Numerical posterior distribution error control and expected Bayes Factors in the Bayesian Uncertainty Quantification of inverse problems

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Abstract

In bayesian UQ most relevant cases of forward maps (FM, or regressor function) are defined in terms of a system of (O, P)DE’s with intractable solutions. These necessarily involve a numerical method to find approximate versions of such solutions which lead to a numerical/approximate posterior distribution. In the past decade, several results have been published on the regularity conditions required to ensure converge of the numerical to the theoretical posterior. However, more practical guidelines are needed to ensure a suitable working numerical posterior. Capistrán et al. (2016) prove for ODEs that the Bayes Factor (BF) of the approximate vs the theoretical model tends to 1 in the same order as the numerical method approximation order. In this work we generalize the latter paper in that we consider 1) the use of expected BFs, 2) also PDEs, 3) correlated observations, which results in, 4) more practical and workable guidelines in a more realistic multidimensional setting. The main result is a bound on the absolute global errors to be tolerated by the FM numerical solver, which we illustrate with some examples. Since the BF is kept near 1 we expect that the resulting numerical posterior is basically indistinguishable from the theoretical posterior, even though we are using an approximate numerical FM. The method is illustrated with an ODE and a PDE example, using synthetic data.

KEYWORDS: Inverse Problems, Bayesian Inference, Bayes factors, ODE solvers, PDE solvers.

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1 Introduction

Bayesian Uncertainty Quantification (UQ) has attracted substantial attention in recent years, covering a wide range of applications both in well-established fields as well as in emerging areas. Some recent examples may be found in Zhu et al. (2011); Cai et al. (2011); Fall et al. (2011); Chama et al. (2012); Nissinen et al. (2011); Kozawa et al. (2012); Cui et al. (2011a); Wan and Zabaras (2011); Hazelton (2010); Kaipio and Fox (2011). For reviews on the subject see Kaipio and Fox (2011); Watzenig and Fox (2009); Woodbury (2011); Fox et al. (2013).

The usual parametric (finite dimensional) Bayesian formulation of Inverse Problems, in broad terms, is that given a Forward Map (FM) $F_\theta$, a noise model is assumed for the observations $y_j \sim G_\sigma(F_\theta(j))$, for some noise level $\sigma$ and typically additive gaussian errors with known standard deviation $\sigma$ are assumed. This observation model creates a probability density of all data $Y$ given all parameters $\Phi$ namely $P_Y|\Phi(y|\theta,\sigma)$. For fixed data $y$ this forms the likelihood, regarding the latter as a function of $\theta, \sigma$, and is the basis of the statistical analysis of Inverse Problems. Using Bayesian inference one establishes a prior distribution $P_\Phi(\theta,\sigma)$ and defines the posterior distribution

$$P_{\Phi|Y}(\theta,\sigma|y) = \frac{P_{Y|\Phi}(y|\theta,\sigma)P_\Phi(\theta,\sigma)}{P_Y(y)}.$$ 

(1)

This probability distribution on the unknowns $\theta$ and $\sigma$ quantifies the uncertainty on the possible values for these parameters coherent with the data $y$. However, the common denominator in this particular Bayesian inference problem is that we do not have an analytical or computationally simple and precise implementation of the FM.

Instead, a numerical approach is required to create a solver and find a numerical approximation of the FM $F_\theta^\alpha$, for some discretization parameter $\alpha$ (eg. step size, grid norm, terms in a series, etc. concrete examples will be given in section 2). Since we can only use the numeric approximation, this in turn leads to a numeric likelihood $P_{Y|\Phi}^\alpha(y|\theta,\sigma)$ and therefore a numeric posterior

$$P_{\Phi|Y}^\alpha(\theta,\sigma|y) = \frac{P_{Y|\Phi}^\alpha(y|\theta,\sigma)P_\Phi(\theta,\sigma)}{P_Y^\alpha(y)}.$$ 

(2)

$P_Y^\alpha(y) = \int P_{Y|\Phi}^\alpha(y|\theta,\sigma)P_\Phi(\theta,\sigma)d\theta d\sigma$ and $P_Y(y) = \int P_{Y|\Phi}(y|\theta,\sigma)P_\Phi(\theta,\sigma)d\theta d\sigma$ are the normalization constants of the two models, also called the marginal
likelihoods of data $\mathbf{y}$.

Numerical methods are designed so as, if the discretization tends to zero $|\alpha| \to 0$, for some norm or functional $| \cdot |$, then the numeric FM tends to the theoretical FM at some order $O(|\alpha|^p)$. This is the global error control for the numerical method or solver, which we discuss in detail in section 2.1. However, it is of great interest to prove that the same happens with the theoretical vs the numeric posteriors in (1) and (2) respectively, in order to make sense of our Bayesian approach.

Recently a number of papers have dealt with this problem in a theoretical sense by establishing regularity conditions so as

$$\lim_{|\alpha| \to 0} ||P^{\alpha}_{\Phi|\mathbf{Y}}(\theta, \sigma|\mathbf{y}) - P_{\Phi|\mathbf{Y}}(\theta, \sigma|\mathbf{y})|| = 0,$$

for some (e.g. Hellinger) measure metric $|| \cdot ||$; see Cotter et al. (2010) for a review. This forms a sound theoretical basis for the Bayesian analysis of inverse problems. However, in applications we have to choose a discretization $\alpha$. More practical guidelines are needed to choose the numerical solver precision and how this controls the level of approximation between $P^{\alpha}_{\Phi|\mathbf{Y}}(\theta, \sigma|\mathbf{y})$ and $P_{\Phi|\mathbf{Y}}(\theta, \sigma|\mathbf{y})$.

