Dynamically Orthogonal approximation of time dependent random PDEs

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Part I: Problem Setting and Motivation

Topic: Many engineering/physical problems are described by mathematical models in which, however, the parameters are affected by a considerable amount of uncertainty, due e.g. to measurement errors, limited data availability or intrinsic variability of the phenomenon itself.

Probabilistic framework: The uncertain input data are described in terms of random variables or space/time varying random fields in a complete probability space $(\Omega, \mathcal{A}, \mathcal{P})$, where Ω is the set of outcomes, $\mathcal{A}$ a σ-algebra and $P : \mathcal{A} \to [0, 1]$ a probability measure.

Mathematical Model: Time dependent PDEs with random parameters:

$$\begin{cases} \frac{\partial}{\partial t}u(x,t,\omega) = \mathcal{L}[u(x,t,\omega),\omega], & x \in D,\ t \in \mathcal{T},\ \omega \in \Omega \\ u(x,t=0,\omega) = u_0(x,\omega), & x \in D,\ \omega \in \Omega, \\ u(x,t,\omega) = h(x,t), & x \in \partial D,\ t \in \mathcal{T},\ \omega \in \Omega \end{cases} \tag{1}$$

where $\mathcal{L}$ is a general (linear or non-linear) differential operator, $x \in D \subset \mathbb{R}^d, 1 \le d \le 3$, is the spatial coordinate and t is the time variable in $\mathcal{T} \equiv [0, T]$.

Sources of randomness: coefficients in the equations, initial conditions and forcing terms.

Difficulties in the numerical approximation:

- course of dimensionality: the number of random input variables is often large and typically the computational effort grows exponentially with the dimension of the probability space $\Rightarrow$ For N large, numerically solving the system (1) might be unfeasible.
- long-time integration: The probabilistic structure of the solution u in (1) may significantly deviate in time from that of the input parameters. It follows that the parameters-to-solution map may become more and more complex to approximate as time evolves $\Rightarrow$ Approximations that makes use of fixed (spatial or stochastic) basis functions might require an increasing numbers of terms in time to keep good accuracy level (deteriorating convergence rate).

Goal: Dynamical low rank approximation.

Analytical results: The best S rank approximation of the solution in norm $L^2(D) \times L^2(\Omega)$ is given by the truncated Karhunen-Lòeve expansion $\left(u_S^{KL}\right)$ of u at any time. In practice the optimal S dimensional approximation subspace is difficult to characterize and evolves in time. However the truncated Karhunen-Lòeve expansion provides an analytical lower bound for the approximation error of low rank approximation methods.

Part II: Dynamically Orthogonal Approximation

The Dynamically Orthogonal approximation (DO, proposed e.g. in [2]) consists in a reduced basis approach with bases that evolve in time. The approximate solution is defined as:

$$u_S(x,t;\,\omega) \;=\; \bar{u}_S(x,t) \;+\; \sum_{i=1}^{S} Y_i(t;\,\omega)U_i(x,t) \tag{2}$$

where:

- $\bar{u}_S(x,t) \;\cong\; \mathbb{E}[u(x,t;\,\omega)]$,
- $\{U_i(x,t)\}_{i=1}^S$ are deterministic orthonormal functions in $\mathrm{L}^2(\mathrm{D})$,
- $\{Y_i(t;\,\omega)\}_{i=1}^S$ are zero mean stochastic processes in $\mathrm{L}^2(\Omega)$.

The uniqueness of the representation is provided by imposing the so called *Dynamically Orthogonal condition* [2]:

$$< \frac{\partial U_i(\cdot,t)}{\partial t},\, U_j(\cdot,t) >= 0 \qquad \forall i,\, j \,=1,\ldots S\ \forall t \in [0,\,\mathrm{T}] \tag{3}$$

By performing a Galerkin projection of the governing equation (1), one derives dynamic equations for each term in (2).

DO system

$$\frac{\partial \bar{u}_S(x,\,t)}{\partial t} \;=\; \mathbb{E}[\mathcal{L}(u_S(\cdot,t;\,\omega);\,\omega)] \tag{4}$$

$$\sum_{i=1}^{S} \frac{\partial U_i(x,\,t)}{\partial t}\mathbf{C}_{ij}(t) \;=\; \Pi_{\mathcal{U}}^{\perp}\mathbb{E}[\mathcal{L}(u_S(\cdot,t;\,\omega);\,\omega)Y_j(t;\,\omega)] \qquad \forall j = 1,\ldots,S \tag{5}$$

$$\frac{\partial Y_i(t;\,\omega)}{\partial t} \;=< \mathcal{L}^*(u_S(\cdot,t;\,\omega);\,\omega),\, U_i(\cdot,t) > \qquad \forall i = 1,\ldots,S \tag{6}$$

