D-optimal Bayesian Interrogation for Parameter and Noise Identification of Recurrent Neural Networks

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Abstract. We introduce a novel online Bayesian method for the identification of a family of noisy recurrent neural networks (RNNs). We develop Bayesian active learning technique in order to optimize the interrogating stimuli given past experiences. In particular, we consider the unknown parameters as stochastic variables and use the D-optimality principle, also known as '*infomax method*', to choose optimal stimuli. We apply a greedy technique to maximize the information gain concerning network parameters at each time step. We also derive the D-optimal estimation of the additive noise that perturbs the dynamical system of the RNN. Our analytical results are approximation-free. The analytic derivation gives rise to attractive quadratic update rules.

1 Introduction

When studying online systems it is of high relevance to facilitate fast information gain concerning the system [1,2]. As an example, consider the research on real neurons. In one of the experimental paradigms, researchers look for the stimulus that maximizes the response of the neuron [3,4]. Another approach searches for stimulus distribution that maximizes mutual information between stimulus and response [5]. A recent technique assumes that the unknown system belongs to the family of generalized linear models [6] and treats the parameters as probabilistic variables. Then the goal is to find the optimal stimuli by maximizing mutual information between the parameter set and the response of the system.

We are interested in the active learning [7,8,9,10] of noisy recurrent artificial neural networks (RNNs), when we have the freedom to interrogate the network and to measure the responses. Our framework is similar to the generalized linear model (GLM) approach used by [6]: we would like to choose interrogating, or '*control*' inputs in order to (i) identify the parameters of the network and (ii) estimate the additive noise efficiently. From now on, we use the terms *control* and *interrogation* interchangeably; control is the conventional expression, whereas the word interrogation expresses our aims better. We apply online Bayesian learning [11,12,13,14] to accomplish our task. For Bayesian methods prior updates often lead to intractable posterior distributions such as a mixture of exponentially numerous distributions. Here, we show that in our model computations are both tractable and approximation-free. Further, the emerging learning rules are simple. We also show that different stimuli are needed for the same RNN

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model depending on whether the goal is to estimate the weights of the RNN or the additive noise that perturbs the RNN. Hereafter we will refer to this noise as the 'driving noise' of the RNN.

Our approach, which optimizes control online in order to gain maximum information concerning the parameters, falls into the realm of Optimal Experimental Design, or Optimal Bayesian Design [15,1,16,17,18]. Several optimality principles have been worked out and their efficiencies have been studied extensively in the literature. For a review see, e.g., [19]. Our approach corresponds to the so-called D-optimality [20,21], which is equivalent to the information maximization (infomax) principle applied by [6]. We use both terms, the term *D-optimality* and the term *infomax*, to designate our approach. To the best of our knowledge, D-optimality has not been applied to the typical non-spiking stochastic artificial recurrent neural network model that we treat here.

The contribution of this paper can be summarized as follows: We use the D-optimality (infomax) principle and derive cost functions and algorithms for (i) the parameter learning of the stochastic RNN and (ii) the estimation of its driving noise. We show that, (iii) using the D-optimality interrogation technique, these two tasks are not compatible with each other: greedy control signals derived from the D-optimality principle for parameter estimation are suboptimal (basically the worst possible) for the estimation of the driving noise and vice versa. We show that (iv) D-optimal cost functions lead to simple greedy optimization rules both for the parameter estimation and for the noise estimation, respectively. Investigation of non-greedy multiple step optimizations, which may achieve more efficient estimation of the network parameters and the noise, seems difficult and is beyond the scope of the present paper. However, (v) for the task of estimating the driving noise we introduce a non-greedy multiple step look-ahead heuristics.

The paper is structured as follows: In Section 2 we introduce our model. Section 3 concerns the Bayesian equations of the RNN model. Section 4 derives the optimal control for its parameter identification starting from the D-optimality (infomax) principle. Section 5 deals with our second task, when the goal is the estimation of the driving noise of the RNN. The paper ends with a short discussion and some conclusions (Section 6).

2 The Model

We introduce our model here. Let $P(\mathbf{e}) = \mathcal{N}_{\mathbf{e}}(\mathbf{m}, \mathbf{V})$ denote the probability density of a normally distributed stochastic variable $\mathbf{e}$ with mean $\mathbf{m}$ and covariance matrix $\mathbf{V}$. Let us assume that we have d simple computational units called '*neurons*' in a recurrent neural network:

$$\mathbf{r}_{t+1} = g\left(\sum_{i=0}^{I} \mathbf{F}_i \mathbf{r}_{t-i} + \sum_{j=0}^{J} \mathbf{B}_j \mathbf{u}_{t+1-j} + \mathbf{e}_{t+1}\right), \tag{1}$$

where $\{\mathbf{e}_t\}$, the driving noise of the RNN, denotes temporally independent and identically distributed (i.i.d.) stochastic variables and $P(\mathbf{e}_t) = \mathcal{N}_{\mathbf{e}_t}(\mathbf{0}, \mathbf{V})$, $\mathbf{r}_t \in \mathbb{R}^d$ represents the observed activities of the neurons at time t. Let $\mathbf{u}_t \in \mathbb{R}^c$ denote the control signal at time t. The neural network is formed by the weighted delays represented by matrices $\mathbf{F}_i$ ($i = 0, \ldots, I$) and $\mathbf{B}_j$ ($j = 0, \ldots, J$), which connect neurons to each other and also the control components to the neurons, respectively. Control can also be seen as the means of interrogation, or the stimulus to the network [6]. We assume that function $g : \mathbb{R}^d \to \mathbb{R}^d$ in (1) is known and invertible. The

computational units, the neurons, sum up weighted previous neural activities as well as weighted control inputs. These sums are then passed through identical non-linearities according to Eq. (1). Our goal is to estimate the parameters $\mathbf{F}_i \in \mathbb{R}^{d \times d}$ $(i = 0, \ldots, I)$, $\mathbf{B}_j \in \mathbb{R}^{d \times c}$ $(j = 0, \ldots, J)$ and the covariance matrix $\mathbf{V}$, as well as the driving noise $\mathbf{e}_t$ by means of the control signals.

In artificial neural network terms, (1) is in the form of *rate code models*. In our rate code model, noise, control, and the recurrent activities influence the firing rates similarly. We show that analytic cost functions emerge for this model that are free of approximation.

