The connection between Bayesian estimation of a Gaussian random field and RKHS
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Abstract—Reconstruction of a function from noisy data is often formulated as a regularized optimization problem over an infinite-dimensional reproducing kernel Hilbert space (RKHS). The solution describes the observed data and has a small RKHS norm. When the data fit is measured using a quadratic loss, this estimator has a known statistical interpretation. Given the noisy measurements, the RKHS estimate represents the posterior mean (minimum variance estimate) of a Gaussian random field with covariance proportional to the kernel associated with the RKHS. In this paper, we provide a statistical interpretation when more general losses are used, such as absolute value, Vapnik or Huber. Specifically, for any finite set of sampling locations (including where the data were collected), the MAP estimate for these locations.

This connection establishes a firm statistical foundation for several stochastic approaches used to estimate unknown regularizations. To illustrate this, we develop a numerical scheme that implements a Bayesian estimator with an absolute value loss. This estimator is used to learn a function from measurements contaminated by outliers.

Index Terms—kernel based regularization; Gaussian processes; representer theorem; reproducing kernel Hilbert spaces; regularization networks; support vector regression; Markov chain Monte Carlo

I. INTRODUCTION

Minimizing a regularized functional with respect to a reproducing kernel Hilbert space (RKHS) \( \mathcal{H} \) is a popular approach to reconstruct a function \( F: \mathcal{X} \rightarrow \mathbb{R} \) from noisy data; e.g. see [1], [2], [3], [4]. To be specific, regularization in \( \mathcal{H} \) estimates \( F \) using \( \hat{F} \) defined by

\[
\hat{F} = \arg \min_{F \in \mathcal{H}} \left( \sum_{i=1}^{N} V_i [y_i - F(x_i)] + \| F \|^2_{\mathcal{H}} \right),
\]

where \( \gamma \in \mathbb{R}^+ \) is the regularization parameter, \( \mathcal{X} \) is a set (finite or infinite), \( x_i \in \mathcal{X} \) is the location where \( y_i \in \mathbb{R} \) is measured, \( V_i: \mathbb{R} \rightarrow \mathbb{R}^+ \) is the loss function for \( y_i \), and \( \| \cdot \|_{\mathcal{H}} \) is the RKHS norm induced by the positive definite reproducing kernel \( K: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R} \), see [1]. Here \( y_i \) is the ith element of a vector \( y \). Note however that \( x_i \) is the ith measurement location (not the ith element of a vector \( x \)), and \( V_i \) is the loss function corresponding to the ith residual.

One of the important features of the above approach is that, even if the dimension of \( \mathcal{H} \) is infinite, the solution belongs to a finite-dimensional subspace. In fact, under mild assumptions on the loss, according to the representer theorem [5], [6], \( \hat{F} \) in (1) is the sum of kernel sections \( K_i: \mathcal{X} \rightarrow \mathbb{R} \) defined by \( K_i(x) = K(x_i, x) \). To be specific,

\[
\hat{F}(\cdot) = \sum_{i=1}^{N} \hat{c}_i K_i(\cdot),
\]

where \( \hat{c} \) is defined by

\[
\hat{c} = \arg \min_{c \in \mathbb{R}^N} \left( \sum_{i=1}^{N} V_i \left( y_i - \sum_{j=1}^{N} K(x_i, x_j) c_j \right) + \gamma c^T \mathbf{K} c \right).
\]

Here and below, \( \mathbf{K} \in \mathbb{R}^{N \times N} \) denotes the kernel matrix, or Gram matrix, defined by \( K_{ij} = K(x_i, x_j) \). When the component loss functions \( V_i(\cdot) \) are quadratic, the problem in (1) admits a zero-mean Gaussian random field with a prior covariance proportional to \( K \), and that \( K \) is independent of the white Gaussian measurement noise. Then, given the measurements, for every \( x \) the value \( \hat{F}(x) \) is the posterior mean, and hence the minimum variance estimate of \( F(x) \), e.g. see subsection 2.3 of [8]. This connection, briefly reviewed in Section III, is well known in the literature and was initially studied in [9] in the context of spline regression, see also [3], [10], [11]. This connection can be proved using the representer theorem, which also yields the closed form solutions of the coefficients \( \hat{c}_i \) in (2):

\[
\hat{c}_i = (\mathbf{K} + \gamma \mathbf{I}_N)^{-1} y_i,
\]

where \( y \in \mathbb{R}^N \) is the vector of measurements \( y_i \) and \( \mathbf{I}_N \) is the \( N \times N \) identity matrix.

