Bayesian Optimization of Hyperparameters when the Marginal Likelihood is Estimated by MCMC

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Abstract

Bayesian models often involve a small set of hyperparameters determined by maximizing the marginal likelihood. Bayesian optimization is a popular iterative method where a Gaussian process posterior of the underlying function is sequentially updated by new function evaluations. An acquisition strategy uses this posterior distribution to decide where to place the next function evaluation. We propose a novel Bayesian optimization framework for situations where the user controls the computational effort, and therefore the precision of the function evaluations. This is a common situation in econometrics where the marginal likelihood is often computed by Markov Chain Monte Carlo (MCMC) methods, with the precision of the marginal likelihood estimate determined by the number of MCMC draws. The proposed acquisition strategy gives the optimizer the option to explore the function with cheap noisy evaluations and therefore finds the optimum faster. Prior hyperparameter estimation in the steady-state Bayesian vector autoregressive (BVAR) model on US macroeconomic time series data is used for illustration. The proposed method is shown to find the optimum much quicker than traditional Bayesian optimization or grid search.

Keywords: Acquisition strategy, Optimized precision, Steady-state BVAR, US example.

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1 Introduction

The trend in econometrics is to use increasingly more flexible models that can give a richer description of the economy under investigation. As the model complexity increases, the estimation problems get more involved and computationally costly MCMC methods are often used to sample from the posterior distribution.

Most models involve a relatively small set of hyperparameters that needs to be chosen by the user. As an example, consider the steady-state BVAR model of Villani (2009), which is widely used among practitioners and professional forecasters (see e.g. Gustafsson et al. (2016) and Stockhammar and Österholm (2017)) and is used in Section 4 for illustration. The choice of prior distribution in BVARs is often reduced to the selection of a small set of prior hyperparameters. Some of these hyperparameters can be specified subjectively by experts, for example, the steady-state is usually given rather informative subjective priors. Other prior hyperparameters control the smoothness/shrinkage properties of the model and are less easy to specify subjectively. Giannone et al. (2015) proposed to treat these hard-to-specify prior hyperparameters as unknown parameters and explore the joint posterior of the hyperparameters, the VAR dynamics, and the shock covariance matrix. This is a statistically elegant approach but can be computationally costly, and most practitioners seem to prefer to fix the hyperparameters before estimating the other model parameters. Carriero et al. (2012) propose a brute force approach where the marginal likelihood is evaluated over a grid. This is very computationally demanding, and the vast majority of applications instead use conventional values for the hyperparameters, dating back to Doan et al. (1984). However, the conventional values were found to be optimal on a specific historical dataset and are likely to be suboptimal for other datasets.

Hence, there is a real practical demand for a fast method for optimizing the marginal likelihood over a set of hyperparameters. However, the marginal likelihood is rarely available in closed form. The BVARs with conjugate priors considered in Carriero et al. (2012) are an exception, but already the steady-state VAR needs MCMC methods to evaluate the marginal likelihood. This makes the optimization problem challenging since every evaluation of the marginal likelihood requires a full MCMC run.

Bayesian optimization (BO) is an iterative optimization technique originating from machine learning. BO is particularly suitable for optimization of costly noisy functions in small to moderate dimensional parameter spaces (Brochu et al., 2010; Snoek et al., 2012) and is therefore well suited for marginal likelihood optimization. The method treats the underlying function as an unknown object that can be inferred by Bayesian inference by evaluating the function at a finite number of points. A Gaussian process prior expresses the Bayesian prior beliefs about the underlying function, often just containing the information that the function is believed to has a certain degree of smoothness. Bayes theorem is then used to sequentially update the Gaussian process posterior after each new function evaluation.
Bayesian optimization uses the most recently updated posterior of the function to decide where to optimally place the next function evaluation. This so-called acquisition strategy is a trade-off between: i) exploiting the available knowledge about the function to improve the current maxima and ii) exploring the function to reduce the posterior uncertainty.

Our paper proposes a framework for Bayesian optimization for the setting where the user can control the precision and computational cost of each function evaluation. The typical scenario that we have in mind is when the marginal likelihood is computed by MCMC. This is a very common situation in econometrics using, for example, the estimators in Chib (1995), Chib and Jeliazkov (2001) and Geweke (1999). The precision of the marginal likelihood estimate at each evaluation point is then chosen by the user via the number of MCMC iterations. This makes it possible to use occasional cheap noisy evaluations of the marginal likelihood to quickly explore the marginal likelihood over hyperparameter space during the optimization. Our proposed acquisition strategy can be seen as jointly deciding where to place the new evaluation but also how much computational effort to spend in obtaining the estimate. We implement this strategy by a stopping rule for the MCMC sampling combined with an auxiliary prediction model for the computation effort at any new evaluation point; the auxiliary prediction model is learned during the course of the optimization.

We apply the method to the steady-state BVAR and demonstrate that the new acquisition strategy finds the optimal hyperparameters faster than traditionally used acquisition functions. It is also substantially faster than a grid search and finds a better optimum.

The outline of the paper is as follows. Section 2 introduces the hyperparameter estimation problem and presents Chib’s marginal likelihood estimator from Gibbs sampling. Section 3 gives the necessary background on Gaussian processes and Bayesian optimization and introduces our new Bayesian optimization framework. Section 4 assesses the performance of the proposed algorithm in empirical examples. The final section concludes and the appendix gives implementation details.

2 Hyperparameter estimation

Hyperparameters in Bayesian econometric models can have a large effect on empirical results and have to be selected with care. The method proposed here is generally applicable and will be presented in full generality, but we will consider selection of hyperparameters in the popular class of Bayesian vector autoregressive models (BVARs) as our running example.

2.1 Hyperparameter estimation

Consider the standard BVAR model

$$y_t = \sum_{k=1}^{K} \Pi_k y_{t-k} + \varepsilon_t,$$
where \( \{\varepsilon_t\}_{t=1}^T \) are iid \( N(0, \Sigma) \). A simplified version of the Minnesota prior (see e.g. Karlsson (2013)) without cross-equation shrinkage is of the form

\[
(\Pi, \Sigma) \sim MNIW(\Pi, \Omega_\Pi, S, \nu),
\]

with

\[
\Sigma \sim IW(S, \nu), \quad \text{vec}(\Pi')\Sigma \sim N(\text{vec}(\Pi'), \Sigma \otimes \Omega_\Pi).
\]

where \( \text{vec}(\Pi) \) and \( \Omega_\Pi \) denotes the prior mean and covariance of the coefficient matrix, \( S \) is the prior scale matrix with the prior degrees of freedom, \( \nu \). The diagonal elements of \( \Omega_\Pi \) are given by

