The Cross Gramian
An Overview and Open Problems

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1. Obligatory Notation

2. Cross Gramian Flavors

3. Cross Gramian Related Open Problems
   - I. Galerkin projection error bound
   - II. $\mathcal{H}_2$ optimized cross Gramian
   - III. Nonlinear cross Gramians

4. Cross Gramians for Gas Transport
Nonlinear Parametric Input-Output Systems:

\[
\begin{align*}
\dot{x}(t) &= f(x(t), u(t), \theta) \\
y(t) &= g(x(t), u(t), \theta)
\end{align*}
\]

Linear Input-Output System:

\[
\begin{align*}
\dot{x}(t) &= Ax(t) + Bu(t) \\
y(t) &= Cx(t)
\end{align*}
\]

- $M := \text{dim}(u(t))$
- $N := \text{dim}(x(t))$
- $Q := \text{dim}(y(t))$
- $P := \text{dim}(\theta)$
Reduced Nonlinear Input-Output Systems:

\[
\dot{x}_r(t) = f_r(x_r(t), u(t), \theta_r)
\]
\[
y_r(t) = g_r(x_r(t), u(t), \theta_r)
\]

Reduced Linear Input-Output System:

\[
\dot{x}_r(t) = A_r x_r(t) + B_r u(t)
\]
\[
y_r(t) = C_r x_r(t)
\]

- \(n := \text{dim}(x_r(t)) \ll \text{dim}(x(t))\)
- \(p := \text{dim}(\theta_r) \ll \text{dim}(\theta)\)
- \(\|y(\theta) - y_r(\theta_r)\| \ll 1\)
Reduced Nonlinear Input-Output Systems:

\[
\begin{align*}
\dot{x}_r(t) &= V_1 f(U_1 x_r(t), u(t), \Pi_1 \theta_r) \\
y_r(t) &= g(U_1 x_r(t), u(t), \Pi_1 \theta_r)
\end{align*}
\]

Reduced Linear Input-Output System:

\[
\begin{align*}
\dot{x}_r(t) &= (V_1 A U_1) x_r(t) + (V_1 B) u(t) \\
y_r(t) &= (C U_1) x_r(t)
\end{align*}
\]

- \(U_1 \in \mathbb{R}^{N \times n}, V_1 \in \mathbb{R}^{n \times N}, V_1 U_1 = 1, x_r(t) = V_1 x(t)\)
- \(\Pi_1 \in \mathbb{R}^{P \times p}, \Lambda_1 \in \mathbb{R}^{p \times P}, \Lambda_1 \Pi_1 = 1, \theta_r = \Lambda_1 \theta\)
- Hyperreduction is a different story.
Hankel Operator

Evolution Operator (infinite rank!)\(^1\)

\[ S(u) := C \int_0^\infty e^{At} Bu(t) dt \]

Controllability Operator:

\[ C(u) := \int_0^\infty e^{At} Bu(-t) dt \]

Observability Operator:

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

Hankel Operator (finite rank!)\(^2\):

\[ H := \mathcal{O} \circ C \]

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\(^1\) A.C. Antoulas. *Approximation of Large-Scale Dynamical Systems*. Vol. 6 of Advances in Design and Control, SIAM, 2005.

Hankel Operator (maps past inputs to future outputs):

\[ H := O \circ C \]

Cross Gramian\(^3\) (note it’s generally not a Gramian matrix!):

\[ W_X := C \circ O = \int_0^\infty e^{At} BC e^{At} \, dt \]

\[ \Leftrightarrow AW_X + W_X A = -BC \]

- \( \lambda_i(A) < 0 \)
- \( M \overset{!}{=} Q \)
- \( \text{tr}(W_X) = \text{tr}(H) \)
- \( W_X : \mathbb{R}^N \rightarrow \mathbb{R}^N \)

\(^3\)K.V. Fernando. **Covariance and Gramian matrices in control and systems theory.** University of Sheffield, 1983.
Relation to Balanced Truncation

Symmetric System:

\[ OC = (OC)^* \Rightarrow W_X^2 = CC^*O^*O = WCW_O \]

Cross Gramian is equivalent to balanced truncation.

