Westfälische Wilhelms-Universität Münster

REDUCED BAYESIAN INVERSION

Reducing Bayesian Inverse Problems with Balanced Truncation

Applied Mathematics Münster

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Synopsis

Combined reduction enables the concurrent reduction of state and parameter space dimensions, which accelerates the integration. Here the reduction of state space is based upon experimental observations which are balanced against a models output. The parameter space is reduced based on the identifiability inside the model. In a Bayesian inversion setting with undetermined posterior parameter distributions, the estimation duration can be significantly shortened.

Balanced Truncation

Control Systems

As an underlying model to the (Bayesian) inversion, control systems are considered:

$$\dot{x} = f(x, u, \theta)$$
$$y = g(x, u, \theta).$$

First, to introduce balanced truncation the focus is narrowed to linear control systems:

$$\dot{x} = Ax + Bu$$
$$y = Cx.$$

The empirical gramians are based on the same approach, yet allow nonlinear and thus more general control systems.

Controllability + Observability

Controllability quantifies how well a state can be driven by input or control. The controllability gramian W_C characterizes the controllability of a linear system and is computed as the smallest semi-positive definite solution of the Lyapunov equation:

$$AW_C + W_C A^T = -BB^T.$$

Observability quantifies how well a change in state is reflected by the outputs. The observability gramian W_O characterizes the observability of a linear system and is computed as the smallest semi-positive definite solution of the Lyapunov equation:

$$A^T W_O + W_O A = -C^T C.$$

Balanced Truncation

The Hankel operator maps past inputs to future outputs via the impulse response:

$$H(t) = \int_{-\infty}^{0} C e^{A(t-\tau)} B u(\tau) d\tau.$$

The singular values of the Hankel operator σ_i indicate the importance of the associated state to the system dynamics. To determine the least controllable and least observable states, the controllability and observability gramians are balanced by a similarity transformation that balances the systems components (A, B, C). Truncating the balancing transformation U, V with $VW_C V^T = U^T W_O U = \sigma_i$, the reduced linear system is given by (VAU, VB, CU).

Empirical Gramians

Empirical Controllability Gramian

The empirical controllability gramian ([1]) is computed by averaging the outer product of state time-series centered around the steady state $\bar{x}$:

$$W_C = \frac{1}{|Q_u||R_u|} \sum_{h=1}^{|Q_u|} \sum_{i=1}^{|R_u|} \sum_{j=1}^{m} \frac{1}{c_h^2} \int_0^\infty \Psi^{hij}(t) dt$$
$$\Psi^{hij}(t) = (x^{hij}(t) - \bar{x})(x^{hij}(t) - \bar{x})^* \in \mathbb{R}^{n \times n}.$$

x^{hij} is a state time-series generated using the perturbed input $u^{hij}(t) = c_h S_i e_j u(t) + \bar{u}$ based on the perturbation sets:

$$E_u = \{e_i \in \mathbb{R}^j; \|e_i\| = 1; e_i e_{j \neq i} = 0; i = 1, \dots, m\}$$
$$R_u = \{S_i \in \mathbb{R}^{j \times j}; S_i^* S_i = \mathbb{1}; i = 1, \dots, s\}$$
$$Q_u = \{c_i \in \mathbb{R}; c_i > 0; i = 1, \dots, q\}.$$

For linear systems the empirical controllability gramian equals the classic controllability gramian, but since being based on snapshots extends also to nonlinear systems!

Empirical Observability Gramian

The empirical observability gramian ([1]) is computed by averaging the inner product of output time-series centered around the steady state output $\bar{y}$:

$$W_O = \frac{1}{|Q_x||R_x|} \sum_{k=1}^{|Q_x|} \sum_{l=1}^{|R_x|} \frac{1}{d_k^2} T_l \int_0^\infty \Psi^{kl}(t) dt \; T_l^*$$
$$\Psi^{kl}_{ab} = (y^{kla}(t) - \bar{y})^* (y^{klb}(t) - \bar{y}) \in \mathbb{R}.$$

y^{kla} is an output time-series generated using the perturbed initial state $x_0^{kla} = d_k S_l f_a + \bar{x}$ based on the perturbation sets:

$$E_x = \{f_i \in \mathbb{R}^n; \|f_i\| = 1; f_i f_{j \neq i} = 0; i = 1, \dots, n\}$$
$$R_x = \{T_i \in \mathbb{R}^{n \times n}; T_i^* T_i = \mathbb{1}; i = 1, \dots, t\}$$
$$Q_x = \{d_i \in \mathbb{R}; d_i > 0; i = 1, \dots, r\}.$$

For linear systems the empirical observability gramian equals the classic observability gramian, but since being based on snapshots extends also to nonlinear systems!

Empirical Identifiability Gramian

A system can be augmented by a constant state for each parameter with the parameter value as initial state:

$$\dot{x}_a = \begin{pmatrix} \dot{x} \\ \dot{\theta} \end{pmatrix} = \begin{pmatrix} f(x, u, \theta) \\ 0 \end{pmatrix}$$
$$x_a(0) = \begin{pmatrix} x_0 \\ \theta \end{pmatrix}.$$

Then the empirical identifiability gramian ([2]) is given as the empirical observability gramian of this augmented system:

$$W_{O,a} = \begin{pmatrix} W_O & W_M \\ W_M^* & W_P \end{pmatrix}.$$

The lower right block with size according to the parameter space dimension comprises the observability of the parameters:

$$W_I = W_P - W_M^* W_O^{-1} W_M \approx W_P.$$

Parameters can then be reduced by truncation based on the singular values of W_I.

