AA216/CME345: MODEL REDUCTION

Projection-based Model Order Reduction

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Outline

- Ordinary Differential Equation (ODE)

$$\frac{d\mathbf{w}}{dt}(t) = \mathbf{f}(\mathbf{w}(t), t) \tag{1}$$

  - $\mathbf{w} \in \mathbb{R}^N$: State variable
  - initial condition: $\mathbf{w}(0) = \mathbf{w}_0$

- Output equation

$$\mathbf{y}(t) = \mathbf{g}(\mathbf{w}(t), t) \tag{2}$$

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- Note the absence of a parameter dependence for now

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- The state variable – or simply, the state – can be written exactly as a linear combination of vectors spanning $\mathcal{S}$

$$\mathbf{w}(t) = q_1(t)\mathbf{v}_1 + \cdots + q_{k_{\mathcal{S}}}(t)\mathbf{v}_{k_{\mathcal{S}}}$$

  - $\mathbf{V}_{\mathcal{S}} = [\mathbf{v}_1 \ \cdots \ \mathbf{v}_{k_{\mathcal{S}}}] \in \mathbb{R}^{N \times k_{\mathcal{S}}}$ is a **time-invariant** basis for $\mathcal{S}$
  - $(q_1(t), \cdots, q_{k_{\mathcal{S}}}(t))$ are the **generalized coordinates** for $\mathbf{w}(t)$ in $\mathcal{S}$
  - $\mathbf{q}(t) = [q_1(t) \ \cdots \ q_{k_{\mathcal{S}}}(t)]^T \in \mathbb{R}^{k_{\mathcal{S}}}$ is the **reduced-order state vector**

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- In matrix form, the above expansion can be written as

$$\boxed{\mathbf{w}(t) = \mathbf{V}_{\mathcal{S}}\mathbf{q}(t)}$$

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- Substituting the above subspace approximation in Eq. (1) and in Eq. (2) leads to

$$\begin{aligned} \frac{d}{dt}(\mathbf{V}\mathbf{q}(t)) &= \mathbf{f}(\mathbf{V}\mathbf{q}(t), t) + \mathbf{r}(t) \\ \mathbf{y}(t) &\approx \mathbf{g}(\mathbf{V}\mathbf{q}(t), t) \end{aligned}$$

where $\mathbf{r}(t)$ is the residual due to the subspace approximation

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- Over-determined system $(k < N)$

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- Let $\mathbf{V}$ be a matrix in $\mathbb{R}^{N\times k}$
  - $\mathbf{V}$ is an **orthogonal (orthonormal) matrix** if and only if

$$\boxed{\mathbf{V}^T\mathbf{V} = \mathbf{I}_k}$$

Definition

A matrix $\mathbf{\Pi} \in \mathbb{R}^{N \times N}$ is a **projection** matrix (or projective matrix, idempotent matrix) if

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  - $\mathbf{\Pi}$ is diagonalizable (follows from the previous consequence)
  - let k be the rank of $\mathbf{\Pi}$: then, there exists a basis $\mathbf{X}$ such that

$$\mathbf{\Pi} = \mathbf{X} \begin{bmatrix} \mathbf{I}_k & \\ & \mathbf{0}_{N-k} \end{bmatrix} \mathbf{X}^{-1}$$

(follows from the two previous consequences)

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- $\mathbf{\Pi}$ defines the **projection onto** $\mathcal{S}_1$ **parallel to** $\mathcal{S}_2$

$$\boxed{\mathbb{R}^N = \mathcal{S}_1 \oplus \mathcal{S}_2}$$

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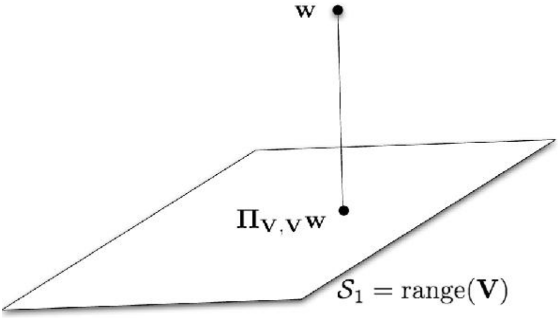
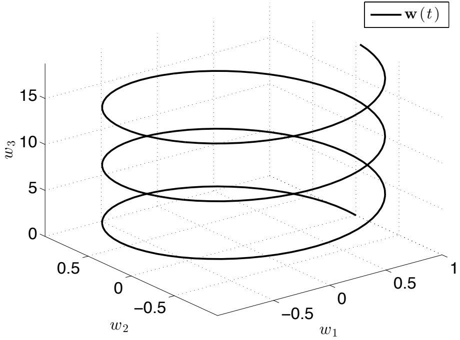


