Calculation of Hessian under Constraints

with Applications to Bayesian System Identification

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# Abstract

In Bayesian system identification with globally identifiable models, the posterior (i.e., given data) probability density function (PDF) of model parameters can be approximated by a Gaussian PDF. The most probable value (MPV) of the parameters is equal to the mean of the Gaussian PDF. It maximises the posterior PDF, or equivalently, minimises the negative of logarithm (NL) of the posterior PDF. The covariance matrix of the Gaussian PDF is equal to the Hessian of the NL at the MPV. Model parameters can be subjected to constraints, which must be accounted for in the calculation of the posterior covariance matrix. In applications such as modal identification, existing strategies define a set of free parameters and map them to the model parameters so that the constraints are always satisfied. The Hessian of the NL with respect to the free parameters is obtained and then transformed to give the posterior covariance matrix of the model parameters where constraints are accounted for. Analytical expressions for this Hessian are complicated because of the composite actions of the NL and the mapping; and this creates significant burden in computer coding. In this work, a theoretical framework is developed for evaluating the Hessian of a function under constraints in a systematic manner. It is applied to obtain new analytical expressions for evaluating the posterior covariance matrix in Bayesian operational modal analysis. The resulting expressions are simpler than existing ones based on direct differentiation. They allow problems with similar mathematical structures to be computer-coded in a coherent manner. Numerical examples are presented to illustrate consistency and computational aspects.

**Keywords**: Bayesian system identification; constraint; Hessian; Lagrange multiplier; operational modal analysis;

# Introduction

System identification aims at identifying the parameters of a mathematical model from measured data. It is under intensive research in many disciplines, e.g., structural dynamics in mechanical and civil engineering [1][2][3][4][5]. Bayesian approach offers a fundamental means to address uncertainties in system identification [6][7][8]. In this approach, identification results are encapsulated in the ‘posterior’ (i.e., given data) probability distribution of parameters. Let  be a vector of parameters to be identified and  denotes the measured data. Without much loss of generality,  and  are assumed to be continuous-valued. According to Bayes’ Theorem, the posterior probability density function (PDF) of  for given  is

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where  is the ‘prior distribution’, reflecting the analyst’s knowledge in the absence (or without using the information) of data;  is a normalizing constant, immaterial to the distribution of ;  is the ‘likelihood function’, which is the PDF of  for a given . For convenience in analysis and computation, the posterior PDF is often written as

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where

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is called the ‘negative logarithm function’ (NL) in this work.

One major task in Bayesian system identification is the determination of the statistics associated with the posterior PDF. The computational strategy depends on the topology of the posterior PDF, which reflects whether the data has provided sufficient information for identifying the parameters [9][10]. For ‘globally identifiable problems’, which is typical in well-posed problems, the posterior PDF has a unique maximum in the interior of the parameter space. The location of the maximum is the posterior ‘most probable value’ (MPV), , at which  is minimised. Approximating  by a second order Taylor series about  leads to a Gaussian approximation of  with a mean equal to  and a covariance matrix  equal to the inverse of the Hessian of  at the MPV, i.e.,

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where

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and the hat ‘^’ denotes that the Hessian is evaluated at the MPV.

Depending on how the system identification problem is formulated, there can be constraints among some of the model parameters. For example, in modal identification, mode shapes are subjected to scaling constraints. The entries of the covariance matrix of process noise in a state-space model are subjected to symmetry constraints. While constraints can be handled by proper parameterisation or Lagrange multipliers in the determination of MPV, the problem is more non-trivial for the posterior covariance matrix. Simply taking the Hessian of the NL with respect to (w.r.t.) the original parameters (which are under constraints) at the MPV does not give the right answer.

