Gramian Based Model Reduction of Large-scale Dynamical Systems

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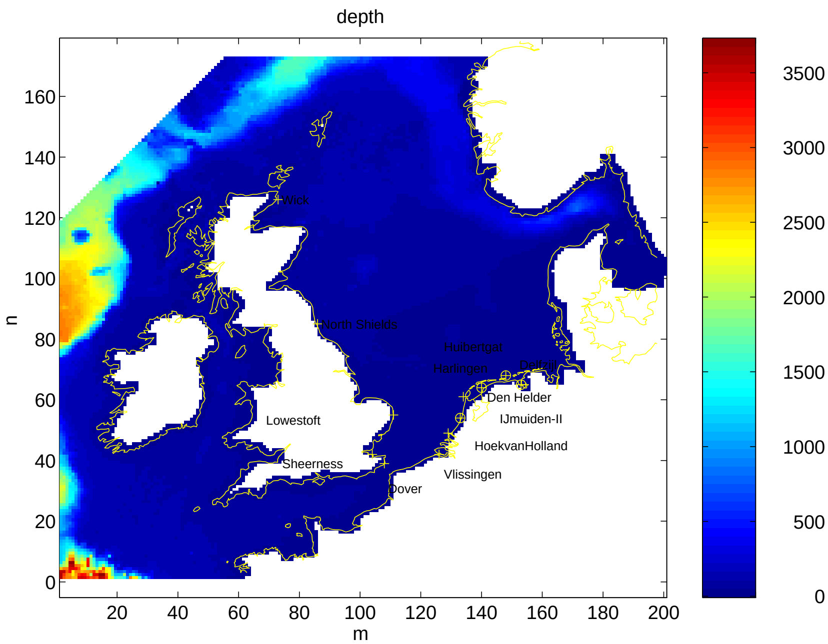
- Origin and motivation
  Ex: Storm surge forecasting
- Typical techniques (Gramians)
  Linear time-invariant
  Linear time-varying
  Non-linear
- Numerical/Algorithmic issues (Krylov)

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

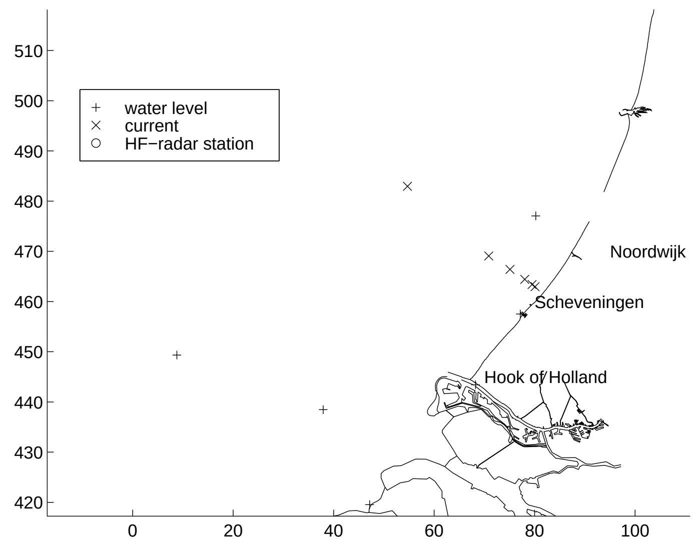
$x(t) \doteq [h(t), v_x(t), v_y(t)]$ satisfies the shallow water equations

$$\begin{aligned} \partial x(t)/\partial t &= F(x(t), w(t)) \\ y(t) &= G(x(t), v(t)) \end{aligned}$$

