t,$$

where \mathbf{A}_t is a 30×20 Toeplitz matrix with 7 diagonals corresponding to 7 structure components:

$$\mathbf{A}_t = \begin{pmatrix} \alpha_1 & \alpha_5 & \alpha_6 & \alpha_7 & 0 & 0 & 0 & 0 & 0 & \cdots \\ \alpha_2 & \alpha_1 & \alpha_5 & \alpha_6 & \alpha_7 & 0 & 0 & 0 & 0 & \cdots \\ \alpha_3 & \alpha_2 & \alpha_1 & \alpha_5 & \alpha_6 & \alpha_7 & 0 & 0 & 0 & \cdots \\ \alpha_4 & \alpha_3 & \alpha_2 & \alpha_1 & \alpha_5 & \alpha_6 & \alpha_7 & 0 & 0 & \cdots \\ 0 & \alpha_4 & \alpha_3 & \alpha_2 & \alpha_1 & \alpha_5 & \alpha_6 & \alpha_7 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

Each of the structure components was randomly generated from a uniform distribution on the interval $[0, 1]$, and their specific values to 3 digits of accuracy are given in the following table:

i	1	2	3	4	5	6	7
α_i	0.721	0.578	0.579	0.080	0.810	0.919	0.921

The components of the 20×1 vector \mathbf{x}_t were also randomly generated from a uniform distribution on the interval $[0, 1]$ and are given by (to 3 digits of accuracy):

i	1	2	3	4	5	6	7	8	9	10
$\mathbf{x}_t(i)$	0.533	0.745	0.996	0.833	0.134	0.389	0.732	0.380	0.221	0.853
i	11	12	13	14	15	16	17	18	19	20
$\mathbf{x}_t(i)$	0.224	0.684	0.331	0.988	0.028	0.658	0.160	0.621	0.028	0.623

The observed vector and structure components vector are given by

$$\begin{aligned}\mathbf{b}_o &= \mathbf{b}_t + \mathbf{w}, \\ \boldsymbol{\alpha}_o &= \boldsymbol{\alpha}_t + \mathbf{e},\end{aligned}$$

where $\mathbf{w} \sim N(\mathbf{0}, \sigma_w^2 \mathbf{I}_m)$ and $\mathbf{e} \sim N(\mathbf{0}, \sigma_e^2 \mathbf{I}_p)$.

Each of the standard deviations σ_w and σ_e has three possible values: 10^{-1} , 10^{-2} , and 10^{-3} . For each of the 9 options we generated 200 realizations of the perturbation vectors \mathbf{w} and \mathbf{e} according to the chosen standard deviations and computed the average of the estimation error $\|\hat{\mathbf{x}} - \mathbf{x}_t\|$ for the LS, STLS, and STML estimates (the last two were computed by the MATLAB function `fminunc` with an initial vector chosen as the least squares solution). Since, as was already mentioned, the STML is in a sense a regularization of the STLS estimate with a special choice of regularizer, we also computed the corresponding results for two popular regularized estimates:

1. TIK-GCV—Tikhonov solution $(\mathbf{A}^T \mathbf{A} + \lambda \mathbf{I})^{-1} \mathbf{A}^T \mathbf{b}$, where λ is chosen by the generalized cross validation (GCV) criteria [22] implemented by the MATLAB function `gcv` from the “regularization tools” package [25], and
2. LSQR—the LSQR solution computed with the MATLAB function `lsqr` with tolerance set to $m\sigma_w^2 = 30\sigma_w^2$. The output of LSQR with low tolerance can be considered as a regularized solution.

The mean over 200 runs for each of the 9 settings are summarized in the following table (the boldfaced numbers represent the best results of the corresponding row):

σ_e	σ_w	LS	STLS	STML	LSQR	TIK-GCV
1e-3	1e-3	0.0580	0.0523	0.0522	0.0580	0.0689
	1e-2	0.3700	0.3700	0.3688	0.2659	0.2210
	1e-1	3.6452	3.6459	3.6330	1.3980	0.9557
1e-2	1e-3	0.4181	0.2902	0.2635	0.4181	0.2821
	1e-2	0.5815	0.5612	0.4825	0.4140	0.3457
	1e-1	3.9612	4.0894	3.1000	1.3994	0.9892
1e-1	1e-3	1.4679	1.7391	0.9853	1.4645	1.0027
	1e-2	2.6212	5.0213	0.9767	1.2341	1.3078
	1e-1	9.8396	34.0736	1.1731	1.4044	1.1444

Clearly, the STML estimate provides better results than LS and STLS. The reason for that might be the inherent regularization of this estimate. For large values of σ_e the STLS estimate usually behaves worse than LS, while the STML solution is better by an order of magnitude. It can also be seen that the STML estimate was competitive to the two other regularized solvers (LSQR and TIK-GCV). In particular, it gave the best

results for low values of σ_w and also when $\sigma_e = 10^{-1}$, $\sigma_w = 10^{-2}$. In other words, when the uncertainty in \mathbf{A} is substantial with respect to the uncertainty in \mathbf{b} , the STML is superior to standard regularization methods. The Tikhonov solution was better in all other cases. We also note that the BFGS method implemented in `fminunc` did not converge for a small percentage of the runs (for either STLS or STML). Specifically, in each of the 9 scenarios, we performed between 202 and 207 runs in order to obtain the required 200 results (since in 2–7 runs the BFGS method did not converge for either the STLS or STML problem). We also noticed through additional numerical experiments that the observations that (1) STML outperforms STLS and (2) the gap increases as σ_e grows are typical and only mildly depend on the initial values of \mathbf{A}_t and \mathbf{x}_t .

In our second example, we consider the discretization of the famous Phillips test problem which is an integral equation of the first kind [35]. The exact system was obtained from the “regularization tools” package [25]. The problem consists of a symmetric Toeplitz matrix with 17 diagonals corresponding to 9 structure components. Each structure component was perturbed proportionally to its magnitude in the following manner: for every $i = 1, \dots, 9$, the structure component α_i ($i = 1, \dots, 9$) was changed to $\alpha_i(1 + e_i)$, where $e_i \sim N(0, 0.02)$. We also chose $\sigma_w = 0.001$. Since the problem here corresponds to a 32×32 square measurement matrix, the STLS solution coincides with LS. We compared the STML estimate with the STLS solution and the Tikhonov solution whose parameter is chosen via GCV. A representative run is given in Figure 3.1. Evidently, the STML and TIK-GCV estimates fit the true signal reasonably, whereas the STLS solution behaves erratically.

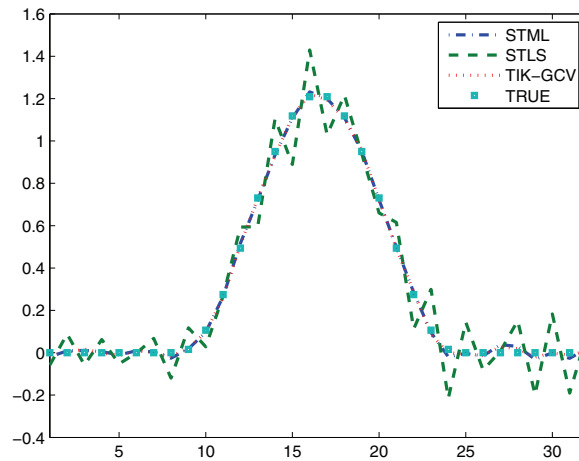


FIG. 3.1. The true signal versus the STLS, Tikhonov (with parameter choice via GCV), and STML estimates.

4. The matrix-restricted structure. As we have seen in the previous section, computation of the STML estimate amounts to solving a nonconvex optimization problem. Therefore, in general, there is no method that efficiently finds the global minimum. In this section we discuss a special structure in which the STML problem can be reduced into a single-variable minimization.

4.1. Definition and problem reduction. Suppose that the errors in the model matrix \mathbf{A} are of the form \mathbf{DEC} , where $\mathbf{D} \in \mathbb{R}^{m \times p}$, $\mathbf{C} \in \mathbb{R}^{l \times n}$ are known matrices and $\mathbf{E} \in \mathbb{R}^{p \times l}$ is unknown. This structure, which we will refer to as a *matrix-restricted* structure, allows us to model various interesting special cases. For example, the choice

$$(4.1) \quad \mathbf{D} = \begin{pmatrix} \mathbf{I}_{m_1} \\ \mathbf{0}_{(m-m_1) \times m_1} \end{pmatrix}, \mathbf{C} = \mathbf{I}_n,$$

corresponds to the situation in which the first m_1 rows of \mathbf{A} are contaminated by noise, while the remainder $m - m_1$ rows are noise free. The choice $\mathbf{D} = \mathbf{I}_m$, $\mathbf{C} = (\mathbf{0}_{n_1}, \mathbf{I}_{n-n_1})$, corresponds to the scenario in which the first n_1 columns of \mathbf{A} are error free while the remaining $n - n_1$ are noisy. Finally, the TML problem can be recovered by assuming $\mathbf{D} = \mathbf{I}_m$, $\mathbf{C} = \mathbf{I}_n$.

The matrix-restricted structure was analyzed in the context of STLS in [4] where it was shown that for such a structure the problem can be reduced into a single-variable minimization, and that under some additional conditions the one-dimensional objective is unimodal. Another closely related structure discussed in the context of the STLS problem is the *restricted* case [41] in which the matrix and right-hand side perturbations are jointly assumed to have the “DEC” structure. The STLS problem in this setting can be solved using the restricted singular value decomposition [41]. In this section we show that much like the STLS, the STML problem with matrix-restricted structure can be reduced into a single-variable problem.