\[
\lambda_{ii} = \frac{\lambda_1^2}{(l \lambda_3 s_r)^2}, \quad \text{for lag } l \text{ of variable } r, \quad i = (l - 1)p + r,
\]

where \( \lambda_1 \) controls the overall shrinkage and \( \lambda_3 \) the lag-decay shrinkage set by the user, \( s_r \) denotes the estimated standard deviation of variable \( r \). The fact that we do not use the additional cross-equation shrinkage hyperparameter, \( \lambda_2 \), makes this prior conjugate to the VAR likelihood, a fact that will be important in the following. It has been common practice to use standard values that dates back to Doan et al. (1984), but there has been a renewed interest to find values that are optimal for the given application (see e.g. Giannone et al. (2015), Carriero et al. (2012), and Bańbura et al. (2010)). Two main approaches have been proposed. First, Giannone et al. (2015) proposed to sample from the joint posterior distribution using the decomposition

\[
p(\beta, \theta|y_{1:T}) = p(\beta|\theta, y_{1:T})p(\theta|y_{1:T}),
\]

where \( p(\theta|y_{1:T}) \) is the marginal posterior distribution of the hyperparameters. The algorithm samples from \( p(\theta|y_{1:T}) \) using Metropolis-Hastings (MH) and then samples directly from \( p(\beta|\theta, y_{1:T}) \) for each \( \theta \) draw by drawing \( \Pi \) and \( \Sigma \) from the Normal-Inverse Wishart distribution. There are some limitations to using this approach. First, the \( p(\theta|y_{1:T}) \) can be multimodal and it can be hard to find a good MH proposal density, making the sampling time-consuming. Second, it has been our experience that practitioners view hyperparameter selection similar to model selection, and want to determine a fixed value for \( \theta \) once and for all early in the model building process.

Carriero et al. (2012) instead propose an exhaustive grid search to find the \( \theta \) that maximizes \( p(\theta|y_{1:T}) \) and then uses that optimal \( \theta \) throughout the remaining analysis. The obvious drawback here is that a grid search is very costly, especially with more than a couple of hyperparameters.

A problem with both the approach in Giannone et al. (2015) and Carriero et al. (2012) is that \( p(\theta|y_{1:T}) \) is often not available in closed form. This is true e.g. for the Minnesota prior with cross-equation shrinkage since the prior is no longer conjugate, and is also true
for the steady-state BVAR (Villani, 2009). However, MCMC can often be used to get a noisy estimate of \( p(\theta | y_{1:T}) \) at any \( \theta \), usually at a sizeable computational cost.

A common approach to select hyperparameters is to maximize the marginal likelihood, 
\[
p(y_{1:T} | \theta) = \int p(y_{1:T} | \theta, \beta) p(\beta | y_{1:T}) \ d\beta,
\]
which is equivalent to maximizing the posterior distribution of the hyperparameters under a flat hyper-prior, as is noted in both Carriero et al. (2012) and Giannone et al. (2015).

### 2.2 Estimating the marginal likelihood

Neither the posterior of the hyperparameters nor the marginal likelihood are tractable for most models. Chib (1995) proposes an accurate way of computing a simulation consistent estimate of the marginal likelihood when the posterior can be obtained via Gibbs sampling, which is the case for many econometric models. Chib and Jeliazkov (2001) extend Chib’s estimator to when the posterior is simulated from with MH. Chib’s (1995) estimator is based on the following identity obtained by inverting Bayes’s theorem:

\[
m(y) = \frac{p(y | \theta)p(\theta)}{p(\theta | y)}.
\]

Consider, for example, the steady-state BVAR model, which can be sampled using a three-block Gibbs sampler, see Villani (2009). The joint posterior of the three-block model can be factorized, and evaluated in a point \( \beta^* \) as:

\[
p_\theta(\beta_1^*, \beta_2^*, \beta_3^* | y) = p_\theta(\beta_1^* | \beta_2^*, \beta_3^*, y)p_\theta(\beta_2^* | \beta_3^*, y)p_\theta(\beta_3^* | y).
\]

Now, \( p_\theta(\beta_1^* | \beta_2^*, \beta_3^*, y) \) is a full conditional distribution, w.r.t. the hyperparameters in \( \theta \), which we have available in closed form, and

\[
p_\theta(\beta_3^* | y) = \int p_\theta(\beta_3^* | \beta_1, \beta_2, y)p_\theta(\beta_1, \beta_2 | y)d\beta_1 d\beta_2
\]

can be estimated by \( G^{-1} \sum_{i=1}^N p_\theta(\beta_3^* | \beta_1^{(i)}, \beta_2^{(i)}, y) \) using the MCMC chains \( \left\{ \beta_1^{(i)}, \beta_2^{(i)} \right\}_{i=1}^G \).

Further, \( p_\theta(\beta_2^* | \beta_3^*, y) \) can easily be obtained by running a reduced version on the same Gibbs sampler, but this time, we fix \( \beta_3 \) to \( \beta_3^* \) in every Gibbs iteration. We can then estimate \( p_\theta(\beta_2^* | \beta_3^*, y) = \int p_\theta(\beta_2^* | \beta_1, \beta_3^*, y)p_\theta(\beta_1 | \beta_3^*, y)d\beta_1 \) by \( G^{-1} \sum_{i=1}^G p_\theta(\beta_2^* | \beta_1^{(i)}, \beta_3^*, y) \), where \( \left\{ \beta_1^{(i)} \right\}_{i=1}^G \) are draws from the reduced Gibbs sampler. Chib (1995) also derives asymptotic standard errors for the estimator. For more details regarding the Chib estimator, see Appendix A.
3 Bayesian optimization of hyperparameters

3.1 Gaussian processes

Since Bayesian optimization is a relatively unknown method in econometrics, we give an introduction here to Gaussian processes and their use in Bayesian optimization.

A Gaussian process (GP) is a (possibly infinite) collection of random variables such that any subset is jointly distributed according to a multivariate normal distribution, see e.g. Williams and Rasmussen (2006).

