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Empirical Gramians 4 MOR

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Motivation

Research Question from Systems Neuroscience:

- How are various regions of the brain connected?
- Are there universal network (sub-)structures?

Mathematical Setting:

- Inverse Problem
- Parametric Input-Output System
- Nonlinear Dynamics

Rough Outline

Numerical Challenges:

- Large-Scale Models
- Multi-Many-Query Setting
- High-Dimensional Parameter-Spaces

Approach:

- System-Theoretic Ansatz
- "Data-Driven"
- Combined State and Parameter Reduction
- Reduce First, Infer Later

Contents

Model + Reduction

Full Order Model (FOM):

$$\dot{x}(t) = f(x(t), u(t))$$
$$y(t) = g(x(t), u(t))$$
$$x(0) = x_0$$

- $M := \dim(u(t))$
- $N := \dim(x(t)) \gg 1$
- $O := \dim(y(t))$
- $f : \mathbb{R}^N \times \mathbb{R}^M \to \mathbb{R}^N$
- $g : \mathbb{R}^N \times \mathbb{R}^M \to \mathbb{R}^O$

Reduced Order Model (ROM):

$$\dot{x}_r(t) = f_r(x_r(t), u(t))$$
$$y_r(t) = g_r(x_r(t), u(t))$$
$$x_r(0) = x_{r,0}$$

- $n := \dim(x_r(t)) \ll N$
- $\dim(y_r(t)) = O$
- $\|y - y_r\| \ll 1$
- $f : \mathbb{R}^n \times \mathbb{R}^M \to \mathbb{R}^n$
- $g : \mathbb{R}^n \times \mathbb{R}^M \to \mathbb{R}^O$

Model Order Reduction

Actual Input-Output Mapping:

$$u \mapsto x \mapsto y$$

Relevant Input-Output Mapping:

$$u \mapsto y$$

Reduction Rationale:

- $\dim(x(t)) \gg 1$
- $\dim(u(t)) \ll \dim(x(t))$
- $\dim(y(t)) \ll \dim(x(t))$

ROM Construction

Generic ROM:

$$\dot{x}_r(t) = f_r(x_r(t), u(t))$$
$$y_r(t) = g_r(x_r(t), u(t))$$
$$x_r(0) = x_{r,0}$$

Projection-Based ROM:

$$\dot{x}_r(t) = Vf(Ux(t), u(t))$$
$$y_r(t) = g(Ux(t), u(t))$$
$$x_r(0) = Vx_0$$

- $U \in \mathbb{R}^{N \times n}$
- $V \in \mathbb{R}^{n \times N}$
- $VU = \mathbb{1}$ (Petrov-Galerkin)
- $VU = \mathbb{1}, V = U^T$ (Galerkin)

System Gramians

1. Controllability Gramian
2. Observability Gramian
3. Cross Gramian

Linear System Theory

Linear State-Space System:

$$\dot{x}(t) = Ax(t) + Bu(t)$$
$$y(t) = Cx(t)$$
$$x(0) = x_0$$

- $A \in \mathbb{R}^{N \times N}$
- $B \in \mathbb{R}^{N \times M}$
- $C \in \mathbb{R}^{O \times N}$

Controllability + Observability

Solution Operator:

$$S(u)(t) = \int_0^t C\,\mathrm{e}^{A\tau}\,Bu(\tau)\mathrm{d}\tau = y(t)$$

Hankel Operator:

$$H(u)(t) = \int_0^t C\,\mathrm{e}^{A\tau}\,Bu(-\tau)\mathrm{d}\tau$$

Finite Rank because of Rank Nullity [Francis'87]:

$$H = \mathcal{O} \circ \mathcal{C}$$

Controllability Gramian

Controllability:

How well can the states be driven by input.

Controllability Operator:

$$\mathcal{C}(u) = \int_{-\infty}^{0} \mathrm{e}^{-At} Bu(t)\mathrm{d}t$$

Controllability Gramian:

$$W_C := \mathcal{C}\mathcal{C}^*$$

Observability Gramian

Observability:

How well changes in the state are reflected by the output.

