Error-Covariance Analysis of the Total Least Squares Problem

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This paper derives and analyzes the estimate error-covariance associated for both the non-stationary and stationary noise process cases with uncorrelated element-wise components for the total least squares problem. The non-stationary case is derived directly from the associated unconstrained total least squares loss function. The stationary case is derived by using a linear expansion of the total least squares estimate equation, which involves a first order expansion of the associated singular value decomposition matrices. The actual solution for the error-covariance is evaluated at the true variables, which are unknown in practice. Two common approaches to overcome this difficulty are used; the first involves using the measurements directly and the second involves using the estimates which are more accurate than the measurements. This paper shows that using the latter greatly simplifies the error-covariance solution for the stationary case. Simulation results are shown to quantify the theoretical derivations.

I. Introduction

Total least squares[1] (TLS) expands upon standard least squares by incorporating noise not only in the measurements but also in the basis functions themselves. Several applications of TLS exist in the real world. A common one is identification of linear and nonlinear systems. For example, consider the following scalar discrete-time system with constant sampling interval: $y_{k+1} = \Phi y_k + \Gamma u_k$, where Φ and Γ are constant scalar variables, and y_k and u_k are the output and input, respectively at time t_k. It is desired to estimate Φ and Γ from measurements of y_k. A one-time step approach can be used to estimate these variances using a simple linear least square approach.[2] The basis function matrix is a function of both the measurements and inputs using this approach. The measurements are processed using sensor data, which always have noise associated with them; the input may also have noise because a closed-loop control system may be involved and the input may be a function of the measurements too. A more realistic example involves the Eigensystem Realization Algorithm (ERA),[3] which provides a balanced realization of the discrete-time multi-input-multi-output discrete-time system matrices. In the ERA solution measurements are also used in the Hankel matrix, which is akin to the basis function matrix. Other applications involve fuzzy system identification of an industrial gas engine power plant,[4] blind deconvolution problems as encountered in image deblurring when both the image and the blurring function have uncertainty,[5] and applications to astronomy and geodesy.[6]

Since noise exists in the basis functions then the standard least squares solution is not optimal from both a minimum variance and maximum likelihood point of view. Thus a different loss function must be used other than the standard least squares loss function. The "errors-in-variables" estimator shown in Ref. 7 coincides with the TLS solution. This indicates that the TLS estimate is a strongly consistent estimate for large samples, which leads to an asymptotic unbiasedness property. Ordinary least squares with errors in the basis functions produces biased estimates as the sample size increases. However, the error-covariance of TLS is larger than the ordinary least squares error-covariance, but by increasing the noise in the measurements the bias of ordinary least squares becomes more important and even the dominating term.[8] Also, it is has

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been shown that weighted least squares and TLS yield asymptotically equivalent results as the perturbation level goes to zero.[9]

The covariance of the estimate errors in the standard linear least squares problem is straightforward to derive. Standard least squares can easily be shown to produce an efficient estimate, i.e. its state error-covariance achieves the Cramér-Rao lower bound.[2] The equivalence of the TLS to maximum likelihood estimation is shown in Refs. 10 and 11. A Cramér-Rao lower bound is derived in Ref. 11, however isotropic errors are assumed for the errors in both the basis functions and measurements, i.e. the overall covariance matrix is given by a scalar times identity. In this paper more generalized and realistic noise models are assumed. In particular, the errors in both the measurements and basis functions are not assumed to be isotropic in nature and can obey either a non-stationary or stationary process. The only assumption here is that the errors are element-wise uncorrelated, which is true for many systems. The Cramér-Rao lower bound is first derived, which is valid for both the non-stationary and stationary noise process cases. Then, a perturbation approach of the TLS loss function is employed to prove that the associated covariance matrix achieves the Cramér-Rao lower bound to within first-order terms. The TLS estimate for the stationary noise case involves performing a singular value decomposition (SVD) of an augmented matrix involving the basis functions and measurements. The derivation of the error-covariance follows directly from the SVD matrix solution. Unlike the non-stationary noise case, a matrix inverse is not required to compute the error-covariance for the stationary noise case.

The organization of this paper proceeds as follows. First, a review of maximum likelihood estimation is given with a particular emphasis on the linear least squares problem. The Cramér-Rao lower inequality is also shown. Then, the relationship of TLS to maximum likelihood estimation is shown. Next, error-covariance expressions for both the non-stationary and stationary cases are derived. Finally, simulation results are shown to validate the derived error-covariance expressions.

II. Maximum Likelihood Estimation

The maximum likelihood (ML) approach yields estimates for the unknown quantities which maximize the probability of obtaining the observed set of data. In this section a review of ML estimation for the standard linear least squares solution is given, which includes a review of the Cramér-Rao inequality. Then the ML formulation for the TLS problem is formally shown. The Cramér-Rao inequality is then derived for the non-stationary noise process case, assuming no correlations exist between element-wise errors of the measurements and basis functions.

A. Linear Least Squares Review

Consider the following model linear model:

$$\tilde{\mathbf{y}} = H\,\mathbf{x} + \Delta\mathbf{y} \tag{1}$$

where H is an $m \times n$ matrix which contains no errors and $\Delta\mathbf{y}$ is an $m \times 1$ vector which is a zero-mean Gaussian white-noise process with covariance R. The goal of the least squares problem is to determine an estimate for the $n \times 1$ vector $\mathbf{x}$, with $n \leq m$.

The mean of the $m \times 1$ measurement $\tilde{\mathbf{y}}$, denoted by $\boldsymbol{\mu}$, is computed by taking the expectation of Eq. (1), which gives $\boldsymbol{\mu} = H\,\mathbf{x}$. Then the covariance of $\tilde{\mathbf{y}}$ is given by

$$\text{cov}\left\{\tilde{\mathbf{y}}\right\} \triangleq E\left\{(\tilde{\mathbf{y}} - \boldsymbol{\mu})(\tilde{\mathbf{y}} - \boldsymbol{\mu})^T\right\} \tag{2}$$

where $E\{\,\}$ denotes expectation. Carrying out the computation in Eq. (2) gives $\text{cov}\left\{\tilde{\mathbf{y}}\right\} = R$. Hence the conditional density function of $\tilde{\mathbf{y}}$ given $\mathbf{x}$ is

$$p(\tilde{\mathbf{y}}|\mathbf{x}) = \frac{1}{(2\pi)^{m/2}\left[\det(R)\right]^{1/2}} \exp\left\{-\frac{1}{2}(\tilde{\mathbf{y}} - H\mathbf{x})^T R^{-1} (\tilde{\mathbf{y}} - H\mathbf{x})\right\} \tag{3}$$

In the ML approach an estimate of $\mathbf{x}$, denoted by $\hat{\mathbf{x}}$, is sought that maximizes Eq. (3). Due to the monotonic aspect of the function, the ML solution can be accomplished by also taking the natural logarithm of Eq. (3), which yields

$$\ln\left[p(\tilde{\mathbf{y}}|\mathbf{x})\right] = -\frac{1}{2}(\tilde{\mathbf{y}} - H\mathbf{x})^T R^{-1} (\tilde{\mathbf{y}} - H\mathbf{x}) - \frac{m}{2}\ln(2\pi) - \frac{1}{2}\ln\left[\det(R)\right] \tag{4}$$

The last two terms of the right-hand side of Eq. (4) can be ignored since they are independent of $\mathbf{x}$. Minimizing the negative of Eq. (4) is equivalent to maximizing it. Therefore, ignoring terms independent of $\mathbf{x}$ leads to the following loss function which is minimized to determine the estimate:

$$J(\hat{\mathbf{x}}) = \frac{1}{2}\left(\tilde{\mathbf{y}} - H\hat{\mathbf{x}}\right)^T R^{-1}\left(\tilde{\mathbf{y}} - H\hat{\mathbf{x}}\right) \tag{5}$$

The solution for this minimization problem leads directly to the classical least squares solution for the estimate:

$$\hat{\mathbf{x}}(\tilde{\mathbf{y}}) \equiv \hat{\mathbf{x}} = (H^T R^{-1} H)^{-1} H^T R^{-1} \tilde{\mathbf{y}} \tag{6}$$

The mean of $\hat{\mathbf{x}}$ is given by $\mathbf{x}$, which means the estimator is unbiased. The error-covariance of $\hat{\mathbf{x}}$ is given by

$$\text{cov}\{\hat{\mathbf{x}}\} = (H^T R^{-1} H)^{-1} \tag{7}$$

which can be used to develop 3σ bounds on the expected estimate errors.

The Cramér-Rao inequality[12] can be used to provide a lower bound on the expected errors between the estimated quantities and the true values from the known statistical properties of the measurement errors. The theory was proved independently by Cramér and Rao, although it was found earlier by Fisher[13] for the special case of a Gaussian distribution. The Cramér-Rao inequality for an unbiased estimate $\hat{\mathbf{x}}$ is given by

$$P \triangleq E\left\{(\hat{\mathbf{x}} - \mathbf{x})(\hat{\mathbf{x}} - \mathbf{x})^T\right\} \geq F^{-1} \tag{8}$$

where the Fisher information matrix (FIM), F, is given by

$$F = E\left\{\left(\frac{\partial}{\partial \mathbf{x}} \ln[p(\tilde{\mathbf{y}}|\mathbf{x})]\right)\left(\frac{\partial}{\partial \mathbf{x}} \ln[p(\tilde{\mathbf{y}}|\mathbf{x})]\right)^T\right\} \tag{9}$$

The partial derivatives are assumed to exist and to be absolutely integrable. A formal proof of the Cramér-Rao inequality requires using the "conditions of regularity" (see Ref. 14 for details). It is clear that the estimate in Eq. (6) achieves the Cramér-Rao lower bound and is thus an efficient estimator.

Maximum likelihood has many desirable properties. A few of the useful ones are now discussed. First, a ML estimator is a consistent estimator, which means $\hat{\mathbf{x}}(\tilde{\mathbf{y}})$ converges in a probabilistic sense to the truth, $\mathbf{x}$, for large samples. This states that the estimate is unbiased for large samples. Second, a ML estimator is asymptotically efficient, which means that $\hat{\mathbf{x}}(\tilde{\mathbf{y}})$ achieves the Cramér-Rao lower bound for large samples.

Oftentimes, as is seen many times throughout this paper, the estimate equation is nonlinear in both its functional parameters and random errors. To determine the error-covariance matrix, P, in Eq. (8) a classical first-order expansion of the nonlinear functions can be used.[2] This is best illustrated by example. Suppose that a random function is given $\hat{\mathbf{z}} = \mathbf{f}(\hat{\mathbf{p}})$, with $\hat{\mathbf{p}} = \mathbf{p} + \boldsymbol{\delta}\mathbf{p}$, where $\boldsymbol{\delta}\mathbf{p}$ is a zero-mean Gaussian noise process with covariance denoted by P_{pp}. To within first order the covariance of $\hat{\mathbf{z}}$, denoted by P_{zz}, is computed using the Jacobian of $\mathbf{f}$, and is given by

$$P_{zz} = \left[\left.\frac{\partial \mathbf{f}}{\partial \hat{\mathbf{p}}}\right|_{\text{truth}}\right] P_{pp} \left[\left.\frac{\partial \mathbf{f}}{\partial \hat{\mathbf{p}}}\right|_{\text{truth}}\right]^T \tag{10}$$

This Jacobian is evaluated at the true values, which are replaced with measured or estimated values in practice. It is important to note that Eq. (10) is valid only for an unbiased estimate.

B. Total Least Squares

For the general problem, the TLS model is given by

$$\tilde{\mathbf{y}} = \mathbf{y} + \Delta\mathbf{y} \tag{11a}$$

$$\tilde{H} = H + \Delta H \tag{11b}$$

where $\tilde{\mathbf{y}}$ is an $m \times 1$ measurement vector, $\mathbf{y}$ is its respective true value, $\Delta\mathbf{y}$ is the measurement noise, $\tilde{H}$ is an $m \times n$ matrix of basis functions with random errors, H is its respective true value, and ΔH represents the errors to the model H. Define the following $m \times (n+1)$ matrix:

$$\tilde{D} \triangleq \begin{bmatrix} \tilde{H} & \tilde{\mathbf{y}} \end{bmatrix} \tag{12}$$

The TLS problem seeks an optimal estimate of the $n \times 1$ vector $\mathbf{x}$, denoted by $\hat{\mathbf{x}}$ with $\hat{\mathbf{y}} = \hat{H}\hat{\mathbf{x}}$, where $\hat{\mathbf{y}}$ is the estimate of $\mathbf{y}$ and $\hat{H}$ is the estimate of H, which maximizes

$$p(\tilde{D}|D) = \frac{1}{(2\pi)^{m/2}\left[\det\left(R\right)\right]^{1/2}} \exp\left\{-\frac{1}{2}\text{vec}^T(\tilde{D}^T - D^T)\, R^{-1}\text{vec}(\tilde{D}^T - D^T)\right\} \tag{13}$$

where $D \triangleq [H \;\; \mathbf{y}]$, which satisfies $D\,\mathbf{z} = \mathbf{0}$ with $\mathbf{z} \triangleq [\mathbf{x}^T \;\; -1]^T$, and vec denotes a vector formed by stacking the consecutive columns of the associated matrix, and R is the covariance matrix. Unfortunately because H now contains errors the constraint $\hat{\mathbf{y}} = \hat{H}\,\hat{\mathbf{x}}$ must also be added to the maximization problem. The negative log-likelihood now leads to the following loss function:

$$J(\hat{D}) = \frac{1}{2}\text{vec}^T(\tilde{D}^T - \hat{D}^T)\, R^{-1}\text{vec}(\tilde{D}^T - \hat{D}^T), \quad \text{s.t.} \quad \hat{D}\,\hat{\mathbf{z}} = \mathbf{0} \tag{14}$$

where $\hat{\mathbf{z}} \triangleq [\hat{\mathbf{x}}^T \;\; -1]^T$ and $\hat{D} \triangleq [\hat{H} \;\; \hat{\mathbf{y}}]$ denotes the estimate of D. For a unique solution it is required that the rank of $\hat{D}$ be n, which means $\hat{\mathbf{z}}$ spans the null space of $\hat{D}$.

III. Error-Covariance Derivation

In this section the estimate error-covariance is derived for two cases in the TLS problem. The first assumes that the errors are element-wise, i.e. the rows of the matrix $\tilde{D}$, uncorrelated but allows the covariance to vary in time, i.e. non-stationary errors. The case covers a wide variety of problems, which is also used to develop a sequential least squares solution for the linear least squares problem.[2] The second case assumes that the errors are element-wise uncorrelated with stationary errors.

A. Element-Wise Uncorrelated and Non-Stationary Case

For this case the covariance matrix is given by the following block diagonal matrix:

$$R = \text{blkdiag}\begin{bmatrix}\mathcal{R}_1 & \cdots & \mathcal{R}_m\end{bmatrix} \tag{15}$$

where each $\mathcal{R}_i$ is an $(n+1)\times(n+1)$ matrix given by

$$\mathcal{R}_i = \begin{bmatrix}\mathcal{R}_{hh_i} & \mathcal{R}_{hy_i} \\ \mathcal{R}_{hy_i}^T & \mathcal{R}_{yy_i}\end{bmatrix} \tag{16}$$

where $\mathcal{R}_{hh_i}$ is an $n \times n$ matrix, $\mathcal{R}_{hy_i}$ is $n \times 1$ vector and $\mathcal{R}_{yy_i}$ is a scalar. Partition the matrix ΔH and the vector $\Delta\mathbf{y}$ by their rows:

$$\Delta H = \begin{bmatrix}\boldsymbol{\delta}\mathbf{h}_1^T \\ \boldsymbol{\delta}\mathbf{h}_2^T \\ \vdots \\ \boldsymbol{\delta}\mathbf{h}_m^T\end{bmatrix}, \quad \Delta\mathbf{y} = \begin{bmatrix}\delta y_1 \\ \delta y_2 \\ \vdots \\ \delta y_m\end{bmatrix} \tag{17}$$

where each $\boldsymbol{\delta}\mathbf{h}_i$ has dimension $n \times 1$ and each δy_i is a scalar. The partitions in Eq. (16) are then given by

$$\mathcal{R}_{hh_i} = E\left\{\boldsymbol{\delta}\mathbf{h}_i\boldsymbol{\delta}\mathbf{h}_i^T\right\} \tag{18a}$$
$$\mathcal{R}_{hy_i} = E\left\{\delta y_i\boldsymbol{\delta}\mathbf{h}_i\right\} \tag{18b}$$
$$\mathcal{R}_{yy_i} = E\left\{\delta y_i^2\right\} \tag{18c}$$

Note that each $\mathcal{R}_i$ is allowed to be a fully populated matrix so that correlations between the errors in the individual i^{th} row of ΔH and the i^{th} element of $\Delta\mathbf{y}$ can exist. When $\mathcal{R}_{hy_i}$ is zero then no correlations exist.

