WESTFÄLISCHE WILHELMS-UNIVERSITÄT MÜNSTER

APPLIED MATHEMATICS MÜNSTER

Model Reduction for Inverse Network Models

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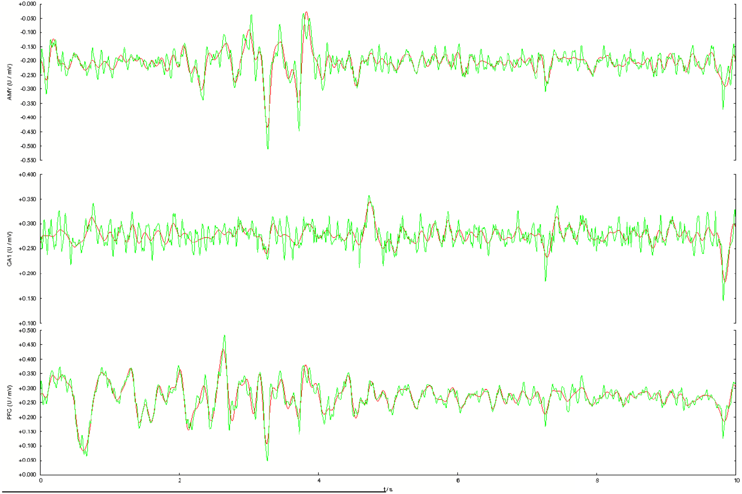
Motivation

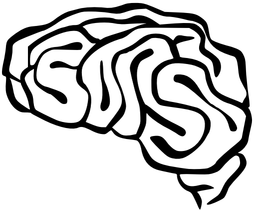
Intracranial EEG and tuned model output[1]:



[1] [Himpe'11]

Application

- Effective Connectivity
- Causal Connectivity
- Learning / Unlearning



- Experiments (EEG/MEG, fMRI/fNIRS)
- Deduce Connectivity

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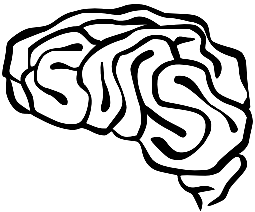
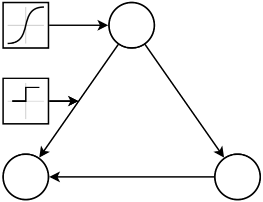


- Network Model
- Dynamical System
- Control System



- Experiments (EEG/MEG, fMRI/fNIRS)
- Deduce Connectivity

- Large-Scale
- Inverse Problem

Control Systems

Linear Dynamical System

$$\begin{aligned} \dot{x}(t) &= Ax(t) \qquad x \in \mathbb{R}^N,\ A \in \mathbb{R}^{N \times N} \\ x(0) &= x_0 \end{aligned} \tag{1}$$

(1) A is the adjacency matrix of a weighted directed graph.

Control Systems

Linear Dynamical System

$$\dot{x}(t) = Ax(t) \qquad x \in \mathbb{R}^N,\ A \in \mathbb{R}^{N\times N} \qquad (1)$$
$$x(0) = x_0$$

Linear Control System

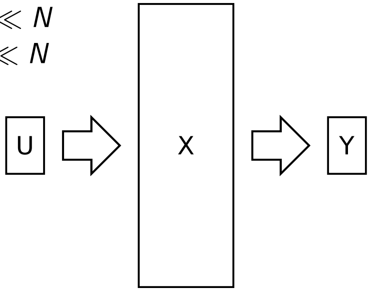
$$\dot{x}(t) = Ax(t) + Bu(t) \qquad u \in \mathbb{R}^M,\ B \in \mathbb{R}^{N\times M}$$
$$y(t) = Cx(t) \qquad x \in \mathbb{R}^N,\ A \in \mathbb{R}^{N\times N}$$
$$x(0) = x_0 \qquad y \in \mathbb{R}^O,\ C \in \mathbb{R}^{O\times N}$$

(1) A is the adjacency matrix of a weighted directed graph.

Model Reduction

Context:

- $N = \dim(x) \gg 1$
- $M = \dim(u) \ll N$
- $O = \dim(y) \ll N$



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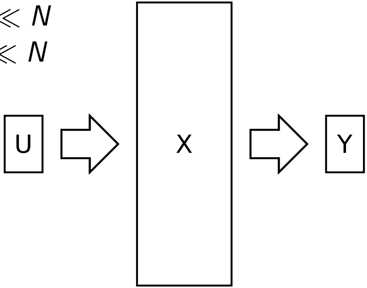
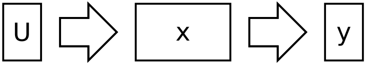


Reduced Order Model:



- $M \ll N$
- $\|Y - y\| \ll 1$

Linear Model Reduction

Aim:

1. Identifiy important and less important states.
2. Compute projection sorting states by importance.
3. Truncate neglectable states.