- Example: Helix in 3D ($N = 3$)
  - let $\mathbf{w}(t) \in \mathbb{R}^3$ define a curve parameterized by $t \in [0, 6\pi]$ as follows

$$\mathbf{w}(t) = \begin{bmatrix} w_1(t) \\ w_2(t) \\ w_3(t) \end{bmatrix} = \begin{bmatrix} \cos(t) \\ \sin(t) \\ t \end{bmatrix}$$



- Orthogonal projection onto
  - range($\mathbf{V}$) = span($\mathbf{e}_1, \mathbf{e}_2$)

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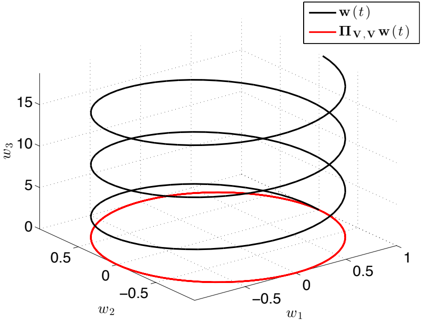

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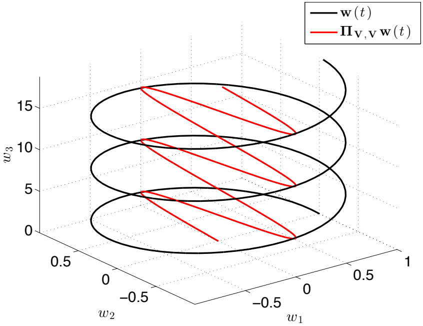

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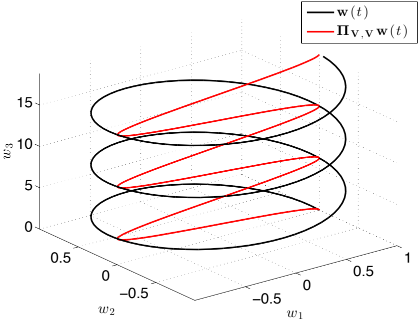

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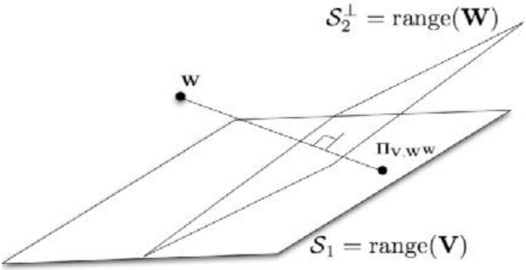

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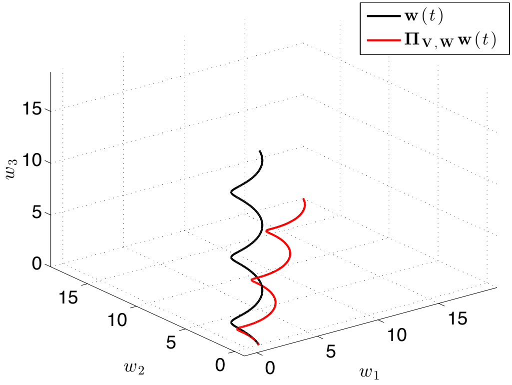
  - projected helix equation
$$\mathbf{\Pi}_{\mathbf{V},\mathbf{W}}\mathbf{w}(t) = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \cos(t) \\ \sin(t) \\ t \end{bmatrix} = \begin{bmatrix} \cos(t) + t \\ \sin(t) + t \\ 0 \end{bmatrix}$$


$\mathbf{w}(t)$
$\mathbf{\Pi}_{\mathbf{V},\mathbf{W}}\,\mathbf{w}(t)$
w_3
15
10
5
0
w_2
15
10
5
0
w_1
0
5
10
15