Partition the matrices $\tilde{D}$, $\hat{D}$ and $\tilde{H}$, and the vector $\tilde{\mathbf{y}}$ by their rows:

$$\tilde{D} = \begin{bmatrix}\tilde{\mathbf{d}}_1^T \\ \tilde{\mathbf{d}}_2^T \\ \vdots \\ \tilde{\mathbf{d}}_m^T\end{bmatrix}, \quad \hat{D} = \begin{bmatrix}\hat{\mathbf{d}}_1^T \\ \hat{\mathbf{d}}_2^T \\ \vdots \\ \hat{\mathbf{d}}_m^T\end{bmatrix}, \quad \tilde{H} = \begin{bmatrix}\tilde{\mathbf{h}}_1^T \\ \tilde{\mathbf{h}}_2^T \\ \vdots \\ \tilde{\mathbf{h}}_m^T\end{bmatrix}, \quad \tilde{\mathbf{y}} = \begin{bmatrix}\tilde{y}_1 \\ \tilde{y}_2 \\ \vdots \\ \tilde{y}_m\end{bmatrix} \tag{19}$$

where each $\tilde{\mathbf{d}}_i$ and $\hat{\mathbf{d}}_i$ has dimension $(n+1)\times 1$, each $\tilde{\mathbf{h}}_i$ has dimension $n\times 1$ and each $\tilde{y}_i$ is a scalar. For the element-wise uncorrelated and non-stationary case, the constrained loss function in Eq. (14) can be converted to an equivalent unconstrained one.[15,16] Here, a simplified version of this is shown. For the element-wise uncorrelated and non-stationary case, the loss function in Eq. (14) reduces down to

$$J(\hat{\mathbf{x}}) = \frac{1}{2}\sum_{i=1}^{m}(\tilde{\mathbf{d}}_i - \hat{\mathbf{d}}_i)^T \mathcal{R}_i^{-1}(\tilde{\mathbf{d}}_i - \hat{\mathbf{d}}_i), \quad \text{s.t.} \quad \hat{\mathbf{d}}_j^T\hat{\mathbf{z}} = 0, \quad j = 1, 2, \ldots, m \tag{20}$$

The loss function is rewritten into an unconstrained one by determining a solution for $\hat{\mathbf{d}}_i$ and substituting its result back into Eq. (20). To accomplish this task the loss function is appended using Lagrange multipliers, which gives the following loss function:

$$J'(\hat{\mathbf{d}}_i) = \lambda_1\hat{\mathbf{d}}_1^T\hat{\mathbf{z}} + \lambda_2\hat{\mathbf{d}}_2^T\hat{\mathbf{z}} + \cdots + \lambda_m\hat{\mathbf{d}}_m^T\hat{\mathbf{z}} + \frac{1}{2}\sum_{i=1}^{m}(\tilde{\mathbf{d}}_i - \hat{\mathbf{d}}_i)^T\mathcal{R}_i^{-1}(\tilde{\mathbf{d}}_i - \hat{\mathbf{d}}_i) \tag{21}$$

where each λ_i is a Lagrange multiplier. Taking the partial of Eq. (21) with respect to each $\hat{\mathbf{d}}_i$ leads to the following m necessary conditions:

$$\mathcal{R}_i^{-1}\hat{\mathbf{d}}_i - \mathcal{R}_i^{-1}\tilde{\mathbf{d}}_i + \lambda_i\hat{\mathbf{z}} = \mathbf{0}, \quad i = 1, 2, \ldots, m \tag{22}$$

Left multiplying Eq. (22) by $\hat{\mathbf{z}}^T\mathcal{R}_i$ and using the constraint $\hat{\mathbf{d}}_i^T\hat{\mathbf{z}} = 0$ leads to

$$\lambda_i = \frac{\hat{\mathbf{z}}^T\tilde{\mathbf{d}}_i}{\hat{\mathbf{z}}^T\mathcal{R}_i\,\hat{\mathbf{z}}} \tag{23}$$

Substituting Eq. (23) into Eq. (22) leads to

$$\hat{\mathbf{d}}_i = \left[I_{(n+1)\times(n+1)} - \frac{\mathcal{R}_i\hat{\mathbf{z}}\,\hat{\mathbf{z}}^T}{\hat{\mathbf{z}}^T\mathcal{R}_i\,\hat{\mathbf{z}}}\right]\tilde{\mathbf{d}}_i \tag{24}$$

where $I_{(n+1)\times(n+1)}$ is an $(n+1)\times(n+1)$ identity matrix. If desired the specific estimates for $\mathbf{h}_i$ and y_i, denoted by $\hat{\mathbf{h}}_i$ and $\hat{y}_i$, respectively, are given by

$$\hat{\mathbf{h}}_i = \tilde{\mathbf{h}}_i - \frac{(\mathcal{R}_{hh_i}\hat{\mathbf{x}} - \mathcal{R}_{hy_i})e_i}{\hat{\mathbf{z}}^T\mathcal{R}_i\,\hat{\mathbf{z}}} \tag{25a}$$

$$\hat{y}_i = \tilde{y}_i - \frac{(\mathcal{R}_{hy_i}^T\hat{\mathbf{x}} - \mathcal{R}_{yy_i})e_i}{\hat{\mathbf{z}}^T\mathcal{R}_i\,\hat{\mathbf{z}}} \tag{25b}$$

where $e_i \triangleq \tilde{\mathbf{h}}_i^T\hat{\mathbf{x}} - \tilde{y}_i$. Substituting Eq. (24) into Eq. (20) yields the following unconstrained loss function:

$$J(\hat{\mathbf{x}}) = \frac{1}{2}\sum_{i=1}^{m}\frac{(\tilde{\mathbf{d}}_i^T\hat{\mathbf{z}})^2}{\hat{\mathbf{z}}^T\mathcal{R}_i\,\hat{\mathbf{z}}} \tag{26}$$

Note that Eq. (26) represents a non-convex optimization problem. The necessary condition for optimality gives

$$\frac{\partial J(\hat{\mathbf{x}})}{\partial\hat{\mathbf{x}}} = \sum_{i=1}^{m}\frac{e_i\,\tilde{\mathbf{h}}_i}{\hat{\mathbf{x}}^T\mathcal{R}_{hh_i}\hat{\mathbf{x}} - 2\mathcal{R}_{hy_i}^T\hat{\mathbf{x}} + \mathcal{R}_{yy_i}} - \frac{e_i^2(\mathcal{R}_{hh_i}\hat{\mathbf{x}} - \mathcal{R}_{hy_i})}{(\hat{\mathbf{x}}^T\mathcal{R}_{hh_i}\hat{\mathbf{x}} - 2\mathcal{R}_{hy_i}^T\hat{\mathbf{x}} + \mathcal{R}_{yy_i})^2} = \mathbf{0} \tag{27}$$

A closed-form solution is not possible for $\hat{\mathbf{x}}$. An iteration procedure is provided using:[10]

$$\hat{\mathbf{x}}^{(j+1)} = \left[\sum_{i=1}^{m}\frac{\tilde{\mathbf{h}}_i\tilde{\mathbf{h}}_i^T}{\gamma_i(\hat{\mathbf{x}}^{(j)})} - \frac{e_i^2(\hat{\mathbf{x}}^{(j)})\mathcal{R}_{hh_i}}{\gamma_i^2(\hat{\mathbf{x}}^{(j)})}\right]^{-1}\left[\sum_{i=1}^{m}\frac{\tilde{y}_i\tilde{\mathbf{h}}_i}{\gamma_i(\hat{\mathbf{x}}^{(j)})} - \frac{e_i^2(\hat{\mathbf{x}}^{(j)})\mathcal{R}_{hy_i}}{\gamma_i^2(\hat{\mathbf{x}}^{(j)})}\right] \tag{28a}$$

$$\gamma_i(\hat{\mathbf{x}}^{(j)}) \triangleq \hat{\mathbf{x}}^{(j)T}\mathcal{R}_{hh_i}\hat{\mathbf{x}}^{(j)} - 2\mathcal{R}_{hy_i}^T\hat{\mathbf{x}}^{(j)} + \mathcal{R}_{yy_i} \tag{28b}$$

$$e_i(\hat{\mathbf{x}}^{(j)}) \triangleq \tilde{\mathbf{h}}_i^T\hat{\mathbf{x}}^{(j)} - \tilde{y}_i \tag{28c}$$

where $\hat{\mathbf{x}}^{(j)}$ denotes the estimate at the j^{th} iteration. Typically the initial estimate is obtained by employing the closed-form solution algorithm for the element-wise uncorrelated and non-stationary case (shown later), using the average of all the covariances in that algorithm.

1. Derivation Based on Fisher Information Matrix

Because the ML estimator is asymptotically efficient, the covariance matrix can be approximated by the inverse of the FIM. If the estimate is unbiased and maximizes the likelihood then its associated covariance is identical to the inverse of the FIM.[2] To derive the FIM for the TLS estimate $\hat{\mathbf{x}}$, it is possible to determine the FIM for the TLS estimate $\hat{D}$ from the likelihood function given by Eq. (13) and then retrieve the FIM for $\hat{\mathbf{x}}$ from it. It is difficult, however, to derive the FIM for $\hat{D}$ because of the constraint $D\,\mathbf{z} = \mathbf{0}$ with $\mathbf{z} \triangleq [\mathbf{x}^T \;\; -1]^T$, which explicitly involves $\mathbf{x}$. The FIM for the joint TLS estimate of $\{\mathbf{x},\; H\}$ will be derived instead.

The likelihood function in Eq. (13) is now treated as a function of $\{\mathbf{x}, H\}$:

$$p(\tilde{D}|\mathbf{x}, H) = \frac{1}{(2\pi)^{m/2}\left[\det(R)\right]^{1/2}} \exp\left\{-\frac{1}{2}\text{vec}^T\left(\tilde{D}^T - D^T(\mathbf{x},\, H)\right) R^{-1}\text{vec}\left(\tilde{D}^T - D^T(\mathbf{x},\, H)\right)\right\} \tag{29}$$

with $D(\mathbf{x},\, H) \triangleq [H \quad H\mathbf{x}]$. In the element-wise uncorrelated and non-stationary case, because $\tilde{\mathbf{d}}_i$ and $\tilde{\mathbf{d}}_j$, $i \neq j$, are independent of each other, the likelihood function reduces to

$$\begin{aligned} p(\tilde{D}|\mathbf{x}, H) &= \frac{1}{\prod_{i=1}^{m}\left[\det(2\pi\mathcal{R}_i)\right]^{1/2}} \exp\left\{-\frac{1}{2}\sum_{i=1}^{m}\left(\tilde{\mathbf{d}}_i - \mathbf{d}_i(\mathbf{x}_i,\, \mathbf{h}_i)\right)^T \mathcal{R}_i^{-1}\left(\tilde{\mathbf{d}}_i - \mathbf{d}_i(\mathbf{x}_i,\, \mathbf{h}_i)\right)\right\} \\ &= \prod_{i=1}^{m} p\left(\tilde{\mathbf{d}}_i|\mathbf{x}, \mathbf{h}_i\right) \end{aligned} \tag{30}$$

with $\mathbf{d}_i(\mathbf{x}_i,\, \mathbf{h}_i) \triangleq [\mathbf{h}_i^T \;\; \mathbf{h}_i^T\mathbf{x}]^T$ and

$$p(\tilde{\mathbf{d}}_i|\mathbf{x}, \mathbf{h}_i) \triangleq \frac{1}{\left[\det(2\pi\mathcal{R}_i)\right]^{1/2}} \exp\left\{-\frac{1}{2}\left(\tilde{\mathbf{d}}_i - \mathbf{d}_i(\mathbf{x}_i,\, \mathbf{h}_i)\right)^T \mathcal{R}_i^{-1}\left(\tilde{\mathbf{d}}_i - \mathbf{d}_i(\mathbf{x}_i,\, \mathbf{h}_i)\right)\right\} \tag{31}$$

Now, the FIM of the likelihood function $p(\tilde{\mathbf{d}}_i|\mathbf{x}, \mathbf{h}_i)$ is derived. Define

$$\mathbf{a}_i \triangleq \begin{bmatrix} \mathbf{x} \\ \mathbf{h}_i \end{bmatrix}, \quad p(\tilde{\mathbf{d}}_i|\mathbf{a}_i) \triangleq p(\tilde{\mathbf{d}}_i|\mathbf{x}, \mathbf{h}_i), \quad \mathbf{d}_i(\mathbf{a}_i) \triangleq \mathbf{d}_i(\mathbf{x}, \mathbf{h}_i) \tag{32}$$

The FIM, F_i^a, for $\mathbf{a}_i$ is

$$F_i^a = E\left\{\left(\frac{\partial}{\partial \mathbf{a}_i}\ln[p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)]\right)\left(\frac{\partial}{\partial \mathbf{a}_i}\ln[p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)]\right)^T\right\} \tag{33}$$

The natural logarithm of $p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)$ is

$$\ln[p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)] = -\frac{1}{2}\left(\tilde{\mathbf{d}}_i - \mathbf{d}_i(\mathbf{a}_i)\right)^T \mathcal{R}_i^{-1}\left(\tilde{\mathbf{d}}_i - \mathbf{d}_i(\mathbf{a}_i)\right) - \frac{1}{2}\ln\det(2\pi R_i) \tag{34}$$

Taking partials of the natural logarithm of $p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)$ leads to

$$\frac{\partial}{\partial \mathbf{a}_i}\ln[p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)] = \begin{bmatrix} 0_{n\times n} & \mathbf{h}_i \\ I_{n\times n} & \mathbf{x} \end{bmatrix} \mathcal{R}_i^{-1}\left(\tilde{\mathbf{d}}_i - \mathbf{d}_i(\mathbf{a}_i)\right) \tag{35}$$

where $0_{n\times n}$ and $I_{n\times n}$ denote the n-dimensional null matrix and identify matrix, respectively. Because $E\left\{\tilde{\mathbf{d}}_i - \mathbf{d}_i(\mathbf{a}_i)\right\} = \mathbf{0}$, then

$$E\left\{\frac{\partial}{\partial \mathbf{a}_i}\ln[p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)]\right\} = \begin{bmatrix} 0_{n\times n} & \mathbf{h}_i \\ I_{n\times n} & \mathbf{x} \end{bmatrix} \mathcal{R}_i^{-1} E\left\{\left(\tilde{\mathbf{d}}_i - \mathbf{d}_i(\mathbf{a}_i)\right)\right\} = \mathbf{0} \tag{36}$$

This means the regularity condition

$$E\left\{\frac{\partial}{\partial \mathbf{a}_i}\ln[p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)]\right\} \triangleq \int \frac{\partial}{\partial \mathbf{a}_i}\ln[p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)]\, p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)\, d\tilde{\mathbf{d}}_i = \int \left[\frac{\partial p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)}{\partial \mathbf{a}_i}\right] d\tilde{\mathbf{d}}_i = \mathbf{0} \tag{37}$$

is satisfied, which is prerequisite for the derivation of the Cramér-Rao lower bound. Post-multiplying $\partial \ln[p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)]/\partial \mathbf{a}_i$ by its transpose leads to

$$\left(\frac{\partial}{\partial \mathbf{a}_i} \ln[p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)]\right)\left(\frac{\partial}{\partial \mathbf{a}_i} \ln[p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)]\right)^T = \begin{bmatrix} 0_{n\times n} & \mathbf{h}_i \\ I_{n\times n} & \mathbf{x} \end{bmatrix} \mathcal{R}_i^{-1} \left(\tilde{\mathbf{d}}_i - \mathbf{d}_i(\mathbf{a}_i)\right)\left(\tilde{\mathbf{d}}_i - \mathbf{d}_i(\mathbf{a}_i)\right)^T \mathcal{R}_i^{-1} \begin{bmatrix} 0_{n\times n} & \mathbf{h}_i \\ I_{n\times n} & \mathbf{x} \end{bmatrix}^T \tag{38}$$

Taking the expectation and using

$$E\left\{\left(\tilde{\mathbf{d}}_i - \mathbf{d}_i(\mathbf{a}_i)\right)\left(\tilde{\mathbf{d}}_i - \mathbf{d}_i(\mathbf{a}_i)\right)^T\right\} = \mathcal{R}_i \tag{39}$$

leads to

$$F_i^a = E\left\{\left(\frac{\partial}{\partial \mathbf{a}_i} \ln[p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)]\right)\left(\frac{\partial}{\partial \mathbf{a}_i} \ln[p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)]\right)^T\right\} = \begin{bmatrix} 0_{n\times n} & \mathbf{h}_i \\ I_{n\times n} & \mathbf{x} \end{bmatrix} \mathcal{R}_i^{-1} \begin{bmatrix} 0_{n\times n} & \mathbf{h}_i \\ I_{n\times n} & \mathbf{x} \end{bmatrix}^T \tag{40}$$

Since the regularity condition is met, the FIM F_i^a can be derived using an alternative form, given by

$$F_i^a = -E\left\{\frac{\partial^2}{\partial \mathbf{a}_i \partial \mathbf{a}_i^T} \ln\left[p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)\right]\right\} \tag{41}$$

Taking the partial of both sides of Eq. (35) leads to

$$\frac{\partial^2}{\partial \mathbf{a}_i \partial \mathbf{a}_i^T} \ln\left[p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)\right] = -\begin{bmatrix} 0_{n\times n} & \mathbf{h}_i \\ I_{n\times n} & \mathbf{x} \end{bmatrix} \mathcal{R}_i^{-1} \begin{bmatrix} 0_{n\times n} & \mathbf{h}_i \\ I_{n\times n} & \mathbf{x} \end{bmatrix}^T + \frac{\partial}{\partial \mathbf{a}_i^T}\left\{\begin{bmatrix} 0_{n\times n} & \mathbf{h}_i \\ I_{n\times n} & \mathbf{x} \end{bmatrix} \mathcal{R}_i^{-1} \left(\tilde{\mathbf{d}}_i - \mathbf{d}_i(\mathbf{a}_i)\right)\right\} \tag{42}$$

Because the expectation of the second term vanishes, then

$$F_i^a = -E\left\{\frac{\partial^2}{\partial \mathbf{a}_i \partial \mathbf{a}_i^T} \ln\left[p(\tilde{\mathbf{d}}_i|\mathbf{a}_i)\right]\right\} = \begin{bmatrix} 0_{n\times n} & \mathbf{h}_i \\ I_{n\times n} & \mathbf{x} \end{bmatrix} \mathcal{R}_i^{-1} \begin{bmatrix} 0_{n\times n} & \mathbf{h}_i \\ I_{n\times n} & \mathbf{x} \end{bmatrix}^T \tag{43}$$

Equation (43) is identical to Eq. (40).