Observability Operator:

$$\mathcal{O}(x_0)(t) = C\,\mathrm{e}^{At}\,x_0$$

Observability Gramian:

$$W_O := \mathcal{O}^*\mathcal{O}$$

Balancing + Truncation

Hankel Singular Values [Hladnik & Omladic'88]:

$$\lambda(H^* H) = \lambda(\mathcal{C}^* \mathcal{O}^* \mathcal{O} \mathcal{C}) = \lambda(\mathcal{C} \mathcal{C}^* \mathcal{O}^* \mathcal{O})$$

Balancing Transformation:

$$W_C W_O \stackrel{SVD}{=} UDV \rightarrow \begin{pmatrix} U_1 & U_2 \end{pmatrix}, \begin{pmatrix} V_1 \\ V_2 \end{pmatrix}$$

Practically (i.e.: [Benner et al.'10]):

- Compute Low-Rank Factors
- of Lyapunov Equation Solutions

Cross Gramian [Fernando & Nicholson'83]

Defined for Square Systems:

$$W_X := \mathcal{C}\mathcal{O}$$

For Symmetric Systems holds:

$$\begin{aligned} H &= H^* \\ \Rightarrow \mathcal{O}\mathcal{C} &= (\mathcal{O}\mathcal{C})^* \\ \Rightarrow \mathcal{C}\mathcal{C}^*\mathcal{O}^*\mathcal{O} &= \mathcal{C}(\mathcal{O}\mathcal{C})^*\mathcal{O} \\ &= \mathcal{C}(\mathcal{O}\mathcal{C})\mathcal{O} \\ &= (\mathcal{C}\mathcal{O})(\mathcal{C}\mathcal{O}) \end{aligned}$$

Approximate Balancing + Direct Truncation

For symmetric systems:

$$W_X^2 = W_C W_O$$
$$\Rightarrow |\lambda(W_X)| = \sqrt{\lambda(W_C W_O)}$$

Direct Truncation:

$$W_X \overset{SVD}{=} UDV \to \begin{pmatrix} U_1 & U_2 \end{pmatrix} \to V_1 = U_1^T$$

Stability Preserving [Rowley et al.'04]:

$$\begin{aligned} W_X W_X^T &= \mathcal{C}\mathcal{O}(\mathcal{O}\mathcal{C})^* \\ &= \mathcal{C}\mathcal{O}\mathcal{O}^*\mathcal{C}^* \\ &= \mathcal{C}(\mathcal{O}\mathcal{O}^*)\mathcal{C}^* \end{aligned}$$

Non-Symmetric Cross Gramian [H. & Ohlberger'15 (Submitted)]

Breadcrumbs:

- A SISO System is always symmetric
- Utilize Decentralized Control [Moaveni & Khaki Sedigh'06]
- Reduce "Average" SISO System

Average Cross Gramian for Non-Square / Non-Symmetric Systems:

$$W_Z := \int_0^\infty e^{At} \sum_{m=1}^{M} B_{*,m} \sum_{o=1}^{O} C_{o,*} e^{At} \,\mathrm{d}t$$

Data-Driven Gramian-Based Reduced Order Modelling

Shopping List:

- "Few" Solutions affordable, Many Solutions needed
- "Good" Time-Domain Approximation
- Known Operating Region
- Nonlinear Systems (!)

Original Gramian Computation [Moore'81]

Controllability Gramian:

$$X(t) = \begin{pmatrix} x_1(t) & x_2(t) & \dots & x_M(t) \end{pmatrix}$$
$$W_C = \int_0^\infty X(t)X^T(t)\mathrm{d}t$$

Observability Gramian:

$$Y(t) = \begin{pmatrix} y_1(t) & y_2(t) & \dots & y_N(t) \end{pmatrix}$$
$$W_O = \int_0^\infty Y^T(t)Y(t)\mathrm{d}t$$

Empirical Gramians [Lall et al.'99]

System Gramians:

$$W_C = \int_0^\infty (e^{At} B)(e^{At} B)^T \mathrm{d}t,$$
$$W_O = \int_0^\infty (C e^{At})^T (C e^{At}) \mathrm{d}t,$$
$$W_X = \int_0^\infty (e^{At} B)(C e^{At}) \mathrm{d}t.$$

- Formalizes Operating Region.
- Systematic simulations
- with perturbed impulse responses
- and perturbed initial values.
- Equality of Empirical and "Classic" System Gramians.

