Bayesian Nonparametric Estimation of Milky Way Parameters Using Matrix-Variate Data, in a New Gaussian Process Based Method

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Abstract: In this paper we develop an inverse Bayesian approach to find the value of the unknown model parameter vector that supports the real (or test) data, where the available data is matrix-variate. The data is represented as an unknown function of the model parameters, where this high-dimensional function is modelled using a high-dimensional Gaussian Process (GP). The model for the function is trained using available training data and inverted by Bayesian means, to estimate the sought value of the model parameter vector at which the test data is realised. We achieve a closed-form expression for the posterior of the unknown parameter vector and the parameters of the invoked GP, given test and training data. For posterior inference we use the recently advanced Transformation-based Markov Chain Monte Carlo (TMCMC). We perform model fitting by comparing the observed data with predictions made at different summaries of the posterior probability of the model parameter vector. As a supplement, we undertake a leave-one-out cross validation of our method. The method is illustrated via the estimation of Milky Way feature parameter vector using available real and simulated stellar velocity data matrices.

Keywords and phrases: Supervised learning, Inverse problems, Gaussian Process, Matrix-variate Normal, Transformation-based MCMC.

1. Introduction

The method of science is typified by attempts at learning the unknown model parameter vector, given observed data. The data is expressed as a function of the sought model parameter vector $S$ where this functional relationship between data and the unknown value of $S$ is not necessarily known.

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This unknown function can be trained using available “training data” and subsequently inverted to provide an estimate for the unknown value of $S$ at which the measured data, i.e. test data, is realised, where such test data is contrasted with “training data”, by which we imply data generated at chosen values of $S$ (for example, via simulations or obtained as archival data).

The learning of a high-dimensional function from available training data, using standard non-parametric methods (such as spline fitting or wavelet based learning)—either in the Bayesian or classical approach—is expected to be unsatisfactory for various reasons. The most acute of these is that modelling high-dimensional functions using splines/wavelets require restrictive assumptions and in particular, may fail to adequately take into account the correlation structure between the component functions. Using splines/wavelets in high dimensions leads to an increase in the complexity of the task of learning the unknown function from the data, and in particular of inverting it to achieve the sought value of $S$ that supports the real data. Furthermore, the classical approach has been criticised on the ground that it ignores parameter uncertainty, in that the approach provides only a point estimate of the set of model parameters. Such a worry can however be addressed in a Bayesian framework. An added advantage of the Bayesian approach is that priors on the unknown parameters can bring in extra information into the model. Thus, in principle, a training data set of comparatively smaller size than that required in the classical approach, will be adequate in the Bayesian paradigm.

Solving for the value of $S$ that supports the real or test data requires operating the inverse of the learnt function on the test data. The existence and uniqueness of such solution can be questioned given that the problem may not even be well-posed in a Hadamard sense (Hofmann, 2011; Kabani, 2008; Tarantola, 2005). The problem may even be ill-conditioned since errors in the measurement may exist. Such worries about ill-posedness and ill-conditioning are mitigated in the Bayesian framework (Carreira-Perpin, 2001; Stuart, 2013) in which the equivalent of the solution suggested above is the computation of the posterior probability of the sought value of $S$, given the test and training data. Given the inherent inadequacies of learning using splines/wavelets discussed above, we opt to model the unknown functional relationship between data and model parameter $S$ with a high-dimensional Gaussian Process ($GP$).

Any set of scalar data points generated by a scalar valued $GP$ is jointly distributed as a multivariate normal. Similarly, a set of vector-variate measurements generated by a vector valued $GP$ is distributed jointly as matrix normal, parametrised by a mean matrix and a left and right covariance matrix; these matrix-values parameters correspond to the mean and covariance structure of the $GP$. On the other hand, if the data is matrix-variate, it is expressed as an unknown matrix-variate function of $S$, which if modelled by a matrix-variate Gaussian Process ($GP$) would imply that one realisation from such a matrix-variate $GP$ would be the set of the observed matrices that will be jointly distributed as 3-way tensor normal, parametrised by a mean matrix and 3 covariance matrices (Hoff, 2011). It is with the motivation of reducing the need to learn the parameters of 3 covariance matrices from the data, to 2, that we vectorise our intrinsically matrix-valued data sets. This leads to the functional relationship between the data and model parameter vector being rendered vector-valued, modelled by a vector-variate $GP$, a set of realisations from which is jointly matrix normal, parametrised by matrix-variate parameters that we intend to learn from the data, along with the unknown $S$.

In this paper, we present a generic method that allows for the Bayesian non-parametric learning of an unknown model parameter vector, given matrix-variate data. The developed methodology is illustrated via an application to estimate a Milky Way feature parameter vector, given the available matrix-variate stellar velocity data. In the context of this application, we demonstrate the effec-
tiveness of our Gaussian Process based method with much smaller data sets than were used in the past. The other major advantage of this presented method is that it readily allows for the expansion of dimensionality of the model parameter vector and is capable of taking measurement errors into account.

The rest of the paper is structured as follows. In Section 2, we present the details of the modelling strategy that we adopt. The treatment of measurement errors within the modelling is discussed in Section 2.6. In Section 3 we discuss the application via which the new method is illustrated while details of the inference are discussed in Section 3.1. Section 4 contains results obtained from using available real and training data. We compare the obtained results with the estimates available in the astronomical literature in Section 4.1. Section sec:modelfit presents results of model fitting by comparing test data with predictions made at different summaries of the posterior of the model parameter vector $S$. The paper is rounded up with a discussions section.

2. Model

Let $j$ number of measurements of a $k$-dimensional variable be available; this vector variable is referred to below as the “observable”. Thus the measurements of this observable constitute a $j \times k$-dimensional matrix. We refer to the measured data as test data and seek the unknown value $s^{(new)}$ of model parameter $S$ at which it is realised. Let data be generated at $n$ known values of $S$: $s^*_1, \ldots, s^*_n$. Then $\{s^*_1, \ldots, s^*_n\}$ is the design set and $s^*_i$ is the $i$-th design vector at which the $i$-th synthetic data matrix is generated, $i = 1, 2, \ldots, n$. Then these $n$ synthetic data matrices comprise a training data set. Here a data matrix is $j \times k$-dimensional. As motivated in the introductory section, we express the relation between the data $V$ and unknown model parameter vector $S$ as $V = \xi(S)$, where $\xi(\cdot)$ is an unknown function. We train the model for $\xi(\cdot)$ using the training data and invert the function using Bayesian means to estimate the unknown $s^{(new)}$ at which the real, i.e. the test data is realised.

Indeed the matrix-variate nature of the data prompts this functional relationship to be modelled by a matrix-variate $\mathcal{GP}$, but as delineated in the introductory section, that would require that realisations from this $\mathcal{GP}$—such as the $n$ number of $j \times k$-dimensional data matrices—are jointly distributed as 3-way tensor normal. However in this exercise, we choose to simplify the learning by rephrasing the intrinsically $j \times k$-dimensional matrix-valued data sets as $jk$-dimensional vectors. Such vectorisation allows us to avoid the need for learning the parametrisation of the 3 covariance matrices that characterise the 3-way tensor normal density, in favour of parametrising the 2 covariance matrices of the matrix-normal distribution; such learning is difficult in general when the problem does not manifest sparsity and reduction in the number of unknown parameters is welcomed. In this treatment a measurement is rendered vector-valued, as $\xi(\cdot)$ is vector-valued and $\xi(\cdot)$ can be modelled by a vector-variate $\mathcal{GP}$ so that realisations from this $\mathcal{GP}$ are jointly matrix normal.