On the other hand Capistrán et al. (2016) present an approach to address the above problem using Bayes factors (BF; the odds in favor) of the numerical model vs the theoretical model (further details will be given in section 2). With equal prior probability for both models, this BF is $P^{\alpha}_{\Phi|\mathbf{Y}}(\mathbf{y}) / P_{\Phi|\mathbf{Y}}(\mathbf{y})$. In an ODE framework, these odds are proved in Capistrán et al. (2016) to converge to 1 (that is, both models would be equal) in the same order as the numerical solver used. For high order solvers Capistrán et al. (2016) illustrates, by reducing the step size in the numerical solver, that there should exist a point at which the BF is basically 1, but for fixed discretization $\alpha$ (step size) greater than zero. This is the main point made by Capistrán et al. (2016): it could be possible to calculate, for solver orders of 2 or more, a threshold for the tolerance such that the numerical posterior is basically equal to the theoretical posterior so, although we are using an approximate FM, the resulting posterior is error free. Capistrán et al. (2016) illustrate, with some examples, that such optimal solver discretization leads to basically no differences in the numerical and the theoretical posterior (since the BF is basically 1). Moreover, since for most solvers its computational complexity goes to infinity as $|\alpha| \to 0$, using the optimal $\alpha$ led in their examples to a 90% save in CPU time.
However, Capistrán et al. (2016) still has a number of shortcomings. First, it depends crucially on estimating the normalizing constants $P_{Y}(y)$ from Monte Carlo samples of the unnormalized posterior, for a range of discretizations $|\alpha|$. This is a very complex estimation problem and is the subject of current research and is in fact very difficult to reliably estimate these normalizing constants in mid to high dimension problems. Second, Capistrán et al. (2016) approach is as yet incomplete since one would need to decrease $|\alpha|$ systematically, calculating $P_{Y}(y)$ to eventually estimate $P_{Y}(y)$, which in turn will pin point a discretization at which both models are indistinguishable. Being this a second complex estimation problem, the main difficulty here is that one has already calculated the posterior for small $|\alpha|$ and therefore it renders useless the selection of the optimal step size.

To improve on Capistrán et al. (2016), the idea of this paper is to consider the expected value of the BFs, before data is observed. We will try to bound this expected BF to find general guidelines to establish error bounds on the numerical solver, depending on the specific problem at hand and the sample design used, but not on particular data. These guidelines will be solely regarding the forward map and, although conservative, represent useful bounds to be used in practice.

We do not discuss in this paper the infinite dimension counterpart of this approach, of interest when inference is needed over function spaces as it is the case in some general PDE inverse problems, see for example Cotter et al. (2009); Dunlop and Stuart (2015) and references therein. As mentioned above, we restrict ourselves to the finite dimensional parametric case where we establish our results.

The paper is organized as follows. Our formal setting will be discussed in section 2. In section 3 we present our main result, including several comments of some implications and practical guidelines for its use. In sections 4 and 5 we present prove of concept examples, considering an ODE and a PDE, respectively. In both cases, using error estimated on the numeric forward maps we were able to very substantially reduce CPU time while obtaining basically the same posterior. Finally, a discussion of the paper is presented in section 6.
2 Setting

Assume that we observe a process \( y = (y_1, \ldots, y_n) \) at locations \( x_1, \ldots, x_n \in D \subset \mathbb{R}^m \). This is a general setting, to include ODEs and PDEs and other inverse problems, in which the domain may include, for example, space and time: \( x_i = [(z_{ix}, z_{iy}), t_i] \). That is, \( x_i \) is an observation at coordinates \( (z_{ix}, z_{iy}) \) and at time \( t_i \), etc.

We assume that the Forward Map \( F_\theta : \mathbb{R}^m \rightarrow \mathbb{R}^q \) is well defined for all parameters \( \theta \) where \( \theta \in A \subset \mathbb{R}^d \). Typically, as mentioned above, \( F_\theta(x) \), for all \( x \in D \), is the solution of a system of ODE’s or PDE’s. This means that \( F_\theta(x) \) are the \( q \) state variables representing the solution of the ODE or PDE system, with parameters \( \theta \), at location \( x \). In many cases, especially dealing with PDEs, the actual unknown is a function in which the inference problem at hand is infinite dimensional. As mentioned in the introduction, in this paper we confine ourselves to the finite dimensional parametric problem, that is, the unknown is \( \theta \) of dimension \( d \). The initial or boundary conditions are taken as known, although these may be turned to be part of the unknown parameters, using common techniques.

Let \( f : \mathbb{R}^q \rightarrow \mathbb{R} \) be the observational functional, in the sense that \( y_i \) is an observation of \( f(F_\theta(x_i)) \). For example, \( f(F_\theta(x_i)) \) is one particular state variable, for which we have observations. We only consider univariate observations at each location \( x_i \).