Empirical Controllability Gramian [Lall et al.'99]

$$W_C = \sum_{q \in Q_U} \int_0^\infty X^q(t) \otimes X^q(t) \mathrm{d}t$$

- $\otimes$ symbolizes the dyadic product
- Q_U is the set of impulse perturbations

Empirical Observability Gramian [Lall et al.'99]

$$W_{O,ij} = \sum_{q \in Q_X} \int_0^\infty \langle Y^{q,i}(t), Y^{q,j}(t) \rangle \mathrm{d}t$$

- $\langle \cdot, \cdot \rangle$ symbolizes the standard inner product
- Q_X is the set of initial state perturbations

Empirical Linear Cross Gramian [Baur et al.'15 (Submitted)]

$$W_Y = \sum_{q \in Q_U} \int_0^\infty X^q(t) \otimes Z^q(t) \mathrm{d}t$$

- $\otimes$ symbolizes the dyadic product
- Z is an adjoint system's state trajectory

Empirical Cross Gramian [H. & Ohlberger'14]

$$W_{X,ij} = \sum_{q \in Q_U \times Q_X} \sum_{k=1}^{J=O} \int_0^\infty \langle X_i^{q,k}(t), Y_k^{q,j}(t) \rangle \mathrm{d}t$$

- $\langle \cdot, \cdot \rangle$ symbolizes the standard inner product
- Adjoint free nonlinear empirical cross gramian

Parametric Model Order Reduction

Parametric FOM:

$$\dot{x}(t) = f(x(t), u(t), \theta)$$
$$y(t) = g(x(t), u(t), \theta)$$
$$x(0) = x_0$$

- $P := \dim(\theta)$
- $f : \mathbb{R}^N \times \mathbb{R}^M \times \mathbb{R}^P \to \mathbb{R}^N$
- $g : \mathbb{R}^N \times \mathbb{R}^M \times \mathbb{R}^P \to \mathbb{R}^O$

Parametric ROM:

$$\dot{x}_r(t) = f_r(x_r(t), u(t), \theta)$$
$$y_r(t) = g_r(x_r(t), u(t), \theta)$$
$$x_r(0) = x_{r,0}$$

- $\|y(\theta) - y_r(\theta)\| \ll 1$
- $f : \mathbb{R}^n \times \mathbb{R}^M \times \mathbb{R}^P \to \mathbb{R}^n$
- $g : \mathbb{R}^n \times \mathbb{R}^M \times \mathbb{R}^P \to \mathbb{R}^O$

Parameter Aware State Reduction [Sun & Hahn'06]

The Empirical Gramian Way:

$$\overline{W}_X = \sum_{\theta_h \in \Theta_h} W_X(\theta_h)$$

Mathematical Justification:

- Interpret parameters as constant inputs.
- A natural extension for the empirical controllability gramian,
- for linear systems with linear parametrization.

Combined State and Parameter Reduction

Parameter Reduction:

$$\dot{x}(t) = f(x(t), u(t), \theta_r)$$
$$y(t) = g(x(t), u(t), \theta_r)$$
$$x(0) = x_0$$

Combined Reduction:

$$\dot{x}_r(t) = f_r(x_r(t), u(t), \theta_r)$$
$$y_r(t) = g_r(x_r(t), u(t), \theta_r)$$
$$x_r(0) = x_{r,0}$$