3 Bayesian Approach

Here we embed the estimation task into the Bayesian framework. First, we introduce the following notations: $\mathbf{x}_{t+1} = [\mathbf{r}_{t-I}; \ldots; \mathbf{r}_t; \mathbf{u}_{t-J+1}; \ldots; \mathbf{u}_{t+1}]$, $\mathbf{y}_{t+1} = g^{-1}(\mathbf{r}_{t+1})$, $\mathbf{A} = [\mathbf{F}_I, \ldots, \mathbf{F}_0, \mathbf{B}_J, \ldots, \mathbf{B}_0] \in \mathbb{R}^{d \times m}$. With these notations, model (1) reduces to a linear equation

$$\mathbf{y}_t = \mathbf{A}\mathbf{x}_t + \mathbf{e}_t. \tag{2}$$

To fulfill our goal, the online estimation of the unknown quantities (parameter matrix $\mathbf{A}$, noise $\mathbf{e}_t$ and its covariance matrix $\mathbf{V}$), we rely on Bayes' method. We assume that prior knowledge is available and we update our posteriori knowledge on the basis of the observations. Control will be chosen at each instant to provide maximal expected information concerning the quantities we have to estimate. Starting from an arbitrary prior distribution of the parameters the posterior distribution needs to be computed. This can be highly complex, however, so approximations are common in the literature. For example, assumed density filtering, when the computed posterior is projected to simpler distributions, has been suggested [22,23,11]. We shall use the method of conjugated priors [24] instead. For matrix $\mathbf{A}$ we assume a matrix valued normal distribution prior. For covariance matrix $\mathbf{V}$ inverted Wishart (IW) distribution will be our prior. One can show for these choices that the functional form of the posteriori distributions is not affected.

We define the normally distributed matrix valued stochastic variable $\mathbf{A} \in \mathbb{R}^{d \times m}$ by using the following quantities: $\mathbf{M} \in \mathbb{R}^{d \times m}$ is the expected value of $\mathbf{A}$. $\mathbf{V} \in \mathbb{R}^{d \times d}$ is the covariance matrix of the rows, and $\mathbf{K} \in \mathbb{R}^{m \times m}$ is the so-called precision parameter matrix that we shall modify in accordance with the Bayesian update. They are both positive semi-definite matrices. The density function of the stochastic variable $\mathbf{A}$ is defined as:

$$\mathcal{N}_{\mathbf{A}}(\mathbf{M}, \mathbf{V}, \mathbf{K}) = \frac{|\mathbf{K}|^{d/2}}{|2\pi\mathbf{V}|^{m/2}} \exp(-\frac{1}{2}tr((\mathbf{A} - \mathbf{M})^T \mathbf{V}^{-1}(\mathbf{A} - \mathbf{M})\mathbf{K})),$$

where tr, $|\cdot|$, and superscript T denote the trace operation, the determinant, and transposition, respectively. See e.g. [25,26]. We assume that $\mathbf{Q} \in \mathbb{R}^{d \times d}$ is a positive definite matrix and $n > 0$. Using these notations, the density of the Inverted Wishart distribution with parameters $\mathbf{Q}$ and n is as follows [25]:

$$\mathcal{IW}_{\mathbf{V}}(\mathbf{Q}, n) = \frac{1}{Z_{n,d}} \frac{1}{|\mathbf{V}|^{(d+1)/2}} \left| \frac{\mathbf{V}^{-1}\mathbf{Q}}{2} \right|^{n/2} \exp(-\frac{1}{2}tr(\mathbf{V}^{-1}\mathbf{Q})),$$

where $Z_{n,d} = \pi^{d(d-1)/4} \prod_{i=1}^{d} \Gamma((n+1-i)/2)$ and $\Gamma(.)$ denotes the gamma function.

Now, one can rewrite model (2) as follows:

$$P(\mathbf{A}|\mathbf{V}) = \mathcal{N}_{\mathbf{A}}(\mathbf{M}, \mathbf{V}, \mathbf{K}), \tag{3}$$

$$P(\mathbf{V}) = \mathcal{IW}_{\mathbf{V}}(\mathbf{Q}, n), \tag{4}$$

$$P(\mathbf{e}_t|\mathbf{V}) = \mathcal{N}_{\mathbf{e}_t}(\mathbf{0}, \mathbf{V}), \tag{5}$$

$$P(\mathbf{y}_t|\mathbf{A}, \mathbf{x}_t, \mathbf{V}) = \mathcal{N}_{\mathbf{y}_t}(\mathbf{A}\mathbf{x}_t, \mathbf{V}). \tag{6}$$

4 The Infomax Approach for Parameter Learning

Let us compute the parameter estimation strategy for task (1) (i.e., for task (3)-(6)) as prescribed by the infomax principle. Let us introduce two shorthands; $\boldsymbol{\theta} = \{\mathbf{A}, \mathbf{V}\}$, and $\{\mathbf{x}\}_i^j = \{\mathbf{x}_i, \ldots, \mathbf{x}_j\}$. We choose the control value in (1) at each instant such that it provides the most expected information concerning the unknown parameters. Assuming that $\{\mathbf{x}\}_1^t$, $\{\mathbf{y}\}_1^t$ are given, according to the infomax principle our goal is to compute

$$\arg \max_{\mathbf{u}_{t+1}} I(\boldsymbol{\theta}, \mathbf{y}_{t+1}; \{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^t), \tag{7}$$

where $I(a, b; c)$ denotes the mutual information of stochastic variables a and b for fixed parameters c. Let $H(a|b; c)$ denote the conditional entropy of variable a conditioned on variable b and for fixed parameter c. Note that

$$I(\boldsymbol{\theta}, \mathbf{y}_{t+1}; \{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^t) = H(\boldsymbol{\theta}; \{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^t) - H(\boldsymbol{\theta}|\mathbf{y}_{t+1}; \{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^t),$$

holds [27] and $H(\boldsymbol{\theta}; \{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^t) = H(\boldsymbol{\theta}; \{\mathbf{x}\}_1^t, \{\mathbf{y}\}_1^t)$ is independent from $\mathbf{u}_{t+1}$, hence our task is reduced to the evaluation of the following quantity:

$$\arg \min_{\mathbf{u}_{t+1}} H(\boldsymbol{\theta}|\mathbf{y}_{t+1}; \{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^t) = \tag{8}$$

$$= \arg \min_{\mathbf{u}_{t+1}} - \int d\mathbf{y}_{t+1} P(\mathbf{y}_{t+1}|\{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^t) \int d\boldsymbol{\theta} P(\boldsymbol{\theta}|\{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^{t+1}) \log P(\boldsymbol{\theta}|\{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^{t+1}).$$

In order to solve this minimization problem we need to evaluate $P(\mathbf{y}_{t+1}|\{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^t)$, the posterior $P(\boldsymbol{\theta}|\{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^{t+1})$, and the entropy of the posterior, that is $\int d\boldsymbol{\theta} P(\boldsymbol{\theta}|\{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^{t+1}) \log P(\boldsymbol{\theta}|\{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^{t+1})$, where $P(a|b)$ denotes the conditional probability of variable a given condition b. The main steps of these computations are provided below.