Thus, we find it more useful to consider the $j$ number of measurements of the $k$-dimensional observable, as a $jk$-dimensional observed vector $v^{(test)}$. This test data is realised at the unknown value $s^{(new)}$ of $S$. Again, a $j \times k$-dimensional synthetic data matrix is treated as a $jk$-dimensional synthetic data vector $v_i$, $i = 1, 2, \ldots, n$, along the lines of the observed data. Then all the $n$ synthetic data vectors together comprise the training data $D_s = (v_1; v_2; \ldots; v_n)^T$ where the training data $D_s$ is generated at the chosen values $\{s^*_1, \ldots, s^*_n\}$ of $S$. Given our treatment of $v_i$ as a $jk$-dimensional vector, the training data set $D_s$ is a matrix with $n$ rows and $jk$ columns.

Thus in this treatment, we have $n$ $jk$-dimensional synthetic data vectors (inputs), each generated at a chosen value of the model parameter vector (target), i.e. we have the $n$ observations
(v_1, s_1^*, \ldots, (v_n, s_n^*)), and the aim is to predict the unknown model parameter vector s^{(new)} at which the input is the test data, i.e. the data vector v^{(test)}. In this paradigm of supervised learning akin to the discussion in Neal (1998), a predictive distribution of s^{(new)} is sought, conditioned on the test data v^{(test)} and the training data D_s = (v_1|v_2, \ldots, v_n)^T.

We begin the discussion on the model by elaborating on the detailed structure of the used GP. In this section we ignore measurement errors and present our model of these n vector-variate functions. Later in Section 2.6, we delineate the method used to take measurement uncertainties on board.

As the data are vectorised in this treatment as jk-dimensional vectors, we recall that ξ(·) is also rendered a jk-variate vector function whose ℓ-th component function is ξ_ℓ(·). Then we can write v_i = ξ(s_i) := (ξ_i(s_i), \ldots, ξ_{jk}(s_i))^T, ∀ i = 1, \ldots, n. We model the jk-dimensional function ξ(·) with a jk-dimensional GP. One realisation from this high-dimensional GP is \{ξ(s_1), ξ(s_2), \ldots, ξ(s_n)\}. Then the joint distribution of \{ξ(s_1), ξ(s_2), \ldots, ξ(s_n)\} is matrix normal, with adequate parametrisation. We represent this as

\[
\{ξ(s_1), ξ(s_2), \ldots, ξ(s_n)\} \sim \mathcal{MN}_{n,jk}(μ, A, Ω),
\] (2.1)

where the mean matrix of this matrix normal distribution is the n × jk-dimensional matrix μ, the left covariance matrix is the n × n-dimensional A and the right covariance matrix is the jk × jk-dimensional matrix Ω. These individual matrix-variate parameters of this distribution stem from the parametrisation of the high-dimensional GP that is used to model ξ(·) and we discuss such parametrisation below. Before proceeding to that, we note that Equation 2.1 is the same as saying that the likelihood is matrix normal.

2.1. Parameters of the matrix-normal distribution

Assuming ξ(·) to be continuous, the applicability of a stationary covariance function is expected to suffice. We choose to implement the popularly used square exponential covariance function (Rasmussen and Williams, 2006; Santner et al., 2003; Scholkopf and Smola, 2002). This covariance function is easy to implement and renders the sampled functions smooth and infinitely differentiable. Also, we relax the choice of a zero mean function though that is another popular choice. Instead we choose to define the mean function in a way that is equivalent to the suggestion that the data is viewed as centred around a linear model with the residuals characterised by a vector-variate GP (A. O’Hagan, 1978; Cressie, 1993). We then integrate over all such possible global intercepts to arrive at a result that is more general than if the mean is fixed at zero. An advantage of the non-zero mean function is that in the limit of the smoothness parameters (characterising the smoothness of the functions sampled from this GP) approaching large values, the random function reduces to a linear regression model. This appears plausible, as distinguished from the result that in this limit of very large smoothness, the random function will concur with the errors, as in models with a zero mean function.

The non-zero mean function μ(·) of the GP is represented as factored into a matrix H that bears information about its shape and another (B) that tells us about its strength or the extent to which this chosen mean function deviates from being zero. Thus, μ(·) := H B, where

\[
H^T := [h^{(m \times 1)}(s_1), \ldots, h^{(m \times 1)}(s_n)], \quad \text{with}
\]

m := d + 1

\[
h^{(m \times 1)}(s_i) = (1, s_i^{(1)}, s_i^{(2)}, \ldots, s_i^{(d)})^T
\] (2.2)
where \( s_i = (s_i^{(1)}, s_i^{(2)}, \ldots, s_i^{(d)})^T \) for \( i = 1, \ldots, n \) and we have recalled the suggestion that such a non-zero mean function be expressed in terms of a few basis functions (Rasmussen and Williams, 2006), (prompting us to choose to fix this functional form such that \( h(s) := (1, s)^T \) for all values of \( S \)). A similar construct was used by Blight and Ott (1975) who performed a \( GP \)-based polynomial regression analysis. Thus, in our treatment, \( h(\cdot) \) is a \((d + 1)\)-dimensional vector. The coefficient matrix \( B \) is

\[
B = (\beta_{11}, \ldots, \beta_{j1}, \ldots, \beta_{1k}, \ldots, \beta_{jk})
\]

where for \( p = 1, \ldots, j, p' = 1, \ldots, k, \beta_{pp'} \) is an \( m \)-dimensional column vector. As we choose to set \( m = d + 1 \), \( B \) is a matrix with \( d + 1 \) rows and \( jk \) columns.

The covariance function of the \( GP \) is again represented as factored into a matrix \( \Omega \) that tells us about the strength or amplitude of the covariance and another \( A \) that bears information about its shape. The amplitude matrix \( \Omega \) is \( jk \times jk \)-dimensional and is defined as

\[
\Omega = \Sigma \otimes C
\]

where \( \Sigma \) is the \( j \times j \) matrix telling us the amplitude of the covariance amongst the \( j \) different observations, for each of the \( k \) components of the data vector, at a fixed value of \( S \). On the other hand, \( C \) is the \( k \times k \) matrix giving the amplitude of covariance amongst the \( k \) different components of the vector-valued observable, at each of the \( j \) observations, at a given value of \( S \). We realise that under the assumption of Gaussian errors in the measurements, the error variance matrix will be added to \( \Omega \). We discuss this in detail later in Section 2.6.

The shape of the covariance function is borne by the matrix \( A \) which is \( n \times n \)-dimensional. Given our choice of square exponential covariance function, it is defined as

\[
A^{(n \times n)} := [a(\cdot, \cdot)], \quad \text{where} \\
a(s, s') \equiv \exp\{-\frac{1}{2}(s - s')^T Q (s - s')\},
\]

for any 2 values \( s \) and \( s' \) of \( S \). Here, \( Q^{(d \times d)} \) represents the inverse of the scale length that underlies correlation between functions at any two values of the function variable. In other words, \( Q \) is the matrix of the smoothness parameters. Thus, \( Q \) is a matrix that bears information about the smoothness of the sampled functions; it is a diagonal matrix consisting of \( d \) non-negative smoothness parameters denoted by \( b_1, \ldots, b_d \). In other words, we assume the same smoothness for each component function of \( \xi(\cdot) \). This smoothness is determined by the parameters \( b_1, \ldots, b_d \). We will learn these smoothness parameters in our work from the data. Of course, though we say that the smoothness is learnt in the data, the underlying effect of the choice of the square exponential covariance function on the smoothness of the sampled functions is acknowledged. Indeed, as Snelson (2007) states, one concern about the square exponential function is that it renders the functions sampled from it as artificially smooth. An alternative covariance function, such as the Matern class of covariances (Matern, 1986; Snelson, 2007; Tilmann Gneiting and William Kleiber and Martin Schlather, 2010), could give rise to sampled functions that are much rougher than those obtained using the square exponential covariance function, for the same values of the hyperparameters of amplitude and scale that characterise these covariance functions (see Chapter 1 of Snelson’s thesis).

