Gramian Based Model Reduction of Large-scale Dynamical Systems

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• Origin and motivation
  Ex: Storm surge forecasting

• Typical techniques (Gramians)
  Linear time-invariant
  Linear time-varying
  Non-linear

• Numerical/Algorithmic issues (Krylov)
Storm surge forecasting in the North Sea

see Verlaan-Heemink ’97

Problem
Using measurements predict the state of the North Sea variables in order to operate the sluices in due time (6h.)

Solution
\[ x(t) = [h(t), u_x(t), u_y(t)] \] satisfies the shallow water equations

\[
\begin{align*}
\frac{\partial x(t)}{\partial t} &= F(x(t), w(t)) \\
y(t) &= G(x(t), v(t))
\end{align*}
\]

with measurements \( y(t) \) and noise processes \( v(.), w(.) \)
\[ \Rightarrow \text{estimate and predict } \hat{x}(t) \text{ using Kalman filtering} \]
Some data: very few measurements (x’s and +’s)

but discretized state is very large-scale (60,000 variables)
Nevertheless it works ...

Reconstruction works well around estuarium
Visualisation of computed variance of the error

Standard deviation of filter using 8 measurement locations

Standard deviation of filter using measurement locations
(1 used for validation)
Suppose a "good" discretization $x(.) \in \mathbb{R}^N$ is given

Dynamical systems modeled via explicit equations

$$x(t) \in \mathbb{R}^N, N >> m, p$$

**discretize**

**continuous-time**

\[
\begin{align*}
\dot{x}(t) &= G(x(t), u(t)) \\
y(t) &= H(x(t), u(t))
\end{align*}
\]

**discrete-time**

\[
\begin{align*}
x(k + 1) &= G(x(k), u(k)) \\
y(k) &= H(x(k), u(k))
\end{align*}
\]

**linearize**

\[
\begin{align*}
\dot{x}(t) &= A(t)x(t) + B(t)u(t) \\
y(t) &= C(t)x(t) + D(t)u(t)
\end{align*}
\]

**freeze time**

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

Many control problems require $\approx N^3/ (\Delta t)$ operations.
Because of cubic complexity in $N \Rightarrow$ model reduction
Linear Time Invariant Systems

Given "large model" \( \{A_{NN}, B_{Nm}, C_{pN}\} \)

\[
\begin{aligned}
\dot{x}(t) &= Ax(t) + Bu(t) \\
y(t) &= Cx(t) + Du(t),
\end{aligned}
\]

\( u(t) \in \mathbb{R}^m, y(t) \in \mathbb{R}^p, x(t) \in \mathbb{R}^N, N << m, p \)

find "small model" \( \{\hat{A}_{nn}, \hat{B}_{nm}, \hat{C}_{pn}\} \) with \( n << N \)

\[
\begin{aligned}
\dot{\hat{x}}(t) &= \hat{A}\hat{x}(t) + \hat{B}u(t) \\
\hat{y}(t) &= \hat{C}\hat{x}(t) + \hat{D}u(t),
\end{aligned}
\]

driven by the same input \( u(t) \) with small error

\[ \|y(t) - \hat{y}(t)\| \]

Model reduction = find a smaller model, i.e. \( n << N \):

- approximation problem
- stability is important
- measure is important
How to capture the essence of the system?

Transfer functions and norms

\[ H(s) = C(sI_N - A)^{-1}B + D, \quad \hat{H}(s) = \hat{C}(sI_n - \hat{A})^{-1}\hat{B} + \hat{D}, \]

are \( p \times m \) rational matrices

try to match frequency responses

by minimizing their difference using

\[ \|H(\cdot) - \hat{H}(\cdot)\|_{\infty} = \sup_{\omega} \sigma_{max}\{H(j\omega) - \hat{H}(j\omega)\} \]

Theory:

- balanced truncation (Moore ’81)
- optimal Hankel norm approximation (Adamian-Arov-Krein ’71, Glover ’90)
- interpolation (Gragg-Lindquist ’83)

Other references: Gallivan-Grimme-VanDooren, Jaimoukha-Kasanelly, Villemagne-Skelton, Boley, Craig, Freund-Feldman, Sorensen-Antoulas, ...
Why $\| \cdot \|_\infty$ norm?