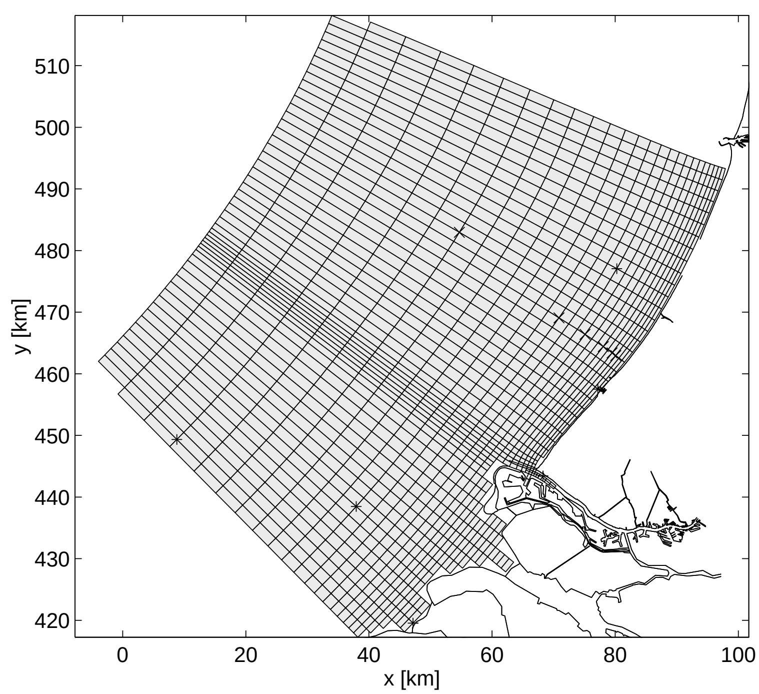
with measurements $y(t)$ and noise processes $v(.), w(.)$

$\Longrightarrow$ estimate and predict $\hat{x}(t)$ using Kalman filtering

Some data : very few measurements (x's and $+$'s)



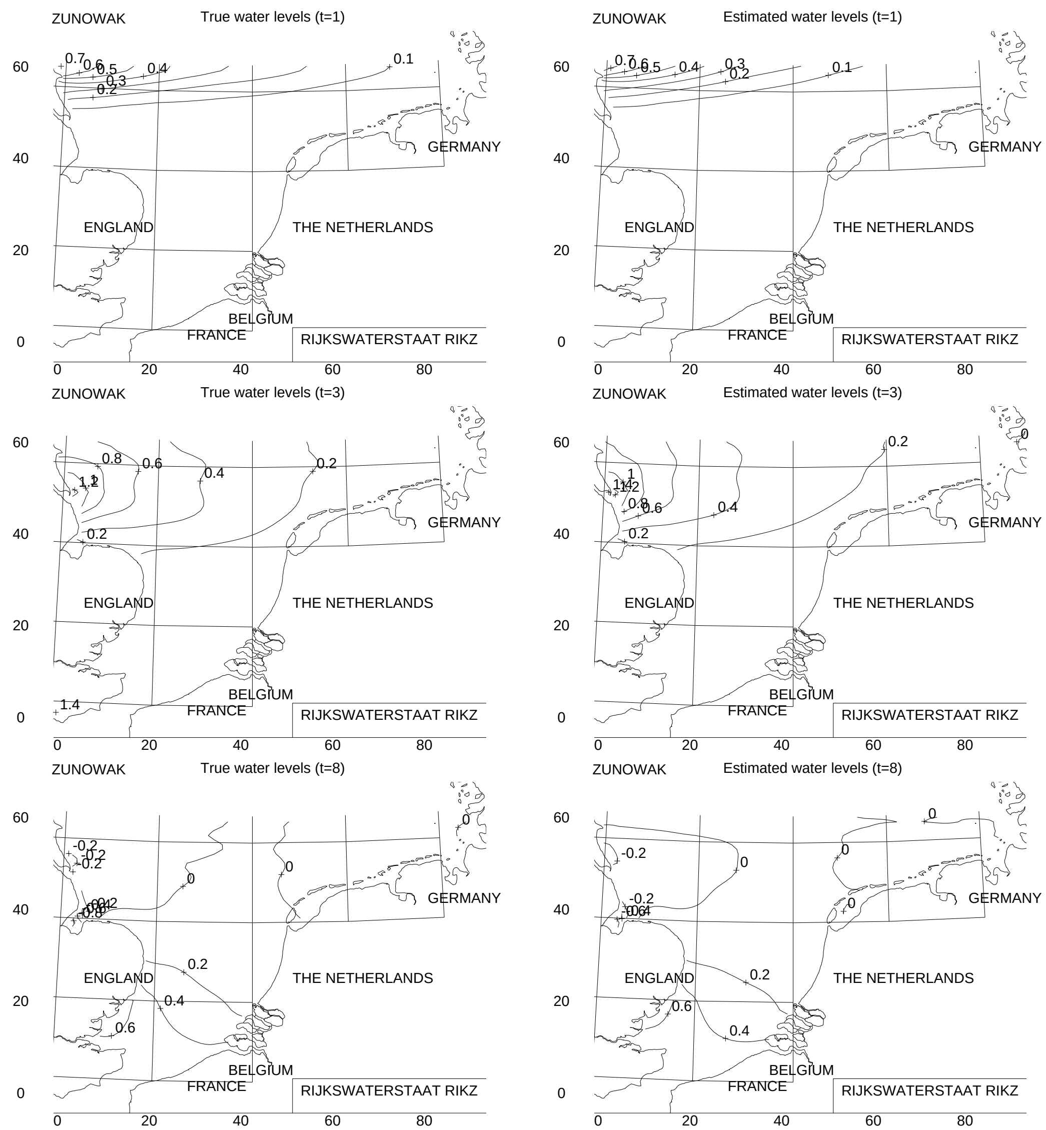
but discretized state is very large-scale (60.000 variables)