Let \( \omega_{r\ell} \) denote the \((r, \ell)\)-th element of \( \Omega \), \( c_{r\ell} \) the \((r, \ell)\)-th element of \( C \) and let \( \sigma_{r\ell} \) denote the \((r, \ell)\)-th element of \( \Sigma \). Let the \( \ell \)-th component function of \( \xi(\cdot) \) be \( \xi_\ell(\cdot) \) with \( \ell = m_1 k + m_2 \), where
\( \ell = 1, \ldots, jk \) and \( m_2 = 1, 2, \ldots, k \), \( m_1 = 0, 1, \ldots, j - 1 \). Then the correlation between the components of \( \xi(\cdot) \) yields the following correlation structures:

\[
\text{corr} \left( \xi_{1k+m_2}(s_i), \xi_{i'k+m_1'}(s_i) \right) = \frac{\sigma_{m_1 m_1'}}{\sqrt{\sigma_{m_1 m_1} \sigma_{m_1' m_1'}}} \quad \forall \ m_2, i \quad \text{and} \quad m_1 \neq m_1' \tag{2.6}
\]

\[
\text{corr} \left( \xi_{1k+m_2}(s_i), \xi_{i'k+m_2'}(s_i) \right) = \frac{c_{m_2 m_2'}}{\sqrt{c_{m_2 m_2} c_{m_2' m_2'}}} \quad \forall \ m_1, i \quad \text{and} \quad m_2 \neq m_2' \tag{2.7}
\]

\[
\text{corr} \left( \xi_{1k+m_2}(s_i), \xi_{i'k+m_1'}(s_i) \right) = \frac{c_{m_2 m_1'}}{\sqrt{c_{m_2 m_2} c_{m_2' m_1'}}} \quad \forall i, m_1 \neq m_1', m_2 \neq m_2' \tag{2.8}
\]

\[
\text{corr} \left( \xi_{\ell}(s_1), \xi_{\ell}(s_2) \right) = a(s_1, s_2) \quad \forall \ \ell \quad \text{and} \quad s_1 \neq s_2 \tag{2.9}
\]

The 1st of the above 4 equations shows the correlation between the component functions for the same component of the vector-valued observable at 2 (of the \( j \)) different measurements, taken at a given value of the \( S \). For a given measurement, the correlation between 2 different components of (the \( k \) components of) the observable is given by the 2nd equation above. For a given value of \( S \), if we seek the correlation between the component functions for 2 different measurements of 2 different components of the observables, this is provided in the 3rd equation. The correlation between component functions for 2 different values of \( S \) is given in the last of the above 4 equation. Then these 4 correlations give the full correlation structure amongst components of \( \xi(\cdot) \).

### 2.2. Likelihood

We have just discussed the details of the matrix normal distribution that is the joint distribution of realisations from the high-dimensional \( \mathcal{GP} \) under consideration. Here we write the likelihood of the matrix-variate parameters of this matrix normal distribution, given the training data \( D_s \).

The training data is the \( n \times jk \)-dimensional matrix \( D_s = (v_1; v_2; \ldots; v_n)^T \) where \( v_i \) is the \( jk \)-dimensional synthetic motion vector generated at design vector \( s_i^* \), \( i = 1, 2, \ldots, n \). Here \( v_i^T \) can be expressed as a function of the \( i \)-th design vector \( s_i^* \), as in \( v_i = \xi(s_i^*) \). To express the likelihood, we recall that the distribution of the training data \( \{v_1, v_2, \ldots, v_n\} \), i.e. the joint distribution of \( \{\xi(s_1^*), \xi(s_2^*), \ldots, \xi(s_n^*)\} \) is matrix normal (Equation 2.1). In order to achieve this likelihood, we rewrite the \( S \)-dependent parameters of this matrix normal distribution at the values of \( S \) at which the training data \( D_s \) is realised, i.e. in terms of the design vectors. Thus, we define

- the \( n \times jk \)-dimensional mean function \( H_DB \), where the linear form of the mean structure is contained in \( H_D^{(n \times m)} := [h^{(m \times 1)}(s_1^*), \ldots, h^{(m \times 1)}(s_n^*)] \) (and the coefficient matrix \( B \) is defined in Equation 2.3).

- the square exponential factor in the covariance matrix \( A_D^{(n \times n)} := [\exp\{-(s^* - s'^*)^TQ(s^* - s'^*)\}] \) (see Equation 2.5).

Then it follows from the matrix normal distribution of in Equation 2.1, with mean function defined in Equation 2.2 and Equation 2.3, and covariance matrix defined using Equation 2.5 and Equation 2.4, that \( D_s \) is distributed as matrix normal with mean matrix \( H_DB \), left covariance matrix \( A_D \) and right covariance matrix \( \Omega \), i.e.

\[
[D_s \mid B, C, \Sigma, Q] \sim \mathcal{MN}_{n,jk}(H_DB, A_D, \Omega) \tag{2.10}
\]
Thus, using known ideas about the matrix normal distribution - see Dawid (1981), Carvalho and West (2007) - we write

$$[D_s | B, C, Σ, Q] = \frac{1}{(2\pi)^{njk} |A_D|^{1/2} |Ω|^{1/2}} \exp \left\{ -\frac{1}{2} tr \left[ Ω^{-1} (D_s - H_D B)^T A_D^{-1} (D_s - H_D B) \right] \right\}$$

(2.11)

The interpretation of the above is that the $r$-th row of $[D_s | B, Σ, C, Q]$ is multivariate normal with mean corresponding to row of the mean matrix $H_D B$ and with covariance matrix $Ω$. Rows $r$ and $ℓ$ of $[D_s | B, Σ, C, Q]$ has covariance matrix $a(s_r, s_ℓ)Ω$. Similarly, the $ℓ$-th column of it is distributed as multivariate normal with mean being the $ℓ$-th column of $H_D B$ and with covariance matrix $ω_ℓ,ℓA_D$, where $ω_r,ℓ$ denotes the $(r, ℓ)$-th element of $Ω$. The covariance between columns $r$ and $ℓ$ is given by the matrix $ω_{r,ℓ}A_D$.

2.3. Estimating $s^{(new)}$

In order to predict the unknown model parameter vector $s^{(new)}$ when the input is the measured real data vector $v^{(test)}$, we would need the posterior predictive distribution of $s^{(new)}$, given $v^{(test)}$ and the training data $D_s$. This posterior predictive is usually computed by integrating over all the matrix-variate $GP$ parameters realised at the chosen design vectors $s_1^*, \ldots, s_n^*$.

While it is possible to analytically integrate over $B$ and $C$, $Σ$ and $Q$ cannot be analytically integrated out. In fact, we find it useful to learn the $d$ smoothing parameters i.e. the $d$ diagonal elements of $Q$, given the data. Thus, one useful advantage of our method is that the smoothness of the process does not need to be imposed by hand, but can be learnt from the data, if desired.

Given that we are then learning of $s^{(new)}$, $Σ$ and $Q$, we rephrase our motivation as seeking to compute the joint posterior probability of $s^{(new)}$, $Q$ and $Σ$, conditional on the real data and the training data, for a choice of the design set. In fact, we achieve a closed form expression of this joint posterior of $s^{(new)}$, $Q$ and $Σ$, by integrating over the other hyperparameters, namely, the amplitude of the mean function ($B$) and the matrix $C$ that bears information about covariance between different components of the data vector for each of the $j$ observations, at a fixed value of $S$. From this closed form expression, the marginal posterior probability densities of $Q$, $Σ$ and any of the $d$ components of the $s^{(new)}$ vector can be obtained, using the transformation based MCMC sampling method (Dutta and Bhattacharya, 2013) that we adopt.

Thus, for a given choice $s_1^*, \ldots, s_n^*$ of the design vectors, the posterior distribution $[s^{(new)}, Σ, Q | v^{(test)}, D_s]$ is sought, by marginalising $[s^{(test)}, Σ, Q, B, C | v^{(test)}, D_s]$ over the process matrices $B$ and $C$.