- $P := \dim(\theta) \gg 1$
- $p := \dim(\theta_r) \ll P$
- $\|y(\theta) - y(\theta_r)\| \ll 1$
- $f : \mathbb{R}^N \times \mathbb{R}^M \times \mathbb{R}^p \to \mathbb{R}^N$
- $g : \mathbb{R}^N \times \mathbb{R}^M \times \mathbb{R}^p \to \mathbb{R}^O$

- $\|y(\theta) - y_r(\theta_r)\| \ll 1$
- $f : \mathbb{R}^n \times \mathbb{R}^M \times \mathbb{R}^p \to \mathbb{R}^n$
- $g : \mathbb{R}^n \times \mathbb{R}^M \times \mathbb{R}^p \to \mathbb{R}^O$

(Empirical) Joint Gramian [H. & Ohlberger'14]

Augmented System:

$$\begin{pmatrix} \dot{x}(t) \\ \dot{\theta}(t) \end{pmatrix} = \begin{pmatrix} f(x(t), u(t), \theta) \\ 0 \end{pmatrix}$$

$$y(t) = g(x(t), u(t), \theta)$$

$$\begin{pmatrix} x(0) \\ \theta(0) \end{pmatrix} = \begin{pmatrix} x_0 \\ \theta \end{pmatrix}$$

Cross Gramian of Augmented System (Joint Gramian):

$$W_J = \begin{pmatrix} W_X & W_M \\ W_m & W_\theta \end{pmatrix}$$

Uncontrollable Parameters:

$$W_m = 0$$

$$W_\theta = 0$$

(Empirical) Cross-Identifiability Gramian [H. & Ohlberger'14]

Schur-Complement of W_θ (Cross-Identifiability Gramian):

$$W_{\ddot{I}} = 0 - \frac{1}{2} W_M^T (W_X + W_X^T)^{-1} W_M$$

$W_{\ddot{I}}$ encodes the "observability" of parameters.

Parameter Projection as Principal Components:

$$W_{\ddot{I}} \overset{SVD}{=} \Pi \Delta \Lambda \rightarrow \Pi = \begin{pmatrix} \Pi_1 & \Pi_2 \end{pmatrix}$$

Cross-Gramian-Based Combined State and Parameter Reduction

State-space projection:

$$W_X \overset{TSVD}{=} U_1 D_1 V_1$$

Parameter-space projection:

$$W_{\ddot{I}} \overset{TSVD}{=} \Pi_1 \Delta_1 \Lambda_1$$

Combined state and parameter ROM:

$$\begin{aligned} \dot{x}_r(t) &= U_1^T f(U_1 x_r(t), u(t), \Pi_1 \theta_r), \\ y_r(t) &= g(U_1 x_r(t), u(t), \Pi_1 \theta_r), \\ x_r(0) &= U_1^T x_0, \\ \theta_r &= \Pi_1^T \theta \end{aligned}$$

Numerical Experiments

1. Benchmark model
2. Test System

- Combined State and Parameter Reduction
- Joint L_2 State and Parameter Norm
- Nonlinear Parametric Systems
- Netbook computable

emgr - Empirical Gramian Framework (Version: 3.6, 10/2015)

Empirical Gramians:

- Empirical Controllability Gramian
- Empirical Observability Gramian
- Empirical Linear Cross Gramian
- Empirical Cross Gramian
- Empirical Sensitivity Gramian
- Empirical Identifiability Gramian
- Empirical Joint Gramians

Features:

- Custom Solver Interface
- Non-Symmetric Cross Gramian
- Compatible with OCTAVE and MATLAB
- Vectorized and Parallelizable
- Open Source License (BSD 2-Clause)