One way to account for constraints is to define a set of ‘free parameters’ and map them to the model parameters so that the constraints are always satisfied. The Hessian w.r.t. the free parameters is obtained and then transformed to give the posterior covariance matrix of the model parameters where constraints are accounted for. This mapping approach has been adopted in the derivation of analytical expressions for evaluating the posterior covariance matrix in Bayesian operational modal analysis (OMA), e.g., [11] for single setup data (see also [12]) and [13] for multiple setup data. The case for single setup data is the conventional setting in OMA where all degrees of freedom (DOFs) are synchronously measured during the same time period. The case for multiple setup data is demanded in practice where it is desired to obtain the mode shape comprising more DOFs than the number of available synchronous data channels (limited by, e.g., the number the sensors). In both cases, the constraint arises from mode shape scaling. Due to the composite action of the NL and the mapping function, the expressions are generally complicated, which creates burden in the development of computer codes. This motivated the present work to develop a more systematic method for deriving or calculating the Hessian under constraints. Two formulas are developed. The first formula is applicable for general parameter values. It allows the derivatives of the NL and the mapping function to be computer-coded separately. The second formula is applicable at the MPV. It is expressed in a compact form via Lagrange multiplier concepts. The proposed theory is applied to obtain new analytical expressions for evaluating the posterior covariance matrix in Bayesian operational modal analysis. The resulting procedures are simpler than existing ones based on direct differentiation.

# Transformation of covariance matrix

Let  be a set of parameters subjected to  independent constraints:

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The posterior covariance matrix of  under constraints can be calculated via the covariance matrix of a set of ‘free’ (i.e., unconstrained) parameters. Let  be a function that maps the vector of free parameters  to  so that the constraints are always satisfied, i.e.,

 for any ,  (

Since there are  parameters in  and they are subjected to  constraints, the dimension of the admissible space is . The number of parameters in  must then be

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As in Section 1, let  be the NL when the Bayesian system identification problem is formulated in terms of . When the problem is formulated in terms of , the NL for  is given by the composite function

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The MPV of  is related to the MPV of  by , where the hat ‘^’ denotes the MPV. Under Gaussian approximation of the posterior PDF of , its posterior covariance matrix is the inverse of the Hessian of  at . From this, the posterior covariance matrix of  can be obtained by transformation of variables. Let  and  be uncertain variations in  and  from their MPV, respectively. To the first order,

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where  denotes the gradient of  at the MPV. The posterior covariance matrix of  is then given by

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where  is the posterior covariance matrix of , equal to the inverse of  (Hessian of  at the MPV). Due to the mapping ,  () only has rank  and so is singular when . Nevertheless this singularity is immaterial to the posterior uncertainty of  because uncertainty variations in  result in variations in  that are orthogonal to the singular directions [14]. Consequently,

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where ‘’ denotes the ‘pseudo-inverse’, i.e., evaluated via eigenvector representation ignoring the  zero eigenvalue components arising from constraints. Since  is a composite function of , its Hessian (w.r.t. ) is analytically more complicated to derive than the Hessian of  (w.r.t. ).

# Outline of theory

For the ease of reading, in this section we first outline the key theoretical results in this paper. Mathematical proofs are provided in the appendix.

For general , we show that the Hessian of  can be expressed in terms of the gradients and Hessians of  and  by (Section 7.1)

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where ‘’ denotes the Kronecker product;  denotes the  identity matrix;

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denotes respectively the gradient and Hessian of  w.r.t.  and evaluated at ;

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denote respectively the gradient and Hessian of . Note that  is a vector-valued function. In (15),  and  are defined in a generalised manner by viewing the operators  and via the Kronecker product as  and , respectively. This generalisation is consistent with the ordinary definition when the function is a scalar.

