Westfälische Wilhelms-Universität Münster

Applied Mathematics Münster

Efficient Cross-Gramian-Based State and Parameter Reduction

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Application

We do:

- Model Order Reduction
- Parameter Identification / Sensitivity Analysis
- **Combined Reduction**

for:

- Brain Connectivity Models
- Network Models
- (Discretized) Partial Differential Equations

Control Systems

Linear Control System:

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

- Input / Control: $u \in \mathbb{R}^M$
- State: $x \in \mathbb{R}^N$
- Output: $y \in \mathbb{R}^O$
- System Matrix: $A \in \mathbb{R}^{N \times N}$
- Input Matrix: $B \in \mathbb{R}^{N \times M}$
- Output Matrix: $C \in \mathbb{R}^{O \times N}$

Model Order Reduction

Original System:

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

Have:

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

Reduced Order System:

$$\dot{\tilde{x}} = \tilde{A}\tilde{x} + \tilde{B}u$$
$$\tilde{y} = \tilde{C}\tilde{x}$$
$$\tilde{x}(0) = \tilde{x}_0$$

Want:

- $\dim(\tilde{x}) \ll \dim(x)$
- $\|y - \tilde{y}\| \ll 1$

Controllability & Observability [Moore'81]

Controllability:

Controllability Operator:

$$\mathcal{C}(u) := \int_0^\infty e^{At} B u(t) \mathrm{d}t$$

Controllability Gramian:

$$W_C := \mathcal{C}\mathcal{C}^* = \int_0^\infty e^{At} B B^T e^{A^T t} \mathrm{d}t \Leftrightarrow A W_C + W_C A^T = -B B^T$$

Observability:

Observability Operator:

$$\mathcal{O}(x_0) := C e^{At} x_0$$

Observability Gramian:

$$W_O := \mathcal{O}^*\mathcal{O} = \int_0^\infty e^{A^T t} C^T C e^{At} \mathrm{d}t \Leftrightarrow A^T W_O + W_O A = -C^T C$$

$\rightarrow$ Balanced Truncation

Cross Gramian [Fernando & Nicholson'83]

Cross Gramian:

$$W_X := \mathcal{C}\mathcal{O} = \int_0^\infty e^{At} B C e^{At} \mathrm{d}t \Leftrightarrow AX + XA = -BC$$

$$\rightarrow \text{Approximate Balancing}$$

- System must be square:

$$\dim(B) = \dim(C^T).$$

- If system is symmetric, thus

$$Ce^A B = (Ce^A B)^T,$$

- Abs of the eigenvalues of W_X equal the Hankel singular values,

$$W_X^2 = W_C W_O.$$

- SISO systems are always symmetric:

$$Ce^A B \in \mathbb{R}\,.$$

Controllability-Based Cross Gramian [Fernando & Nicholson'85]

Controllability Gramian:

$$W_C := \mathcal{C}\mathcal{C}^* = \int_0^\infty e^{At} B B^T e^{A^T t} \mathrm{d}t$$

Adjoint Augmented System:

$$\begin{pmatrix} \dot{x} \\ \dot{x}^* \end{pmatrix} = \begin{pmatrix} A & 0 \\ 0 & A^T \end{pmatrix} \begin{pmatrix} x \\ x^* \end{pmatrix} + \begin{pmatrix} B \\ C^T \end{pmatrix} u'$$

Controllability Gramian of Adjoint Augmented System:

$$W_C^+ = \begin{pmatrix} W_C & W_X \\ W_X^T & W_O \end{pmatrix}$$

Cross-Gramian-Based State Reduction

Cross Gramian:

$$W_X := \int_0^\infty e^{At} B C e^{At} \mathrm{d}t$$

Direct Truncation:

$$W_X \overset{SVD}{=} UDV^T$$

$$\sigma_1 > \sigma_2 > \ldots > \sigma_k \gg \sigma_{k+1} > \ldots > \sigma_N$$

$$\rightarrow U = \begin{pmatrix} U_1 & U_2 \end{pmatrix}$$

(State-)Reduced System:

$$\tilde{A} = U_1^T A U_1$$

$$\tilde{B} = U_1^T B$$

$$\tilde{C} = C U_1$$

$$\tilde{x}_0 = U_1^T x_0$$

Empirical Gramians [Lall'99]

System Gramians:

$$W_C = \int_0^\infty e^{At}B(e^{At}B)^T \mathrm{d}t$$

$$W_O = \int_0^\infty e^{A^T t}C^T(e^{A^T t}C^T)^T \mathrm{d}t$$

Empirical Gramians:

$$\hat{W}_C = \int_0^\infty x(t)x(t)^T \mathrm{d}t$$

$$\hat{W}_O = \int_0^\infty x^*(t)x^*(t)^T \mathrm{d}t$$

Note:

- Empirical computations (of impulse responses).
- Equal to classic gramians for linear systems.
- Extend to nonlinear systems.