Assume that the *a priori* distributions $P(\mathbf{A}|\mathbf{V}, \{\mathbf{x}\}_1^t, \{\mathbf{y}\}_1^t) = \mathcal{N}(\mathbf{A}|\mathbf{M}_t, \mathbf{V}, \mathbf{K}_t)$ and $P(\mathbf{V}|\{\mathbf{x}\}_1^t, \{\mathbf{y}\}_1^t) = \mathcal{IW}_{\mathbf{V}}(\mathbf{Q}_t, n_t)$ are known. Then the posterior distribution of $\boldsymbol{\theta}$ is:

$$P(\mathbf{A}, \mathbf{V}|\{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^{t+1}) = \frac{P(\mathbf{y}_{t+1}|\mathbf{A}, \mathbf{V}, \mathbf{x}_{t+1})P(\mathbf{A}|\mathbf{V}, \{\mathbf{x}\}_1^t, \{\mathbf{y}\}_1^t)P(\mathbf{V}|\{\mathbf{x}\}_1^t, \{\mathbf{y}\}_1^t)}{P(\mathbf{y}_{t+1}|\{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^t)}$$

$$= \frac{\mathcal{N}_{\mathbf{y}_{t+1}}(\mathbf{A}\mathbf{x}_{t+1}, \mathbf{V})\mathcal{N}_{\mathbf{A}}(\mathbf{M}_t, \mathbf{V}, \mathbf{K}_t)\mathcal{IW}_{\mathbf{V}}(\mathbf{Q}_t, n_t)}{\int_{\mathbf{A}} \int_{\mathbf{V}} \mathcal{N}_{\mathbf{y}_{t+1}}(\mathbf{A}\mathbf{x}_{t+1}, \mathbf{V})\mathcal{N}_{\mathbf{A}}(\mathbf{M}_t, \mathbf{V}, \mathbf{K}_t)\mathcal{IW}_{\mathbf{V}}(\mathbf{Q}_t, n_t))}.$$

This expression can be rewritten in a more useful form: let $\mathbf{K} \in \mathbb{R}^{m \times m}$ and $\mathbf{Q} \in \mathbb{R}^{d \times d}$ be positive definite matrices. Let $\mathbf{A} \in \mathbb{R}^{d \times m}$, and let us introduce the density function of the

matrix valued Student-t distribution [28,26] as follows:

$$\mathcal{T}_{\mathbf{A}}(\mathbf{Q}, n, \mathbf{M}, \mathbf{K}) = \frac{|\mathbf{K}|^{d/2}}{\pi^{dm/2}} \frac{Z_{n+m,d}}{Z_{n,d}} \frac{|\mathbf{Q}|^{n/2}}{|\mathbf{Q} + (\mathbf{A} - \mathbf{M})\mathbf{K}(\mathbf{A} - \mathbf{M})^T|^{(m+n)/2}},$$

Now, we need the following lemma:

Lemma 41

$$\mathcal{N}_{\mathbf{y}}(\mathbf{Ax}, \mathbf{V})\mathcal{N}_{\mathbf{A}}(\mathbf{M}, \mathbf{V}, \mathbf{K})\mathcal{IW}_{\mathbf{V}}(\mathbf{Q}, n) = \mathcal{N}_{\mathbf{A}}((\mathbf{MK} + \mathbf{yx}^T)(\mathbf{xx}^T + \mathbf{K})^{-1}, \mathbf{V}, \mathbf{xx}^T + \mathbf{K}) \times$$
$$\times \mathcal{IW}_{\mathbf{V}}\left(\mathbf{Q} + (\mathbf{y} - \mathbf{Mx})\left(1 - \mathbf{x}^T(\mathbf{xx}^T + \mathbf{K})^{-1}\mathbf{x}\right)(\mathbf{y} - \mathbf{Mx})^T, n + 1\right) \times$$
$$\times \mathcal{T}_{\mathbf{y}}\left(\mathbf{Q}, n, \mathbf{Mx}, 1 - \mathbf{x}^T(\mathbf{xx}^T + \mathbf{K})^{-1}\mathbf{x}\right).$$

Proof. It is easy to show that the following equations hold:

$$\mathcal{N}_{\mathbf{y}}(\mathbf{Ax}, \mathbf{V})\mathcal{N}_{\mathbf{A}}(\mathbf{M}, \mathbf{V}, \mathbf{K}) = \mathcal{N}_{\mathbf{A}}(\mathbf{M}^+, \mathbf{V}, \mathbf{xx}^T + \mathbf{K})\mathcal{N}_{\mathbf{y}}(\mathbf{Mx}, \mathbf{V}, \gamma),$$
$$\mathcal{N}_{\mathbf{A}}(\mathbf{M}, \mathbf{V}, \mathbf{K})\mathcal{IW}_{\mathbf{V}}(\mathbf{Q}, n) = \mathcal{IW}_{\mathbf{V}}(\mathbf{Q} + \mathbf{H}, n + 1)\mathcal{T}_{\mathbf{A}}(\mathbf{Q}, n, \mathbf{M}, \mathbf{K}), \qquad (9)$$

where $\mathbf{M}^+ = (\mathbf{MK} + \mathbf{yx}^T)(\mathbf{xx}^T + \mathbf{K})^{-1}$, $\gamma = 1 - \mathbf{x}^T(\mathbf{xx}^T + \mathbf{K})^{-1}\mathbf{x}$, $\mathbf{H} = (\mathbf{A} - \mathbf{M})\mathbf{K}(\mathbf{A} - \mathbf{M})^T$ for the sake of brevity. Then we have

$$\mathcal{N}_{\mathbf{y}}(\mathbf{Mx}, \mathbf{V}, \gamma)\mathcal{IW}_{\mathbf{V}}(\mathbf{Q}, n) = \mathcal{IW}_{\mathbf{V}}(\mathbf{Q} + (\mathbf{y} - \mathbf{Mx})\gamma(\mathbf{y} - \mathbf{Mx})^T, n + 1)\mathcal{T}_{\mathbf{y}}(\mathbf{Q}, n, \mathbf{Mx}, \gamma),$$

and the statement of the lemma follows.