The next step is to derive the FIM for $\hat{\mathbf{x}}$. The total Fisher information for $\hat{\mathbf{x}}$ will be denoted by F and the Fisher information corresponding to a single measurement $\tilde{\mathbf{d}}_i$ will be denoted by F_i. Because $\tilde{\mathbf{d}}_i$ and $\tilde{\mathbf{d}}_j$ are independent of each other and $\mathbf{h}_i$ and $\mathbf{h}_j$ are different for $i \neq j$, then $F = \sum_{i=1}^m F_i$. To see this, consider the partition of F_i^a:

$$F_i^a \triangleq \begin{bmatrix} F_{xx_i} & F_{xh_i} \\ F_{xh_i}^T & F_{hh_i} \end{bmatrix} = \begin{bmatrix} \begin{bmatrix} 0_{n\times n} & \mathbf{h}_i \end{bmatrix} \mathcal{R}_i^{-1} \begin{bmatrix} 0_{n\times n} \\ \mathbf{h}_i^T \end{bmatrix} & \begin{bmatrix} 0_{n\times n} & \mathbf{h}_i \end{bmatrix} \mathcal{R}_i^{-1} \begin{bmatrix} I_{n\times n} \\ \mathbf{x}^T \end{bmatrix} \\ \begin{bmatrix} I_{n\times n} & \mathbf{x} \end{bmatrix} \mathcal{R}_i^{-1} \begin{bmatrix} 0_{n\times n} \\ \mathbf{h}_i^T \end{bmatrix} & \begin{bmatrix} I_{n\times n} & \mathbf{x} \end{bmatrix} \mathcal{R}_i^{-1} \begin{bmatrix} I_{n\times n} \\ \mathbf{x}_i^T \end{bmatrix} \end{bmatrix} \tag{44}$$

and the augmented FIM for $[\hat{\mathbf{x}}^T, \hat{\mathbf{h}}_1^T, \ldots, \hat{\mathbf{h}}_m^T]^T$:

$$\mathcal{F} \triangleq \begin{bmatrix} \mathcal{F}_{xx} & \mathcal{F}_{xh} \\ \mathcal{F}_{xh}^T & \mathcal{F}_{hh} \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^m F_{xx_i} & F_{xh_1} & \cdots & F_{xh_m} \\ F_{xh_1}^T & F_{hh_1} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ F_{xh_1}^T & 0 & \cdots & F_{hh_m} \end{bmatrix} \tag{45}$$

Note that F_{xx_i} are rank-one matrices, F_{hh_i} are nonsingular, and for $m \geq n$, $\mathcal{F}$ is nonsingular. Applying the matrix inversion lemma to $\mathcal{F}$ leads to

$$\begin{aligned} F^{-1} = \mathcal{F}_{xx} &= \left(\sum_{i=1}^m F_{xx_i} - \begin{bmatrix} F_{xh_1} & \cdots & F_{xh_m} \end{bmatrix} \begin{bmatrix} F_{hh_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & F_{hh_m} \end{bmatrix}^{-1} \begin{bmatrix} F_{xh_1}^T \\ \vdots \\ F_{xh_m}^T \end{bmatrix}\right)^{-1} \\ &= \left(\sum_{i=1}^m \left(F_{xx_i} - F_{xh_i} F_{hh_i}^{-1} F_{xh_i}^T\right)\right)^{-1} \end{aligned} \tag{46}$$

or equivalently $F = \sum_{i=1}^{m} F_i$, where

$$F_i = F_{xx_i} - F_{xh_i} F_{hh_i}^{-1} F_{xh_i}^T \tag{47}$$

Note that F_i are rank-one.

For the F_i^a in Eq. (43), F_i satisfies

$$(F_i^a)^\dagger = \begin{bmatrix} F_i^\dagger & * \\ * & * \end{bmatrix} \tag{48}$$

where $*$ denote matrices of appropriate dimensions and $\dagger$ denotes the Penrose-Moore pseudoinverse. Taking the pseudoinverse of Eq. (43) leads to

$$(F_i^a)^\dagger = \left(\begin{bmatrix} 0_{n\times n} & \mathbf{h}_i \\ I_{n\times n} & \mathbf{x} \end{bmatrix}^\dagger \right)^T \mathcal{R}_i \begin{bmatrix} 0_{n\times n} & \mathbf{h}_i \\ I_{n\times n} & \mathbf{x} \end{bmatrix}^\dagger \tag{49}$$

It can be shown that

$$\begin{bmatrix} 0_{n\times n} & \mathbf{h}_i \\ I_{n\times n} & \mathbf{x} \end{bmatrix}^\dagger = \begin{bmatrix} -\dfrac{\mathbf{x}\mathbf{h}_i^T}{h_i^2} & I_{n\times n} \\ \dfrac{\mathbf{h}_i^T}{h_i^2} & 0_{n\times n} \end{bmatrix} \tag{50}$$

with $h_i^2 = \mathbf{h}_i^T \mathbf{h}$. So,

$$(F_i^a)^\dagger = \begin{bmatrix} -\dfrac{\mathbf{h}\mathbf{x}_i^T}{h_i^2} & \dfrac{\mathbf{h}_i^T}{h_i^2} \\ I_{n\times n} & 0_{n\times n} \end{bmatrix} \mathcal{R}_i \begin{bmatrix} -\dfrac{\mathbf{x}\mathbf{h}_i^T}{h_i^2} & I_{n\times n} \\ \dfrac{\mathbf{h}_i^T}{h_i^2} & 0_{n\times n} \end{bmatrix} = \begin{bmatrix} \dfrac{(\mathbf{z}^T \mathcal{R}_i \mathbf{z})}{h_i^4} \mathbf{h}_i \mathbf{h}_i^T & \dfrac{1}{h_i^2} \mathbf{h}_i (\mathbf{x}^T R_{hh_i} - R_{hy_i}^T) \\ \dfrac{1}{h_i^2} (R_{hh_i} \mathbf{x} - R_{hy_i}) \mathbf{h}_i^T & R_{hh_i} \end{bmatrix} \tag{51}$$

Since $(F_i)^\dagger$ is the upper-left block of $(F_i^a)^\dagger$, then

$$(F_i)^\dagger = \frac{(\mathbf{z}^T \mathcal{R}_i \mathbf{z})}{h_i^4} \mathbf{h}_i \mathbf{h}_i^T = \frac{(\mathbf{z}^T \mathcal{R}_i \mathbf{z})}{h_i^2} \frac{\mathbf{h}_i}{h_i} \frac{\mathbf{h}_i^T}{h_i} \tag{52}$$

and

$$F_i = \frac{h_i^2}{(\mathbf{z}^T \mathcal{R}_i \mathbf{z})} \left(\frac{\mathbf{h}_i}{h_i} \frac{\mathbf{h}_i^T}{h_i} \right)^\dagger = \frac{h_i^2}{(\mathbf{z}^T \mathcal{R}_i \mathbf{z})} \left(\frac{\mathbf{h}_i}{h_i} \frac{\mathbf{h}_i^T}{h_i} \right) = \frac{\mathbf{h}_i \mathbf{h}_i^T}{\mathbf{z}^T R_i \mathbf{z}} \tag{53}$$

Therefore,

$$F = \sum_{i=1}^{m} \frac{\mathbf{h}_i \mathbf{h}_i^T}{\mathbf{z}^T \mathcal{R}_i \, \mathbf{z}} \tag{54}$$

Finally, the error covariance matrix of $\hat{\mathbf{x}}$ is given by $P \approx F^{-1}$. If $\mathcal{R}_{hh_i}$ and $\mathcal{R}_{hy_i}$ are both zero, meaning no errors exist in the measured basis functions, then the FIM reduces down to

$$F = \sum_{i=1}^{m} \mathcal{R}_{yy_i}^{-1} \mathbf{h}_i \mathbf{h}_i^T \tag{55}$$

which is equivalent to the FIM for the standard least squares problem.

2. Derivation Based on First-Order Linearization

The error-covariance is now derived using the approach shown by Eq. (10). First it must be shown that the estimate is unbiased. Let the estimate be given by its true value plus a perturbation: $\hat{\mathbf{x}} = \mathbf{x} + \boldsymbol{\delta}\mathbf{x}$. The individual numerator parts of Eq. (26) are then given by

$$\begin{aligned} (\tilde{\mathbf{d}}_i^T \hat{\mathbf{z}})^2 &= (\tilde{\mathbf{h}}_i^T \hat{\mathbf{x}} - \tilde{y}_i)^2 \\ &= \bar{e}_i^2 + 2\bar{e}_i (\tilde{\mathbf{h}}_i^T \boldsymbol{\delta}\mathbf{x}) + (\tilde{\mathbf{h}}_i^T \boldsymbol{\delta}\mathbf{x})^2 \end{aligned} \tag{56}$$

The individual denominator parts of Eq. (26) are given by

$$\hat{\mathbf{z}}^T \mathcal{R}_i \, \hat{\mathbf{z}} = \mathbf{z}^T \mathcal{R}_i \, \mathbf{z} + \boldsymbol{\delta}\mathbf{x}^T \mathcal{R}_{hh_i} \boldsymbol{\delta}\mathbf{x} + 2\mathbf{b}_i^T \boldsymbol{\delta}\mathbf{x} \tag{57}$$

Using the binomial series for a second-order expansion of $(\hat{\mathbf{z}}^T \mathcal{R}_i \, \hat{\mathbf{z}})^{-1}$ leads to the approximation

$$(\hat{\mathbf{z}}^T \mathcal{R}_i \, \hat{\mathbf{z}})^{-1} \approx (\mathbf{z}^T \mathcal{R}_i \, \mathbf{z})^{-1} - (\boldsymbol{\delta}\mathbf{x}^T \mathcal{R}_{hh_i} \boldsymbol{\delta}\mathbf{x} + 2\mathbf{b}_i^T \boldsymbol{\delta}\mathbf{x})(\mathbf{z}^T \mathcal{R}_i \, \mathbf{z})^{-2} + (\boldsymbol{\delta}\mathbf{x}^T \mathcal{R}_{hh_i} \boldsymbol{\delta}\mathbf{x} + 2\mathbf{b}_i^T \boldsymbol{\delta}\mathbf{x})^2 (\mathbf{z}^T \mathcal{R}_i \, \mathbf{z})^{-3} \tag{58}$$

Substituting Eqs. (56) and (58) into Eq. (26), and retaining terms dependent only up to second order in $\boldsymbol{\delta}\mathbf{x}$ yields

$$J(\boldsymbol{\delta}\mathbf{x}) = \sum_{i=1}^{m} \frac{2\bar{e}_i(\tilde{\mathbf{h}}_i^T \boldsymbol{\delta}\mathbf{x}) + (\tilde{\mathbf{h}}_i^T \boldsymbol{\delta}\mathbf{x})^2}{\mathbf{z}^T \mathcal{R}_i \, \mathbf{z}} - \frac{\bar{e}_i^2 \boldsymbol{\delta}\mathbf{x}^T \mathcal{R}_{hh_i} \boldsymbol{\delta}\mathbf{x} + 2\bar{e}_i^2 \mathbf{b}_i^T \boldsymbol{\delta}\mathbf{x} + 4\bar{e}_i \boldsymbol{\delta}\mathbf{x}^T \mathbf{b}_i \tilde{\mathbf{h}}_i^T \boldsymbol{\delta}\mathbf{x}}{(\mathbf{z}^T \mathcal{R}_i \, \mathbf{z})^2} + \frac{4\bar{e}_i^2 \boldsymbol{\delta}\mathbf{x}^T \mathbf{b}_i \mathbf{b}_i^T \boldsymbol{\delta}\mathbf{x}}{(\mathbf{z}^T \mathcal{R}_i \, \mathbf{z})^3} \tag{59}$$

Taking the partial with respect to $\boldsymbol{\delta}\mathbf{x}$ and setting to resultant to zero for the necessary condition for optimality gives

$$\frac{\partial J(\boldsymbol{\delta}\mathbf{x})}{\partial \boldsymbol{\delta}\mathbf{x}} = \left\{ \sum_{i=1}^{m} \frac{\tilde{\mathbf{h}}_i \tilde{\mathbf{h}}_i^T}{\mathbf{z}^T \mathcal{R}_i \, \mathbf{z}} - \frac{\bar{e}_i \left[\bar{e}_i \mathcal{R}_{hh_i} + 2(\mathbf{b}_i \tilde{\mathbf{h}}_i^T + \tilde{\mathbf{h}}_i \mathbf{b}_i^T) \right]}{(\mathbf{z}^T \mathcal{R}_i \, \mathbf{z})^2} + \frac{4\bar{e}_i^2 \mathbf{b}_i \mathbf{b}_i^T}{(\mathbf{z}^T \mathcal{R}_i \, \mathbf{z})^3} \right\} \boldsymbol{\delta}\mathbf{x} + \sum_{i=1}^{m} \frac{\bar{e}_i \tilde{\mathbf{h}}_i}{\mathbf{z}^T \mathcal{R}_i \, \mathbf{z}} - \frac{\bar{e}_i^2 \mathbf{b}_i}{(\mathbf{z}^T \mathcal{R}_i \, \mathbf{z})^2} = \mathbf{0} \tag{60}$$

This equation can be used to develop a nonlinear least squares iteration to determine the estimate, with the correction given by

$$\boldsymbol{\delta}\mathbf{x} = \left\{ \sum_{i=1}^{m} \frac{\tilde{\mathbf{h}}_i \tilde{\mathbf{h}}_i^T}{\mathbf{z}^T \mathcal{R}_i \, \mathbf{z}} - \frac{\bar{e}_i \left[\bar{e}_i \mathcal{R}_{hh_i} + 2(\mathbf{b}_i \tilde{\mathbf{h}}_i^T + \tilde{\mathbf{h}}_i \mathbf{b}_i^T) \right]}{(\mathbf{z}^T \mathcal{R}_i \, \mathbf{z})^2} + \frac{4\bar{e}_i^2 \mathbf{b}_i \mathbf{b}_i^T}{(\mathbf{z}^T \mathcal{R}_i \, \mathbf{z})^3} \right\}^{-1} \left(\sum_{i=1}^{m} \frac{\bar{e}_i^2 \mathbf{b}_i}{(\mathbf{z}^T \mathcal{R}_i \, \mathbf{z})^2} - \frac{\bar{e}_i \tilde{\mathbf{h}}_i}{\mathbf{z}^T \mathcal{R}_i \, \mathbf{z}} \right) \tag{61}$$