The linear model corresponding to the matrix-restricted structure is

$$(4.2) \quad \mathbf{b} = (\mathbf{A} + \mathbf{DEC})\mathbf{x} + \mathbf{w}.$$

Denoting the i th column of \mathbf{D} by \mathbf{d}_i ($i = 1, \dots, p$) and the j th row of \mathbf{C} by \mathbf{c}_j ($j = 1, \dots, l$), we can rewrite (4.2) as

$$(4.3) \quad \mathbf{b} = \left(\mathbf{A} + \sum_{i=1}^p \sum_{j=1}^l e_{ij} \mathbf{A}_{ij} \right) \mathbf{x} + \mathbf{w},$$

where e_{ij} is the (i, j) th component of \mathbf{E} and $\mathbf{A}_{ij} = \mathbf{d}_i \mathbf{c}_j^T$. The special structure of \mathbf{A}_{ij} allows us to simplify the STML problem.

LEMMA 4.1. *The STML problem corresponding to the linear model with $e_{i,j} \sim N(0, \sigma_e)$ and $w_i \sim N(0, \sigma_w)$ is*

$$(4.4) \quad \min_{\mathbf{x} \in \mathbb{R}^n} \{ \log \det \boldsymbol{\Sigma}_{\mathbf{x}} + (\mathbf{Ax} - \mathbf{b})^T \boldsymbol{\Sigma}_{\mathbf{x}}^{-1} (\mathbf{Ax} - \mathbf{b}) \},$$

where

$$\boldsymbol{\Sigma}_{\mathbf{x}} = \sigma_e^2 \|\mathbf{Cx}\|^2 \mathbf{DD}^T + \sigma_w^2 \mathbf{I}_m.$$

Proof. All we need to compute is the matrix $\boldsymbol{\Sigma}_{\mathbf{x}}$ for the matrix-restricted structure. By (4.3) it follows that

$$\begin{aligned} \sum_{i=1}^p \sum_{j=1}^l \mathbf{A}_{ij} \mathbf{x} \mathbf{x}^T \mathbf{A}_{ij}^T &= \sum_{i=1}^p \sum_{j=1}^l \mathbf{d}_i \mathbf{c}_j^T \mathbf{x} \mathbf{x}^T \mathbf{c}_j \mathbf{d}_i^T = \sum_{i=1}^p \sum_{j=1}^l \mathbf{x}^T \mathbf{c}_j \mathbf{c}_j^T \mathbf{x} \mathbf{d}_i \mathbf{d}_i^T \\ &= \mathbf{x}^T \left[\sum_{j=1}^l \mathbf{c}_j \mathbf{c}_j^T \right] \mathbf{x} \sum_{i=1}^p \mathbf{d}_i \mathbf{d}_i^T = \mathbf{x}^T \mathbf{C}^T \mathbf{Cx} \mathbf{DD}^T = \|\mathbf{Cx}\|^2 \mathbf{DD}^T, \end{aligned}$$

proving the result. \square

4.2. An equivalent one-dimensional problem. In order to solve problem (4.4), we can use the same methodology that was used in [42]. This allows us to convert the problem into a single-variable minimization and then use a one-dimensional solver.

We begin by noting that (4.4) can be rewritten as:

$$(4.5) \quad \min_{\alpha \geq 0} G(\alpha),$$

where $G(\alpha)$ is defined as:

$$(4.6) \quad G(\alpha) \equiv \min_{\mathbf{x}} \{ \log \det \mathbf{\Gamma}_\alpha + (\mathbf{Ax} - \mathbf{b})^T \mathbf{\Gamma}_\alpha^{-1} (\mathbf{Ax} - \mathbf{b}) : \|\mathbf{Cx}\|^2 = \alpha \},$$

with

$$\mathbf{\Gamma}_\alpha = \sigma_e^2 \alpha \mathbf{DD}^T + \sigma_w^2 \mathbf{I}_m.$$

An evaluation of the function $G(\cdot)$ requires the solution of a minimization problem of a quadratic function subject to a single quadratic equality constraint. This is a special case of the class of *generalized trust region subproblems* (GTRS) which consists of minimizing a general quadratic function (possibly indefinite) subject to a general quadratic constraint. It is known that under mild conditions GTRS problems possess necessary and sufficient optimality conditions, and that—as a result—they can be solved efficiently [34].

The function $G(\cdot)$ is not convex or unimodal, and therefore, general one-dimensional solvers are not guaranteed to reach the global minimum. However, it is usually simpler to solve one-dimensional optimization problems than multivariate ones. An interesting property is that every local minimum point of (4.5) corresponds to at least one local minimum of the multivariate problem (4.4). The reverse claim does not hold true, which means that local optima points of the multivariate problem (4.4) might vanish in the transition to the one-dimensional problem (4.5). This property is summarized in Theorem 4.2 below. The proof is very similar to the proof of Theorem 4.1 of [4] and is included here for completeness.

THEOREM 4.2. *Let α_0 be a local minimum of the single-variable problem (4.5), and let \mathbf{x} be an optimal solution of (4.6) with $\alpha = \alpha_0$. Then \mathbf{x} is a local minimum of problem (4.4).*

Proof. Since α_0 is a local minimum of (4.5), there exists an interval $I = [\alpha_0 - \delta, \alpha_0 + \delta]$ such that $G(\alpha_0) \leq G(\alpha)$ for every $\alpha \in I \cap [0, \infty]$. Let \mathbf{x}_0 be an optimal solution of (4.6) with $\alpha = \alpha_0$ as stated in the theorem. Our objective is to show that \mathbf{x}_0 is a local minimum of (4.4). Let $\mathbf{x} \in \mathbb{R}^n$ satisfy $\|\mathbf{x} - \mathbf{x}_0\| \leq \rho$, where $\rho = \min\{1, \frac{\delta}{2\lambda_{\max}(\mathbf{C}^T \mathbf{C})(\|\mathbf{x}_0\| + 1)}\}$. By the mean value theorem, there exists $\lambda \in [0, 1]$ such that

$$\mathbf{x}^T \mathbf{C}^T \mathbf{C} \mathbf{x} - \mathbf{x}_0^T \mathbf{C}^T \mathbf{C} \mathbf{x}_0 = 2[\mathbf{x}_0 + \lambda(\mathbf{x} - \mathbf{x}_0)]^T \mathbf{C}^T \mathbf{C} (\mathbf{x} - \mathbf{x}_0)$$

so that

$$\begin{aligned} |\mathbf{x}^T \mathbf{C}^T \mathbf{C} \mathbf{x} - \mathbf{x}_0^T \mathbf{C}^T \mathbf{C} \mathbf{x}_0| &\leq 2\lambda_{\max}(\mathbf{C}^T \mathbf{C}) \|\mathbf{x}_0 + \lambda(\mathbf{x} - \mathbf{x}_0)\| \|\mathbf{x} - \mathbf{x}_0\| \\ &\leq 2\lambda_{\max}(\mathbf{C}^T \mathbf{C})(\|\mathbf{x}_0\| + \|\mathbf{x} - \mathbf{x}_0\|) \|\mathbf{x} - \mathbf{x}_0\| \\ &\leq 2\lambda_{\max}(\mathbf{C}^T \mathbf{C})(\|\mathbf{x}_0\| + 1)\rho \leq \delta. \end{aligned}$$

Now, since $\mathbf{x}_0^T \mathbf{C}^T \mathbf{C} \mathbf{x}_0 = \alpha_0$ it follows that $\mathbf{x}^T \mathbf{C}^T \mathbf{C} \mathbf{x} \in I \cap [0, \infty]$, and as a result

$$G(\mathbf{x}^T \mathbf{C}^T \mathbf{C} \mathbf{x}) \geq G(\alpha_0).$$

Finally, let $g(\cdot)$ be the objective function of problem (4.4). Then

$$g(\mathbf{x}) \geq G(\mathbf{x}^T \mathbf{C}^T \mathbf{C} \mathbf{x}) \geq G(\alpha_0) = G(\mathbf{x}_0^T \mathbf{C}^T \mathbf{C} \mathbf{x}_0) = g(\mathbf{x}_0),$$

establishing the result. \square

The following example demonstrates that indeed local minima points might vanish in the passage to the one-dimensional problem.

Example. Consider the STML problem with (randomly generated) data

$$\mathbf{A} = \begin{pmatrix} -0.69 & 0.96 \\ 0.70 & 0.88 \\ 1.14 & 0.21 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 1.34 \\ 1.52 \\ 0.87 \end{pmatrix}, \quad \mathbf{C} = \begin{pmatrix} 0.89 & 1.19 \\ -2.30 & -2.01 \end{pmatrix},$$

$$\mathbf{D} = \begin{pmatrix} 1.16 & 0.42 & -0.58 \\ 0.84 & 0.46 & 0.16 \\ 0.97 & 0.16 & 0.12 \end{pmatrix},$$

and $\sigma_e = \sigma_w = 1$. This example was randomly generated by choosing the components of \mathbf{b} , \mathbf{A} , \mathbf{C} , and \mathbf{D} from a standard normal distribution (using the MATLAB function `randn`) and then rounded to have only two digits after the decimal point. Approximately 10% of the problems generated in this manner had the property of having multiple local minima, and this example is one such instance.