State-Space Symmetric System:

\[ A = A^T, \quad C = B^T \Rightarrow CO = CC^* = O^*O \]

All system Gramians are equal.
Approximate balancing\textsuperscript{4} via singular value decomposition:

\[ W_X \overset{\text{SVD}}{=} UDV \]

Direct Truncation (Galerkin projection):

\[ U_1 := U_{:,1:n}, \quad \sum_{i=1}^{n} D_{ii} < \varepsilon \]

\[ V_1 := U_{1}^\top \]

Non-Symmetric Cross Gramian

Cross Gramian of a square MIMO as sum of SISOs:

\[
W_X = \sum_{i=1}^{M} \int_{0}^{\infty} e^{At} B_{:,i} C_{:,i} e^{At} \, dt
\]

Non-Symmetric Cross Gramian \(^5\) (Cross Gramian of average system):

\[
W_Z := \sum_{i=1}^{M} \sum_{j=1}^{Q} \int_{0}^{\infty} e^{At} B_{:,i} C_{:,j} e^{At} \, dt
\]

\[
= \int_{0}^{\infty} e^{At} \left( \sum_{i=1}^{M} B_{:,i} \right) \left( \sum_{j=1}^{Q} C_{:,j} \right) e^{At} \, dt
\]

- Motivated by Decentralized Control
- Stability Preserving (since all SISO systems are symmetric)

Primal-Dual System:

\[
\begin{pmatrix}
\dot{x}(t) \\
\dot{z}(t)
\end{pmatrix} = 
\begin{pmatrix}
A & 0 \\
0 & A^T
\end{pmatrix}
\begin{pmatrix}
x(t) \\
z(t)
\end{pmatrix} + 
\begin{pmatrix}
B \\
C^T
\end{pmatrix}
\begin{pmatrix}
u(t) \\
v(t)
\end{pmatrix}
\]

→ \( W_C = \begin{pmatrix}
W_C & W_X \\
W_X^T & W_O
\end{pmatrix} \)

- Primal Impulse Response: \( g_x(t) = e^{At} B \)
- Dual Impulse Response: \( g_z(t) = e^{A^T t} C^T \)

Empirical Linear Cross Gramian\(^6\):

\[
W_X = \int_0^\infty (e^{At} B)(e^{A^T t} C^T)^T dt \approx \int_0^\infty x(t)z(t)^T dt =: W_Y
\]

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Empirical Cross Gramian\textsuperscript{7}:

\[
\hat{W}_X := \frac{1}{M} \sum_{m=1}^{M} \int_{0}^{\infty} \Psi_{ij}^m(t) dt \in \mathbb{R}^{N \times N}
\]

\[
\Psi_{ij}^m(t) = (x_i^m(t) - \bar{x}_i^m)(y_j^m(t) - \bar{y}_j^m) \in \mathbb{R}
\]

- \(x^i(t)\) is a state trajectory with a perturbed \(i\)-th input.
- \(y^m(t)\) is an output trajectory with a perturbed \(m\)-th initial state.
- Applicable to nonlinear systems: only \(x^i(t)\) and \(y^m(t)\) required.
- Equal to linear cross Gramian for linear systems.
- Efficient empirical non-symmetric cross Gramian.

Augmented System:

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

\[ y(t) = g(x(t), u(t), \theta(t)) \]

Joint Gramian\(^4\) (Empirical Cross Gramian of the Augmented System):

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

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

\[ W_I := -W_M^T W_X^{-1} W_M \]
Empirical Gramians

- Applicable to any system that can be simulated:
  - Nonlinear systems
  - Parametric systems
  - Time-varying systems
- Basic idea is averaging.
- Simple computation.
- Allows high-dimensional parameter spaces.
- Enables combined state and parameter reduction\(^8\).

More info on empirical Gramians:


Combined reducibility for the nonlinear RC cascade benchmark\textsuperscript{9}.

\textsuperscript{9}MORwiki. \textbf{Nonlinear RC Ladder}. http://modelreduction.org/index.php/Nonlinear_RC_Ladder
Combined reducibility for the hyperbolic network model\textsuperscript{10}.

Combined reducibility for the EEG dynamic causal model\textsuperscript{11}.

