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### Application of the Riemannian Levenberg-Marquardt Algorithm to off-line System Identification

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# Application of the Riemannian Levenberg–Marquardt Algorithm to Off–line System Identification \*

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## Abstract

In a companion paper, [26], a Riemannian version of the Levenberg–Marquardt algorithm for the minimization of a nonlinear sum of squares over a Riemannian differentiable manifold, in a coordinate independent way, has been developed. Here, this algorithm applied to simulated examples from the field of (off–line) identification of linear multivariable models from measured output data.

First it is indicated that linear multivariable system identification is a topic which may quite well involve the minimization of a criterion function over a Riemannian manifold. This is a consequence of the fact that (a) the space of candidate models of a fixed order  $n$  exhibits a differentiable manifold structure which is not Euclidean [5, 15]; (b) this manifold can be endowed with various Riemannian metrics [12, 27]; (c) when using a prediction error criterion in identification, the function to be minimized often has the form of a (nonlinear) sum of squares [19, 31].

Next, overlapping parametrizations for the model class are considered, related to different choices for the structural indices, based on nice selections. A structure switching algorithm due to [23, 24] is discussed.

Using all these ingredients, off–line simulation experiments are carried out. Two different  $\ell^2$ –induced Riemannian metrics are used and the results are compared to the outcomes of the Gauss–Newton method and the non–Riemannian versions of the Levenberg–Marquardt algorithm. It is found that the Riemannian version of the Levenberg–Marquardt algorithm is more robust than the other methods, provided an adequate Riemannian metric is chosen. Thus, this advanced algorithm seems most profitable in “difficult” situations, where numerical problems easily occur.

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# 1 Introduction

This paper is concerned with an application of a Riemannian version of the Levenberg–Marquardt algorithm, as developed in the companion paper [26], to the field of off-line system identification. There we are dealing with the problem of estimating parameters in order to identify a model from available measurement data. Most available estimation procedures are based on the concept of trying to minimize an associated criterion function that expresses the misfit of a candidate model. Commonly used criterion functions often fall into the class of *prediction error criteria* (cf., e.g., [19] and [31]). The most popular one consists of the sum of squares of the prediction errors that emerge when applying the available measurement data to the candidate model with the objective of one-step-ahead prediction of future outputs. One can get to this criterion in various ways, e.g. via the principle of maximum likelihood.

In many of these situations, the parameter space actually corresponds to only a *part* of the set of candidate models that one has in mind. Indeed, it is a known fact that various model sets that are commonly being used, such as the sets of linear multivariable models of a fixed finite order  $n$ , do not form Euclidean spaces, but *differentiable manifolds* instead (cf. [5]). In the multivariable case it has been proved that one cannot restrict to just *one* continuous canonical form for this manifold as it can never capture all candidate models (cf. [15]). One therefore has to consider several structures instead, and their related (pseudo-)canonical forms, which provide a set of overlapping parameter charts for the differentiable manifold under consideration. Smooth differentiable manifolds can always be endowed with a Riemannian metric (cf. [4]), and for this particular application several choices are discussed in [12, 27]. This leads us to a situation where a nonlinear sum of squares has to be minimized over a Riemannian manifold, which is covered by a set of overlapping coordinate charts, thus making the results of [26] applicable.

In Sect. 2 we state the identification problem of estimating a linear multivariable model of a given fixed order  $n$  on the basis of a prediction error criterion. We also give a description of the model class, involving its manifold structure, overlapping parametrizations, structure selection strategy and choice of Riemannian metric. Main references within this context are [23, 24, 12, 14, 28, 27]. The actual calculation of the Riemannian metric tensors is discussed in detail in App. A.

Sect. 3 contains the results of experiments carried out with the Riemannian versions of the Levenberg–Marquardt algorithm, which are compared to the results for the Gauss–Newton method and for a non-Riemannian version of Levenberg–Marquardt. Efficient implementation of the Riemannian algorithms for these examples, which handle large amounts of data, asks for an alternative organization of certain calculations, as discussed in [26, App. B]. We restrict ourselves to experiments with *simulated* data, which gives us the possibility for direct comparison with the underlying data generating models. Sect. 4 concludes the paper.

## 2 Multivariable off-line system identification with Riemannian metrics, using a prediction error criterion

This section is concerned with the problem setting of an application of the Riemannian version of the Levenberg-Marquardt algorithm (as developed in [26], based on [22]) in the field of off-line linear multivariable system identification. More details about this approach can be found in [27]. We shall be occupied with the following problem, which is adopted from [29].

### 2.1 Problem statement and parametrization of the model class

We suppose we are studying some stochastic vector output process  $y = \{y(t)\}_{t \in \mathbb{Z}}$  of dimension  $p$  of, e.g., some physical or economical system. It is our intention to find a mathematical model that describes the joint temporal dynamics of the process components  $y_1(t), \dots, y_p(t)$  as good as possible. This model might then be used for various purposes, such as prediction of future outputs, construction of a controller, etc.

To achieve this, we suppose we have a record of size  $T$  of observations of process  $y$  at our disposal, that is, we have the measurements  $\{y(t)\}_{t=1,2,\dots,T}$ . Moreover, we make some assumptions about process  $y$ , in order to limit the complexity of our problem, while keeping its practical applicability broad enough. These are the following:

1.  $y$  is a stationary  $p$ -dimensional Gaussian vector process of zero mean, with rational spectral density;
2.  $y$  is purely non deterministic;
3.  $y$  is a full rank process.

Then, following [29], it is a central result in stochastic system theory that such a process can always be represented by a linear, finite dimensional recursive scheme of the following type (called innovations form):

$$\begin{cases} x(t+1) = Ax(t) + Bw(t) \\ y(t) = Cx(t) + w(t) \end{cases} \quad (t \in \mathbb{Z}), \quad (2.1)$$

where  $A$ ,  $B$  and  $C$  are matrices of suitable dimension and  $\{w(t)\}_{t \in \mathbb{Z}}$  is a  $p$ -dimensional white Gaussian sequence of zero mean, with covariance matrix  $\Omega > 0$ , say.

Due to the assumption of  $y$  having full rank, we can assume without loss of generality that the matrix triple  $(A, B, C)$  is minimal, i.e.  $(A, B)$  is reachable and  $(C, A)$  is observable. In that case the dimension  $n$  of the state process  $x = \{x(t)\}_{t \in \mathbb{Z}}$  equals the order (or McMillan degree) of the system. From the assumption that  $y$  is purely non deterministic we have that the spectrum  $\sigma(A)$  of  $A$ , i.e. the set of eigenvalues of  $A$ , is contained in the open unit disk in  $\mathbb{C}$ :

$$\sigma(A) \subset \{s \in \mathbb{C} \mid |s| < 1\}. \quad (2.2)$$

Any matrix with this property is called *asymptotically stable*.

One can eliminate the state process from representation (2.1) to obtain the following input-output relation:

$$y(t) = \sum_{k=0}^{\infty} H_k w(t-k), \quad t \in \mathbb{Z}. \quad (2.3)$$

Here the matrices  $H_k$  are the Markov matrices, given by

$$\begin{cases} H_0 = I \\ H_k = CA^{k-1}B \quad (k = 1, 2, \dots). \end{cases} \quad (2.4)$$

We define the infinite matrix  $H$ , the weighting pattern or impulse response of the system, by

$$H := [H_0, H_1, H_2, \dots]. \quad (2.5)$$

and the infinite column vector  $w^t$ , containing all "past" values of  $w(t)$ , by

$$w^t := \begin{bmatrix} w(t) \\ w(t-1) \\ \vdots \end{bmatrix}, \quad t \in \mathbf{Z}. \quad (2.6)$$

Hence we can write the input-output relation as:

$$y(t) = H w^t, \quad t \in \mathbf{Z}. \quad (2.7)$$

The requirements mentioned so far are still not sufficient to have a unique representation of the form (2.1) describing the output process  $y(t)$ . Basically, there are two sources of nonuniqueness. The first source is that there are in general several pairs  $(H, w^t)$  generating the same process  $y(t)$  via equation (2.7). There is a way to overcome this problem, namely by choosing a *special kind* of innovations representation. For the state space innovations representation (2.1) the corresponding innovations can be represented via a recursive scheme:

$$\begin{cases} x(t+1) = (A - BC)x(t) + By(t) \\ w(t) = -Cx(t) + y(t) \end{cases} \quad (t \in \mathbf{Z}). \quad (2.8)$$

The innovations representation that we choose is required to have the property of being *causally invertible*, meaning that one can write  $\{w(t)\}_{t \in \mathbf{Z}}$  as

$$w(t) = \sum_{k=0}^{\infty} G_k y(t-k), \quad t \in \mathbf{Z}, \quad (2.9)$$

where the matrices  $G_k$  are defined by:

$$\begin{cases} G_0 = I \\ G_k = -C(A - BC)^{k-1}B \quad (k = 1, 2, \dots). \end{cases} \quad (2.10)$$

The requirement of causal invertibility imposes the additional constraint on  $A$ ,  $B$  and  $C$  that matrix  $(A - BC)$  must be *stable*, that is, its eigenvalues are required to lie inside the *closed* unit disk in  $\mathbf{C}$ . Later in this section we shall restrict ourselves to the case where  $(A - BC)$  is *asymptotically* stable for reasons of convenience: the associated prediction error filter then becomes asymptotically stable and the problem is easier to handle. Notice that this only excludes a "thin" set from the general case.

The second source of nonuniqueness stems from the freedom left in choosing a basis for the state space  $\mathbf{R}^n$ . Indeed, it is easily seen that any basis transformation of the state space does not affect input-output relation (2.3). This brings us to calling two minimal matrix triples  $(A, B, C)$  and  $(\bar{A}, \bar{B}, \bar{C})$  of order  $n$  (*i/o*-)equivalent if there exists a nonsingular matrix  $T \in \mathbf{R}^{n \times n}$  such that

$$(\bar{A}, \bar{B}, \bar{C}) = (TAT^{-1}, TB, CT^{-1}). \quad (2.11)$$

The space of all  $n \times n$  nonsingular matrices is denoted by  $Gl(n)$ . The *equivalence classes* generated by the equivalence relation above are also called *orbits* under the action of the general linear group  $Gl(n)$ . What one should do to obtain uniqueness of the innovations representation is to parametrize the set of equivalence classes. The problem here is that in the multivariable case it is impossible to use only one global Euclidean parametrization. (Cf. [15].)