Nevertheless it works ...

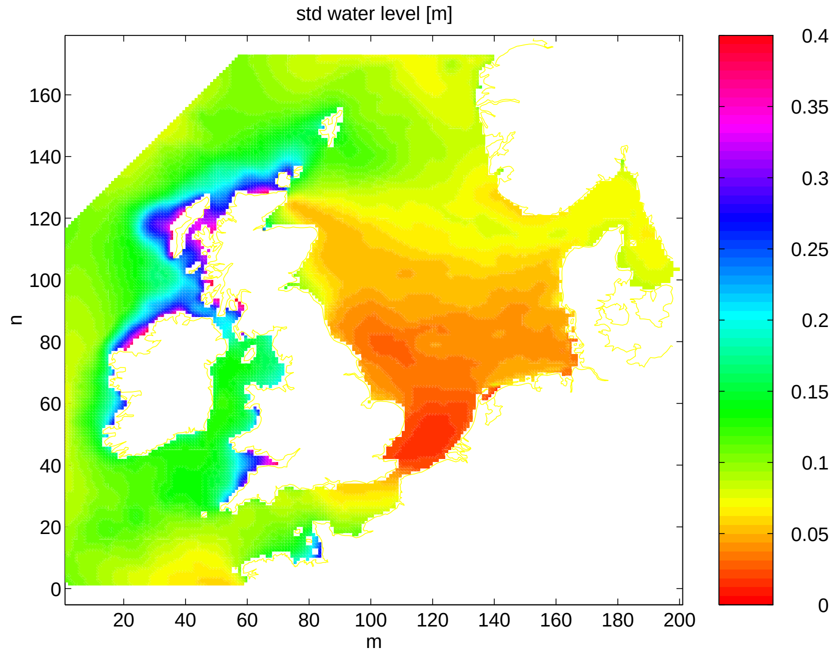
True water levels

Estimated water levels

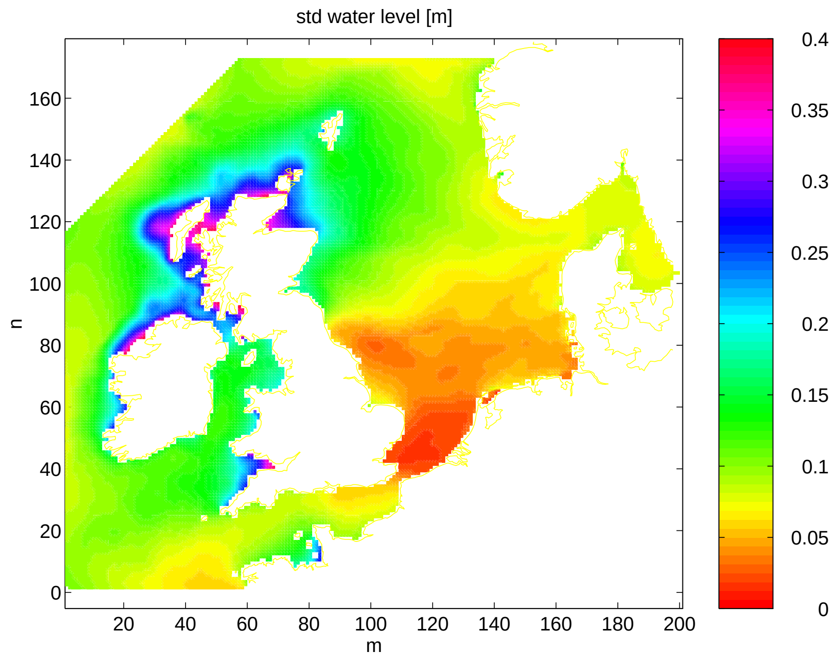


Reconstruction works well around estuarium

Visualisation of computed variance of the error



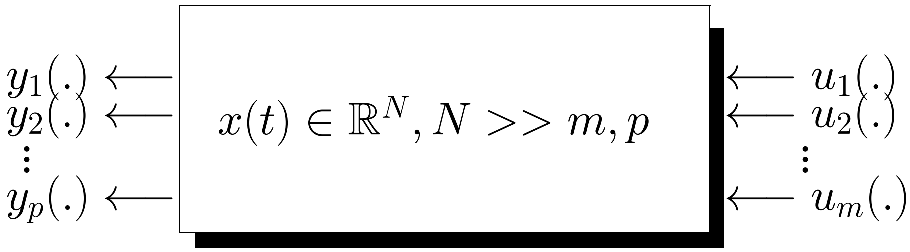
Standard deviation of filter using 8 measurement locations



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



$$\stackrel{\text{discretize}}{\Longrightarrow}$$

continuous-time

$$\begin{cases} \dot{x}(t) = G(x(t), u(t)) \\ y(t) = H(x(t), u(t)) \end{cases}$$

discrete-time

$$\begin{cases} x(k+1) = G(x(k), u(k)) \\ y(k) = H(x(k), u(k)) \end{cases}$$

$\Downarrow$ linearize $\Downarrow$

$$\begin{cases} \dot{x}(t) = A(t)x(t) + B(t)u(t) \\ y(t) = C(t)x(t) + D(t)u(t) \end{cases} \qquad \begin{cases} x(k+1) = A(k)x(k) + B(k)u(k) \\ y(k) = C(k)x(k) + D(k)u(k) \end{cases}$$

$\Downarrow$ freeze time $\Downarrow$