A Gaussian process, denoted by \( f(x) \sim \mathcal{GP}(m(x), k(x, x')) \), can be seen as a probability distribution over functions \( f: \mathcal{X} \rightarrow \mathbb{R} \) that is completely specified by its mean function, \( m(x) \equiv \mathbb{E}f(x) \), and its covariance function, \( \mathbb{C}(f(x), f(x')) \equiv k(x, x') \), where \( x \) and \( x' \) are two arbitrary input values to \( f(\cdot) \). Note that the covariance function specifies the covariance between any two function values, \( f(x_1) \) and \( f(x_2) \). A popular covariance function is the squared exponential (SE):

\[
k(x, x') = \sigma^2_f \exp\left(-\frac{|x - x'|^2}{2\ell^2}\right),
\]

where \( |x - x'| \) is the Euclidean distance between the two points; the covariance function is specified by its two kernel hyperparameters, the scale parameter \( \sigma_f > 0 \) and the length scale \( \ell > 0 \). The scale parameter \( \sigma_f \) govern the variability of the function and the length scale determines how fast the correlation between two function values taper off with the distance \( |x - x'| \), see Figure 1. The covariance function \( k(x, x') \) can be used to compute the covariance matrix for any subset of function values. The fact that any finite sampling of function values \( \{f(x_n) \mid x_n \in \mathcal{X}\}_{n=1}^N \) constitutes a multivariate normal distribution on \( \mathbb{R}^N \) allows for the convenient conditioning and marginalization properties of the multivariate normal distribution. Decisions regarding the kernel functions are important when working
with GPs, and there are a few standard alternatives to choose from. An increasingly popular alternative to the squared exponential kernel is the Matérn kernel, see e.g. Matérn (1960) and Williams and Rasmussen (2006). The Matérn kernel has an additional hyperparameter, $\nu > 0$, in addition to the length scale $\ell$ and scale $\sigma_f$, such that the process is $k$ times mean square differentiable if $\nu > k$. Hence, $\nu$ controls the smoothness of the process and it can be shown that the Matérn kernel approaches the SE kernel as $\nu \to \infty$ (Williams and Rasmussen, 2006). The SE kernel is therefore considered too smooth for many applications. Our approach is directly applicable for any valid kernel function, but we will use the popular Matérn $\nu = 5/2$ kernel in our applications:

$$k_{\nu=5/2}(r) = \sigma_f^2 \left( 1 + \frac{\sqrt{5}r}{\ell} + \frac{5r^2}{3\ell^2} \right) \exp \left( -\frac{\sqrt{5}r}{\ell} \right),$$

where $r = |x - x'|$. The Matérn 5/2 has two continuous derivatives which is often a requirement for Newton-type optimizers and is often recommended for Bayesian optimization (Snoek et al., 2012). To find the optimal value for the $\sigma_f$ and $\ell$, the method of MacDonald et al. (2015) is used.

### 3.2 Bayesian optimization

Bayesian optimization is distinct from other optimization methods in that it constructs a probabilistic model for $f$, which it then uses to solve the optimization problem. The main use of a probabilistic model on $f$ is that we can quantify the uncertainty of our function in different regions of the function space to select optimal future evaluation points. Such utility functions are referred to as acquisition functions in the Bayesian optimization literature (see e.g. Brochu et al., 2010 and Snoek et al., 2012) and are generally denoted by $a(x)$.

An intuitively sensible acquisition rule is to select a new evaluation point that maximizes the probability of obtaining a higher function value than the current maximum, $f_{\text{max}}$, i.e. the Probability of Improvement (PI):

$$PI(x) \equiv P(f(x) > f_{\text{max}}) = \Phi \left( \frac{m(x) - f_{\text{max}}}{s(x)} \right),$$

where $f_{\text{max}}$ is the maximum value of the function obtained so far. $m(x)$ and $s(x)$ are the posterior mean and standard deviation of $f$ in the point $x$, conditional on the available function evaluations, and $\Phi$ denotes the cumulative standard normal distribution. The PI criterion will choose the point which is most probable to give an improvement but does so without regard to the size of the improvement. For this reason, the Expected Improvement
(EI) is usually preferred:

\[
EI(x) = (m(x) - f_{\text{max}})\Phi \left( \frac{m(x) - f_{\text{max}}}{s(x)} \right) + s(x)\phi \left( \frac{m(x) - f_{\text{max}}}{s(x)} \right),
\]

(1)

where \( \phi \) denotes the density function of the standard normal distribution. We can see from (1) that the first part is associated with the magnitude of our predicted improvement and the second part is related to the uncertainty of our function in that area. Thus, the EI provides a deterministic way to select a new point where the decision incorporates the trade-off between high expected improvement (exploitation) and to learn more about the underlying function (exploration). This is illustrated in Figure 2, where the black line shows the true objective function, the blue line denotes the posterior mean of the GP, and the pink-shaded regions show 95\% posterior probability bands for \( f \). The red dashed lines indicate the position of the current maximum, red (small) dots show historical function evaluations, and the green (large) dot denotes the current evaluation. The lower part shows the EI acquisition function evaluated for each \( x \). As we start in the top-left corner, we can see that the algorithm starts to climb towards the maximum (upper part), and the EI acquisition function (lower part) indicates that there is a high expected improvement by moving further to the right. After further improvements (top-right plot followed by bottom-left plot), the algorithm has found an \( x \) close to the maximum such that further expected improvement is low in the middle \( x \)-region. The EI strategy then suggests that it is worth to explore the endpoints where there is still high uncertainty. In the final (lower-right) figure, the uncertainty at the endpoints is removed, and the algorithm will continue a more thorough search in the region close to the maximum until it is stopped.
However, acquisition rules like PI or EI do not take into account that different evaluation points can be more or less costly. To introduce the notation of cost into the acquisition strategy, Snoek et al. (2012) proposed Expected Improvement per second, $EIS(x) \equiv EI(x)/c(x)$, where $c: \mathcal{X} \to \mathbb{R}^+$ is a duration function that measures the evaluation time at input $x$ in seconds. More generally, we can define $a(x)/c(x)$ as an effort-aware acquisition function. The duration function is typically unknown and Snoek et al. (2012) proposed to estimate it alongside $f$ using an additional Gaussian process for $\log c(x)$.

### 3.3 Bayesian optimization with optimized precision

EIS assumes that the duration (or the cost) of function evaluations are unknown, but fixed for a given input $x$; once we visit $x$, the cost of the function estimate $\hat{f}(x)$ is given. However, the user can often choose the duration spent to obtain a certain precision in the estimate; for example by increasing the number of MCMC iterations when the marginal likelihood is estimated by MCMC. This perspective opens up for strategies that not only optimize for the next evaluation point, but also optimize over the computational resources, or equivalently,
the precision of the estimate $\hat{f}(x)$. We formally extend BO by modeling the function evaluations with a heteroscedastic GP

$$\hat{f}(x) = f(x) + \epsilon, \; \epsilon \sim N(0, \sigma^2(G))$$

$$f \sim G\mathcal{P}(\mu(x), k(x, x')),$$

where the noise variance $\sigma^2(G)$ is now an explicit function of the number of MCMC iterations, $G$, or some other duration measure. Hence the user can now choose both where to place the next evaluation and the effort spent in computing it by maximizing

$$\tilde{a}(x, G) \equiv a(x)/G,$$

with respect both $x$ and $G$, where $a(x)$ is a baseline acquisition function, for example EI.

