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Generalized source-conditions and uncertainty bounds for deconvolution problems

JD Rezac¹, A Dienstfrey¹, N Vlajic², and A Chijioke², PD Hale¹

¹National Institute of Standards and Technology, Boulder CO, USA

²National Institute of Standards and Technology, Gaithersburg MD, USA

E-mail: jacob.rezac@nist.gov, andrew.dienstfrey@nist.gov, paul.hale@nist.gov, nicholas.vlajic@nist.gov, akobuije.chijioke@nist.gov

Abstract. Many problems in time-dependent metrology can be phrased mathematically as a deconvolution problem. In such a problem, measured data is modeled as the convolution of a known system response function with an unknown source signal. The goal of deconvolution is to estimate the unknown source signal given knowledge about the system response function. A well-studied method for calculating this estimate is Tikhonov regularized deconvolution which attempts to balance the average difference between the estimated solution and true source signal with the variance in the estimated solution. In this article we study this so-called biasvariance tradeoff in the context of estimating a source measured by a high speed oscilloscope. By assuming we have bounds on the true source's Fourier coefficients and a structural model for the uncertainties in the system response function, we derive pointwise-in-time confidence intervals on the true signal based on the estimated signal. We demonstrate the new technique with simulations relevant to the high speed measurement context.

1. Introduction

Time-dependent measurands are becoming increasingly important in metrology as practitioners move away from parameter-dependent descriptions of measurands and towards a characterization of the functional form of the time-varying signal. Such models are useful in a number of measurement applications such as pressure, force, and torque metrology, and measurement of high speed waveforms used for communication systems [2]. In this article, we discuss the measurement of time-dependent objects using linear time invariant systems. Ideally, this process is modeled as

$$y_{*}(t) = \int_{-\infty}^{\infty} a_{*}(t-\tau) x_{*}(\tau) \,\mathrm{d}\tau,$$
(1)

where $y_*(t)$ indicates noise-free output, $a_*(t)$ is the system response, and $x_*(t)$ is the input signal. Equation (1) is unreasonable in practice as measurements contain noise and the system response is itself also subject to uncertainty. A more complete continuous model is

$$y(t) = \int_{-\infty}^{\infty} a(t-\tau)x(\tau) \,\mathrm{d}\tau = y_*(t) + n(t), \tag{2}$$

where $a(t) \approx a_*(t)$ represents uncertainty on the system response and n(t) represents additive noise. In practice it is natural to work with discrete samples in time. We write the discrete

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problem as a matrix system

$$\mathbf{y} = \mathbf{A}\mathbf{x} = \mathbf{A}_*\mathbf{x}_* + \boldsymbol{\delta} + \mathbf{n},\tag{3}$$

where $\boldsymbol{\delta}$ represents discretization error, and $\mathbf{y} = [y(t_0), y(t_1), \dots, y(t_N)]^T$ is a vector composed of measured data (and similarly for \mathbf{x} and \mathbf{n}). For simplicity we set $\boldsymbol{\delta} = \mathbf{0}$.

The deconvolution problem we treat below is to estimate $x_*(t)$ given measurements of y(t)and a(t). Deconvolution is notoriously unstable, and some form of regularization is needed to stabilize the inversion in the presence of noise. The Tikhonov formalism used henceforth defines a one-parameter family of estimates $\hat{\mathbf{x}}_{\lambda}$ given by

$$\hat{\mathbf{x}}_{\lambda} = \left(\mathbf{A}^T \mathbf{A} + \lambda^2 \mathbf{L}^T \mathbf{L}\right)^{-1} \mathbf{A}^T \mathbf{y} = \mathbf{A}_{\lambda}^{\dagger} \mathbf{y}$$
(4)

in which an auxiliary penalty operator \mathbf{L} is used to impose prior assumptions on \mathbf{x} . Here $\lambda > 0$ is a scalar parameter. We assume λ has been determined by auxiliary considerations and is held fixed for purposes of the statistical analysis. In our calculations below \mathbf{L} is a periodized, second-difference matrix which corresponds to a standard smoothness condition. There are many interpretations of $\hat{\mathbf{x}}_{\lambda}$ and we refer to the literature for discussion [7, 6].

To better understand uncertainties in $\hat{\mathbf{x}}_{\lambda}$, we take into account uncertainties in both measured data and the system response function. As the measurement noise is modeled by a random variable, this randomness is propagated into $\hat{\mathbf{x}}_{\lambda}$ and it is natural to partition the uncertainty into contributions arising from variance and bias. Our uncertainty analysis then follows subject to assumptions on: noise statistics, a spectral bound on the true source $x_*(t)$, and a perturbation bound on the true convolution kernel $a_*(t)$. For noise statistics we assume discrete white noise and the analysis is classical. The spectral assumption on $x_*(t)$ has been used previously to derive a bias bound for regularized deconvolution in metrology contexts [5, 4]. Although not noted in those papers, this type of assumption has a history in regularization analysis and is referred to as a source condition [1]. The novelty of the present work consists of representing the uncertainty on the deconvolution kernel as a controlled perturbation, and thereby generalizing source condition analysis to encompass contributions from uncertainties in the system response.