One way to deal with this problem is presented in [23, 24]. The approach taken there consists of defining a set of *overlapping parametrizations* of which each element covers a part of the model space, such that together they cover all. Of course, along with this approach one has to provide a criterion for switching between these parametrizations. We will discuss this work in more detail. Suppose we are given a stochastic system of the form (2.1), with  $(A, B, C)$  minimal of order  $n$ ,  $A$  and  $(A - BC)$  asymptotically stable and  $\{w(t)\}_{t \in \mathbf{Z}}$  a white Gaussian sequence with zero mean and

positive definite covariance matrix  $\Omega$ . As before, its Markov matrices are denoted by  $H_0, H_1, H_2, \dots$ . We define *reachability matrix*  $R$  and *observability matrix*  $O$  corresponding to  $(A, B, C)$  by

$$R = [B, AB, \dots, A^{n-1}B], \quad O = \begin{bmatrix} C \\ CA \\ \vdots \\ CA^{n-1} \end{bmatrix}. \quad (2.12)$$

Minimality of  $(A, B, C)$  requires that  $\text{rank}(R) = \text{rank}(O) = n$ . For  $k \in \{1, 2, \dots\} \cup \{\infty\}$  we further define blockwise Hankel matrices  $\mathcal{H}_k$  as

$$\mathcal{H}_k = \begin{bmatrix} H_1 & H_2 & \dots & H_k \\ H_2 & H_3 & \dots & H_{k+1} \\ \vdots & \vdots & & \vdots \\ H_k & H_{k+1} & \dots & H_{2k-1} \end{bmatrix}. \quad (2.13)$$

It is easily seen that the following relation holds:

$$\mathcal{H}_n = OR. \quad (2.14)$$

The blockwise Hankel matrices are all invariant under the action of  $\mathcal{G}l(n)$ , whereas  $R$  and  $O$  are not. Also,  $\text{rank}(\mathcal{H}_k) = n$  for all  $k \geq n$ .

One can construct different parametrizations for (parts of) the model space by choosing different bases for the row space of  $\mathcal{H}_\infty$ . In each parametrization there are  $2np$  independent parameters involved, which is obvious from the fact that the space of all matrix triples  $(A, B, C)$  has dimension  $n^2 + 2np$  and the space  $\mathcal{G}l(n)$  has dimension  $n^2$ . The overlapping parametrizations of [23, 24] make use of so called *nice selections*. A nice selection is defined as a set of  $n$  positive integers (a multi-index) with the property that if  $j > p$  is in the set then also  $j - p$  is in the set. In the present case the extra property that all the integers  $1, 2, \dots, p$  are in the set is required to hold (because the output process  $y$  is assumed to be of full rank). A way to visualize a nice selection is offered by the so-called Young diagram (see e.g. [12, Sect.2.3.5]). In analogy with this diagram we can draw a matrix of squares (a "crate diagram"), in which for each element of the nice selection we put a cross in its corresponding square, when numbering the squares from 1 to  $np$ , column after column. For instance, with  $n = 7, p = 4$  and nice selection  $\{1, 2, 3, 4, 6, 7, 10\}$  one gets the diagram

×						
×	×	×				
×	×					
×						

Conversely, to each such diagram with the property that it contains exactly  $n$  crosses placed in such a way that the first column is filled completely and that there are no spaces between crosses in the same row, corresponds a nice selection. From this observation it is easy to calculate the number of different nice selections as  $\binom{n-1}{p-1}$ .

A nice selection is used to denote the numbers of the rows of  $\mathcal{H}_\infty$  which should serve as a basis for its row space. Of course, for this purpose these rows must be linearly independent. Although, for a given matrix  $\mathcal{H}_\infty$ , this need not be the case for every possible nice selection, one can always obtain a nice selection with such property. For instance, it is a well-known fact that if one selects the first  $n$  linearly independent rows of  $\mathcal{H}_\infty$ , thereby checking for dependencies with earlier rows only, one obtains the *observability* or *Kronecker indices*, which constitute a nice selection.

From the choice of basis for the row space of  $\mathcal{H}_\infty$  by means of a nice selection it is possible to construct matrices  $A, B$  and  $C$  which correspond to the blocks (the Markov matrices) of  $\mathcal{H}_\infty$ . These matrices then have the following structure.

- \* Matrix  $A$  consists of  $(n - p)$  fixed rows and  $p$  parameter rows (thus containing  $np$  parameters). The fixed rows are unit row vectors, with the unit element subsequently on places  $p + 1, \dots, n$ . The row numbers of the  $p$  parameter rows can be obtained from the diagram. For this, one has to number the squares in which there is a cross, column after column, from 1 to  $n$ . Then the numbers on the end of each row denote the parameter row numbers. For the example above this gives the diagram

1							
2	5	7					
3	6						
4							

so the numbers of the parameter rows are 1, 4, 6 and 7. Consequently, matrix  $A$  in that case takes the form

$$A = \begin{pmatrix} * & * & * & * & * & * & * \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ * & * & * & * & * & * & * \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ * & * & * & * & * & * & * \\ * & * & * & * & * & * & * \end{pmatrix},$$

where the stars denote the parameter locations.

- \* Matrix  $B$  consists of parameters only. Since  $B$  is of size  $n \times p$ , it also contains  $np$  parameters.
- \* Matrix  $C$  is fixed, and for all nice selections the same. It has the form

$$C = ( I \ O ),$$

with  $I$  denoting the  $p \times p$  identity matrix and  $O$  the  $p \times (n - p)$  zero matrix.

It is easy to switch between two such parametrizations. Starting from a matrix triple  $(A, B, C)$  in one representation, the transformation matrix  $T$  bringing it to matrix triple  $(TAT^{-1}, TB, CT^{-1})$  in the second representation consists of the rows of the observability matrix  $O$  (see (2.12)) with row numbers that are in the second nice selection. (Notice that in this case  $CT^{-1}$  is always equal to  $C$ .) For more information on these parametrizations one can consult, e.g., [9] and [27].

Now we turn to the switching mechanism. This is an important topic, because although almost every system can be represented via all parametrizations (all parametrizations are so to say generic), one can encounter severe numerical difficulties if one does not select a parametrization properly. For instance, if, in some parametrization, one is dealing with a system that is close to a system that cannot be represented in that parametrization, the corresponding rows of the blockwise Hankel matrix will be almost singular and yield an ill-conditioned basis. As pointed out in [23, 24], one should use a nice selection that leads to matrices  $A$ ,  $B$  and  $C$  for which the positive definite solution  $P$  of the discrete-time Lyapunov equation

$$P - APA^T = BB^T \tag{2.15}$$

is well-conditioned.

*Remark* This is also suggested by the observation that, by construction, all parametrizations we use lead to matrix triples  $(A, B, C)$  for which  $(C, A)$  is observable. Minimality is therefore achieved when  $(A, B)$  is reachable. This means that  $R$  (see (2.12)) must have full rank. This property is

closely connected to Lyapunov equation (2.15): if one defines the infinite reachability matrix  $R^\infty$  for  $(A, B, C)$  by  $R^\infty := [B, AB, A^2B, \dots]$  then the solution  $P$  of (2.15) can be written as  $P = R^\infty (R^\infty)^T$ . Therefore, if  $R$  (and consequently  $R^\infty$ ) is almost singular, matrix  $P$  will be ill-conditioned.

The following *heuristic* algorithm is used to select a better parametrization if the current one is recognized to behave badly.

1. Compute the positive definite solution  $P$  of (2.15).
2. Factorize  $P$  as  $P = LDL^T$ , where  $L$  is unit lower triangular and  $D$  is diagonal (with positive elements on its main diagonal).
3. Compute  $W := OL$ , with  $O$  denoting the observability matrix of the system (see formula (2.12)).
4. Select  $n$  rows from  $W$  in such a way that:
  - the  $n$  row numbers constitute a nice selection;
  - weighted Gram-Schmidt orthogonalization applied to these rows, with diagonal matrix  $D$  containing the weights, will lead to a factorization  $\tilde{L}Q$  where  $\tilde{L}$  is unit lower triangular and  $\tilde{D} := QDQ^T$  is diagonal ( $\tilde{D} > 0$ ), for which the conditioning of  $\tilde{D}$  is better than the conditioning of  $D$ .
5. The corresponding rows of  $O$  yield transformation matrix  $T$ .

Here, there are two things that need further explanation. First, we remark that the conditioning of  $P$  is evaluated by inspection of the (relative) magnitude of the diagonal elements of  $D$ , instead of via the eigenvalues. The  $LD$ -factorization in step 2 serves for this purpose; an algorithm can be found in [3]. Second, step 4 of the algorithm needs further discussion. If one uses transformation matrix  $T$  to go from one parametrization to another, then, in the notation of step 4,  $P$  transforms from  $LDL^T$  to  $TLDL^T T^T$ , which is equal to  $\tilde{L}QDQ^T \tilde{L}^T = \tilde{L}\tilde{D}\tilde{L}^T$ . Thus, the new conditioning can be evaluated via  $\tilde{D}$ . Now, step 4 is organized as follows.

- 4a. Select rows  $1, 2, \dots, p$  from  $W$  (these must always be selected, since we want to get a nice selection).
- 4b. There are  $p$  candidates among the remaining rows of  $W$  which can be added to the set of currently selected rows, without destroying the structure needed for a nice selection. From these candidates we select the one which will lead to the largest new element of  $\tilde{D}$ , when added to the set.
- 4c. Perform weighted Gram-Schmidt orthogonalization to the selected rows from  $W$ . If the number of currently selected rows is still less than  $n$ , continue with step 4b.

One should realize that this algorithm provides no guarantee for finding the best parametrization. It contains a *heuristic* element, which is incorporated in the way the new nice selection is obtained. Once a row from  $W$  is selected, it cannot be removed from the new basis anymore, although it might turn out to match not so well with new rows to be selected, and there might be better combinations possible. However, the described method seems to work well in practice. We remark that an algorithm for weighted Gram-Schmidt orthogonalization can be found in [3].

We shall use the overlapping parametrizations described above to parametrize the matrix triples  $(A, B, C)$  that we will encounter in the identification algorithm that we are going to apply, together with the model structure selection procedure just explained. First however, we will introduce some more mathematics, and digress on the construction of a differentiable manifold endowed with a Riemannian metric, representing the model space.