A formal statistical model for more general loss functions (e.g., the Vapnik \( \varepsilon \)-insensitive loss used in support vector regression [12], [13], [14]) is missing from the literature. After interpreting the \( V_i \) as alternative statistical models for the observation noise, many papers argue that \( \hat{F} \) in (1) can be viewed as a maximum a posteriori (MAP) estimator assuming a priori probability density of \( F \) is proportional to \( \exp (-\| F \|^2_{\mathcal{H}}) \), e.g. [13] Section 7]. These kinds of statements are informal, since in an infinite-dimensional function space the concept of probability density is not well defined, see e.g. [15] for a thorough treatment of Gaussian measures. The main
contribution of this note is to provide a rigorous statistical model that justifies \( \hat{F} \) as an estimate of a Gaussian random field.

This connection provides a firm statistical foundation for several stochastic approaches for estimating unknown regularization parameters. Examples of such parameters include \( \gamma \) in \( \ell_1 \) and possibly other parameters used to specify \( K \). To illustrate, we develop a Bayesian estimator equipped with the absolute value \( \ell_1 \) loss using the Markov chain Monte Carlo (MCMC) framework \cite{16}. The estimator recovers a function starting from measurements contaminated by outliers, and compares favorably with the tuning approach recently proposed in \cite{17} where \( \gamma \) is determined using CP-like statistics and the concept of equivalent degrees of freedom.

The structure of the paper is as follows. In Section II we formulate the statistical model. In Section III we review the connection between regularized estimation in RKHS and estimation in the quadratic case, and then extend this connection to more general losses. Section IV uses this connection to describe Bayesian approaches that estimate regularization parameters. A numerical experiment is then reported in Section V to illustrate the theoretical results. Section VI contains a summary and conclusion. The proofs are presented in Section VII.

II. STATISTICAL MODEL

Here and below, \( \mathbf{E}[\cdot] \) indicates the expectation operator, and given (column) random vectors \( u \) and \( v \), we define

\[
\text{cov}(u,v) = \mathbf{E}[(u - \mathbf{E}[u])(v - \mathbf{E}[v])^T].
\]

We assume that the measurements \( y_i \) are obtained by measuring the function \( F \) at sampled points \( x_i \) in the presence of additive noise, i.e.,

\[
y_i = F(x_i) + e_i, \quad i = 1, \ldots, n,
\]

where each \( x_i \) is a known sampling location. We make the following assumptions:

**Assumption 1:** We are given a known positive definite autocovariance function \( K \) on \( X \times X \) and a scalar \( \lambda > 0 \) such that for any sequence of points \( \{x_j: j = 1, \ldots, J\} \), the vector \( f = [F(x_1), \ldots, F(x_J)] \) is a Gaussian random variable with mean zero and covariance given by

\[
\text{cov}(f_j, f_k) = \lambda K(x_j, x_k).
\]

A random function \( F \) that satisfies Assumption 1 is often referred to as a zero-mean Gaussian random field on \( X \).

**Assumption 2:** We are given a sequence of measurement pairs \( (x_i, y_i) \in X \times R \) and corresponding loss functions \( V_i \) for \( i = 1, \ldots, N \). In addition, we are given a scalar \( \sigma > 0 \) such that

\[
\mathbf{p}(y|F) \propto \prod_{i=1}^{N} \exp \left( -\frac{V_i[y_i - F(x_i)]}{2\sigma^2} \right).
\]

Furthermore, the measurement noise random variables \( e_i = y_i - F(x_i) \) are independent of the the random function \( F \).

For example, \( V_i(r) = r^2 \) corresponds to Gaussian noise, while using \( V_i(r) = |r| \) corresponds to Laplacian noise. These loss functions (and corresponding standardized densities) are pictured in Figure 1. The statistical interpretation of an \( \epsilon \)-insensitive \( V_i \) in terms of Gaussians with mean and variance described by suitable random variables can be found in \cite{18}.

III. ESTIMATION IN REPRODUCING KERNEL HILBERT SPACES

A. Gaussian measurement noise

We first consider the case of Gaussian measurement noise; i.e., \( V_i(r) = r^2 \). This corresponds to modeling the \( \{e_i\} \) as i.i.d. Gaussian random variables with variance \( \sigma^2 \). In view of the independence of \( F \) and \( e \), it turns out that \( F(x) \) and \( y \) are jointly Gaussian for any \( x \in X \). Hence, the posterior \( \mathbf{p}(F|y) \) is also Gaussian. The mean and variance for this posterior can be calculated using the following proposition \cite{8}.