2. Uncertainty Analysis

Since we treat the true source as a deterministic function, we can define the bias-variance decomposition of the expected mean square error (MSE) of our estimator by^1

$$\mathbb{E}\big[(\hat{\mathbf{x}}_{\lambda} - \mathbf{x}_{*})^{2}\big] = (\mathbb{E}[\hat{\mathbf{x}}_{\lambda}] - \mathbf{x}_{*})^{2} + \mathbb{E}\big[(\hat{\mathbf{x}}_{\lambda} - \mathbb{E}[\hat{\mathbf{x}}_{\lambda}])^{2}\big] = \operatorname{bias}\left(\hat{\mathbf{x}}_{\lambda}\right)^{2} + \mathbb{V}\operatorname{ar}(\hat{\mathbf{x}}_{\lambda}).$$

Recalling the measurement model (3) and the Tikhonov inversion (4), and assuming $\mathbb{E}[\mathbf{n}] = \mathbf{0}$ and $\mathbb{V}ar(\mathbf{n}) = \mathbf{\Sigma}$, we have the explicit expressions

bias
$$(\hat{\mathbf{x}}_{\lambda}) = \left(\mathbf{A}_{\lambda}^{\dagger}\mathbf{A}_{*} - \mathbf{I}\right)\mathbf{x}_{*}$$
 and $\mathbb{V}\operatorname{ar}(\hat{\mathbf{x}}_{\lambda}) = (\mathbf{A}_{\lambda}^{\dagger})^{T}\boldsymbol{\Sigma}\mathbf{A}_{\lambda}^{\dagger}.$ (5)

2.1. Variance

While the statistical analysis shown above is valid for any random model for \mathbf{n} , we refine this further by assuming that \mathbf{n} is distributed as discrete white-noise with mean zero and constant variance, $\mathbf{n} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$. In this case $\hat{\mathbf{x}}_{\lambda}$ is also multivariate Gaussian fully described by its mean and covariance

$$\mathbb{E}[\hat{\mathbf{x}}_{\lambda}] = \mathbf{x}_{*} + \text{bias}\left(\hat{\mathbf{x}}_{\lambda}\right) \qquad \text{and} \qquad \mathbb{V}\text{ar}(\hat{\mathbf{x}}_{\lambda}) = \sigma^{2}(\mathbf{A}_{\lambda}^{\dagger})^{T}\mathbf{A}_{\lambda}^{\dagger}.$$

¹ The squared vector operation is to be interpreted as an outer-product $\hat{\mathbf{x}}_{\lambda}^2 = \hat{\mathbf{x}}_{\lambda} \hat{\mathbf{x}}_{\lambda}^T$ for the expectation computations, and element-wise for the bias terms. Hence, $\operatorname{bias}(\hat{\mathbf{x}}_{\lambda})^2$ is a vector which may be interpreted as a diagonal matrix depending on context, and $\operatorname{Var}(\hat{\mathbf{x}}_{\lambda})$ is the complete covariance matrix.

The Gaussian assumption allows for a precise statement of coverage intervals. Introducing a vector for the matrix diagonal $\mathbf{v}_{\lambda} = \text{diag}\left((\mathbf{A}_{\lambda}^{\dagger})^{\mathrm{T}}\mathbf{A}_{\lambda}^{\dagger}\right)$, using the fact that the marginal variances of a multivariate Gaussian are given by this diagonal, for each t_j we have a $100(1-\alpha)\%$ confidence interval of the form (interpreting the vector probability equation as marginals on each element)

$$1 - \alpha = \mathbb{P}\left(\left|\hat{\mathbf{x}}_{\lambda} - \mathbf{x}_{*} - \operatorname{bias}\left(\hat{\mathbf{x}}_{\lambda}\right)\right| \le z_{\alpha/2}\sigma\sqrt{\mathbf{v}_{\lambda}}\right) \ge \mathbb{P}\left(\left|\hat{\mathbf{x}}_{\lambda} - \mathbf{x}_{*}\right| \le \left|\operatorname{bias}\left(\hat{\mathbf{x}}_{\lambda}\right)\right| + z_{\alpha/2}\sigma\sqrt{\mathbf{v}_{\lambda}}\right) \quad (6)$$

Thus, a confidence band of size $|\text{bias}(\hat{\mathbf{x}}_{\lambda})| + z_{\alpha/2}\sigma\sqrt{\mathbf{v}_{\lambda}}$ centered on the inversion $\hat{\mathbf{x}}_{\lambda}$ will necessarily contain the true solution with specified probability. Since \mathbf{x}_* is unknown, so is bias $(\hat{\mathbf{x}}_{\lambda})$. In the next section we discuss how to bound the bias contribution to this confidence interval.