The expected value of the matrix on the left-hand side of Eq. (60) is given by

$$E\left\{ \sum_{i=1}^{m} \frac{\tilde{\mathbf{h}}_i \tilde{\mathbf{h}}_i^T}{\mathbf{z}^T \mathcal{R}_i \, \mathbf{z}} - \frac{\bar{e}_i \left[\bar{e}_i \mathcal{R}_{hh_i} + 2(\mathbf{b}_i \tilde{\mathbf{h}}_i^T + \tilde{\mathbf{h}}_i \mathbf{b}_i^T) \right]}{(\mathbf{z}^T \mathcal{R}_i \, \mathbf{z})^2} + \frac{4\bar{e}_i^2 \mathbf{b}_i \mathbf{b}_i^T}{(\mathbf{z}^T \mathcal{R}_i \, \mathbf{z})^3} \right\} = \sum_{i=1}^{m} \frac{\mathbf{h}_i \mathbf{h}_i^T}{\mathbf{z}^T \mathcal{R}_i \, \mathbf{z}} \tag{62}$$

where $E\{\bar{e}_i^2\} = \mathbf{z}^T \mathcal{R}_i \, \mathbf{z}$, and $E\{\bar{e}_i \tilde{\mathbf{h}}_i\} = \mathbf{b}_i$ and $E\{\bar{e}_i \tilde{\mathbf{h}}_i^T\} = \mathbf{b}_i^T$ have been used. They are true because

$$\begin{aligned} E\{\bar{e}_i^2\} = E\left\{ (\tilde{\mathbf{h}}_i^T \mathbf{x} - \tilde{y}_i)^2 \right\} &= E\left\{ [(\mathbf{h}_i + \boldsymbol{\delta}\mathbf{h}_i)^T \mathbf{x} - \mathbf{h}_i^T \mathbf{x} - \delta y_i]^2 \right\} \\ &= E\left\{ (\mathbf{x}^T \boldsymbol{\delta}\mathbf{h}_i - \delta y_i)^2 \right\} \\ &= \mathbf{x}^T \mathcal{R}_{hh_i} \mathbf{x} - 2\mathbf{x}^T \mathcal{R}_{hy_i} + \mathcal{R}_{yy_i} \\ &= \mathbf{z}^T \mathcal{R}_i \, \mathbf{z} \end{aligned} \tag{63}$$

$$\begin{aligned} E\left\{ \bar{e}_i \tilde{\mathbf{h}}_i \right\} &= E\left\{ [(\mathbf{h}_i + \boldsymbol{\delta}\mathbf{h}_i)^T \mathbf{x} - (y_i + \delta y_i)](\mathbf{h}_i + \boldsymbol{\delta}\mathbf{h}_i) \right\} \\ &= (\mathbf{h}_i^T \mathbf{x} - y_i)\mathbf{h}_i + \mathcal{R}_{hh_i} \mathbf{x} - \mathcal{R}_{hy_i} \\ &= \mathbf{b}_i \end{aligned} \tag{64}$$

Also note

$$E\left\{ \sum_{i=1}^{m} \frac{\bar{e}_i \tilde{\mathbf{h}}_i}{\mathbf{z}^T \mathcal{R}_i \, \mathbf{z}} - \frac{\bar{e}_i^2 \mathbf{b}_i}{(\mathbf{z}^T \mathcal{R}_i \, \mathbf{z})^2} \right\} = \sum_{i=1}^{m} \frac{\mathbf{b}_i}{\mathbf{z}^T \mathcal{R}_i \, \mathbf{z}} - \frac{\mathbf{b}_i}{\mathbf{z}^T \mathcal{R}_i \, \mathbf{z}} = \mathbf{0} \tag{65}$$

Equations (60), (62) and (65) indicate that

$$\left[\sum_{i=1}^{m} \frac{\mathbf{h}_i \mathbf{h}_i^T}{\mathbf{z}^T \mathcal{R}_i \, \mathbf{z}} \right] E\left\{ \boldsymbol{\delta}\mathbf{x} \right\} = \mathbf{0} \tag{66}$$

As stated previously linearly independent basis function should be employed in practice. For this case the matrix in Eq. (66) is never singular and $E\{\boldsymbol{\delta}\mathbf{x}\} = \mathbf{0}$ must be true. Thus the TLS estimator produces an unbiased estimate to within first-order terms.

The error-covariance is now derived using Eq. (10), where the estimate follows from Eq. (27). Three error sources are present: the first is $\boldsymbol{\delta}\mathbf{x}$ which is the error on $\hat{\mathbf{x}}$, the second is $\boldsymbol{\delta}\mathbf{h}_i$ which is the error on $\tilde{\mathbf{h}}_i$, and the third is δy_i which is the error on $\tilde{y}_i$. Define the expression in Eq. (27) by $\mathbf{g} \triangleq \partial J(\hat{\mathbf{x}})/\partial \hat{\mathbf{x}} = \mathbf{0}$. The partial of $\mathbf{g}$ with respect to $\hat{\mathbf{x}}$ is given by

$$
\begin{aligned}
-\frac{\partial^2 \ln[p(\tilde{\mathbf{d}}|\mathbf{x})]}{\partial \mathbf{x}\, \partial \mathbf{x}^T} = \sum_{i=1}^{m} \frac{\tilde{\mathbf{h}}_i \tilde{\mathbf{h}}_i^T}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} &- \frac{2\bar{e}_i [\tilde{\mathbf{h}}_i\, (\mathcal{R}_{hh_i}\mathbf{x} - \mathcal{R}_{hy_i})^T + (\mathcal{R}_{hh_i}\mathbf{x} - \mathcal{R}_{hy_i})\, \tilde{\mathbf{h}}_i^T]}{(\mathbf{z}^T \mathcal{R}_i\, \mathbf{z})^2} \\
&- \frac{\mathcal{R}_{hh_i} \bar{e}_i^2}{(\mathbf{z}^T \mathcal{R}_i\, \mathbf{z})^2} + \frac{4\bar{e}_i^2 (\mathcal{R}_{hh_i}\mathbf{x} - \mathcal{R}_{hy_i})(\mathcal{R}_{hh_i}\mathbf{x} - \mathcal{R}_{hy_i})^T}{(\mathbf{z}^T \mathcal{R}_i\, \mathbf{z})^3} \\
&+ \frac{\mathcal{R}_{hh_i}}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} - \frac{2(\mathcal{R}_{hh_i}\mathbf{x} - \mathcal{R}_{hy_i})(\mathcal{R}_{hh_i}\mathbf{x} - \mathcal{R}_{hy_i})^T}{(\mathbf{z}^T \mathcal{R}_i\, \mathbf{z})^2}
\end{aligned} \tag{67}
$$

According to Eq. (10) this partial is evaluated at the true values. Since $y_i = \mathbf{h}_i^T \mathbf{x}$ then

$$
\left.\frac{\partial \mathbf{g}}{\partial \hat{\mathbf{x}}}\right|_{\text{truth}} = \sum_{i=1}^{m} \frac{\mathbf{h}_i \mathbf{h}_i^T}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} \tag{68}
$$

The partial of $\mathbf{g}$ with respect to $\tilde{\mathbf{h}}_i$ evaluated at the true values is given

$$
\left.\frac{\partial \mathbf{g}}{\partial \tilde{\mathbf{h}}_i}\right|_{\text{truth}} = \sum_{i=1}^{m} \frac{\mathbf{h}_i \mathbf{x}^T}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} \tag{69}
$$

The partial of $\mathbf{g}$ with respect to $\tilde{y}_i$ evaluated at the true values is given

$$
\left.\frac{\partial \mathbf{g}}{\partial \tilde{y}_i}\right|_{\text{truth}} = -\sum_{i=1}^{m} \frac{\mathbf{h}_i}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} \tag{70}
$$

Then to within first order the following equation is given:

$$
-\left(\sum_{i=1}^{m} \frac{\mathbf{h}_i \mathbf{h}_i^T}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}}\right) \boldsymbol{\delta}\mathbf{x} = \sum_{i=1}^{m} \frac{\mathbf{h}_i \mathbf{x}^T \boldsymbol{\delta}\mathbf{h}_i}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} - \frac{\mathbf{h}_i \delta y_i}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} \tag{71}
$$

The error-covariance, $P \triangleq E\left\{\boldsymbol{\delta}\mathbf{x}\, \boldsymbol{\delta}\mathbf{x}^T\right\}$, is derived from

$$
P = F^{-1} E\left\{\left[\sum_{i=1}^{m} \frac{\mathbf{h}_i (\mathbf{x}^T \boldsymbol{\delta}\mathbf{h}_i - \delta y_i)}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}}\right]\left[\sum_{i=1}^{m} \frac{\mathbf{h}_i (\mathbf{x}^T \boldsymbol{\delta}\mathbf{h}_i - \delta y_i)}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}}\right]^T\right\} F^{-1} \tag{72}
$$

where F is given by Eq. (54). Since element-wise uncorrelated terms are assumed, then the expectation in Eq. (72) reduces down to

$$
E\left\{\left[\sum_{i=1}^{m} \frac{\mathbf{h}_i (\mathbf{x}^T \boldsymbol{\delta}\mathbf{h}_i - \delta y_i)}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}}\right]\left[\sum_{i=1}^{m} \frac{\mathbf{h}_i (\mathbf{x}^T \boldsymbol{\delta}\mathbf{h}_i - \delta y_i)}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}}\right]^T\right\} = E\left\{\sum_{i=1}^{m} \frac{\mathbf{h}_i \mathbf{h}_i^T (\mathbf{x}^T \boldsymbol{\delta}\mathbf{h}_i - \delta y_i)^2}{(\mathbf{z}^T \mathcal{R}_i\, \mathbf{z})^2}\right\} \tag{73}
$$

Using $E\{(\mathbf{x}^T \boldsymbol{\delta}\mathbf{h}_i - \delta y_i)^2\} = \mathbf{z}^T \mathcal{R}_i\, \mathbf{z}$ leads to

$$
P = F^{-1} \left(\sum_{i=1}^{m} \frac{\mathbf{h}_i \mathbf{h}_i^T}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}}\right) F^{-1} = F^{-1} \tag{74}
$$

Comparing Eqs. (54) and (74) shows that the Cramér-Rao lower bound is achieved to within first-order terms.

The FIM is evaluated at the respective true values for $\mathbf{h}_i$ and $\mathbf{x}$, which are not available in practice. Either the estimated or measured values are typically used in their place. The expected errors induced by using the measured values are now shown. The estimate is again written by $\hat{\mathbf{x}} = \mathbf{x} + \boldsymbol{\delta}\mathbf{x}$ where the covariance of $\boldsymbol{\delta}\mathbf{x}$ is given by P. The estimate of the FIM, denoted by $\hat{F}$, using the measured values can now be written as

$$\hat{F} = \sum_{i=1}^{m} \frac{(\mathbf{h}_i + \boldsymbol{\delta}\mathbf{h}_i)(\mathbf{h}_i + \boldsymbol{\delta}\mathbf{h}_i)^T}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z} + \boldsymbol{\delta}\mathbf{x}^T \mathcal{R}_{hh_i} \boldsymbol{\delta}\mathbf{x} + 2(\mathcal{R}_{hh_i}\mathbf{x} - \mathcal{R}_{hy_i})\boldsymbol{\delta}\mathbf{x}} \tag{75}$$

Using Eq. (58) leads to the approximation

$$\hat{F} \approx \sum_{i=1}^{m} \frac{(\mathbf{h}_i + \boldsymbol{\delta}\mathbf{h}_i)(\mathbf{h}_i + \boldsymbol{\delta}\mathbf{h}_i)^T}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} - \frac{[\boldsymbol{\delta}\mathbf{x}^T \mathcal{R}_{hh_i} \boldsymbol{\delta}\mathbf{x} + 2(\mathcal{R}_{hh_i}\mathbf{x} - \mathcal{R}_{hy_i})\boldsymbol{\delta}\mathbf{x}](\mathbf{h}_i + \boldsymbol{\delta}\mathbf{h}_i)(\mathbf{h}_i + \boldsymbol{\delta}\mathbf{h}_i)^T}{(\mathbf{z}^T \mathcal{R}_i\, \mathbf{z})^2} \tag{76}$$

Computing $\delta F \triangleq E\{\hat{F}\} - F$ gives

$$\delta F = \sum_{i=1}^{m} \frac{\mathcal{R}_{hh_i}}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} - \frac{\mathrm{Tr}(P\, \mathcal{R}_{hh_i})(\mathbf{h}_i \mathbf{h}_i^T + \mathcal{R}_{hh_i})}{(\mathbf{z}^T \mathcal{R}_i\, \mathbf{z})^2} \tag{77}$$

The relative magnitudes of the terms in Eq. (77) and the FIM, given by the inverse of Eq. (54), are now compared. If the signal-to-noise ratio is large then $||\mathbf{h}_i \mathbf{h}_i^T||_F = \mathbf{h}_i^T \mathbf{h}_i >> ||\mathcal{R}_{hh_i}||_{\mathrm{F}}$. Thus the first term on the right-hand side of Eq. (77) is negligible. Also, $\mathcal{R}_{hh_i}$ in second term on the right-hand side of Eq. (77) can be neglected since $\mathbf{h}_i \mathbf{h}_i^T$ is added to it. Thus, the second term on the right-hand side of Eq. (77) is negligible if the following inequality holds:

$$\frac{\mathbf{h}_i^T \mathbf{h}_i}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} >> \frac{\mathrm{Tr}(P\, \mathcal{R}_{hh_i})\mathbf{h}_i^T \mathbf{h}_i}{(\mathbf{z}^T \mathcal{R}_i\, \mathbf{z})^2} \tag{78}$$

The term $\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}$ is equal to $\mathrm{Tr}(\mathbf{x}\, \mathbf{x}^T \mathcal{R}_{hh_i}) - 2\mathcal{R}_{hy_i}^T \mathbf{x} + \mathcal{R}_{yy_i}$. Since $\mathcal{R}_{yy_i} > 0$ then Eq. (78) will hold if the following holds:

$$\mathrm{Tr}(\mathbf{x}\, \mathbf{x}^T \mathcal{R}_{hh_i}) >> \mathrm{Tr}(P\, \mathcal{R}_{hh_i}) + 2\mathcal{R}_{hy_i}^T \mathbf{x} \tag{79}$$

Even if the cross-correlations given by $\mathcal{R}_{hh_i}$ are on the same order as the terms given in $\mathcal{R}_{hh_i}$ the fact that the signal-to-noise ratio is large and the estimate errors are small will make the inequality in Eq. (79) hold. Therefore, the errors induced by using the measured values to compute the error-covariance are higher-order in nature and thus are negligible. Also, if estimates are used in place of measurements, then $\mathcal{R}_i$, along with its partitions, in Eq. (77) is replaced with the covariance of the estimates.