Fourier transforms of signals:

$$u_f(\omega) = \mathcal{F}u(t), \quad y_f(\omega) = \mathcal{F}y(t), \quad \hat{y}_f(\omega) = \mathcal{F}\hat{y}(t)$$

yields

$$y_f(\omega) = H(j\omega)u_f(\omega), \quad \hat{y}_f(\omega) = \hat{H}(j\omega)u_f(\omega).$$

and hence a bound for $e(t) \doteq [y(t) - \hat{y}(t)]$:

$$\mathcal{F}e(t) = e_f(\omega) = [H(j\omega) - \hat{H}(j\omega)]u_f(\omega).$$

Minimize worst case error $\|e_f(\omega)\|_2$ for $\|u_f(\omega)\|_2 = 1$ by minimizing

$$\|H(.) - \hat{H}(.)\|_\infty \doteq \sup_\omega \|H(j\omega) - \hat{H}(j\omega)\|_2,$$

but this is a difficult norm to handle!
Use Hankel norm instead of $\| \cdot \|_\infty$ approximations

Consider the mapping “past inputs” $\Rightarrow$ “future outputs”

**Continuous-time**

\[
y(t) = \int_{-\infty}^{0} C e^{A(t-\tau)} B u(\tau) d\tau = C e^{At} \cdot \int_{0}^{\infty} e^{A\tau} B u(-\tau) d\tau,
\]

\[
y(t) = C e^{At} x(0), \quad x(0) = \int_{0}^{\infty} e^{A\tau} B u(-\tau) d\tau.
\]

**Discrete-time**

\[
y(k) = \sum_{-\infty}^{0} C A^{(k-j)} B u(j) = C A^k \cdot \sum_{0}^{\infty} A^j B u(-j),
\]

\[
y(k) = C A^k x(0), \quad x(0) = \sum_{0}^{\infty} A^j B u(-j).
\]
$N \times N$ Gramians derived from the Hankel map

From $y([0, \infty)) = O x(0), \quad x(0) = C u((\infty, 0))$, define the dual maps $O^* : y([0, \infty)) \mapsto x(0), \quad C^* : x(0) \mapsto u((\infty, 0))$ and the (observability and controllability) Gramians

$$G_o = O^* O, \quad G_c = C C^*$$

**Continuous-time**

$$G_o = \int_0^{+\infty} (Ce^{At})^T (Ce^{At}) dt, \quad G_c = \int_0^{+\infty} (e^{At} B)(e^{At} B)^T dt,$$

**Discrete-time**

$$G_o = \sum_{k=0}^{+\infty} (CA^k)^T (CA^k), \quad G_c = \sum_{k=0}^{+\infty} (A^kB)(A^kB)^T,$$

Gramians can be viewed as “energy functions”

- $G_c$ for past inputs $\mapsto x(0)$
- $G_o$ for $x(0) \mapsto$ future outputs

Perform ordered eigendecomposition $\Lambda = T^{-1}(G_c G_o)T$ (with $\lambda_n \gg \lambda_{n+1}$) and project on the first $n$ coordinates:

$$T^{-1} A T \doteq \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \quad T^{-1} B \doteq \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}, \quad C T \doteq \begin{bmatrix} C_1 & C_2 \end{bmatrix}.$$

$$\{\hat{A}, \hat{B}, \hat{C}\} \doteq \{A_{11}, B_1, C_1\}$$
Interpolating the frequency response $H(\omega)$ seems a good idea since Parseval’s theorem implies

$$G_o = \frac{1}{2\pi} \int_{-\infty}^{+\infty} (-j\omega I - A^T)^{-1} C^T C (j\omega I - A)^{-1} d\omega,$$

$$G_c = \frac{1}{2\pi} \int_{-\infty}^{+\infty} (j\omega I - A)^{-1} BB^T (-j\omega I - A^T)^{-1} d\omega.$$

and

$$G_o = \frac{1}{2\pi} \sum_{-\infty}^{+\infty} (e^{-j\omega I} - A^T)^{-1} C^T C (e^{j\omega I} - A)^{-1}$$

$$G_c = \frac{1}{2\pi} \sum_{-\infty}^{+\infty} (e^{j\omega I} - A)^{-1} BB^T (e^{-j\omega I} - A^T)^{-1}.$$