- Start from a HDM for the problem of interest

$$\boxed{\begin{array}{rcl} \dfrac{d\mathbf{w}}{dt}(t) & = & \mathbf{f}(\mathbf{w}(t), t) \\ \mathbf{y}(t) & = & \mathbf{g}(\mathbf{w}(t), t) \\ \mathbf{w}(0) & = & \mathbf{w}_0 \end{array}}$$

  - $\mathbf{w} \in \mathbb{R}^N$: Vector of state variables
  - $\mathbf{y} \in \mathbb{R}^q$: Vector of output variables (typically $q \ll N$)
  - $\mathbf{f}(\cdot, \cdot) \in \mathbb{R}^N$: Completes the specification of the HDM-based problem

- The goal is to construct a **Projection-based Reduced-Order Model** (PROM)

$$\begin{aligned} \frac{d\mathbf{q}}{dt}(t) &= \mathbf{f}_r(\mathbf{q}(t), t) \\ \mathbf{y}(t) &\approx \mathbf{g}_r(\mathbf{q}(t), t) \end{aligned}$$

  where
  - $\mathbf{q} \in \mathbb{R}^k$: **Vector of reduced-order state variables**, $k \ll N$
  - $\mathbf{y} \in \mathbb{R}^q$: Vector of output variables
  - $\mathbf{f}_r(\cdot, \cdot) \in \mathbb{R}^k$: Completes the description of the PROM
- The discussion of the initial condition is deferred to later

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  - be computationally tractable
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  - preserve as many properties of the HDM as possible

- Recall the residual $\mathbf{r}(t) \in \mathbb{R}^{N \times k}$ introduced by approximating $\mathbf{w}(t)$ as $\mathbf{V}\mathbf{q}(t)$

$$\mathbf{V}\frac{d\mathbf{q}}{dt}(t) = \mathbf{f}\left(\mathbf{V}\mathbf{q}(t), t\right) + \mathbf{r}(t) \Leftrightarrow \mathbf{r}(t) = \mathbf{V}\frac{d\mathbf{q}}{dt}(t) - \mathbf{f}\left(\mathbf{V}\mathbf{q}(t), t\right)$$

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- Constrain this residual to be orthogonal to a subspace $\mathcal{W}$ defined by a **test basis** $\mathbf{W} \in \mathbb{R}^{N \times k}$ – that is, compute $\mathbf{q}(t)$ such that

$$\boxed{\mathbf{W}^T \mathbf{r}(t) = \mathbf{0}}$$

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- This leads to the *descriptive form* of the governing equations of the **Petrov-Galerkin** PROM

$$\boxed{\mathbf{W}^T\mathbf{V}\frac{d\mathbf{q}}{dt}(t) = \mathbf{W}^T\mathbf{f}(\mathbf{Vq}(t), t)}$$

- Assume that $\mathbf{W}^T\mathbf{V}$ is non-singular: In this case, the PROM can be re-written in the *non-descriptive form*

$$\boxed{\begin{array}{rcl} \frac{d\mathbf{q}}{dt}(t) & = & (\mathbf{W}^T\mathbf{V})^{-1}\mathbf{W}^T\mathbf{f}(\mathbf{V}\mathbf{q}(t), t) \\ \mathbf{y}(t) & \approx & \mathbf{g}(\mathbf{V}\mathbf{q}(t), t) \end{array}}$$

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- After the above reduced-order equations have been solved, the subspace approximation of the high-dimensional state vector can be reconstructed, if needed, as follows

$$\boxed{\mathbf{w}(t) \approx \mathbf{Vq}(t)}$$

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- If in addition $\mathbf{V}$ is orthogonal, the reduced-order equations become

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- Special case: **Linear Time-Invariant (LTI)** systems

$$\begin{aligned} \mathbf{f}(\mathbf{w}(t), t) &= \mathbf{A}\mathbf{w}(t) + \mathbf{B}\mathbf{u}(t) \\ \mathbf{g}(\mathbf{w}(t), t) &= \mathbf{C}\mathbf{w}(t) + \mathbf{D}\mathbf{u}(t) \end{aligned}$$