Input-To-Output map:

$$u \longmapsto x \longmapsto y$$

Linear Model Reduction

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Input-To-Output map:

$$u \longmapsto x \longmapsto y$$

Input-To-State map:

$$u \longmapsto x$$

Controllability

State-To-Output map:

$$x \longmapsto y$$

Observability

Controllability & Observability

Impulse Response:

$$G(t) = Ce^{At}B,\ t > 0$$

Hankel Operator:

$$H = \int_0^\infty Ce^{At}Bdt$$

Controllability Operator:

$$C = \int_0^\infty e^{At}Bdt$$

Observability Operator:

$$O = \int_0^\infty Ce^{At}dt$$

Controllability Gramian:

$$W_C := CC^*$$

Observability Gramian:

$$W_O := O^*O$$

$$\sigma_i := \lambda(H) = \sqrt{\lambda(W_O W_C)}$$

Balanced Truncation[2]

Controllability Gramian W_C:

Lyapunov equation:

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

If $\mathrm{Re}(\lambda(A)) < 0$):

$$W_C = \int_0^\infty e^{At} BB^T e^{A^T t} dt$$

Observability Gramian W_O:

Lyapunov equation:

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

If $\mathrm{Re}(\lambda(A)) < 0$):

$$W_O = \int_0^\infty e^{A^T t} C^T C e^{At} dt$$

Balancing: Sort by least controllable AND least observable states.

$$\exists U, V : UV = \mathbb{1}, VW_C V^T = U^T W_O U = \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix}$$

[2] [Moore'81]

Direct Truncation[4] (Approximate Balancing)

Cross Gramian[3] W_X**:**

Sylvester equation:

$$AW_X + W_X A = -BC$$

If $\mathrm{Re}(\lambda(A)) < 0$):

$$W_X = \int_0^\infty e^{At} B C e^{At} dt$$

NO balancing required!

$$W_O W_C = W_X^2 \Rightarrow \sigma_i = |\lambda(W_X)| \Rightarrow W_X = UDV \approx U \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix} V$$

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[3] Assume $\Sigma = \{A, B, C\}$ symmetric $\Leftarrow CA^{-1}B$ symmetric!

[4] Review in [Antoulas'05]

Truncation

1 $$\begin{cases} \dot{x} = Ax + Bu \\ y = Cx \\ x(0) = x_0 \end{cases}$$

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

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4
$$\begin{cases} \dot{x} = \begin{pmatrix} \tilde{A}_{11} & \tilde{A}_{12} \\ \tilde{A}_{21} & \tilde{A}_{22} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} \tilde{B}_1 \\ \tilde{B}_2 \end{pmatrix} u \\ y = \begin{pmatrix} \tilde{C}_1 & \tilde{C}_2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ x(0) = \begin{pmatrix} \tilde{x}_{0,1} \\ \tilde{x}_{0,2} \end{pmatrix} \end{cases}$$

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---

5 $$\begin{cases} \dot{\tilde{x}} = \tilde{A}_{11}\tilde{x}_1 + \tilde{B}_1 u \\ \tilde{y} = \tilde{C}_1\tilde{x}_1 \\ \tilde{x}(0) = \tilde{x}_{0,1} \end{cases}$$

Nonlinear Control Systems

Linear Control System

$$\dot{x}(t) = Ax(t) + Bu(t) \qquad u \in \mathbb{R}^M,\ B \in \mathbb{R}^{N\times M}$$

$$y(t) = Cx(t) \qquad x \in \mathbb{R}^N,\ A \in \mathbb{R}^{N\times N}$$

$$x(0) = x_0 \qquad y \in \mathbb{R}^O,\ C \in \mathbb{R}^{O\times N}$$

General Control System

$$\dot{x}(t) = f(x(t), u(t)) \qquad u \in \mathbb{R}^M,$$

$$y(t) = g(x(t), u(t)) \qquad x \in \mathbb{R}^N,\ f : \mathbb{R}^N \times \mathbb{R}^M \to \mathbb{R}^N$$

$$x(0) = x_0 \qquad y \in \mathbb{R}^O,\ g : \mathbb{R}^N \times \mathbb{R}^M \to \mathbb{R}^O$$

What now?

Empirical Gramians[5]

- Empirical Controllability Gramian: $W_C = \langle \int_0^\infty x_U(t) x_U^*(t) dt \rangle_U$
- Empirical Observability Gramian: $W_O = \langle \int_0^\infty \rho(y_X^*(t) y_X(t)) dt \rangle_X$
- Empirical Cross Gramian: $W_X = \langle \int_0^\infty \varphi(x_U(t), y_X(t)) dt \rangle_{U \times X}$

with perturbation spaces

1. U for perturbing the input u,
2. X for perturbing the initial state x_0

assembled from

- rotations (orthogonal matrices),
- scaling (real numbers),
- for each input / state (unit normal vectors),

determined by the operating range of the underlying contol system.