What technique to use? The discrete-time case:

$$\begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \end{bmatrix} = OC \begin{bmatrix} u_{-1} \\ u_{-2} \\ u_{-3} \\ \vdots \end{bmatrix} = \begin{bmatrix} C \\ CA \\ CA^2 \\ \vdots \end{bmatrix} \begin{bmatrix} B & AB & A^2B & \ldots \\ u_{-1} \\ u_{-2} \\ u_{-3} \\ \vdots \end{bmatrix}$$

... suggests to use Krylov spaces!

$$\mathcal{K}_j(M, R) = \text{Im} \{ R, MR, M^2R, \ldots, M^{j-1}R \}$$
Rational interpolation and moment matching

Let \( X \) and \( Y \) define a projector \( (Y^TX = I_n) \) and

\[
\{ \hat{A}, \hat{B}, \hat{C}, D \} = \{ Y^TAX, Y^TB, CX, D \}
\]

Taylor series of \( H(s) = C(sI - A)^{-1}B + D \) around \( \infty \)

\[
H(s) = H_0 + H_1s^{-1} + H_2s^{-2} + \cdots,
\]

where the moments \( H_i \) are equal to:

\[
H_0 = D, \quad H_i = CA_i^{-1}B, \ i = 1, 2, ...
\]

The reduced order model \( \hat{H}(s) = \hat{C}(sI - \hat{A})^{-1}\hat{B} + \hat{D} \) has a similar expansion

\[
\hat{H}(s) = \hat{H}_0 + \hat{H}_1s^{-1} + \hat{H}_2s^{-2} + \cdots,
\]

with moments \( \hat{H}_i \) :

\[
\hat{H}_0 = \hat{D}, \quad \hat{H}_i = \hat{C}A_i^{-1}\hat{B}, \ i = 1, 2, ...
\]

Moment matching of both models (Padé approximation) is obtained by using Krylov spaces (Gragg-Lindquist ’83)
**Theorem:** Let \( m = p, Y^T X = I_n \) and assume

\[
\text{Im} X = \text{Im} \left[ B, AB, A^2 B, \ldots A^{k-1} B \right],
\]

\[
\text{Im} Y = \text{Im} \left[ C^T, A^T C^T, A^{2T} C^T, \ldots A^{(k-1)T} C^T \right]
\]

then the first \( 2k \) moments match:

\[
H_j = \hat{H}_j, \quad j = 1, \ldots, 2k.
\]

Rational Krylov methods extend this to several points \( \sigma_i \):
multipoint (Padé) approximations are obtained by just using modified Krylov spaces:
(Gallivan-Grimme-VanDooren '97)

\[
\text{Im} X = \bigcup_i \mathcal{K}_{j_i} \{(A - \sigma_i I)^{-1}, (A - \sigma_i I)^{-1} B\}
\]

\[
\text{Im} Y = \bigcup_i \mathcal{K}_{j_i} \{(A^T - \sigma_i I)^{-1}, (A^T - \sigma_i I)^{-1} C^T\}
\]

in the above theorem
Comparison “Optimal” and rational approximations

15th order approximation of 120th order CD player

Legend: ··· Hankel norm — Balanced truncation - - Rational Krylov

| Errors | \(|T(\cdot) - \hat{T}(\cdot)| | ln(|T(\cdot) - \hat{T}(\cdot)|) |
|--------|------------------|------------------|
| Hankel | 0.02             | 6.1              |
| Balanc.| 0.04             | 4.1              |
| Rat. Kr.| 4.02           | 1.5              |