2.4. Priors used

We use uniform prior on $B$ and a simple non-informative prior on $C$, namely, $π(C) \propto |C|^{-(j+1)/2}$. As for the priors on the other parameters, we assume uniform prior on $Q$ and use the non-informative prior $π(Σ) \propto |Σ|^{-(k+1)/2}$. The prior information available in the literature will be considered to select the prior on $s^{(new)}$; below we use uniform priors on all components of the $s^{(new)}$ vector (see Section 4 for greater details in regard to the application that we discuss later).
2.5. Posterior of $s^{(new)}$ given training and test data

Since our interest lies in estimating $s^{(new)}$, given the real (test) data and the simulated (training) data, as well as in learning the smoothness parameter matrix $Q$ and the matrix $\Sigma$ that bears the covariance amongst the $j$ observables, we compute the joint posterior probability density $[s^{(new)}, Q, \Sigma | v^{(test)}, D_s]$. As expressed above, we achieve this by writing $[s^{(new)}, B, C, Q, \Sigma | v^{(test)}, D_s]$ and marginalise over $B$ and $C$.

To construct an expression for this posterior distribution, we first collate the training and test data to construct the augmented data set $D_{aug} = (H_{aug}^T)^T$. Then the set of values of the model parameter vector $S$ that supports $D_{aug} = \{s_1^*, \ldots, s_n^*, s^{(new)}\}$ of which only $s^{(new)}$ is unknown.

We next write the $S$-dependent matrix-value parameters at those values of $S$ at which the augmented data set is realised. Thus we define

- $H_{D_{aug}}^{(n+1) \times m} := [h_s, h_t, \ldots, h_s, h_t, (s_1^*, s_n^*)]$, where our choice of the functional form of $h_s$ has been given in Section 2 and we also set $m = d + 1$,
- $A_{D_{aug}}^{(n+1) \times (n+1)} := [\exp(-(s'_i - s'_j)^T Q (s'_i - s'_j))]$ where $s'_i$ and $s'_j$ are members of the set $\{s_1^*, \ldots, s_n^*, s^{(new)}\}$,
- $M_{aug} := A_{D_{aug}}^{-1} - A_{D_{aug}}^{-1} H_{D_{aug}} H_{D_{aug}}^{-1} H_{D_{aug}} A_{D_{aug}}^{-1}$,
- $(D_{aug}^T M_{aug} D_{aug})^{(jk \times jk)} := [M_{tu}^j, t, u = 1, \ldots, k]$, where $M_{aug, tu}$ is a matrix with $j$ rows and $j$ columns. Given $\Sigma$, we define $m = d + 1$ and $\psi_{tu}^{-1}$ as the $(t, u)$-th element of $\Sigma^{-1}$, so that $(n + 1 - m) k \psi_{tu}^{-1}$.

The priors used on $B, C, Q, \Sigma$ and $s^{(new)}$ are listed in Section 2.4. Using these, we observe that

$$
[s^{(new)}, Q, B, \Sigma, C | v^{(test)}, D_s] \propto D_{aug}^{(n+1) \times m} \times \exp \left[ \frac{1}{2} \Omega^{-1} \Omega^{-1} D_{aug} \right] \times \exp \left[ \frac{1}{2} \Omega^{-1} \Omega^{-1} B^{-1} \Omega^{-1} B^{-1} \right] \times \exp \left[ \frac{1}{2} \Omega^{-1} \Omega^{-1} H_{D_{aug}} H_{D_{aug}}^{-1} H_{D_{aug}} A_{D_{aug}}^{-1} A_{D_{aug}}^{-1} \right] \times \exp \left[ \frac{1}{2} \Omega^{-1} \Omega^{-1} A_{D_{aug}}^{-1} A_{D_{aug}}^{-1} A_{D_{aug}}^{-1} \right]
$$

(2.12)

where we have recalled Equation 2.11.

Marginalising $[s^{(new)}, Q, B, \Sigma, C | v^{(test)}, D_s]$ (as expressed in Equation 2.12) over $B$ and $C$ yields the joint posterior $[s^{(new)}, Q, \Sigma | v^{(test)}, D_s]$, the form of which is obtained as follows:

$$
[s^{(new)}, Q, \Sigma | v^{(test)}, D_s] = \int \int [s^{(new)}, Q, B, \Sigma, C | v^{(test)}, D_s] dB dC
$$

(2.13)
Thus, we obtain a closed-form expression of the joint posterior of $s^{(new)}$, $Q$, $\Sigma$, given training and test data, for a given choice of the design matrix (Equation 2.13), up to a normalising constant. The $GP$ prior is strengthened by the $n$ number of samples taken from it at the training stage. We sample from the achieved posterior using MCMC techniques to achieve the marginal posterior probabilities of $Q$, $\Sigma$ or any component of $s^{(new)}$, given all data. We conduct posterior inference using the TMCMC methodology (Dutta and Bhattacharya, 2013) that works by constructing proposals that are deterministic bijective transformations of a random vector drawn from a chosen distribution.

### 2.6. Errors in measurement

In our application, the errors in the measurements are small and will be ignored for the rest of the analysis. In general, when errors in the measurements that comprise the training data and the test data are not negligible, we assume Gaussian measurement errors $\varepsilon_t$, in $v_t$, with $t = 1, 2, \ldots$, such that $\varepsilon_t \sim N_{jk}(0, \varsigma)$, where $\varsigma = \Sigma_1 \otimes \Sigma_2$; $\Sigma_1, \Sigma_2$ being positive definite matrices. If both $\Sigma_1$ and $\Sigma_2$ are chosen to be diagonal matrices, then $\varsigma$ is a diagonal matrix; assuming same diagonal elements would simplify $\varsigma$ to be of the form $\phi \times I$, where $I$ is the $jk \times jk$-th order identity matrix. This error variance matrix $\varsigma$ must be added to $\Omega$ before proceeding to the subsequent calculations. TMCMC can be then be used to update $\varsigma$.

3. Case study

Curiosity about the nature of the Milky Way parameter space that we earthlings live in, is only natural. Here we focus on the learning of those Milky Way parameters that can be invoked to bear influence upon the observed motions of individual stars in the neighbourhood of the Sun. Astrophysical modelling indicates that in the solar neighbourhood, effects of different features of the Milky Way are relevant (Antoja et al., 2009; Chakrabarty, 2007; Minchev et al., 2009). Such features include an elongated bar-like structure made of stars (the stellar bar) that rotates at the centre of the Galaxy, and the spiral pattern of the Galaxy (see Figure 1 of supplementary section S-1). Thus, the motions of stars in the solar neighbourhood are affected by the parameters that define these Galactic features. Included in these feature parameters are the locations of the observer of such motions - we from Earth observe such motions and the observed stellar velocities are affected by where in the Galaxy we are. On astronomical scales, the Earth’s location in the Milky Way is equivalent to the location of the Sun inside the Galaxy. Our location in the Galaxy is given by the angular separation of the Sun from a chosen line inside the system (an identified axis of the aforementioned stellar bar) and the distance from the Sun to the centre of the Galaxy. These location parameters of the observer, as well as parameters of the bar, spiral pattern and other Milky Way features, can be brought to bear influence upon the motions of stars that are observed. Such parameters also include rates of rotation of the spiral pattern ($\Omega_s$) and that of the bar ($\Omega_b$), etc. In fact, the number of relevant feature parameter demands expansion to include parameters that have hitherto been ignored from astrophysical modelling of the available stellar data.

Given that these galactic feature parameters affect the solar neighbourhood, if motions of a sample of stars in this neighbourhood are measured, such data will harbour information about these feature parameters. Then, inversion of such measured motions will allow for the learning of the unknown feature parameters. This approach has been adopted in the modelling of our galaxy, to result in the estimation of the angular separation of the Sun from a chosen axis of the bar and the distance of the
Sun from the Galactic centre (Dehnen, 2000; Fux, 2001; Minchev et al., 2010; Simone et al., 2004). The other relevant feature parameters are typically held constant in such modelling.