## 2.2 The model class as a Riemannian differentiable manifold

Let  $m, n$  and  $p$  be positive integers. We define the following spaces:

$$\mathcal{H}_{m,p} := \{(H_0, H_1, H_2, \dots) \mid H_i \in \mathbb{R}^{p \times m} \ (i = 0, 1, 2, \dots)\}, \quad (2.16)$$

$$\mathcal{H}_{m,p}^a := \{(H_0, H_1, H_2, \dots) \mid H_i \in \mathbb{R}^{p \times m} \ (i = 0, 1, 2, \dots); \text{trace} \sum_{i=0}^{\infty} H_i H_i^T < \infty\}, \quad (2.17)$$

$$S^n := \{\{s(t)\}_{t \in \mathbb{Z}} \mid s(t) \in \mathbb{R}^n \ (t \in \mathbb{Z})\}, \quad (2.18)$$

$$S_0^n := \{\{s(t)\}_{t \in \mathbb{Z}} \mid s(t) \in \mathbb{R}^n \ (t \in \mathbb{Z}); \exists t_0 \in \mathbb{Z} : s(t) = 0, \forall t < t_0\}, \quad (2.19)$$

$$\mathcal{L}_0^{m,p} := \{F : S_0^m \rightarrow S_0^p \mid F \text{ is linear and shift-invariant}\}. \quad (2.20)$$

On each of these spaces the operations addition and scalar multiplication are defined as usual, in a “pointwise” fashion. The operations on  $\mathcal{H}_{m,p}^a$  and  $S_0^n$  are defined via  $\mathcal{H}_{m,p}$  and  $S^n$  respectively, by restriction. Notice that  $\mathcal{H}_{m,p}^a$  and  $S_0^n$  are closed under these operations.

The shift-invariance property referred to in the definition of  $\mathcal{L}_0^{m,p}$  is defined as follows. Let  $\delta_n$  denote the (forward) shift-operator acting on elements of  $S^n$ , defined by

$$\delta_n(\{s(t)\}_{t \in \mathbb{Z}}) = \{u(t)\}_{t \in \mathbb{Z}} \quad \text{with } u(t) = s(t+1), \quad \forall t \in \mathbb{Z}. \quad (2.21)$$

Then a mapping  $F : S_0^m \rightarrow S_0^p$  is called (forward) shift-invariant if for all  $s \in S_0^m$  we have that

$$F(\delta_m(s)) = \delta_p(F(s)). \quad (2.22)$$

(One could as well define a backward shift-operator; since we are considering sequences over  $\mathbb{Z}$  this is the inverse of the forward one. In the present case, forward and backward shift-invariance are seen to be equivalent, hence we can simply speak about shift-invariance.)

On  $\mathcal{H}_{m,p}^a$  we further define an inner product  $\langle \cdot, \cdot \rangle_{\ell^2}$  by

$$\langle H, \tilde{H} \rangle_{\ell^2} := \text{trace} \sum_{i=0}^{\infty} H_i \tilde{H}_i^T, \quad (2.23)$$

where  $H = (H_0, H_1, H_2, \dots)$  and  $\tilde{H} = (\tilde{H}_0, \tilde{H}_1, \tilde{H}_2, \dots)$ . This makes  $\mathcal{H}_{m,p}^a$  into a Hilbert space. Of course the inner product induces a norm on  $\mathcal{H}_{m,p}^a$ , denoted by  $\|\cdot\|_{\ell^2}$  and satisfying

$$\|H\|_{\ell^2} := \langle H, H \rangle_{\ell^2}^{1/2} = (\text{trace} \sum_{i=0}^{\infty} H_i H_i^T)^{1/2}, \quad (2.24)$$

for  $H = (H_0, H_1, H_2, \dots) \in \mathcal{H}_{m,p}^a$ .

Next, we associate with every element  $H$  of  $\mathcal{H}_{m,p}$  an element  $F^{(H)}$  of  $\mathcal{L}_0^{m,p}$  via the mapping  $\tau_{m,p}$  defined by

$$\tau_{m,p} : \mathcal{H}_{m,p} \rightarrow \mathcal{L}_0^{m,p},$$

$$\tau_{m,p}(H) = F^{(H)},$$

with  $F^{(H)}(u) = y$  for  $u = \{u(t)\}_{t \in \mathbb{Z}} \in S_0^m$  and  $y = \{y(t)\}_{t \in \mathbb{Z}} \in S_0^p$  defined by the formula:

$$y(t) = \sum_{i=0}^{\infty} H_i u(t-i), \quad \forall t \in \mathbb{Z}. \quad (2.25)$$

It is easily verified that  $\tau_{m,p}$  yields a linear injection from  $\mathcal{H}_{m,p}$  into  $\mathcal{L}_0^{m,p}$ . Therefore we identify each element  $H$  of  $\mathcal{H}_{m,p}$  with its corresponding element  $F^{(H)}$  of  $\mathcal{L}_0^{m,p}$ . (The image of  $\mathcal{H}_{m,p}$  under  $\tau_{m,p}$  can be described as the subset of  $\mathcal{L}_0^{m,p}$  consisting of all *causal* mappings, that is, mappings  $F$  such that if  $u(t) = 0$  for all  $t < t_0$  then also  $(Fu)(t) = 0$  for all  $t < t_0$ .)

We now define the mapping  $\tau_{m,p}^a$  from  $\mathcal{H}_{m,p}^a$  in  $\mathcal{L}_0^{m,p}$  as the restriction of  $\tau_{m,p}$  to the domain  $\mathcal{H}_{m,p}^a$ .

Its image is denoted by  $\mathcal{L}_{m,p}^a$ , and we identify the spaces  $\mathcal{H}_{m,p}^a$  and  $\mathcal{L}_{m,p}^a$ . In this way we have a norm on  $\mathcal{L}_{m,p}^a$ , induced by the norm  $\|\cdot\|_{\ell^2}$ . We write

$$\|F^{(H)}\|_{\ell^2} := \|(\tau_{m,p}^a)^{-1}(F^{(H)})\|_{\ell^2}. \quad (2.26)$$

Now we turn to an alternative way of describing subsets of  $\mathcal{H}_{m,p}^a$  (or equivalently  $\mathcal{L}_{m,p}^a$ ). For this, we consider discrete-time, linear, time-invariant, asymptotically stable, deterministic systems  $\Sigma$  of finite McMillan degree, of the form

$$\Sigma = \begin{cases} x(t+1) = Ax(t) + Bu(t) \\ y(t) = Cx(t) + Du(t) \end{cases} \quad (t \in \mathbb{Z}), \quad (2.27)$$

where  $\{x(t)\}_{t \in \mathbb{Z}} \in S_0^n$ ,  $\{u(t)\}_{t \in \mathbb{Z}} \in S_0^m$ ,  $\{y(t)\}_{t \in \mathbb{Z}} \in S_0^p$ ,  $A \in \mathbb{R}^{n \times n}$ ,  $B \in \mathbb{R}^{n \times m}$ ,  $C \in \mathbb{R}^{p \times n}$ ,  $D \in \mathbb{R}^{p \times m}$ , with the additional requirements that  $A$  is asymptotically stable and that the representation is minimal, i.e.  $(A, B)$  is reachable and  $(C, A)$  is observable. (Notice our requirement  $\{x(t)\}_{t \in \mathbb{Z}} \in S_0^n$ . This implies that for each input  $\{u(t)\}_{t \in \mathbb{Z}} \in S_0^m$  there exists  $t_0 \in \mathbb{Z}$  such that the system is at rest for  $t < t_0$ . This is why we can write  $\{y(t)\}_{t \in \mathbb{Z}} \in S_0^p$ .)

We denote a system  $\Sigma$  of the form and with the properties above as  $\Sigma = (A, B, C, D)$ . The set of all such systems, with fixed parameters  $m, n$  and  $p$ , is denoted by  $L_{m,n,p}^{m,a}$ :

$$L_{m,n,p}^{m,a} := \{(A, B, C, D) \mid A \in \mathbb{R}^{n \times n}, B \in \mathbb{R}^{n \times m}, C \in \mathbb{R}^{p \times n}, D \in \mathbb{R}^{p \times m}, \\ (A, B, C) \text{ is minimal, } A \text{ is asymptotically stable}\}. \quad (2.28)$$

We regard systems basically as *input-output mappings*. For a system  $\Sigma$  of the form above the associated input-output mapping is given by formula (compare (2.3)):

$$y(t) = \sum_{i=0}^{\infty} H_i(\Sigma)u(t-i), \quad \forall t \in \mathbb{Z}, \quad (2.29)$$

where the matrices  $H_i(\Sigma)$  ( $i = 0, 1, 2, \dots$ ) are the Markov matrices (compare (2.4)), defined by

$$\begin{cases} H_0(\Sigma) = D, \\ H_i(\Sigma) = CA^{i-1}B \quad (i = 1, 2, \dots). \end{cases} \quad (2.30)$$

As before, we have that two systems  $\Sigma = (A, B, C, D)$  and  $\tilde{\Sigma} = (\tilde{A}, \tilde{B}, \tilde{C}, \tilde{D})$  from  $L_{m,n,p}^{m,a}$  are called *(i/o)-equivalent* if they correspond to the same input-output mapping. Again,  $\Sigma$  and  $\tilde{\Sigma}$  are equivalent if and only if there exists  $T \in \mathcal{G}l(n)$  such that  $(\tilde{A}, \tilde{B}, \tilde{C}, \tilde{D}) = (TAT^{-1}, TB, CT^{-1}, D)$ . The set of equivalence classes on  $L_{m,n,p}^{m,a}$ , the orbits under the action of  $\mathcal{G}l(n)$ , induced by the equivalence relation is defined as the quotient space

$$M_{m,n,p}^{m,a} := L_{m,n,p}^{m,a} / \mathcal{G}l(n). \quad (2.31)$$

Now we can define an injective mapping  $\rho_{m,n,p}$  from  $M_{m,n,p}^{m,a}$  to  $\mathcal{L}_{m,p}^a$  by

$$\rho_{m,n,p}(\tilde{\Sigma}) = F^{(H)}, \quad (2.32)$$

with  $H = (H_0(\tilde{\Sigma}), H_1(\tilde{\Sigma}), H_2(\tilde{\Sigma}), \dots)$ , the sequence of Markov matrices corresponding to any representative element of the equivalence class  $\tilde{\Sigma}$  from  $M_{m,n,p}^{m,a}$ .

We define the space  $M_{m,p}^{m,a}$  as the space of all input-output mappings generated by systems of the form under consideration, with fixed input and output dimensions  $m$  and  $p$  and finite McMillan degree  $n$ .

$$M_{m,p}^{m,a} := \bigcup_{n=0}^{\infty} M_{m,n,p}^{m,a}, \quad (2.33)$$

where  $M_{m,0,p}^{m,a}$  denotes the zero system (corresponding to a sequence of zero Markov matrices). Identifying the sets  $M_{m,n,p}^{m,a}$  ( $n = 0, 1, 2, \dots$ ) and their union  $M_{m,p}^{m,a}$  with their respective images in  $\mathcal{L}_{m,p}^a$ , we can think of these sets of systems as being imbedded in Hilbert space  $\mathcal{H}_{m,p}^a$ . Thus the

norm on  $\mathcal{H}_{m,p}^a$  also induces a norm on the space  $M_{m,p}^{m,a}$  (but only a *metric* and not a norm on the spaces  $M_{m,n,p}^{m,a}$  ( $n = 1, 2, \dots$ ), since these are not closed under the linear operations).