The covariance of $\hat{\mathbf{h}}_i$ and variance of $\hat{y}_i$ are now derived, which are defined by $P_{hh_i} = E\{(\hat{\mathbf{h}}_i - E\{\hat{\mathbf{h}}_i\})(\hat{\mathbf{h}}_i - E\{\hat{\mathbf{h}}_i\})^T\}$ and $P_{yy_i} = E\{(\hat{y}_i - E\{\hat{y}_i\})(\hat{y}_i - E\{\hat{y}_i\})^T\}$, respectively. The cross-covariance $P_{hy_i} = E\{(\hat{\mathbf{h}}_i - E\{\hat{\mathbf{h}}_i\})(\hat{y}_i - E\{\hat{y}_i\})^T\}$ is also derived which is used to derive the covariance of $\hat{\mathbf{d}}_i$. These covariances are useful for many applications. For example, the estimate $\hat{y}_i$ may be employed in a Kalman filter to provide filtered estimates. The correct variance of $\hat{y}_i$ is need to ensure proper tuning in the Kalman filter design. Using $\hat{\mathbf{x}} = \mathbf{x} + \boldsymbol{\delta}\mathbf{x}$ and Eq. (58), as well as $\tilde{\mathbf{h}}_i = \mathbf{h}_i + \boldsymbol{\delta}\mathbf{h}_i$ and $\tilde{y}_i = y_i + \delta y_i$, in Eq. (25a) gives

$$\begin{aligned}\hat{\mathbf{h}}_i = \mathbf{h}_i + \boldsymbol{\delta}\mathbf{h}_i &- \frac{(\mathcal{R}_{hh_i}\mathbf{x} + \mathcal{R}_{hh_i}\boldsymbol{\delta}\mathbf{x} - \mathcal{R}_{hy_i})(\mathbf{h}_i^T \boldsymbol{\delta}\mathbf{x} + \mathbf{h}_i^T \boldsymbol{\delta}\mathbf{h}_i - \delta y_i)}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} \\ &+ \frac{(\mathcal{R}_{hh_i}\mathbf{x} + \mathcal{R}_{hh_i}\boldsymbol{\delta}\mathbf{x} - \mathcal{R}_{hy_i})(\mathbf{h}_i^T \boldsymbol{\delta}\mathbf{x} + \mathbf{h}_i^T \boldsymbol{\delta}\mathbf{h}_i - \delta y_i)(\boldsymbol{\delta}\mathbf{x}^T \mathcal{R}_{hh_i}\boldsymbol{\delta}\mathbf{x} + 2\mathbf{b}_i^T \boldsymbol{\delta}\mathbf{x})}{(\mathbf{z}^T \mathcal{R}_i\, \mathbf{z})^2}\end{aligned} \tag{80}$$

Retaining terms up to second order only, then

$$E\left\{\hat{\mathbf{h}}_i\right\} = \mathbf{h}_i - \frac{\mathcal{R}_{hh_i} P\, \mathbf{h}_i}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} + \frac{2(\mathbf{h}_i^T P\, \mathbf{b}_i)\mathbf{b}_i}{(\mathbf{z}^T \mathcal{R}_i\, \mathbf{z})^2} \tag{81}$$

The last two terms on the right-hand side of Eq. (81) are second order in nature. Thus, to within first order $E\{\hat{\mathbf{h}}_i\} = \mathbf{h}_i$, which indicates that the estimate is unbiased. Define the following matrices:

$$M_{h_i} \triangleq \begin{bmatrix} I_{n\times n} - \dfrac{\mathbf{b}_i \mathbf{x}^T}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} & \dfrac{\mathbf{b}_i}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} \end{bmatrix} \tag{82a}$$

$$N_{h_i} \triangleq \frac{\mathbf{b}_i \mathbf{h}_i^T}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} \tag{82b}$$

$$M_{y_i} \triangleq \begin{bmatrix} -\dfrac{\beta_i \mathbf{x}^T}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} & 1 + \dfrac{\beta_i}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} \end{bmatrix} \tag{82c}$$

$$N_{y_i} \triangleq \frac{\beta_i \mathbf{h}_i^T}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} \tag{82d}$$

where $\beta_i \triangleq \mathcal{R}_{hy_i}^T \mathbf{x} - \mathcal{R}_{yy_i}$ and $I_{n\times n}$ is an $n \times n$ identity matrix. Then the covariance of $\hat{\mathbf{h}}_i$ up to first-order terms is given by

$$P_{hh_i} = M_{h_i}\mathcal{R}_i M_{h_i}^T + N_{h_i} P\, N_{h_i}^T \tag{83}$$

The term $N_{h_i} P\, N_{h_i}^T$ is often much smaller than $M_{h_i}\mathcal{R}_i M_{h_i}^T$ and can be ignored in most cases. In a similar fashion the expected value of $\hat{y}_i$ can be shown to be given by

$$E\left\{\hat{y}_i\right\} = y_i - \frac{\mathcal{R}_{hy_i}^T P\, \mathbf{h}_i}{\mathbf{z}^T \mathcal{R}_i\, \mathbf{z}} + \frac{2(\mathbf{h}_i^T P\, \mathbf{b}_i)\beta_i}{(\mathbf{z}^T \mathcal{R}_i\, \mathbf{z})^2} \tag{84}$$

As before the estimate is unbiased to within first order. Then the variance of $\hat{y}_i$ up to first-order terms is given by

$$P_{yy_i} = M_{y_i}\mathcal{R}_i M_{y_i}^T + N_{y_i} P\, N_{y_i}^T \tag{85}$$

Also, the cross-covariance is given by

$$P_{hy_i} = M_{h_i}\mathcal{R}_i M_{y_i}^T + N_{h_i} P\, N_{y_i}^T \tag{86}$$

Finally, the covariance of $\hat{\mathbf{d}}_i$, denoted by P_{dd_i}, is given by

$$P_{dd_i} = \begin{bmatrix} P_{hh_i} & P_{hy_i} \\ P_{hy_i}^T & P_{yy_i} \end{bmatrix} \tag{87}$$

The matrices in Eqs. (82) should be computed using the estimated values in practice because they are derived using $\mathbf{h}_i^T \mathbf{x} - \mathbf{y}_i = 0$. The estimates also obey $\hat{\mathbf{h}}_i^T \hat{\mathbf{x}}_i - \hat{\mathbf{y}}_i = 0$ by virtue of the required constraint in Eq. (14), but using the measurements with $\tilde{\mathbf{h}}_i^T \hat{\mathbf{x}}_i - \tilde{\mathbf{y}}_i = 0$ is not zero in practice. Therefore it is more accurate to use the estimates rather than the measurements to compute these matrices. Also, note that P_{dd_i} can be written by

$$P_{dd_i} = \begin{bmatrix} M_{h_i} & N_{h_i} \\ M_{y_i} & N_{y_i} \end{bmatrix} \begin{bmatrix} \mathcal{R}_i & 0_{(n+1)\times n} \\ 0_{(n+1)\times n}^T & P \end{bmatrix} \begin{bmatrix} M_{h_i} & N_{h_i} \\ M_{y_i} & N_{y_i} \end{bmatrix}^T \tag{88}$$

where $0_{(n+1)\times n}$ is an $(n+1) \times n$ matrix of zeros. This shows that P_{dd_i} is a singular matrix, which is due to the constraint $\hat{\mathbf{d}}_i^T \hat{\mathbf{z}} = 0$.

B. Element-Wise Uncorrelated and Stationary Case

For this case R is assumed to have a block diagonal structure of the form

$$R = \text{blkdiag}\begin{bmatrix} \mathcal{R} & \cdots & \mathcal{R} \end{bmatrix} \tag{89}$$

where $\mathcal{R}$ is an $(n+1) \times (n+1)$ matrix. The solution to this problem is presented in Ref. 10. First the Cholesky decomposition of $\mathcal{R}$ is taken: $\mathcal{R} = C^T C$ where C is defined as an upper block diagonal matrix. Partition the inverse as

$$C^{-1} = \begin{bmatrix} C_{11} & \mathbf{c} \\ \\ \mathbf{0}^T & c_{22} \end{bmatrix} \tag{90}$$

where C_{11} is an $n \times n$ matrix, $\mathbf{c}$ is an $n \times 1$ vector and c_{22} is a scalar. The solution is given by taking the singular value decomposition of the following matrix:

$$\tilde{D}C^{-1} = \tilde{U}\tilde{S}\tilde{V}^T \tag{91}$$

where the reduced form is used, with $\tilde{S} = \text{diag}\begin{bmatrix} \tilde{s}_1 & \cdots & \tilde{s}_{n+1} \end{bmatrix}$, $\tilde{U}$ is an $m \times (n+1)$ matrix and $\tilde{V}$ is an $(n+1) \times (n+1)$ matrix partitioned in a similar manner as the C^{-1} matrix:

$$\tilde{V} = \begin{bmatrix} \tilde{V}_{11} & \tilde{\mathbf{v}} \\ \\ \tilde{\mathbf{w}}^T & \tilde{v}_{22} \end{bmatrix} \tag{92}$$

The total least squares solution assuming an isotropic error process, i.e. $\mathcal{R}$ is a scalar times identity matrix, is

$$\hat{\mathbf{x}}_{\rm I} = -\tilde{v}_{22}^{-1}\tilde{\mathbf{v}} \tag{93}$$

The final solution is then given by

$$\hat{\mathbf{x}} = c_{22}^{-1}(C_{11}\hat{\mathbf{x}}_{\rm I} - \mathbf{c}) \tag{94}$$

Clearly if the error process is isotropic then $\hat{\mathbf{x}} = \hat{\mathbf{x}}_{\rm I}$, because $C_{11} = \sigma^{-2}I_{n\times n}$ where $I_{n\times n}$ is an $n\times n$ identity matrix, $\mathbf{c} = \mathbf{0}$ and $c_{22} = \sigma^{-2}$ where σ^2 is the variance associated with the isotropic process. The estimate for D is given by

$$\hat{D} = \tilde{U}_n \tilde{S}_n \tilde{V}_n^T C \tag{95}$$

where $\tilde{U}_n$ is the truncation of the matrix $\tilde{U}$ to $m\times n$, $\tilde{S}_n$ is the truncation of the matrix $\tilde{S}$ to $n\times n$, and $\tilde{V}_n$ is the truncation of the matrix $\tilde{V}$ to $(n+1)\times n$.

The solution summary is as follows. First form the augmented matrix, $\tilde{D}$, in Eq. (12) and take the Cholesky decomposition of the covariance $\mathcal{R}$. Take the inverse of C and obtain the matrix partitions shown in Eq. (90). Then take the reduced-form singular value decomposition of the matrix $\tilde{D}C^{-1}$, as shown in Eq. (91), and obtain the matrix partitions shown in Eq. (92). Obtain the isotropic solution using Eq. (93) and obtain the final solution using Eq. (94).

The error-covariance for the estimate in Eq. (94) is derived. For this case the FIM in Eq. (54) simplifies to

$$F = \frac{1}{\mathbf{z}^T\mathcal{R}\,\mathbf{z}}\sum_{i=1}^{m}\mathbf{h}_i\mathbf{h}_i^T \tag{96}$$

This requires an inverse of an $n\times n$ matrix. Note that if $\mathcal{R}$ is isotropic then Eq. (96) matches with the result shown in Ref. 11. Since a closed-form solution exists for the element-wise uncorrelated and stationary case, then an approximation for the error-covariance can be derived directly from the solution. The derivation begins by applying perturbations to the vector $\tilde{\mathbf{v}}$ and scalar $\tilde{v}_{22}$:

$$\tilde{\mathbf{v}} = \mathbf{v} + \boldsymbol{\delta}\mathbf{v} \tag{97a}$$

$$\tilde{v}_{22} = v_{22} + \delta v_{22} \tag{97b}$$

where $\mathbf{v}$ is the true value of $\tilde{\mathbf{v}}$, $\boldsymbol{\delta}\mathbf{v}$ is its respective perturbation, v_{22} is the true value of $\tilde{v}_{22}$, and δv_{22} is its respective perturbation. Using the binomial series the first-order expansion of $(v_{22}+\delta v_{22})^{-1}$ is given by

$$(v_{22}+\delta v_{22})^{-1} \approx v_{22}^{-1} - v_{22}^{-2}\,\delta v_{22} \tag{98}$$

Substituting Eqs. (97) and (98) into Eq. (93) and ignoring higher-order terms leads to

$$\hat{\mathbf{x}}_{\rm I} - \mathbf{x}_{\rm I} \approx -v_{22}^{-1}\boldsymbol{\delta}\mathbf{v} + v_{22}^{-2}\delta v_{22}\,\mathbf{v} \tag{99}$$

where $\mathbf{x}_{\rm I} \triangleq -v_{22}^{-1}\mathbf{v}$. Assuming that $\boldsymbol{\delta}\mathbf{v}$ and δv_{22} are random variables leads to the following error-covariance matrix for the isotropic total least squares solution:

$$\begin{aligned} P_{\rm I} &\triangleq E\left\{(\hat{\mathbf{x}}_{\rm I}-\mathbf{x}_{\rm I})(\hat{\mathbf{x}}_{\rm I}-\mathbf{x}_{\rm I})^T\right\} \\ &= v_{22}^{-2}E\left\{\boldsymbol{\delta}\mathbf{v}\,\boldsymbol{\delta}\mathbf{v}^T\right\} + v_{22}^{-4}\mathbf{v}\,\mathbf{v}^T E\left\{\delta v_{22}^2\right\} - v_{22}^{-3}E\left\{\delta v_{22}\boldsymbol{\delta}\mathbf{v}\right\}\mathbf{v}^T - v_{22}^{-3}\mathbf{v}E\left\{\delta v_{22}\boldsymbol{\delta}\mathbf{v}^T\right\} \end{aligned} \tag{100}$$

Using $\mathbf{x} = c_{22}^{-1}(C_{11}\mathbf{x}_{\rm I} - \mathbf{c})$ and Eq. (94) leads to

$$\hat{\mathbf{x}} - \mathbf{x} = c_{22}^{-1}C_{11}(\hat{\mathbf{x}}_{\rm I} - \mathbf{x}) \tag{101}$$

Therefore, the error-covariance matrix for the total least squares solution is given by

$$P \triangleq E\left\{(\hat{\mathbf{x}}-\mathbf{x})(\hat{\mathbf{x}}-\mathbf{x})^T\right\} = c_{22}^{-2}C_{11}P_{\rm I}\,C_{11}^T \tag{102}$$

Note that $P_{\rm I}$ is evaluated at the true values, $\mathbf{v}$ and v_{22}, which are not available in practice. These can be replaced with $\tilde{\mathbf{v}}$ and $\tilde{v}_{22}$ in practice, which leads to higher-order error effects that can be ignored for large signal-to-noise ratios as stated previously.

The expectations in Eq. (100) now need to be derived to complete the derivation of the error-covariance. Using Eq. (91) and the fact that the errors are stationary gives

$$C^{-T} E\left\{\tilde{\mathbf{d}}_i \tilde{\mathbf{d}}_i^T\right\} C^{-1} = C^{-T} \mathcal{R}\, C^{-1} = C^{-T} C^T C\, C^{-1} = I_{(n+1)\times(n+1)} \tag{103}$$

where C^{-T} is defined as the transpose of the inverse of C. The goal here is to compute the following quantity:

$$B \triangleq \begin{bmatrix} E\left\{\boldsymbol{\delta}\mathbf{v}\, \boldsymbol{\delta}\mathbf{v}^T\right\} & E\left\{\delta v_{22} \boldsymbol{\delta}\mathbf{v}\right\} \\ E\left\{\delta v_{22} \boldsymbol{\delta}\mathbf{v}^T\right\} & E\left\{\delta v_{22}^2\right\} \end{bmatrix} \tag{104}$$

Let $\tilde{\mathbf{p}} \triangleq [\tilde{\mathbf{v}}^T \;\; \tilde{v}_{22}]^T$. Using the analogy from Eq. (10), together with Eq. (103), the matrix B is approximated using the following matrix:

$$\tilde{B} = \left[\frac{\partial \tilde{\mathbf{p}}}{\partial \mathrm{vec}(\tilde{D}^T)}\right] \left[\frac{\partial \tilde{\mathbf{p}}}{\partial \mathrm{vec}(\tilde{D}^T)}\right]^T \tag{105}$$

where "measured" values are used in place of estimated values, which again leads to higher-order error effects that can be ignored for large signal-to-noise ratios.

A method to compute the Jacobian of the singular value decomposition is shown in Ref. 17, which is reviewed here. The derivatives of the singular values are given by

$$\frac{\partial \tilde{s}_k}{\partial \tilde{d}_{ij}} = \tilde{u}_{ik}\, \tilde{v}_{jk} \tag{106}$$

where $\tilde{s}_k$ is the k^{th} diagonal element of the matrix $\tilde{S}$, $\tilde{d}_{ij}$ is ij^{th} element of $\tilde{D}$, $\tilde{u}_{ik}$ is the ik^{th} element of $\tilde{U}$, and $\tilde{v}_{jk}$ is the jk^{th} element of $\tilde{V}$. To determine the partials of the matrices $\tilde{U}$ and $\tilde{V}$, first the following set of linear equations must be solved for $\omega^{ij}_{\tilde{U}_{k\ell}}$ and $\omega^{ij}_{\tilde{V}_{k\ell}}$:

$$\tilde{s}_\ell\, \omega^{ij}_{\tilde{U}_{k\ell}} + \tilde{s}_k\, \omega^{ij}_{\tilde{V}_{k\ell}} = \tilde{u}_{ik}\, \tilde{v}_{j\ell} \tag{107a}$$

$$\tilde{s}_k\, \omega^{ij}_{\tilde{U}_{k\ell}} + \tilde{s}_\ell\, \omega^{ij}_{\tilde{V}_{k\ell}} = -\tilde{u}_{i\ell}\, \tilde{v}_{jk} \tag{107b}$$

where $\omega^{ij}_{\tilde{U}_{k\ell}}$ and $\omega^{ij}_{\tilde{V}_{k\ell}}$ are the $k\ell^{\text{th}}$ elements of the skew symmetric matrices $\Omega^{ij}_{\tilde{U}}$ and $\Omega^{ij}_{\tilde{V}}$, respectively. Note because these matrix are skew symmetric then only the upper triangular elements need to be computed to determine the matrices. The partials are then given by

$$\frac{\partial \tilde{U}}{\partial \tilde{d}_{ij}} = \tilde{U}\, \Omega^{ij}_{\tilde{U}} \tag{108a}$$

$$\frac{\partial \tilde{V}}{\partial \tilde{d}_{ij}} = -\tilde{V}\, \Omega^{ij}_{\tilde{V}} \tag{108b}$$

More details can be found in Ref. 17.