In the astronomical literature, Milky Way feature parameters in the solar neighbourhood have been explored via simulation based studies (Englmaier and Gerhard, 1999; Fux, 1997) while similar estimation is performed using other (astronomical) model-based studies (Aumer and Binney, 2009; Golubov, 2012; Perryman, 2012). Chakrabarty (2007) attempted estimation of the sought Galactic parameters via a test of hypothesis exercise. A non-parametric frequentist test was designed to test for the null that the observed data is sampled from the estimated density of the \(i\)-th synthetic data generated at the \(i\)-th chosen value of the Milky Way feature parameter vector \(S\). The \(p\)-value of the used test statistic was recorded for each \(i = 1, 2, \ldots, n\) where \(n\) such choices of \(s\) were made. The choices of \(s\) at which the highest \(p\)-values were obtained, were considered better supported by the observed data. Hence the empirical distribution of these \(p\)-values in the space of \(S\), was used to provide interval estimates of the Milky Way feature vector. However, the method requires computational effort and is highly data intensive since the best match is sought over a very large collection of training data points. This shortcoming had compelled Chakrabarty (2007) to resort to an unsatisfactory coarse gridding of the space of \(S\). This problem gets acute enough for the method to be rendered useless when the dimensionality of the vector \(S\) that we hope to learn, increases. Moreover, the method of quantification of uncertainty of the estimate of the location is also unsatisfactory, dependent crucially on the binning details, which in turn is bounded by cost and memory considerations.

In the methodology discussed above we attempt an estimate of the unknown Milky Way feature parameter vector \(S \in \mathbb{R}^d\) using the sampled discrete stellar velocity data. In our application, the dimensionality of \(S\) is 2 as we estimate the coordinates of the radial location \(r_\odot\) of the Sun with respect to the Galactic centre and the angular separation \(\phi_\odot\) of the Sun-Galactic centre line from a pre-set line in the Milky Way disk (see Figure 1 in supplementary section S-1). Then for the Sun, \(R = r_\odot\) and \(\Phi = \phi_\odot\) where the variable \(R\) gives radial distance from the Galactic centre of any point on the disk of the Milky Way and the variable \(\Phi\) gives the angular separation of this point from this chosen pre-set line. The reason for restricting our application to the case of \(d=2\) is the existence of simulated stellar velocity data (aka training data) generated by scanning over chosen guesses for \(r_\odot\) and \(\phi_\odot\), with all other feature parameters held constant. If simulated data distinguished by choices of other Milky Way feature parameters become available, then the implementation of such data as training data will be possible, allowing then for the learning of Milky way parameters in addition to \(r_\odot\) and \(\phi_\odot\). In this method, computational costs are the only concern in extending to cases of \(d > 2\); extending to a higher dimensional \(S\) only linearly scales computational costs (Section 6).

Also, the stellar velocity vector is 2-dimensional, i.e. \(k=2\) in this application. Then the measured data in this application is a \(j \times 2\)-dimensional matrix. In our Bayesian approach, a much smaller \(j (=50)\) allows for inference on the unknown value \(s^{(\text{new})}\) of the Milky Way feature parameter vector, than \(j \sim 3000\) that is demanded by the aforementioned calibration approach used by Chakrabarty (2007).

In this application, the available data include the observed or real data and 4 sets of synthetic (or training) data sets obtained via dynamical simulations of each of 4 distinct base astronomical models of our galaxy advanced by Chakrabarty (2007). As the analysis is performed with each training data set at a time, we do not include reference to the corresponding base model in the used notation. The simulated data presented in Chakrabarty (2007) that we use here, is generated at 216 distinct values of \(S\), i.e. \(n=216\). Thus, our design set comprises the 216 chosen values of \(S\): \(s_1^* \ldots s_{216}^*\). For each
of the 4 base astrophysical models, at each chosen \( s^*_i \), 50 2-dimensional stellar velocity vectors are generated from dynamical simulations of that astrophysical model (of the Milky Way), performed at that value of \( S \). These 50 2-dimensional velocity vectors are treated in our work as a \( 50 \times 2 = 100 \)-dimensional motion vector \( v_i; i = 1, \ldots, 216 \). Then at the 216 design vectors, \( s^*_1, \ldots, s^*_216 \), 216 motion vectors are generated: \( v_1, \ldots, v_{216} \). Then the training data in our work comprises all such motion vectors and is represented as \( D_s(216 \times 100) \). The real or test data is treated in our work as the 100-dimensional motion vector \( v^{(\text{test})} \).

As said above, there are 4 distinct training data sets available from using the 4 base astronomical models of the Milky Way, as considered by Chakrabarty (2007). The choice of the base astrophysical model is distinguished by the ratio of the rates of rotation of the spiral to the bar, \( \Omega_s/\Omega_b \). That this ratio is relevant to stellar motions in the Galaxy is due to the fact that \( \Omega_s/\Omega_b \) can crucially control the degree of chaos in the Galactic model\(^1\). Thus, the 4 base astrophysical models are differently chaotic. This results in 4 distinct simulated velocity data sets \( D_s^{(1)}, D_s^{(2)}, D_s^{(3)}, D_s^{(4)} \) that bear the effects of such varying degrees of chaos, each generated at the chosen design set \( \{ s^*_1, \ldots, s^*_n \} \).

Details of the dynamical simulations performed on the 4 astrophysical models are given in the supplementary section S-2.

### 3.1. Details of our implementation of TMCMC

In TMCMC, high-dimensional parameter spaces are explored by constructing bijective deterministic transformations of a low-dimensional random vector. The random vector of which a proposal density is a transformation of, can be chosen to be of dimensionality between 1 and the dimensionality of the parameters under the target posterior. The acceptance ratio in TMCMC does not depend upon the distribution of the chosen random vector. In our application we use TMCMC to update the entire block \((s^{(\text{new})}, Q, \Sigma)\) at the same time using additive transformations of a one-dimensional random variable \( \epsilon \sim N(0, 1)I_{\{ \epsilon > 0 \}} \). In the \( t \)-th iteration, the state of the unknown parameters is \((s^{(\text{new};t)}, Q^{(t)}, \Sigma^{(t)}) := \varphi^{(t)} \). We update \( \varphi^{(t)} \) by setting, with probabilities \( \pi_j \) and \((1 - \pi_j)\), \( \varphi_j^{(t+1)} = \varphi_j^{(t)} \pm c_j \epsilon \) (forward transformation) and \( \varphi_j^{(t+1)} = \varphi_j^{(t)} - c_j \epsilon \) (backward transformation), respectively, where, for \( j = 1, \ldots, d, \pi_j \) are appropriately chosen probabilities and \( c_j \) are appropriately chosen scaling factors. Assume that for \( j_1 \in \mathcal{U}, \varphi_{j_1}^{(t)} \) gets the positive transformation, while for \( j_2 \in \mathcal{U}^c, \varphi_{j_2}^{(t)} \) gets the backward transformation. Here \( \mathcal{U} \cup \mathcal{U}^c = \{1, \ldots, d^*\} \), where \( d^* = 2d + \frac{k(k+1)}{2} \). The proposal \( \varphi^{(t+1)} \) is accepted with acceptance probability given in Supplementary Section S-3.

Once the proposal mechanism and the initial values are decided, we discard the next 100,000 iterations of our final TMCMC run as burn-in and stored the next 1,000,000 iterations for inference. For each model it took approximately 6 hours on a laptop to generate 1,100,000 TMCMC iterations.