(and similarly the b. c.) where, being $\mathcal{U} \;=\; span \;<\; U_1(x,t),\ldots,U_S(x,t) \;>$, $\Pi_{\mathcal{U}}^{\perp}$ is the orthogonal projection operator in $L^2(D)$ to the complement of $\mathcal{U}$, i.e. $\Pi_{\mathcal{U}}^{\perp}[v] = v - \sum_{i=1}^{S} \langle v, U_i\rangle\, U_i$,
$\mathbf{C}$ is the covariance matrix of the random variables $\{Y_i\}_{i=1}^S$,
$\mathcal{L}^*(u(x,t,\omega),\omega) = \mathcal{L}(u(x,t,\omega),\omega) - \mathbb{E}\left[\mathcal{L}(u(x,t,\cdot))\right]$.
The initial conditions are imposed to be equal to the best S rank approximation of u_0.

Variational Formulation

Let $\mathcal{H}$ be a Hilbert space such that $u(t) \in \mathcal{H} \otimes \mathrm{L}^2(\Omega),\ \forall t \in \mathcal{T}$.

Definitions and notations:

S-rank function: any square integrable random field $u_S = \bar{u} + u^* = \bar{u}(x) + \mathbf{U}^T(x)\mathbf{Y}(\omega)$ with

- $\bar{u}(x) \in \mathcal{H}$,
- $\mathbf{U} = (U_1, \cdots, U_S) \in [H]^S$ a vector with orthogonal components in $L^2(D)$.
- $\mathbf{Y} = (Y_1, \cdots, Y_S) \in [\mathrm{L}^2(\Omega)]^S$ a vector of uncorrelated random components in $L^2(\Omega)$ with zero mean and positive variance, such that $\mathrm{rank}(\mathbf{C}) = S$

$\boldsymbol{\mathcal{M}_S} \subset \mathcal{H} \otimes \mathrm{L}^2(\Omega)$ is the manifold of all the zero mean S-rank functions.
$\boldsymbol{\mathcal{T}_{u_S^*}\mathcal{M}_S}$ is the tangent space to $\boldsymbol{\mathcal{M}_S}$ at u_S^*. **Orthogonal projection onto $\boldsymbol{\mathcal{T}_{u_S^*}\mathcal{M}_S}$:** $\forall v \in \mathcal{H} \otimes \mathrm{L}^2(\Omega)$, with $v^* = v - \mathbb{E}[v]$, and $u_S^* \in \mathcal{M}_S$

$$P_{u_S^*}(v) = P_{u_S^*}(v^*) = \mathbf{U}^T \left\langle v^*, \mathbf{U}^T \right\rangle + (\Pi_{\mathcal{U}}^{\perp}\{\mathbb{E}[v^*\mathbf{Y}^T]\}\mathbf{C}^{-1})^T\mathbf{Y}$$

Equivalent formulation of the DO approach: The DO approximation corresponds to a Galerkin projection, namely the DO approximate solution is the S rank random field that minimizes the residual of the governing equation in $\boldsymbol{\mathcal{T}_{u_S^*(t)}\mathcal{M}_S}$ at any time instant, i.e.:

Weak Formulation. *At each $t \in \mathcal{T}$, find $u_S(\cdot,t,\cdot) = \bar{u}_S(\cdot,t) + u_S^*(\cdot,t,\cdot)$ with $(\bar{u}_S, u_S^*) \in \mathcal{H} \times \mathcal{M}_S$ such that:*

$$\mathbb{E}\left[\left\langle \frac{\partial u_S(\cdot,t,\cdot)}{\partial t} \;-\; \mathcal{L}(u_S(\cdot,t,\cdot)),\, v \right\rangle\right] = 0, \quad \forall v : (\bar{v}, v^*) \in \mathcal{H} \times \mathcal{T}_{u_S^*(t)}\mathcal{M}_S$$

or equivalently:

$$\frac{\partial u_S(x,t,\omega)}{\partial t} = \mathbb{E}\left[\mathcal{L}(u_S(x,t,\cdot)\right] + P_{u_S^*(t)}(\mathcal{L}^*(u_S(x,t,\omega)))$$

REMARK: The DO variational formulation is the analogue of the **Dirac-Frenkel Variational Principle** used e.g. for

- **MCTDH** approximation of deterministic Schrodinger equations [see e.g. *C. Lubich* et al.],
- **Dynamical Low Rank** approximation of evolution tensor equations [see e.g. *O. Koch, C. Lubich*].

Error Analysis

Let u be the solution of a linear parabolic PDE with stochastic diffusion coefficient. Then, under suitable assumptions, the DO approximation error can be bounded in terms of best approximation error.