Equation (13) is applicable for any . In fact, it is applicable for any function  that need not even be related to constraints. Due to the Kronecker product in the second term, the expression involves multiplying large matrices which are sparse. Generally,  does not vanish at the MPV due to the presence of constraints. The value of  at the MPV is not equal to the first term in (13). Using Lagrange multiplier concepts and the fact that  does satisfy the constraints in (7), we show further that the Hessian of  at the MPV is given by (Section 7.2)

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where

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is the ‘Lagrangian’;  are Lagrange multipliers;

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is the Hessian of  at the MPV;

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We also show that the posterior covariance matrix of  in (12) is invariant to the choice of the constraint functions  and mapping . Specifically, it is shown that (Section 7.3)  remains the same when  is replaced by  for any monotonic scalar function  with  and a non-zero derivative at . On the other hand, if one works with a new set of admissible free parameters  instead of , the resulting posterior covariance matrix of  remains the same (Section 7.4).

# Applications to Bayesian modal identification

Equation (16) allows the posterior covariance matrix of the set of model parameters  under constraints to be derived and calculated in a systematic manner. Using this formula, the derivatives of the NL  and the mapping function  can be handled separately. The derivatives of  are simpler than those of  because it does not involve any constraints.

In this section, we apply (16) to derive new expressions for calculating the posterior covariance matrix of parameters for Bayesian ambient modal identification (also known as ‘operational modal analysis’) with single setup data [11] and multiple setup data [13]. These methods make use of the Fast Fourier Transform (FFT) of ambient data in a selected frequency band around the subject modes of interest. See [15] for the pioneering paper and [16] for a review. Examples of recent field applications include [17][18][19][20][21][22]. Although the approach is applicable for general multiple (possibly close) modes [23], the discussion here is limited to well-separated modes. The new expressions allow easier and more systematic computer-coding of identification uncertainty.

In Bayesian modal identification, the prior PDF is assumed to be a constant because it is slowly varying compared to the likelihood function for typical data size encountered in applications. The posterior PDF is then directly proportional to the likelihood function, i.e.,

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where

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## Single setup data

In the single setup setting [11], let  (each  vector) be the time history of ambient acceleration data measured at  degrees of freedom (DOFs) of the subject structure. The scaled FFT of  at frequency  is defined as

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where  and  (sec) is the sampling interval. For long stationary data, it can be shown that the FFTs at different frequencies are asymptotically independent and jointly complex Gaussian with zero mean and a covariance equal to the power spectral density (PSD) matrix [24]. Correspondingly, using the scaled FFT  in a selected frequency band around the subject mode of interest, the NL is given by

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where the sum is over the frequencies in the selected band with  FFT points;  is the theoretical PSD matrix of data for given . Assuming a single mode in the selected band,

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where  denotes the  identity matrix;  () is the mode shape confined to the measured DOFs;  and  are respectively the PSD of the modal force and prediction error (e.g., measurement noise), both assumed to be constant in the selected band;

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is the dynamic amplification factor,  (Hz) is the natural frequency and  is the damping ratio (assuming classical damping). The mode shape is assumed to be scaled to have unit Euclidean norm, i.e., . Using the eigenvector representation of , the NL can be rewritten as a quadratic function of , which is found to facilitate analysis and computation:

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where

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The set of parameters  comprises , , ,  and , subjected to the constraint . Let  comprises the parameters other than the mode shape. In the context of the theory in Section 3, one can take

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so that  for any . Using (16),

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where  is the Hessian of the NL in (28) (ignoring constraint) at the MPV; and, using (19),

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is the value of the Lagrange multiplier at the MPV. Direct differentiation and evaluating at the MPV gives

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where  denotes a  zero matrix (similar notation for others);  denotes the gradient w.r.t. ;  denotes the value of  at the MPV. It remains to determine . The derivatives of  w.r.t. , ,  and  are the same as those derived in [11] because these parameters are not subjected to constraints. The derivatives of  w.r.t.  are now simpler, because they no longer need to account for the norm constraint. Let an indexed variable denote a derivative w.r.t. the variable. Direct differentiation of (28) and evaluating at the MPV gives

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The derivatives of  in (29) w.r.t. , ,  and  can be derived easily and are omitted here. Comparing the formulae here with those presented in Appendices I and II of [11], the derivatives involving the mode shapes are significantly simplified because they no longer involve the terms resulting from differentiation of  w.r.t.  by chain-rule. Such effect is now accounted by the Lagrange multiplier and the gradient . This makes computer-coding easier.