Rational approximation looks better on a logarithmic scale
Approximate the (discrete) time-varying systems

\[
\begin{align*}
    x(k + 1) &= A(k)x(k) + B(k)u(k) \\
    y(k) &= C(k)x(k) + D(k)u(k)
\end{align*}
\]

by a lower order models of same type. We notice that

\[
\begin{bmatrix}
    y(k) \\
    y(k+1) \\
    y(k+2) \\
    \vdots
\end{bmatrix}
= \begin{bmatrix}
    C(k) \\
    C(k+1)A(k) \\
    C(k+2)A(k+1)A(k) \\
    \vdots
\end{bmatrix} x(k),
\]

\[
x(k) = \begin{bmatrix}
    u(k-1) \\
    u(k-2) \\
    u(k-3) \\
    \vdots
\end{bmatrix}
\]

which again suggests Krylov. Use low rank approximations

\[
G_o(k) \approx S_o(k)S_o^T(k), \quad G_c(k) \approx S_c(k)S_c^T(k),
\]

where \( S_o(k) \) and \( S_c(k) \) are \( N \times n \) matrices

Such approximations are obtained e.g. by keeping only the \( n \) dominant singular vectors at step \( k \) of the Krylov recurrence:

\[
S_c(k) = \text{SVD}_n [B(k), A(k)S_c(k-1)]
\]
Let’s go back to the Storm Surge example

The important matrix in this Kalman filtering problem is

$$P(k) = \mathcal{E}\{(x(k) - \hat{x}(k))(x(k) - \hat{x}(k))^T\}$$

which represents the “error covariance” of the estimation.

If we approximate

$$P(k) \approx S(k)S(k)^T, \quad S(k) \in \mathbb{R}^{N \times n},$$

then we obtain the recurrence

$$S(k + 1) \Leftarrow SVD_n \left[ \begin{array}{ccc} R(k) & C(k)S(k) & 0 \\ 0 & A(k)S(k) & B(k)Q(k) \end{array} \right]$$

where the new factor $S(k + 1)$ stays of rank $n$ by a projection (using the SVD).

The only big matrix involved here is the sparse matrix $A(k)$ which is multiplied with only $n$ columns

Verlaan-Heemink ’97
Consider the discrete-time system
\[
\begin{cases}
x(k + 1) = G(x(k), u(k)) \\
y(k) = H(x(k), u(k)).
\end{cases}
\]

One could linearize along a “nominal” trajectory \((x(k), u(k))\) and get \(A(\cdot), B(\cdot), C(\cdot), D(\cdot)\) from Taylor expansion of \(G(\cdot, \cdot), H(\cdot, \cdot)\).

**Simpler idea (POD)**: (Holmes-Lumley-Berkooz ’96)

Use the “energy function” \(G : = \sum_{k=k_i}^{k_f} x(k)x(k)^T\).

From
\[x(k + 1) = A(k)x(k)\]
with initial conditions \(x(k_i)\), we have
\[x(k) = \Phi(k, k_i)x(k_i)\).

Therefore \(G\) looks like a Gramian :
\[
\sum_{k=k_i}^{k_f}(\Phi(k, k_i)x(k_i))(\Phi(k, k_i)x(k_i))^T.
\]

Now project on its dominant subspace (POD)
Example: Use POD in CVD reactor (Ly-Tran '99)

Schematic representation of a horizontal quartz reactor in a steel confinement shell

Compute state trajectories for one "typical" input:

Snap shots of "typical" states

Ten dominant "states"
Concluding remarks

- large-scale is typically sparse
- time-stepping (simulation) is cheaper than control (optimization)
- find an “energy function” that is “cheap” and project on its dominant features

Future work

- find error bounds “on the fly”
- incorporate projections in closed loop

Further reading


See also SIAM short course notes on http://www.auto.ucl.ac.be/~vdooren/