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  - reduced-order LTI operators

$$
\begin{aligned}
\mathbf{A}_r &= (\mathbf{W}^T\mathbf{V})^{-1}\mathbf{W}^T\mathbf{A}\mathbf{V} \in \mathbb{R}^{k\times k}, \ k \ll N \\
\mathbf{B}_r &= (\mathbf{W}^T\mathbf{V})^{-1}\mathbf{W}^T\mathbf{B} \in \mathbb{R}^{k\times p} \\
\mathbf{C}_r &= \mathbf{C}\mathbf{V} \in \mathbb{R}^{q\times k} \\
\mathbf{D}_r &= \mathbf{D} \in \mathbb{R}^{q\times p}
\end{aligned}
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$$\mathbf{w}(0) - \mathbf{V}\mathbf{q}(0) = (\mathbf{I}_N - \mathbf{V}(\mathbf{W}^T\mathbf{V})^{-1}\mathbf{W}^T)\mathbf{w}_0$$

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- Alternative: use an affine approximation $\mathbf{w}(t) = \mathbf{w}(0) + \mathbf{V}\mathbf{q}(t)$ (see Homework $\#1$)

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  - the associated initial condition is

$$\tilde{\mathbf{w}}(0) = \mathbf{V}\mathbf{q}(0) = \mathbf{V}(\mathbf{W}^T\mathbf{V})^{-1}\mathbf{W}^T\mathbf{w}(0)$$

- Recall the projector $\mathbf{\Pi_{V,W}}$

$$\mathbf{\Pi_{V,W}} = \mathbf{V}(\mathbf{W}^T\mathbf{V})^{-1}\mathbf{W}^T$$

Definition

Equivalent HDM

$$\begin{aligned} \frac{d\tilde{\mathbf{w}}}{dt}(t) &= \mathbf{\Pi_{V,W}}\mathbf{f}(\tilde{\mathbf{w}}(t), t) \\ \tilde{\mathbf{y}}(t) &= \mathbf{g}(\tilde{\mathbf{w}}(t), t) \end{aligned}$$

with the initial condition

$$\tilde{\mathbf{w}}(0) = \mathbf{\Pi_{V,W}}\mathbf{w}(0)$$

The equivalent dynamical function is

$$\tilde{\mathbf{f}}(\cdot,\cdot) = \mathbf{\Pi_{V,W}}\mathbf{f}(\cdot,\cdot)$$

- Consider the Petrov-Galerkin PROM

$$\begin{aligned}\frac{d\mathbf{q}}{dt}(t) &= (\mathbf{W}^T\mathbf{V})^{-1}\mathbf{W}^T\mathbf{f}(\mathbf{V}\mathbf{q}(t), t)\\ \mathbf{y}(t) &\approx \mathbf{g}(\mathbf{V}\mathbf{q}(t), t)\\ \mathbf{q}(0) &= (\mathbf{W}^T\mathbf{V})^{-1}\mathbf{W}^T\mathbf{w}(0)\end{aligned}$$

Lemma

Choosing two different bases $\mathbf{V}'$ and $\mathbf{W}'$ that respectively span the same subspaces $\mathcal{V}$ and $\mathcal{W}$ results in the same reconstructed solution $\mathbf{w}(t)$

In other words, subspaces are more important than bases ...

- Consequences
  - given a HDM, a corresponding PROM is uniquely defined by its associated Petrov-Galerkin projector $\mathbf{\Pi}_{\mathbf{V},\mathbf{W}}$

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  - $\mathcal{W}$ and $\mathcal{V}$ belong to the **Grassmann manifold** $\mathcal{G}(k, N)$, which is the set of all subspaces of dimension k in $\mathbb{R}^N$

- Question: Can we characterize the **error** of the solution computed using a PROM relative to the solution obtained using the HDM?

$$\begin{aligned}\mathcal{E}_{\text{PROM}}(t) &= \mathbf{w}(t) - \tilde{\mathbf{w}}(t) \\ &= \mathbf{w}(t) - \mathbf{V}\mathbf{q}(t)\end{aligned}$$