Reduced Inversion

Prediction + Experimental Observability

Introduced by [3], the Inference for Prediction approach extends the concept of balanced truncation of controllability gramian and observability gramian to balancing experimentally observed data and model simulations. Experiment Observability $W_{O,E}$ is computed as the empirical observability gramian based on the experimentally observed output. Prediction Observability $W_{O,P}$ is computed as the empirical observability gramian based on simulations of the underlying model.

Combined Reduction

For a combined reduction of state and parameter spaces, first, the parameter space is reduced via a projection based on the singular values of the identifiability gramian W_I of an augmented prediction observability gramian $W_{O,P,a}$. Then, the state space dimension is reduced using balanced truncation. As opposed to regular balanced truncation of controllability and observability gramian $\sigma_i = \sqrt{\lambda(W_C W_O)}$, here the prediction and experiment observability gramian $\xi_i = \sqrt{\lambda(W_{O,E} W_{O,P})}$ are balanced and truncated.

Data-Driven Reduction

Since the empirical gramians are solely based on evaluating time-series not only synthetic simulations, but also experimental data can be used to assemble these gramian matrices. Usually only the systems output is accessible to measurement, thus only the observability gramian is employed. If the system is symmetric controllability information can be corporated too. The prediction observability evaluates simulations of the model, thus also the empirical cross gramian and empirical joint gramian, see [4], apply.

Experiments

Application

For reconstruction of connectivity between brain regions of which the individual regions activity level is measured using EEG the DCM-EEG model ([5]) is available:

$$\ddot{x} = \hat{A}x + A_\theta \tanh K_\theta x + Bu$$
$$y = Cx.$$

The parametrized Hyperbolic Network Model with parametrized system matrix is a simplified version, chosen here as underlying model:

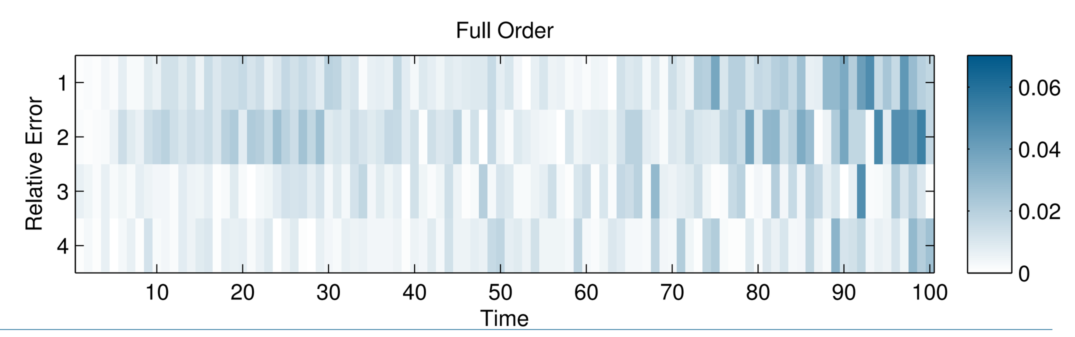
$$\dot{x} = A_\theta \tanh x + Bu$$
$$y = Cx.$$

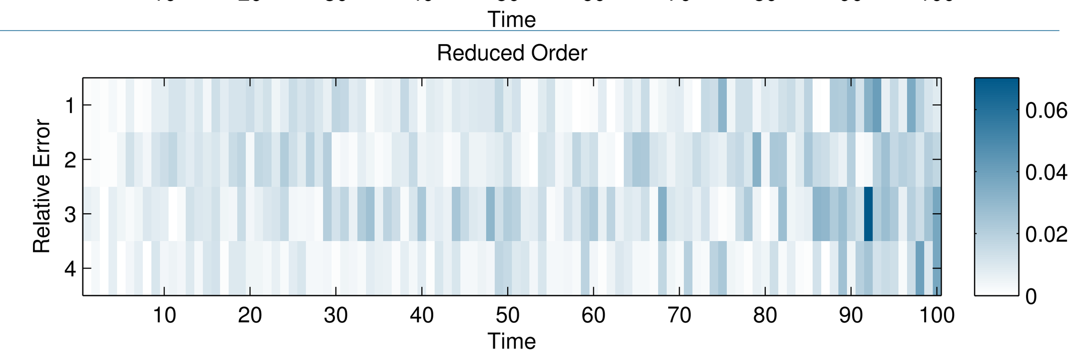
Synthetic Experimental Data

For randomly generated parameters a model simulation is generated for impulsive input to which Gaussian noise is added to provide the experimentally observed data. The systems dimensions are set to 4 inputs and outputs, 16 states and thus 256 parameters. The (Bayesian) inversion is performed assuming a stable system matrix A and flat priors. Averaged over 10 random systems, the results are:

	Offline Time	Online Time	Relative Error
Full Order	$0s$	$18.7s$	0.0148
Reduced Order	$21.9s$	$4.8s$	0.0146

Error in Full and Reduced Simulations





Read Me

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[2] D. Geffen et al. Observability Based Parameter Identifiability for Biochemical Reaction Networks. *Proceedings of the ACC*:2130–2135 (2008).
[3] C. Lieberman and K. Willcox. Goal-Oriented Inference: Approach, Linear Theory, and Application to Advection Diffusion. *SIAM Journal on Scientific Computing* 34.4(2012):A1880–A1904,
[4] C. Himpe and M. Ohlberger. Cross-Gramian Based Combined State and Parameter Reduction. *Preprint*, arXiv:1302.0634 (2013).
[5] R.J. Moran et al. Dynamic causal models of steady-state responses. *NeuroImage*, 44:796-811 (2009).

- Source code available at: http://j.mp/acces13 under open source license and compatible with MATLAB and OCTAVE