We assume gaussian errors on the observations, however, we consider the possibility of correlated observations, namely, let \( f_\theta = (f(F_\theta(x_1)), \ldots, f(F_\theta(x_n)))' \) then

\[
\mathbf{y} \mid \theta, \sigma^{-2}, \mathbf{A} \sim N_n(f_\theta, \sigma^{-2} \mathbf{A}),
\]

where \( \sigma^{-2} \mathbf{A} \) is the precision matrix (inverse of the variance-covariance matrix) of the \( n \)-dimensional Gaussian distribution with mean \( f_\theta \). \( \mathbf{A}^{-1} \) is a correlation matrix with some correlation structure on \( D \). \( \mathbf{A}^{-1} \) will be taken as known, but \( \sigma^2 \) will be considered unknown in general. This is a particular covariance structure, very common in time series or spatial statistics. Indeed, if \( \mathbf{A} = \mathbf{I} \) we go back to the common uncorrelated error structure. A specific example is to use a correlation function \( \rho \) an a metric \( d(x_i, x_j) \) in \( D \) to give \( \mathbf{A}^{-1} = (\rho(d(x_i, x_j))) \), and therefore correlation decreases as the location points separate. This is an isotropic correlation structure. Many other structures may be considered and this has been extensively studied in the statistics literature [Christakos (1992)]. Note that the marginal distribution...
for the observations is

\[ y_i = f(F_\theta(x_i)) + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma b_i), \]  

(3)

where \( b_i^2 = |A^{-1}|_{ii} \), that is, \( \sigma b_i \) is the standard error of the noise.

Let also \( f_\alpha = (f(F_\theta^\alpha(x_1)), \ldots, f(F_\theta^\alpha(x_n)))' \) and \( y | \theta, \sigma^2, A \sim N_n(f_\theta^\alpha, \sigma^{-2} A) \) for the numerical model. From this the likelihood of the approximated model is

\[ P_{Y|\theta}(y|\theta, \sigma) = (2\pi\sigma^2)^{-\frac{n}{2}} |A|^{-\frac{1}{2}} \exp \left\{ -\frac{1}{2\sigma^2} (y - f_\theta^\alpha)'A(y - f_\theta^\alpha) \right\}, \]  

(4)

with the corresponding expression for the exact model.

Regarding the prior distribution for the parameters \( P_\Phi(\theta, \sigma) \), we assume that \( P_\Phi(\theta, \sigma) = g(\sigma)P_\Theta(\theta) \). A common and reasonable assumption in which the prior on the observational noise is independent of the prior regarding the actual model parameters.

### 2.1 Global Error Control

We assume we use a numerical method to obtain an approximation of the Forward Map, that is \( F_\theta^\alpha(x_i) \), for some discretization \( \alpha \). As a general setting for approximation strategies, the numerical method or solver discretization \( \alpha \) may now be multidimensional. We assume that the global error control of the solver states that

\[ ||F_\theta^\alpha(x_i) - F_\theta(x_i)|| \leq K_{x_i, \theta}|\alpha|^p, \]  

(5)

for some functional \( |\cdot| \) for the discretization. That is, the solver is of order \( p \). For example \( \alpha = (\Delta x, \Delta t) \) in finite element PDE solvers, etc. and, perhaps \( |\alpha| = \sup |\alpha_i| \). In section [1] we present an ODE example in which \( \alpha = \Delta t \), ie. the time step size, \( |\cdot| \) is the identity and the solver has order \( p = 4 \). Moreover, in section [5] we present a PDE example where \( \alpha = (\Delta x, \Delta t) \), \( |\alpha| = \Delta x \) and the solver has order \( p = 2 \).

Using this asymptotic behavior of the global error and assuming that \( f \) is differentiable, we can write

\[ f(F_\theta^\alpha(x)) - f(F_\theta(x)) = \nabla f(F_\theta(x))(F_\theta^\alpha(x) - F_\theta(x)) + O(|\alpha|^{2p}) = O(|\alpha|^p). \]  

(6)
for all $x \in D$ and $\theta \in A$. We further assume that $\nabla f$ is bounded and that $K_{x_i, \theta} < K'$ for all locations $x_i$ and all $\theta \in A$. From this we conclude that the global error is

$$|f(F_{\theta}^\alpha(x_i)) - f(F_{\theta}(x_i))| \leq K|\alpha|^p,$$

for some global $K$. This approximation is also of order $p$.

### 2.2 Bayes Factors

As mentioned in the introduction the Bayes Factor (BF) of the exact vs the approximated model, for some fixed data $y$ is $\frac{P_Y(y)}{P_Y(y)}$. Assuming an equal prior probability for both models, the BF is the posterior odds of one model against the other (ie. $\frac{p}{1-p}$ with $p = \frac{P_Y^\alpha(y)}{P_Y(y) + P_Y(y)}$ the posterior probability of the numerical model with discretization $\alpha$). In terms of model equivalence an alternative expression conveying the same odds is

$$\frac{1}{2} \left| 1 - \frac{P_Y^\alpha(y)}{P_Y(y)} \right|.$$

We will call the above absolute deviance of the BF from 1 the “ABF”. In terms of the Jeffreys scale if the ABF is less than 1 (ie. $1 \leq \text{BF} \leq 3$) the difference regarding both models is “not worth more than a bare mention” [KASS and RAFTERY 1995, Jeffreys 1961]. An even more stringent requirement would be an ABF less than $\frac{1}{20} = 0.05$, for example, to practically ensure no difference in both the numerical and the approximated posteriors. In the next section we see how to bound the expected ABF in terms of the absolute maximum global error for the numeric FM.

### 3 Main result

We now present our main result.