A complication with maximization of $\tilde{a}(x, G)$ is that while we typically know that $\sigma(G) = O(1/\sqrt{G})$ in Monte Carlo or MCMC, the exact numerical standard error depends on the integrated autocorrelation time (IACT) of the MCMC chain. Note that the evaluation points can, for example, be hyperparameters in the prior, where different values can give rise to varying degrees of well-behaved posteriors, so we cannot expect the IACT to be constant over the hyperparameter space. Rather than maximizing $\tilde{a}(x, G)$ with respect to both $x$ and $G$ directly, we propose to implement the algorithm in an alternative way that achieves a similar effect. The idea includes stopping the evaluation early whenever the function evaluation turns out to be hopelessly low with a low probability of improvement over the current $f_{\text{max}}$.

For a given $x$ we let $G$ increase, in batches of a fixed size, until

$$\text{PI}(x) \equiv \Phi \left( \frac{\hat{m}^{(g)}(x) - f_{\text{max}}}{\hat{s}^{(g)}(x)} \right) < \alpha,$$

for some small value, $\alpha$, or until $G$ reaches a predetermined upper bound, $\bar{G}$. Where $\hat{m}^{(g)}(x)$ and $\hat{s}^{(g)}(x)$ denotes the posterior mean and standard deviation of the GP evaluated at $x$ in the $g$:th MCMC iteration. Note that both the posterior mean $m(x)$ and standard deviation $s(x)$ are functions of the noise variance, which in turn is a function of $G$. The posterior distribution for $f(x)$ is hence continuously updated as $G$ grows until $1 - \alpha$ of the posterior mass of $f(x)$ is concentrated below $f_{\text{max}}$, at which point the evaluation stops. The optimization approach is insensitive to the choice of $\alpha$, as long as it is a relatively small number. We now propose to maximize the following acquisition function based on early stopping

$$\tilde{a}_\alpha(x) = a(x)/\hat{G}_\alpha(x),$$

where $\hat{G}_\alpha(x)$ is a prediction of the number of MCMC draws needed at $x$ before the evaluation stops, with the probability $\alpha$ as the threshold for stopping. We emphasize that early stopping is here used in a subtle way, not only as a simple rule to short-circuit useless computations, but also in the planning of future computations; the mere possibility of early stopping can make the algorithm try an $x$ which does not have the highest $a(x)$, but which is expected to
be cheap and is therefore worth a try. This effect that comes via $\sigma^2(G)$ is not present in the EIS of Snoek et al. (2012) where the cost is fixed and is not influenced by the probability model on $f$.

Although one can use any model to predict $G$, we will here fit a GP regression model to the logarithm of the number of MCMC draws, $\log G_j$ for $j = 1, ..., J$ in the $J$ previous evaluations

$$\log G_j = h(z_j) + \varepsilon_j, \varepsilon_j \sim iid N(0, \psi^2)$$

$$h \sim GP(m_G(z), k_G(z, z')),$$

where $z_j$ is a vector of covariates. The hyperparameters, $x_{1:J}$, themselves may be used as predictors of $\hat{G}(x)$, but also $D(x) = \hat{m}(x) - f_{\text{max}}$ and $s(x)$ are likely to have predictive power for $G$, as well as $u(x) = (\hat{m}(x) - f_{\text{max}})/s(x)$. We will use $z_j = (x_j, D(j)(x_j), s(j)(x_j), u(j)(x_j))$ in our applications, where the superscript over $j$ denotes the BO iteration. Note that the prediction for $G$ is taken to be $\hat{G} = \exp(m_G(z))$, in our case, which correspond to the median of a log-normal distribution.

**Algorithm 1.** Bayesian Optimization with Optimized Precision (BOOP)

**input**

- an estimator $\hat{f}(x)$ of the function to be maximized, and its standard error function $\sigma(G)$.
- $j_0$ initial points $x_{1:j_0} \equiv (x_1, \ldots, x_{j_0})$, a vector of corresponding function evaluations, $\hat{f}(x_{1:j_0})$, and standard errors $\sigma^2(G_{1:j_0})$.
- a baseline acquisition function $a(x)$, and early stopping thresholding probability $\alpha$.

**initialization**

Estimate the function $f(x)$ together with the standard error $\sigma(G)$ at some $j_0$ initial points $x_{1:j_0} \equiv (x_1, \ldots, x_{j_0})$.

**for** $j$ from $j_0 + 1$ until convergence **do:**

a) Estimate the heteroscedastic GP for $f$ based on past evaluations

$$\hat{f}(x_{1:(j-1)}) = f(x_{1:(j-1)}) + \epsilon, \epsilon \sim N(0, \Sigma_{1:(j-1)})$$

$$f(x) \sim GP(m(x), k(x, x')),$$

where $\Sigma_{1:(j-1)} \equiv \text{Diag}(\sigma^2(G_1), \ldots, \sigma^2(G_{j-1}))$.

b) Estimate the GP for $\log G$ based on past evaluations

$$\log G_{1:(j-1)} = h(z_{1:(j-1)}) + \varepsilon, \varepsilon \sim N(0, \psi^2 I)$$

$$h(z) \sim GP(m_G(z), k_G(z', z)),$$

where the elements of $z$ are functions of $x$. Return the point prediction $\hat{G}_\alpha(x)$.

c) Optimize the acquisition function $\hat{a}_\alpha(x) = a(x)/\hat{G}_\alpha(x)$ to select the next point, $x_j$.

d) Compute $\hat{f}(x_j)$ and $\sigma^2(G_j)$ by early stopping at thresholding probability $\alpha$.

e) Update the datasets in a) with $(x_j, \hat{f}(x_j), \sigma^2(G_j))$ and in b) with $(z_j, \log G_j)$.

We will use the term **Bayesian Optimization with Optimized Precision** (BOOP) for BO.
methods that optimize $\tilde{a}_\alpha(x)$ in (3), and more specifically BOOP-EI when EI is used as the baseline acquisition function, $a(x)$. The whole procedure is described in Algorithm 1. The specific Chib estimator of the log marginal likelihood used in the applications in Section 4 is detailed in the appendix in Algorithm 2, implementation of the early stopping step is straightforward in its application.

Note that (2) assumes that $\hat{f}(x)$ is an unbiased estimator at any $x$ and for any MCMC sample size. We performed a small simulation exercise that shows that the Chib estimator is approximately unbiased after a few iterations, see Figure 7 in Appendix A. See also Section 5 for some ideas to extended the current methods to biased estimators.