More info at: `http://gramian.de`

Benchmark Model

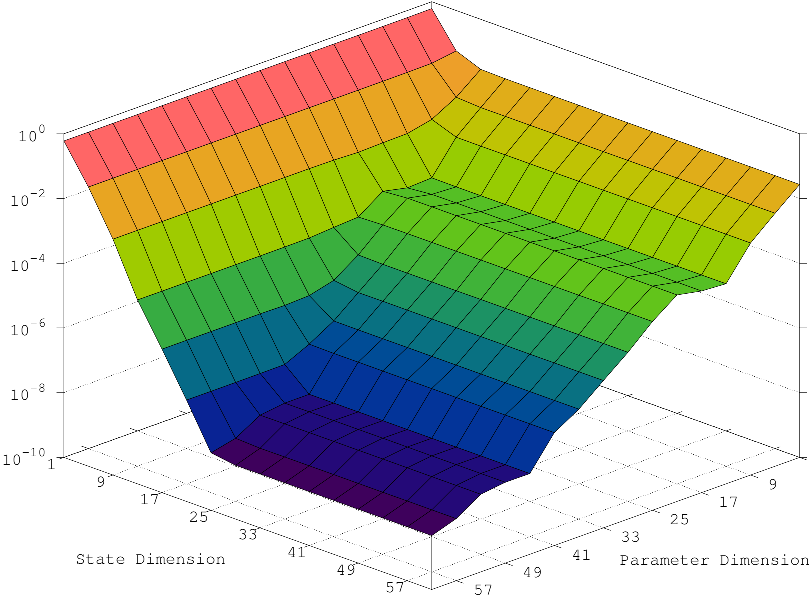
Nonlinear RC Ladder[1]:

$$\dot{x}(t) = \nabla(\nabla g_\theta(x(t))) + Bu(t)$$
$$y(t) = x_1(t)$$

- SISO system
- $g_\theta(x) = (\exp(40x) - 1) + \theta x$
- $N = 64$
- $P = 64$

[1] Listed in the MORwiki: `modelreduction.org/index.php/Nonlinear_RC_Ladder`

Relative $L_2 \otimes L_2$ Output Error



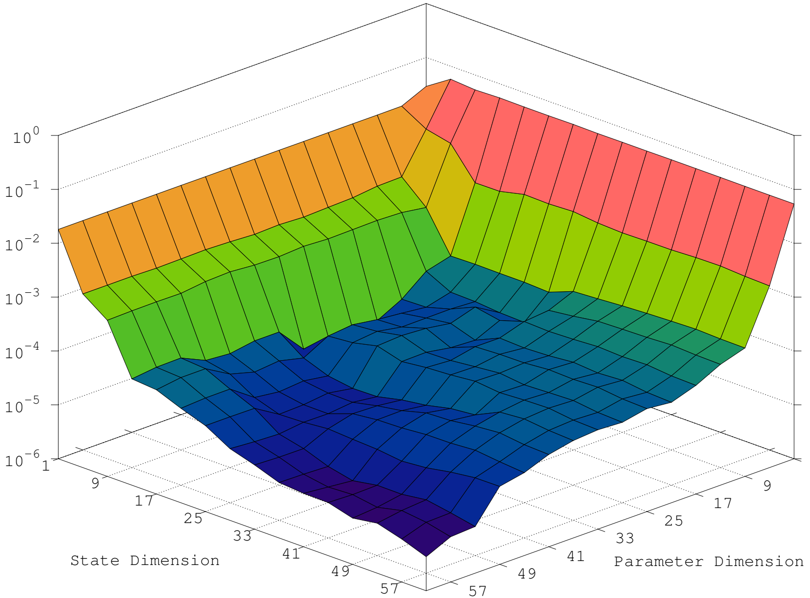
Test Model

Hyperbolic Network Model:

$$\dot{x}(t) = A\tanh(K(\theta)x(t)) + Bu(t)$$
$$y(t) = Cx(t)$$

- SISO System
- $K_{ij} = \theta_i \delta_{ij}$
- $N = 64$
- $P = 64$

Relative $L_2 \otimes L_2$ Output Error



Outlook

Communication Avoiding Parallelization

tl;dl

- Cross-gramian-based model reduction,
- for parametrized nonlinear systems,
- using the empirical cross gramian.

`http://gramian.de`

Thanks!

Get the Companion Code: `http://j.mp/mor4mems15`

MORwiki

Contents:

- Methods
- Benchmarks
- Software
- Events
- References

modelreduction.org