## Multiple setup data

In the multiple setup setting [13], it is assumed that ambient vibration data is collected from  setups, each performed in different time periods and measuring a possibly different set of DOFs. Modal properties other than the mode shape can possibly vary in different setups. The ‘local mode shape’ in Setup , i.e., confined to the measured DOFs in the setup, is denoted by  (). The ‘global mode shape’  () covers the measured DOFs in all setups. It is scaled to have unit norm, i.e., . Each  is related to  by , where  () is a selection matrix. The -entry of  is 1 if the th data channel in Setup  measures DOF  of .

Let  () be the ambient time history data in Setup  and  ( complex) be the collection of scaled FFTs in the selected band:

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where  (sec) is the sampling interval. Using the FFTs from all setups, the NL is given by

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where, for Setup , analogous to (25),

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 is the number of FFT points in the selected band;

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 (Hz) is the natural frequency,  is the damping ratio,  is the modal force PSD and  is the prediction error PSD. The set of modal parameters  comprises  and , subjected to unit norm constraint .

Using the theory in Section 3, it is possible to leverage on the computer code for single setup problem in Section 4.1 to calculate the posterior covariance matrix for multiple setup problem. For this purpose, the NL should be written in terms of a local mode shape that has unit norm, which has been assumed in the single setup setting. This can be done by defining the normalised local mode shape  and the corresponding modal force PSD  so that  in (41) is written as

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and now . The NL for each setup can then be written in exactly the same form as in (28) for a single setup:

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where

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Define the set of parameters in Setup  as

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so that

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Let  denote the set of parameters in Setup  other than the local mode shape, i.e.,

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Define  (free parameters),  (model parameters under constraints),  (mapping function satisfying constraints) and  (vector of constraint functions) as

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These definitions are specially designed to facilitate derivations and computations. Here,  has  free parameters;  has  parameters () under constraints among  and ; and  contains the  constraints. Check that  for any . Since  are explicitly contained in , they can be treated as independent variables when taking partial derivatives of . The partial derivative of  w.r.t.  is zero because  depends on  only through , but  has already been included in . Nevertheless,  is deliberately included in , for otherwise it is difficult to express systematically in  the constraints among the local mode shapes . Since  instead of  appears in the expression of  in (44), the gradient and Hessian of  w.r.t.  in (46) is equal to those of the NL for single setup problem with unit norm constraint in the local mode shape. These can be computed using the same computer code developed for the single setup problem.

The derivatives of  and  at the MPV can be obtained by direct differentiation:

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By noting that , the gradient and Hessian of  w.r.t.  at the MPV can be partitioned as

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These can be computed using the computer code for the single setup problem (with unit norm constraint on ). The gradient and Hessian of  at the MPV are related to those of  by

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In addition to the advantage from simplicity of expressions in the case of single setup, the formulation further reduces substantially the computer-coding effort by making use of the program developed for single setup. Computer-coding for the series of formulae in Section 3 of [13] is completely bypassed.

# Illustrative examples

In this section, numerical examples for single setup and multiple setup data are presented to investigate the consistency and computational aspect of the proposed method. Consistency is about the correctness of the formulation and is demonstrated by comparing the posterior covariance matrix calculated from the proposed method and finite different method (FDM). Computational aspect is investigated by comparing the computational time of the proposed method with the previous methods [11][12][13] and the FDM. To see how computational time scales with problem size, it is investigated w.r.t. the number of DOFs for single setup data and w.r.t. the number of setups for multiple setup data.

