

Adjoint formulation for manifold-reduced system

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Original governing equation

We refer to the original governing equation as a priori projected system:

$$\begin{aligned}\frac{d\mathbf{x}}{dt} &= \mathbf{P}(\mathbf{x}; \theta) \cdot \mathbf{F}(\mathbf{x}; \theta) \\ \mathbf{P}(\mathbf{x}; \theta) &= \mathbf{I} - \mathbf{V}_f \mathbf{U}_f \\ \mathbf{J} = \nabla_x \mathbf{F} &= \begin{bmatrix} \mathbf{V}_s & \mathbf{V}_f \end{bmatrix} \begin{bmatrix} \Lambda_{ss} & 0 \\ 0 & \Lambda_{ff} \end{bmatrix} \begin{bmatrix} \mathbf{U}_s \\ \mathbf{U}_f \end{bmatrix}\end{aligned}\tag{1}$$

where $\theta \in \mathbb{R}^{N_c}$ is the control parameter. For other notations, refer to the original document.

Observable and its sensitivity

We have the observable as a functional of state variable \mathbf{x} :

$$\mathcal{O}[\mathbf{x}] = \int_0^T o(\mathbf{x}) dt,$$

and we would like to measure its sensitivity to control parameters,

$$\begin{aligned}\nabla_\theta \mathcal{O} &= \int_0^T \nabla_x o \cdot \nabla_\theta \mathbf{x} dt + \int_0^T \nabla_\theta o dt \\ &= \langle \nabla_x o, \nabla_\theta \mathbf{x} \rangle + \int_0^T \nabla_\theta o dt,\end{aligned}\tag{2}$$

where the inner product is defined on \mathbb{R}^N ,

$$\langle \mathbf{a}, \mathbf{b} \rangle = \int_0^T a_i b_i dt$$

with Einstein notation for indices.

Sensitivity equation

To obtain the sensitivity (2), the sensitivity of the solution $\nabla_\theta \mathbf{x}$ needs to be computed. It can be obtained by solving the linearized equation from (1). From now on the equations are expressed in index notation to avoid the ambiguity.

- i, j, k : the index on \mathbb{R}^N space
- c : the index on control space \mathbb{R}^{N_c}
- l : the index on fast manifold space \mathbb{R}^{N_f}

$$\begin{aligned}
\frac{d}{dt} \partial_c x_i &= \partial_c (P_{ij} F_j) \\
&= \partial_k (P_{ij} F_j) \partial_c x_k + \partial_c (P_{ij} F_j) \\
&= [\partial_k P_{ij} \cdot F_j + P_{ij} \cdot \partial_k F_j] \partial_c x_k + \partial_c P_{ij} F_j + P_{ij} \partial_c F_j
\end{aligned} \tag{3}$$

$$\begin{aligned}
\partial_k P_{ij} &= -\partial_k V_{il} U_{lj} - V_{il} \partial_k U_{lj} \\
\partial_c P_{ij} &= -\partial_c V_{il} U_{lj} - V_{il} \partial_c U_{lj}
\end{aligned} \tag{4}$$

Adjoint formulation

We define a constraint functional \mathcal{H} as the inner product of adjoint variable and (3),

$$\begin{aligned}
\mathcal{H} &= \left\langle \mathbf{x}^\dagger, \frac{d}{dt} \partial_c x_i - [\partial_k P_{ij} \cdot F_j + P_{ij} \cdot \partial_k F_j] \partial_c x_k - \partial_c P_{ij} F_j - P_{ij} \partial_c F_j \right\rangle \\
&\equiv 0.
\end{aligned} \tag{5}$$

Since \mathcal{H} is always equivalent to 0 as (3) holds, we add (5) to the sensitivity (2),

$$\nabla_\theta \mathcal{O} = \langle \nabla_x \mathcal{O}, \nabla_\theta \mathbf{x} \rangle + \int_0^T \nabla_\theta \mathcal{O} \, dt = \langle \nabla_x \mathcal{O}, \nabla_\theta \mathbf{x} \rangle + \mathcal{H} + \int_0^T \nabla_\theta \mathcal{O} \, dt$$

which can be expressed in index-wise notation,

$$\begin{aligned}
\nabla_\theta \mathcal{O} &= \langle \nabla_x \mathcal{O}, \nabla_\theta \mathbf{x} \rangle + \mathcal{H} + \int_0^T \nabla_\theta \mathcal{O} \, dt \\
&= \langle \partial_i \mathcal{O}, \partial_c x_i \rangle + \left\langle x_i^\dagger, \frac{d}{dt} \partial_c x_i \right\rangle - \left\langle x_i^\dagger, [\partial_k P_{ij} \cdot F_j + P_{ij} \cdot \partial_k F_j] \partial_c x_k \right\rangle \\
&\quad - \left\langle x_i^\dagger, \partial_c P_{ij} F_j \right\rangle - \left\langle x_i^\dagger, P_{ij} \partial_c F_j \right\rangle + \int_0^T \partial_c \mathcal{O} \, dt
\end{aligned}$$