**Proposition 3:** Suppose \( u \) and \( v \) are jointly Gaussian random vectors. Then, \( \mathbf{p}(u|v) \) is also Gaussian with mean and autocovariance given by

\[
\mathbf{E}(u|v) = \mathbf{E}(u) + \text{cov}(u,v)\text{cov}(v,v)^{-1}[v - \mathbf{E}(v)],
\]

\[
\text{cov}(u,v|v) = \text{cov}(u,v) - \text{cov}(u,v)\text{cov}(v,v)^{-1}\text{cov}(v,v) .
\]

Suppose Assumptions 1 and 2 hold with \( V_i(r) = r^2 \) and \( K_i \) as given in (2) for \( i = 1, \ldots, N \). It follows that \( y \) is Gaussian. Applying Proposition 3 with \( u = F(x) \) and \( v = y \), we obtain

\[
\mathbf{E}(u) = 0, \quad \mathbf{E}(v) = 0, \quad \text{and}
\]

\[
\mathbf{E}(F(x)|y) = \lambda [K_1(x) \ldots K_N(x)](\lambda K + \sigma^2 I_N)^{-1} y .
\]

Using the notation \( \gamma = \sigma^2/\lambda \), one obtains

\[
\mathbf{E}(F(x)|y) = [K_1(x) \ldots K_N(x)](\lambda K + \gamma I_N)^{-1} y ,
\]

\[
= \sum_{i=1}^{N} \hat{c}_i K_i(x) .
\]

where \( \hat{c} \) is computed using (4). This shows that in the Gaussian case the minimum variance estimate coincides with \( \hat{F} \) defined by (1). We formalize this result in the following proposition.

**Proposition 4:** Suppose that \( F \) satisfies Assumption 1 and \( \mathbf{p}(y|F) \) satisfies Assumption 2 with \( V_i(r) = r^2 \). Then the minimum variance estimate of \( F(x) \) given \( y \) is \( \hat{F}(x) \) defined by (1), with \( \gamma = \sigma^2/\lambda \) and \( \mathcal{H} \) the RKHS induced by \( K \).
B. Non-Gaussian measurements: MAP estimate

We now consider what happens when the Gaussian assumptions on \(e_i\) are removed. If the probability density function for \(F\) was well defined and given by

\[
p(F) \propto \exp\left(-\frac{\|F\|_{\mathcal{H}}^2}{2\lambda}\right),
\]

then the posterior density conditional on the data would be

\[
p(F|y) \propto \exp\left(-\frac{\sum_{i=1}^{N} V_i[y_i - F(x_i)]^2}{2\sigma^2} - \frac{\|F\|_{\mathcal{H}}^2}{2\lambda}\right).
\]

In this case, the negative log of \(p(F|y)\) would be proportional to the objective in (1). Hence, one could immediately conclude that \(\hat{F}\) is the MAP estimator. Unfortunately, the posterior density of \(F\) on a function space is not well defined. However, one can consider the MAP estimates corresponding to any finite sample of \(F\) that includes the observations \(y_i\) (since these are finite dimensional estimation problems). The following proposition shows that \(\hat{F}\) solves all such problems.

**Proposition 5:** Suppose that \(F\) satisfies Assumption 1 and \(p(y|F)\) satisfies Assumption 2. Let \(\{x_i : i = N+1, \ldots, N+M\}\) be an arbitrary set of points in \(\mathcal{X}\) where \(M\) is a given non-negative integer, and define

\[
f = [F(x_1), \ldots, F(x_{N+M})]^T.
\]

Then the MAP estimate for \(f\) given \(y\) is

\[
\arg\max_f p(y|f)p(f) = [\hat{F}(x_1), \ldots, \hat{F}(x_{N+M})]^T,
\]

where \(\hat{F}\) is defined by (1), with \(\gamma = \sigma^2/\lambda\) and \(\mathcal{H}\) is the RKHS induced by \(K\).

C. Non-Gaussian measurements: minimum variance estimate

When considering non-Gaussian measurement loss functions, the minimum variance estimate \(E[F(\cdot)|y]\) and the MAP estimate \(\hat{F}(\cdot)\) are different.

**Example 6:** Consider the case where \(N = 1, M = 0, V_i(r) = |r|, y = 1, and \lambda = 1, \sigma = 1, K(x_1,x_1) = 1\). For this case, \(f = F(x_1)\), and the MAP estimate for \(f\) given \(y\) is

\[
\hat{f} = \arg\min_f (f^2 + |1 - f|) = 1/2.
\]

Define \(A > 0\) by

\[
A = \int_{-\infty}^{+\infty} \exp(-f^2 - |1 - f|) \, df.
\]

The difference between the minimum variance estimate and the MAP estimate is (see Appendix VII-D for details)

\[
E(F(y)) - \hat{f} = \frac{\exp(-3/4)}{A} \int_{-\infty}^{+\infty} \frac{\exp(1 - 2s) - 1}{s^2} \, ds.
\]

For \(s > 1/2\), the integrand in (6) is negative, so the right hand side is negative, and \(E(F(y)) < \hat{f}\).