In Figure 4.1 the contour plot is presented on the left image and the function $G(\cdot)$ is presented on the right image. The function G is presented here only for values in the range $[0, 2]$, but a plot of this function for larger values reveals that it is increasing for values in the range $(2, \infty)$. The global optimum is attained at $\tilde{\mathbf{x}} = (-0.1188, 0.4537)$ with value 2.4314. It can also be seen from the contour plot that there exists a local minimum at $\hat{\mathbf{x}} = (-0.3343, 0.0208)$, and its value is 3.5524. The interesting fact is that the function $G(\cdot)$ has only one local minimum point (and hence also global) that is attained at $\alpha = 0.5963$ which matches the global optimum $\tilde{\mathbf{x}}$. Therefore, in this example, we can see that $\hat{\mathbf{x}}$ vanishes in the process of passing to the one-dimensional formulation.

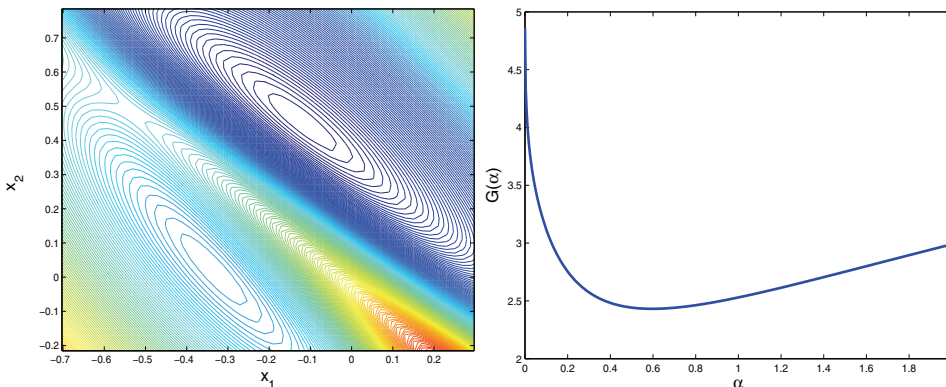


FIG. 4.1. A contour plot of the two-dimensional problem (left) and the corresponding one-dimensional formulation (right).

Recall that, in fact, we reformulated the STML problem as a one-dimensional bilevel optimization problem. That is, each evaluation of the objective function $G(\alpha)$

requires the solution of another optimization problem. In the unstructured case, i.e., when $\mathbf{D} = \mathbf{C} = \mathbf{I}$, it was shown in [43] that the TML can be recast as a minimization of a one-dimensional unimodal *explicit* function.

5. Circulant-based structures. Two classes of matrices that appear in applications are circulant matrices and block circulant with circulant blocks (BCCB). The first class appears in one-dimensional deconvolution problems with periodic boundary conditions, while the class of BCCB matrices emerges in two-dimensional deconvolution problems (such as image deblurring) with periodic boundary conditions [2, 26]. In this section we show that when the model matrix has one of these structures, the STML can be found by solving a unimodal single-variable optimization problem.

In section 5.1 we present necessary notation, as well as a complex relaxation of the corresponding optimization problem. In section 5.3 we decompose the complex relaxation into one-dimensional complex-valued problems, which are later transformed into one-dimensional unimodal real-valued problems in section 5.4. The consequence is that a global optimum point of the complex relaxation can be found efficiently. In section 5.5 we show that the complex relaxation has at least one real-valued solution which implies that the original real-valued problem can be solved efficiently.

5.1. Basic definitions and notation. Although our primary interest in the context of this paper is to consider real-valued matrices and vectors, we will need to deal with the complex domain in our analysis. Therefore, in this section we use the notation \mathbb{F} to stand for the underlying number field which is either the real number field \mathbb{R} or the complex number field \mathbb{C} .

The class of $n \times n$ circulant matrices consists of all $n \times n$ matrices in which each row is a cyclic right shift of the previous row. That is, an $n \times n$ circulant matrix is of the form

$$(5.1) \quad \mathcal{T}^{(1)}(\mathbf{c}) \equiv \begin{pmatrix} c_1 & c_2 & c_3 & \cdots & c_n \\ c_n & c_1 & c_2 & \cdots & c_{n-1} \\ c_{n-1} & c_n & c_1 & \cdots & c_{n-2} \\ \vdots & \vdots & \vdots & & \vdots \\ c_2 & c_3 & c_4 & \cdots & c_1 \end{pmatrix} \quad (\mathbf{c} \in \mathbb{F}^n).$$

The linear operator $\mathcal{T}^{(1)} : \mathbb{F}^n \rightarrow \mathbb{F}^{n \times n}$ can also be written as

$$\mathcal{T}^{(1)}(\mathbf{c}) = \sum_{j=1}^n c_j \mathbf{A}_j^{(1)},$$

where $\mathbf{A}_j^{(1)} = \mathbf{S}_n^{j-1}$, with \mathbf{S}_n being the $n \times n$ ‘‘cyclic shift matrix’’ defined by $\mathbf{S}_n = \mathcal{T}^{(1)}((0, 1, 0, 0, \dots, 0)^T)$.

The set of circulant matrices over the number field \mathbb{F} is given by

$$(5.2) \quad \mathcal{L}^{(1)}(\mathbb{F}) = \left\{ \mathcal{T}^{(1)}(\mathbf{c}) : \mathbf{c} \in \mathbb{F}^n \right\}.$$

We will always assume that the circulant matrices are of size $n \times n$ with a known n . The representation (5.2) will be referred to as the *algebraic* representation of the set.

A well-known property of the set of $n \times n$ circulant matrices over the complex number field, $\mathcal{L}^{(1)}(\mathbb{C})$, is that they are exactly the matrices which are diagonalizable

by the unitary discrete Fourier transform (DFT) matrix \mathbf{F}_n [18]. That is, we can also write a *spectral* representation of $\mathcal{L}^{(1)}(\mathbb{C})$ by

$$(5.3) \quad \mathcal{L}^{(1)}(\mathbb{C}) = \{\mathbf{F}_n^* \text{diag}(\boldsymbol{\lambda}) \mathbf{F}_n : \boldsymbol{\lambda} \in \mathbb{C}^n\}.$$

An $mn \times mn$ BCCB matrix with n^2 blocks of size $m \times m$ has the form

$$\begin{pmatrix} \mathbf{C}_1 & \mathbf{C}_2 & \mathbf{C}_3 & \cdots & \mathbf{C}_n \\ \mathbf{C}_n & \mathbf{C}_1 & \mathbf{C}_2 & \cdots & \mathbf{C}_{n-1} \\ \mathbf{C}_{n-1} & \mathbf{C}_n & \mathbf{C}_1 & \cdots & \mathbf{C}_{n-2} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ \mathbf{C}_2 & \mathbf{C}_3 & \mathbf{C}_4 & \cdots & \mathbf{C}_1 \end{pmatrix},$$

where $\mathbf{C}_1, \dots, \mathbf{C}_n \in \mathcal{L}^{(1)}(\mathbb{F})$. We denote the set of all such matrices by $\mathcal{L}^{(2)}(\mathbb{F})$. The algebraic representation of $\mathcal{L}^{(2)}(\mathbb{F})$ is given by

$$\mathcal{L}^{(2)}(\mathbb{F}) = \{\mathcal{T}^{(2)}(\mathbf{c}) : \mathbf{c} \in \mathbb{F}^{mn}\},$$

where the linear operator $\mathcal{T}^{(2)} : \mathbb{F}^{mn} \rightarrow \mathbb{F}^{mn \times mn}$ is defined by

$$(5.4) \quad \mathcal{T}^{(2)}(\mathbf{c}) = \sum_{k=1}^{mn} c_k \mathbf{A}_k^{(2)}.$$

The mn structure matrices $\mathbf{A}_1^{(2)}, \dots, \mathbf{A}_{mn}^{(2)}$ are the mn Kronecker products $\mathbf{S}_n^j \otimes \mathbf{S}_m^i$, $i = 0, \dots, m-1, j = 1, \dots, n-1$ (in some order). Similar to the circulant case, $\mathcal{L}^{(2)}(\mathbb{C})$ also has a spectral representation,

$$\mathcal{L}^{(2)}(\mathbb{C}) = \{(\mathbf{F}_n \otimes \mathbf{F}_m)^* \text{diag}(\boldsymbol{\lambda}) (\mathbf{F}_n \otimes \mathbf{F}_m) : \boldsymbol{\lambda} \in \mathbb{C}^{mn}\};$$

that is, BCCB matrices are exactly the matrices which are diagonalizable by the unitary two-dimensional DFT matrix $\mathbf{F}_n \otimes \mathbf{F}_m$. We will assume throughout the section that the BCCB matrices consist of n^2 blocks of $m \times m$ matrices and that m and n are known.

One more property that will be important in our analysis is that for every $k = 1, 2$ and $\mathbf{c} \in \mathbb{F}^{p_k}$,

$$\|\mathcal{T}^{(k)}(\mathbf{c})\|_F^2 = p_k \|\mathbf{c}\|^2.$$

To summarize our notation, we consider two structures $\mathcal{L}^{(k)}(\mathbb{F}), k = 1, 2$, given by

$$(5.5) \quad \mathcal{L}^{(k)}(\mathbb{F}) = \left\{ \mathcal{T}^{(k)}(\mathbf{c}) = \sum_{i=1}^{p_k} c_i \mathbf{A}_i^{(k)} : \mathbf{c} \in \mathbb{F}^{p_k} \right\}, \quad k = 1, 2,$$

where

$$p_1 = n, p_2 = mn.$$

Over the complex domain, each of these spaces consists of matrices that are all diagonalizable by the same unitary matrix:

$$(5.6) \quad \mathcal{L}^{(k)}(\mathbb{C}) = \left\{ \mathbf{Q}_{(k)}^* \text{diag}(\boldsymbol{\lambda}) \mathbf{Q}_{(k)} : \boldsymbol{\lambda} \in \mathbb{F}^{p_k} \right\},$$

where

$$(5.7) \quad \mathbf{Q}_{(1)} = \mathbf{F}_n, \quad \mathbf{Q}_{(2)} = \mathbf{F}_n \otimes \mathbf{F}_m.$$

In the derivations below, we consider both structures simultaneously. The index k , that takes the values 1 or 2, will indicate the identity of the structure (1, circulant; 2, BCCB).