Figure 3 illustrates the early stopping part of BOOP in a toy example. The upper left graph illustrates the situation at the first BOOP iteration. The black lines show the true unknown function. The three red dots denote initial evaluations and the large green dot is the fourth evaluation obtained by $N = 4$ MCMC iterations. The inferred Gaussian process posterior for $f$ based on these four evaluations are plotted as mean $\hat{m}(x)$ (blue line) and 95% posterior intervals (pink shaded area). We can see that the 95% posterior interval at the current $x$ includes $f_{\text{max}}^{(1)}$ (dotted red line), the highest function value observed so far and it therefore worthwhile to increase the number of MCMC iterations for this $x$. Moving one graph to the right we see that after $N = 6$ MCMC iterations the 95% posterior interval still includes $f_{\text{max}}^{(1)}$, and we move one more graph to the right for $N = 8$ iterations. Here we conclude that the sampled point is almost certainly not an improvement and we move on to a new evaluation point. The new evaluation point is found by maximizing the BOOP-EI acquisition function in (3) with updated effort prediction function $\hat{G}(z)$ in Equation 4 and is depicted by the green dot in leftmost graph in the second row of Figure 3. Following the progress in the second row, we see that it takes only $N=6$ samples to conclude that the function value is almost certainly lower than the current maximum at the second BO iteration. Finally, in the third row, we can see that the point is sampled with high variance at the beginning, but as we increase $N$ it becomes clear that this $x$ is indeed is an improvement.
4 Empirical applications

In this section we apply the tools described in the previous sections on the steady-state BVAR of Villani (2009). This model has been widely used among practitioners and forecasters of macroeconomic variables, see e.g. Gustafsson et al. (2016) and the references therein. Giannone et al. (2015) show that finding the right values for the hyperparameters in BVARs can significantly improve forecasting performance. Moreover, Bańbura et al. (2010) show that different degree of shrinkage (controlled by the hyperparameters) is necessary under different model specifications.

4.1 The steady-state BVAR

The steady-state BVAR model of Villani (2009) is given by:

$$\Pi(L)(y_t - \Psi x_t) = \varepsilon_t,$$

where $\varepsilon_t \sim \text{iid} N(0, \Sigma)$, $E[y_t] = \Psi x_t$. In particular, if we assume that $x_t = 1 \quad \forall t$, then $\Psi$ is the overall mean of the process. We take the prior distribution to be:

- $p(\Sigma) \sim \Sigma^{-(n+1)/2}$
- $\text{vec}(\Pi) \sim N(\theta_{\Pi}, \Omega_{\Pi})$
- $\Psi \sim N(\theta_{\Psi}, \Omega_{\Psi})$.
where $\theta_\Psi$ and $\Omega_\Psi$ are the mean and covariance matrix for the steady states which we set informative according to Table 1. The prior mean for the lag-dynamics, $\theta_\Pi$, is explained in the coming subsection and the prior covariance matrix for the dynamics, $\Omega_\Pi$, is constructed using

$$\omega_{ii} = \begin{cases} \lambda_1^2 \left( \frac{1}{(l_{\lambda 3})^2} \right), & \text{for own lag } l \text{ of variable } r, \ i = (l - 1)n + r, \\ \frac{(\lambda_1 \lambda_2 s_{r})^2}{(l_{\lambda 3} s_{r})^2}, & \text{for cross-lag } l \text{ of variable } r \neq j, \ i = (l - 1)n + j, \end{cases}$$

where $\omega_{ii}$ is the diagonal elements of $\Omega_\Pi$. We also assume prior independence, following Villani (2009). The hyperparameters that we optimize over are; the overall-shrinkage parameter $\lambda_1$, the cross-lag shrinkage $\lambda_2$, and the lag-decay parameter $\lambda_3$.

The steady-state BVAR is non-linear in the parameters, but the posterior distribution of the model parameters can be sampled with a simple Gibbs sampling scheme (Villani, 2009). The marginal likelihood, together with its empirical standard error, can be estimated by the method in Chib (1995) as explained in Section 2.2 and detailed in Appendix A.

### 4.2 Data and model settings

Table 1 describes the data used in our applications which are also used in Giannone et al. (2015). It contains 23 macroeconomic variables for which two subsets are selected to represent a medium-sized model with 7 variables and a large model that contains 22 of the variables (real investment is excluded). Before the analysis, the consumer price index and the five-year bond rate were transformed from monthly to a quarterly frequency. All series are transformed such that they become stationary according to the augmented Dickey-Fuller test. This is necessary for the data to be consistent with the prior assumption of a steady-state. The number of lags is chosen according to the HQ-criteria, Hannan and Quinn (1979) and Quinn (1980). This resulted in $p = 2$ lags for both the medium-sized- and the large model.

We set the prior mean of the coefficient matrix, $\Pi$, to values that reflect some persistence on the first lag, but also that all the time series are stationary. E.g. the prior mean on the first lag of the FED interest rate and the GDP-deflator is set to 0.6, while others are set to zero in the medium-sized model. Lags longer than 1 and cross-lags all have zero prior means. The priors for the steady-states are set informative to the values listed in Table 1, these values follow suggestions from the literature for most variables, see e.g. Louzis (2019) and Österholm (2012). There were a few variables where we could not find theoretical values for either the mean or the standard deviation, in those cases, we set them close to their empirical counterparts.
Table 1: Data description.

| Variable                  | Mnemonic(FRED) | Transform      | Medium | Freq  | Prior          |
|---------------------------|----------------|----------------|--------|-------|----------------|
| Real GDP                  | GDPCI          | 400 x diff-log | x      | Q     | (2.5;3.5)      |
| GDP deflator              | GDPCTPI        | 400 x diff-log | x      | Q     | (1.5;2.5)      |
| FED funds rate            | FEDFUNDS       | -              | x      | Q     | (4.3;5.2)      |
| Consumer price index      | CPIAUCSL       | 400 x diff-log | M      | Q     | (1.5;2.5)      |
| Commodity prices          | PPIACO         | 400 x diff-log | Q      | Q     | (1.5;2.5)      |
| Industrial production     | INDPRO         | 400 x diff-log | Q      | Q     | (2.3;3.7)      |
| Employment                | PAYEMS         | 400 x diff-log | Q      | Q     | (2.5;3.5)      |
| Employment, service       | SRVPRD         | 400 x diff-log | Q      | Q     | (1.5;2.5)      |
| Real consumption          | PCECC96        | 400 x diff-log | x      | Q     | (2.5;3.5)      |
| Real investment           | GDPIC1         | 400 x diff-log | x      | Q     | (2.3;3.7)      |
| Real residential investment| PRFIx          | 400 x diff-log | Q      | Q     | (1.5;4.5)      |
| Non-residential investment| PNFIx          | 400 x diff-log | Q      | Q     | (1.5;4.5)      |
| Personal consumption expenditure, price index | PCECTPI | 400 diff-log | x | Q | (1.5;4.5) |
| Gross private domestic investment, price index | GPDICTPDI | 400 x diff-log | Q | Q | (1.5;4.5) |
| Capacity utilization      | TCU            | diff           | Q      |       | (79.3;80.7)    |
| Consumer expectations     | UMCSERTx       | diff           | Q      |       | (-0.5;0.5)     |
| Hours Worked              | HOANBS         | 400 x diff-log | x      | Q     | (2.5;3.5)      |
| Real compensation/hour    | AHETPIx        | 400 x diff-log | x      | Q     | (1.5;2.5)      |
| One year bond rate        | GS1            | diff           | Q      |       | (-0.5;0.5)     |
| Five year bond rate       | GS5            | diff           | M      |       | (-0.5;0.5)     |
| SP 500                    | S&P 500        | 400 x diff-log | Q      |       | (-2.2)         |
| Effective exchange rate   | TWEXMMTH       | 400 x diff-log | Q      |       | (-1.1)         |
| M2                        | M2REAL         | 400 x diff-log | Q      |       | (5.5;6.5)      |