**Theorem 3.1** For the Expected ABF (EABF) we have that

$$||P_Y(\cdot) - P_Y^\alpha(\cdot)||_{TV} = \int \frac{1}{2} \left| 1 - \frac{P_Y^\alpha(y)}{P_Y(y)} \right| P_Y(y)dy \leq \sqrt{\frac{1}{2\pi} \frac{n}{\sigma^*} K|\alpha|^p \frac{b_i}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} |a_{ij}|},$$

where $\sigma^* = \left( \int \frac{1}{g(\sigma)}d\sigma \right)^{-1}$.
Proof 3.1 As in Capistrán et al. (2016) define the likelihood ratio

\[ R_\alpha(\theta) = \frac{P^\alpha_{Y|\Phi}(y|\theta, \sigma)}{P_Y(y|\theta, \sigma)}. \]

Using (4) and after a simple manipulation we see that

\[ R_\alpha(\theta) = \exp \left[ -\frac{1}{2} \sigma^2 \{ -2(f^\alpha_\theta - f_\theta)'A(y - f_\theta) + (f^\alpha_\theta - f_\theta)'A(f^\alpha_\theta - f_\theta) \} \right]. \]

Let \( D^\alpha_\theta = (f^\alpha_\theta - f_\theta)' \). Using (7) we have

\[ ||D^\alpha_\theta A|| < ||D^\alpha_\theta||_2||A||_2 = O(|\alpha|^{2p}) \] (9)

where \( ||A||_2 \) refers to the induced \( L_2 \) matrix norm. Therefore for \( |\alpha| \) small

\[ R_\alpha(\theta) - 1 = \frac{1}{\sigma^2} D^\alpha_\theta A(y - f_\theta) + O(|\alpha|^{2p}) \]

since \( e^{-x} = 1 - x + O(x^2) \) for \( |x| \) small. Note now that

\[ P^\alpha_Y(y) = P_Y(y) + \int P_{Y|\Phi}(y|\theta, \sigma)(R_\alpha(\theta) - 1)P_\Phi(\theta, \sigma)d\theta d\sigma. \]

Dividing by \( P_Y(y) \) we have

\[ \left| 1 - \frac{P^\alpha_Y(y)}{P_Y(y)} \right| = \int \left( \frac{1}{\sigma^2} D^\alpha_\theta A(y - f_\theta) + O(|\alpha|^{2p}) \right) P_{Y|\Phi}(\theta, \sigma|y)d\theta d\sigma \]
\[ \leq \frac{1}{\sigma^2} \int |D^\alpha_\theta A(y - f_\theta)| P_{Y|\Phi}(\theta, \sigma|y)d\theta d\sigma + |O(|\alpha|^{2p})|. \] (10)

Now for the EABF we have

\[ \int \left| 1 - \frac{P^\alpha_Y(y)}{P_Y(y)} \right| P_Y(y)dy \leq \frac{1}{\sigma^2} \int \int |D^\alpha_\theta A(y - f_\theta)| P_{Y|\Phi}(y|\theta, \sigma)dy P_\Phi(\theta, \sigma)d\theta d\sigma, \]

ignoring the higher order term. Let \( u = D^\alpha_\theta A \) with \( u = (u_i) \), then

\[ \sigma^{-2} |D^\alpha_\theta A(y - f_\theta)| = \sigma^{-2} \sum_{i=1}^{n} u_i(y_i - f(F_\theta(x_i))) \leq \frac{1}{\sigma} \sum_{i=1}^{n} |u_i|b_i \frac{|y_i - f(F_\theta(x_i))|}{\sigma b_i}. \] (11)
Since \( \int \frac{|x|}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \, dx = \sqrt{\frac{2}{\pi}} \) we have

\[
\left| 1 - \frac{P_Y(y)}{P_Y(y)} \right| P_Y(y) \, dy \leq \sqrt{\frac{2}{\pi}} \int \frac{b_i}{\sigma} \sum_{i=1}^{n} |u_i| P_\Theta(\theta, \sigma) \, d\theta \, d\sigma,
\]

and therefore

\[
\int \frac{1}{2} \left| 1 - \frac{P_Y^*(y)}{P_Y(y)} \right| P_Y(y) \, dy \leq \sqrt{\frac{1}{2\pi}} \frac{b_i}{\sigma^*} \sqrt{\sum_{i=1}^{n} |u_i| P_\Theta(\theta) \, d\theta} = \sqrt{\frac{1}{2\pi}} \frac{b_i}{\sigma^*} \int \|D_\theta^a A\|_1 P_\Theta(\theta) \, d\theta.
\]

From (7) note that

\[
|u_i| \leq K |\alpha|^p \sum_{j=1}^{n} |a_{ij}|
\]

and from this we obtain the result.

**Corollary 3.2** The EABF tends to zero in the same order as the numerical solver, that is \( O(|\alpha|^p) \); the same happens to the ABF assuming

\[
\int \left| y_i - f(F_\Theta(x_i)) \right| \frac{1}{\sigma b_i} P_{\Theta/Y}(\theta, \sigma|y) \, d\theta \, d\sigma < \infty.
\]

for all \( x_i \).

**Proof 3.2** The result is immediate for the EABF since the bound in (8) is \( O(|\alpha|^p) \). For the ABF use (10) and (11) to obtain the result.

### 3.1 Remarks on Theorem 3.1

- Note that if, as in many inverse problems formulations, the gaussian observation noise variance \( \sigma^2 \) assumed known, then we could think that its prior is a Dirac delta and indeed \( \sigma^* = (\int \frac{1}{2} g(s) \, ds)^{-1} = \sigma \). In fact, we assume in the examples in sections 4 and 5 that \( \sigma \) is known.