Using this lemma, we can compute the posterior probabilities. Let us introduce the following quantities:

$$\gamma_{t+1} = 1 - \mathbf{x}_{t+1}^T(\mathbf{x}_{t+1}\mathbf{x}_{t+1}^T + \mathbf{K}_t)^{-1}\mathbf{x}_{t+1},$$
$$n_{t+1} = n_t + 1,$$
$$\mathbf{M}_{t+1} = (\mathbf{M}_t\mathbf{K}_t + \mathbf{y}_{t+1}\mathbf{x}_{t+1}^T)(\mathbf{x}_{t+1}\mathbf{x}_{t+1}^T + \mathbf{K}_t)^{-1},$$
$$\mathbf{Q}_{t+1} = \mathbf{Q}_t + (\mathbf{y}_{t+1} - \mathbf{M}_t\mathbf{x}_{t+1})\gamma_{t+1}(\mathbf{y}_{t+1} - \mathbf{M}_t\mathbf{x}_{t+1})^T. \qquad (10)$$

For the posterior probabilities we have determined that

$$P(\mathbf{A}|\mathbf{V}, \{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^{t+1}) = \mathcal{N}_{\mathbf{A}}(\mathbf{M}_{t+1}, \mathbf{V}, \mathbf{x}_{t+1}\mathbf{x}_{t+1}^T + \mathbf{K}_t), \qquad (11)$$
$$P(\mathbf{V}|\{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^{t+1}) = \mathcal{IW}_{\mathbf{V}}(\mathbf{Q}_{t+1}, n_{t+1}), \qquad (12)$$
$$P(\mathbf{y}_{t+1}|\{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^t) = \mathcal{T}_{\mathbf{y}_{t+1}}(\mathbf{Q}_t, n_t, \mathbf{M}_t\mathbf{x}_{t+1}, \gamma_{t+1}).$$

Having done so, we can compute the entropy of the posterior distribution of $\boldsymbol{\theta} = \{\mathbf{A}, \mathbf{V}\}$ by means of the following lemma:

Lemma 42 *The entropy of a stochastic variable with density function $P(\mathbf{A}, \mathbf{V}) = \mathcal{N}_{\mathbf{A}}(\mathbf{M}, \mathbf{V}, \mathbf{K})\mathcal{IW}_{\mathbf{V}}(\mathbf{Q}, n)$ assumes the form $-\frac{d}{2}\ln|\mathbf{K}| + (\frac{m+d+1}{2})\ln|\mathbf{Q}| + f_1(d, n)$, where $f_1(d, n)$ depends only on d and n.*

Proof. Let $vec(\mathbf{A})$ denote a vector of dm dimensions where the $(d(i-1)+1)^{th}, \ldots, (id)^{th}$ $(1 \le i \le m)$ elements of this vector are equal to the elements of the ith column of matrix $\mathbf{A} \in \mathbb{R}^{d \times m}$ in the appropriate order. Let $\otimes$ denote the Kronecker-product. It is known that for $P(\mathbf{A}) = \mathcal{N}_{\mathbf{A}}(\mathbf{M}, \mathbf{V}, \mathbf{K})$, $P(vec(\mathbf{A})) = \mathcal{N}_{vec(\mathbf{A})}(vec(\mathbf{M}), \mathbf{V} \otimes \mathbf{K}^{-1})$ holds [26]. Using the well-known formula for the entropy of a multivariate and normally distributed variable [27] and applying the relation $|\mathbf{V} \otimes \mathbf{K}^{-1}| = |\mathbf{V}|^m / |\mathbf{K}|^d$, we have that

$$H(\mathbf{A}; \mathbf{V}) = \frac{1}{2} \ln |\mathbf{V} \otimes \mathbf{K}^{-1}| + \frac{dm}{2} \ln(2\pi e) = \frac{m}{2} \ln |\mathbf{V}| - \frac{d}{2} \ln |\mathbf{K}| + \frac{dm}{2} \ln(2\pi e).$$

Exploit certain properties of the Wishart distribution, we compute the entropy of distribution $\mathcal{IW}_{\mathbf{V}}(\mathbf{Q}, n)$. The density of the Wishart distribution is defined by

$$\mathcal{W}_{\mathbf{V}}(\mathbf{Q}, n) = \frac{1}{Z_{n,d}} |\mathbf{V}|^{(n-d-1)/2} \left| \frac{\mathbf{Q}^{-1}}{2} \right|^{n/2} \exp\left(-\frac{1}{2} tr(\mathbf{V}\mathbf{Q}^{-1})\right).$$

Let Ψ denote the digamma function, and let $f_2(d, n) = -\sum_{i=1}^{d} \Psi(\frac{n+1-i}{2})) - d \ln 2$. Replacing $\mathbf{V}^{-1}$ with $\mathbf{S}$, we have for the Jacobian that $|\frac{d\mathbf{V}}{d\mathbf{S}}| = |\frac{d\mathbf{S}^{-1}}{d\mathbf{S}}| = |\mathbf{S}|^{-(d+1)}$ [25]. To proceed we use that $E_{\mathcal{W}_{\mathbf{S}}(\mathbf{Q},n)}\mathbf{S} = n\mathbf{Q}$, and $E_{\mathcal{W}_{\mathbf{S}}(\mathbf{Q},n)} \ln |\mathbf{S}| = \ln |\mathbf{Q}| - f_2(d, n)$, [29] and substitute them into $E_{\mathcal{IW}_{\mathbf{V}}(\mathbf{Q},n)} \ln |\mathbf{V}|$, and $E_{\mathcal{IW}_{\mathbf{V}}(\mathbf{Q},n)} tr(\mathbf{Q}\mathbf{V}^{-1})$:

$$E_{\mathcal{IW}_{\mathbf{V}}(\mathbf{Q},n)} \ln |\mathbf{V}| =$$

$$= \int \frac{1}{Z_{n,d}} \frac{1}{|\mathbf{V}|^{(d+1)/2}} \left| \frac{\mathbf{V}^{-1}\mathbf{Q}}{2} \right|^{n/2} \exp\left(-\frac{1}{2} tr(\mathbf{V}^{-1}\mathbf{Q})\right) \ln |\mathbf{V}| d\mathbf{V}$$

$$= -\int \frac{1}{Z_{n,d}} |\mathbf{S}|^{(d+1)/2} \left| \frac{\mathbf{S}\mathbf{Q}}{2} \right|^{n/2} \exp\left(-\frac{1}{2} tr(\mathbf{S}\mathbf{Q})\right) \ln |\mathbf{S}| |\mathbf{S}|^{-d-1} d\mathbf{S}$$

$$= -\int \frac{1}{Z_{n,d}} |\mathbf{S}|^{(n-d-1)/2} \left| \frac{\mathbf{Q}}{2} \right|^{n/2} \exp\left(-\frac{1}{2} tr(\mathbf{S}\mathbf{Q})\right) \ln |\mathbf{S}| d\mathbf{S}$$

$$= -E_{\mathcal{W}_{\mathbf{S}}(\mathbf{Q}^{-1},n)} \ln |\mathbf{S}|$$

$$= \ln |\mathbf{Q}| + f_2(d, n). \tag{13}$$

One can also show that

$$E_{\mathcal{IW}_{\mathbf{V}}(\mathbf{Q},n)} tr(\mathbf{Q}\mathbf{V}^{-1}) =$$

$$= \int \frac{1}{Z_{n,d}} \frac{1}{|\mathbf{V}|^{(d+1)/2}} \left| \frac{\mathbf{V}^{-1}\mathbf{Q}}{2} \right|^{n/2} \exp\left(-\frac{1}{2} tr(\mathbf{V}^{-1}\mathbf{Q})\right) tr(\mathbf{Q}\mathbf{V}^{-1}) d\mathbf{V}$$