The table shows the 23 US macroeconomic time series from the FRED database used in the empirical analysis. The column named Prior contains the steady-state mean ± one standard deviation.

4.3 Experimental setup

We consider three competing optimization strategies: (I) an exhaustive grid-search, (II) Bayesian optimization with the EI acquisition function (BO-EI), and (III) our BOOP-EI algorithm. In each approach, we use the restrictions \( \lambda_1 \in (0, 5) \), \( \lambda_2 \in (0, 1) \), and \( \lambda_3 \in (0, 5) \). In the grid-search, \( \lambda_1 \) and \( \lambda_2 \) move in steps of 0.05 and \( \lambda_3 \) moves in steps of 0.1, yielding in total 10000 marginal likelihood evaluations. For the Bayesian optimization algorithm, we set the number of evaluations to 150, and we use two random draws as initial values for the GPs.

For (I) and (II) we use in total 10000 Gibbs iterations with 2500 as a burn-in sample in each model evaluation. For (III) we draw 3000 Gibbs samples where we burn 2500 and use the rest to calculate the probability of improvement PI, by doing this we ensure that the estimated marginal likelihood will be approximately unbiased (see Figure 7 in Appendix A).
If \( P_i < \alpha \) we accept the draw with relatively large standard errors, otherwise we generate a new batch (of size 200) of Gibbs samples and again check the criteria. As a consequence, the total number of Gibbs iterations will vary between 3000 and 10 000 in each of the 150 BO-iterations. The application is robust to the choice of \( \alpha \), as long as it is a reasonably low number, in this study we use \( \alpha = 0.001 \). This means that the probability of improvement should be very low before we stop the MCMC run. We run method (II) and (III) ten times and report the results in Figure 6 and Table 2.

For comparison, we will also use the standard values of the hyperparameters used in e.g. the BEAR-toolbox, Dieppe et al. (2016), \( \lambda_1 = 0.1, \lambda_2 = 0.5, \) and \( \lambda_3 = 1 \), as a benchmark. The methods are compared with respect to i) how well the optimized hyperparameters maximizes the marginal likelihood, and ii) how much computational resources that has to be spent in the optimization.

### 4.4 Results for the medium-sized model

Table 2: Optimization Results Medium Steady-State BVAR.

|                     | Standard | BO-EI     | BOOP-EI   | Grid      |
|---------------------|----------|-----------|-----------|-----------|
| Log ML              | -3099.28 | -3069.01  | -3068.84  | -3069.03  |
| Gibbs iterations    | -        | 1.5 \* 10^6 | 405750     | 10^9      |
| Avg. iter to 90%    | -        | 9 \* 10^5  | 431061     | -         |
| Model evaluations   | -        | 150       | 150       | 10^5      |
| \( \lambda_1 \)     | 0.1      | 0.30      | 0.27      | 0.3       |
| \( \lambda_2 \)     | 0.5      | 0.38      | 0.43      | 0.4       |
| \( \lambda_3 \)     | 1        | 0.69      | 0.76      | 0.9       |

The table compares different methods for hyperparameter optimization in the medium-sized steady-state BVAR. Each method is run 10 times and the reported hyperparameters for each method are the best ones over the 10 runs. The reported duration measures are averages taken over all runs. The third row in the table show the number of iterations it takes (on average) to close 90% of the gap between the log ML from standard values and the maximum. The marginal likelihood of the selected models were re-estimated using 100,000 Gibbs iterations with 40,000 as a burn-in.

Table 2 summarizes the results of the medium size BVAR model. We see that all three optimization strategies find hyperparameters that yield substantially higher log marginal likelihood than the standard values. We can also see that both Bayesian optimization methods yield as good hyperparameters as the grid search at only a small fraction of the computational cost. It is also clear from Table 2 that a substantial amount of computations can be gained via our new acquisition strategy. It is interesting to note that the values for \( \lambda_1 \) and \( \lambda_2 \) are similar for all three optimization approaches but that \( \lambda_3 \) differs to some extent. This is due to the flatness of the log marginal likelihood in that area.

Figure 4 displays the log marginal likelihood surfaces over the grid of \((\lambda_1, \lambda_2)\)-values used in the grid search. Each subgraph is for a fixed value of \( \lambda_3 \in \{0.1, 1, 2, 5\} \). The red dot indicates the maximum log marginal likelihood for the given \( \lambda_3 \), and the green dot indicates the standard values. In all four sub-graphs, we can see that the standard values
are located outside the high-density regions, relatively far from the maximum (except when the lag-decay shrinkage parameter, \( \lambda_3 \), is 0.1). A comparison of Figures 4 and 5 shows that the GP’s predicted log marginal likelihood surface is quite accurate already after merely 150 evaluations; this is quite impressive considering that Bayesian optimization tries to find the maximum in the fastest way, and does not aim to have high precision in low-density areas.

Figure 4: Log marginal likelihood surfaces over a fine grid of \((\lambda_1, \lambda_2)\)-values. The different panels are: (a) \( \lambda_3 = 0.1 \), (b) \( \lambda_3 = 1 \), (c) \( \lambda_3 = 2 \), (d) \( \lambda_3 = 5 \). The red dot denotes the maximum log marginal likelihood value for the given \( \lambda_3 \), and the green dot indicates the standard values.
Figure 5: GP predictions of the hyperparameter surfaces in Figure 4 based on 150 evaluations.

Figure 6 shows that BOOP-EI finds higher values of the log marginal likelihood much faster than plain BO with EI acquisitions. From Table 2 we can see that BOOP-EI uses less than a third of the MCMC iterations compared to BO-EI for a full run. To close 90% of the gap between the standard values and the maximum it takes about half the time for BOOP-EI. Interesting to note is that BO-EI leads to (on average) a higher number of improvements on the way to the maximum; while BOOP-EI gives fewer improvements but of larger magnitude; the strategy of cheaply exploring new territories before locally optimizing the function pays off.