Consider synthetic data generated according to

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where  is the modal acceleration satisfying , with natural frequency  rad/sec (1 Hz) and damping ratio 1%;  is the modal excitation modelled as a Gaussian white noise with a PSD of 1.6 $μg/\sqrt{Hz }$;  is the channel noise modelled as a Gaussian white noise vector with i.i.d. components and a PSD of 1 $μg/\sqrt{Hz}$. Data is generated at a sampling rate of 100 Hz for 1000 seconds. To allow direct investigation w.r.t. the number of DOFs, the mode shapes value of all measured DOFs are assumed to be identical, i.e., . For single setup data, the data with  measured DOFs simply comprises the first  DOFs. For multiple setup data, each setup is assumed to have four measured DOFs. DOFs 1 and 2 are assigned as the reference DOFs. For  setups, the measured DOFs in different setups are assumed to be {1,2,3,4}, {1,2,5,6}, {1,2,7,8}, …, {1,2, }.

## Consistency

To demonstrate consistency, the posterior covariance matrix calculated by the proposed method is compared with that by FDM. For each entry in the posterior covariance matrix, the ratio of the value by FDM to that by the proposed method is calculated. The average of the absolute values of ratios for all entries is used as a measure for checking numerical consistency, the closer to 1 the better. In applying FDM, the finite difference from the MPV  (at which the Hessian should be evaluated) in the multi-dimensional space of  is parameterised as , where  is a dimensionless scalar step size. Figure 1 shows the average ratio for single setup data with 100 DOFs. Figure 2 shows the ratio for multiple setup data with 10 setups. It is clear that as the step size  decreases, the ratio converges to 1, demonstrating consistency of the proposed method. For both single setup and multiple setup data, other cases for different DOFs or number of setups have been verified similarly.



**Figure 1 Average ratio of the entries in the posterior covariance matrix calculated by FDM to that by the proposed method, single setup data with 100 DOFs.**



**Figure 2 Average ratio of the entries in the posterior covariance matrix calculated by FDM to that by the proposed method, multiple setup data with 10 setups.**

## Computational time

To investigate the computational aspect, Figure 3 shows the computational time required by the proposed method, the previous method [11][12] and the FDM for the single setup data versus the number of measured DOFs. A desktop computer (HP Elite Desk, i5-4590T, 2GHz) was used. The computational times of the proposed and previous method are similar, while that of the FDM is substantially longer. The computational time for multiple setup data is shown in Figure 4, where the results are plotted w.r.t. the number of setups. The computational time of the proposed method is slightly shorter than that of the previous method [13] but they grow at a similar rate with the number of setups. Similar to the case of single setup, FDM requires substantially longer computational time. While in reality the computational time may depend on the particular programming approach or skills of the programmer, the results here suggest that the computational times of the proposed method and the previous one are of the same order of magnitude. As mentioned before, the intended merit of the proposed method lies in the systematic and simplified nature of the programming effort required.



**Figure 3 Computational time, single setup data**



**Figure 4 Computational time, multiple setup data**

# Conclusions

A general theory has been developed for deriving and calculating the Hessian of a scalar function under multiple constraints where the derivatives of the function and constraints can be handled separately, allowing a systematic and efficient treatment in computer coding. Motivated by uncertainty quantification in Bayesian system identification, the theory has been applied to derive new analytical expressions for evaluating the posterior covariance matrix of ambient modal identification with single setup and multiple setup data. The framework allows the calculations for multiple setup data to leverage on those already developed for single setup data, therefore eliminating mathematically repetitive computer coding. The numerical examples demonstrate the consistency and computational aspect of the proposed method. While the computational times required by the proposed method and previous methods are of the same order of magnitude, the merit of the proposed method lies in the systematic and simplified nature of the required programming effort.

# Appendix. Derivations

In this appendix, derivations are provided for the results outlined in Section 3.

## Hessian for general parameter value

Here, we derive (13) that expresses the Hessian of  in terms of the gradients and Hessians of  and  for general . We first show that the gradient of  is given by

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Let  and . For simplicity in notation, omit dependence on variables. For ,

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Assembling this result row-wise for ,



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which proves (58).