$$\begin{cases} \dot{x}(t) = Ax(t) + Bu(t) \\ y(t) = Cx(t) + Du(t) \end{cases} \qquad \begin{cases} x(k+1) = Ax(k) + Bu(k) \\ y(k) = Cx(k) + Du(k) \end{cases}$$

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" $\{A_{NN}, B_{Nm}, C_{pN}\}$

$$\begin{cases} \dot{x}(t) = Ax(t) + Bu(t) \\ y(t) = Cx(t) + Du(t), \end{cases}$$

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

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

$$\begin{cases} \dot{\hat{x}}(t) = \hat{A}\hat{x}(t) + \hat{B}u(t) \\ \hat{y}(t) = \hat{C}\hat{x}(t) + \hat{D}u(t), \end{cases}$$

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

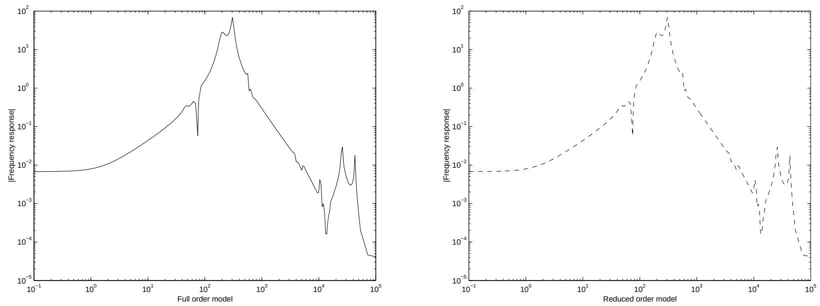
How to capture the essence of the system ?

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

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

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 $\| \, . \, \|_\infty$ 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 !