---

\(^1\)For example, it is well known in chaos theory that when \( \Omega_s/\Omega_b \) is such that one of the radii at which the bar and the stellar disk resonate, concurs with a radius at which the spiral and the stellar disk resonate, global chaos is set up in the system (G. Walker and J. Ford, 1969). Chakrabarty and Sideris (2008) have corroborated that the degree of chaos is maximal in the astrophysical Galactic model marked by such a ratio (\( \Omega_s/\Omega_b=22/55 \)). They report that in models marked by slightly lower (\( \Omega_s/\Omega_b=18/55 \)) or higher (\( \Omega_s/\Omega_b=25/55 \)) values of this ratio, chaos is still substantial. In the Galactic model that precludes the spiral however, chaos was quantified to be minimal. It is these 4 states of chaos - driven by the 4 values of \( \Omega_s/\Omega_b \) - that mark the 4 astrophysical models as distinct.
4. Results using real data

The training data that we use was obtained by Chakrabarty (2007), by choosing the solar radial location from the interval [1.7, 2.3] in model units. This explains the motivation for selecting the bounds on $r_\odot$ to be the edges of this interval. Here, values of distances are expressed in the units implemented in the base astrophysical models of the Milky Way. However, to make sense of the results we have obtained, these model units will need to be scaled to provide values in real astronomical units of distances inside galaxies, such as the “kiloparsec” (abbreviated as “kpc”). A distance of 1 in model unit scales to $\frac{R}{r_\odot}$-kpc, where $R$ is the solar radius obtained in independent astronomical studies (Binney and Merrifield, 1998, $R=8$kpc) and $\hat{r}_\odot$ is the estimate of the solar radius in our work. The ulterior aim in estimating the solar radius is in estimating the rotational frequency $\Omega_b$ of the bar, where $\Omega_b = \frac{v_0}{R}$, with $v_0=220$kms$^{-1}$ and $R=8$kpc. Then, we get $\Omega_b = \frac{220}{\frac{8}{\hat{r}_\odot}}$kms$^{-1}$/kpc.

See Section S-1 of the attached supplementary material to see a schematic representation of the central bar in the Galaxy and Section S-2 for details of the scaling between the model units and real astronomical units.

Our other estimate is of the angular separation between the long axis of the bar and the line that joins the Sun to the Galactic centre. It is suggested in past astronomical modelling work to be an acute angle (Chakrabarty, 2007; Englmaier and Gerhard, 1999; Fux, 2001). Indeed, the training data used here was generated in simulations performed by Chakrabarty (2007), in which $\phi_\odot$ is chosen from the interval $[0, 90^\circ]$. This motivates the consideration of the interval of $[0, 90^\circ]$ for the angular location of the Sun.

Given the bounds on $r_\odot$ and $\phi_\odot$ presented above, in our TMCMC algorithm, we reject those moves that suggest $r_\odot$ and $\phi_\odot$ values that fall outside these presented intervals.

The 4 astrophysical models of the Galaxy that were used to generate the 4 training data sets, are marked by the same choice of the value of $\Omega_s$, and the background Galactic model parameters, while they are distinguished by the varying choices of the ratio $\Omega_s : \Omega_b$, where the Galactic spiral pattern rotates with rate $\Omega_s$. In fact, the astrophysical model bar_6 is the only one that does not include the influence of the spiral pattern while the other three astrophysical models include the influence of both the bar and the spiral. For the astrophysical models sp3bar3_18, sp3bar3 and sp3bar3_25, $\Omega_s : \Omega_b$ is respectively set to $18\Omega_b/55$, $22\Omega_b/55$, $25\Omega_b/55$. The physical effect of this choice is to induce varying levels of chaoticity in the 4 astrophysical models. Thus, Chakrabarty and Sideris (2008) confirmed that of the 4 models, bar_6 manifests very low chaoticity while sp3bar3 manifests maximal chaos, though both sp3bar3_18, sp3bar3_25 are comparably chaotic.

Ancillary real data needs to be brought in to judge the relative fit amongst the astrophysical base models. In fact, Chakrabarty (2007) brought in extra information to perform model selection. Such information was about the observed variance of the components of stellar velocities and this was used to rule out the model bar_6 as physically viable, though the other three models were all acceptable from the point of view of such ancillary observations that are available. This led to the inference that $\Omega_s \in [18\Omega_b/55, 25\Omega_b/55]$.

It is to be noted that if there was 1 data set and we were trying to fit 4 different models to that same data, then it is very much possible that for this 1 data set, the average of 4 models could have been achieved. However, here we are dealing with 4 base models, each of which is giving rise to a distinct training data set, in fact under mutually contradicting physics. Therefore, such model averaging is
The marginal posterior densities of \((r_\odot, \phi_\odot)\) corresponding to the 4 base astrophysical models of the Milky Way, are shown in Figures 1, 2, 3 and 4. It merits mention that the multimodality manifest in the marginal posterior distributions in 3 of the 4 base models is not an artifact of inadequate convergence but is a direct fallout of the marked amount of chaoticity in all 3 base models except in the model \(\text{bar}_6\), (Chakrabarty and Sideris, 2008). In Section S-6, we discuss the connection between chaos and consistency of multiple observer locations with available stellar velocity data.

Table 1 presents the posterior mode, the 95% highest posterior density (HPD) credible region of \(r_\odot\) and \(\phi_\odot\) respectively, associated with the four base models. Here \(r_\odot\) is expressed in the model units of length, i.e. in units of \(r_{CR}\). \(\phi_\odot\) is expressed in degrees. The HPDs are computed using the methodology discussed in Carlin and Louis (1996). Disjoint HPD regions, characterise the highly multi-modal posterior distributions of the unknown location. Using the 95% HPDs of the estimate \(r_\odot\) expressed in model units, and using the independently known astronomical measurement of the solar radial location as 8kpc, the bar rotational frequency \(\Omega_b\) is computed (see third enumerated point discussed above) in Table 1.

Summaries of the posteriors (mean, variance and 95% credible interval) of the smoothness parameters \(b_1, b_2\) and \(\Sigma\) are presented in Tables 2, 3. Notable in all these tables are the small posterior variances of the quantities in question; this is indicative of the fact that the data sets we used, in spite of the relatively smaller size compared to the astronomically large data sets used in the previous approaches in the literature, are very much informative, given our vector-variate GP-based Bayesian approach. Owing to our Gaussian Process approach, the posterior of \(\Sigma\) should be close to the null matrix \textit{a posteriori} if the choice of the design set and the number of design points are adequate.
Quite encouragingly, Table 3, shows that indeed Σ is close to the null matrix a posteriori, for all the four models, signifying that the unknown velocity function has been learned well in all the cases.

### 4.1. Comparison with results in astrophysical literature

The estimates of the angular separation of the long axis of the bar from the Sun-Galactic centre line and the rotation rate of the bar compare favourably with results obtained by Chakrabarty (2007), Englmaier and Gerhard (1999), Debattista et al. (2002), Benjamin et al. (2005), Antoja et al. (2011). A salient feature of our implementation is the vastly smaller data set that we needed to invoke than any of the methods reported in the astronomical literature, in order to achieve the learning of the two-dimensional vector $S$ - in fact while in the calibration approach of Chakrabarty (2007), the required sample size is of the order of 3,500, in our work, this number is 50. Thus, data sufficiency issues, when a concern, are well tackled by our method.

| Model       | $r_\odot$ (in units of $r_{CR}$) | $\Omega_b$ (in $\text{kms}^{-1}/\text{kpc}$) | $\phi_\odot$ |
|-------------|----------------------------------|---------------------------------|--------------|
|             | Mode 95% HPD                      | Mode 95% HPD                    | Mode 95% HPD |
| $\text{bar6}$ | 2.20 [2.04, 2.30]                | [56.1, 63.25]                  | 23.50 [21.20, 25.80] |
| $\text{sp3bar3}$ | 1.73 [1.70, 2.26] ∪ [2.27, 2.28] | [46.75, 62.15] ∪ [62.45, 62.7] | 18.8 [9.6, 61.5] |
| $\text{sp3bar3}_{18}$ | 1.76 [1.70, 2.29]                | [46.75, 62.98]                | 32.5 [17.60, 79.90] |
| $\text{sp3bar3}_{25}$ | 1.95 [1.70, 2.15]                | [46.75, 59.12]                | 37.6 [28.80, 40.40] |
Upon the analyses of the viable astrophysical models of the Galaxy, Chakrabarty (2007) reported the result that $r_⊙ \in [1.9375, 2.21]$ in model units while $φ_⊙ \in [0°, 30°]$, where these ranges correspond to the presented uncertainties on the estimates, which were however, rather unsatisfactorily achieved (see Section 2). The values of the components of $S$, learnt in our work, overlap well with these results. As mentioned above, the models $sp3bar\_3\_18$, $sp3bar\_3$ and $sp3bar\_3\_25$ are distinguished by distinct values of the ratios of the rotational rates of the spiral pattern $Ω_3$ to that of the bar ($Ω_b$) in the Galaxy. Then the derived estimate for $Ω_b$ (Table 1) suggests values of $Ω_3$ of the Milky Way spiral.