5.2. The STML problem. Our goal is to find efficient methods for calculating the STML estimate corresponding to each of the two linear models

$$(5.8) \quad \mathbf{b} = (\mathbf{A} + \mathcal{T}^{(k)}(\mathbf{c}))\mathbf{x} + \mathbf{w},$$

where $\mathbf{A} \in \mathcal{L}^{(k)}(\mathbb{R})$ and $\mathbf{b} \in \mathbb{R}^{p_k}$ are known and $\mathbf{w} \in \mathbb{R}^{p_k}$ and $\mathbf{c} \in \mathbb{R}^{p_k}$ are the unknown perturbations. The STML associated with the model (5.8) is the solution to

$$(5.9) \quad (P_{\mathbb{R}}) : \min_{\mathbf{x}} \left\{ (\mathbf{A}\mathbf{x} - \mathbf{b})^T \left[\Sigma_{\mathbf{x}}^{(k)} \right]^{-1} (\mathbf{A}\mathbf{x} - \mathbf{b}) + \log \det \Sigma_{\mathbf{x}}^{(k)} : \mathbf{x} \in \mathbb{R}^{p_k} \right\},$$

where

$$\Sigma_{\mathbf{x}}^{(k)} = \sigma_e^2 \sum_{i=1}^{p_k} \mathbf{A}_i^{(k)} \mathbf{x}\mathbf{x}^T \left[\mathbf{A}_i^{(k)} \right]^T + \sigma_w^2 \mathbf{I}$$

for every $\mathbf{x} \in \mathbb{R}^{p_k}$.

Analyzing (5.9) turns out to be difficult since the spectral representation (5.6) holds only over the complex domain and not over the real domain. We therefore begin by solving (5.9) over the complex domain; namely, we consider the problem

$$(5.10) \quad (P_{\mathbb{C}}) : \min_{\mathbf{x}} \left\{ (\mathbf{A}\mathbf{x} - \mathbf{b})^* \left[\Sigma_{\mathbf{x}}^{(k)} \right]^{-1} (\mathbf{A}\mathbf{x} - \mathbf{b}) + \log \det \Sigma_{\mathbf{x}}^{(k)} : \mathbf{x} \in \mathbb{C}^{p_k} \right\},$$

where the definition of $\Sigma_{\mathbf{x}}^{(k)}$ is extended to the complex domain as follows:

$$\Sigma_{\mathbf{x}}^{(k)} = \sigma_e^2 \sum_{i=1}^{p_k} \mathbf{A}_i^{(k)} \mathbf{x}\mathbf{x}^* \left[\mathbf{A}_i^{(k)} \right]^* + \sigma_w^2 \mathbf{I}$$

for every $\mathbf{x} \in \mathbb{C}^{p_k}$. We will call problem $(P_{\mathbb{C}})$ the *convex relaxation* of $(P_{\mathbb{R}})$. This terminology is consistent with the one presented in [7].

Clearly, if the solution to (5.10) turns out to be real, then it will also be the STML estimate. In the next subsections we will show that the convex counterpart can be solved exactly; namely, a global optimum can be found. We also prove that (5.10) has at least one optimal solution that is real. If, in addition, there is a solution to $\mathbf{A}\mathbf{x} = \mathbf{b}$, then (5.10) has a unique solution which coincides with the STML. Therefore, solving (5.10) will often result in the true STML estimate.

Our strategy for solving (5.10) is to first show that it can be decomposed into p_k one-dimensional complex-valued problems. We then show that the solution to each such problem can be found by solving a one-dimensional unimodal real-valued problem. This implies that the global optimum can be found exactly.

5.3. Solving (P_C) . In order to decompose (P_C) of (5.10) into a set of one-dimensional problems, we exploit the spectral decomposition of $\Sigma_{\mathbf{x}}^{(k)}$.

PROPOSITION 5.1. *Let $\mathbf{x} \in \mathbb{C}^{p_k}$. Then*

$$(5.11) \quad \Sigma_{\mathbf{x}}^{(k)} = \mathbf{Q}_{(k)}^* \text{diag} \left([p_k \sigma_e^2 |\tilde{x}_i|^2 + \sigma_w^2]_{i=1}^{p_k} \right) \mathbf{Q}_{(k)},$$

where $\tilde{\mathbf{x}} = \mathbf{Q}_{(k)} \mathbf{x}$ and $\mathbf{Q}_{(k)}$ is given by (5.7).

Note that Proposition 5.1 implies that $\Sigma_{\mathbf{x}}^{(k)} \in \mathcal{L}^{(k)}(\mathbb{C})$ for every $\mathbf{x} \in \mathbb{C}^{p_k}$.

The proof of Proposition 5.1 relies on the following lemma whose simple and technical proof is omitted.

LEMMA 5.2. *Let m, p be positive integers, and let $\mathbf{v} \in \mathbb{C}^m$, $\mathbf{Z} \in \mathbb{C}^{m \times p}$, and $d > 0$. Then the optimal value of the following minimization problem in the variables $\boldsymbol{\alpha} \in \mathbb{C}^p$*

$$(5.12) \quad \min_{\boldsymbol{\alpha}} \|\mathbf{v} + \mathbf{Z}\boldsymbol{\alpha}\|^2 + d\|\boldsymbol{\alpha}\|^2$$

is

$$(5.13) \quad d\mathbf{v}^*(d\mathbf{I} + \mathbf{Z}\mathbf{Z}^*)^{-1}\mathbf{v}.$$

We are now ready to prove Proposition 5.1.

Proof. Let $\mathbf{x} \in \mathbb{C}^{p_k}$ be fixed. Consider the optimization problem (5.12) with arbitrary $\mathbf{v} \in \mathbb{C}^{p_k}$ and constant $d = \frac{\sigma_w^2}{\sigma_e^2}$, and let $\mathbf{Z} \in \mathbb{C}^{p_k \times p_k}$ be given by

$$\mathbf{Z} = \left(\mathbf{A}_1^{(k)} \mathbf{x}, \mathbf{A}_2^{(k)} \mathbf{x}, \dots, \mathbf{A}_{p_k}^{(k)} \mathbf{x} \right).$$

By Lemma 5.2, the optimal value of problem (5.12) is given by

$$\frac{\sigma_w^2}{\sigma_e^2} \mathbf{v}^* \left(\frac{\sigma_w^2}{\sigma_e^2} \mathbf{I} + \sum_{i=1}^{p_k} \mathbf{A}_i^{(k)} \mathbf{x} \mathbf{x}^* [\mathbf{A}_i^{(k)}]^* \right)^{-1} \mathbf{v},$$

which is the same as

$$(5.14) \quad \sigma_w^2 \mathbf{v}^* \left[\Sigma_{\mathbf{x}}^{(k)} \right]^{-1} \mathbf{v}.$$

To find a different expression for the optimal value of problem (5.12), let us rewrite it explicitly:

$$\min \left\{ \left\| \mathbf{v} + \sum_{i=1}^{p_k} \alpha_i \mathbf{A}_i^{(k)} \mathbf{x} \right\|^2 + d\|\boldsymbol{\alpha}\|^2 : \boldsymbol{\alpha} \in \mathbb{C}^{p_k} \right\},$$

which is the same as

$$\min \left\{ \left\| \mathbf{v} + \mathcal{T}^{(k)}(\boldsymbol{\alpha}) \mathbf{x} \right\|^2 + \frac{d}{p_k} \|\mathcal{T}^{(k)}(\boldsymbol{\alpha})\|^2 : \boldsymbol{\alpha} \in \mathbb{C}^{p_k} \right\}.$$

Using the notation (5.5), it follows that we can also write the above as

$$(5.15) \quad \min \left\{ \left\| \mathbf{v} + \mathbf{W}\mathbf{x} \right\|^2 + \frac{d}{p_k} \|\mathbf{W}\|^2 : \mathbf{W} \in \mathcal{L}^{(k)}(\mathbb{C}) \right\}.$$

Now, using the spectral representation of $\mathcal{L}^{(k)}(\mathbb{C})$ given in (5.6), we make the change of variables $\mathbf{W} = \mathbf{Q}_{(k)}^* \text{diag}(\boldsymbol{\lambda}) \mathbf{Q}_{(k)}$, where $\boldsymbol{\lambda} \in \mathbb{C}^{p_k}$, which combined with the unitarity property of $\mathbf{Q}_{(k)}$, transforms problem (5.15) into

$$(5.16) \quad \min \left\{ \|\tilde{\mathbf{v}} + \text{diag}(\boldsymbol{\lambda})\tilde{\mathbf{x}}\|^2 + \frac{d}{p_k} \|\boldsymbol{\lambda}\|^2 : \boldsymbol{\lambda} \in \mathbb{C}^{p_k} \right\},$$

where $\tilde{\mathbf{v}} = \mathbf{Q}_{(k)} \mathbf{v}$ and $\tilde{\mathbf{x}} = \mathbf{Q}_{(k)} \mathbf{x}$. Problem (5.16) is separable and can be written as

$$(5.17) \quad \min \left\{ \sum_{i=1}^{p_k} \left(|\tilde{v}_i + \lambda_i \tilde{x}_i|^2 + \frac{d}{p_k} |\lambda_i|^2 \right) : \boldsymbol{\lambda} \in \mathbb{C}^{p_k} \right\}.$$