Using this imbedding in Hilbert space one can prove that the spaces  $M_{m,n,p}^{m,a}$  are *differentiable manifolds*, see for instance [11, 12, 13] and the references given there. The norm  $\|\cdot\|_{\ell^2}$  defined on  $M_{m,p}^{m,a}$  provides us with a *Riemannian metric* on these manifolds. This is so, because the derivative of a smooth curve of systems on  $M_{m,n,p}^{m,a}$  at a point  $\Sigma = (A, B, C, D)$  can be regarded as an element of  $M_{m,p}^{m,a}$ . Consequently, the norm  $\|\cdot\|_{\ell^2}$  induces a norm on the tangent space to  $M_{m,n,p}^{m,a}$  at  $\Sigma$ . This can be seen as follows (cf. [12, Sect.5.2]).

Recall that the addition of two systems is already defined via addition of corresponding sequences of Markov matrices. A system  $(\bar{A}, \bar{B}, \bar{C}, \bar{D})$ , not necessarily in minimal form, that has a sequence of Markov matrices being the sum of the sequences of Markov matrices of systems  $(A, B, C, D)$  and  $(\tilde{A}, \tilde{B}, \tilde{C}, \tilde{D})$ , of McMillan degree  $n$  and  $\tilde{n}$  respectively, is given by the relations

$$\bar{A} = \begin{pmatrix} A & 0 \\ 0 & \tilde{A} \end{pmatrix}, \bar{B} = \begin{pmatrix} B \\ \tilde{B} \end{pmatrix}, \bar{C} = (C \quad \tilde{C}), \bar{D} = D + \tilde{D}. \quad (2.34)$$

Any minimal representation of this system will therefore be of McMillan degree  $\leq n + \tilde{n}$ . Notice that matrix  $\bar{A}$  is asymptotically stable if  $A$  and  $\tilde{A}$  are so.

Next, let  $\Sigma(t) = (A(t), B(t), C(t), D(t))$  denote a differentiable curve on  $M_{m,n,p}^{m,a}$ , parametrized by  $t \in \mathbb{R}$  and satisfying  $\Sigma(0) = \Sigma = (A, B, C, D)$ . Let the tangent vector at  $\Sigma$  in the direction of the curve be denoted by  $[\dot{A}, \dot{B}, \dot{C}, \dot{D}]$ . The derivative of the curve at  $\Sigma$  is denoted by  $\dot{\Sigma}$  and given by the expression

$$\dot{\Sigma} = \lim_{t \rightarrow 0} \frac{\Sigma(t) - \Sigma(0)}{t}. \quad (2.35)$$

Here, one considers the right hand side as a limit of systems in  $M_{m,p}^{m,a}$  (all of McMillan degree  $\leq 2n$ ). As reported in [12] one can derive the formula

$$\dot{\Sigma} = \left( \begin{pmatrix} A & 0 \\ \dot{A} & A \end{pmatrix}, \begin{pmatrix} B \\ \dot{B} \end{pmatrix}, (\dot{C} \quad C), \dot{D} \right). \quad (2.36)$$

We denote the norm on the tangent space at  $\Sigma$ , induced by the norm  $\|\cdot\|_{\ell^2}$  on  $M_{m,p}^{m,a}$ , by  $\|\cdot\|_{g_{\Sigma}}$ . This norm satisfies the formula

$$\|[\dot{A}, \dot{B}, \dot{C}, \dot{D}]\|_{g_{\Sigma}} = \|\dot{\Sigma}\|_{\ell^2} \quad (2.37)$$

In principle it is now possible to calculate for a given system  $\Sigma = (A, B, C, D)$  the corresponding Riemannian metric tensor, using formula (2.36). We denote the matrix representing this tensor at  $\Sigma$  by  $R_{\Sigma}$ . In App. A we discuss in more detail the actual calculation of  $R_{\Sigma}$  when using the overlapping parametrizations of [23, 24]. Related information may be found in [27]. The Riemannian metric described above is seen to be induced by the  $\ell^2$ -norm for  $m \times p$  matrices, regarded as elements of the vector space  $\mathbb{R}^{m \times p}$ . This then explains the subscript  $\ell^2$  for the norms used throughout this section.

As a matter of fact, one can think of many other Riemannian metrics on the system manifold. An important alternative for the procedure described above results from assuming the standpoint that the objects that should be close are not really the true system and the identified model, but instead their corresponding representations of the innovations, which we call the *prediction error filters*. (Of course, this standpoint is closely related to a future use of the final identified model for one-step-ahead output prediction purposes.) In this case one can use matrices  $G_k$  (see (2.10)) instead of the usual Markov matrices  $H_k$ . The computational consequences of this alternative approach are also discussed in App. A.

Further alternatives derive from the use of alternative inner products on  $\mathcal{H}_{m,p}^a$  instead of (2.23). For instance, one can use different weighting factors, thereby stressing the importance of a good fit with respect to certain impulse response matrices. Thus, one can arrive at, for example, what is called the *Hilbert-Schmidt-Hankel* (HSH-)norm, or the *exponential* (e-)norm. (These are also briefly discussed in [12] and [27].) Of course, one can again assume the two different standpoints, leading to a wide variety of choices. In this paper we will restrict to the  $\ell^2$ -norm, for *both* standpoints.

### 2.3 Off-line identification using a prediction error criterion

We now turn to the topic of off-line identification algorithms. As discussed before we are considering systems of the form (2.1), which we can rewrite as representations for the innovations (2.8):

$$\begin{cases} x(t+1) = (A - BC)x(t) + By(t) \\ w(t) = -Cx(t) + y(t) \end{cases} \quad t \in \mathbb{Z}.$$

The optimal linear predictor for  $y(t)$  based on all past observations  $\dots, y(t-2), y(t-1)$  is given by  $\hat{y}(t|t-1) = Cx(t)$ . Consequently,  $w(t)$  can be interpreted as the *prediction error* for  $y(t)$  at time  $t$ . Notice that the above equations do not involve the error covariance matrix  $\Omega$ , but only  $A$ ,  $B$  and  $C$ . We use the parametrizations discussed previously to represent these matrices. Within one parametrization we collect all  $2np$  parameters in one parameter vector, denoted by  $\theta$  (or at time  $t$  by  $\theta_t$ ). Instead of writing  $(A, B, C)$  we will write  $(A(\theta), B(\theta), C(\theta))$  when the dependence on the parameter vector is involved. Notice that we actually use parametrizations where  $C$  does *not* depend on  $\theta$ , but is constant.

As remarked in [12, Sect.6.2.2], it follows from the properties of the steady state Kalman filter that among the set of all admissible parameter vectors  $\theta$ , the "true" parameter vector  $\hat{\theta}$  (corresponding to the state space representation of the underlying process  $\{y(t)\}_{t \in \mathbb{Z}}$ ) constitutes a *unique global minimum* for the criterion function  $V(\theta)$ , defined by

$$V(\theta) := \frac{1}{2} E \|w(\theta, t)\|^2 = \frac{1}{2} E w(\theta, t)^T w(\theta, t), \quad (2.38)$$

where the expectation is taken with respect to the true probability law. (See also [1], [10], [14, 28].) Therefore, an off-line identification algorithm can be obtained, in analogy with gradient methods for unconstrained minimization, by adjusting in each iteration  $k$  the current parameter estimate  $\theta_k$  in the direction of the negative gradient of  $V(\theta)$  at  $\theta_k$ . The gradient  $\frac{\partial V}{\partial \theta}(\theta)$  is given by the following relation:

$$\frac{\partial V}{\partial \theta}(\theta) = E \frac{\partial w(\theta, t)^T}{\partial \theta} w(\theta, t), \quad (2.39)$$

again with the expectation taken with respect to the true probability law.

One can obtain relations for the quantities  $\frac{\partial w(\theta, t)}{\partial \theta}$  by partial differentiation of the equations representing the innovations. This yields

$$\begin{cases} \frac{\partial x(\theta, t+1)}{\partial \theta^i} = \left( \frac{\partial A(\theta)}{\partial \theta^i} - \frac{\partial B(\theta)}{\partial \theta^i} C \right) x(\theta, t) + (A - BC) \frac{\partial x(\theta, t)}{\partial \theta^i} + \frac{\partial B(\theta)}{\partial \theta^i} y(t), \\ \frac{\partial w(\theta, t)}{\partial \theta^i} = -C \frac{\partial x(\theta, t)}{\partial \theta^i}, \end{cases} \quad (t \in \mathbb{Z}), \quad (i = 1, 2, \dots, 2np), \quad (2.40)$$

where  $\theta = (\theta^1, \theta^2, \dots, \theta^{2np})^T$ . The matrices  $\frac{\partial A(\theta)}{\partial \theta^i}$  and  $\frac{\partial B(\theta)}{\partial \theta^i}$  are all very sparse: at most one element of each matrix will be nonzero. By taking together the equations representing the innovations and all equations (2.40) one can define an augmented state space system with state vector  $\xi(\theta, t)$  at time  $t$  (see [12, Sect.6.2.2]).  $\xi(\theta, t)$  consists of the state  $x(\theta, t)$  and its partial derivatives with respect to the components of  $\theta$

$$\xi(\theta, t) = \left( x(\theta, t)^T, \frac{\partial x(\theta, t)^T}{\partial \theta^1}, \dots, \frac{\partial x(\theta, t)^T}{\partial \theta^{2np}} \right)^T. \quad (2.41)$$

We call this augmented system the *extended prediction error filter*. Its output consists of the prediction error  $w(\theta, t)$  and the quantity  $\frac{\partial w(\theta, t)}{\partial \theta}$ . Because it is impossible to calculate  $\frac{\partial V}{\partial \theta}(\theta)$  (the probability law is unknown) one has to *approximate* this gradient, using the extended filter output above. It is important to realize that in order to have an algorithm that really produces prediction errors  $w(t)$ , one must reprocess *all* available data (until time  $T$ ), after each change in the parameter estimate.

One has to provide initial values for the algorithm. The extended state vector  $\xi(t)$  will in general be set to zero (the effect of an initial condition will extinguish for asymptotically stable filters, like we are using). However, one cannot put  $\theta_0$  equal to zero, since it must be made sure that the corresponding representation is still minimal. Non-minimality will result in singularity of the

Riemannian metric tensor, something that has to be avoided. Therefore one really has to come up with an appropriate initial estimate.