- The bound in Theorem 3.1 is a result of the uniform bound for the error in the numerical solver, as stated in (7). However, a more precise and at least theoretically interesting bound would be using the integral in the rhs of (12)

\[
\int \|D_\theta^a A\|_1 P_\Theta(\theta) \, d\theta < C.
\]
With this one may obtain an expected bound for the EABF. Since it is an expected and not an uniform bound, potentially we may allow more solver error in regions with less a priori mass, etc.

However, our present approach considers using a simpler global bound uniform for all $\theta$, perhaps less precise, but importantly not adding more computational burden on problems already computationally very demanding, as explained in the next remark.

- If we set the absolute uniform global error as $|f(F_0^\alpha(x_i)) - f(F_\theta(x_i))| \leq K_0 = K|\alpha|^p$ and, as explained in section 2.2 if we let the $EABF \leq \frac{1}{20} = 0.05$ we expect nearly no difference in the numerical and the theoretical posterior. For uncorrelated data we have $a_{ij} = \delta_{i,j}$ and therefore $\frac{k}{n} \sum_{i=1}^{n} \sum_{i=1}^{n} |a_{ij}| = 1$. Then, setting $\sqrt{\frac{1}{2\pi} \frac{nK_0}{\sigma^*}} \leq \frac{1}{20}$ we need

$$K_0 \leq \frac{k}{n}\sigma^* \quad (14)$$

where $k = \frac{1}{20} \sqrt{2\pi} \approx 0.12$. That is, we may tolerate an absolute uniform error of up to 12% of the expected standard deviation observation noise for $n = 1$, 0.12% for $n = 10$, 0.012% for $n = 100$ etc. Reasonably, in the light of this analysis of the Bayesian inverse problems, the tolerated error in the numerical solver is put in terms of the observational noise expected and the sample size. When more noise is expected more error may be tolerated and as the sample size increases the numerical solver needs to be more precise.

This is the main application of our theorem, the uniform global error to be accepted should be bounded in terms of the observational noise and sample size considered and not solely as a property of the forward map at hand. Our bound could be conservative, but it is intended to be an useful and applicable tool serving as a reference for the numerical solver precision.

- Note that the bound in (7) may be realized during computation. That is, the solver may be applied and its error estimated at the design points $x_i$, when needing the FM for some specific $\theta$. If the required bound is exceeded then the discretization $\alpha$ could be altered to comply with the error bound. That is, in practice there is no need to establish (7) theoretically, but rather by a careful strategy for actual global error.
estimation (in the numerical analysis literature these error estimates are derived from the so called output or \textit{a posteriori} error estimates, but here we use a different name for obvious reasons). The posterior distribution in most cases is sampled using MCMC, which requires the approximated likelihood at each of many iterations; an automatic process of global error estimation and control will be required in order to comply with (7).

- The result in the corollary regarding the ABF means that, for any fixed data $\mathbf{y}$ the BF $\frac{P^a(\mathbf{y})}{P^b(\mathbf{y})}$ tends to one in the same order as the solver order, that is $O(|\alpha|^p)$. This is a more general version of the main result of Capistrán et al. (2016) using the assumption

$$\int \left| \frac{y_i - f(F_\theta(x_i))}{\sigma_{b_i}} \right| P_\Phi(\theta, \sigma | \mathbf{y}) d\theta d\sigma < \infty$$

(i.e. the posterior expected standardzied absolute residuals are bounded). In Capistrán et al. (2016) they assumed instead that the parameter space $A$ is compact, which implies the above. The setting in Capistrán et al. (2016) is only for ODE’s while ours considers more general forward maps, including ODEs and PDEs.

### 4 Example using an ODE: Logistic growth

As a prove of concept, we base our first numerical study on the logistic growth model which is a common model of population growth in ecology, medicine, among many other applications (Foryś and Marciniak-Czochra, 2003). Let $X(t)$ be, for example, the size of a tumor to time $t$. The logistic growth dynamics are governed by the following differential equation

$$\frac{dX}{dt} = rX(t)(1 - X(t)/K), \quad X(0) = X_0$$

(15)

with $r$ being the growth rate and $K$ the carrying capacity e.g. $\lim_{t \to \infty} X(t) = K$. The ODE in (15) has an explicit solution equal to

$$X(t) = \frac{KX_0}{X_0 + (K - X_0)e^{-rt}}.$$
We simulate a synthetic data set with the error model $y_i = X(t_i) + \varepsilon_i$, where $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$, and the following parameters $X(0) = 100$, $r = 1$, $K = 1000$, $\sigma = 30$. The data are plotted in Figure 1. We consider 26 observations at times $t_i$ regularly spaced between 0 and 10. Capistrán et al. (2016) also studied this example.

Since we have an analytic solution, if we run a numerical solver on the system we may calculate the maximum absolute error of the solver, $K_0$ in (14), exactly by comparing with the analytic solution. Moreover, in Appendix A we explain how the global error may be estimated using Runge-Kutta solver methods. We run a Cash–Karp RK method, of order 5 (Cash and Karp, 1990), which enables us to produce and estimate $\hat{K}_0$ of $K_0$.

The error bound for the FM as stated in (14) is $\frac{k}{\|\mathbf{K}\|_{\infty}} \approx 0.13$. The ODE with the initial condition defines our forward map $\tilde{F}_\theta$ ($q = p = 1$) and we take $f(x) = x$ as the observational functional. To sample from the posterior distribution we use a generic MCMC algorithm called the t-walk (Christen and Fox, 2010).