The following proposition shows that the minimum variance estimate \(E[F(\cdot)|y]\) and the MAP estimate \(\hat{F}(\cdot)\) belong to the same subspace of \(\mathcal{H}\), namely, the linear span of the functions \(K_i(\cdot), i = 1, \ldots, N\).

**Proposition 7:** Suppose that \(F\) satisfies Assumption 1 and \(p(y|F)\) satisfies Assumption 2. Define

\[
g = [F(x_1), \ldots, F(x_N)]^T, \quad \hat{d} = K^{-1}E(g|y)\cdot
\]

For each \(x \in \mathcal{X}\) the minimum variance estimate of \(F(x)\) is

\[
E[F(x)|y] = \sum_{i=1}^{N} \hat{d}_i K_i(x).
\]

Note that, given \(\sigma\) and \(\lambda\), the vector \(E(g|y)\) can be approximated using the relation

\[
p(g|y) \propto \exp\left(-\frac{\sum_{i=1}^{N} V_i[y_i - g_i]}{2\sigma^2} - \frac{g^T K^{-1} g}{2\lambda}\right)
\]

together with random sampling technique such as MCMC.

IV. FUNCTION AND REGULARIZATION PARAMETER ESTIMATION

In real applications, the regularization parameter \(\gamma = \sigma^2/\lambda\) is typically unknown and needs to be inferred from data. In the case of Gaussian measurement noise, this problem is often solved by exploiting the stochastic interpretation given by Proposition 4. For example, following an empirical Bayes approach, the marginal likelihood can be computed analytically and the unknown parameters (often called hyperparameters) can be estimated by optimizing this likelihood, e.g. see [19] and [11] Subsection 5.4.1. \(\gamma\) is then set to its estimated value, and \(\hat{F}\) in (1) is obtained using equations (4) and (2). Propositions 5 and 7 provide the statistical foundations that extend this technique to non-Gaussian measurement noise.

In the more general case of Assumption 2 (non-Gaussian measurement noise) the marginal likelihood cannot be computed analytically. Let \(\eta\) denote the vector of unknown hyperparameters (\(\sigma\) and/or \(\lambda\)) and recall the notation \(g = [F(x_1), \ldots, F(x_N)]^T\). Following a Bayesian approach, we model \(\eta\) as a random vector with prior probability density \(p(\eta)\). The conditional density for the data \(y\) and the unknown function samples \(g\), given the hyperparameters \(\eta\) is

\[
p(y,g|\eta) = \prod_{i=1}^{N} \frac{1}{\sigma\sqrt{\lambda}} \exp\left(-\frac{V_i[y_i - g_i]}{2\sigma^2} - \frac{g^T K^{-1} g}{2\lambda}\right).
\]

The difficulty underlying the estimation of \(\eta\) is that \(p(\eta|y)\) is not, in general, available in closed form. One possibility is to use stochastic simulation techniques, e.g. MCMC [16] or particle filters [20], which can sample from \(p(\eta,g|y)\) provided that a suitable proposal density for \(\eta\) and \(g\) can be designed. An MCMC scheme for sampling from the posterior for \(g\) and \(\eta\) (corresponding to the \(\ell_1\) measurement model) is described in Appendix VII-E and applied in section VII below. Proposition 7 is especially important because it shows how to compute \(E[F(x)|y]\) for any \(x\) from the minimum variance estimate for \(g\). Similary, given an estimate of \(\eta\), we can use Proposition 5 to compute the corresponding \(\hat{F}(x)\) for any \(x\).
V. SIMULATION EXAMPLE

We consider the simulated problem in [17, Section 5.1]. The unknown function to be estimated is

$$F_0(x) = \exp[\sin(8x)], \quad 0 \leq x \leq 1$$

which is displayed as the thick line in the bottom two panels of Fig. 2. This function is reconstructed from the measurements

$$y_i = F_0(x_i) + e_i \quad \text{with} \quad x_i = (i-1)/63, \quad i = 1, \ldots, 64.$$  

We include two Monte Carlo experiments each consisting of 300 function reconstructions. In the first experiment, for each reconstruction, measurements $y_i$ are generated using $e_i \sim N(0, 0.09)$. A typical data set is plotted as circles in the bottom left panel of Fig. 2. In the second experiment, we simulate the presence of outliers by adding, with probability 0.1, a random offset equal to $\pm 3$ to each measurement generated in the first experiment. A typical data set is plotted as circles in the bottom right panel of Fig. 2.