Differentiating with respect to λ_i for every $i = 1, \dots, p_k$, we obtain that the optimal solution is attained at

$$\lambda_i = -\frac{\overline{\tilde{x}_i} \tilde{v}_i}{|\tilde{x}_i|^2 + \frac{d}{p_k}}.$$

Substituting the above expression back into the objective function of (5.17), we obtain the following expression for the optimal value:

$$(5.18) \quad \frac{d}{p_k} \sum_{i=1}^{p_k} \frac{|\tilde{v}_i|^2}{|\tilde{x}_i|^2 + \frac{d}{p_k}} = \frac{d}{p_k} \mathbf{v}^* \left[\mathbf{Q}_{(k)}^* \text{diag} \left(\frac{1}{|\tilde{x}_i|^2 + \frac{d}{p_k}} \right) \mathbf{Q}_{(k)} \right] \mathbf{v}.$$

We arrived at two different expressions—(5.14) and (5.18)—for the same quantity (the optimal value of problem (5.12)). As a result, these two expressions are obviously the same:

$$\sigma_w^2 \mathbf{v}^* \left[\boldsymbol{\Sigma}_{\mathbf{x}}^{(k)} \right]^{-1} \mathbf{v} = \frac{d}{p_k} \mathbf{v}^* \left[\mathbf{Q}_{(k)}^* \text{diag} \left(\frac{1}{|\tilde{x}_i|^2 + \frac{d}{p_k}} \right) \mathbf{Q}_{(k)} \right] \mathbf{v}.$$

Since the above equality is satisfied for every $\mathbf{v} \in \mathbb{C}^{p_k}$, it follows that

$$\sigma_w^2 \left[\boldsymbol{\Sigma}_{\mathbf{x}}^{(k)} \right]^{-1} = \frac{d}{p_k} \mathbf{Q}_{(k)}^* \text{diag} \left(\frac{1}{|\tilde{x}_i|^2 + \frac{d}{p_k}} \right) \mathbf{Q}_{(k)},$$

which after taking the inverse of both sides gives the desired identity (5.11). □

Using Proposition 5.1 we can now decompose (5.10) into p_k one-dimensional problems over the complex domain. To this end we assume that the observed matrix \mathbf{A} also belongs to the underlying structure, that is, $\mathbf{A} \in \mathcal{L}^{(k)}(\mathbb{R})$.

THEOREM 5.3 (decomposition for circulant and BCCB structures). *Let $\boldsymbol{\alpha}$ be the eigenvalues of \mathbf{A} defined by the relation*

$$(5.19) \quad \mathbf{A} = \mathbf{Q}_{(k)}^* \text{diag}(\boldsymbol{\alpha}) \mathbf{Q}_{(k)},$$

where $\mathbf{Q}_{(k)}$ is defined by (5.7). Then every solution to problem $(P_{\mathbb{C}})$ (see (5.10)) is given by $\mathbf{x} = \mathbf{Q}_{(k)}^* \tilde{\mathbf{x}}$, where for every $i = 1, \dots, p_k$, the i th component of $\tilde{\mathbf{x}}$, \tilde{x}_i , is an optimal solution to the one-dimensional complex-valued problem

$$(5.20) \quad \min_{\tilde{x}_i \in \mathbb{C}} \left\{ \frac{|\alpha_i \tilde{x}_i - \tilde{b}_i|^2}{p_k \sigma_e^2 |\tilde{x}_i|^2 + \sigma_w^2} + \log(p_k \sigma_e^2 |\tilde{x}_i|^2 + \sigma_w^2) \right\},$$

with $\tilde{\mathbf{b}} = \mathbf{Q}_{(k)} \mathbf{b}$.

Proof. Plugging the expression (5.11) for $\Sigma_{\mathbf{x}}^{(k)}$ into problem $(P_{\mathbb{C}})$ and using the unitarity property of $\mathbf{Q}_{(k)}$, we obtain the following equivalent formulation:

$$(5.21) \quad \min_{\mathbf{x}} \left\{ (\mathbf{Q}_{(k)} \mathbf{A} \mathbf{x} - \mathbf{Q}_{(k)} \mathbf{b})^* \text{diag} \left([p_k \sigma_e^2 |\tilde{x}_i|^2 + \sigma_w^2]_{i=1}^{p_k} \right)^{-1} (\mathbf{Q}_{(k)} \mathbf{A} \mathbf{x} - \mathbf{Q}_{(k)} \mathbf{b}) \right. \\ \left. + \log \det \left[\text{diag} \left([p_k \sigma_e^2 |\tilde{x}_i|^2 + \sigma_w^2]_{i=1}^{p_k} \right) \right] : \mathbf{x} \in \mathbb{C}^{p_k} \right\}.$$

Note that

$$\mathbf{Q}_{(k)} \mathbf{A} \mathbf{x} - \mathbf{Q}_{(k)} \mathbf{b} = \mathbf{Q}_{(k)} \mathbf{A} \mathbf{Q}_{(k)}^* \mathbf{Q}_{(k)} \mathbf{x} - \tilde{\mathbf{b}} = \text{diag}(\alpha) \tilde{\mathbf{x}} - \tilde{\mathbf{b}}.$$

Making the change of variables $\tilde{\mathbf{x}} = \mathbf{Q}_{(k)} \mathbf{x}$ and using the above identity, problem (5.21) reduces to the separable problem

$$\min_{\tilde{\mathbf{x}} \in \mathbb{C}^{p_k}} \left\{ \sum_{i=1}^{p_k} \left[\frac{|\alpha_i \tilde{x}_i - \tilde{b}_i|^2}{p_k \sigma_e^2 |\tilde{x}_i|^2 + \sigma_w^2} + \log(p_k \sigma_e^2 |\tilde{x}_i|^2 + \sigma_w^2) \right] \right\},$$

establishing the desired result. \square

Theorem 5.3 implies that a solution to $(P_{\mathbb{C}})$ can be constructed via the following three stages:

1. Find the eigenvalues of \mathbf{A} given by the relation (5.19), and compute $\tilde{\mathbf{b}} = \mathbf{Q}_{(k)} \mathbf{b}$.
2. For each $i = 1, \dots, p_k$ find $\tilde{x}_i \in \mathbb{C}$ which is an optimal solution of (5.20).
3. An optimal solution of $(P_{\mathbb{C}})$ is given by $\mathbf{x} = \mathbf{Q}_{(k)}^* \tilde{\mathbf{x}}$.

It remains to discuss how to solve (5.20). This is the topic of the next section.

5.4. Solution of the one-dimensional problem. Our objective is to show how to solve for each $i = 1, \dots, p_k$ the one-dimensional problem (5.20), that is, how to solve problems of the form

$$(5.22) \quad \min_{z \in \mathbb{C}} \left\{ f(z) \equiv \frac{|az - b|^2}{c|z|^2 + d} + \log(c|z|^2 + d) \right\},$$

where $a, b \in \mathbb{C}$ and $c, d \in \mathbb{R}_{++}$.

Note that since (5.22) is over the complex domain, it is essentially a two-dimensional problem of the real domain (taking the real and imaginary part as the variables). In this section we will show how to further reduce the problem into the following one-dimensional minimization problem over the *real* domain:

$$(5.23) \quad \min_{y \geq 0} \left\{ g(y) \equiv \frac{|a|^2 y - 2|ab| \sqrt{y} + |b|^2}{cy + d} + \log(cy + d) \right\}.$$

The equivalence between (5.22) and (5.23) is established in Lemma 5.4 below. It is also proven that the new one-dimensional problem (5.23) is strictly unimodal, which means that it is possible to efficiently find its global minimum. The proof of this lemma and the subsequent results in this section mainly involve a rather technical analysis of one-dimensional problems and are therefore relegated to the appendices. In the lemma, we use the following notation. For a complex number $z \in \mathbb{C}$ the sign function is given by

$$\text{sgn}(z) \equiv \begin{cases} \frac{z}{|z|}, & z \neq 0, \\ 0, & z = 0. \end{cases}$$

Note that $|\operatorname{sgn}(z)| = 1$ for any nonzero z .

LEMMA 5.4 (equivalence of (5.22) and (5.23)). (i) *If $ab \neq 0$, then \tilde{y} is an optimal solution of (5.23) if and only if $z = \operatorname{sgn}(\bar{a}b)\sqrt{\tilde{y}}$ is an optimal solution of (5.22).*

(ii) *If $ab = 0$, then \tilde{y} is an optimal solution of (5.23) if and only if $z = \omega\sqrt{\tilde{y}}$ is an optimal solution of (5.22) for every $\omega \in \mathbb{C}$ satisfying $|\omega| = 1$.*

Proof. See Appendix B. \square

Remark 5.1. A direct consequence from Lemma 5.4 is that if a and b are real, then problem (5.22) has a real optimal solution.

The key properties of (5.23) are summarized in the following lemma.