$$= \int \frac{1}{Z_{n,d}} |\mathbf{S}|^{(d+1)/2} \left| \frac{\mathbf{S}\mathbf{Q}}{2} \right|^{n/2} \exp\left(-\frac{1}{2} tr(\mathbf{S}\mathbf{Q})\right) tr(\mathbf{Q}\mathbf{S}) |\mathbf{S}|^{-d-1} d\mathbf{S},$$

$$= \int \frac{1}{Z_{n,d}} |\mathbf{S}|^{(n-d-1)/2} \left| \frac{\mathbf{Q}}{2} \right|^{n/2} \exp\left(-\frac{1}{2} tr(\mathbf{S}\mathbf{Q})\right) tr(\mathbf{Q}\mathbf{S}) d\mathbf{S},$$

$$= E_{\mathcal{W}_{\mathbf{S}}(\mathbf{Q}^{-1},n)} tr(\mathbf{Q}\mathbf{S}),$$

$$= tr(\mathbf{Q}\mathbf{Q}^{-1}n) = nd \tag{14}$$

We calculate the entropy of stochastic variable $\mathbf{V}$ with distribution $\mathcal{IW}_{\mathbf{V}}(\mathbf{Q}, n)$. It follows from Eq. (13) and Eq. (14) that

$$H(\mathbf{V}) =$$

$$= -E_{\mathcal{IW}_{\mathbf{V}}(\mathbf{Q},n)} \left[-\ln(Z_{n,d}) + \frac{n}{2} \ln \left| \frac{\mathbf{Q}}{2} \right| - \frac{n+d+1}{2} \ln |\mathbf{V}| - \frac{1}{2} tr(\mathbf{V}^{-1}\mathbf{Q}) \right]$$

$$= \ln(Z_{n,d}) - \frac{n}{2} \ln \left| \frac{\mathbf{Q}}{2} \right| + \frac{n+d+1}{2} \left[\ln |\mathbf{Q}| - \sum_{i=1}^{d} \Psi(\frac{n+1-i}{2})) - d\ln 2 \right] + \frac{nd}{2}$$

$$= \frac{d+1}{2} \ln |\mathbf{Q}| + f_3(d, n),$$

where $f_3(d, n)$ depends only on d and n.

Given the results above, we complete the computation of entropy $H(\mathbf{A}, \mathbf{V})$ as follows:

$$H(\mathbf{A}, \mathbf{V}) = H(\mathbf{A}|\mathbf{V}) + H(\mathbf{V}) = H(\mathbf{V}) + \int d\mathbf{V} \mathcal{IW}_{\mathbf{V}}(\mathbf{Q}, n) H(\mathbf{A}; \mathbf{V})$$

$$= \int d\mathbf{V} \mathcal{IW}_{\mathbf{V}}(\mathbf{Q}, n) \left(\frac{m}{2} \ln |\mathbf{V}| - \frac{d}{2} \ln |\mathbf{K}| + \frac{dm}{2} \ln(2\pi e) \right) + H(\mathbf{V})$$

$$= -\frac{d}{2} \ln |\mathbf{K}| + \frac{dm}{2} \ln(2\pi e) + \frac{m}{2} [\ln |\mathbf{Q}| + f_2(d, n)] + \frac{d+1}{2} \ln |\mathbf{Q}| + f_3(d, n)$$

$$= -\frac{d}{2} \ln |\mathbf{K}| + (\frac{m+d+1}{2}) \ln |\mathbf{Q}| + f_1(d, n).$$

This is exactly what was claimed in Lemma 42.

Lemmas 41 and 42 lead to the following:

Corrolary 43 *For the entropy of a stochastic variable with posterior distribution $P(\mathbf{A}, \mathbf{V}|\mathbf{x}, \mathbf{y})$ it holds that*

$$H(\mathbf{A}, \mathbf{V}; \mathbf{x}, \mathbf{y}) = -\frac{d}{2} \ln |\mathbf{x}\mathbf{x}^T + \mathbf{K}| + f_1(d, n) + (\frac{m+d+1}{2}) \ln |\mathbf{Q} + (\mathbf{y} - \mathbf{M}\mathbf{x})\gamma(\mathbf{y} - \mathbf{M}\mathbf{x})^T|.$$

We note that the following lemma also holds:

Lemma 44

$$\int \mathcal{T}_{\mathbf{y}}(\mathbf{Q}, n, \boldsymbol{\mu}, \gamma) \ln |\mathbf{Q} + (\mathbf{y} - \boldsymbol{\mu})\gamma(\mathbf{y} - \boldsymbol{\mu})^T| d\mathbf{y}$$

is independent from both $\boldsymbol{\mu}$ and γ,

and thus we can compute the conditional entropy expressed in (8):

Lemma 45

$$H(\mathbf{A}, \mathbf{V}|\mathbf{y}; \mathbf{x}) = \int p(\mathbf{y}|\mathbf{x}) H(\mathbf{A}, \mathbf{V}; \mathbf{x}, \mathbf{y}) d\mathbf{y} = -\frac{d}{2} \ln |\mathbf{x}\mathbf{x}^T + \mathbf{K}| + g_1(\mathbf{Q}, d, n).$$

where $g_1(\mathbf{Q}, d, n)$ depends only on $\mathbf{Q}$, d and n.

Collecting all the terms, we arrive at the following *intriguingly simple* expression

$$\mathbf{u}_{t+1^{opt}} = \arg\min_{\mathbf{u}_{t+1}} \int p\left(\mathbf{y}_{t+1}|\{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^t\right) H(\mathbf{A}, \mathbf{V}|\{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^t, \mathbf{y}_{t+1}) d\mathbf{y}_{t+1}$$

$$= \arg\min_{\mathbf{u}_{t+1}} -\frac{d}{2} \ln |\mathbf{x}_{t+1}\mathbf{x}_{t+1}^T + \mathbf{K}_t| = \arg\max_{\mathbf{u}_{t+1}} \mathbf{x}_{t+1}^T \mathbf{K}_t^{-1} \mathbf{x}_{t+1}, \tag{15}$$

where

$$\mathbf{x}_{t+1} \doteq [\mathbf{r}_{t-I}; \ldots; \mathbf{r}_t; \mathbf{u}_{t-J+1}; \ldots; \mathbf{u}_{t+1}],$$

and we used that $|\mathbf{x}\mathbf{x}^T + \mathbf{K}| = |\mathbf{K}|(1 + \mathbf{x}^T\mathbf{K}^{-1}\mathbf{x})$ according to the Matrix Determinant Lemma [30]. We assume a bounded domain $\mathcal{U}$ for the control, which is necessary to keep the maximization procedure of (15) finite. This is, however, a reasonable condition for all practical applications. So,

$$\mathbf{u}_{t+1^{opt}} = \arg\max_{\mathbf{u}\in\mathcal{U}} \mathbf{x}_{t+1}^T \mathbf{K}_t^{-1} \mathbf{x}_{t+1}, \tag{16}$$

In what follows D-optimal control will be referred to as *'infomax interrogation scheme'*. The steps of our algorithm are summarized in Table 1.