Both experiments compare three different methods for modeling the measurement noise and estimating the kernel scale factor $\lambda$ (described below). All the methods model the function correlations by using a cubic spline kernel shifted by 1 to deal with non null initial conditions of $f$ at 0, i.e. $K(x_i, x_j)$ equals

$$(x_j + 1)(x_j + 1)\min(x_i + 1, x_j + 1) - \min(x_i + 1, x_j + 1)^3 \over 2 - 6$$

[3, Chapter 1]. In addition, once an estimate for $\lambda$ is determined, all methods use the MAP estimator [1] to reconstruct the function $F_0(x)$ by solving the problem in equation (3).

- $L_2+OML$: The measurement noise is modeled by a quadratic loss with $\sigma^2 = 0.09$. (During the second experiment, the outliers represent unexpected model deviations.) For each reconstruction, the kernel scale factor $\lambda$ is estimated using marginal likelihood optimization [11, section 5.4.1].

- $L_1+Bayes$: The measurement noise is modeled by the $\ell_1$ loss with $\sigma$ chosen so the variance of the corresponding Laplace distribution is 0.09. The kernel scale factor $\lambda$ is estimated by following the Bayesian approach discussed (for non-Gaussian noise) in section [17]. More details can be found in Appendix VII-E. Once the estimate for $\lambda$ is determined, the problem in (3) is solved using the interior point method described in [21].

- $L_1+EDF$: The measurement noise is modeled by the $\ell_1$ loss with $\sigma$ chosen so the variance of the corresponding Laplace distribution is 0.09. The kernel scale factor $\lambda$ is estimated using the approach described in [17]; i.e., relying on $C_p$-like statistic and the concept of equivalent degrees of freedom (EDF). The notation $C$ in [17, eq. 1], corresponds to $\sigma^{-2}/2$ in this paper. The objective in [17, eq. 19] is optimized on a grid containing 50 values of $\log_{10}(C)$ uniformly distributed on $[1, 6]$. The number of degrees of freedom entering [17, eq. 19], as a function of $C$, is determined at every run as described in [17, Remark 1] (with $\varepsilon = 0$).

The top panels of Fig. 2 are boxplots of the 300 relative errors defined by

$$\sqrt{\sum_{i=1}^{64} |F_0(x_i) - \hat{F}(x_i)|^2 \over \sum_{i=1}^{64} F_0^2(x_i)}$$

for the three different methods. In absence of outliers (top left panel), all the methods provide accurate function reconstructions, and the $L_2+OML$ method performs best. The bottom left panel contains the results of a single reconstruction using the $L_2+OML$ and $L_1+Bayes$ methods.

The situation dramatically changes in presence of outliers (top right panel). As expected, the errors for the $L_2+OML$ method increase significantly. The estimate obtained by the $L_2+OML$ method for a single reconstruction is displayed in the bottom right panel (solid line). It is apparent that the quadratic loss is very vulnerable to unexpected model deviations. On the other hand the estimate obtained by $L_1+Bayes$ method is much closer to the truth. This remarkable performance is confirmed by the top right panel. The errors corresponding to the $L_1+Bayes$ method with outliers is similar to the performance obtained in the absence of outliers. In addition, the $L_1+Bayes$ method outperforms the $L_1+EDF$ method.

Removal 8: The MCMC scheme discussed in the last part of Appendix VII-E was also used to compute the minimum variance estimate of $F$. The performance of this estimator is virtually identical to that of $L_1+Bayes$. Once the MCMC samples are computed, there is very little extra computation required to obtain the minimum variance estimate of $F$. In addition, it does not require the somewhat complex optimization procedure described in [21].

Removal 9: We also considered a third experiment, where the true value of the noise variance, i.e. $\sigma^2 = 0.99$, is provided to the three estimators. The average error of the $L_2+OML$ method decreases from 0.52 to 0.21, while that of the $L_1+EDF$ method decreases from 0.24 to 0.15. The average error of the $L_1+Bayes$ method does not change significantly, staying around 0.1 in both the second and third experiments.

VI. CONCLUSION

When the RKHS induced by $K$ is infinite-dimensional, the realizations of the Gaussian random field with autocovariance $K$ do not fall in $\mathcal{H}$ with probability one, see [22, eq. 34] and also [23, 24, 25] for generalizations. A simple heuristic argument illustrating this fact can be also found in Chapter 1 of [3]. The intuition here is that the realizations of $F$ are much less regular than functions in the RKHS whose kernel is equal to the autocovariance $K$. On the other hand, in the case of Gaussian measurement noise, $\hat{F}$ defined in (1) is the minimum variance estimate; see Proposition 4. In this note we proved a formal connection between Bayesian estimation and the more general case prescribed by Assumption 2. Given the training set $\{\{(x_i, y_i)\}$, for any finite set of locations which include the training locations $\{x_i\}$, the MAP estimate of $F$ at the locations is the RKHS estimate evaluated at these locations. We have also shown that the MAP estimate of $F$ and the minimum variance estimate of $F$ belong to the finite dimensional subspace (of the RKHS) induced by the
covariance $K$ at the training locations. (These results can be extended to more general cases by using more general versions of the Representer Theorem \textsuperscript{(2)}. This link between statistical estimation and RKHS regularization provides a foundation for the application of statistical approaches to joint estimation of the function and the regularization parameters. The simulation example in this paper illustrates the utility of this connection.