Our purpose of adjoint formulation is to avoid calculation of $\partial_c x_k$. The adjoint formulation is required for first two terms of \mathcal{H} :

$$\bullet \left\langle x_i^\dagger, \frac{d}{dt} \partial_c x_i \right\rangle$$

$$\begin{aligned}
\left\langle x_i^\dagger, \frac{d}{dt} \partial_c x_i \right\rangle &= \int_0^T x_i^\dagger \frac{d}{dt} \partial_c x_i \, dt \\
&= x_i^\dagger \partial_c x_i \Big|_0^T - \int_0^T \frac{d}{dt} x_i^\dagger \partial_c x_i \, dt \\
&= x_i^\dagger \partial_c x_i \Big|_0^T - \left\langle \frac{d}{dt} x_i^\dagger, \partial_c x_i \right\rangle
\end{aligned}$$

$$\begin{aligned}
& \bullet \left\langle x_i^\dagger, [\partial_k P_{ij} \cdot F_j + P_{ij} \cdot \partial_k F_j] \partial_c x_k \right\rangle \\
& \quad \left\langle x_i^\dagger, [\partial_k P_{ij} \cdot F_j + P_{ij} \cdot \partial_k F_j] \partial_c x_k \right\rangle \\
& = \int_0^T x_i^\dagger [\partial_k P_{ij} \cdot F_j + P_{ij} \cdot \partial_k F_j] \partial_c x_k dt \\
& = \int_0^T x_k^\dagger [\partial_i P_{kj} \cdot F_j + P_{kj} \cdot \partial_i F_j] \partial_c x_i dt \\
& = \left\langle [\partial_i P_{kj} \cdot F_j + P_{kj} \cdot \partial_i F_j] x_k^\dagger, \partial_c x_i \right\rangle
\end{aligned}$$

where nothing except the index exchange between i and k has been done, which corresponds to the transpose of the matrix $\in \mathbb{R}^N \times \mathbb{R}^N$.

Substituting these two terms, we obtain the dual expression for the sensitivity,

$$\begin{aligned}
\nabla_\theta \mathcal{O} &= \langle \nabla_x o, \nabla_\theta \mathbf{x} \rangle + \mathcal{H} + \int_0^T \nabla_\theta o dt \\
&= \langle \partial_i o, \partial_c x_i \rangle + \left\langle x_i^\dagger, \frac{d}{dt} \partial_c x_i \right\rangle - \left\langle x_i^\dagger, [\partial_k P_{ij} \cdot F_j + P_{ij} \cdot \partial_k F_j] \partial_c x_k \right\rangle \\
&\quad - \left\langle x_i^\dagger, \partial_c P_{ij} F_j \right\rangle - \left\langle x_i^\dagger, P_{ij} \partial_c F_j \right\rangle + \int_0^T \partial_c o dt \\
&= \langle \partial_i o, \partial_c x_i \rangle - \left\langle \frac{d}{dt} x_i^\dagger, \partial_c x_i \right\rangle - \left\langle [\partial_i P_{kj} \cdot F_j + P_{kj} \cdot \partial_i F_j] x_k^\dagger, \partial_c x_i \right\rangle \\
&\quad + x_i^\dagger \partial_c x_i \Big|_0^T - \left\langle x_i^\dagger, \partial_c P_{ij} F_j \right\rangle - \left\langle x_i^\dagger, P_{ij} \partial_c F_j \right\rangle + \int_0^T \partial_c o dt \\
&= \left\langle -\frac{d}{dt} x_i^\dagger - [\partial_i P_{kj} \cdot F_j + P_{kj} \cdot \partial_i F_j] x_k^\dagger + \partial_i o, \partial_c x_i \right\rangle \\
&\quad + x_i^\dagger \partial_c x_i \Big|_0^T - \left\langle x_i^\dagger, \partial_c P_{ij} F_j \right\rangle - \left\langle x_i^\dagger, P_{ij} \partial_c F_j \right\rangle + \int_0^T \partial_c o dt
\end{aligned}$$

First term in the equation above is now the new constraint functional, i.e. the adjoint equation, and the other four terms are equivalent to the sensitivity $\nabla_\theta \mathcal{O}$. As long as the adjoint equation equals to 0, $\partial_c x_i$ needs not be computed. Regarding the second term $x_i^\dagger \partial_c x_i$, we don't really have the information about $\partial_c \mathbf{x}$ at T , nor use the final condition of \mathbf{x} as a control parameter. This provides us with the final condition for \mathbf{x}^\dagger ,

$$\mathbf{x}^\dagger = 0 \quad \text{at } t = T$$

Therefore, the sensitivity $\nabla_\theta \mathcal{O}$ can be computed by solving the following adjoint system:

$$\begin{aligned}
\frac{d}{dt} x_i^\dagger &= -[\partial_i P_{kj} \cdot F_j + P_{kj} \cdot \partial_i F_j] x_k^\dagger + \partial_i o \\
\partial_k P_{ij} &= -\partial_k V_{il} U_{lj} - V_{il} \partial_k U_{lj} \\
\mathbf{x}^\dagger &= 0 \quad \text{at } t = T \\
\partial_c \mathcal{O} &= -x_i^\dagger \partial_c x_i \Big|_{t=0} - \left\langle x_i^\dagger, \partial_c P_{ij} F_j \right\rangle - \left\langle x_i^\dagger, P_{ij} \partial_c F_j \right\rangle + \int_0^T \partial_c o dt \\
\partial_c P_{ij} &= -\partial_c V_{il} U_{lj} - V_{il} \partial_c U_{lj}
\end{aligned}$$