The necessary approximations are then organized as follows. We initialize the extended prediction error filter as indicated above, so that the extended filter output involves *prediction errors* (denoted by  $e(t)$  to distinguish them from the innovations  $w(t)$  that they are approximating) together with their partial derivatives with respect to the parameters  $\theta^i$  (denoted by  $\frac{\partial e(t)}{\partial \theta^i}$ ; these are exact). Instead of  $V(\theta)$  we try to minimize  $V_T(\theta)$ , defined as the following approximation of  $V(\theta)$ :

$$V_T(\theta) = \frac{1}{2} \sum_{t=1}^T \|e(\theta, t)\|^2. \quad (2.42)$$

This is a *prediction error criterion* (see e.g. [19], [31] for a more general account of such criteria). The gradient of  $V_T(\theta)$  is given by

$$\frac{\partial V_T(\theta)}{\partial \theta} = \sum_{t=1}^T \frac{\partial e(\theta, t)^T}{\partial \theta} e(\theta, t). \quad (2.43)$$

These are calculable expressions and it is possible to minimize  $V_T(\theta)$  by means of numerical algorithms. The main observation to make is that  $V_T(\theta)$  is in fact a (nonlinear) *sum of squares*, which follows easily if we stack all prediction errors  $e(t, \theta)$  in one big column vector of dimension  $pT$ . Thus, we are dealing with a *nonlinear least squares problem*, to which we can apply the methods of Gauss-Newton, (Riemannian) Levenberg-Marquardt, (Riemannian) steepest descent, etc., as explained in the companion paper [26]. Indeed, as we have shown, the space over which  $V_T$  is to be minimized is a Riemannian manifold for which a covering of overlapping parameter charts is available, together with a switching mechanism, and on which various Riemannian metrics can be chosen. This concludes the discussion of our theoretical framework for the experiments presented in the next section.

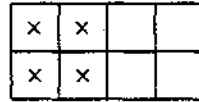
### 3 Computer Experiments and Results

We shall presently discuss the results of a number of computer experiments that have been carried out with respect to the identification problem introduced in Sect. 2. The set-up of these experiments is as follows.

Using computer simulation we have generated samples of 2000 datapoints for three different systems, all linear, asymptotically stable and minimum phase, of order  $n = 4$  and with  $p = 2$  (the number of (stochastic) inputs and outputs; there are no exogenous inputs). From these three samples we have constructed three extra samples of size 1000, by selecting the first 1000 datapoints in each case. This to make it possible to acquire some information about the influence of the sample size on the identification results.

The choice of  $n$  and  $p$  is based upon a trade-off between required computing time and complexity of the structure of the problem. (The larger the value of  $n$  is, the more datapoints are needed to obtain reasonable estimates for the true underlying system parameters and the more parameters are to be estimated, so that more computing time is required. On the other hand, then also more overlapping charts are needed to cover the system manifold and the problem becomes more interesting and involved.) For  $n = 4$  and  $p = 2$  there are three possible structures, as described in App. A and indicated below. The total number of parameters to be estimated is  $2np = 16$ .

The characteristics of the data generating systems are the following. For all three data generating systems the *structure* (given by the observability indices) corresponds to a diagram of the form (see Sect. 2 for an interpretation):



Thus, the system matrices  $A$ ,  $B$  and  $C$  are parametrized by

$$A = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \theta_1 & \theta_2 & \theta_3 & \theta_4 \\ \theta_5 & \theta_6 & \theta_7 & \theta_8 \end{pmatrix} \quad B = \begin{pmatrix} \theta_9 & \theta_{13} \\ \theta_{10} & \theta_{14} \\ \theta_{11} & \theta_{15} \\ \theta_{12} & \theta_{16} \end{pmatrix} \quad C = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad (3.1)$$

In these three situations we constructed the driving white noise to be Gaussian, 2-dimensional, zero mean with *unit covariance*, that is

$$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (3.2)$$

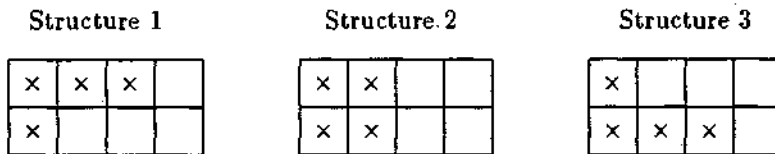
Within this set-up, the three data generating systems are then characterized by, respectively, the "true" parameter vectors

$$\theta_*^{(1)} = (0.3, -0.1, 0.4, 0.0, -0.3, -0.2, 0.0, 0.3, -0.1, 0.0, 0.2, 0.3, -0.2, -0.3, 0.2, 0.4)^T$$

$$\theta_*^{(2)} = (0.1, -0.3, 0.1, 0.1, -0.3, -0.7, 0.1, -0.1, 0.1, 0.2, -0.2, -0.1, -0.1, 0.1, 0.1, 0.1)^T$$

$$\theta_*^{(3)} = (0.3, 0.1, -0.2, -0.3, -0.4, 0.2, -0.1, -0.2, 0.2, -0.1, -0.2, 0.15, -0.2, -0.1, -0.2, -0.1)^T$$

The three possible structures by which linear systems of order 4 with 2 inputs and outputs can be described are numbered, via their corresponding diagrams, according to



Thus, the data generating systems described above all correspond to what is called structure 2. We have applied a number of identification algorithms, all starting from the same 4 different initial

points. They are given by

$$\begin{aligned}\theta_0^{(1)} &= (0.2, -0.4, 0.0, 0.2, -0.4, -0.8, 0.2, 0.0, 0.0, 0.3, -0.1, -0.2, -0.2, 0.2, 0.2, 0.0)^T \\ \theta_0^{(2)} &= (0.0, 0.1, 0.1, -0.1, -0.2, 0.1, 0.0, -0.1, 0.1, -0.2, 0.1, -0.1, 0.0, -0.1, 0.1, -0.2)^T \\ \theta_0^{(3)} &= (0.4, -0.2, 0.3, -0.1, -0.2, -0.1, -0.1, -0.1, 0.2, -0.2, 0.1, 0.1, -0.3, -0.2, 0.3, 0.1)^T \\ \theta_0^{(4)} &= (0.5, 0.0, 0.1, -0.1, -0.2, 0.1, -0.3, -0.1, 0.1, 0.2, -0.3, -0.1, 0.0, -0.2, 0.0, -0.2)^T\end{aligned}$$

where  $\theta_0^{(1)}$ ,  $\theta_0^{(3)}$  and  $\theta_0^{(4)}$  are in structure 2, and  $\theta_0^{(2)}$  is in structure 1.

The minimization methods under consideration all contain the "on-line" structure selecting strategy of [23, 24], described in Sect. 2.

There are 4 identification algorithms we have studied:

**RLM1** The *Riemannian Levenberg-Marquardt* method, with Riemannian metric derived from the  $\ell^2$ -norm on Hilbert space and imbedding as described in Sect. 2 (this is called the *i/o*-imbedding; see also App. A).

**RLM2** The *Riemannian Levenberg-Marquardt* method, with Riemannian metric derived from the  $\ell^2$ -norm on Hilbert space but an alternative imbedding taking the prediction error filters as our point of departure (this is called the *o/i*-imbedding; see Sect. 2 and App. A).

**LM** The *standard Levenberg-Marquardt* method, i.e. with the Euclidean metric on each parameter chart separately.

**GN** The *damped Gauss-Newton* method, where step-sizes are halved until a decrease in the function value is obtained.

In Tables 1-6 the results of the identification experiments are collected, showing the number of iterations needed to reach a local minimum in each situation.

In these tables, a *single star* indicates that the method *crashed* after the given number of iterations. In all cases this was due to the fact that the estimated model contained an unstable matrix  $A$ , despite our definition of the admissible model area. In such situations, the numerical procedure for calculating the solution to a Lyapunov equation, as required by the structure selection algorithm, generates numerical overflows, as can be seen from the formulas presented in App. A.3. One should notice that these problems occurred for *all methods except RLM1*. This is a consequence of the fact that the Riemannian metric induced by the  $\ell^2$ -norm on Hilbert space when using the *i/o*-embedding "explodes" if  $A$  becomes unstable (i.e., some eigenvalues tend to infinity). Therefore, the Riemannian metric used in RLM1 *automatically* enforces asymptotic stability of  $A$ . However, the Riemannian metric for RLM2 enforces only asymptotic stability of  $A - BC$ , whereas LM and GN do not enforce any stability at all. Of course, one could try to prevent those situations via imposing further restrictions on the steplength, e.g. by using the same "halving" strategy as already implemented for the GN method. But then most likely convergence to points *on the boundary* of the admissible area would occur, simply because this boundary is not a natural consequence of the intrinsic problem structure. Solutions obtained this way would not be acceptable in practice either, but would require extra analysis in order to be recognized as such.

method	starting point			
	$\theta_0^{(1)}$	$\theta_0^{(2)}$	$\theta_0^{(3)}$	$\theta_0^{(4)}$
RLM1	76	28	16	31**
RLM2	7*	24	17	14*
LM	1*	26	17	21
GN	3*	6	27	6*

Table 1. Numbers of iterations for 1000 datapoints generated via system based on  $\theta_0^{(1)}$ .

method	starting point			
	$\theta_0^{(1)}$	$\theta_0^{(2)}$	$\theta_0^{(3)}$	$\theta_0^{(4)}$
RLM1	46	20	14	36**
RLM2	8*	20	13	> 100
LM	1*	21	15	19
GN	51**	21	15	29**

Table 2. Numbers of iterations for 2000 datapoints generated via system based on  $\theta_*^{(1)}$ .

method	starting point			
	$\theta_0^{(1)}$	$\theta_0^{(2)}$	$\theta_0^{(3)}$	$\theta_0^{(4)}$
RLM1	9	22	25	15
RLM2	9	24*	23	19
LM	9	18	14	15
GN	13	3*	21	22

Table 3. Numbers of iterations for 1000 datapoints generated via system based on  $\theta_*^{(2)}$ .

method	starting point			
	$\theta_0^{(1)}$	$\theta_0^{(2)}$	$\theta_0^{(3)}$	$\theta_0^{(4)}$
RLM1	15	28	28	23
RLM2	17	31	26	27
LM	17	23	19	25
GN	26	48	33	34

Table 4. Numbers of iterations for 2000 datapoints generated via system based on  $\theta_*^{(2)}$ .

method	starting point			
	$\theta_0^{(1)}$	$\theta_0^{(2)}$	$\theta_0^{(3)}$	$\theta_0^{(4)}$
RLM1	33	45	41	32
RLM2	59	45	41	48
LM	1*	44	40	42
GN	1*	> 100	> 100	61

Table 5. Numbers of iterations for 1000 datapoints generated via system based on  $\theta_*^{(3)}$ .

method	starting point			
	$\theta_0^{(1)}$	$\theta_0^{(2)}$	$\theta_0^{(3)}$	$\theta_0^{(4)}$
RLM1	15	19	11	14
RLM2	19	21	11	14
LM	38	25	12	14
GN	20	14	14	15

Table 6. Numbers of iterations for 2000 datapoints generated via system based on  $\theta_*^{(3)}$ .