  - assume here a Galerkin projection and an associated orthogonal basis
    - $\mathbf{V}^T\mathbf{V} = \mathbf{I}_k$
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    - $\mathbf{V}^T\mathbf{V} = \mathbf{I}_k$
    - projector $\mathbf{\Pi}_{\mathbf{V},\mathbf{V}} = \mathbf{V}\mathbf{V}^T$
- the error vector can be decomposed into **two orthogonal components**

$$\begin{aligned}\mathcal{E}_{\text{PROM}}(t) &= \mathbf{w}(t) - \mathbf{\Pi}_{\mathbf{V},\mathbf{V}}\mathbf{w}(t) + \mathbf{\Pi}_{\mathbf{V},\mathbf{V}}\mathbf{w}(t) - \mathbf{V}\mathbf{q}(t) \\ &= \left(\mathbf{I}_N - \mathbf{\Pi}_{\mathbf{V},\mathbf{V}}\right)\mathbf{w}(t) + \mathbf{V}\left(\mathbf{V}^T\mathbf{w}(t) - \mathbf{q}(t)\right) \\ &= \mathcal{E}_{\mathbf{V}^\perp}(t) + \mathcal{E}_{\mathbf{V}}(t)\end{aligned}$$

- Error component orthogonal to $\mathbf{V}$

$$\boxed{\mathcal{E}_{\mathbf{V}^\perp}(t) = \left(\mathbf{I}_N - \mathbf{\Pi}_{\mathbf{V},\mathbf{V}}\right)\mathbf{w}(t)}$$

Interpretation: The exact trajectory does not strictly belong to $\mathcal{V} = \text{range}(\mathbf{V}) \Rightarrow$ *projection error*

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Interpretation: An “equivalent” but *different* dynamical system is solved $\Rightarrow$ *modeling error*

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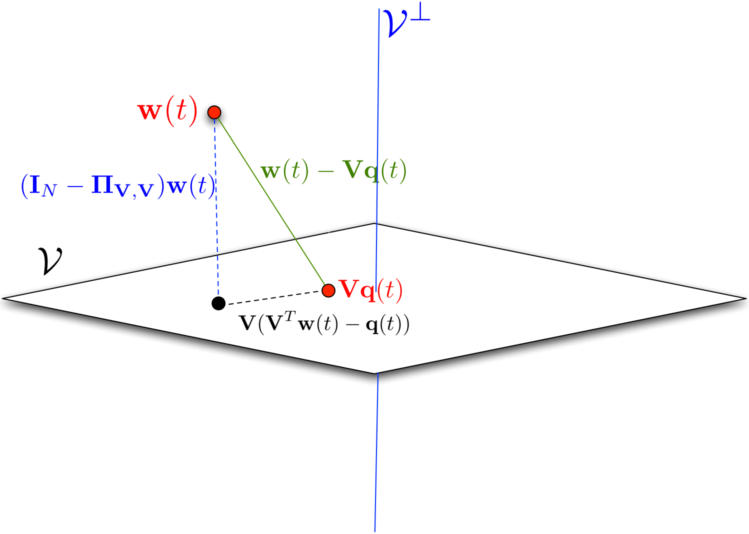
- Note that $\mathcal{E}_{\mathbf{V}^\perp}(t)$ can be computed without executing the PROM and therefore can provide an **a priori** error estimate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$\mathbf{w}(t) - \mathbf{V}\mathbf{q}(t)$
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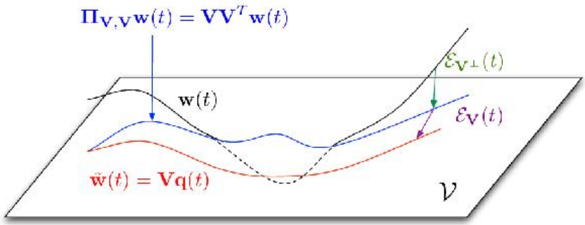

Adapted from *A New Look at Proper Orthogonal Decomposition*, Rathiman and Petzold, SIAM Journal of Numerical Analysis, Vol. 41, No. 5, 2003.