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5 [Lall'99],[Hahn'02],[Streif'06],[Himpe'13a]

Empirical Gramians II

Note:

- For linear systems, the "empirical" equal the "classic" gramians.
- Computation requires only basic matrix and vector operations.

General Projection Framework:

$$\dot{\tilde{x}}(t) = Vf(U\tilde{x}(t), u(t))$$
$$\tilde{y}(t) = g(U\tilde{x}(t), u(t))$$
$$\tilde{x}(0) = Vx_0$$

Thus, **Nonlinear Model Reduction** can also use

- Balanced Truncation,
- Direct Truncation.

The same tools as for linear model reduction.

Parameter Reduction

Parametrized Control System

$$\dot{x}(t) = f(x(t), u(t), \theta) \qquad u \in \mathbb{R}^M,\ \theta \in \mathbb{R}^P$$

$$y(t) = g(x(t), u(t), \theta) \qquad x \in \mathbb{R}^N,\ f : \mathbb{R}^N \times \mathbb{R}^M \times \mathbb{R}^P \to \mathbb{R}^N$$

$$x(0) = x_0 \qquad y \in \mathbb{R}^O,\ g : \mathbb{R}^N \times \mathbb{R}^M \times \mathbb{R}^P \to \mathbb{R}^O$$

Aim:

1. Identifiy important and less important parameters.
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1. Identifiy important and less important states.
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Parameter Reduction

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$$y(t) = g(x(t), u(t), \theta) \qquad x \in \mathbb{R}^N,\ f : \mathbb{R}^N \times \mathbb{R}^M \times \mathbb{R}^P \to \mathbb{R}^N$$

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1. Identifiy important and less important states.
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Handle parameters as:

- constant inputs
- constant states

More Empirical Gramians[6]

Empirical Sensitivity Gramian (Controllability-Based) W_S :

$$\hat{u} = \begin{pmatrix} u \\ \theta \end{pmatrix} \rightarrow \dot{x} = f(x, \hat{u}) = f(x, u) + \sum_{k=1}^{P} f(x, \theta_k) \rightarrow W_S = \delta_{i,j} \operatorname{trace}(W_{C,i})$$

Empirical Identifiability Gramian (Observability-Based) W_I :

$$\hat{x} = \begin{pmatrix} x \\ \theta \end{pmatrix} \rightarrow \dot{\hat{x}} = f(\hat{x}, u) = \begin{pmatrix} f(x, u, \theta) \\ 0 \end{pmatrix}, \hat{x}(0) = \begin{pmatrix} x_0 \\ \theta \end{pmatrix} \Rightarrow W_I = S(\hat{W}_O)$$

Empirical Joint Gramian (Cross-Gramian-Based) W_J :

$$\hat{x} = \begin{pmatrix} x \\ \theta \end{pmatrix} \rightarrow \dot{\hat{x}} = f(\hat{x}, u) = \begin{pmatrix} f(x, u, \theta) \\ 0 \end{pmatrix}, \hat{x}(0) = \begin{pmatrix} x_0 \\ \theta \end{pmatrix} \Rightarrow W_{\dot{I}} = \bar{S}(W_J := \hat{W}_X)$$

[6] [Sun'06], [Geffen'08], [Himpe'13a]

Combined Reduction

Controllability-Based

1. Compute W_S
   $\rightarrow W_C$
2. Decompose W_S
3. Truncate θ
4. Compute W_O
5. Balance W_C, W_O
6. Decompose W_{CO}
7. Truncate x

Observability-Based

1. Compute W_I
   $\rightarrow W_O$
2. Decompose W_I
3. Truncate θ
4. Compute W_C
5. Balance W_C, W_O
6. Decompose W_{CO}
7. Truncate x

Cross-Gramian-Based

1. Compute $W_{\ddot{I}}$
   $\rightarrow W_X$
2. Decompose $W_{\ddot{I}}$
3. Truncate θ
4. Decompose W_X
5. Truncate x

emgr - Empirical Gramian Framework[7]

Gramians:

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

Features:

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

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

[7] see [Himpe'13]

Numerical Experiment

Hyperbolic Network Model[8]:

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

Dimensions:

- $\dim(u) = \{4, 5, 6, 7, 8\}$
- $\dim(y) = \dim(u)$
- $\dim(x) = \{16, 25, 36, 49, 64\},\ \dim(\tilde{x}) \overset{!}{=} \dim(u)$
- $\dim(\theta) = \dim(x)^2,\ \dim(\tilde{\theta}) \overset{!}{=} \dim(\tilde{x})^2$

[8] [Quan'01]

Setup

Synthetic Data:

1. Generate random network (θ) with ensured stability of $A(\theta)$.
2. Integrate System to obtain system output.
3. Add Gaussian noise to output.