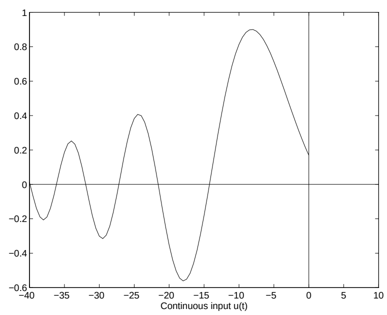
Use Hankel norm instead of $\|.\|_\infty$ approximations

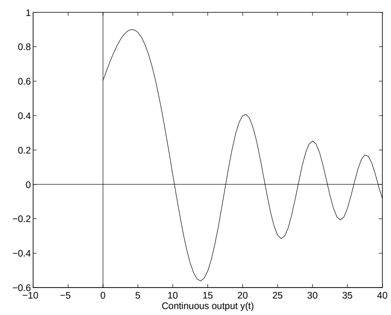
Consider the mapping "past inputs" $\Longrightarrow$ "future outputs"

Continuous-time

$$y(t) = \int_{-\infty}^{0} Ce^{A(t-\tau)}Bu(\tau)d\tau = Ce^{At} \cdot \int_{0}^{\infty} e^{A\tau}Bu(-\tau)d\tau,$$

$$y(t) = Ce^{At}x(0), \quad x(0) = \int_{0}^{\infty} e^{A\tau}Bu(-\tau)d\tau.$$

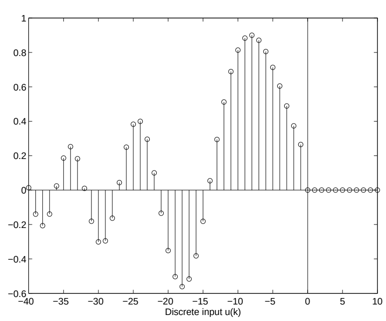


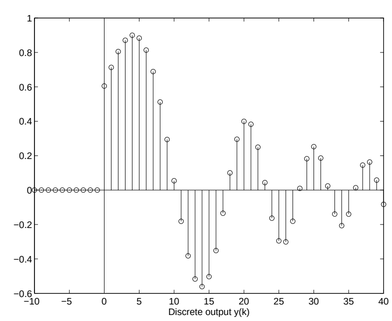


Discrete-time

$$y(k) = \sum_{-\infty}^{0} CA^{(k-j)}Bu(j) = CA^{k} \cdot \sum_{0}^{\infty} A^{j}Bu(-j),$$

$$y(k) = CA^{k}x(0), \quad x(0) = \sum_{0}^{\infty} A^{j}Bu(-j).$$





$N \times N$ Gramians derived from the Hankel map

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

$$G_o \doteq \mathcal{O}^*\mathcal{O}, \quad G_c \doteq \mathcal{C}\mathcal{C}^*$$

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

$$G_o = \sum_0^{+\infty} (CA^k)^T (CA^k), \quad G_c = \sum_0^{+\infty} (A^kB)(A^kB)^T,$$

Gramians can be viewed as "energy functions"
G_c for past inputs $\longrightarrow x(0)$
G_o for $x(0) \longrightarrow$ future outputs

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

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

$$\{\hat{A}, \hat{B}, \hat{C}\} \doteq \{A_{11}, B_1, C_1\}$$

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 :

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

... suggests to use Krylov spaces !

$$\mathcal{K}_j(M,R) = \text{Im}\left\{R, MR, M^2R, \dots, M^{j-1}R\right\}$$

Rational interpolation and moment matching

Let X and Y define a projector ($Y^T X = I_n$) and

$$\left\{\hat{A}, \hat{B}, \hat{C}, D\right\} = \{Y^T A X, Y^T B, C X, D\}$$

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

$$H(s) = H_0 + H_1 s^{-1} + H_2 s^{-2} + \cdots ,$$

where the **moments** H_i are equal to :

$$H_0 = D, \quad H_i = C A^{i-1} B, \ i = 1, 2, ...$$

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

$$\hat{H}(s) = \hat{H}_0 + \hat{H}_1 s^{-1} + \hat{H}_2 s^{-2} + \cdots ,$$

with moments $\hat{H}_i$:

$$\hat{H}_0 = \hat{D}, \quad \hat{H}_i = \hat{C} \hat{A}^{i-1} \hat{B}, \ i = 1, 2, ...$$

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

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

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

then the first $2k$ moments match :

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

■

Rational Krylov methods extend this to several points σ_i :

multipoint (Padé) approximations are obtained by just using modified Krylov spaces : (Gallivan-Grimme-VanDooren '97)