LEMMA 5.5 (properties of problem (5.23)). (i) *The solution of (5.23) is attained.*

(ii) *If \tilde{y} is an optimal solution of (5.23), then $\tilde{y} \leq M$, where*

$$M = \begin{cases} \frac{|b|^2}{|a|^2}, & a \neq 0, \\ \frac{d}{c} \left(e^{|b|^2/d} - 1 \right), & a = 0. \end{cases}$$

(iii) *The objective function $g(\cdot)$ of (5.23) is strictly unimodal over $[0, \infty)$. In particular, the optimal solution of (5.23) is unique.*

Proof. See Appendix C. \square

Lemma 5.5 shows that the one-dimensional problem (5.23) is a problem of minimizing a unimodal function over a closed and bounded interval $[0, M]$. Therefore, it is possible to efficiently find the global minimum of (5.23) by invoking any one of the one-dimensional solvers for unimodal functions (such as golden section or parabolic interpolation). By Lemma 5.4, this also means that it is possible to efficiently find the global optimal solution of the one-dimensional complex-valued problem (5.22).

We can also formulate a very simple condition under which the optimal solution of (5.22) is unique.

THEOREM 5.6 (uniqueness of the optimal solution of $(P_{\mathbb{C}})$). *If the linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$ has a solution, then problem $(P_{\mathbb{C}})$ has a unique solution.*

Proof. See Appendix D. \square

5.5. Solution of $(P_{\mathbb{R}})$. Recall that our basic assumptions are that $\mathbf{A} \in \mathcal{L}^{(k)}(\mathbb{R})$ and $\mathbf{b} \in \mathbb{R}^{pk}$, so the data of the problem is real-valued. Our analysis in the previous section was on the complex-valued problem $(P_{\mathbb{C}})$. The next result shows that problem $(P_{\mathbb{C}})$ has at least one real-valued solution, thus establishing the equivalence of problems $(P_{\mathbb{R}})$ and $(P_{\mathbb{C}})$ in the sense that at least one optimal solution of problem $(P_{\mathbb{C}})$ is the optimal solution of problem $(P_{\mathbb{R}})$. The proof of the theorem below demonstrates explicitly how to find the real solution.

THEOREM 5.7. *Problem $(P_{\mathbb{C}})$ has at least one real-valued optimal solution $\mathbf{x} \in \mathbb{R}^{pk}$.*

Proof. We will prove the result for $k = 1$, that is, for the circulant case. The proof for the BCCB case ($k = 2$) is similar. We use the following notation:

$$\dot{A}_n = \{\mathbf{z} \in \mathbb{C}^n : z_1 \in \mathbb{R}, z_{j+1} = \overline{z_{n+1-j}}, j = 1, \dots, n-1\}.$$

The proof relies on the following two properties:

A. $\mathbf{w} \in \mathbb{R}^n \Leftrightarrow \mathbf{F}_n \mathbf{w} \in \dot{A}_n$.

B. Given a circulant matrix $\mathbf{C} \in \mathcal{L}^{(1)}(\mathbb{C})$, with a spectral decomposition $\mathbf{C} = \mathbf{F}_n^* \operatorname{diag}(\boldsymbol{\lambda}) \mathbf{F}_n$, the following holds: \mathbf{C} is real-valued ($\mathbf{A} \in \mathcal{L}^{(1)}(\mathbb{R})$) if and only if $\boldsymbol{\lambda} \in \dot{A}_n$ (see [13]).

Let $\boldsymbol{\alpha}$ be the eigenvalues vector of \mathbf{A} defined by the relation

$$(5.24) \quad \mathbf{A} = \mathbf{F}_n^* \operatorname{diag}(\boldsymbol{\alpha}) \mathbf{F}_n.$$

Then by Theorem 5.3, every solution to problem $(P_{\mathbb{C}})$ is given by $\mathbf{x} = \mathbf{F}_n^* \tilde{\mathbf{x}}$, where for every $i = 1, \dots, n$, the i th component of $\tilde{\mathbf{x}}$, \tilde{x}_i , is an optimal solution to the one-dimensional complex-valued problem

$$(5.25) \quad (E_i) \quad \min_{\tilde{x}_i \in \mathbb{C}} \left\{ \frac{|\alpha_i \tilde{x}_i - \tilde{b}_i|^2}{n\sigma_e^2 |\tilde{x}_i|^2 + \sigma_w^2} + \log(n\sigma_e^2 |\tilde{x}_i|^2 + \sigma_w^2) \right\},$$

where $\tilde{\mathbf{b}} = \mathbf{F}_n \mathbf{b}$. By properties A and B we have that $\alpha_1, \tilde{b}_1 \in \mathbb{R}$, and it holds that for every $j = 1, \dots, n-1$,

$$\alpha_{j+1} = \overline{\alpha_{n+1-j}}, \quad \tilde{b}_{j+1} = \overline{\tilde{b}_{n+1-j}}.$$

From the latter properties combined with Remark 5.1, it follows that (E_1) has a real optimal solution, and in addition it holds that if \hat{x}_{j+1} is an optimal solution of (E_{j+1}) , then $\overline{\hat{x}_{j+1}}$ is an optimal solution of (E_{n+1-j}) . Therefore, $\tilde{\mathbf{x}}$ can be chosen to reside in $\tilde{\mathbb{A}}$, and as a consequence, the corresponding solution $\mathbf{x} = \mathbf{F}_n^* \tilde{\mathbf{x}}$ is real-valued. \square

Note that combining the latter result with the uniqueness theorem, Theorem 5.6, it follows that if the linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$ has a solution, then the unique solution of problem $(P_{\mathbb{C}})$ is real-valued.

5.6. An image deblurring example. We conclude this section with an image deblurring example illustrating the potential of the STML estimate for problems with periodic boundary conditions. First recall that circulant and BCCB matrices are necessarily square, and therefore, if the corresponding matrices are invertible, the STLS and LS estimates coincide with the naïve solution to the linear system. Thus, in this case, the STLS essentially ignores the uncertainty in the model matrix. This is in contrast to the STML estimate which, in the same setting, does take into consideration the uncertainty in the model matrix and does not utilize any additional information.

Consider the 256×256 cameraman gray image (top left image of Figure 5.1) scaled so that all the pixels are in the interval $[0, 1]$. We blur it with a Gaussian point spread function (PSF) of dimension 31×31 with standard deviation 2 implemented by the command `psfGauss([31,31],2)` from [26]. The blurring is performed under the assumption of periodic boundary conditions so that the “true” linear system can be described by

$$\mathbf{b}_t = \mathbf{A}_t \mathbf{x}_t,$$

where \mathbf{A}_t has a BCCB structure, \mathbf{x}_t is the “vectorized” true image (that is, a vector obtained by stacking the column of the true image), and \mathbf{b}_t is the vectorized blurred, but noiseless, image. We assume that the blurring operator is not exactly known and that the observed PSF is constructed by adding a 31×31 matrix with components independently generated from a zero-mean normal distribution with standard deviation 10^{-4} . The observed image is constructed by adding to each of the components of \mathbf{b}_t a zero-mean normally distributed random variable with standard deviation 10^{-3} , and it is displayed on the top left image of Figure 5.1.

The top right image of Figure 5.1 is the very poor quality naïve solution, which as mentioned above, coincides with the STLS estimate. The bottom left image is the reconstruction using Tikhonov with the regularization parameter chosen according to GCV (abbreviated as before as TIK-GCV), and the bottom right image is the STML solution (with $\sigma_e = 10^{-4}$, $\sigma_w = 10^{-3}$). Both TIK-GCV and STML provide images which are very close to the original. The STML solution is slightly better in



FIG. 5.1. *Deblurring of the cameraman. Top left: blurred and noisy image. Top right: naïve reconstruction which coincides with the STLS estimate. Bottom left: Tikhonov with GCV parameter choice. Bottom right: the STML solution.*

the sense that its relative error $\|\mathbf{x}_t - \mathbf{x}_{\text{STML}}\|/\|\mathbf{x}_t\|$ is 0.092, while the relative error of the Tikhonov solution is equal to 0.1021. This example was given as an illustration of the potential of the STML technique; extensive numerical experiments on image deblurring problems is beyond the scope of the current paper.

6. Conclusion. This paper presented and analyzed a new solution technique called STML for solving structured approximate linear systems $\mathbf{Ax} \approx \mathbf{b}$ in which both \mathbf{A} and \mathbf{b} are uncertain. The ML interpretation of the estimate was described under suitable normality assumptions and was compared to the statistical meaning of the well-known STLS method. We demonstrated via several examples the advantage of the STML technique over the STLS estimate. Computing the STML involves solving a nonconvex problem. As a result, theoretically, only stationary points are guaranteed to be found by general-purpose optimization methods. Several structures in which the STML problem can be significantly reduced, and even globally solved, were presented.

Unfortunately, it does not seem likely that the global optimal solution of the problem can be found efficiently for all possible structures. Therefore, an important line of future research is to seek new and useful structures in which the problem can be solved by some specialized numerical scheme.