- Again, consider the case of an orthogonal Galerkin projection
- One can derive an ODE governing the behavior of the error component lying in $\mathcal{V}$ in terms of that lying in $\mathcal{V}^\perp$

$$\boxed{\begin{array}{rcl} \dfrac{d\mathcal{E}_{\mathbf{V}}}{dt}(t) & = & \mathbf{\Pi}_{\mathbf{V},\mathbf{V}}\left(\mathbf{f}(\mathbf{w}(t),t) - \mathbf{f}(\mathbf{w}(t) - \mathcal{E}_{\mathbf{V}}(t) - \mathcal{E}_{\mathbf{V}^\perp}(t),t)\right) \\ \mathcal{E}_{\mathbf{V}}(0) & = & \mathbf{0} \end{array}}$$

- In the case of an **autonomous linear system**

$$\boxed{\frac{d\mathbf{w}}{dt}(t) = \mathbf{A}\mathbf{w}(t)}$$

the error ODE has the simple form

$$\boxed{\frac{d\mathcal{E}_{\mathbf{V}}}{dt}(t) = \mathbf{\Pi}_{\mathbf{V},\mathbf{V}}\left(\mathbf{A}\mathcal{E}_{\mathbf{V}}(t)\right) + \mathbf{\Pi}_{\mathbf{V},\mathbf{V}}\left(\mathbf{A}\mathcal{E}_{\mathbf{V}^\perp}(t)\right)}$$

where $\mathcal{E}_{\mathbf{V}^\perp}(t)$ acts as a **forcing term**

- Then, one can then derive the following error bound

Theorem

$$\boxed{\|\mathcal{E}_{PROM}(t)\| \leq \left(\|F(T, \mathbf{V}^T\mathbf{A}\mathbf{V})\|_2 \|\mathbf{V}^T\mathbf{A}\mathbf{V}^\perp\|_2 + 1\right) \|\mathcal{E}_{\mathbf{V}^\perp}(t)\|}$$

where $\|\cdot\|$ *denotes the* $\mathcal{L}_2\left([0, T], \mathbb{R}^N\right)$ *function norm,* $\|f\|_2 = \sqrt{\int_0^T \|f(\tau)\|_2^2 d\tau}$, *and* $F(T, \mathbf{M})$ *denotes the linear operator defined by*

$$\begin{aligned} F(T, \mathbf{M}) : \mathcal{L}_2\left([0, T], \mathbb{R}^N\right) &\rightarrow \mathcal{L}_2\left([0, T], \mathbb{R}^N\right) \\ \mathbf{u} &\longmapsto t \longmapsto \left(\int_0^t e^{\mathbf{M}(t-\tau)}\mathbf{u}(\tau) d\tau\right) \end{aligned}$$

- Error bounds for the nonlinear case can be found in *A New Look at Proper Orthogonal Decomposition*, Rathiman and Petzold, SIAM Journal of Numerical Analysis, Vol. 41, No. 5, 2003

- If $\mathbf{A}$ is **symmetric** and the projection is an **orthogonal Galerkin** projection, the stability of the HDM is preserved during the reduction process (Hint: Consider the equivalent HDM and analyze the sign of $\frac{d}{dt}(\tilde{\mathbf{w}}^T\tilde{\mathbf{w}})$)

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- However, if $\mathbf{A}$ is not symmetric, the stability of the HDM is not preserved: For example, consider a linear HDM characterized by the following unsymmetric matrix

$$\mathbf{A} = \begin{bmatrix} 1 & -3.5 \\ 0.6 & -2 \end{bmatrix}$$

  - consider next the reduced-order basis $\mathbf{V}$

$$\mathbf{V} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

- If $\mathbf{A}$ is **symmetric** and the projection is an **orthogonal Galerkin** projection, the stability of the HDM is preserved during the reduction process (Hint: Consider the equivalent HDM and analyze the sign of $\frac{d}{dt}(\tilde{\mathbf{w}}^T\tilde{\mathbf{w}})$)
- However, if $\mathbf{A}$ is not symmetric, the stability of the HDM is not preserved: For example, consider a linear HDM characterized by the following unsymmetric matrix

$$\mathbf{A} = \begin{bmatrix} 1 & -3.5 \\ 0.6 & -2 \end{bmatrix}$$

  - the eigenvalues of $\mathbf{A}$ are $\{-0.1127, -0.8873\}$ (stable model)
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  - $\mathbf{A}_r = [1]$ and therefore the Galerkin PROM is not asymptotically stable