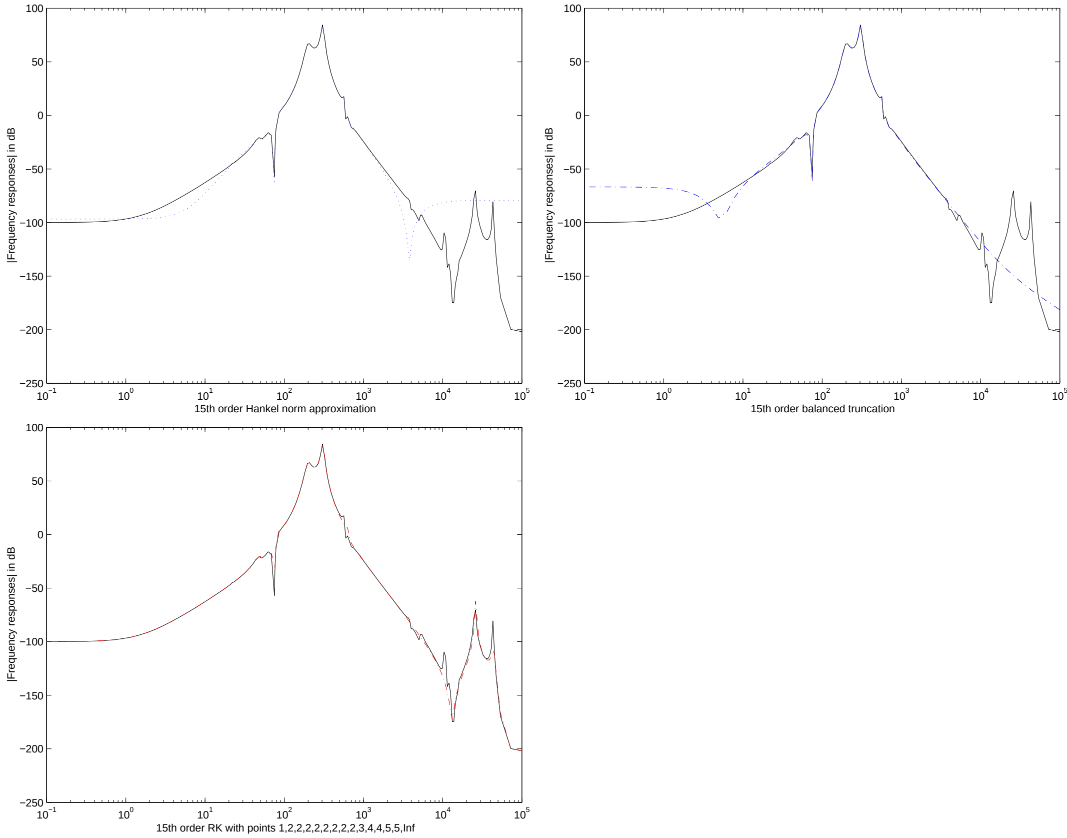
$$\text{Im}X = \bigcup_i \mathcal{K}_{j_i}\{(A - \sigma_i I)^{-1}, (A - \sigma_i I)^{-1}B\}$$

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

in the above theorem

Comparison “Optimal” and rational approximations

15th order approximation of 120 th order CD player



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

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

Rational approximation looks better on a logarithmic scale

Time-varying systems

Approximate the (discrete) time-varying systems

$$\begin{cases} x(k+1) = A(k)x(k) + B(k)u(k) \\ y(k) = C(k)x(k) + D(k)u(k) \end{cases}$$

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

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

$x(k) =$

$$\begin{bmatrix} B_{(k-1)} & A_{(k-1)}B_{(k-2)} & A_{(k-1)}A_{(k-2)}B_{(k-3)} & \dots \end{bmatrix} \begin{bmatrix} u(k-1) \\ u(k-2) \\ u(k-3) \\ \vdots \end{bmatrix}$$

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 :

$$S_c(k) = SVD_n\left[B(k), A(k)S_c(k-1)\right]$$

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

$$S(k+1) \Leftarrow SVD_n \begin{bmatrix} R(k) & C(k)S(k) & 0 \\ 0 & A(k)S(k) & B(k)Q(k) \end{bmatrix}$$

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

Time-varying linearized problems

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 $A(.), B(.), C(.), D(.)$ from Taylor expansion of $G(., .), H(., .)$

Simpler idea (POD) : (Holmes-Lumley-Berkooz '96)

Use the "energy function" $G \doteq \sum_{k=k_i}^{k_f} x(k)x(k)^T$.