Another point that merits mentions is that the estimates of $r_⊙$ and $φ_⊙$ presented by Chakrabarty (2007) exclude the model $sp3bar\_3$ which could not be used to yield estimates given the highly scattered nature of the corresponding $p$-value distribution. Likewise, in our work, the same model manifests maximal multi-modality amongst the others, but importantly, our approach allows for the representation of the full posterior density using which, the computation of the 95% HPDs is performed.

That the new method is able to work with smaller velocity data sets, is an important benefit, particularly in extending the application to galaxies other than our own, in which small numbers of individual stars are going to be tracked in the very near future for their velocities, under observational programmes such as PANStarrs (Johnston et al., 2009) and GAIA (Kucinskas et al., 2005; Lindegren et al., 2007, http://www.rssd.esa.int/index.php?project=GAIA&page=index); the sample sizes of measured stellar velocity vectors in these programmes will be much smaller in external galaxies than what has been possible in our own. At the same time, our method is advanced as a template for the analysis of the stellar velocity data that is available for the Milky Way, with the aim of learning a high-dimensional Galactic parameter vector; by extending the scope of the dynamical simulations of the Galaxy, performed on different astrophysical models of the Milky Way, the Milky Way models will be better constrained. The mission GAIA - a mission of the European Space Agency - is set to provide large sets of stellar velocity data all over the Milky Way. Our

### Table 2

Summary of the posterior distributions of the smoothness parameters $b_1, b_2$ for the 4 models.

| Model    | $b_1$ Mean | $b_1$ Var | $b_1$ 95% CI | $b_2$ Mean | $b_2$ Var | $b_2$ 95% CI |
|----------|------------|-----------|--------------|------------|-----------|--------------|
| $bar_3$  | 0.9598155  | 3.15 × 10^{-9} | [0.959703, 0.959879] | 1.005078  | 2.85 × 10^{-9} | [1.004985, 1.005142] |
| $sp3bar\_3$ | 0.8739616  | 6.72 × 10^{-7}  | [0.872347, 0.875052] | 1.003729  | 8.98 × 10^{-7}  | [1.002500, 1.005500] |
| $sp3bar\_3\_18$ | 0.9410686  | 1.46 × 10^{-5}  | [0.938552, 0.955264] | 0.999010  | 4.08 × 10^{-6}  | [0.997219, 1.004945] |
| $sp3bar\_3\_25$ | 0.7597931  | 5.64 × 10^{-10} | [0.759743, 0.759833] | 0.992174  | 2.89 × 10^{-9}  | [0.992067, 0.992246] |

### Table 3

Summary of the posterior distribution of the diagonal and one non-diagonal element of $Σ$, from the 4 base astrophysical models.

| Model    | $σ_{11}$ Mean | $σ_{11}$ Var | $σ_{11}$ 95% CI | $σ_{22}$ Mean | $σ_{22}$ Var | $σ_{22}$ 95% CI | $σ_{12}$ Mean | $σ_{12}$ Var | $σ_{12}$ 95% CI |
|----------|---------------|--------------|-----------------|---------------|--------------|-----------------|---------------|--------------|----------------|
| $bar_3$  | [5.40 × 10^{-8}, 4.0 × 10^{-4}] | 6.20 × 10^{-8}, 4.76 × 10^{-4} | [0, 1.30 × 10^{-5}] |               |              |                 |               |              |                |
| $sp3bar\_3$ | [3.66 × 10^{-3}, 1.03 × 10^{-2}] | 6.53 × 10^{-5}, 1.83 × 10^{-2} | [−6.40 × 10^{-5}, 2.68 × 10^{-4}] |               |              |                 |               |              |                |
| $sp3bar\_3\_18$ | [1.45 × 10^{-3}, 1.68 × 10^{-4}] | 1.29 × 10^{-5}, 1.50 × 10^{-1} | [−1.19 × 10^{-3}, 2.16 × 10^{-3}] |               |              |                 |               |              |                |
| $sp3bar\_3\_25$ | [1.21 × 10^{-4}, 5.69 × 10^{-4}] | 1.13 × 10^{-4}, 5.21 × 10^{-4} | [−1.00 × 10^{-6}, 1.50 × 10^{-5}] |               |              |                 |               |              |                |
method, in conjunction with astrophysical models, can allow for fast learning of local and global model parameters of the Galaxy.

5. Model fitting

In this section we compare the observed test velocity data with predictions that we make at a summary \(\hat{s}\) of the posterior of the model parameter vector \(S\). To achieve this, we first need to provide a suitable estimator of the function \(\xi(\cdot)\). We attempt to write the conditional distribution of \(\xi(\hat{s})\) given the augmented data \(D_a\) made of training data \(D_s\) augmented by \(v^{(\text{test})}\) that we consider realised at \(S = \hat{s}\), where we choose \(\hat{s}\) to be the median \(s^{(\text{median})}\) of the posterior of \(S\) given \(D_a\), the mode \(s^{(\text{mode})}\) of this posterior or \(s^{(u)}, u=1,2,3,4\)—the end points of the disjoint 95% HPD region of the posterior of \(S\) (see Table 1).

Since \(\{\xi(\hat{s}), \xi(s_1), \ldots, \xi(s_n), \xi(\hat{s})\}\) is jointly matrix-normal, \(\xi(\hat{s})|\xi(s_1), \ldots, \xi(s_n), \xi(\hat{s}) = [\xi(\hat{s})|D_s]\) is \(jk\)-variate normal. The mean function of this distribution at different \(\tilde{s}\) is then compared to the test data. Thus, the estimate of the function that we seek is \(E[\xi(S)|D_s, S, Q]\), given the dependence of \(\xi(\cdot)\) on the smoothness parameters (elements of \(Q\)) that we anticipate.

However, we only know the conditional of \(\xi(\cdot)\) on all the \(GP\) parameters, including the ones that we do not learn from the data, namely \(B\) and \(C\). So we need to marginalise \(\xi(\cdot) \mid \Sigma, B, C, Q, D_s\) over \(B\) and \(C\). To achieve this, we need to invoke the conditional distribution of \(B\) and \(C\) with respect to the other \(GP\) parameters and \(D_s\). We recall the priors on the \(GP\) parameters \(B, \Sigma, C\) (from Section 2.4) to write \(\pi(B, \Sigma, C) \propto |\Sigma|^{-(k+1)/2} |C|^{-(j+1)/2}\). It then follows that

\[
[B \mid \Sigma, C, Q, D_s] \sim N_{m,jk}(\hat{B}_{GLS}, (H^T_D A_D^{-1} H_D)^{-1}, \Omega),
\]

where, \(\hat{B}_{GLS} = (H^T_D A_D^{-1} H_D)^{-1}(H^T_D A_D^{-1} B D_s)\). Marginalising the \(jk\)-variate normal that is the conditional \(\xi(\cdot) \mid B, \Sigma, C, Q, D_s\) over \(B\) (using Equation 5.1) it can be shown that

\[
\xi(\cdot) \mid \Sigma, C, Q, D_s \sim N_{jk}(\mu_2(\cdot), a_2(\cdot, \cdot)\Omega),
\]

where

\[
\mu_2(\cdot) = \hat{B}_{GLS}h(\cdot) + (D_s - H_D \hat{B}_{GLS})^T A_D^{-1} \sigma D(\cdot);
\]

\[
a_2(s_1, s_2) = a_1(s_1, s_2) + [h(s_1) - H^T_D A_D^{-1} s D(s_1)]^T (H^T_D A_D^{-1} H_D)^{-1} [h(s_2) - H^T_D A_D^{-1} s D(s_2)].
\]

We define \((n-m)\hat{\Omega}_{GLS} = (D_s - H_D \hat{B}_{GLS})^T A_D^{-1} (D_s - H_D \hat{B}_{GLS}), \) i.e. \((n-m)\hat{\Omega}_{GLS} = D_s^T M D_s\), with \(M = A_D^{-1} - A_D^{-1} H_D (H^T_D A_D^{-1} H_D)^{-1} H_D A_D^{-1}\).