Regarding the numerical solver we start with a large step size of 0.1, that would maintain numerical stability, and calculate $\hat{K}_0$ and $K_0$. If the solution does not comply with the bound as calculated by the estimate, that is $\hat{K}_0 > 0.13$, a new solution is attempted by reducing the step size by half,
until the Runge-Kutta estimated global absolute errors is within the bound, \( \hat{K}_0 \leq 0.13 \). The results are shown in figure 2. Moreover, a fine step size Runge-Kutta solver was also ran with step size of 0.005, for comparisons. No difference was observed in both posterior distributions, and the posterior mean and MAP estimators were basically identical. However, a 93\% save was obtain by reducing CPU time from approximately 100 to 7 min, with 40,000 MCMC iterations.

Since in this case an analytic solution is available we also calculate the exact maximum absolute error \( K_0 \). The average estimated error was \( 7.8 \cdot 10^{-3} \) while the average exact error was \( 3.8 \cdot 10^{-5} \), for the adaptive step size method as describe above. For the fixed time step method we had estimated and average errors \( 2.1 \cdot 10^{-8} \) and \( 6.2 \cdot 10^{-12} \), respectively. In both cases our error estimates where some orders of magnitude higher than the true errors. Certainly the fine (fixed) step solver is quite more precise reaching more than 5 orders of magnitude larger precision. However, in the light of theorem 3.1 this increase precision is not worth the great increase in CPU time since indeed results are basically the same using a coarser solver. And a 93\% CPU time reduction was obtained nevertheless our error estimates where two orders of magnitude higher. Numerical errors are now viewed, not in a context free situation, but in the context of this inverse problem, relative to sample size and expected observational errors, by using the bound in (14).

5 Example using a PDE: Burgers’ equation

Burgers’ is a fundamental PDE with many applications in fluid mechanics, acoustics, traffic flow modeling, among others LeVeque (2002).

Let us consider the Riemann problem for the viscous Burgers’ equation

\[
\begin{align*}
    u_t + uu_z &= \epsilon u_{zz} \\
    u(z, 0) &= \begin{cases} 
      u_L & z < z_0 \\
      u_R & z_0 < z,
    \end{cases}
\end{align*}
\]

where \( u_L, u_R, z_0 \) and \( \epsilon \) are real numbers. The direct problem is to compute \( u = u(z, t) \) solving the initial value problem (16). We assume \( u_L > u_R \) which would correspond to a shock wave in the inviscid limit \( \epsilon = 0 \).

Using the Cole-Hopf transformation we can obtain the solution of problem
Figure 2: Logistic growth example marginal posterior distributions of \(r\) (a) and \(K\) (b), \(\sigma = 30\). For a fine step size of 0.005 (blue histograms) we obtain basically the same results (green histograms) as starting from a step size of 0.1 and restricting the estimated maximum absolute error to the proposed bound, that is \(\hat{K}_0 \leq \frac{k}{2n} \sigma = 0.13\). A 92% CPU time reduction was obtained, from approximately 103 to 7 min, running 40,000 iterations of the MCMC.

in closed form to obtain

\[
    u(z, t) = u_L - \frac{u_L - u_R}{1 + q(z - z_0, t) \exp\left(-\frac{u_L - u_R}{2\epsilon}(z - z_0 - ct)\right)}
\]  \tag{17}

where \(q(z, t) = \frac{\text{erfc}(z - u_R t / \sqrt{4\epsilon t})}{\text{erfc}(z - u_L t / \sqrt{4\epsilon t})}\) and \(c = (u_L + u_R) / 2\); see Chapter 4 of Whitham \cite{Whitham1999}, for details.

The inference problem is to estimate \(\theta = (u_L - u_R, z_0)\) given observations \(u_j = u(z_1, t_j)\) at a fixed point in space \(z_1\) for \(j = 1, \ldots, k\). That is, the locations are \(x_j = (z_1, t_j)\). As in the previous example, the observation operator \(f(\cdot)\) is the identity.

To numerically solve the Riemann problem in \cite{LeVeque2002}, we use a classical second-order accurate finite-volume implementation of the viscous Burgers’ equation with piecewise linear slope reconstruction with outflow boundary conditions, see Leveque \cite{LeVeque2002}. In this case, we build a grid with both space and time steps, namely \(\alpha = (\Delta z, \Delta t)\). The standard procedure is to fix \(\Delta z\) and the temporal grid is determined by a Courant-Friedricks-Levy condition

\[
    \Delta t_n = c \frac{\Delta z}{\max |u(\cdot, t_{n-1})|}. \tag{18}
\]
In the numerical example below we use $c = 0.1$. In this case $|\alpha| = \Delta z$ and $p = 2$, that is, the numerical method is order 2, $O(|\alpha|^2)$. Moreover, error estimates may be obtained from this solution, as explained in Appendix B.

Using the analytic solution in (17) and the error estimates, we can establish the exact error $K_0$ and its estimate $\hat{K}_0$ as in the previous example. From $\hat{K}_0$ we check if the adaptive method is within the bounds established in (14). Note that, in the current case $\hat{K}_0 \approx K_0$, provided $K_0$ is estimated through interpolation, as shown in Appendix B.

Again we use synthetic data using the observation point $z_1 = 2.0$, $n = 6$, $t = \{0.0, 0.1, 0.2, 0.3, 0.4, 0.5\}$ and $\sigma = 0.0115$ (we choose this standard error to obtain a signal-to-noise ratio of 100). The true parameter values are $u_R = 2$, $u_L = 1$, $z_0 = 1$.