The procedure to compute the partials can be computationally expensive. However, for the total least squares problem, only the partial of the last column of $\tilde{V}$, i.e. the vector $\tilde{\mathbf{p}}$, is required which significantly reduces the computations. Specifically only the last column of $\Omega^{ij}_{\tilde{V}}$ is required. The first step is to compute elements of the $(n+1)\times 1$ vector $\boldsymbol{\omega}^{ij} = [\omega^{ij}_1 \;\; \cdots \;\; \omega^{ij}_n \;\; 0]^T$, with

$$\omega^{ij}_k = \frac{1}{\tilde{s}_k^2 - \tilde{s}_{n+1}^2} (\tilde{s}_k\, \tilde{u}_{ik}\, \tilde{v}_{j\,n+1} + \tilde{s}_{n+1}\, \tilde{u}_{i\,n+1}\, \tilde{v}_{jk}) \tag{109}$$

for $k = 1, 2\ \ldots, n$. Then the following $(n+1)\times(n+1)$ matrix is formed:

$$\Omega_i \triangleq \left[\boldsymbol{\omega}^{i1} \,|\, \;\; \cdots \;\; |\, \boldsymbol{\omega}^{i\,n+1}\right] \tag{110}$$

Using the block diagonal structure of R allows Eq. (105) to be computed simply by

$$\tilde{B} = \tilde{V} \left[\sum_{i=1}^{m} \Omega_i\, \Omega_i^T\right] \tilde{V}^T \tag{111}$$

Partition the matrix $\tilde{B}$ into

$$\tilde{B} = \begin{bmatrix} \tilde{B}_{11} & \tilde{\mathbf{b}} \\ \\ \tilde{\mathbf{b}}^T & \tilde{b}_{22} \end{bmatrix} \tag{112}$$

where $\tilde{B}_{11}$ is an $n \times n$ matrix, $\tilde{\mathbf{b}}$ is an $n \times 1$ vector and $\tilde{b}_{22}$ is a scalar. Equation (100), evaluated using the tilde quantities, is now given by

$$P_{\mathrm{I}} = \tilde{v}_{22}^{-2} \left[\tilde{B}_{11} + \tilde{v}_{22}^{-2} \tilde{b}_{22} \tilde{\mathbf{v}}\, \tilde{\mathbf{v}}^T - \tilde{v}_{22}^{-1} (\tilde{\mathbf{b}}\, \tilde{\mathbf{v}}^T + \tilde{\mathbf{v}}\, \tilde{\mathbf{b}}^T) \right] \tag{113}$$

Then the error-covariance can now be computed using Eq. (102):

$$P = \tilde{v}_{22}^{-2} c_{22}^{-2} C_{11} \left[\tilde{B}_{11} + \tilde{v}_{22}^{-2} \tilde{b}_{22} \tilde{\mathbf{v}}\, \tilde{\mathbf{v}}^T - \tilde{v}_{22}^{-1} (\tilde{\mathbf{b}}\, \tilde{\mathbf{v}}^T + \tilde{\mathbf{v}}\, \tilde{\mathbf{b}}^T) \right] C_{11}^T \tag{114}$$

In the error-covariance approximation the "measured" quantities are used in place of the true variables. Instead, the estimated values can be used. Note that Eq. (95) is equal to $\hat{D} = \tilde{U} \tilde{\tilde{S}} \tilde{V}^T C$, where $\tilde{\tilde{S}}$ is given by $\tilde{S}$ with $\tilde{s}_{n+1} = 0$. Therefore, Eq. (109) can be approximated by setting $\tilde{s}_{n+1} = 0$, which yields the following expression:

$$\omega_k^{ij} = \tilde{u}_{ik}\, \tilde{v}_{j\,n+1} / \tilde{s}_k \tag{115}$$

Define $\tilde{U}_n$ from Eq. (95) by its rows:

$$\tilde{U}_n = \begin{bmatrix} \tilde{\mathbf{u}}_1^T \\ \mathbf{u}_2^T \\ \vdots \\ \tilde{\mathbf{u}}_m^T \end{bmatrix} \tag{116}$$

Using Eqs. (115) and (116) allows Ω_i to be simply written by

$$\Omega_i = \begin{bmatrix} \tilde{\mathbf{v}} \\ \tilde{v}_{22} \end{bmatrix}^T \otimes \begin{bmatrix} \tilde{S}_n^{-1} \tilde{\mathbf{u}}_i \\ 0 \end{bmatrix} \tag{117}$$

where $\tilde{S}_n$ is defined in Eq. (95). Using Eq. (117) to compute Ω_i reduces the computational load while still producing accurate results. The error-covariance in Eq. (114) is valid for any sample size under the small noise assumption. Both Eqs. (96) and (114) require a summation of terms over m, but Eq. (114) does not require a matrix inverse of an $n \times n$ matrix to compute the error-covariance. Thus Eq. (114) is preferred over the inverse of Eq. (96) to compute the error-covariance.

A sequential algorithm for the TLS estimate involving the element-wise uncorrelated and stationary case is possible. Denote the point m by $k+1$. Suppose that the TLS algorithm is executed on data up to and including point k, and denote the estimate at that point by $\hat{\mathbf{x}}_k$. Next, suppose that a new set of data, denoted by $\tilde{\mathbf{d}}_{k+1}$, is now available. Then append the matrix $\tilde{D} C^{-1}$ with a new row $\tilde{\mathbf{d}}_{k+1}^T C^{-1}$. A sequential solution can be obtained using an SVD update of the appended matrix[18] to yield the estimate at point $k+1$, denoted by $\hat{\mathbf{x}}_{k+1}$. Several alternatives to this approach are shown in Ref. 19, two of which are now summarized. Using a small batch up to some point k, perform a QR decomposition on the matrix $\tilde{D} C^{-1}$. Denote the resulting R matrix from this composition as R_k. Using a new set of data $\tilde{\mathbf{d}}_{k+1}$ form the following $1 \times (n+1)$ vector:

$$\mathbf{s}^T = -\tilde{\mathbf{d}}_{k+1}^T R_k \tag{118}$$

Next perform a QR decomposition on the vector $[1 \;\; \mathbf{s}^T]^T$ and denote the resulting $(n+2) \times (n+2)$ Q matrix by Q_{k+1}. Then update R_k^{-1} to obtain R_{k+1}^{-1} by

$$\begin{bmatrix} \mathbf{p} & R_{k+1}^{-1} \end{bmatrix} = \begin{bmatrix} \mathbf{0}_{(n+1)\times 1} & R_k^{-1} \end{bmatrix} Q_{k+1} \tag{119}$$

where $\mathbf{0}_{(n+1)\times 1}$ is an $(n+1) \times 1$ vector of zeros and $\mathbf{p}$ is an $(n+1) \times 1$ vector not needed for the solution. Then perform an SVD decomposition on the matrix R_{k+1} and compute $\hat{\mathbf{x}}_{\mathrm{I}_{k+1}}$ using Eq. (93) employing the V matrix from the resulting SVD decomposition of R_{k+1}. Finally, compute $\hat{\mathbf{x}}_{k+1}$ using Eq. (94) so that

$$\hat{\mathbf{x}}_{k+1} = c_{22}^{-1} (C_{11} \hat{\mathbf{x}}_{\mathrm{I}_{k+1}} - \mathbf{c}) \tag{120}$$

An approximate solution is also possible that does not involve an SVD decomposition. Using R_{k+1}^{-1} form the following matrix:

$$E_{k+1} = R_{k+1}^{-1} R_{k+1}^{-T} = \begin{bmatrix} E_{11_{k+1}} & \mathbf{e}_{k+1} \\ \\ \mathbf{e}_{k+1}^T & e_{22_{k+1}} \end{bmatrix} \tag{121}$$

where $E_{11_{k+1}}$ is an $n \times n$ matrix, $\mathbf{e}_{k+1}$ is an $n \times 1$ vector and $e_{22_{k+1}}$ is a scalar. Using the previous estimate $\hat{\mathbf{x}}_{\mathrm{I}_k}$ the new estimate is approximated by

$$\hat{\mathbf{x}}_{\mathrm{I}_{k+1}} = \frac{\mathbf{e}_{k+1} - E_{11_{k+1}} \hat{\mathbf{x}}_{\mathrm{I}_k}}{\mathbf{e}_{k+1}^T \hat{\mathbf{x}}_{\mathrm{I}_k} - e_{22_{k+1}}} \tag{122}$$

This approximation is very good if $\hat{\mathbf{x}}_{\mathrm{I}_{k+1}}$ is close to $\hat{\mathbf{x}}_{\mathrm{I}_k}$, otherwise an iteration is required.[19] Equation (120) is then used to compute the TLS estimate.

A sequential covariance expression can be derived from Eq. (120) using the SVD solution or the approximate solution given by Eq. (122), however a simpler and less computationally expensive approach uses the Fisher information directly. The FIM using data up to and including the point k is given by

$$F_k = \sum_{i=1}^{k} \frac{\mathbf{h}_i \mathbf{h}_i^T}{\mathbf{z}_k^T \mathcal{R}\, \mathbf{z}_k} \tag{123}$$

Then the FIM using data up to and including the point $k+1$ is given by

$$F_{k+1} = \frac{\mathbf{h}_{k+1} \mathbf{h}_{k+1}^T}{\mathbf{z}_{k+1}^T \mathcal{R}\, \mathbf{z}_{k+1}} + F_k \tag{124}$$

Using $P_k = F_k^{-1}$ and applying the matrix inversion lemma on Eq. (124) yields

$$P_{k+1} = \left(I_{n\times n} - \frac{P_k \mathbf{h}_{k+1} \mathbf{h}_{k+1}^T}{\mathbf{h}_{k+1}^T P_k \mathbf{h}_{k+1} + \mathbf{z}_{k+1}^T \mathcal{R}\, \mathbf{z}_{k+1}} \right) P_k \tag{125}$$

Equation (125) requires an inverse of a scalar quantity and thus is computationally efficient. Once again the estimated or measured values are used to compute P_{k+1} in practice.

IV. Examples

This section shows four examples. The first two involve curve fitting a set of data with one case involving stationary noise processes and the other case involving non-stationary noise processes. The next example involves a robot navigation problem. The last example involves bearings-only estimation with uncertain base points.

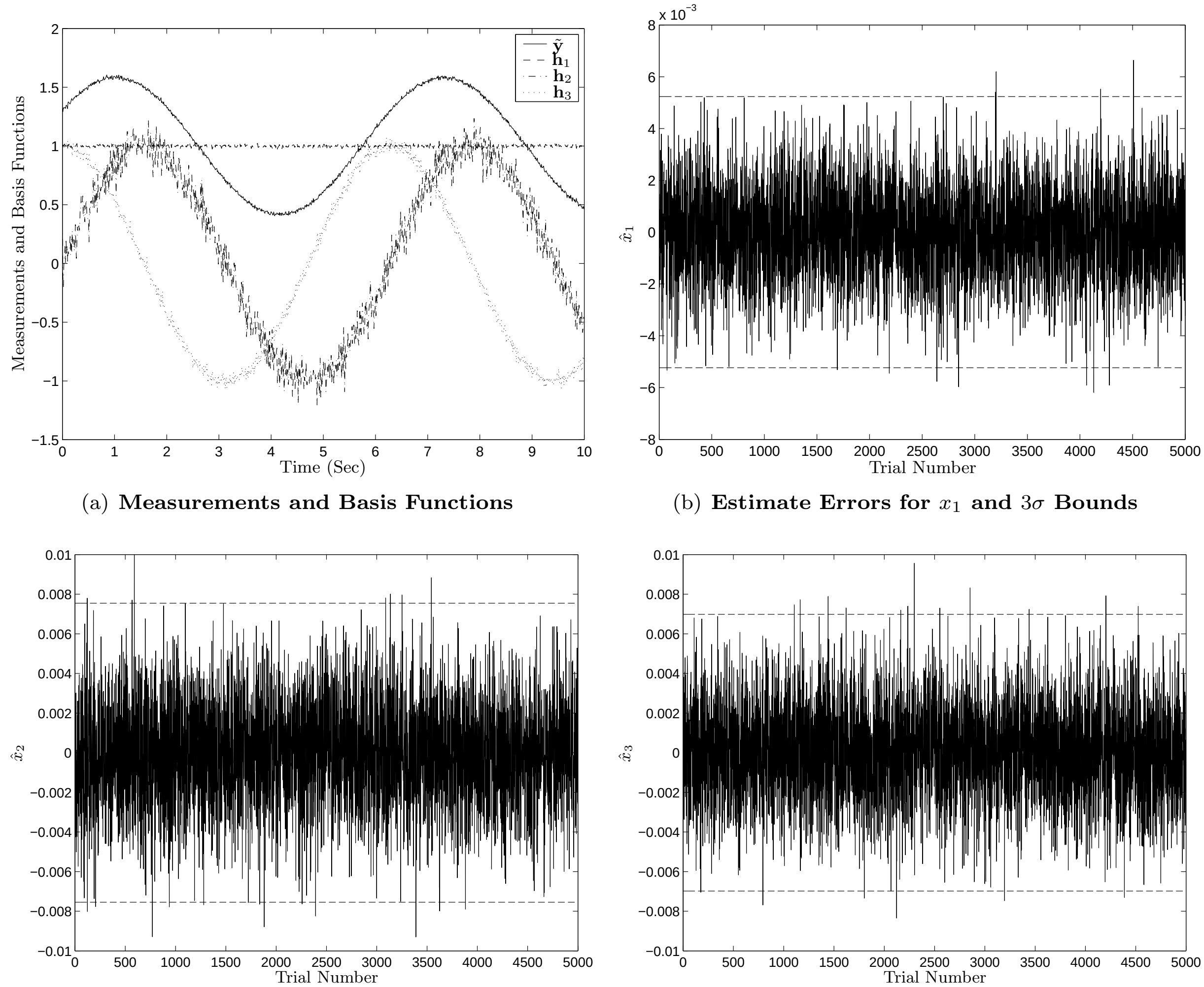
A. Curve Fitting with Stationary Errors

An example is shown here that involves using total least squares to estimate the coefficients of a polynomial function with stationary errors. The true H and $\mathbf{x}$ quantities are given by

$$H = \begin{bmatrix} 1 & \sin(t) & \cos(t) \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} 1 \\ 0.5 \\ 0.3 \end{bmatrix} \tag{126}$$

A fully populated $\mathcal{R}$ matrix is used in this example, with

$$\mathcal{R} = \begin{bmatrix} 1\times10^{-4} & 1\times10^{-6} & 1\times10^{-5} & 1\times10^{-9} \\ 1\times10^{-6} & 1\times10^{-2} & 1\times10^{-7} & 1\times10^{-6} \\ 1\times10^{-5} & 1\times10^{-7} & 1\times10^{-3} & 1\times10^{-6} \\ 1\times10^{-9} & 1\times10^{-6} & 1\times10^{-6} & 1\times10^{-4} \end{bmatrix} \tag{127}$$



(a) **Measurements and Basis Functions**

(b) **Estimate Errors for x_1 and 3σ Bounds**

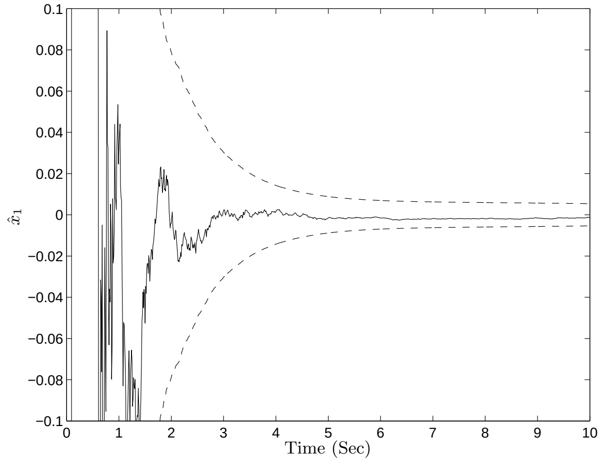
(c) **Estimate Errors for x_2 and 3σ Bounds**

(d) **Estimate Errors for x_3 and 3σ Bounds**

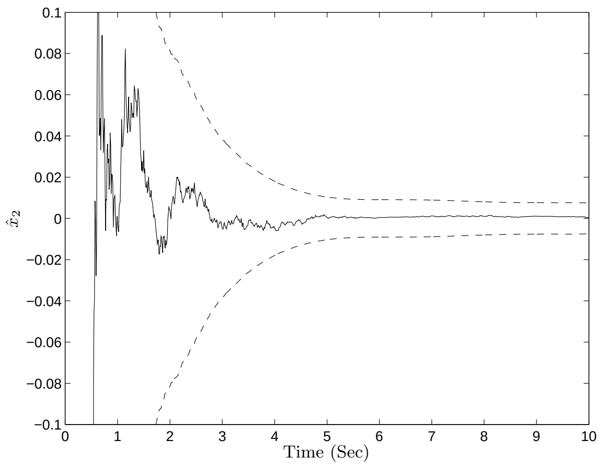
Figure 1. Total Least Squares Simulation Results: Stationary Case

Synthetic measurements are generated using a sampling interval of 0.01 seconds to a final time of 10 seconds. The estimate is determined using Eq. (94) and the error-covariance is determined using Eq. (114).