We consider the mean of \(\mu_2(\cdot)\) of the conditional posterior given by (5.3) as a suitable estimator of the velocity function in our case. Note that \(\mu_2\) involves the unknown smoothness parameters \(\{b_1, b_2\}\); we plug-in the corresponding posterior medians \((0.874254, 1.003545)\) for these.

It is important to mention that though the mean and variance in Equations 5.3 and Equation 5.4 were developed using \(D_s\), in our construction of the velocity function estimator \(\mu_2, D_a\) is implemented, where \(D_a\) is obtained by augmenting \(D_s\) with \(v^{(\text{test})}\) that is realised at \(S = \hat{s}\). The underlying theory remains the same as above.

It is important to note that \(\mu_2(S)\), where \(S\) is the unknown location, is a random variable, and even though the posterior of \(\Sigma\) is concentrated around the null matrix, the variance of \(\mu_2(S)\) is not
0, thanks to the fact that $S$ does not have 0 variance. Consequently, the posterior variance of $\xi(S)$ does not have 0 variance. To see this formally, note that

$$\begin{align*}
V & \text{ar}[\xi(S)|\mathcal{D}_a] = V \text{ar}[E \{\xi(S)|\Sigma, C, Q, S, \mathcal{D}_a\}] + E[V \text{ar}[\xi(S)|\Sigma, C, Q, S, \mathcal{D}_a]] \\
& = V \text{ar}[\mu_2(S)|\mathcal{D}_a] + E[a_2(S, S)|\Omega|\mathcal{D}_a].
\end{align*}$$ (5.5)

Since the posterior $[\Sigma|\mathcal{D}_a]$ is concentrated around the $k \times k$-dimensional null matrix, it follows that the posterior $[\Omega|\mathcal{D}_a]$ is also concentrated around the $jk \times jk$-dimensional null matrix. Hence, in (5.5), $E[a_2(S, S)|\Omega|\mathcal{D}_a] \approx 0$. However, the first part of (5.5), $V \text{ar}[\mu_2(S)|\mathcal{D}_a]$, is strictly (and significantly) positive, showing that the variance of the posterior of $\xi(S)$ is significantly positive.

The above result shows that it should not be expected that the observed test velocity data $v^{(\text{test})}$ will be predicted accurately by $\mu_2(s)$, for any given $s$. This is in contrast with the usual Gaussian process emulators, where the argument of the unknown function is non-random, so that if the posterior of the function variance is concentrated around 0, then the posterior variance of the emulator would be close to 0.

In Figure 5 we illustrate, in the case of sp3bar3 (the most chaotic model), the degree of agreement of $\mu_2(s)$ with $v^{(\text{test})}$ for different choices of $s$. We compare with $v^{(\text{test})}$ the predictions $\mu_2(s^{(\text{mode})})$, $\mu_2(\tilde{s})$ and $\mu_2(s^{(\text{median})})$; $u = 1, 2, 3, 4$. Here, $s^{(\text{mode})} = (1.73, 18.8^\circ)$ is the (component-wise) posterior mode and $\tilde{s} = (2.2, 35^\circ)$ is a point somewhat close to the (component-wise) posterior median $s^{(\text{median})} = (1.994478, 33.59429^\circ)$ (grid-point closest to $s^{(\text{median})}$).

As observed in Figure 5 the best fit of $v^{(\text{test})}$ has been provided by $\mu_2(\tilde{s})$ where $\tilde{s}$ is close to the median $s^{(\text{median})}$; as the point $(s^{(\text{median})}, v^{(\text{test})})$ is in the training data constituting $\mu_2$, this is to be expected. The estimators $\mu_2(s^{(\text{mode})})$ and $\mu_2(s^{(1)})$ perform somewhat reasonably, but the remaining estimators $\mu_2(s^{(u)})$; $u = 2, 3, 4$ do not perform adequately, signifying the effect of variability of our estimator due the posterior of $S$.

While it is the randomness of the argument $S$ of the unknown function $\xi(\cdot)$ that causes the variability of our estimator, such variability is highest in the most chaotic of the 4 base astrophysical models (sp3bar3), and least in the only non-chaotic base astrophysical model (bar b). A similar exercise of predicting $v^{(\text{test})}$ using the training data simulated from this non-chaotic base model gives excellent fits at all the aforementioned used values of $S$; see Figure 6.

6. Discussions

Computational complexity scales only linearly with the dimensionality of the unknown model parameter $S$. Thus, porting a training data comprised of $n$ independent values of $S$, $s_i, i = 1, \ldots, n$, where $s_i$ is a $d$-dimensional vector, $d > 2$, is not going to render the computational times infeasible. This allows for the learning of high-dimensional model parameter vectors in our method.

In contrast to the situation with increasing the dimensionality of the unknown model parameter, increasing the dimensionality of the measurable will but imply substantial increase in the run time, since the relevant computational complexity then scales non-linearly, as about $O(k^3)$, (in addition to the cost of $k$ square roots), where $k$ is the dimensionality of the observed variable. This is because of the dimensionality of the aforementioned $\Sigma$ matrix is $k \times k$, and the inverse of this enters the computation of the posterior via the definition $C_{GLS,aug}$. Thus, for example, increasing the dimensions of the measurable from 2 to 4 increases the run time 8-fold, which is a large jump in the required run time. However, for most applications, we envisage the expansion of the dimensionality
of the unknown model parameter, i.e. \(d\), rather than that of the measurable, i.e. \(k\). Thus, the method is expected to yield results within acceptable time frames, for most practical applications.

The other major benefit of our work is that it allows for organic learning of the smoothness parameters, rather than results being subject to ad hoc choices of the same.

As more Galactic simulations spanning a greater range of model parameters become available, the rigorous learning of such Milky Way parameters using our method will become possible, given the available stellar velocity data. This will enhance the quality of our knowledge about our own galaxy. That our method allows for such learning even for under-abundant systems, is encouraging for application of a similar analysis to galaxies other than our own, in which system parameters may be learnt using the much smaller available velocity data sets, compared to the situation in our galaxy.

**Supplementary material**

Some background details on the application to the Milky Way are discussed in Section S-1 of the attached supplementary material. Section S-2 discusses the details of the dynamical simulations that
lead to the training data set used in our supervised learning of the Milky Way feature parameters. In Section S-3 we present details of the TMCMC methodology that we use here. S-4 discusses the cross-validation of our model and methodology, on simulated as well the real stellar velocity data. The effect of chaos on the modality of the posterior distributions of our unknowns is discussed in Section S-5.

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![Figure 6](image.png)

**Fig 6.** Prediction of $v^{\text{(test)}}$ for model bar6: plots of 2 components of $\mu_2(s)$ against $v^{\text{(test)}}$ for $s = \tilde{s}$ (2 adjacent panels on the left hand side of the top row), $s^{(\text{mode})}$ (2 panels on the right of top row), $s^{(1)}$ (2 panels on the left in the lower row), $s^{(2)}$ (2 panels on the left in the lower row).
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