Summary

- Governing equation

$$\begin{aligned}\frac{d\mathbf{x}}{dt} &= \mathbf{P}(\mathbf{x}; \theta) \cdot \mathbf{F}(\mathbf{x}; \theta) \\ \mathbf{P}(\mathbf{x}; \theta) &= \mathbf{I} - \mathbf{V}_f \mathbf{U}_f \\ \mathbf{J} = \nabla_x \mathbf{F} &= \begin{bmatrix} \mathbf{V}_s & \mathbf{V}_f \end{bmatrix} \begin{bmatrix} \Lambda_{ss} & 0 \\ 0 & \Lambda_{ff} \end{bmatrix} \begin{bmatrix} \mathbf{U}_s \\ \mathbf{U}_f \end{bmatrix}\end{aligned}\tag{6}$$

- Observable and its sensitivity

$$\begin{aligned}\mathcal{O}[\mathbf{x}; \theta] &= \int_0^T o(\mathbf{x}; \theta) dt \\ \nabla_\theta \mathcal{O} &= \langle \nabla_x o, \nabla_\theta \mathbf{x} \rangle + \int_0^T \nabla_\theta o \, dt\end{aligned}\tag{7}$$

- Adjoint equation

$$\begin{aligned}\frac{d}{dt} x_i^\dagger &= -\partial_i (P_{kj} F_j) x_k^\dagger + \partial_i o \\ &= [\partial_i P_{kj} \cdot F_j + P_{kj} \cdot \partial_i F_j] x_k^\dagger + \partial_i o \\ \partial_k P_{ij} &= -\partial_k V_{il} U_{lj} - V_{il} \partial_k U_{lj} \\ \mathbf{x}^\dagger &= 0 \quad \text{at } t = T\end{aligned}\tag{8}$$

- i, j, k : the index on \mathbb{R}^N space
- c : the index on control space \mathbb{R}^{N_c}
- l : the index on fast manifold space \mathbb{R}^{N_f}

- Adjoint-based sensitivity

$$\begin{aligned}\partial_c \mathcal{O} &= -x_i^\dagger \partial_c x_i \Big|_{t=0} - \left\langle x_i^\dagger, \partial_c (P_{ij} F_j) \right\rangle + \int_0^T \partial_c o \, dt \\ &= -x_i^\dagger \partial_c x_i \Big|_{t=0} - \left\langle x_i^\dagger, \partial_c P_{ij} F_j \right\rangle - \left\langle x_i^\dagger, P_{ij} \partial_c F_j \right\rangle + \int_0^T \partial_c o \, dt \\ \partial_c P_{ij} &= -\partial_c V_{il} U_{lj} - V_{il} \partial_c U_{lj}\end{aligned}\tag{9}$$

Comments on solving the adjoint equation

In solving the adjoint equation (8), we may first think of the same manifold-reduction as we do for the governing equation. That is, we can decompose \mathbf{x}^\dagger into slow and fast manifolds according to the matrix

$$-\partial_i (P_{kj} F_j) = -[\partial_i P_{kj} \cdot F_j + P_{kj} \cdot \partial_i F_j],$$

and reduce the system onto slow manifolds.

Although, this procedure may not be necessary and rather redundant. On this matter you should

have a better knowledge, but I guess manifold reduction is usually required for a nonlinear system which is very stiff until it reaches the slow manifolds. On the other hand, the adjoint system (8), although time-variant, it is basically a linear system. Of course I cannot guarantee that its stiffness is always smaller than that of the original nonlinear system. But I hope a direct time-integration for (8) may be possible in an efficient way, but simpler than just following the same decomposition for nonlinear systems.

Another minor comment is regarding the derivatives $\nabla_x(\mathbf{P} \cdot \mathbf{F})$ and $\nabla_\theta(\mathbf{P} \cdot \mathbf{F})$. Using automatic differentiation, I don't know which one will be more efficient and simple whether decomposing further the terms inside the parentheses or not. In other words, there are two options to compute the derivatives:

$$\begin{aligned} & \nabla(\mathbf{P} \cdot \mathbf{F}) \\ & \text{or} \\ & \nabla \mathbf{P} \cdot \mathbf{F} + \mathbf{P} \cdot \nabla \mathbf{F} \end{aligned}$$