Theorem. [3] *Assume that $0 \le t \le \bar{t}$ the best rank S approximation $u_S^{KL}(t) \in \left(H^2(D) \cap H_0^1(D)\right) \otimes L^2(\Omega)$ is continuously differentiable in time and $\sigma_{min}(u_S^{KL}(t)) \ge \rho > 0$. Then $\exists \hat{t} \in (0,\ \bar{t}]$ such that:*

$$\|u_S^{DO}(t) - u(t)\|_0^2 + \underline{a}\int_0^t |u_S^{DO}(\tau) - u_S^{KL}(\tau)|_1^2 d\tau \le 2\alpha e^{2\beta(t)} \int_0^t \|u_S^{KL}(\tau) - u(\tau)\|_1^2 d\tau, \tag{7}$$

for all $0 < t \le \hat{t}$. $\|.\|_1$, $(|.|_1)$ denotes the (semi) norm in $H^1(D) \otimes L^2(\Omega)$, $\|.\|_0$ the norm in $L^2(D) \otimes L^2(\Omega)$. $\beta(t)$ depends on $\frac{1}{\rho}$ and $\|\mathcal{L}^*(u_S^{KL}(\tau))\|_0$, $\|\mathcal{L}^*(u(\tau))\|_0$, $\|\mathcal{L}^*(u_S^{DO}(\tau))\|_0$ $\|\dot{u}_S^{KL}(\tau)\|_0$ that are bounded under mild assumptions on the data (see [3] for further details),

REMARKS: It has been shown by means of simple analytical examples that the continuous time-differentiability of u_S^{KL} is a strictly necessary condition to get bound (7).

Part III: Numerical aspects

We approximate the deterministic equations (4)-(5) by Finite Elements method and equations (6) by Stochastic Collocation. The time derivative is discretized by a semi-implicit Euler method while both the covariance matrix and the projection operator are treated explicitly in order to linearize and decouple the deterministic equations from the stochastic ones.

Problem: The effective rank of the approximate solution may significantly change in time. This implies that the covariance matrix which couples the set of deterministic equations (5) may, in general, be singular or nearly singular as time evolves.

Strategy: Orthogonalize the stochastic coefficients $\mathbf{Y}$ at each time step before solving system (5). Namely, taken $(\mathbf{V},\ \mathbf{Z})$ such that $\mathbf{U}^T\mathbf{Y} = \mathbf{V}^T\mathbf{Z}$ and $\mathbb{E}[Z_i Z_j] = \delta_{ij}\lambda_i$, only the modes V_i with $\mathbb{E}[Z_i^2] > \epsilon$ evolve, the others remain constant.

Numerical examples

EXAMPLE 1: Linear parabolic PDE with stochastic diffusion coefficient and deterministic initial condition

$$\frac{\partial u(x,t,\omega)}{\partial t} - \mathrm{div}\left(a(x,\omega)\frac{\partial u(x,t,\omega)}{\partial x}\right) = 0, \qquad x \in [0,\ 1],\ t \in \mathcal{T}, \omega \in \Omega \tag{8}$$

$$u(0,t,\omega) = u(1,t,\omega) = 0, \qquad t \in \mathcal{T}, \omega \in \Omega \tag{9}$$

$$u(x,0,\omega) = 10\sin(\pi x) \qquad x \in [0,\ 1], \omega \in \Omega \tag{10}$$

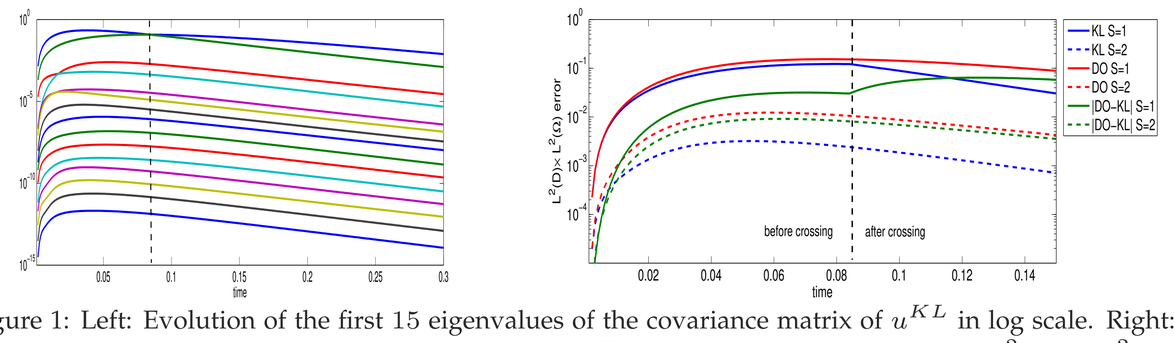

Figure 1: Left: Evolution of the first 15 eigenvalues of the covariance matrix of u^{KL} in log scale. Right: The best approximation error (blue) and the error of the DO approximate solution (red) in $L^2(D) \times L^2(\Omega)$ norm with $S = 1$ (solid line) and $S = 2$ (dotted line), in log scale. In green the $L^2(D) \times L^2(\Omega)$ norm of the difference between u_S^{DO} and u_S^{KL} with $S = 1$ (solid line) and $S = 2$ (dotted line).