Inverse Problem[9]:

1. Offline Phase:
   Compute reduced order model using combined reduction.
2. Online Phase:
   Optimize reduced model using least squares.

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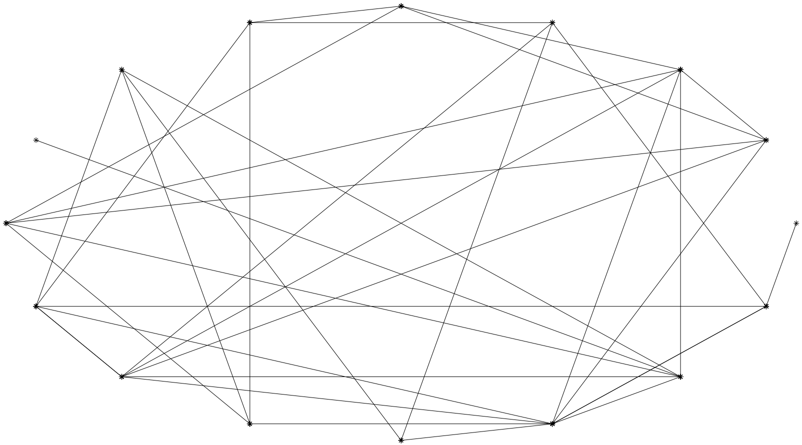
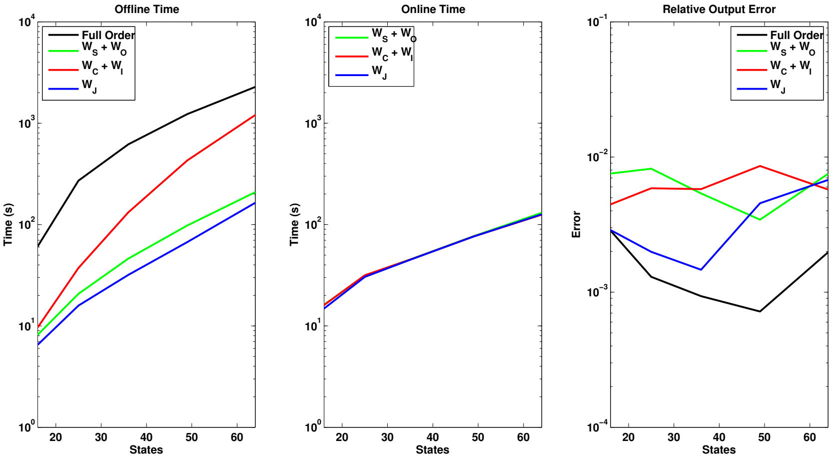
[9] from here on θ is unknown

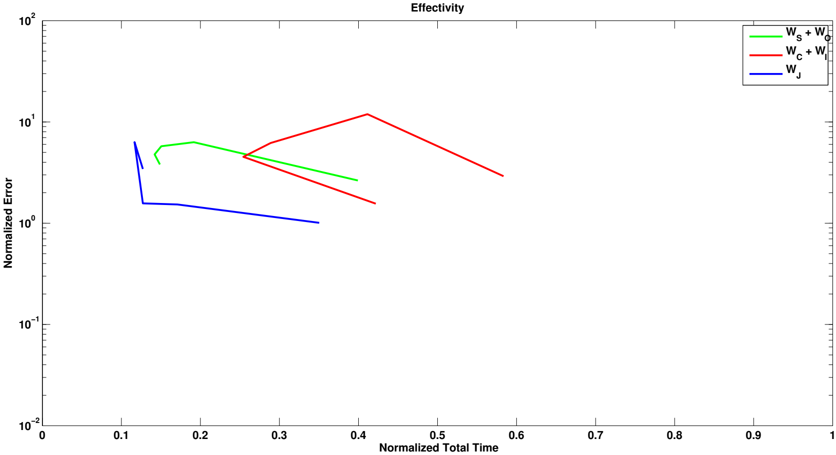
Network (N=16)



Numerical Results



Reduction Effectivity



tl;dl

- Large-Scale Inverse Problems: Model Reduction.
- Model Reduction for Control Systems: Gramian-Based.
- Nonlinear Model Order Reduction: Empirical Gramians.
- Combined Reduction: Reduction of States and Parameters.
- (Empirical) Cross Gramian: very efficient!

- Get the Source Code: `http://j.mp/zifmtn13` .

Thanks!