To show (13), note that

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For , using (58) and the chain rule of differentiation,

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For the first term,

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This implies

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Assembling column-wise for ,

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For the second term in (62),

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If we divide  () column-wise into  partitions of  matrices, then the th partition, say  (), is the rightmost term in the above equation. That is,

  ()

Assembling (66) column-wise for ,

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Assembling (62) column-wise for  and using (65) and (68) gives (13).

## Hessian at MPV

Here, we show that if  satisfies the constraints in (7) then the Hessian of  at the MPV is given by (16). The derivation is based on Lagrange multiplier concepts. The key is to show that at the MPV the second term in (13) becomes

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where a hat ‘^’ denotes that the quantity is evaluated at the MPV.

First recall that  satisfies the constraints in (7):

  for any  ()

Taking the Hessian of (70) w.r.t.  gives a LHS identical to the RHS of (13) except that  is replaced by . This Hessian is zero for any , including the MPV. Thus,

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The second term on the LHS can be expressed in terms of a similar term associated with  as follow. Consider the Lagrangian

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where  contains the Lagrange multipliers. If  minimises  under constraints  (), then there is a  such that  is a stationary point of , i.e.,

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where  denotes the gradient of  w.r.t. . This can be assembled as a matrix equation for :

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Despite the fact that there can be more equations than unknowns (), solution exists for  because  is a linear combination of the rows in . Right-multiplying both sides by  gives a full rank system of dimension , inverting which and taking transpose gives the expression of  in (19). Finally, taking Kronecker product of  with (73) and right-multiplying the resulting expression with  gives, after rearranging,

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Substituting the term  from (71) gives (16).

## Invariance w.r.t. constraint functions

Here, we show that  in (16) remains the same when  is replaced by  for any monotonic scalar function  with  and a non-zero derivative at . Let , . Then  for any  and  imply that  as well. Let  and  be the vectors of Lagrange multipliers at the MPV when the constraint functions are  and , respectively. It is sufficient to show that

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since these are the only terms in (18) affected by the choice of constraint functions.

For any ,

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where

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Evaluating at the MPV and noting ,

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We now evaluate  based on (19) for constraint functions . Using the first equation in (77), at the MPV,

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where

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Then

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This implies

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Using this and the second equation in (79),

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and so

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Taking gradient w.r.t.  on  and evaluating at the MPV gives , and so the first term on the RHS of (85) is zero. Equation (76) then follows.

## Invariance w.r.t. free parameters

Here, we show that if one works with a new set of admissible free parameters  instead of , the resulting posterior covariance matrix of  in (12) remains the same. Let  where  is a transformation; and let . To be admissible,  should be such that  maps  to  so that it always satisfies constraints. Formulating the Bayesian inference problem in terms of , the NL is . Applying (12) but now taking  as the set of free parameters, the posterior covariance matrix of  is given by

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where

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Note that

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Thus, , where the hat ‘^’ denotes that it is evaluated at the MPV. Substituting this and (87) into (86) gives

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On the other hand, consider the singular value (SV) decomposition of  at the MPV:

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where  is a diagonal matrix containing the  singular values of ;  contains in its columns the corresponding orthonormal singular vectors, i.e.,  ( identity matrix). In terms of  and , the pseudo-inverse of  and hence the posterior covariance matrix  of  are given by

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In what follows, we show that  in (90) is equal to  in (93), hence establishing the invariance of the posterior covariance matrix. The derivation involves the SV decomposition of the following matrices, which are introduced first to facilitate presentation:

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where ,  and  () on the RHS of the equations denote the matrices in the SV decomposition. Starting from (90) and substituting  from (91),

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Note that

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 and so the columns of  are orthonormal. This implies that . Substituting into (95),

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since . It can be reasoned from (91) that  and  have the same null space. The null space is orthogonal to the space spanned by the columns in . By writing the identity matrix as  where  contains in its columns an orthonormal basis for the null space, one obtains

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since . Substituting into (97),

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Post-multiplying  by  and noting  gives . Substituting into (99) gives the required result:

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since .

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