We estimate the numerical posterior distribution with a high resolution spatial grid of 512 points for $z \in [0, 4]$, and an adaptive grid, starting with a grid of 128. If the bound is not met then the grid was doubled to 256 and thereafter to 512. We used 20,000 iterations of the twalk MCMC algorithm [Christen and Fox (2010)] to simulate from the posterior distributions using the high-resolution and adaptive grid solvers. The execution time for the high resolution and adaptive grids are respectively 10.95 h and 4.27 h respectively. That is, in this case we obtained a 60% decrease in CPU, again leading to basically the same posterior distribution.

6 Discussion

The Bayesian UQ analysis of inverse problems continues to be a very challenging research topic. In this paper we tried to contribute to the development of this discipline by analyzing the relationship between error in the numerical solver of the differential system under study and the corresponding induced error in the numerical posterior distribution. Once it is established, under regularity conditions, that the numerical posterior distribution tends to the theoretical posterior as the solver error tends to zero, we still need to decide to which precision run the solver. Elaborating on previous work [Capistrán et al. (2016), theorem 3.1] suggest that by carefully choosing a threshold for the global error in the solver we may obtain a posterior distribution that is basically error free. An intuitive perspective on our result is the following: since there is observational error, we may tolerate certain small amount of error in the solver, which will end up blurred by the observational error and
Figure 3: Burgers equation example, marginal posterior distribution for (a) $u_L - u_R$ and (b) $z_0$. Blue histograms are the result of the adaptive grid using our bound, transparent green histogram denotes the posterior distribution from the high resolution grid (see text). Both histograms are basically the same, with a 60% decrease in CPU time.

therefore not noticeable in the posterior distribution.

Indeed, “small” is relative to the data error standard deviation $\sigma$ (and to the sample size), as expressed in (14). This also suggest that, in Bayesian UQ, solver error could be viewed in the perspective of the inference problem at hand, potentially allowing for less precise and less computational demanding solvers that, nevertheless induce basically no error in the resulting posterior distribution and therefore in the uncertainty quantification of the problem at hand.

On the other hand, it is well known that the numerical solver discretization $\alpha$ must be carefully tuned and $|\alpha|$ cannot be increased to arbitrary values. In complex cases, beyond some tight limits for the discretization the numerical solver becomes unstable and results as in (5) cease to be valid. Indeed, solver order and global error control are properties valid for “small” $|\alpha|$. Therefore, in a large set of case studies, little room will be available to decide on an optimal solver discretization. Moreover, in very complex PDE solvers, just changing the discretization is a very demanding enterprise, since there is as yet no automatic and reliable way to define the solver grid, as in for example some spacio-temporal 3D PDE case studies Cui et al. (2011b).

Our examples were proof of concept only, but show promising results.
More importantly, we believe, since the bound in (14) has a simple form, the posterior adaptive control described in both the ODE and the PDE examples could be applied in other case studies. However, this hinges on the availability of reliable, adaptive-like, solver error estimates which, unfortunately, are not always readily available.

A natural continuation of this work is to consider the performance of embedded methods such as Cash-Karp RK45, as well as other feasible alternatives, on stiff ODE problems in this Bayesian context. For PDEs our current interest is on conservation laws approximating the Forward Map by the Discontinuous Galerkin method. For this method, error estimates rest on a solid foundation making our approach promising, see Hesthaven and Warburton (2007); Di Pietro and Ern (2011).

The study of our results in more complex UQ problems is also left for future research. Note also that in many PDE problems the actual unknown is a function, eg. an unknown boundary condition on a scattering problem, needed to be recovered from data. In such a case, the theoretical posterior distribution is infinite dimensional and, as we explained from the onset, we did not consider such case. The proof of our results in such arbitrary space setting is also left for future research.

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A Global error estimation in Runge-Kutta methods

For the reader’s convenience, here we briefly describe how we may estimate the global error in solving the following ODE initial value problem

\[ \frac{X(t)}{dt} = G(t, X, \theta), X(0) = X_0, \]

when using a Runge-Kutta (RK) type numerical method, see Quarteroni et al. (2006) chap. 11 for details. We need the parameters \( \theta \) of the ODE system to be fixed and therefore we write \( G(t, X) = G(t, X, \theta) \) to ease notation.

A RK method can be written as follows. Let \( h > 0 \) be a (time) step size and define a uniform grid such that \( t_{n+1} = t_n + h \). In this case \( |\alpha| = h \). Let \( u_{n+1} = u_n + h \sum_{i=1}^{s} b_i K_i; \) \( u_{n+1} \) is the approximation for \( X(t_n) \) and \( K_i = G(t_n + c_i h, u_n + h \sum_{j=1}^{s} a_{ij} K_j), \quad i = 1, 2, \ldots, s \). \( s \) denotes the number of stages of the method.
The components of the vector $c' = (c_1, c_2, \ldots, c_s)$ need to satisfy $c_i = \sum_{j=1}^{s} a_{ij}, \quad i = 1, 2, \ldots, s$. Let $A = (a_{ij})$ and $b' = (b_1, b_2, \ldots, b_s)$, any RK method is defined by the matrix $A$ and the vectors $b$ and $c$. To have an explicit method we require $a_{ij} = 0$ for $j \geq i$, with $i = 1, 2, \ldots, s$. We used an explicit method in our implementation.