Secondly, a *double star* indicates convergence to a local minimum that is *not a global minimum*. In our experiments, such local minima were always associated with different model structures than those of the data generating systems.

For a good comparison between the results for the different methods we mention that RLM1, RLM2 and LM used Moré's stopping criteria (cf. [26, 22]) whereas GN used Marquardt's (cf. [26, 21]). See [26, Sect. 2, App. C] for a description and testing of their performance. We remark that in the present application Marquardt's stopping criterion tended to be somewhat more on the conservative side than Moré's. But one is faced with the situation that Moré's criteria cannot be used in conjunction with the GN method.

About the different starting points we remark that  $\theta_0^{(3)}$  is closest to  $\theta_*^{(1)}$  and  $\theta_0^{(1)}$  is closest to  $\theta_*^{(2)}$ .  $\theta_0^{(3)}$  and  $\theta_0^{(4)}$  are both relatively close to  $\theta_*^{(3)}$ . This is all clearly reflected by the results of the experiments, as convergence was always quickest from these starting points.

Based on the results of the experiments we conclude the following.

1. The LM method (both standard and Riemannian), is in general more robust than the GN method. This is illustrated by the fact that the GN method crashed more often than any other method and also by the fact that it turned out to be slower in a number of more difficult situations, see e.g. Table 5. Of course, this fact is already well-documented in literature.
2. For well-chosen Riemannian metrics, the Riemannian version of the LM method will be more robust than its non-Riemannian version. As we have seen, method RLM1 is the only method (among the four under investigation) that automatically enforces asymptotic stability of matrix  $A$ . Therefore, certain numerical problems were automatically avoided. In relation to this observation we would like to mention that a second requirement imposed on the set of admissible parameter vectors involves the asymptotic stability of  $A - BC$ . It is due to the fact that instability of  $A - BC$  leads to an unstable prediction error filter, so that the expected criterion values are infinitely large, that this restriction did not lead to serious numerical problems. It is more or less enforced automatically by the choice of minimization criterion. Therefore, automatic enforcement of asymptotic stability of  $A$  seems to be the more urgent prerequisite for an adequate choice of Riemannian metric. We remark that there exist numerous alternative Riemannian metrics with this property, for example obtained via alternative weighting of the Markov matrices in the definition of an inner product on the enveloping Hilbert space (cf. Sect. 2). It is interesting to note that the Riemannian metric that can be defined via the *Fisher information matrix* enforces asymptotic stability of both  $A$  and  $A - BC$ . This is also a good candidate for further investigation. See [25, 14, 28, 27].
3. The lack of built-in "hysteresis" in the structure selection algorithm (as proposed by [5]) caused no problems in our experiments. Such a facility seems only necessary if the optimum corresponds to a model that lies close to the boundary of an area in the admissible space related to a fixed optimal structure. But even then the LM algorithms can terminate appropriately since, as pointed out in [26, Sect. 3], the trust-region size involved in Moré's stopping criteria is independent of the choice of coordinates. In our set-up it is immaterial to which structure the final estimated model corresponds.  
In our experiments, the "correct" structure was usually found within 20 iterations. In a small number of cases convergence within an alternative structure took place.
4. There is an effect of the sample size on the number of iterations required to reach an optimum. In general one would expect the problem to become more smooth if a larger number of data is available and this is what happens for  $\theta_*^{(1)}$  and  $\theta_*^{(3)}$ . The effects for  $\theta_*^{(2)}$  are opposite, but less significant. A more important observation, however, is that despite the availability of a large number of data there can still be alternative local minima and numerical problems for bad starting points. See Table 2.

## 4 Summary and Conclusions

In this paper we have studied an application of the results of the companion paper [26] to the field of system identification. These earlier results involve the development of a Riemannian version of the Levenberg–Marquardt algorithm for the minimization of a nonlinear sum of squares over a Riemannian manifold, together with modifications to make it possible to handle problems with large amounts of data.

In Sect. 2 a theoretical framework for the off-line system identification problem is presented, based on [29, 12, 27], where we restrict ourselves to the use of linear, finite dimensional models of a fixed, prespecified order. We adopt the standard prediction error criterion as our criterion of fit. One may arrive at such a criterion in several ways, e.g. via the principle of maximum likelihood. We are then led to a (large) data fitting problem that falls within the class of nonlinear least squares. It is also exposed how this problem involves Riemannian manifolds: the set of candidate models can be shown to exhibit such a structure and it is pointed out that there are various ways for defining Riemannian metrics on it. The system manifold thus obtained can be covered with overlapping parameter charts, for which a selection strategy, due to [23, 24], is available. This motivates the applicability of the Riemannian Levenberg–Marquardt algorithm. For two different choices of Riemannian metrics the computational aspects, which are rather involved, are treated in App. A.

Then, in Sect. 3, six experiments are considered, carried out with simulated samples of 1000 and 2000 datapoints. The outcomes are analyzed and discussed. As the main result of this paper it can then be stated that the Riemannian Levenberg–Marquardt algorithm can be successfully applied to the off-line system identification problem described in Sect. 2. Provided the Riemannian metric is chosen adequately, the Riemannian Levenberg–Marquardt method is superior to the commonly applied Gauss–Newton method, especially in difficult situations.

## Appendix A : Calculation of Riemannian metric tensors

In this appendix we discuss the calculation of the Riemannian metric tensors for two of the situations encountered in Sect. 2 of this paper. It is therefore assumed that  $(A, B, C)$  has a structure corresponding to one of the (overlapping) parametrizations of [23, 24]. This implies that  $A$  contains parameters in  $p$  of its rows, indicated by integer vector  $pr$  following the convention that  $pr[i]$  denotes the (row) index of the  $i$ -th row containing parameters in  $A$  (for  $i = 1, \dots, p$ ). Matrix  $B$  consists of parameters only and  $C$  is constant and independent of all parameters:  $C = (I, O)$ . The parameters are indexed by subscripts from 1 to  $2np$ , by first going through all parameter rows of  $A$ , then through all columns of  $B$ . They are denoted by  $\theta_1, \dots, \theta_{2np}$ .

For example, if  $n = 4, p = 2$  we have the following three possibilities:

$$pr^T = (3, 4)$$

$$A = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \theta_1 & \theta_2 & \theta_3 & \theta_4 \\ \theta_5 & \theta_6 & \theta_7 & \theta_8 \end{pmatrix}, \quad B = \begin{pmatrix} \theta_9 & \theta_{13} \\ \theta_{10} & \theta_{14} \\ \theta_{11} & \theta_{15} \\ \theta_{12} & \theta_{16} \end{pmatrix}, \quad C = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad (\text{A.1})$$

$$pr^T = (2, 4)$$

$$A = \begin{pmatrix} 0 & 0 & 1 & 0 \\ \theta_1 & \theta_2 & \theta_3 & \theta_4 \\ 0 & 0 & 0 & 1 \\ \theta_5 & \theta_6 & \theta_7 & \theta_8 \end{pmatrix}, \quad B = \begin{pmatrix} \theta_9 & \theta_{13} \\ \theta_{10} & \theta_{14} \\ \theta_{11} & \theta_{15} \\ \theta_{12} & \theta_{16} \end{pmatrix}, \quad C = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad (\text{A.2})$$

$$pr^T = (1, 4)$$

$$A = \begin{pmatrix} \theta_1 & \theta_2 & \theta_3 & \theta_4 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \theta_5 & \theta_6 & \theta_7 & \theta_8 \end{pmatrix}, \quad B = \begin{pmatrix} \theta_9 & \theta_{13} \\ \theta_{10} & \theta_{14} \\ \theta_{11} & \theta_{15} \\ \theta_{12} & \theta_{16} \end{pmatrix}, \quad C = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad (\text{A.3})$$

The positions of the parameter rows are related to so called "nice selections," with respect to the construction of a basis for the row space of the infinite blockwise Hankel matrix associated with the system corresponding to  $(A, B, C)$  (containing its Markov matrices). This limits the number of possibilities for  $pr$ . See also [9, 27].

We shall discuss two situations, namely: (a) the Riemannian metric tensor induced by the  $\ell^2$ -norm on the enveloping Hilbert space for sequences of Markov matrices related to the *system*  $(A, B, C)$  (this is called the *i/o-embedding*); (b) the Riemannian metric tensor induced by the  $\ell^2$ -norm on the enveloping Hilbert space for sequences of Markov matrices related to the corresponding *prediction error filter*  $(A - BC, B, -C)$  (this we call the *o/i-embedding*). In both cases the parameters are contained as described above by  $A$  and  $B$ , so that in particular in situation (b) the *new* matrix triple is *not* brought to one of the overlapping canonical forms.

### A.1 Case 1: Using the i/o-embedding

The Markov matrices associated with an arbitrary triple  $(A, B, C)$  are given by

$$H_k = CA^{k-1}B, \quad \text{for } k \geq 1 \quad (\text{A.4})$$

Following [11, 12, 13], we have that we can associate with any *directional derivative* triple  $[\dot{A}, \dot{B}, \dot{C}]$  at  $(A, B, C)$  the (larger) matrix triple  $(\bar{A}, \bar{B}, \bar{C})$ , where

$$\bar{A} = \begin{pmatrix} A & O \\ \dot{A} & A \end{pmatrix}, \quad \bar{B} = \begin{pmatrix} B \\ \dot{B} \end{pmatrix}, \quad \bar{C} = \begin{pmatrix} \dot{C} & C \end{pmatrix} \quad (\text{A.5})$$

Here the dot denotes differentiation in a certain direction (for instance associated with a curve in the space of systems) at  $(A, B, C)$ . (Compare with Sect. 2.)