Appendix A. Proof of Theorem 3.1. Denote the objective function of (3.4) by f . Note that $f(\mathbf{x} + \mathbf{u}) = f(\mathbf{x})$ for every $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{u} \in V \equiv \text{Null}(\mathbf{A}) \cap \text{Null}(\mathbf{A}_1) \cap \dots \cap \text{Null}(\mathbf{A}_p)$. We can thus restrict the decision variable \mathbf{x} to be in the orthogonal complement of V . This is accomplished by making the change of variables $\mathbf{x} = \mathbf{G}\mathbf{y}$, where \mathbf{G} is a matrix whose columns are a basis for V^\perp . The problem then becomes

$$(A.1) \quad \min_{\mathbf{y}} \{g(\mathbf{y}) \equiv (\tilde{\mathbf{A}}\mathbf{y} - \mathbf{b})^T \tilde{\Sigma}_{\mathbf{x}}^{-1} (\tilde{\mathbf{A}}\mathbf{y} - \mathbf{b}) + \log \det \tilde{\Sigma}_{\mathbf{x}}\},$$

where

$$\tilde{\mathbf{A}} = \mathbf{A}\mathbf{G}, \quad \tilde{\Sigma}_{\mathbf{x}} = \sigma_e^2 \sum_{i=1}^p \tilde{\mathbf{A}}_i \mathbf{y} \mathbf{y}^T \tilde{\mathbf{A}}_i^T + \sigma_w^2 \mathbf{I},$$

with $\tilde{\mathbf{A}}_i = \mathbf{A}_i \mathbf{G}$ for $i = 1, \dots, p$. The problems are equivalent in the sense that \mathbf{y} is an optimal solution of (A.1) if and only if $\mathbf{G}\mathbf{y} + \mathbf{u}$ is an optimal solution of (3.4) for every $\mathbf{u} \in V$. Note that by the construction of $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{A}}_i$, we have that

$$(A.2) \quad \text{Null}(\tilde{\mathbf{A}}) \cap \text{Null}(\tilde{\mathbf{A}}_1) \cap \dots \cap \text{Null}(\tilde{\mathbf{A}}_p) = \{0\}.$$

Now, consider the following decomposition:

$$(A.3) \quad \mathbf{y} = \mathbf{F}\boldsymbol{\eta} + \mathbf{N}\mathbf{v},$$

where \mathbf{F} is a matrix whose columns form a basis for $W = \bigcap_{i=1}^p \text{Null}(\tilde{\mathbf{A}}_i)$ and \mathbf{N} is a matrix whose columns form a basis for W^\perp . Later on, we will use the following properties:

A. $\tilde{\mathbf{A}}\mathbf{F}$ is of full column rank (follows from (A.2)).

B. $\mathbf{N}^T (\sum_{i=1}^p \tilde{\mathbf{A}}_i^T \tilde{\mathbf{A}}_i) \mathbf{N}$ is nonsingular.

In addition, using the definition of \mathbf{F} , we have that $\tilde{\mathbf{A}}_i \mathbf{y} = \tilde{\mathbf{A}}_i \mathbf{N}\mathbf{v}$ for every $i = 1, \dots, p$ so that

$$(A.4) \quad \tilde{\Sigma}_{\mathbf{x}} = \sigma_e^2 \sum_{i=1}^p \tilde{\mathbf{A}}_i \mathbf{N} \mathbf{v} \mathbf{v}^T \mathbf{N}^T \tilde{\mathbf{A}}_i^T + \sigma_w^2 \mathbf{I}.$$

To show that the solution of problem (A.1) is attained, it is enough to show that the level set $\mathcal{L}_\alpha = \{\mathbf{y} : g(\mathbf{y}) \leq \alpha\}$ is nonempty and bounded for some choice of α [10, Proposition 2.1.1] (g is continuous so closedness of the level set is guaranteed). Let α be such that \mathcal{L}_α is nonempty, and let $\mathbf{y} \in \mathcal{L}_\alpha$. First, note that

$$\begin{aligned} \text{Tr}(\tilde{\Sigma}_{\mathbf{x}}) &\stackrel{(A.4)}{=} \text{Tr} \left(\sigma_e^2 \sum_{i=1}^p \tilde{\mathbf{A}}_i \mathbf{N} \mathbf{v} \mathbf{v}^T \mathbf{N}^T \tilde{\mathbf{A}}_i^T + \sigma_w^2 \mathbf{I} \right) \\ &= \sigma_w^2 m + \sigma_e^2 \mathbf{v}^T \mathbf{N}^T \left(\sum_{i=1}^p \tilde{\mathbf{A}}_i^T \tilde{\mathbf{A}}_i \right) \mathbf{N} \mathbf{v} \\ &\geq \sigma_w^2 m + \sigma_e^2 \gamma \|\mathbf{v}\|^2, \end{aligned}$$

where γ is the minimum eigenvalue of $\mathbf{N}^T (\sum_{i=1}^p \tilde{\mathbf{A}}_i^T \tilde{\mathbf{A}}_i) \mathbf{N}$ which is guaranteed to be positive by property B. We use the following notation: for a $k \times k$ matrix \mathbf{M} the

eigenvalues are denoted by $\lambda_1(\mathbf{M}) \geq \lambda_2(\mathbf{M}) \geq \dots \geq \lambda_k(\mathbf{M})$. Also, \mathbf{H} is the matrix given by $\sum_{i=1}^p \tilde{\mathbf{A}}_i \mathbf{N} \mathbf{v} \mathbf{v}^T \mathbf{N}^T \tilde{\mathbf{A}}_i^T$. Using this notation we have

$$\det(\tilde{\Sigma}_{\mathbf{x}}) = \prod_{i=1}^m (\sigma_e^2 \lambda_i(\mathbf{H}) + \sigma_w^2).$$

Since $\lambda_i(\mathbf{H}) \geq 0$ for all i , for every $j = 1, \dots, m$ one has

$$\det(\tilde{\Sigma}_{\mathbf{x}}) \geq \sigma_w^{2(m-1)} (\sigma_e^2 \lambda_j(\mathbf{H}) + \sigma_w^2).$$

Summing these inequalities over $j = 1, \dots, m$, we obtain

$$\begin{aligned} m \det(\tilde{\Sigma}_{\mathbf{x}}) &\geq \sigma_w^{2(m-1)} \left(\sigma_e^2 \sum_{j=1}^m \lambda_j(\mathbf{H}) + \sigma_w^2 m \right) \\ &= \sigma_w^{2(m-1)} \text{Tr}(\tilde{\Sigma}_{\mathbf{x}}) \\ &\geq \sigma_w^{2(m-1)} (\sigma_w^2 m + \sigma_e^2 \gamma \|\mathbf{v}\|^2). \end{aligned}$$

Therefore, since $g(\mathbf{y}) \leq \alpha$, it follows that

$$\sigma_w^{2(m-1)} (\sigma_w^2 m + \sigma_e^2 \gamma \|\mathbf{v}\|^2) \leq m \det(\tilde{\Sigma}_{\mathbf{x}}) = m e^{\log(\det(\tilde{\Sigma}_{\mathbf{x}}))} \leq m e^{g(\mathbf{y})} \leq m e^\alpha,$$

which implies

$$\|\mathbf{v}\|^2 \leq \varepsilon,$$

where $\varepsilon = m \gamma^{-1} \sigma_e^{-2} (\sigma_w^{-2(m-1)} e^\alpha - \sigma_w^2)$. Therefore, \mathbf{v} is bounded.

It remains to show that $\boldsymbol{\eta}$ is bounded. Since $\tilde{\Sigma}_{\mathbf{x}} \succeq \sigma_w^2 \mathbf{I}$, it follows that $\log \det \tilde{\Sigma}_{\mathbf{x}} \geq \log \det(\sigma_w^2 \mathbf{I}) = 2m \log \sigma_w$, which combined with $g(\mathbf{y}) \leq \alpha$ implies that

$$(A.5) \quad (\tilde{\mathbf{A}}\mathbf{y} - \mathbf{b})^T \tilde{\Sigma}_{\mathbf{x}}^{-1} (\tilde{\mathbf{A}}\mathbf{y} - \mathbf{b}) \leq \delta \equiv \alpha - 2m \log \sigma_w.$$

Next, we upper bound the largest eigenvalue of $\tilde{\Sigma}_{\mathbf{x}}$. From the definition of $\tilde{\Sigma}_{\mathbf{x}}$, we have

$$\begin{aligned} \lambda_1(\tilde{\Sigma}_{\mathbf{x}}) &\leq \lambda_1 \left(\sigma_e^2 \sum_{i=1}^p \tilde{\mathbf{A}}_i \mathbf{N} \mathbf{v} \mathbf{v}^T \mathbf{N}^T \tilde{\mathbf{A}}_i^T \right) + \sigma_w^2 \leq \sigma_e^2 \sum_{i=1}^p \lambda_1 \left(\tilde{\mathbf{A}}_i \mathbf{N} \mathbf{v} \mathbf{v}^T \mathbf{N}^T \tilde{\mathbf{A}}_i^T \right) + \sigma_w^2 \\ (A.6) \quad &= \sigma_e^2 \sum_{i=1}^p \|\tilde{\mathbf{A}}_i \mathbf{N} \mathbf{v}\|^2 + \sigma_w^2 \leq \sigma_e^2 \varepsilon \sum_{i=1}^p \lambda_1 \left(\tilde{\mathbf{A}}_i \mathbf{N} \mathbf{N}^T \tilde{\mathbf{A}}_i^T \right) + \sigma_w^2. \end{aligned}$$

Therefore, $\tilde{\Sigma}_{\mathbf{x}}^{-1} \succeq \beta^{-1} \mathbf{I}$, where $\beta = \sigma_e^2 \sum \varepsilon \lambda_1(\tilde{\mathbf{A}}_i \mathbf{N} \mathbf{N}^T \tilde{\mathbf{A}}_i^T) + \sigma_w^2$, which along with (A.5) implies

$$\|\tilde{\mathbf{A}}\mathbf{y} - \mathbf{b}\|^2 \leq \beta \delta.$$

Plugging the decomposition (A.3) into the latter inequality, we obtain $\|\tilde{\mathbf{A}}(\mathbf{F}\boldsymbol{\eta} + \mathbf{N}\mathbf{v}) - \mathbf{b}\| \leq \sqrt{\beta\delta}$. Hence,

$$\|\tilde{\mathbf{A}}\mathbf{F}\boldsymbol{\eta}\| \leq \sqrt{\beta\delta} + \|\tilde{\mathbf{A}}\mathbf{N}\mathbf{v} - \mathbf{b}\| \leq \sqrt{\beta\delta} + \|\tilde{\mathbf{A}}\mathbf{N}\| \|\mathbf{v}\| + \|\mathbf{b}\| \leq \sqrt{\beta\delta} + \|\tilde{\mathbf{A}}\mathbf{N}\| \sqrt{\varepsilon} + \|\mathbf{b}\|.$$

On the other hand, since $\tilde{\mathbf{A}}\mathbf{F}$ is of full column rank, the matrix $\mathbf{F}^T \tilde{\mathbf{A}}^T \tilde{\mathbf{A}}\mathbf{F}$ is nonsingular yielding

$$\|\boldsymbol{\eta}\|^2 \leq \frac{1}{\lambda_{\min}(\mathbf{F}^T \tilde{\mathbf{A}}^T \tilde{\mathbf{A}}\mathbf{F})} \left(\sqrt{\beta\delta} + \|\tilde{\mathbf{A}}\mathbf{N}\| \sqrt{\varepsilon} + \|\mathbf{b}\| \right)^2,$$

proving the boundedness of η . To summarize, since both \mathbf{v} and η are bounded it follows that the level set \mathcal{L}_α is bounded, proving the attainment of the solution.