Combined reducibility for the fMRI dynamic causal model\textsuperscript{12}

I. Direct Truncation Error Bound
II. $H_2$ Optimized Cross Gramian
III. Empirical Cross Gramian vs Nonlinear Cross Gramian
(I.) Distributed Cross Gramian

Column-wise cross Gramian computation:

\[ \hat{W}_X = \left( w_{X,1} \ldots w_{X,N} \right) \]

\[ w_{X,j} = \frac{1}{M} \sum_{m=1}^{M} \int_{0}^{\infty} \psi_{jm}^{i}(t)dt \in \mathbb{R}^{N} \]

\[ \psi_{jm}^{i}(t) = (x_{i}^{m}(t) - \bar{x}_{i}^{m})(y_{j}^{m}(t) - \bar{y}_{j}^{m}) \in \mathbb{R} \]

- Only for empirical cross Gramians \((W_X, W_Y, W_Z, W_J)\)!
- Overcome curse of dimensionality \((W_X \in \mathbb{R}^{N \times N})\).

Hierarchical Approximate Proper Orthogonal Decomposition\(^{13}\)

- Direct distributed computation (of \(U_1\))
- Direct incremental computation (of \(U_1\))
- More on the HAPOD, (see S. Rave’s talk on 2017-08-15, 12:00)

(I.) Direct Truncation Error Bound

Mean Projection Error Bound:

\[ \| W_X - U_1 U_1^T W_X \|_2 \leq \sqrt{\sum_{i=1}^{n} \sigma_i(W_X)^2} \]

State Error Bound\(^{14}\):

\[ \| x(t) - x_r(t) \|_2 \leq c(\| x_0 - U_1 U_1^T x_0 \| + \int_{0}^{\infty} \| R(t) \|_2 \, dt) \]

Tangential Interpolation (using directions: $r^i$ and $l^j$):

$$V_1 := \bigoplus_i C(s_i)r^i, \quad U_1 := \bigoplus_j l^j O(s_j).$$

Frequency Domain Cross Gramian:

$$W_X = \frac{1}{2\pi} \int_{-\infty}^{\infty} (\omega \mathbb{1} - A)^{-1} BC(\omega \mathbb{1} - A)^{-1} d\omega$$

Tangential Cross Gramian:

$$W_{X,rl} := (Cr)(lO) = \frac{1}{2\pi} \int_{-\infty}^{\infty} (\omega \mathbb{1} - A)^{-1} BrlC(\omega \mathbb{1} - A)^{-1} d\omega$$

$$= \int_0^\infty e^{At} (Br)(lC) e^{At} dt$$

$$\rightarrow r_i = l_j = 1 \forall i, j \Rightarrow W_{X,rl} = W_Z$$
Tangential Cross Gramian:

\[
W_{X,rl} = \int_{0}^{\infty} e^{At} BrlC e^{At} \, dt
\]

- What are the “best” directions \( r \) and \( l \)?
- What are desirable properties of \( BrlC \)?
- Can (simplified) balanced gains\(^{15}\) help:

\[
d_i := |\tilde{b}_i \tilde{c}_i| \sigma_i(H)
\]

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Control-Affine Nonlinear System:

\[
\dot{x}(t) = f(x(t)) + g(x(t))u(t) \\
y(t) = h(x(t))
\]

Nonlinear Cross Gramian\(^{16}\) (Solution to a nonlinear Sylvester equation):

\[
\frac{\partial \Phi}{\partial x} f(x) + f(\Phi(x)) = -g(\Phi(x))h(x)
\]

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Explicit nonlinear cross Gramian definition:

\[ \Phi(x_0) := C \circ O(x_0) = ? \]

\[ C(u) = \chi(t), \quad \dot{\chi}(t) = -f(\chi(t)) - g(\chi(t))u(t) \]
\[ O(t) = h(x(t)), \quad \dot{x}(t) = f(x(t)) \]

- Is there an empirical formulation of the nonlinear cross Gramian?
- Is the empirical cross Gramian an approximation to the nonlinear?
1D (Simplified) Isothermal Euler Equations\textsuperscript{17}:

\[
\frac{\partial p}{\partial t} = - \frac{\partial q}{\partial x} \\
\frac{\partial q}{\partial t} = -c^2 \frac{\partial p}{\partial x} - \frac{\lambda}{2D} \frac{q|q|}{p}
\]

- System properties: hyperbolic, nonlinear, coupled.
- Finite difference spatial discretization: DAE.
- Analytic index reduction to implicit ODE.
- Structured projections\textsuperscript{18}:
  - Pressure cross Gramian
  - Mass-flux cross Gramian


Summary

Cross-Gramian-Related Open Problems:

I. Direct Truncation Error Bound
II. $H_2$ Optimized Cross Gramian
III. Empirical vs Nonlinear Cross Gramian

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