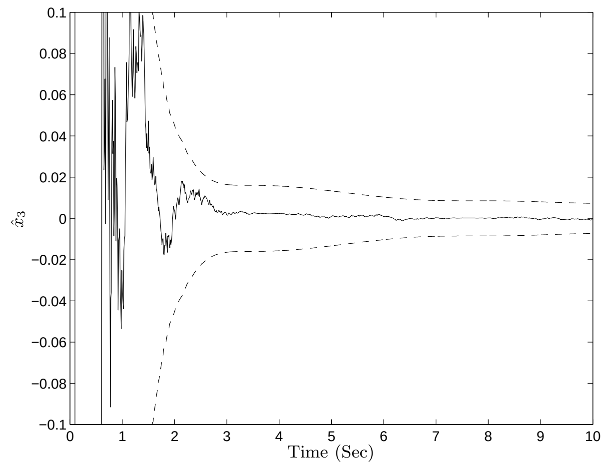
Five thousand Monte Carlo runs are executed in order to compare the actual errors with the computed 3σ bounds using Eq. (114). Figure 1(a) shows the measurements and basis functions with errors. The signal-noise-ratios are modest for this example. Figures 1(b)−1(d) show the errors for the estimates along with their respective computed 3σ bounds. This indicates that Eq. (114) can be used to accurately compute the 3σ bounds. Also, the error-covariance obtained using the inverse of Eq. (96) matches the one obtained using Eq. (114) as expected. A sequential TLS algorithm has also been executed using a batch of the first 10 points to initialize the estimate and error-covariance. Plots of the estimation errors and associated 3σ bounds, computed using Eq. (125), for a single Monte Carlo run are shown in Figures 2(a)−2(c). The computed 3σ clearly bound the actual estimation errors.



(a) **Estimate Errors for x_1 and 3σ Bounds**



(b) **Estimate Errors for x_2 and 3σ Bounds**



(c) **Estimate Errors for x_3 and 3σ Bounds**

Figure 2. Sequential Estimation Errors

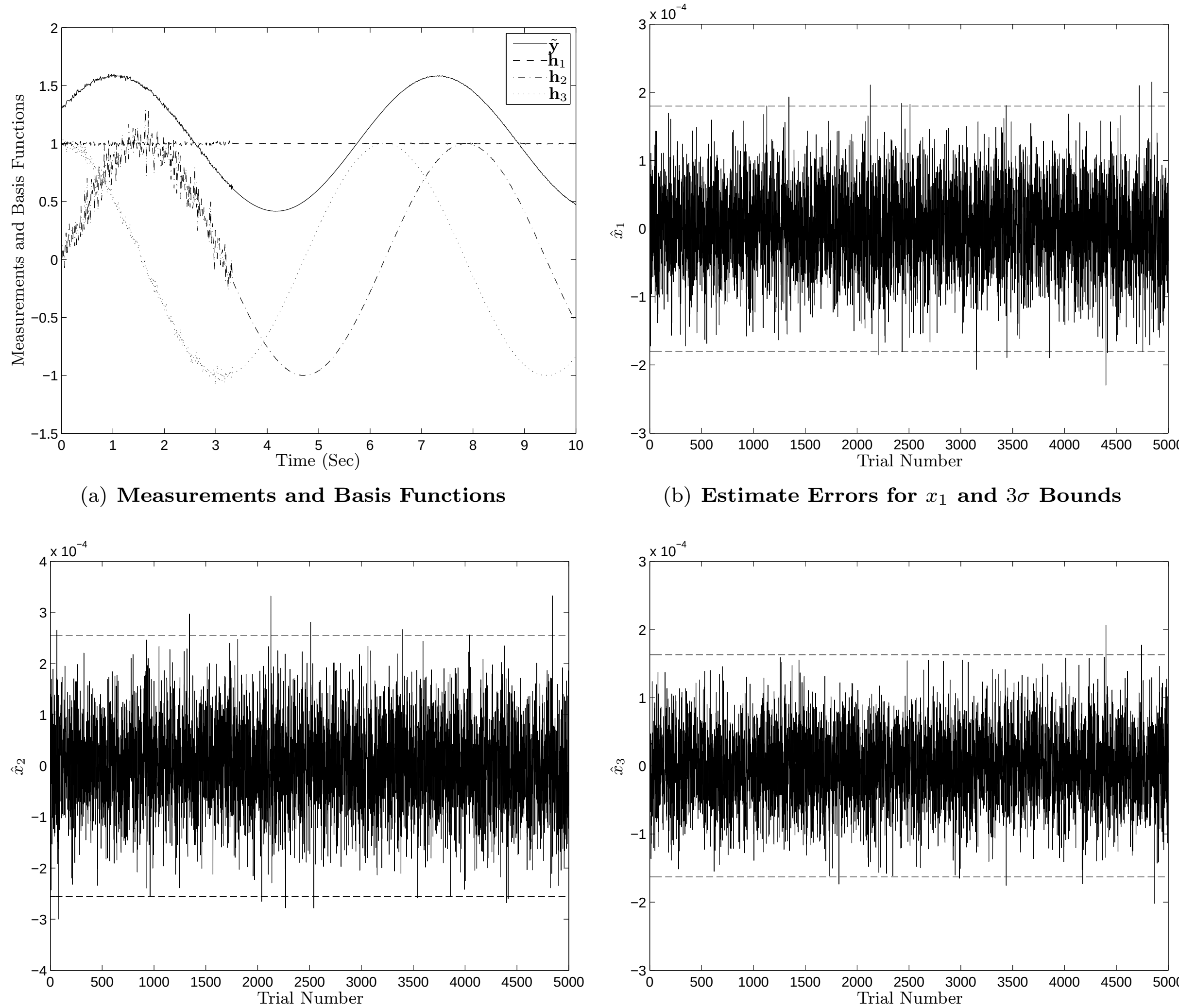
B. Curve Fitting with Non-Stationary Errors

This example is equivalent to the previous one except that a non-stationary process for the errors is used. Three covariance matrices are used, given by

$$\mathcal{R}_1 = \begin{bmatrix} 1\times10^{-4} & 1\times10^{-6} & 1\times10^{-5} & 1\times10^{-9} \\ 1\times10^{-6} & 1\times10^{-2} & 1\times10^{-7} & 1\times10^{-6} \\ 1\times10^{-5} & 1\times10^{-7} & 1\times10^{-3} & 1\times10^{-6} \\ 1\times10^{-9} & 1\times10^{-6} & 1\times10^{-6} & 1\times10^{-4} \end{bmatrix} \tag{128a}$$

$$\mathcal{R}_2 = \begin{bmatrix} 2\times10^{-7} & 8\times10^{-9} & 4\times10^{-8} & 3\times10^{-8} \\ 8\times10^{-9} & 1\times10^{-6} & 3\times10^{-9} & 2\times10^{-9} \\ 4\times10^{-8} & 3\times10^{-9} & 2\times10^{-7} & 5\times10^{-10} \\ 3\times10^{-8} & 2\times10^{-9} & 5\times10^{-10} & 4\times10^{-8} \end{bmatrix} \tag{128b}$$

$$\mathcal{R}_3 = \begin{bmatrix} 6\times10^{-6} & 1\times10^{-6} & 4\times10^{-7} & 4\times10^{-7} \\ 1\times10^{-6} & 3\times10^{-6} & 8\times10^{-7} & 2\times10^{-6} \\ 4\times10^{-7} & 8\times10^{-7} & 3\times10^{-6} & 4\times10^{-7} \\ 4\times10^{-7} & 2\times10^{-6} & 4\times10^{-7} & 4\times10^{-6} \end{bmatrix} \tag{128c}$$



(a) **Measurements and Basis Functions**

(b) **Estimate Errors for x_1 and 3σ Bounds**

(c) **Estimate Errors for x_2 and 3σ Bounds**

(d) **Estimate Errors for x_3 and 3σ Bounds**

Figure 3. Total Least Squares Simulation Results: Non-Stationary Case

The first covariance is used for the first 330 points, the second covariance is used for the next 330 points and the third is used for the remaining points. A plot of the measurements and noisy basis functions is shown in Figure 3(a). As shown by $\mathcal{R}_2$ and $\mathcal{R}_3$ the measurements and basis functions contain significantly lower errors after the first 330 points. The estimate is determined using the iteration procedure shown by Eq. (28) and the error-covariance is determined using Eq. (74), where $\tilde{\mathbf{h}}_i$ is used in place of $\mathbf{h}_i$ and $\hat{\mathbf{z}}$ is used in place of $\mathbf{z}$. Figures 3(b)−3(d) show the errors for the estimates along with their respective computed 3σ bounds. This indicates that Eq. (54) can be used to accurately compute the 3σ bounds for non-stationary errors. The computed error-covariance is given by

$$P = \begin{bmatrix} 3.5916 \times 10^{-9} & 3.9664 \times 10^{-9} & -1.0948 \times 10^{-9} \\ 3.9664 \times 10^{-9} & 7.2525 \times 10^{-9} & -1.2931 \times 10^{-9} \\ -1.0948 \times 10^{-9} & -1.2931 \times 10^{-9} & 2.9468 \times 10^{-9} \end{bmatrix} \tag{129}$$

This matches with the sample error-covariance obtained from the Monte Carlo runs.

The error-covariance using the average of the three covariances for $\mathcal{R}$ in Eq. (114), denoted now by $\bar{P}$, is given by

$$\bar{P} = \begin{bmatrix} 1.0082\times10^{-6} & -3.8986\times10^{-7} & 1.1420\times10^{-7} \\ -3.8986\times10^{-7} & 2.0963\times10^{-6} & -9.7655\times10^{-8} \\ 1.1420\times10^{-7} & -9.7655\times10^{-8} & 1.7888\times10^{-6} \end{bmatrix} \tag{130}$$

Clearly Eq. (129) does not match Eq. (130). This shows that the effect of using a non-stationary process can be profound on the estimation accuracy. It should also be noted that the left-hand side of the inequality in Eq. (79) is five orders of magnitude larger than the right-hand side of Eq. (79) for this case. Thus, using the measured quantities to compute the error-covariance is valid. Another simulation involving only 11 samples, using a sampling interval of 1 second, has also been done. It is found that even with 11 samples the error-covariance in Eq. (74) provides good 3σ bounds. So for this particular simulation case the error-covariance expression assuming an asymptotically efficient condition for the Cramér-Rao lower bound is valid even for a small sample size, which matches the theoretically proven results leading to Eq. (74).

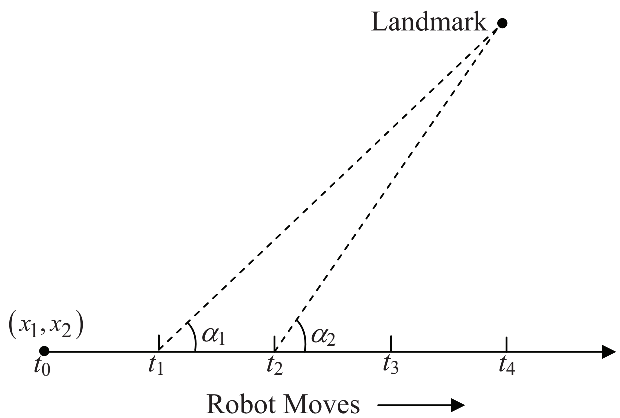


Figure 4. Robot Navigation Problem

C. Robot Navigation

This example uses total least squares to determine the best estimate of a robot's position.[20] A diagram of the simulated robot example is shown in Figure 4. It is assumed that the robot has identified a single landmark with known location in a two-dimensional environment. The robot moves along some straight line with a measured uniform velocity. The goal is to estimate the robot's starting position, denoted by $(x_1,\, x_2)$, relative to the landmark. The landmark is assumed to be located at (0, 0) meters. Angle observations, denoted by α_i, between its direction of heading and the landmark are provided. The angle observation equation follows

$$\cot(\alpha_i) = \frac{x_1 + t_i\, v}{x_2} \tag{131}$$

where t_i is the time at the i^{th} observation time and v is the velocity. The TLS model is given by

$$\mathbf{h}_i = \begin{bmatrix} -1 \\ \cot(\alpha_i) \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad y_i = t_i v \tag{132}$$

so that $y_i = \mathbf{h}_i^T\mathbf{x}$. Measurements of both α_i and v are given by

$$\tilde{\alpha}_i = \alpha_i + \delta\alpha_i \tag{133a}$$

$$\tilde{v}_i = v + \delta v_i \tag{133b}$$

where $\delta\alpha_i$ and δv_i are zero-mean Gaussian white-noise processes with variances σ_α^2 and σ_v^2, respectively. The variances of both the errors in $\cot(\tilde{\alpha}_i)$ and $\tilde{y}_i = t_i\tilde{v}_i$ are required. Assuming $\delta\alpha_i$ is small then the following approximation can be used:

$$\cot(\alpha_i + \delta\alpha_i) \approx \frac{1 - \delta\alpha_i \tan(\alpha_i)}{\tan(\alpha_i) + \delta\alpha_i} \tag{134}$$

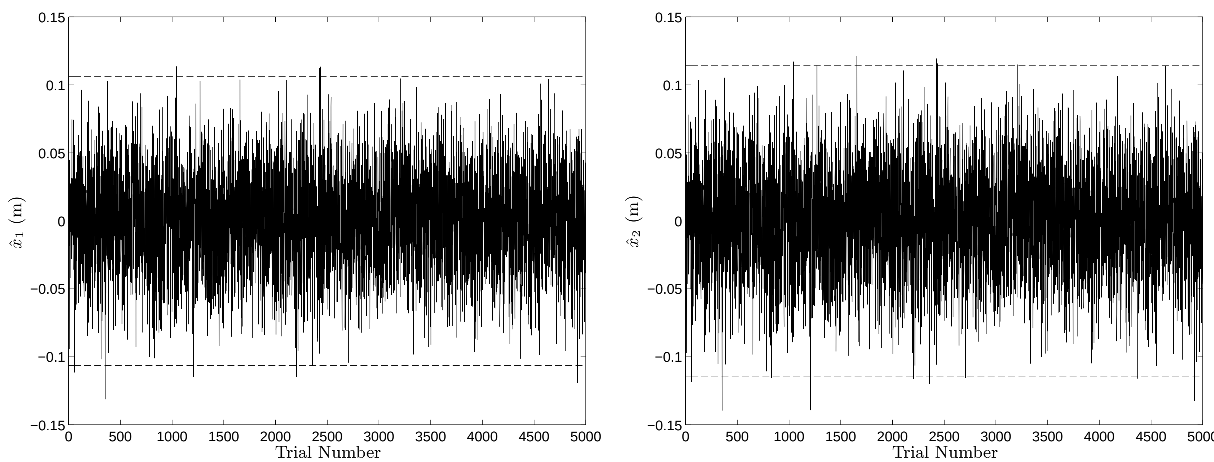
Using the binomial series for a first-order expansion of $(\tan(\alpha_i) + \delta\alpha_i)^{-1}$ leads to

$$
\begin{aligned}
\cot(\alpha_i + \delta\alpha_i) &\approx \frac{[1 - \delta\alpha_i \tan(\alpha_i)][1 - \delta\alpha_i \cot(\alpha_i)]}{\tan(\alpha_i)} \\
&= \cot(\alpha_i) - \delta\alpha_i \csc^2(\alpha_i) + \delta\alpha_i^2 \cot(\alpha_i)
\end{aligned}
\tag{135}
$$

Hence, the variance of the errors for $\cot(\tilde{\alpha}_i)$ is given by $\sigma_\alpha^2 \csc^4(\alpha_i) + 3\sigma_\alpha^4 \cot^2(\alpha_i)$. The variance of the errors for $\tilde{y}_i$ is simply given by $t_i^2 \sigma_v^2$, which grows in time. Therefore, the matrix $\mathcal{R}_i$ is given by

$$
\mathcal{R}_i = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \sigma_\alpha^2 \csc^4(\alpha_i) + 3\sigma_\alpha^4 \cot^2(\alpha_i) & 0 \\ 0 & 0 & t_i^2 \sigma_v^2 \end{bmatrix}
\tag{136}
$$

Since this varies with time the non-stationary TLS solution must be employed. The estimate is determined using the iteration procedure shown by Eq. (28) and the error-covariance is determined using Eq. (74), where $\tilde{\mathbf{h}}_i$ is used in place of $\mathbf{h}_i$ and $\hat{\mathbf{z}}$ is used in place of $\mathbf{z}$. The true values for α_i are also replaced with their respective measured ones to compute $\mathcal{R}_i$ in Eq. (136). Also, note that this matrix is singular but does not cause any issues in the TLS solution.