VII. APPENDIX

A. Lemmas

We begin the appendix with two lemmas which are instrumental in proving Proposition \textsuperscript{5}

\textbf{Lemma 10:} Suppose that $g$ and $h$ are jointly Gaussian random vectors. It follows that

$$\max_h \log p(h|g) = -\log \det \left\{ 2\pi \left[ \text{cov}(h,h) - \text{cov}(h,g)\text{cov}(g,g)^{-1}\text{cov}(g,h) \right] \right\}/2,$$

and this maximum does not depend on the value of $g$.

\textbf{Proof:} The proof comes from well known properties of joint Gaussian vectors, see e.g. \textsuperscript{8}. The conditional density $p(h|g)$ is Gaussian and is given by

$$-2\log p(h|g) = \log \det [2\pi \text{cov}(h,h|g)] + [h - \mathbf{E}(h|g)]^T \text{cov}(h,h|g)^{-1} [h - \mathbf{E}(h|g)],$$

where, recalling also Proposition \textsuperscript{3}

$$\text{cov}(h,h|g) = \text{cov}(h,h) - \text{cov}(h,g)\text{cov}(g,g)^{-1}\text{cov}(g,h).$$

Thus, $\text{cov}(h,h|g)$ does not depend on the value of $g$ (and it would not make sense for it to depend on the value of $h$). Hence, one has

$$\arg \max_h p(h|g) = \mathbf{E}(h|g),$$

$$\max_h \log p(h|g) = -\log \det [2\pi \text{cov}(h,h|g)]/2.$$

This equation, and the representation for $\text{cov}(h,h|g)$ above completes the proof of this lemma.

\textbf{Lemma 11:} Assume that $g$ and $h$ are jointly Gaussian random vectors and that $y$ is a random vector such that $p(y|g,h) = p(y|g)$, and suppose we are given a value for $y$. Define the corresponding estimates for $g$ and $h$ by

$$(g,\hat{h}) = \arg \max_{g,h} p(y|g,h),$$

and assume the above maximizers are unique. It follows that

$$\hat{g} = \arg \max_g p(y|g)p(g),$$

$$\hat{h} = \arg \max_h p(h|g = \hat{g}).$$

Fig. 2. Simulation. Top Boxplot of the 300 relative errors under nominal (top left) and perturbed (top right) conditions. Bottom True function (thick line), noisy output samples (c) and estimates using the $L_2$+OML (solid line) and $L_1$+Bayes (dotted line) estimators under nominal (bottom left) and perturbed (bottom right) conditions.
Proof: We have
\[ p(y,g,h) = p(y|g,h) p(h|g) p(g), \]
\[ \max_{g,h} p(y,g,h) = \max_g \left\{ [p(y|g) p(g)] \max_h p(h|g) \right\}. \]
It follows from Lemma 10 that \( \max_p p(h|g) \) is constant with respect to \( g \). Hence \( \hat{g} = \arg \max_g [p(y|g) p(g)] \), which completes the proof of (8), and
\[ \max_{g,h} p(y,g,h) = p(y|\hat{g}) p(\hat{g}) \max_h p(h|g = \hat{g}), \]
which completes the proof of (9).

B. Proof of Proposition 5

The kernel matrix \( \mathcal{K} \) is positive definite and hence invertible (Assumption 1). Define the random vectors \( g \) and \( h \) by
\[ g = [F(x_1), \ldots, F(x_N)^T, \]
\[ h = [F(x_{N+1}), \ldots, F(x_{N+M})]^T. \]
It follows that \( f \) in Proposition 5 is given by \( f = (g^T, h^T)^T \). Notice that \( p(y|f) = p(y|g) \) and that Lemma 11 can be applied. From (8) and the hypotheses above, we obtain
\[ \hat{g} = \arg \max_g [p(y|g) p(g)], \]
\[ = \arg \max_g \left( \frac{1}{2 \sigma^2} \sum_{i=1}^N y_i - g_i + \frac{g^T \mathcal{K}^{-1} g}{2 \lambda} \right). \]
Using the representation \( g = \mathcal{K} c \) we obtain
\[ \hat{c} = \arg \max_c \left( \frac{1}{2 \sigma^2} \sum_{i=1}^N y_i - \sum_{j=1}^N K(x_i,x_j)c_j + \frac{c^T \mathcal{K} c}{2 \lambda} \right). \]
This agrees with (3), because \( \gamma = \sigma^2 / \lambda \), and thereby shows \( \hat{g} = [\hat{F}(x_1), \ldots, \hat{F}(x_N)]^T \).