The local truncation error $\tau_{n+1}$ at node $t_{n+1}$ of the RK method is defined as the error made in step $n + 1$ of the solver if starting at the exact value $X(t_n)$, that is $\tau_{n+1} = X(t_{n+1}) - X(t_n) - h \sum_{i=1}^{s} b_i K_i$. The RK method is consistent, if $\tau = \max_n |\tau_n| \to 0$ as $h \to 0$. This happens if and only if $\sum_{i=1}^{s} b_i = 1$. The RK method is of order $p$ if $\tau = O(h^{p+1})$ as $h \to 0$ and it is known that $s \geq p$. The global (truncation) error at knot $t_n$ is defined as the error made by the solver, that is $e_n = X(t_n) - u_n$. It is clear that $e_n = \sum_{i=1}^{n} \tau_n$. Under regularity conditions for a RK method of order $p$ we have $K_0 = \max_n |e_n| = O(h^p)$ as $h \to 0$. That is, the maximum absolute global error $K_0$ is of order $p$ as $h \to 0$.

The strategy described here to estimate $e_n$ is to consider two embedded RK methods to solve the system, one with order $p$ and one with order $p - 1$, both with the same number of stages $s$ and the same matrix $A$ and vector $c$, only with different vectors $b$ and $\hat{b}$, respectively.

Let $u_{n+1}$ be the $n + 1$ estimation of $X(t_{n+1})$ of the $p$ order method and let $y_{n+1}$ be obtained by the $p - 1$ order method by starting at $u_n$, namely

$$u_{n+1} = u_n + h \sum_{i=1}^{s} b_i K_i \quad \text{and} \quad y_{n+1} = u_n + h \sum_{i=1}^{s} \hat{b}_i K_i.$$ 

An estimation of the local truncation error at $t_{n+1}$ is $\hat{\tau}_n = u_{n+1} - y_{n+1} = h \sum_{i=1}^{s} (b_i - \hat{b}_i) K_i$ which is basically a byproduct of the $p$ order solver.

The estimate of the global truncation error at knot $t_n$ is then $\hat{e}_n = \sum_{i=1}^{n} \hat{\tau}_n$.

B Global error estimation in the Burgers PDE solver

In order to solve numerically the initial condition problem for the viscous Burgers in [16] we used a second order explicit finite-volume method to handle the advective flux. On the other hand, second order time-stepping is accomplished through Crank-Nicolson updating implicitly in the viscosity
We discretize the solution using homogeneous Neumann conditions on a space interval \( I = [0, 4] \) adding two ghost cells at each endpoint. In order to march in time we enforce the Courant-Friedrichs-Levy condition through the time-stepping rule \( \text{(18)} \) where \( c = 0.1 \) and \( u_h \) is the numerical solution at time \( t \). Discretization is implemented setting a number of space points, e.g. \( N = 2^9 \). Of note, the time step is adapted to obtain the solution at prescribed observation times \( t = \{0.0, 0.1, 0.2, 0.3, 0.4, 0.5\} \).

If we denote the numerical solution by \( u_h \), then the residue is
\[
R_h(u) = \frac{\partial u_h}{\partial t} + u \frac{\partial u_h}{\partial z} - \epsilon \frac{\partial^2 u_h}{\partial z^2}.
\] (19)

We apply our main result using the following after the fact error estimate for continuous approximations to nonlinear viscous hyperbolic conservation laws; see theorem 5.2 of Cockburn \cite{Cockburn}.

Let \( v \) be the entropy solution (of problem \( \text{(16)} \)) and let \( u \) be a continuous approximation. Then
\[
||u(T) - v(T)||_{L^1(\mathbb{R})} \leq \Phi(v_0, u, T) \] (20)

where
\[
\Phi(v_0, u, T) = ||u(0) - v_0||_{L^1(\mathbb{R})} + ||R_h(u)||_{L^1(0, T) \times \mathbb{R}} + C(u) \sqrt{\epsilon}
\]
and
\[
C^2(u) = 8|u|_{L^\infty(0,T;TV(\mathbb{R}))}|u|_{L^1(0,T;TV(\mathbb{R}))}.
\]

Note that the finite volume method that we have used lets the residual go to zero quadratically. Hence, we have the following application of Cockburn theorem. Let \( v(t) \) denote the analytic solution \( \text{(17)} \) of problem \( \text{(16)} \), and let \( u_h \) denote the finite volume solution at times \( t^n \), \( n = 1, ..., N \). Following Cockburn analysis, let us denote by \( \mathcal{U} \) the set of all the interpolates \( u \) such that \( u(t^n) = u_h(t^n) \) for \( n = 1, ..., N \). Then application of Theorem 5.2 of Cockburn gives
\[
||u_h(t^n) - v(t^n)||_{L^1(\mathbb{R})} \leq \inf_{u \in \mathcal{U}} \Phi(v_0, u; t^n), \ n = 1, ..., N
\]

Let us define
\[
r(u_h, t^n) = \frac{\Phi(v_0, u, T)}{||u_h(t^n) - v(t^n)||_{L^1(\mathbb{R})}}.
\] (21)

In order to estimate \( \hat{K}_0 \approx K_0 \) we take \( 2^N + 1 \) grid points on the spatial domain \( z \in [0, 4] \) for \( N = 6, 7, 8, 9, 19 \) and interpolate \( r(u_h, 1) = 1 + K_0 h^2 \), where \( h = 1/\Delta z \).