2.2. Generalized source conditions

An estimate of the bias term is needed to make the confidence bands (6) useful. For simplicity we assume numerical error is negligible and cast our analysis for the continuous system. While details of the true solution $x_*(t)$ and kernel $a_*(t)$ are unknown in practice, we can reasonably introduce controlled assumptions on this lack of knowledge and propagate these uncertainties through the estimation process. Recall that convolution in time is given by a product in the Fourier domain. Since we make assumptions on the Fourier coefficients of $x_*(t)$, we consider our approach to be a generalization of source condition analysis that has been discussed elsewhere in regularization contexts.

There are many cases in which one may assume decay properties of $X_*(f)$. For example, existence of some number of continuous derivatives of $x_*(t)$ implies corresponding orders of algebraic decay of $|X_*(f)| \leq C|f|^{-n}$ as $|f| \to \infty$. More generally, we assume that we have a function B(f) such that $|X_*(f)| \leq B(f)$. This type of assumption has been used in metrology previously, for example in [4, 5].

Concerning the convolution kernel, we assume that its uncertainty may be modeled as a convolutional perturbation of true system,

$$a(t) = a_*(t) + \epsilon \int_{-\infty}^{\infty} r(t-\tau)a_*(\tau) \,\mathrm{d}\tau \qquad \text{and} \qquad A(f) = (1+\epsilon R(f))A_*(f) \tag{7}$$

for some r(t) with $\int |r(t)| dt = 1$ and $0 \le \epsilon \ll 1$. This type of perturbation is reasonable, for example, in situations for which a(t) contains reflections of small magnitude in which case r(t) is a sequence of time-delayed echoes. Since the L_1 norm of r(t) controls the sup-norm of its Fourier transform, $|R(f)| \le 1$.

Transforming the equation for the bias (5) to the Fourier domain, using the source conditions (7), and performing algebra we arrive at

$$|\operatorname{bias} (x_{\lambda}(t_{j}))| = \left| \int_{-\infty}^{\infty} \left(A_{\lambda}^{\dagger}(f)A_{*}(f) - 1 \right) X(f)e^{2\pi i f t_{j}} \, \mathrm{d}f \right|$$
$$\leq \int_{-\infty}^{\infty} \left| \frac{\overline{A(f)}A_{*}(f)}{|A(f)|^{2} + \lambda^{2}|L(f)|^{2}} - 1 \right| |X(f)| \, \mathrm{d}f \leq b_{x,\lambda} + b_{a,\lambda}$$

where

$$b_{x,\lambda} = \lambda^2 \int_{-\infty}^{\infty} \frac{|L(f)|^2 B(f)}{|A(f)|^2 + \lambda^2 |L(f)|^2} \, \mathrm{d}f \quad \text{and} \quad b_{a,\lambda} = \frac{\epsilon}{1 - \epsilon} \int_{-\infty}^{\infty} \frac{|A(f)|^2 B(f)}{|A(f)|^2 + \lambda^2 |L(f)|^2} \, \mathrm{d}f.$$

Substituting the sum of these two bounds into the expression (6) completes the uncertainty analysis for the regularized estimate $\hat{\mathbf{x}}_{\lambda} \approx \mathbf{x}_{*}$. A short calculation demonstrates that $b_{a,\lambda} \to 0$ as $\epsilon \to 0$. We note that the expression for $b_{x,\lambda}$ is basically the same as that derived at separate times [5, 4, 3]. To the best of our knowledge, the expression for $b_{a,\lambda}$ is new.



Figure 1. Reconstructions for SNR=10 (left) and SNR=100 (right). Horizontal axis is unitless time and vertical axis is unitless amplitude.

3. Simulated Examples

A simulated example demonstrates the above uncertainty analysis. We simulate the measurement of a waveform generated by a 3rd order Butterworth filter with a measurement device whose system response function is a 5th order Butterworth filter. Figure 1 shows both estimated and exact solutions along with the estimated 95% confidence interval. We select λ by minimizing estimated MSE. For simplicity, we set B(f) = |X(f)|. We show the deconvolution for both SNR = 10 and SNR = 100, which are reasonable in high speed waveform metrology. In both cases, the exact solution falls within the confidence intervals and that the uncertainty decreases as SNR increases.

4. Conclusions

We have demonstrated that by imposing a condition on the decay of Fourier coefficients of our unknown source and making assumptions on the uncertainties in the system response function, we are able to quantify the uncertainty in our unknown \mathbf{x} as a function of known values. While the idea of bounding Fourier coefficients to better understand uncertainty in Tikhonov estimates has appeared previously, we additionally quantify the MSE of the estimate with these bounds, include an analysis of system uncertainty, and apply a frequentist-style statistical analysis of the results.

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