Finally, by Proposition 3 and Lemma 10, in conjunction with (2), (9), and the expression for \( \hat{g} \) above, we obtain
\[ \hat{h} = \text{cov}(h,g) \text{cov}(g,g)^{-1} \hat{g} = \text{cov}(h,g) (\lambda \mathcal{K})^{-1} \mathcal{K} c, \]
\[ = \begin{pmatrix} K_1(x_{N+1}) & \ldots & K_N(x_{N+1}) \\ \vdots & \ddots & \vdots \\ K_1(x_{N+M}) & \ldots & K_N(x_{N+M}) \end{pmatrix} \begin{pmatrix} \hat{c}_1 \\ \vdots \\ \hat{c}_N \end{pmatrix}, \]
\[ = [\hat{F}(x_{N+1}), \ldots, \hat{F}(x_{N+M})]^T. \]
Combining this with the formula for \( \hat{g} \) above, we conclude
\[ [\hat{F}(x_1), \ldots, \hat{F}(x_{N+M})]^T = \arg \max_f p(y,f), \]
which completes the proof of Proposition 5.

C. Proof of Proposition 7

To obtain the representation (7) we compute \( \mathbf{E}[F(x)|y] \) by first projecting \( F(x) \) onto \( g \) and then onto \( y \), i.e. using the equivalence
\[ \mathbf{E}[F(x)|y] = \mathbf{E} \left( \mathbf{E}[F(x)|g] | y \right). \]
Exploiting Proposition 3 and recalling that \( \text{cov}(g,g) = \mathcal{K} \), the first projection is given by
\[ \mathbf{E}[F(x)|g] = \text{cov}(F(x),g) \text{cov}(g,g)^{-1} g = a^T \mathcal{K}^{-1} g \]
where \( a \in \mathbb{R}^N \) and \( a_i = \text{cov}(F(x),g_i) = K_i(x) \). The second projection yields
\[ \mathbf{E} \left( \mathbf{E}[F(x)|g] | y \right) = a^T \mathcal{K}^{-1} \mathbf{E}[g|y] = \sum_{i=1}^N \hat{d}_i K_i(x) \]
where \( \hat{d} = \mathcal{K}^{-1} \mathbf{E}[g|y] \), which completes the proof.

D. Proof of eq. (6)

It follows from \( N = 1, \gamma = 1, \) that \( c \) is a scalar, \( f = F(x_1) = c \), and using (4) we have
\[ \hat{f} = \hat{c} = \arg \min_c |1 - c| + c^2 = 1/2 \]
It also follows that
\[ p(y|f)p(f) \propto \exp(-f^2 - |1-f|) \]
The minimum variance estimate \( \mathbf{E}(f|y) \), and its difference from the map estimate \( \hat{f} \), are given by
\[ \mathbf{E}(f|y) = \frac{1}{A} \int_{-\infty}^{+\infty} f \exp(-f^2 - |1-f|) df, \]
\[ \mathbf{E}(f|y) - \hat{f} = \frac{1}{A} \int_{-\infty}^{+\infty} (f - 1/2) \exp(-f^2 - 1 + f) df \]
\[ + \frac{1}{A} \int_{-\infty}^{+\infty} (f - 1/2) \exp(-f^2 + 1 - f) df. \]
Multiplying both sides of the equation by \( A \) and using the change of variables \( s = f - 1/2 \), we obtain
\[ A(\mathbf{E}(f|y) - \hat{f}) = \int_{-\infty}^{+\infty} \frac{se^{-(s+1/2)^2+s-1/2} ds + \int_{-\infty}^{+\infty} se^{-(s+1/2)^2-s+1/2} ds}{A} , \]
\[ = \int_{-\infty}^{+\infty} se^{-s^2-3/4} ds + \frac{1}{2} + \int_{-\infty}^{+\infty} se^{-s^2-2s+1/4} ds, \]
\[ = \int_{-\infty}^{+\infty} se^{-s^2-3/4} ds + \int_{-\infty}^{+\infty} se^{-s^2-2s+1/4} ds, \]
\[ = \int_{-\infty}^{+\infty} se^{-s^2-3/4} [e^{1-2s} - 1] ds. \]
This completes the proof of (6).
E. Details of the MCMC scheme for \( L_1 + \text{Bayes} \)

If Assumptions 1 and 2 hold with \( V_j(r) = 2\sqrt{2\sigma |r|} \), the noise \( \varepsilon_i \) is Laplacian with variance \( \sigma^2 \). In this case, it can be difficult to build an efficient MCMC scheme to sample from the posterior of \( \eta \) and \( g \). This is because, a posteriori, the components of \( g \) are generally strongly correlated. It is useful to use to a scale mixture of normals representation because for each normal, the posterior distribution can be useful to use to a scale mixture of normals representation the components of \( \tau \).