From

$$x(k+1) = A(k)x(k)$$

with initial conditions $x(k_i)$, we have

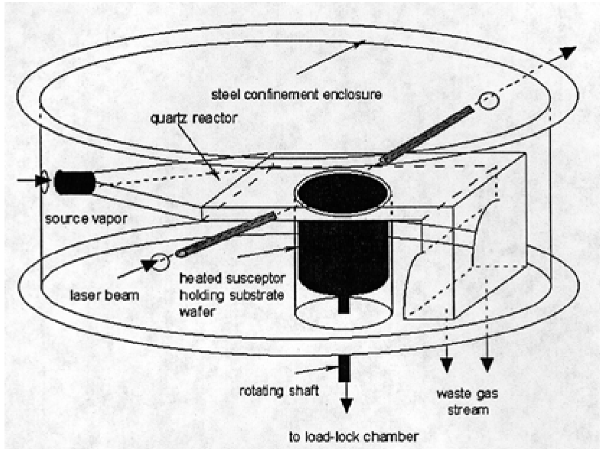
$$x(k) = \Phi(k, k_i)x(k_i).$$

Therefore G looks like a Gramian :

$$\sum_{k=k_i}^{k_f} (\Phi(k, k_i)x(k_i))(\Phi(k, k_i)x(k_i))^T.$$

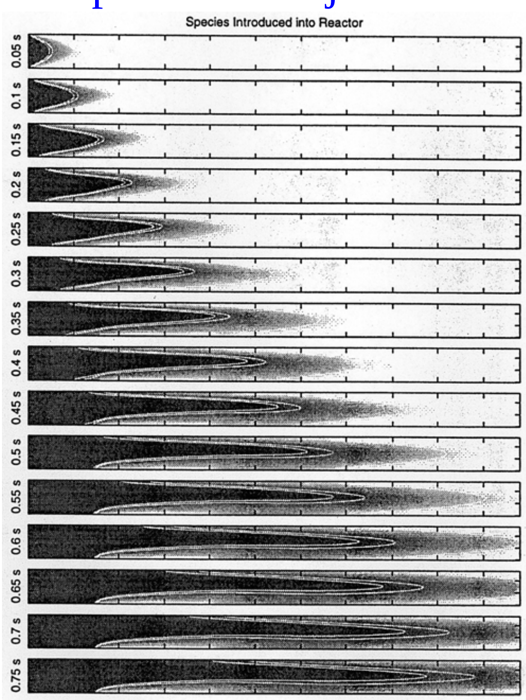
Now project on its dominant subspace (POD)

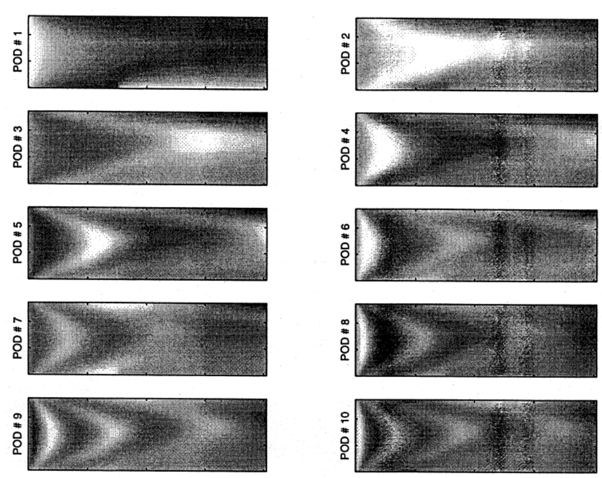
Example : Use POD in CVD reactor (Ly-Tran '99)



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

P. Van Dooren, Gramian based model reduction of large-scale dynamical systems, in *Numerical Analysis 1999*, Chapman and Hall, pp. 231-247, CRC Press, London, 2000.
M. Verlaan and A. Heemink, Tidal flow forecasting using reduced rank square root filters, *Stochastic Hydrology and Hydraulics*, **11**, pp. 349-368, 1997.

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