The space of sequences  $\{H_k\}_{k=1}^{\infty}$  of  $p \times p$  matrices  $H_k$  for which the quantity

$$\text{trace} \left\{ \sum_{k=1}^{\infty} H_k H_k^T \right\} \quad (\text{A.6})$$

is finite (i.e., the infinite sum converges), can be made into a Hilbert space by: (1) introducing the usual linear operations; (2) defining the inner product  $\langle \cdot, \cdot \rangle_{\ell^2}$  between two sequences  $\{H_k\}_{k=1}^{\infty}$  and  $\{\tilde{H}_k\}_{k=1}^{\infty}$  via

$$\langle \{H_k\}_{k=1}^{\infty}, \{\tilde{H}_k\}_{k=1}^{\infty} \rangle_{\ell^2} = \text{trace} \left\{ \sum_{k=1}^{\infty} H_k \tilde{H}_k^T \right\} \quad (\text{A.7})$$

This inner product is related to the  $\ell^2$ -norm on vector spaces, whence the subscript  $\ell^2$ . Indeed, we easily see that

$$\langle \{H_k\}_{k=1}^{\infty}, \{H_k\}_{k=1}^{\infty} \rangle_{\ell^2} = \text{trace} \left\{ \sum_{k=1}^{\infty} H_k H_k^T \right\} = \sum_{k=1}^{\infty} \sum_{i=1}^p \sum_{j=1}^p H_k(i, j)^2 \quad (\text{A.8})$$

If matrix  $A$  is required to be *asymptotically stable*, meaning that all its eigenvalues lie inside the open unit disk, we see that the sequence of Markov matrices associated with  $(A, B, C)$  is an element of the Hilbert space described above and as a matter of fact, the space of *all* sequences of Markov matrices resulting from such triples can be shown to constitute a differentiable manifold imbedded in the Hilbert space just described.

Now that the directional derivative  $[\dot{A}, \dot{B}, \dot{C}]$  at  $(A, B, C)$  can be associated with the system given by matrix triple  $(\dot{A}, \dot{B}, \dot{C})$  and therefore with a sequence of  $p \times p$  Markov matrices as well, we see that we can relate the tangent space to the differentiable manifold of systems at  $(A, B, C)$  with a subspace of the Hilbert space of matrix sequences of size  $p \times p$ . (Notice that if  $A$  is asymptotically stable, then also  $\dot{A}$  has this property.) Therefore, we have an  $\ell^2$ -induced inner product on the tangent space at  $(A, B, C)$ , via this imbedding in Hilbert space. This inner product thus constitutes a Riemannian metric on the manifold of systems (i.e., of canonical matrix triples  $(A, B, C)$ ).

The discussion above is general in the sense that it applies to *all* parametrizations of  $(A, B, C)$ . When restricting to the parametrizations introduced before, we find that  $\dot{C} = 0$  so that the formula of [12] for the inner product of two derivative systems at  $(A, B, C)$  reduces considerably. Noticing that we can rewrite the expression for the inner product as

$$\langle \{H_k\}_{k=1}^{\infty}, \{\tilde{H}_k\}_{k=1}^{\infty} \rangle_{\ell^2} = \text{trace} \left\{ \sum_{k=1}^{\infty} H_k^T \tilde{H}_k \right\} \quad (\text{A.9})$$

(because  $\text{trace}\{H_k \tilde{H}_k^T\} = \text{trace}\{H_k^T \tilde{H}_k\}$ ), we obtain the following formula

$$\begin{aligned} \langle [\dot{A}, \dot{B}, \dot{C}], [\dot{A}', \dot{B}', \dot{C}'] \rangle_{\ell^2} = & \text{trace} \left\{ \dot{B}^T \mathbf{L}(C^T C) \dot{B}' + \right. \\ & + \dot{B}^T \mathbf{L}(A^T \mathbf{L}(C^T C) \dot{A}') B + B^T \mathbf{L}(\dot{A}^T \mathbf{L}(C^T C) A) \dot{B}' + B^T \mathbf{L}(\dot{A}^T \mathbf{L}(C^T C) \dot{A}') B + \\ & \left. + B^T \mathbf{L}(\dot{A}^T \mathbf{L}(A^T \mathbf{L}(C^T C) \dot{A}') A) B + B^T \mathbf{L}(A^T \mathbf{L}(\dot{A}^T \mathbf{L}(C^T C) A) \dot{A}') B \right\} \end{aligned} \quad (\text{A.10})$$

Here, the expression  $\mathbf{L}(K)$  denotes the solution for  $L$  to the (discrete-time) Lyapunov equation

$$L - A^T L A = K \quad (\text{A.11})$$

It is this large formula that we use in our calculation of the Riemannian metric tensor, since we can exploit efficiently the structure of  $A$ ,  $B$  and  $C$ . How exactly this is achieved, will be discussed after the next subsection.

If the Riemannian metric tensor, represented by a matrix of size  $2np \times 2np$ , is split up into 4 blocks of size  $np \times np$  each, then block (1,1) corresponds to the last three terms of the expression above, block (1,2) to the second term, block (2,1) to the third and block (2,2) to the first.

## A.2 Case 2: Using the o/i-imbedding

The prediction error filter associated with system  $(A, B, C)$  corresponds to matrix triple  $(\tilde{A}, \tilde{B}, \tilde{C}) = (A - BC, B, -C)$ . Obviously we have the following relation for the derivatives

$$\dot{\tilde{A}} = \dot{A} - \dot{B}C, \quad \dot{\tilde{B}} = \dot{B}, \quad \dot{\tilde{C}} = -\dot{C} = 0 \quad (\text{A.12})$$

In the present situation we take  $(\tilde{A}, \tilde{B}, \tilde{C})$  as the basis for our calculations and we are concerned with its tangent space. Thus, we consider the sequence of Markov matrices for  $(\tilde{A}, \tilde{B}, \tilde{C})$ , on imposing the extra condition that  $\tilde{A}$  be asymptotically stable. We again have that a derivative system at a prediction error filter can be associated with an augmented linear system, so that we can relate the tangent space to the system manifold at  $(A, B, C)$  to another linear subspace of the Hilbert space discussed before. We can then apply Hanzon's formula for the inner product of two derivative systems, using tildes everywhere. However, we are interested in the parametrization via  $A$  and  $B$ . We get the expression

$$\begin{aligned} \langle [\tilde{A}, \tilde{B}, \tilde{C}], [\dot{\tilde{A}}, \dot{\tilde{B}}, \dot{\tilde{C}}] \rangle_{\ell^2} = & \text{trace} \left\{ \dot{\tilde{B}}^T \tilde{L} (\tilde{C}^T \tilde{C}) \dot{\tilde{B}} + \right. \\ & + \dot{\tilde{B}}^T \tilde{L} (\tilde{A}^T \tilde{L} (\tilde{C}^T \tilde{C}) \dot{\tilde{A}}) \dot{\tilde{B}} + \dot{\tilde{B}}^T \tilde{L} (\tilde{A}^T \tilde{L} (\tilde{C}^T \tilde{C}) \tilde{A}) \dot{\tilde{B}} + \dot{\tilde{B}}^T \tilde{L} (\tilde{A}^T \tilde{L} (\tilde{C}^T \tilde{C}) \dot{\tilde{A}}) \tilde{B} + \\ & \left. + \dot{\tilde{B}}^T \tilde{L} (\tilde{A}^T \tilde{L} (\tilde{A}^T \tilde{L} (\tilde{C}^T \tilde{C}) \dot{\tilde{A}}) \tilde{A}) \tilde{B} + \dot{\tilde{B}}^T \tilde{L} (\tilde{A}^T \tilde{L} (\tilde{A}^T \tilde{L} (\tilde{C}^T \tilde{C}) \tilde{A}) \dot{\tilde{A}}) \tilde{B} \right\} \end{aligned} \quad (\text{A.13})$$

which can be rewritten in terms of  $\dot{A}$ ,  $\dot{B}$ ,  $\dot{A}'$  and  $\dot{B}'$  as:

$$\begin{aligned} \langle [\dot{A}, \dot{B}, \dot{C}], [\dot{A}', \dot{B}', \dot{C}'] \rangle_{\ell^2, o/i} = & \text{trace} \left\{ \dot{B}'^T \tilde{L} (C^T C) \dot{B}' + \dot{B}'^T \tilde{L} (\tilde{A}^T \tilde{L} (C^T C) (\dot{A}' - \dot{B}'C)) B + \right. \\ & + \dot{B}'^T \tilde{L} ((\dot{A} - \dot{B}C)^T \tilde{L} (C^T C) \tilde{A}') \dot{B}' + \dot{B}'^T \tilde{L} ((\dot{A} - \dot{B}C)^T \tilde{L} (C^T C) (\dot{A}' - \dot{B}'C)) B + \\ & + \dot{B}'^T \tilde{L} ((\dot{A} - \dot{B}C)^T \tilde{L} (\tilde{A}^T \tilde{L} (C^T C) (\dot{A}' - \dot{B}'C)) \tilde{A}) B + \\ & \left. + \dot{B}'^T \tilde{L} (\tilde{A}^T \tilde{L} ((\dot{A} - \dot{B}C)^T \tilde{L} (C^T C) \tilde{A}) (\dot{A}' - \dot{B}'C)) B \right\}. \end{aligned} \quad (\text{A.14})$$

Of course,  $\tilde{L}(K)$  now represents the solution for  $\tilde{L}$  to the alternative (discrete-time) Lyapunov equation

$$\tilde{L} - \tilde{A}^T \tilde{L} \tilde{A} = K \quad (\text{A.15})$$

Using this formula, we can calculate the corresponding Riemannian metric tensor. For this, it is desirable to group the terms in the expression. We write