Empirical Cross Gramian

Cross Gramian:

$$\begin{aligned} W_X &:= \int_0^\infty e^{At} B C e^{At} \mathrm{d}t \\ &= \int_0^\infty e^{At} B (e^{A^T t} C^T)^T \mathrm{d}t \end{aligned}$$

Empirical Cross Gramian:

$$W_Y = \int_0^\infty x(t) x^*(t)^T \mathrm{d}t$$

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

Analytic Cross Gramian

$$W_X = \int_0^\infty e^{At} B C e^{At} \mathrm{d}t$$

(Linear) Empirical Cross Gramian

$$W_Y = \int_0^T x(t) x^*(t)^T \mathrm{d}t$$

(Nonlinear) Empirical Cross Gramian

$$W_X' = \frac{1}{|Q_u||R_u| m |Q_x||R_x|} \sum_{h=1}^{|Q_{\boldsymbol{u}}|} \sum_{i=1}^{|R_{\boldsymbol{u}}|} \sum_{j=1}^{m} \sum_{k=1}^{|Q_{\boldsymbol{x}}|} \sum_{l=1}^{|R_{\boldsymbol{x}}|} \frac{1}{c_h d_k} \int_0^\infty T_l \Psi^{hijkl}(t) T_l^T \mathrm{d}t,$$

$$\Psi_{ab}^{hijkl}(t) = f_b^T T_k^T (x^{hij}(t) - \bar{x}) e_i^T S_h^T (y^{kla}(t) - \bar{y})$$

For linear systems: $W_X = W_Y = W_X'$

Balanced Gains [Kabamba'85],[Davidson'86]

Impulse Response Norm:

$$\begin{aligned}
\|y\|_2^2 &= \int_0^\infty y(t)y(t)^T \mathrm{d}t \\
&= \int_0^\infty Ce^{At}B(Ce^{At}B)^T \mathrm{d}t = \int_0^\infty Ce^{At}BB^T e^{A^T t}C^T \mathrm{d}t \\
&= \mathrm{tr}(CW_C C^T) = \mathrm{tr}(B^T W_O B) \overset{\text{SISO only!}}{=} \mathrm{tr}(CW_X B)
\end{aligned}$$

Balanced Gains:

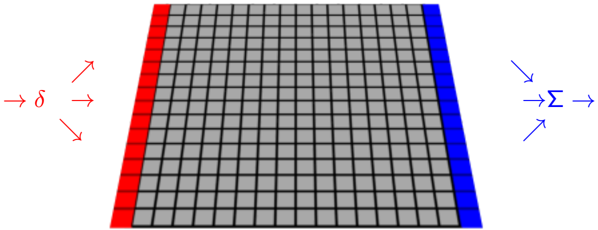
$$\begin{aligned}
\mathrm{tr}(CW_X B) \overset{SVD}{=} \mathrm{tr}(C\,(UDV)\,B) &\overset{Bal.}{\approx} \mathrm{tr}((CU)\,D\,(U^T B)) = \mathrm{tr}(\tilde{C}D\tilde{B}) \\
&= \sum_i |\tilde{c}_i \tilde{b}_i| \sigma_i = \sum_i d_i, \quad \text{Resort}^1 \text{ based on } d_i.
\end{aligned}$$

[1] with Quicksort this is only of complexity $\mathcal{O}(n \log n)$.

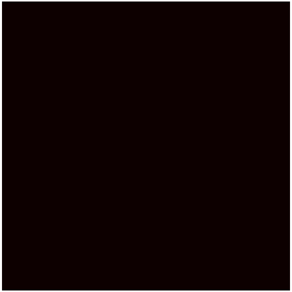
Numerical Experiment

Model:

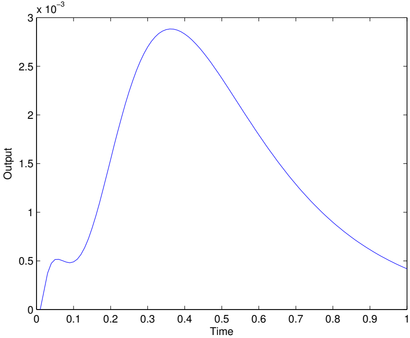
- 2-D Heat Equation
- Unit-Square Domain
- Finite Difference Discretization
- Impulse Input
- Left-Side: Inflow / Input
- Right-Side: Outflow / Output
- Varying diffusion coefficients in every node