(a) **Estimate Errors for x_1 and 3σ Bounds**

(b) **Estimate Errors for x_2 and 3σ Bounds**

Figure 5. Robot Estimation Errors

In the simulation the location of the robot at the initial time is given by $(-10, -10)$ meters and its velocity is given by 1 m/s. The variances are given by $\sigma_\alpha^2 = (0.1\pi/180)^2$ rad^2 and $\sigma_v^2 = 0.01$ m^2/s^2. The final time of the simulation run is 10 seconds and measurements of α and v are taken at 0.01 second intervals. Five thousand Monte Carlo runs are executed in order to compare the actual errors with the computed 3σ bounds using Eq. (74). Figures 5(a) and 5(b) show the errors for the estimates along with their respective computed 3σ bounds. This indicates that Eq. (74) can be used to accurately compute the 3σ bounds. Also, although not shown here, the computed error-covariance using Eq. (74) matches with the sample error-covariance obtained from the Monte Carlo runs.

D. Bearings-Only Point Estimation

Total least squares is applied to estimate the two-dimensional location of a stationary target point using passive bearing measurements. The TLS problem is formulated in Ref. 21, however only stationary errors are assumed. Here a more rigorous development is derived. The problem geometry is depicted in Figure 6. The goal is to estimate the point p from bearings-only measurements, denoted by $\tilde{\theta}_i$. The baseline points, denoted by X_i and Y_i, are assumed to be imprecisely known. The bearing measurement model and baseline

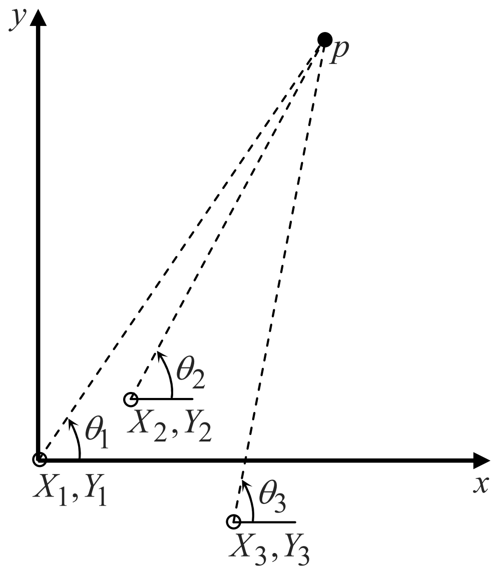


Figure 6. Two-Dimensional Bearings-Only Geometry

point models are given by

$$\tilde{\theta}_i = \theta_i + \delta\theta_i \tag{137a}$$
$$\tilde{X}_i = X_i + \delta X_i \tag{137b}$$
$$\tilde{Y}_i = Y_i + \delta Y_i \tag{137c}$$

where $\delta\theta_i$, δX_i and δY_i are zero-mean Gaussian noise processes with variances $\sigma^2_{\theta_i}$, $\sigma^2_{X_i}$ and $\sigma^2_{Y_i}$, respectively. The observations are modeled as

$$\theta_i = \tan^{-1}\left(\frac{y - Y_i}{x - X_i}\right) \tag{138}$$

Taking the tangent of both sides of Eq. (138) leads to $y_i = \mathbf{h}_i^T \mathbf{x}$, with

$$y_i = -X_i \sin(\theta_i) + Y_i \cos(\theta_i) \tag{139a}$$
$$\mathbf{h}_i = [-\sin(\theta_i) \quad \cos(\theta_i)]^T \tag{139b}$$
$$\mathbf{x} = [x \;\; y]^T \tag{139c}$$

Replacing the true values with the measured values and using the first-order approximations $\sin(\theta_i + \delta\theta_i) = \sin(\theta_i) + \delta\theta_i \cos(\theta_i)$ and $\cos(\theta_i + \delta\theta_i) = \cos(\theta_i) - \delta\theta_i \sin(\theta_i)$, yields the following expressions for $\tilde{y}_i$ and $\tilde{\mathbf{h}}_i$:

$$\begin{aligned} \tilde{y}_i &= -\tilde{X}_i \sin(\tilde{\theta}_i) + \tilde{Y}_i \cos(\tilde{\theta}_i) \\ &= -X_i \sin(\theta_i) + Y_i \cos(\theta_i) - \delta\theta_i X_i \cos(\theta_i) - \delta X_i \sin(\theta_i) - \delta\theta_i \delta X_i \cos(\theta_i) \\ &\quad - \delta\theta_i Y_i \sin(\theta_i) + \delta Y_i \cos(\theta_i) - \delta\theta_i \delta Y_i \sin(\theta_i) \end{aligned} \tag{140a}$$

$$\begin{aligned} \tilde{\mathbf{h}}_i &= [-\sin(\tilde{\theta}_i) \quad \cos(\tilde{\theta}_i)]^T \\ &= [-\sin(\theta_i) - \delta\theta_i \cos(\theta_i) \quad \cos(\theta_i) - \delta\theta_i \sin(\theta_i)]^T \end{aligned} \tag{140b}$$

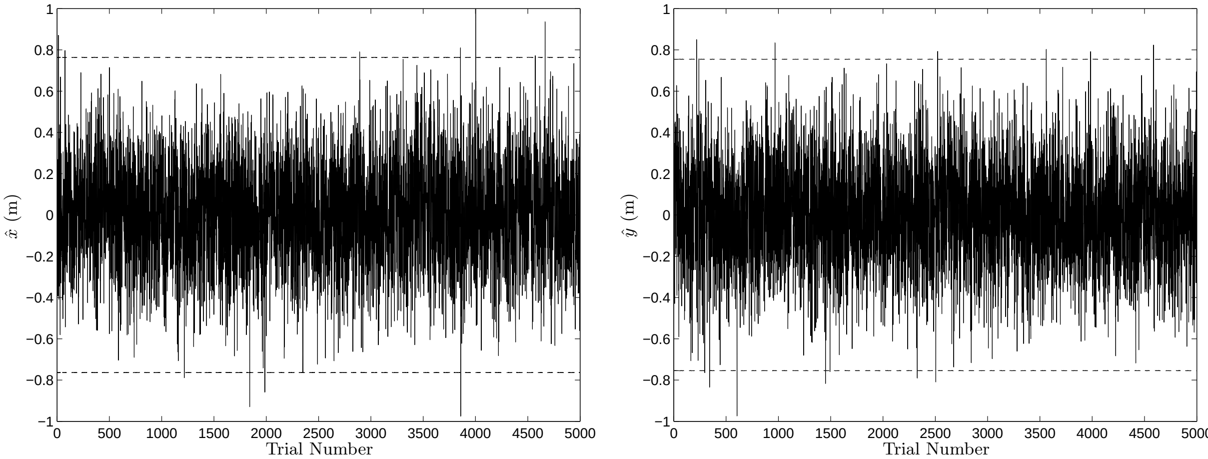
Then the elements of the covariance matrix $\mathcal{R}_i$ are computed to be

$$\mathcal{R}_{yy_i} = \sigma^2_{\theta_i}\{[X_i \cos(\theta_i) + Y_i \sin(\theta_i)]^2 + \sigma^2_{X_i} \cos^2(\theta_i) + \sigma^2_{Y_i} \sin^2(\theta_i)\} + \sigma^2_{X_i} \sin^2(\theta_i) + \sigma^2_{Y_i} \cos^2(\theta_i) \tag{141a}$$

$$\mathcal{R}_{hh_i} = \sigma^2_{\theta_i} \begin{bmatrix} \cos^2(\theta_i) & \sin(\theta_i)\cos(\theta_i) \\ \sin(\theta_i)\cos(\theta_i) & \sin^2(\theta_i) \end{bmatrix} \tag{141b}$$

$$\mathcal{R}_{hy_i} = \sigma^2_{\theta_i} [X_i \cos(\theta_i) + Y_i \sin(\theta_i)] \begin{bmatrix} \cos(\theta_i) \\ \sin(\theta_i) \end{bmatrix} \tag{141c}$$

Note that the covariance matrix does not contain the true locations x and y, unlike other approaches to this problem.[22,23] As before the true values can be replaced with the measured ones to compute the covariance matrix in practice.



(a) **Estimate Errors for x and 3σ Bounds** (b) **Estimate Errors for y and 3σ Bounds**

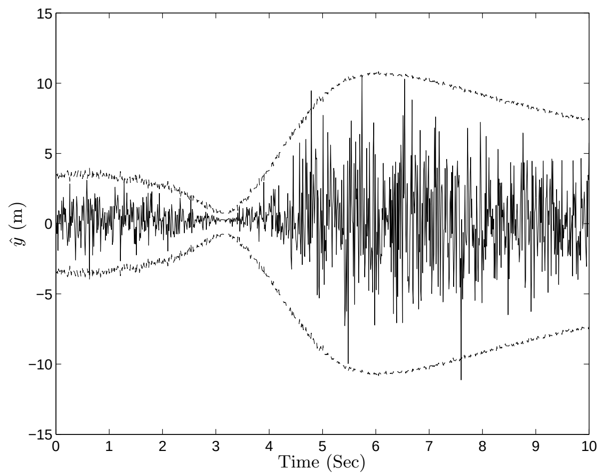
Figure 7. Total Least Squares Bearings-Only Estimation Errors

In the simulation the location of the point p is given at (100, 200) meters. The baseline points are time varying with $X_i = 500\sin(0.01\,t_i)$ and $Y_i = 300\cos(0.2\,t_i)$. The variances are given by $\sigma^2_{\theta_i} = (1\pi/180)^2$ rad^2 and $\sigma^2_{X_i} = \sigma^2_{Y_i} = 25$ m^2 for all i points. The final time of the simulation run is 10 seconds and measurements of $\tilde{\theta}_i$, $\tilde{X}_i$ and $\tilde{Y}_i$ are taken at 0.01 second intervals. Five thousand Monte Carlo runs are executed in order to compare the actual errors with the computed 3σ bounds using Eq. (74). The TLS initial estimate is given by using a standard linear least squares solution with the measurement variance given by Eq. (141a). Figures 7(a) and 7(b) show the errors for the TLS estimates along with their respective computed 3σ bounds. This indicates that Eq. (74) can be used to accurately compute the 3σ bounds. Also, although not shown here, the computed error-covariance using Eq. (74) matches with the sample error-covariance obtained from the Monte Carlo runs. A plot of the output errors and 3σ bounds computed using Eq. (85) for one of the Monte Carlo runs is shown in Figure 8(a). Also plots of the basis function errors and 3σ bounds computed using Eq. (83) are shown in Figures 8(b) and 8(c). Clearly, the derived covariance expressions provide accurate bounds for the actual errors.

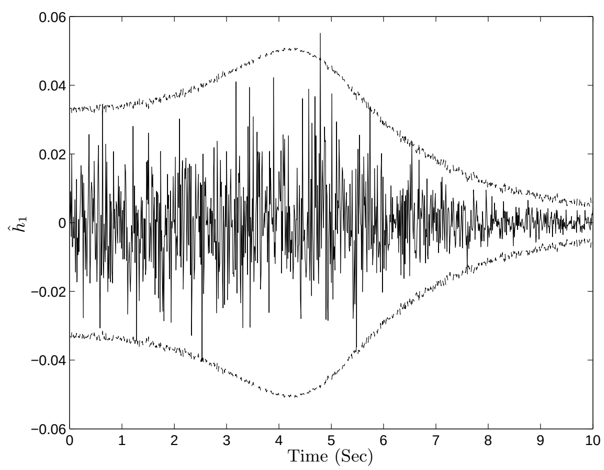
A comparison is made using the standard linear least squares solution with its associated error-covariance. Figures 9(a) and 9(b) show the errors for the linear least squares estimates along with their respective computed 3σ bounds. Comparing these figures to the TLS errors in Figures 7(a) and 7(b) indicates that the linear least squares solution is not optimal and even biased, as discussed in Ref. 21. Clearly the errors in the basis function matrix can cause significant errors if a linear least squares solution is employed over a TLS solution.

V. Conclusions

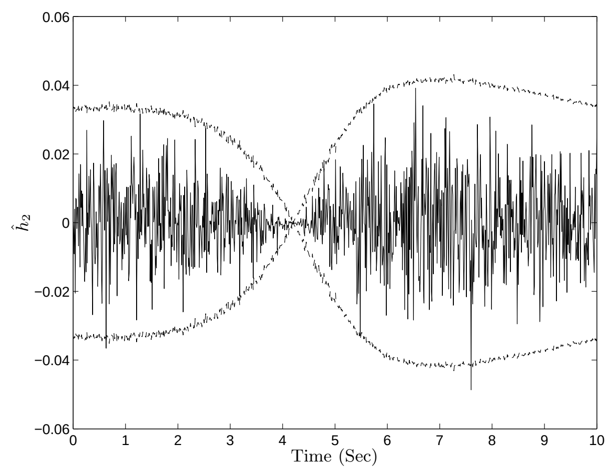
The error-covariances derived here for the total least squares problem provide useful measures to quantify the expected errors in the estimates. A perturbation analysis showed that the derived error-covariance from the associated loss function achieves the Cramér-Rao lower bound. Thus the total least squares estimator is an efficient estimator. An expression for the error-covariance for stationary errors was derived using a perturbation of the closed-form solution. This expression is useful because it does not require a matrix inverse. Simulation results showed that the derived error-covariance expressions provide accurate bounds for the estimate errors.



(a) **Estimate Errors for y and 3σ Bounds**

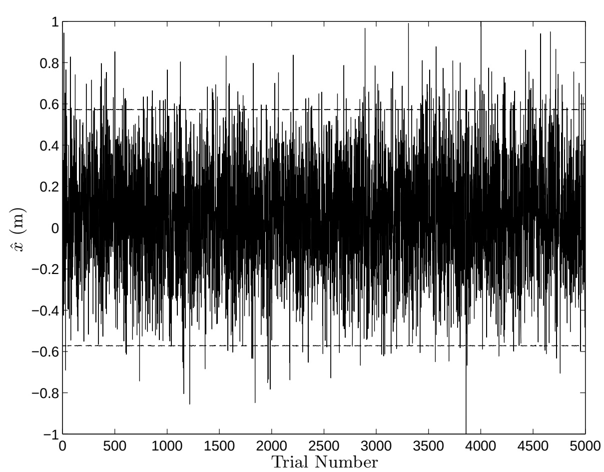


(b) **Estimate Errors for h_1 and 3σ Bounds**

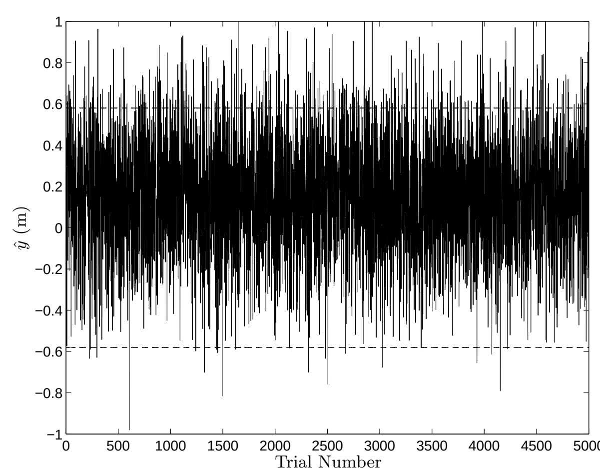


(c) **Estimate Errors for h_2 and 3σ Bounds**

Figure 8. Output and Basis Function Estimation Errors



(a) **Estimate Errors for x and 3σ Bounds**



(b) **Estimate Errors for y and 3σ Bounds**

Figure 9. Linear Least Squares Bearings-Only Estimation Errors

VI. Acknowledgments

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