Because for each normal, the posterior distribution can be represented in closed form. To be specific, each \( p(\varepsilon_i) \) admits the representation \[ p(\varepsilon_i) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{\varepsilon_i^2}{2\sigma^2}\right) \]

Hence, we can model Laplacian noise \( \varepsilon_i \) as a mixture of Gaussians with variances \( \tau_i \) that are exponential random variables of probability density

\[
p(\tau_i) = \begin{cases} 
\exp\left(-\tau_i / \sigma^2\right) / \sigma^2 & \text{if } \tau_i \geq 0 \\
0 & \text{otherwise}
\end{cases}
\]

\[
p(\tau) = p(\tau_1) \cdots p(\tau_N)
\]

We restrict our attention to the case where \( \eta = \lambda \), and use \( \tau = (\tau_1, \ldots, \tau_N)^T \) to denote the independent random variables (which are also independent of \( \lambda \)). We have

\[
p(\tau, \lambda | y) \propto p(y | \tau, \lambda) p(\tau) p(\lambda)
\]

Given \( \tau \) and \( \lambda \), we have the linear Gaussian model \( y = g + \xi \), where \( g \) and \( \xi \) are independently distributed according to

\[
g \sim \mathcal{N}(0, \lambda \mathbf{K}) \quad \text{and} \quad \xi \sim \mathcal{N}(0, \text{diag}(\tau)),
\]

where \( \text{diag}(\tau) \) is the diagonal matrix with \( \tau \) along its diagonal. Notice that \( p(y | \tau, \lambda) \) can be computed in closed form using the classical Gaussian likelihood result; e.g., see subsection 5.4.1. To be specific, using the notation \( C(\tau, \lambda) = \lambda \mathbf{K} + \text{diag}(\tau) \),

\[
p(y | \tau, \lambda) = \frac{1}{\sqrt{2\pi \det[C(\tau, \lambda)]}} \exp\left(-\frac{1}{2} y^T C^{-1}(\tau, \lambda) y\right).
\]

Using an improper flat prior on \( \lambda \geq 0 \), we obtain

\[
p(\tau, \lambda | y) \propto \begin{cases} 
p(y | \tau, \lambda) p(\tau) & \text{if } \lambda \geq 0 \\
0 & \text{otherwise}
\end{cases}
\]

were \( p(y | \tau, \lambda) \) can be computed using (11) and \( p(\tau) \) can be computed using (10). We are now in a position to describe the MCMC scheme used for the \( L_1 + \text{Bayes} \) method in Section V.

The scale factor \( \lambda \), and all the components of \( \tau \) are simultaneously updated using a random walk Metropolis scheme. The proposal density is independent normal increments with standard deviation 30 and \( \sigma^2/30 \) for \( \lambda \) and \( \tau_i \) respectively. This simple scheme has always led to an acceptance rate over 20%. We have assessed that this follows from the fact that the components of \( \lambda \) and \( \tau \) have low correlation a posteriori.

For each function reconstruction, \( L = 10^6 \) MCMC realizations from \( p(\tau, \lambda | y) \) were obtained by the MCMC scheme (which we denote by \( \{\tau^i, \lambda^i\} \) below). Using the convergence diagnostics described in [27], this allowed us to estimate the quantiles \( q = 0.025, 0.25, 0.5, 0.75, 0.975 \) of the marginal posterior of \( \lambda \) with precision \( r = 0.02, 0.05, 0.01, 0.05, 0.02 \), respectively, with probability 0.95.

Now consider recovering the minimum variance estimate \( E[F(x | y)] \). We have seen from Proposition 7 that this reduces to computing \( E(g | y) \). Note that, given a value for \( \lambda \) and \( g \) and \( y \) are jointly Gaussian. Applying Proposition 3

\[
E(g | y : \tau, \lambda) = \text{cov}(g, y | \tau, \lambda) \text{cov}(y, y | \tau, \lambda)^{-1} y,
\]

and \( \{\tau^i, \lambda^i\} \) are the realizations from \( p(\tau, \lambda | y) \) achieved by the MCMC scheme above described above.

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