State + Output



State over Time



emgr - Empirical Gramian Framework

Gramians:

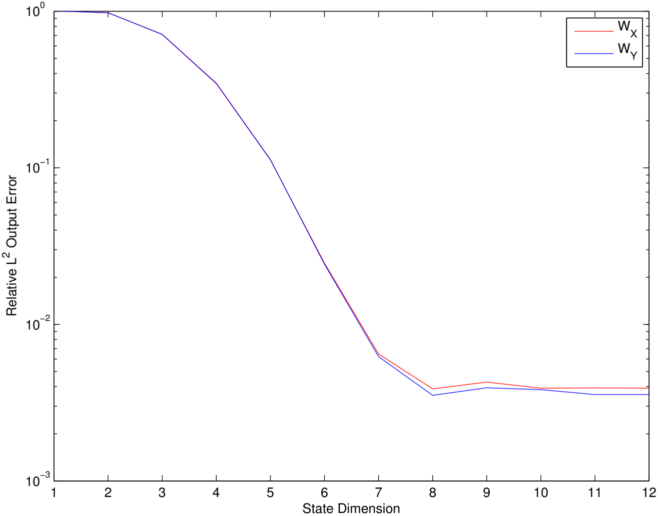
- Empirical Controllability Gramian
- Empirical Observability Gramian
- Empirical Cross Gramian
- Empirical Linear Cross Gramian
- Empirical Sensitivity Gramian
- Empirical Identifiability Gramian
- Empirical Joint Gramian

Features:

- Uniform Interface
- Compatible with MATLAB & OCTAVE (& FREEMAT)
- Vectorized & Parallelizable
- Open-Source licensed

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

Numerical Results (Cross Gramians)

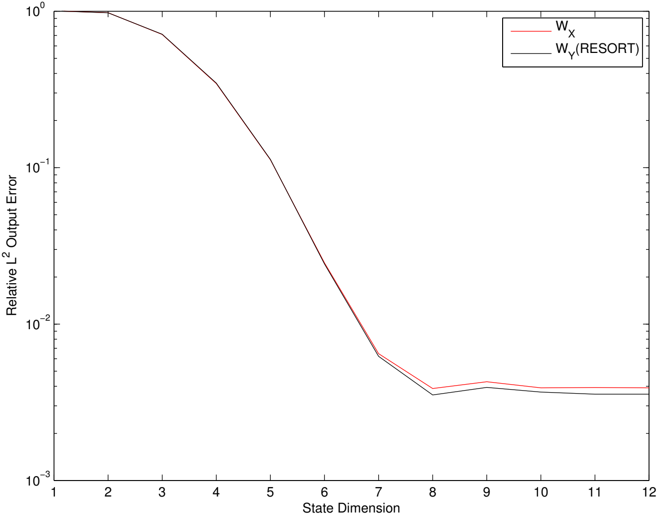


Offline Time [s]:

W_X : 23.9

W_Y : 0.5

Numerical Results (Resorting)



Offline Time [s]:

W_X : 23.9

W_Y^{Resort} : 0.6

Control Systems (Revisited)

Parametrized Linear Control System:

$$\begin{aligned}\dot{x} &= A(\theta)x + Bu \\ y &= Cx \\ x(0) &= x_0\end{aligned}$$

- Input: $u \in \mathbb{R}^M$
- State: $x \in \mathbb{R}^N$
- Output: $y \in \mathbb{R}^O$
- Parameters $\theta \in \mathbb{R}^P$
- System Matrix: $A(\theta) \in \mathbb{R}^{N \times N}$
- Input Matrix: $B \in \mathbb{R}^{N \times M}$
- Output Matrix: $C \in \mathbb{R}^{O \times N}$

Model Order Reduction (Revisited)

Original System:

$$\dot{x} = A(\theta)x + Bu$$
$$y = Cx$$
$$x(0) = x_0$$

Have:

- $\dim(x) \gg 1$
- $\dim(\theta) \gg 1$

Reduced Order System:

$$\dot{\tilde{x}} = \tilde{A}(\tilde{\theta})\tilde{x} + \tilde{B}u$$
$$\tilde{y} = \tilde{C}\tilde{x}$$
$$\tilde{x}(0) = \tilde{x}_0$$

Want:

- $\dim(\tilde{x}) \ll \dim(x)$
- $\dim(\tilde{\theta}) \ll \dim(\theta)$
- $\|y - \tilde{y}\| \ll 1$

Cross-Gramian-Based Parameter Identification [H. & Ohlberger'14]

Parameter Augmented System:

$$\begin{pmatrix} \dot{x} \\ \dot{\theta} \end{pmatrix} = \begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ \theta \end{pmatrix} + \begin{pmatrix} B \\ 0 \end{pmatrix} u$$

$$y = \begin{pmatrix} C & 0 \end{pmatrix} \begin{pmatrix} x \\ \theta \end{pmatrix}$$

$$\begin{pmatrix} x(0) \\ \theta(0) \end{pmatrix} = \begin{pmatrix} x_0 \\ \theta_0 \end{pmatrix}$$

Joint Gramian: (Cross Gramian of Parameter Augmented System)

$$W_J = \begin{pmatrix} W_X & W_M \\ 0 & 0 \end{pmatrix}$$

Cross-Identifiability Gramian: (Schur Complement of Symmetric Part of Joint Gramian)

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

Cross-Gramian-Based Parameter Reduction

Cross-Identifiability Gramian:

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

Direct Truncation:

$$W_{\ddot{I}} \overset{SVD}{=} UDV^T$$

$$\sigma_1 > \sigma_2 > \ldots > \sigma_k \gg \sigma_{k+1} > \ldots > \sigma_N$$

$$\rightarrow U = \begin{pmatrix} U_1 & U_2 \end{pmatrix}$$

Reduced Parameters:

$$\tilde{\theta} = U_1 \theta$$

Cross-Gramian-Based Combined Reduction

Combined State and Parameter Reduction:

1. Compute Joint Gramian W_J
2. Compute from W_J the Cross-Identifiability Gramian $W_{\check{I}}$
3. Compute SVD of Cross-Identifiability Gramian $W_{\check{I}}$
4. "Balance" and Reduce Parameter Dimension
5. Extract the Cross Gramian W_X from W_J
6. Compute SVD of Cross Gramian W_X
7. Balance and Reduce State Dimension

Remember:

- System has to be symmetric!
- Empirical Joint Gramian is just an Empirical Cross Gramian!

Numerical Experiment

Model:

- 2-D Heat Equation
- Unit-Square Domain
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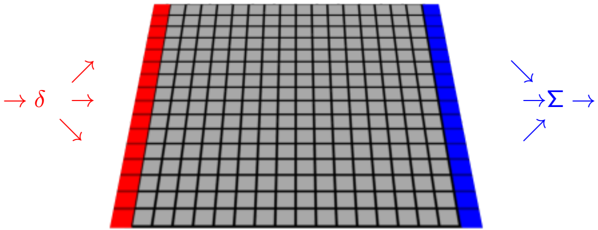
- Right-Side: Outflow / Output
- Parametrization: varying diffusion coefficients in every node



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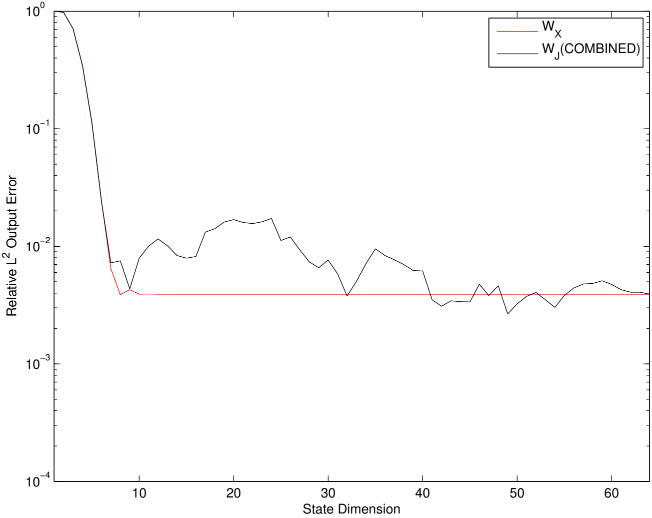
Numerical Results (Combined Reduction)



Offline Time [s]:

W_X : 23.9

W_J : 27.5

tl;dl

Can Do:

- Empirical Cross Gramian (for Linear & Nonlinear Systems)
- Empirical Joint Gramian (& Cross-Identifiability Gramian)

Want To:

- Parametric Controllability-Based Cross Gramian
- Non-Symmetric Cross Gramian

Companion Code: `http://j.mp/eccomas14`

Thanks!