4.5 Results for the large-sized model

We also optimize the parameters of the more challenging large BVAR model containing the 22 different time series, using 200 iterations for both the BO- and BOOP-EI. A complete grid search is too costly here, so we instead compare with parameters obtained from the grid search from the medium-sized BVAR in Section 4.4, which is a realistic strategy in practical work.
Figure 6: Comparison of the convergence speed of the Bayesian optimization methods.

Table 3: Optimization Results Large Steady-State BVAR.

| Hyperparameter | Standard Log ML | Standard Sd log ML | BOOP-EI Log ML | BOOP-EI Sd log ML | BO-EI Log ML | BO-EI Sd log ML | Grid (Medium) Log ML | Grid (Medium) Sd log ML |
|----------------|-----------------|--------------------|----------------|-------------------|--------------|-----------------|---------------------|------------------------|
| Log ML         | −7576.31        | 0.54               | −7458.61       | 0.28              | −7458.19     | 0.42            | −7566.86            | 0.53                   |
| Sd log ML      | 0.54            | 0.28               | 0.42           | 0.58              | 0.53         | 0.3             |                     |                        |
| λ₁             | 0.1             | 0.52               | 0.58           | 0.3               |              |                 |                     |                        |
| λ₂             | 0.5             | 0.11               | 0.08           | 0.4               |              |                 |                     |                        |
| λ₃             | 1               | 1.79               | 1.72           | 0.9               |              |                 |                     |                        |

Hyperparameter optimization in the large steady-state BVAR. The column named Grid are the values obtained from a grid search for the medium size model. The marginal likelihood of the selected models were re-estimated using 100,000 Gibbs iterations with 40,000 as a burn-in.

Table 3 shows that our method, again, finds optimal hyperparameters with substantially larger log ML than standard values, and also much better values than those from the grid search on the medium-sized BVAR. We can also see that the standard values are worse than those of the grid search for the medium-sized model. Finally, note that the hyperparameters selected by BOOP-EI in the large-sized BVAR are quite different from those in the medium-sized model. The optimal λ₁ applies less baseline shrinkage than before, but the lag decay (λ₃) is higher, and in particular, the cross-lag shrinkage, λ₂, is much closer to zero, implying much harder shrinkage towards univariate AR-processes. This latter result strongly suggests that the computationally attractive conjugate prior structure is a highly sub-optimal solution since such a prior requires that λ₂ = 1.
5 Concluding remarks

We propose a new Bayesian optimization method for finding optimal hyperparameters in econometric models. The method can be used to optimize any noisy function where the precision is under the control of the user. We focus on the common situation of maximizing a marginal likelihood evaluated by MCMC, where the precision is determined by the number of MCMC iterations. The ability to choose the precision makes it possible for the algorithm to take occasional cheap and noisy evaluations to explore the marginal likelihood surface, thereby finding the optimum faster.

We assess the performance of the new algorithm by optimizing the prior hyperparameters in the extensively used steady-state BVAR model in both a medium-sized and a large-sized VAR. The method is shown to be practical and competitive to other approaches in that it finds the optimum using a substantially smaller computational budget, and has the potential of being part of the standard toolkit for BVARs. We have focused on optimizing the marginal likelihood, but the method is directly applicable to other utility functions, e.g. the popular log predictive score (Geweke and Keane, 2007 and Villani et al., 2012).

Our approach builds on the assumption that the noisy estimates of the log marginal likelihoods are approximately unbiased, which we show is a reasonable assumption in our case. The unbiasedness of the log marginal likelihood will, however, depend on the combination of MCMC sampler and marginal likelihood estimator, see Adolfson et al. (2007) for some evidence. It would therefore be interesting to extend the method to cases with biased evaluations. One such example in econometrics is Dynamic Stochastic General Equilibrium (DSGE) models (An and Schorfheide, 2007) which are usually analyzed by random walk Metropolis sampling and the marginal likelihood estimated by the modified harmonic estimator (Geweke, 1999). The marginal likelihood estimates are typically very persistent over MCMC iterations in models with many parameters and are therefore only slowly approaching the true marginal likelihood. Since the marginal likelihood trajectory over MCMC iterations is very smooth one can try to predict its evolution and then correct the bias in the marginal likelihood estimates.

Sequential Monte Carlo (SMC) gives unbiased and noisy estimates of the likelihood with precision determined by the number of particles. Extending our method to SMC is non-trivial however since the number of particles cannot be increased adaptively as we do with the MCMC iterations in our algorithm, at least when particle resampling is used. We are currently working on an alternative algorithm in the same spirit as the current proposal which circumvents this complication.
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### A Implementation details for Chib’s marginal likelihood estimator

The marginal likelihood estimator for Gibbs sampling proposed by Chib (1995) has been shown to be very accurate. We will briefly present the estimator here for the case with three blocks in the Gibbs sampler, which is also used in our BVAR application. The idea is that the posterior distribution of the three blocks model can be factorized as

\[
p(\theta_1, \theta_2, \theta_3 | y) = \underbrace{p(\theta_1 | \theta_2, \theta_3, y)}_{(a)} \underbrace{p(\theta_2 | \theta_3, y)}_{(b)} \underbrace{p(\theta_3 | y)}_{(c)}.
\]

If we look at the different parts above; part (a) is a full conditional which is available in closed form. (c) can be estimated in a point using Monte Carlo integration directly from
the Gibbs output

\[ p(\theta_3^*|y) = \int p(\theta_3^*|\theta_1, \theta_2, y) d\theta_1 d\theta_2 \approx \frac{1}{G_1} \sum_{g=1}^{G_1} p(\theta_3^*|\theta_1^{(g)}, \theta_2^{(g)}, y). \]

The only part that is not immediately accessible is part (b), but it can be obtained by running a reduced version of the first Gibbs sampler. Practically, the only thing we do is to fix \( \theta_1 \) at \( \theta_1^* \) and skip this updating step in the reduced Gibbs sampler. Monte Carlo integration can again be used to obtain

\[ p(\theta_2^*|\theta_3^*, y) = \int p(\theta_2^*|\theta_3^*, \theta_1, y) d\theta_1 \approx \frac{1}{G_2} \sum_{g=1}^{G_2} p(\theta_2^*|\theta_3^*, \theta_1^{(g)}, y). \]