Remark: The DO approximation error with $S = 1$ is well controlled by the best approximation error before the crossing between the first two eigenvalues of the covariance matrix of u^{KL}, namely if u_1^{KL} is continuously differentiable in time. After the crossing the DO error degenerates. With $S = 2$, u_2^{KL} is continuously time differentiable in the whole time interval and the control on the DO approximation error is smooth after the crossing as well.

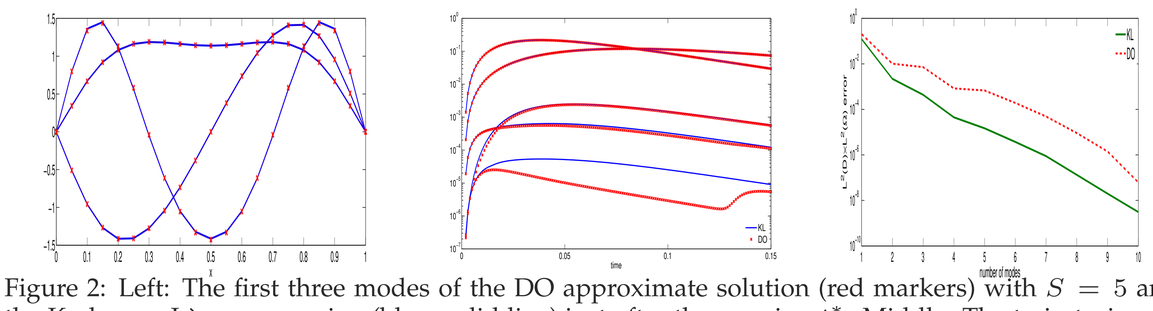

Figure 2: Left: The first three modes of the DO approximate solution (red markers) with $S = 5$ and of the Karhunen-Lòeve expansion (blue, solid line) just after the crossing t^*. Middle: The trajectories of the eigenvalues of the covariance matrix of the stochastic coefficient of u_5^{DO} (red markers) and u_5^{KL} (blue, solid line), in log scale. The first DO and KL modes and eigenvalues are almost indistinguishable. Right: The best approximation error (green) and the error of the DO approximate solution (red, dotted line) in $L^2(D) \times L^2(\Omega)$ norm w.r.t. the number of modes at time $T = 0.1$. The plot shows an exponential convergence rate with respect to the number of modes.

EXAMPLE 2: PDE with non-linear reaction term. (random coefficient and deterministic initial condition)

$$\begin{cases} \dfrac{\partial u(\mathbf{x},t;\omega)}{\partial t} - \Delta u(\mathbf{x},t;\omega) = F(u(\mathbf{x},t;\omega);\omega) & \mathbf{x} \in [0,\ 1]^2,\ t \in \mathrm{T}, \omega \in \Omega \\ \dfrac{\partial u}{\partial \mathbf{n}}(\mathbf{x},t,\omega) = 0, & \mathbf{x} \in \partial\Omega,\ t \in \mathcal{T}, \omega \in \Omega \\ u(\mathbf{x},0;\omega) = u_0(\mathbf{x}) & \mathbf{x} \in [0,\ 1]^2,\ \omega \in \Omega \end{cases} \tag{11}$$

with $F(u) = \beta u(u-1)(\alpha(\omega) - u)$.
The initial condition is a step function and the solutions are a traveling wave with stochastic speed.

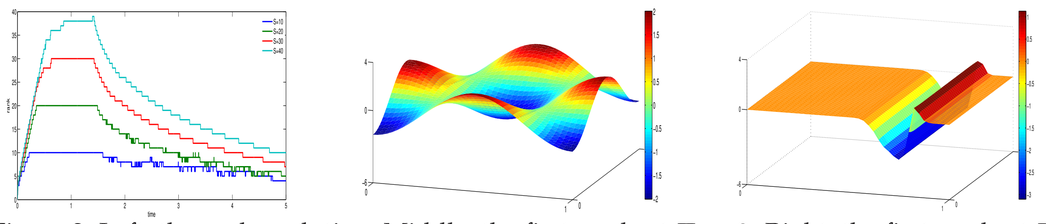

Figure 3: Left: the rank evolution. Middle: the first mode at $T = 0$. Right: the first mode at $T = 0,05$.

Remark: The deterministic modes and the stochastic coefficients of the DO solution adapt in time to the solution. The effective rank of the DO solution evolves in time as well. However this problem is not really suitable for low rank approximation because of the presence of a traveling front at random speed and the DO method is also negatively effected by the frequent crossings of the eigenvalues.

References

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