# Using Adjoint Sensitivity Analysis for decoupling the Polynomial Chaos Expansion from the Curse of Dimensionality

Kyriakos D. Kantarakias* and George Papadakis†

Department of Aeronautics, Imperial College London, Exhibition Road, London, SW7 2AZ, UK

July 9, 2019

*Email: k.kantarakias@imperial.ac.uk
†Email: g.papadakis@imperial.ac.uk

# 1 Test on multiple variables

We have the following set of ODEs

$$\frac{dy}{dt} = -ky \; , \; y(0) = y_0 \tag{1}$$

for which there is an analytic solution available $y(t) = y_0 e^{-kt}$. We are going to slightly modify this problem into a system of decoupled equations

$$\frac{d}{dt}\begin{bmatrix} y_1(t) \\ y_2(t) \\ \vdots \\ y_n(t) \end{bmatrix} = \begin{bmatrix} -k_1 & 0 & \dots & 0 \\ 0 & -k_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & -k_n \end{bmatrix} \begin{bmatrix} y_1(t) \\ y_2(t) \\ \vdots \\ y_n(t) \end{bmatrix} \tag{2}$$

The problem is defined in this variable, multidimensional manner in order to illustrate the ability of adjoint to calculate sensitivities to a large number of uncertain parameters with a computational cost decoupled from the dimension of vector $k$. After solving the system (2), we are going to define the objective function

$$F = \frac{1}{n}\sum_{i=1}^{n}\frac{1}{2}\int_0^T (y_i - y_{target})^2 dt \tag{3}$$

This objective function is the average value of the integral of the mean distance of the trajectory $y(t)$ from a target value $y_{target}$. We are interested in quantifying the effects of uncertainties in the design vector $k = [k_1, k_2, \dots, k_n]^T$ to the objective function. To apply the dPCE we need to compute the sensitivities of this objective function with respect to the design vector $k = [k_1, k_2, \dots, k_n]^T$ using the continuous adjoint method. The augmented objective function is defined as

$$F_{aug} = F + \sum_{i=1}^{n}\int_0^T \Psi_i\Big(\frac{dy_i}{dt} + k_i y_i\Big)dt \tag{4}$$

where $\Psi_i$ refer to the adjoint variables at the direction $n$. We differentiate with respect to the design vector $k$.

$$\delta F_{aug} = \delta F + \delta\sum_{i=1}^{n}\int_0^T \Psi_i\Big(\frac{dy_i}{dt} + k_i y_i\Big)dt \tag{5}$$

where $\delta[.] = \frac{\delta}{\delta s}[.]$ is the sensitivity operator that is commonly used in the continuous adjoint literature. We treat each term separately.

$$\delta F = \delta\frac{1}{N}\sum_{i=1}^{n}\frac{1}{2}\int_0^T (y_i - y_{target})^2 dt = \frac{1}{N}\sum_{i=1}^{n}\frac{1}{2}\int_0^T \delta(y_i - y_{target})^2 dt = \frac{1}{N}\sum_{i=1}^{n}\int_0^T (y_i - y_{target})\delta y_i dt$$

Note that the operator $\delta[.]$ permutes with the time integral because $t$ and $k$ are uncorrelated variables. The same permutation property applies with the adjoint variables $\Psi$.

$$\delta\sum_{i=1}^{n}\int_0^T \Psi_i\Big(\frac{dy_i}{dt} + k_i y_i\Big)dt = \underbrace{\sum_{i=1}^{n}\int_0^T \Psi_i\delta\Big(\frac{dy_i}{dt}\Big)dt}_{T_1} + \underbrace{\sum_{i=1}^{n}\int_0^T \Psi_i\delta(k_i y_i)dt}_{T_2} \tag{6}$$

And we treat both terms of equation (6) individually.

$$
\begin{aligned}
T_1 &= \sum_{i=1}^{n} \int_0^T \Psi_i \delta\Big(\frac{dy_i}{dt}\Big) dt = \sum_{i=1}^{n} [\Psi_i \delta y_i]_0^T - \sum_{i=1}^{n} \int_0^T \frac{d\Psi_i}{dt} \delta y_i dt \\
T_2 &= \sum_{i=1}^{n} \int_0^T \Psi_i \delta(k_i y_i) dt = \sum_{i=1}^{n} \int_0^T \Psi_i y_i \delta k_i dt + \sum_{i=1}^{n} \int_0^T \Psi_i k_i \delta y_i dt
\end{aligned}
\tag{7}
$$

Therefore, equation (5) is written as

$$
\delta F_{aug} = \sum_{i=1}^{n} \Big( \int_0^T \frac{(y_i - y_{target})\delta y_i}{N} dt + [\Psi_i \delta y_i]_0^T - \int_0^T \frac{d\Psi_i}{dt} \delta y_i dt + \int_0^T \Psi_i y_i \delta k_i dt + \int_0^T \Psi_i k_i \delta y_i dt \Big)
\tag{8}
$$

To compute the sensitivities of $F$, we must make the expression of equation (8) must be made independent of variances of the primal variables $y_i$ with respect to the design vector $k$. Therefore, the following FAE must be satisfied,

$$
\frac{d}{dt} \begin{bmatrix} \Psi_1(t) \\ \Psi_2(t) \\ \vdots \\ \Psi_n(t) \end{bmatrix} = \begin{bmatrix} k_1 & 0 & \dots & 0 \\ 0 & k_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & k_n \end{bmatrix} \begin{bmatrix} \Psi_1(t) \\ \Psi_2(t) \\ \vdots \\ \Psi_n(t) \end{bmatrix} + \frac{1}{N} \begin{bmatrix} y_1 - y_{target} \\ y_2 - y_{target} \\ \vdots \\ y_n - y_{target} \end{bmatrix}
\tag{9}
$$

The adjoint boundary conditions are

$$
\Psi_i(T) = 0 \ , \ i = 1, \dots, n
\tag{10}
$$

The expression for the sensitivity derivatives is

$$
\frac{\delta F_i}{\delta k} = \int_0^T \Psi_i y_i dt
\tag{11}
$$

## References