When we have obtained all three parts (a, b, and c) they are put together with the prior and likelihood to obtain an estimate of the log marginal likelihood as

\[ \hat{m}(y) = \log p(y|\theta^*) + \log p(\theta^*) - \log \hat{p}(\theta_1^*, \theta_2^*, \theta_3^*|y), \]

where

\[ \hat{p}(\theta_1^*, \theta_2^*, \theta_3^*|y) = p(\theta_1^*|\theta_2^*, \theta_3^*, y) \hat{p}(\theta_2^*|\theta_3^*, y) \hat{p}(\theta_3^*|y). \]

Chib (1995) also provides a method to compute asymptotic standard errors, which is explained here in the case with three blocks. After running the full- and reduced Gibbs samplers we have the vector process:

\[ h = \left( \begin{array}{c} h_1(\theta_3^*|y) \\ h_2(\theta_2^*|\theta_3^*, y) \end{array} \right) = \left( \begin{array}{c} \hat{p}(\theta_3^*|y) \\ \hat{p}(\theta_2^*|\theta_3^*, y) \end{array} \right). \]

We can now calculate the covariance matrix for \( h \), where it is important to account for autocorrelation in the MCMC draws. Note that due to the procedure of using two separate Gibbs samplers, \( h_1 \) and \( h_2 \) should be approximately independent, see Chib (1995). But the vector notation will be kept for convenience. We should also note that the empirical standard errors are for repeated experiments using the same \( \theta^* \) every time.

Using the vector notation we have

\[ \hat{h} = G^{-1} \sum_{g=1}^{G} h^{(g)} = \left( \begin{array}{c} \hat{p}(\theta_3^*|y) \\ \hat{p}(\theta_2^*|\theta_3^*, y) \end{array} \right). \]

Our objective is now to find the variance of a function of \( \hat{h} \), i.e. \( \psi_1 = \hat{h}_1 \times \hat{h}_2 \) and \( \psi_2 = \ln \hat{h}_1 + \ln \hat{h}_2 \equiv \ln \hat{p}(\theta_3^*|y) + \ln \hat{p}(\theta_2^*|\theta_3^*, y) \). The strategy is to first find the variance of \( \hat{h} \) and then use the delta method to find the variance of our functions.

Since the \( \hat{h} \) inherit the ergodicity from the Gibbs-chains we have that \( \hat{h} \rightarrow \mu \), as \( G \rightarrow \infty \).
almost surely, where $\mu = (p(\theta_3^*|y) + p(\theta_2^*|\theta_3^*, y))'$. Further,

$$\lim_{G \to \infty} G\{E[(\hat{h} - \mu)(\hat{h} - \mu)']\} = 2\pi S(0),$$

where $S(0)$ denotes the spectral density matrix at frequency zero. An estimate of $\Omega \equiv 2\pi S(0)$ can be obtained by the approach of Newey and West (1987). We then have:

$$\Omega_s = G^{-1} \sum_{g=s+1}^{G} (h^{(g)} - \hat{h})(h^{(g+s)} - \hat{h})',$$

then we get

$$\text{var}(\hat{h}) = \frac{1}{G} \left[ \Omega_0 + \sum_{s=1}^{q} \left( 1 - \frac{s}{q+1} \right) (\Omega_s + \Omega_s') \right],$$

where $q$ is a positive integer determining how many autocorrelations to account for. Chib (1995) suggest to (conservatively) use $q = 10$ while we instead fit a vector autoregression to select $q$ to be the lag length to maximize AIC. The variance we are really after is the one for $\psi_2$, and it is obtained by the delta method through:

$$\text{var}(\psi_2) = \left( \frac{\partial \psi_2}{\partial \hat{h}} \right)' \text{var}(\hat{h}) \left( \frac{\partial \psi_2}{\partial \hat{h}} \right),$$

where the gradients consists of the elements $\hat{h}_1^{-1}$ and $\hat{h}_2^{-1}$. To get the empirical standard errors we just take the square root of this expression.

Our methods assumes an unbiased log marginal likelihood estimator. Figure (?) shows that Chib’s estimator is nearly unbiased in the steady-state BVAR already after a few hundred MCMC iterations.
Figure 7: Unbiasedness of Chib’s log marginal likelihood estimator in the steady-state BVAR application. The horizontal axis denotes the number of MCMC draws (excluding 50 observations as burn-in), the blue dots are draws from the sampling distribution of Chib’s estimator for a given MCMC sample size. The red line is the mean of the draws and the blue line represents the true log marginal likelihood, obtained from 100 000 MCMC iterations with 5000 as a burn-in.
Algorithm 2 Chib’s marginal likelihood estimator with standard errors

1 Gibbs 1
(a) Run the first Gibbs-sampler to obtain the full conditional distributions.
(b) Select $\theta^* = (\Pi^*, \Sigma^*, \Psi^*)$ from a high density location.
(c) Use the output to calculate $p(\Psi^*|\Pi^*, \Sigma^*, y)$ and $\hat{p}(\Pi^*|y)$.

2 Gibbs 2
(a) Run the reduced Gibbs-sampler in the same way as the first, but fix $\Pi$ at $\Pi^*$ in every iteration.
(b) Calculate $\hat{p}(\Sigma^*|\Pi^*, y)$.

3 Marginal likelihood
(a) Calculate the likelihood and prior density at $\theta^* = (\Pi^*, \Sigma^*, \Psi^*)$.
(b) Put all the pieces together to obtain
$$\ln \hat{p}(y) = \ln p(y|\Pi^*, \Sigma^*, \Psi^*) + \ln p(\Pi^*, \Sigma^*, \Psi^*) - \ln \hat{p}(\Pi^*|y) - \ln \hat{p}(\Sigma^*|\Pi^*, y) - \ln \hat{p}(\Psi^*|\Pi^*, \Sigma^*, y).$$

4 Empirical standard errors
(a) Compute $\Omega_0$ as $\Omega_s = G^{-1} \sum_{g=s+1}^{G} (h^{(g)} - \hbar^{(g+s)} - \hbar^s)'$, where we set $s = 0$.
(b) Calculate the appropriate autocorrelation order by minimizing AIC for a $VAR(q)$ on $\hbar$. And compute the autocorrelation correction terms $\Omega_s$ for $s = 1, 2, \ldots, q$.
(c) Compute the variance of $\hbar$ as $\text{var}(\hbar) = \frac{1}{G} \left[ \Omega_0 + \sum_{s=1}^{q} \left( 1 - \frac{s}{q+1} \right) (\Omega_s + \Omega'_s) \right]$.
(d) Finally, obtain the variance of $\log$ marginal likelihood by using the delta method as $\text{var}(\psi_2) = \left( \frac{\partial \psi_2}{\partial \hbar} \right)' \text{var}(\hbar) \left( \frac{\partial \psi_2}{\partial \hbar} \right)$, and take the square root.