Appendix B. Proof of Lemma 5.4. Let z be an optimal solution of (5.22). Then by the optimality of z we have

$$f(z) \leq f(\omega z) \text{ for every } \omega \in \mathbb{C} \text{ satisfying } |\omega| = 1,$$

which is the same as

$$\frac{|az - b|^2}{c|z|^2 + d} + \log(c|z|^2 + d) \leq \frac{|a\omega z - b|^2}{c|\omega z|^2 + d} + \log(c|\omega z|^2 + d).$$

The latter inequality reduces to

$$(B.1) \quad \Re((1 - \omega)\bar{a}bz) \geq 0.$$

We will now show that $\bar{a}bz$ is a nonnegative real number. This is obviously true if $z = 0$. Otherwise, we split the analysis into two cases.

Case I. If $ab \neq 0$, then substituting

$$\omega = \frac{\overline{\bar{a}bz}}{|\bar{a}bz|}$$

into (B.1) yields $\Re(\bar{a}bz) \geq |\bar{a}bz|$, implying that $\bar{a}bz$ is a nonnegative real number and, in particular, that $\text{sgn}(z) = \text{sgn}(\bar{a}b)$.

Case II. If $ab = 0$, the function f satisfies $f(\omega z) = f(z)$ for every $z, \omega \in \mathbb{C}$ such that $|\omega| = 1$, and thus ωz is also an optimal solution for every z satisfying $|\omega| = 1$.

A conclusion from the above two cases is that if the minimum of (5.22) is attained at a nonzero solution, then there must be at least one optimal solution z for which $\text{sgn}(z) = \text{sgn}(\bar{a}b)$; consequently, we can make the change of variables $z = \text{sgn}(\bar{a}b)\sqrt{y}$ which transforms problem (5.22) into (5.23).

Appendix C. Proof of Lemma 5.5. (i) Attainment follows from the fact that $g(y) \rightarrow \infty$ as $y \rightarrow \infty$.

(ii) An optimal solution \tilde{y} to (5.23) satisfies

$$\log(c\tilde{y} + d) \leq g(\tilde{y}) \leq g(0) = \frac{|b|^2}{d} + \log(d)$$

so that

$$\tilde{y} \leq \frac{d}{c} \left(e^{|b|^2/d} - 1 \right).$$

If $a \neq 0$, then the following holds:

$$\log(c\tilde{y} + d) \leq g(\tilde{y}) \leq g\left(\frac{|b|^2}{|a|^2}\right) = \log\left(\frac{c|b|^2}{|a|^2} + d\right)$$

so that $\tilde{y} \leq \frac{|b|^2}{|a|^2}$.

(iii) Let y^* be an optimal solution of (5.23). We will show that g is strictly decreasing over $[0, y^*]$ and strictly increasing over $[y^*, \infty)$, thus also establishing that y^* is the unique optimal solution of (5.23). We will prove that the function is strictly

decreasing over $[0, y^*]$. The proof that the function is strictly increasing over $[y^*, \infty)$ is similar and is thus omitted. If $y^* = 0$, then there is nothing to prove. If $y^* > 0$, then let us consider $y_1, y_2 \in [0, y^*]$ such that $y_1 < y_2$ and show that $g(y_1) > g(y_2)$. Since y^* is a minimum point of g over $[0, \infty)$ it follows that $g(y^*) \leq g(y_1)$. Denote $\alpha = g(y_1)$. Then the two inequalities

$$g(y^*) \leq \alpha, g(y_1) \leq \alpha$$

can be rewritten as

$$f_\alpha(y^*) \leq 0, \quad f_\alpha(y_1) \leq 0,$$

where

$$f_\alpha(y) \equiv |a|^2 y - 2|ab|\sqrt{y} + |b|^2 + (cy + d) \log(cy + d) - \alpha(cy + d).$$

Since $y_1 < y_2 < y^*$ it follows that y_2 is a convex combination of y_1 and y^* . Specifically,

$$y_2 = \lambda y_1 + (1 - \lambda)y^*, \quad \lambda = \frac{y^* - y_2}{y^* - y_1}.$$

The function $f_\alpha(\cdot)$ is strictly convex over $[0, \infty)$ (its second derivative is positive), and hence

$$f_\alpha(y_2) = f_\alpha(\lambda y_1 + (1 - \lambda)y^*) < \lambda f_\alpha(y_1) + (1 - \lambda)f_\alpha(y^*) \leq \lambda \cdot 0 + (1 - \lambda) \cdot 0 = 0,$$

which is equivalent to $g(y_2) < \alpha$ so that $g(y_2) < g(y_1)$.

Appendix D. Proof of Theorem 5.6. In order to prove Theorem 5.6 we need to establish two lemmas. The first one—Lemma D.1—is concerned with a sufficient condition for uniqueness of the optimal solution of (5.22). The second one—Lemma D.2—provides a sufficient condition for uniqueness of the optimal solution of (P_C) in terms of the eigenvalues of the model matrix \mathbf{A} and the transformed right-hand side vector $\mathbf{Q}_{(k)}\mathbf{b}$.

LEMMA D.1. *Consider problem (5.22) with $a, b \in \mathbb{C}$ and $c, d \in \mathbb{R}_{++}$. Suppose that either $a \neq 0$ or $a = b = 0$. Then the optimal solution of (5.22) is unique.*

Proof. Note that by Lemma 5.5 the optimal solution of the corresponding one-dimensional real-valued problem (5.23) is always unique. By Lemma 5.4, if $a, b \neq 0$, this also means that problem (5.22) has a unique optimal solution. If $a \neq 0$ and $b = 0$, the objective function of problem (5.22) reduces to

$$\frac{|a|^2|z|^2}{c|z|^2 + d} + \log(c|z|^2 + d),$$

which is increasing with respect to $|z|^2$. Therefore, the unique optimal solution in this case is $z = 0$. If $a = b = 0$, the objective function becomes $\log(c|z|^2 + d)$, which, again, is increasing with respect to $|z|^2$, implying that also in this case the unique optimal solution is $z = 0$. \square

Exploiting the analysis of the one-dimensional problems, we can also formulate a condition under which (P_C) has a unique solution.

LEMMA D.2. *Let $\boldsymbol{\alpha}$ be the eigenvalues vector of \mathbf{A} defined by the relation*

$$\mathbf{A} = \mathbf{Q}_{(k)}^* \text{diag}(\boldsymbol{\alpha}) \mathbf{Q}_{(k)},$$

and let $\tilde{\mathbf{b}} = \mathbf{Q}_{(k)}\mathbf{b}$. Suppose that for every $i = 1, \dots, p_k$ either $\alpha_i \neq 0$ or $\alpha_i = \tilde{b}_i = 0$. Then the optimal solution of problem $(P_{\mathbb{C}})$ is unique.

Proof. By the decomposition theorem, Theorem 5.3, it follows that the optimal solution of problem $(P_{\mathbb{C}})$ is unique if and only if each of the one-dimensional complex-valued problems (5.20) has a unique solution. Invoking Lemma D.1 for each of these problems, the result follows. \square

We are now ready to prove the uniqueness theorem, Theorem 5.6.

The condition of Lemma D.2 translates to the condition that the linear system

$$(D.1) \quad \text{diag}(\boldsymbol{\alpha})\mathbf{z} = \tilde{\mathbf{b}}$$

has a solution. Substituting $\text{diag}(\boldsymbol{\alpha}) = \mathbf{Q}_{(k)}\mathbf{A}\mathbf{Q}_{(k)}^*$, $\tilde{\mathbf{b}} = \mathbf{Q}_{(k)}\mathbf{b}$ in the system (D.1) yields $\mathbf{Q}_{(k)}\mathbf{A}\mathbf{Q}_{(k)}^*\mathbf{z} = \mathbf{Q}_{(k)}\mathbf{b}$, which is equivalent to the system

$$(D.2) \quad \mathbf{A}\tilde{\mathbf{z}} = \mathbf{b}$$

after making the change of variables $\tilde{\mathbf{z}} = \mathbf{Q}_{(k)}^*\mathbf{z}$. We conclude that if the system (D.2) has a solution, then problem $(P_{\mathbb{C}})$ has a unique solution.

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