Table 1: Pseudocode of the algorithm

Control Calculation
$\quad \mathbf{u}_{t+1} = \arg\max_{\mathbf{u}\in\mathcal{U}} \hat{\mathbf{x}}_{t+1}^T \mathbf{K}_t^{-1} \hat{\mathbf{x}}_{t+1}$
$\quad$ where $\hat{\mathbf{x}}_{t+1} = [\mathbf{r}_{t-I}; \ldots; \mathbf{r}_t; \mathbf{u}_{t-J+1}; \ldots; \mathbf{u}_t; \mathbf{u}]$
$\quad$ set $\mathbf{x}_{t+1} = [\mathbf{r}_{t-I}; \ldots; \mathbf{r}_t; \mathbf{u}_{t-J+1}; \ldots; \mathbf{u}_t; \mathbf{u}_{t+1}]$
Observation
$\quad$ observe $\mathbf{r}_{t+1}$, and let $\mathbf{y}_{t+1} = g^{-1}(\mathbf{r}_{t+1})$
Bayesian update
$\quad \mathbf{M}_{t+1} = (\mathbf{M}_t\mathbf{K}_t + \mathbf{y}_{t+1}\mathbf{x}_{t+1}^T)(\mathbf{x}_{t+1}\mathbf{x}_{t+1}^T + \mathbf{K}_t)^{-1}$
$\quad \mathbf{K}_{t+1} = \mathbf{x}_{t+1}\mathbf{x}_{t+1}^T + \mathbf{K}_t$
$\quad n_{t+1} = n_t + 1$
$\quad \gamma_{t+1} = 1 - \mathbf{x}_{t+1}^T(\mathbf{x}_{t+1}\mathbf{x}_{t+1}^T + \mathbf{K}_t)^{-1}\mathbf{x}_{t+1}$
$\quad \mathbf{Q}_{t+1} = \mathbf{Q}_t + (\mathbf{y}_{t+1} - \mathbf{M}_t\mathbf{x}_{t+1})\gamma_{t+1}(\mathbf{y}_{t+1} - \mathbf{M}_t\mathbf{x}_{t+1})^T$

Computation of the inverse $(\mathbf{x}_{t+1}\mathbf{x}_{t+1}^T + \mathbf{K}_t)^{-1}$ in Table 1 can be simplified considerably by the following recursion: let $\mathbf{P}_t = \mathbf{K}_t^{-1}$, then according to the Sherman-Morrison formula [31]

$$\mathbf{P}_{t+1} = (\mathbf{x}_{t+1}\mathbf{x}_{t+1}^T + \mathbf{K}_t)^{-1} = \mathbf{P}_t - \frac{\mathbf{P}_t\mathbf{x}_{t+1}\mathbf{x}_{t+1}^T\mathbf{P}_t}{1 + \mathbf{x}_{t+1}^T\mathbf{P}_t\mathbf{x}_{t+1}}, \tag{17}$$

In this expression matrix inversion disappears and instead only a real number is inverted.

5 Estimating the Noise

One might wish to compute the optimal control for estimating noise $\mathbf{e}_t$ in (1), instead of the identification problem above. Based on (1) and because

$$\mathbf{e}_{t+1} = \mathbf{y}_{t+1} - \sum_{i=0}^{I} \mathbf{F}_i \mathbf{r}_{t-i} - \sum_{j=0}^{J} \mathbf{B}_j \mathbf{u}_{t+1-j}, \tag{18}$$

one might think that the best strategy is to use the optimal infomax control of Table 1, since it provides good estimations for parameters $\mathbf{A} = [\mathbf{F}_I, \ldots, \mathbf{F}_0, \mathbf{B}_J, \ldots, \mathbf{B}_0]$ and so for noise $\mathbf{e}_t$.

Another—and different—thought is the following. At time t, let us denote our estimations as $\hat{\mathbf{e}}_t$, $\hat{\mathbf{F}}_i^t$ (i=0,...,I), and $\hat{\mathbf{B}}_j^t$ (j=0,...,J). Using (18), we have that

$$\mathbf{e}_{t+1} - \hat{\mathbf{e}}_{t+1} = \sum_{i=0}^{I} (\mathbf{F}_i - \hat{\mathbf{F}}_i^t) \mathbf{r}_{t-i} + \sum_{j=0}^{J} (\mathbf{B}_j - \hat{\mathbf{B}}_j^t) \mathbf{u}_{t+1-j}. \tag{19}$$

This hints that the control should be $\mathbf{u}_t = \mathbf{0}$ for all times in order to get rid of the error contribution of matrix $\mathbf{B}_j$ in (19).

Straightforward utilization of D-optimality considerations, opposed to the objective of (7), suggests the optimization of the following quantity:

$$\arg\max_{\mathbf{u}_{t+1}} I(\mathbf{e}_{t+1}, \mathbf{y}_{t+1}; \{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^t),$$

That is, for the estimation of the noise we want to design a control signal $\mathbf{u}_{t+1}$ such that the next output is the best from the point of view of greedy optimization of mutual information between the next output $\mathbf{y}_{t+1}$ and the noise $\mathbf{e}_{t+1}$. It is easy to show that this task is equivalent to the following optimization problem:

$$\arg\min_{\mathbf{u}_{t+1}} \int d\mathbf{y}_{t+1} P(\mathbf{y}_{t+1} | \{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^t) H(\mathbf{e}_{t+1}; \{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^{t+1}), \tag{20}$$

where $H(\mathbf{e}_{t+1}; \{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^{t+1}) = H(\mathbf{Ax}_{t+1}; \{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^{t+1})$, because $\mathbf{e}_{t+1} = \mathbf{y}_{t+1} - \mathbf{Ax}_{t+1}$. To compute this quantity we need the following lemma [26]:

Lemma 51 *If* $P(\mathbf{A}) = \mathcal{N}_{\mathbf{A}}(\mathbf{M}, \mathbf{V}, \mathbf{K})$, *then* $P(\mathbf{Ax}) = \mathcal{N}_{\mathbf{Ax}} \left(\mathbf{Mx}, \mathbf{V}, \left(\mathbf{x}^T \mathbf{K}^{-1} \mathbf{x} \right)^{-1} \right)$