$$\begin{aligned} \langle [\dot{A}, \dot{B}, \dot{C}], [\dot{A}', \dot{B}', \dot{C}'] \rangle_{\ell^2, o/i} = & \text{trace} \left\{ \dot{B}'^T \tilde{L} (\tilde{A}^T \tilde{L} (C^T C) \dot{A}') B + \right. \\ & + \dot{B}'^T \tilde{L} (\tilde{A}^T \tilde{L} (\tilde{A}^T \tilde{L} (C^T C) \tilde{A}) \dot{A}') B + \\ & + \dot{B}'^T \tilde{L} (\tilde{A}^T \tilde{L} (\tilde{A}^T \tilde{L} (C^T C) \dot{A}') \tilde{A}) B + \\ & - \dot{B}'^T \tilde{L} (\tilde{A}^T \tilde{L} (C^T C) \dot{B}'C) B + \\ & - \dot{B}'^T \tilde{L} (\tilde{A}^T \tilde{L} (\tilde{A}^T \tilde{L} (C^T C) \tilde{A}) \dot{B}'C) B + \\ & - \dot{B}'^T \tilde{L} (\tilde{A}^T \tilde{L} (\tilde{A}^T \tilde{L} (C^T C) \dot{B}'C) \tilde{A}) B + \\ & + \dot{B}'^T \tilde{L} (\tilde{A}^T \tilde{L} (C^T C) \tilde{A}) \dot{B}' + \\ & - \dot{B}'^T \tilde{L} (C^T \dot{B}'^T \tilde{L} (C^T C) \dot{A}') B + \\ & - \dot{B}'^T \tilde{L} (\tilde{A}^T \tilde{L} (C^T \dot{B}'^T \tilde{L} (C^T C) \tilde{A}) \dot{A}') B + \\ & - \dot{B}'^T \tilde{L} (C^T \dot{B}'^T \tilde{L} (\tilde{A}^T \tilde{L} (C^T C) \dot{A}') \tilde{A}) B + \\ & + \dot{B}'^T \tilde{L} (\tilde{A}^T \tilde{L} (C^T C) \dot{A}') B + \\ & + \dot{B}'^T \tilde{L} (C^T \dot{B}'^T \tilde{L} (C^T C) \dot{B}'C) B + \\ & + \dot{B}'^T \tilde{L} (\tilde{A}^T \tilde{L} (C^T \dot{B}'^T \tilde{L} (C^T C) \tilde{A}) \dot{B}'C) B + \\ & + \dot{B}'^T \tilde{L} (C^T \dot{B}'^T \tilde{L} (\tilde{A}^T \tilde{L} (C^T C) \dot{B}'C) \tilde{A}) B + \end{aligned} \quad (\text{A.16})$$

$$\begin{aligned}
& -B^T \tilde{\mathbf{L}}(C^T \dot{B}^T \tilde{\mathbf{L}}(C^T C) \tilde{A}) \dot{B}' + \\
& -\dot{B}^T \tilde{\mathbf{L}}(\tilde{A}^T \tilde{\mathbf{L}}(C^T C) \dot{B}' C) B + \\
& + \dot{B}^T \tilde{\mathbf{L}}(C^T C) \dot{B}' \}.
\end{aligned}$$

If the Riemannian metric tensor, represented by a matrix of size  $2np \times 2np$ , is again split up in 4 blocks of size  $np \times np$  each, we get that the (1,1)-block corresponds to the first three terms, the (1,2)-block to terms 4 to 7, block (2,1) to terms 8 to 11 and block (2,2) to terms 12 to 17.

### A.3 Efficient calculation of the Riemannian metric tensors

The terms in the expressions for the Riemannian metric tensors in both situations discussed before can be calculated efficiently by exploiting the structure of matrices  $A$ ,  $B$  and  $C$ . In our formulas we have already accounted for the fact that  $C$  and  $\tilde{C}$  do not depend on any parameters at all, so that  $\dot{C} = \dot{\tilde{C}} = 0$ . For the rest, it is clear that  $\dot{A}$  and  $\dot{B}$  exhibit a special, very sparse structure if we consider partial derivation with respect to one parameter  $\theta_i$  at a time only. Also, we must notice that calculation of any term involves (sometimes repeatedly) the solution of a (discrete-time) Lyapunov equation. Therefore, we shall first discuss how to solve a discrete-time Lyapunov equation in some more detail.

We address the following equation

$$L - A^T L A = K \quad (\text{A.17})$$

where it is assumed that  $A$  is an asymptotically stable matrix. As a consequence of this the solution to such an equation is then *unique* (which is a well-known result), and can formally be expressed as the infinite sum

$$\mathbf{L}(K) = \sum_{k=1}^{\infty} (A^T)^{k-1} K A^{k-1} \quad (\text{A.18})$$

(It is precisely the requirement that  $A$  be asymptotically stable which makes this sum converge.) In order to calculate  $\mathbf{L}(K)$  numerically, we can use the following well-known recursive scheme.

$$\text{initialization:} \quad L(0) = K, \quad M(0) = A \quad (\text{A.19})$$

$$\text{recursion:} \quad L(t+1) = L(t) + M(t)^T L(t) M(t), \quad M(t+1) = M(t)^2 \quad (\text{A.20})$$

Notice that this comes down to

$$L(t) = \sum_{k=1}^{2^t} (A^T)^{k-1} K A^{k-1}, \quad M(t) = A^{(2^t)} \quad (\text{A.21})$$

Therefore, very rapid summation takes place so that relatively few iterations are sufficient for a good approximation to  $\mathbf{L}(K)$ , given by  $L(t)$ .

Next, we mention a number of properties of the Lyapunov equation and its solutions. For all  $K, M \in \mathbf{R}^{n \times n}$  and  $\lambda \in \mathbf{R}$  we have

$$\mathbf{L}(K + M) = \mathbf{L}(K) + \mathbf{L}(M) \quad (\text{A.22})$$

$$\mathbf{L}(\lambda K) = \lambda \mathbf{L}(K) \quad (\text{A.23})$$

$$\mathbf{L}(K^T) = \mathbf{L}(K)^T \quad (\text{A.24})$$

These follow easily from the structure of the equation and the uniqueness of its solution. They will be very useful in representing the solutions to the repeated Lyapunov equations, occurring in the terms for the elements of the Riemannian metric tensors.

We first introduce some more notation. By  $E^{(i,j)}$  we denote the  $(i,j)$ -th ‘‘basis’’ matrix of size  $n \times n$ , that is, the matrix consisting of zeros everywhere, except for the element on location  $(i,j)$  which equals 1. The element at location  $(i,j)$  of matrix  $K$  is denoted by  $K_{(i,j)}$ . The solution to the

Lyapunov equation with  $K = E^{(i,j)}$  is denoted by  $\mathbf{L}(E^{(i,j)}) = L^{(i,j)}$ . Obviously, we can now in general write  $\mathbf{L}(K)$  as

$$\mathbf{L}(K) = \sum_{i=1}^n \sum_{j=1}^n K_{(i,j)} L^{(i,j)} \quad (\text{A.25})$$

Moreover, we have that

$$(L^{(i,j)})^T = L^{(j,i)}, \quad \text{since } (E^{(i,j)})^T = E^{(j,i)} \quad (\text{A.26})$$

We shall pay attention to three special cases, involving the solution to repeated Lyapunov equations.

(i) Consider matrix  $E^{(i,j)}KA$ .

This matrix consists of  $n-1$  zero rows, and only row  $i$  is possibly nonzero. This row is equal to row  $j$  of  $KA$ , that is

$$(E^{(i,j)}KA)_{(m,\ell)} = \begin{cases} 0 & \text{if } m \neq i, \\ \sum_{k=1}^n K_{(j,k)} A_{(k,\ell)} & \text{if } m = i. \end{cases} \quad (\text{A.27})$$

Therefore we get

$$\mathbf{L}(E^{(i,j)}KA) = \sum_{\ell=1}^n \left( L^{(i,\ell)} \left( \sum_{k=1}^n K_{(j,k)} A_{(k,\ell)} \right) \right) \quad (\text{A.28})$$

(ii) Consider matrix  $E^{(i,j)}KE^{(g,h)}$ .

This matrix consists of zeros everywhere, except for possibly the element on place  $(i, h)$  which is equal to  $K_{(j,g)}$ . Thus,  $E^{(i,j)}KE^{(g,h)} = K_{(j,g)}E^{(i,h)}$ . Hence

$$\mathbf{L}(E^{(i,j)}KE^{(g,h)}) = K_{(j,g)}L^{(i,h)} \quad (\text{A.29})$$

(iii) Consider matrix  $A^T \mathbf{L}(E^{(i,j)}KA)E^{(g,h)}$ .

Put  $M = \mathbf{L}(E^{(i,j)}KA)$ , then the matrix above can be written as  $(E^{(h,g)}M^T A)^T$ . Using (i) on this expression yields

$$\mathbf{L}(A^T \mathbf{L}(E^{(i,j)}KA)E^{(g,h)}) = \mathbf{L}(E^{(h,g)}M^T A)^T = \sum_{\ell=1}^n \left( L^{(\ell,h)} \left( \sum_{k=1}^n A_{(k,\ell)} M_{(k,g)} \right) \right) \quad (\text{A.30})$$

But we can also apply (i) to  $M$ . This gives

$$M_{(k,g)} = \sum_{r=1}^n \left( L^{(i,r)}_{(k,g)} \left( \sum_{s=1}^n K_{(j,s)} A_{(s,r)} \right) \right) \quad (\text{A.31})$$

Combining both expressions gives us the final result

$$\mathbf{L}(A^T \mathbf{L}(E^{(i,j)}KA)E^{(g,h)}) = \sum_{\ell=1}^n \left( L^{(\ell,h)} \left( \sum_{k=1}^n A_{(k,\ell)} \sum_{r=1}^n \left( L^{(i,r)}_{(k,g)} \left( \sum_{s=1}^n K_{(j,s)} A_{(s,r)} \right) \right) \right) \right) \quad (\text{A.32})$$

These results are of importance when calculating the terms in the expressions for the Riemannian metric tensors. For this, notice that when we apply partial differentiation with respect to  $\theta_{(i-1)n+j}$  (where  $i \in \{1, \dots, p\}$  and  $j \in \{1, \dots, n\}$ ) we get

$$\dot{A} = \dot{A}^{(i,j)} = E^{(pr(i),j)}, \quad \dot{B} = 0 \quad (\text{A.33})$$

Similarly, if we apply partial differentiation with respect to  $\theta_{np+(i-1)n+j}$  (where  $i \in \{1, \dots, p\}$  and  $j \in \{1, \dots, n\}$ ), we get

$$\dot{B}C = \dot{B}^{(i,j)}C = E^{(j,i)}, \quad \dot{A} = 0 \quad (\text{A.34})$$

Moreover, we have that matrix  $C^T C$  has the structure

$$C^T C = \begin{pmatrix} I & O \\ O & O \end{pmatrix} \quad (\text{A.35})$$

where the identity block is of size  $p \times p$ . Therefore

$$\mathbf{L}(C^T C) = \sum_{i=1}^p L^{(i,i)} \quad (\text{A.36})$$

We finally notice that all terms appearing in the expressions for the elements of the Riemannian metric tensors can be solved with one of the three special forms discussed above. For the Riemannian metric in the second case we must of course use matrices  $\tilde{A}$ ,  $\tilde{B}$  and  $\tilde{C}$ , which comes down to adding tildes in the appropriate places. We also have to make use of the fact that  $\text{trace}\{K^T\} = \text{trace}\{K\}$ , so that the terms where the matrices appear in the opposite order can be rewritten.

Thus, it has become clear how the elements of the Riemannian metric tensors can be calculated, in both cases under consideration, although the actual process of doing so remains quite laborious and time consuming. Possibly symbolic computation of explicit expressions for the elements can lead to a speed up in these cases. Notice that the approach described above might be useful in deriving such expressions.



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