Applying this lemma and using (11) one has that

$$P(\mathbf{Ax}_{t+1} | \mathbf{V}, \{\mathbf{x}\}_1^{t+1}, \{\mathbf{y}\}_1^t) = \mathcal{N}_{\mathbf{Ax}_{t+1}} \left(\mathbf{M}_{t+1} \mathbf{x}_{t+1}, \mathbf{V}, \left(\mathbf{x}_{t+1}^T \mathbf{K}_{t+1}^{-1} \mathbf{x}_{t+1} \right)^{-1} \right) \tag{21}$$

We introduce the notations

$$\tilde{K}_{t+1} = \left(\mathbf{x}_{t+1}^T \mathbf{K}_{t+1}^{-1} \mathbf{x}_{t+1} \right)^{-1} \in \mathbb{R}, \tag{22}$$
$$\lambda_{t+1} = 1 + (\mathbf{Ax}_{t+1} - \mathbf{M}_{t+1} \mathbf{x}_{t+1})^T (\tilde{K}_{t+1} \mathbf{Q}_{t+1}^{-1})(\mathbf{Ax}_{t+1} - \mathbf{M}_{t+1} \mathbf{x}_{t+1}) \in \mathbb{R}$$

and use (9) and (12) for the posterior distribution (21). Then we arrive at

$$P(\mathbf{A}\mathbf{x}_{t+1}|\{\mathbf{x}\}_1^{t+1},\{\mathbf{y}\}_1^t) = \mathcal{T}_{\mathbf{A}\mathbf{x}_{t+1}}\left(\mathbf{Q}_{t+1}, n_{t+1}, \mathbf{M}_{t+1}\mathbf{x}_{t+1}, \tilde{K}_{t+1}\right)$$

$$= \pi^{-d/2}|\tilde{K}_{t+1}^{-1}\mathbf{Q}_{t+1}|^{-1/2}\frac{\Gamma(\frac{n_{t+1}+1}{2})}{\Gamma(\frac{n_{t+1}+1-d}{2})}\lambda_{t+1}^{\frac{n_{t+1}+1}{2}}$$

The Shannon-entropy of this distribution according to [32] equals:

$$H(\mathbf{A}\mathbf{x}_{t+1};\{\mathbf{x}\}_1^{t+1},\{\mathbf{y}\}_1^{t+1}) = f_4(d, n_{t+1}) + \frac{d}{2}\log|\tilde{K}_{t+1}^{-1}| + \log|\mathbf{Q}_{t+1}|$$

where

$$f_4(d, n_{t+1}) = -\log\frac{\Gamma(\frac{n_{t+1}+1}{2})}{\pi^{d/2}\Gamma(\frac{n_{t+1}+1-d}{2})} + \frac{n_{t+1}+1}{2}\left(\Psi\left(\frac{n_{t+1}+1}{2}\right) - \Psi\left(\frac{n_{t+1}+1-d}{2}\right)\right).$$

Using the notations introduced in (10) and in (22) the above expressions can be transcribed as follows:

$$H(\mathbf{A}\mathbf{x}_{t+1};\{\mathbf{x}\}_1^{t+1},\{\mathbf{y}\}_1^{t+1}) = f_4(d, n_{t+1}) - \frac{d}{2}\log|\tilde{K}_{t+1}| + \log|\mathbf{Q}_{t+1}|$$

$$= f_4(d, n_{t+1}) + \frac{d}{2}\log|\mathbf{x}_{t+1}^T(\mathbf{K}_t + \mathbf{x}_{t+1}\mathbf{x}_{t+1}^T)^{-1}\mathbf{x}_{t+1}| + \log|\mathbf{Q}_{t+1}|$$

$$= f_4(d, n_{t+1}) + \frac{d}{2}\log|\mathbf{x}_{t+1}^T(\mathbf{K}_t + \mathbf{x}_{t+1}\mathbf{x}_{t+1}^T)^{-1}\mathbf{x}_{t+1}| +$$

$$+ \log|\mathbf{Q}_t + (\mathbf{y}_{t+1} - \mathbf{M}_t\mathbf{x}_{t+1})\gamma_{t+1}(\mathbf{y}_{t+1} - \mathbf{M}_t\mathbf{x}_{t+1})^T|$$

Now, we are in a position to calculate (20) by applying Lemma 44 as before. We get that

$$\int d\mathbf{y}_{t+1}P(\mathbf{y}_{t+1}|\{\mathbf{x}\}_1^{t+1},\{\mathbf{y}\}_1^t)H(\mathbf{e}_{t+1};\{\mathbf{x}\}_1^{t+1},\{\mathbf{y}\}_1^{t+1}) =$$

$$= g_2(\mathbf{Q}_t, d, n_{t+1}) + \frac{d}{2}\log|\mathbf{x}_{t+1}^T(\mathbf{K}_t + \mathbf{x}_{t+1}\mathbf{x}_{t+1}^T)^{-1}\mathbf{x}_{t+1}|,$$

where $g_2(\mathbf{Q}_t, d, n_{t+1})$ depends only on $\mathbf{Q}_t$, d and n_{t+1}. Thus, we have that

$$\arg\max_{\mathbf{u}_{t+1}} I(\mathbf{e}_{t+1}, \mathbf{y}_{t+1};\{\mathbf{x}\}_1^{t+1},\{\mathbf{y}\}_1^t) = \arg\min_{\mathbf{u}_{t+1}} \log|\mathbf{x}_{t+1}^T(\mathbf{K}_t + \mathbf{x}_{t+1}\mathbf{x}_{t+1}^T)^{-1}\mathbf{x}_{t+1}|$$

$$= \arg\min_{\mathbf{u}_{t+1}} \log\left|\mathbf{x}_{t+1}^T\left(\mathbf{K}_t^{-1} - \frac{\mathbf{K}_t^{-1}\mathbf{x}_{t+1}\mathbf{x}_{t+1}^T\mathbf{K}_t^{-1}}{1 + \mathbf{x}_{t+1}^T\mathbf{K}_t^{-1}\mathbf{x}_{t+1}}\right)\mathbf{x}_{t+1}\right|$$

$$= \arg\min_{\mathbf{u}_{t+1}} \log\left|\frac{\mathbf{x}_{t+1}^T\mathbf{K}_t^{-1}\mathbf{x}_{t+1}}{1 + \mathbf{x}_{t+1}^T\mathbf{K}_t^{-1}\mathbf{x}_{t+1}}\right|$$

$$= \arg\min_{\mathbf{u}_{t+1}} \mathbf{x}_{t+1}^T\mathbf{K}_t^{-1}\mathbf{x}_{t+1}$$

In practice, we perform this optimization in an appropriate domain $\mathcal{U}$. Thus, the D-optimal interrogation scheme for noise estimation is as follows

$$\mathbf{u}_{t+1}^{opt} = \arg\min_{\mathbf{u}\in\mathcal{U}} \mathbf{x}_{t+1}^T\mathbf{K}_t^{-1}\mathbf{x}_{t+1}. \tag{23}$$

It is worth noting that this D-optimal cost function for noise estimation and the D-optimal cost function derived for parameter estimation in (15) are not compatible with each other. Estimating one of them quickly will necessarily delay the estimation of the other.

In Section 5.1 we see that for large enough t values, expression (23) gives rise to control values close to $\mathbf{u}_t = \mathbf{0}$.

5.1 Greedy and Non-Greedy Optimization

Greedy optimization of (23) is simple, provided that $\mathbf{K}_t$ is fixed during the optimization of $\mathbf{u}_{t+1}$. If so, then the optimization task is quadratic. To see this, let us partition matrix $\mathbf{K}_t$ as follows:

$$\mathbf{K}_t = \begin{pmatrix} \mathbf{K}_t^{11} & \mathbf{K}_t^{12} \\ \mathbf{K}_t^{21} & \mathbf{K}_t^{22} \end{pmatrix},$$

where $\mathbf{K}_t^{11} \in \mathbb{R}^{d \times d}, \mathbf{K}_t^{21} \in \mathbb{R}^{m-d \times d}$, $\mathbf{K}_t^{22} \in \mathbb{R}^{m-d \times m-d}$. It is easy to see that if domain $\mathcal{U}$ in (23) is large enough then

$$\mathbf{u}_{t+1}^{opt} = (\mathbf{K}_t^{22})^{-1} \mathbf{K}_t^{21} \mathbf{r}_t. \tag{24}$$

However, for non-greedy solutions, expression $\mathbf{K}_t$ in $\mathbf{x}_{t+1}^T \mathbf{K}_t^{-1} \mathbf{x}_{t+1}$ changes, because it may depend on previous control inputs $\mathbf{u}_1, \ldots, \mathbf{u}_t$, the subject of previous optimization steps. The optimal strategy for long-term non-greedy optimization falls outside of the scope of the present work. Here we propose the following heuristics for this problem: Use the strategy of Table 1 for the first τ steps. It increases $|\mathbf{K}_t|$ quickly in (23). Then after τ-steps switch to the control described in (24). This will decrease the cost function (23) further. We will call this non-greedy interrogation heuristics introduced for noise estimation 'τ-infomax noise interrogation'.

It is worth noting that in the τ-infomax noise interrogation, if the τ switching time is large enough then for large t values $|\mathbf{K}_t^{22}|$ will be large, and hence —according to (24)— the optimal $\mathbf{u}_t$ interrogation will be close to $\mathbf{0}$. The approximation of the 'τ-infomax noise interrogation' when we use the interrogation described in Table 1 for τ steps and then switch to zero-interrogation will be called the 'τ-zero interrogation' scheme.

6 Discussion and Conclusions

We have treated the identification problem of recurrent neural networks described by model (1). We applied active learning to solve this task. In particular, the online D-optimality principle was applied and we investigated the learning properties for parameter and noise estimations. We note that the D-optimal interrogation scheme is also called infomax control in the literature [6]. This name originates from the cost function that optimizes the mutual information.

The GLM model used by [6] is as follows:

$$\mathbf{r}_{t+1} = g \left(\sum_{i=0}^{I} \mathbf{F}_i \mathbf{r}_{t-i} + \sum_{j=0}^{J} \mathbf{B}_j \mathbf{u}_{t+1-j} \right) + \mathbf{e}_{t+1}, \tag{25}$$

where $\{\mathbf{e}_t\}$ is i.i.d. noise with $\mathbf{0} \in \mathbb{R}^d$ mean. The authors model spiking neurons and assume that the main source of the noise is this spiking, which appears at the output of the neurons and adds linearly to the neural activity. They investigated the case in which the observed quantity $\mathbf{r}_t$ had a Poisson distribution. Unfortunately, in this model Bayesian equations become intractable and the estimation of the posterior may be spoiled, because the distribution is projected to the family of normal distributions at each instant. A serious problem with this approach is that the extent of the information loss caused by this approximation is not known. Our stochastic RNN model

$$\mathbf{r}_{t+1} = g\left(\sum_{i=0}^{I} \mathbf{F}_i \mathbf{r}_{-i} + \sum_{j=0}^{J} \mathbf{B}_j \mathbf{u}_{t+1-j} + \mathbf{e}_{t+1}\right),$$

differs only slightly from the GLM model of (25), but it has considerable advantages, as we shall discuss below.

Bayesian designs of different kinds were derived for the linear regression problem in [35]:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\theta} + \mathbf{e} \tag{26}$$
$$P(\mathbf{e}) = \mathcal{N}_{\mathbf{e}}(0, \sigma^2 \mathbf{I}). \tag{27}$$

This problem is similar to ours ((3)-(6)), but while the goal of [35] was to find an optimal design for the explanatory variables $\boldsymbol{\theta}$, we were concerned with the parameter ($\mathbf{X}$ in (26)) and the noise ($\mathbf{e}$) estimation task. In Verdinelli's paper inverted gamma prior and vector-valued normal distribution were assumed on the isotropic noise and on the explanatory variables, respectively. By contrast, we were interested in the matrix-valued coefficients and in general, non-isotropic noises. We used matrix-valued normal distribution for the coefficients and inverted Wishart distribution for the covariance matrix as conjugate priors. Due to the inverted Wishart distribution that we used, the covariance matrix of the noise is not restricted to the isotropic form, but can be general in our case.

The Bayesian online learning framework allowed us to derive analytic results for the greedy optimization of the parameters as well as the driving noise. Optimal interrogation strategies (16) and (23) appeared in attractive, intriguingly simple quadratic forms. We have shown that these two tasks are incompatible with each other. Parameter and noise estimations require the maximization and the minimization of expression $\mathbf{x}_{t+1}^T \mathbf{K}_t^{-1} \mathbf{x}_{t+1}$, respectively.

The problem of non-greedy optimization of the full task has been left open. However, we put forth a heuristic solution for the estimation of the driving noise that we called τ-infomax noise interrogation. It uses the D-optimal interrogation of Table 1 up to τ-steps, and applies the noise estimation control of (23) afterwards. This heuristics decreases the estimation error of the coefficients of matrices $\mathbf{F}$ and $\mathbf{B}$ up to time τ and thus — upon turning off the explorative D-optimization — tries to minimize the estimation error of the value of the noise at time $\tau + 1$. We introduced the τ-zero interrogation scheme and showed that it is a good approximation of the τ-infomax noise scheme for large τ values.

Finally, it seems desirable to determine the conditions under which the algorithms derived from the D-optimal (infomax) principle are both consistent and efficient. The tractable form of our approximation-free results is promising in this respect.

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