Dynamical Low Rank Approximation

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Based on the work in [7].

Outline

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Outline

Introduction

Brief Problem Setting

Consider a random evolutionary PDE with random initial condition and random operator $\mathcal{F}$

$$\dot{u} = \mathcal{F}(u)$$

Monte Carlo Method

- conduct simulations for each realization
- MC requires a lot of sampling

Surrogate Model

- Spectral expansion
  $$u(t, x, \omega) = \sum_{i=1}^{R} U_i(t, x) Y_i(\omega)$$
  Basis functions $\{Y_i\}_{i=1}^{R}$ and deterministic coefficients $\{U_i\}_{i=1}^{R}$
- Reduced basis method
  $$u(t, x, \omega) = \sum_{i=1}^{R} U_i(x) Y_i(t, \omega)$$
  The basis functions $\{U_i\}_{i=1}^{R}$ and the stochastic coefficients $\{Y_i\}_{i=1}^{R}$

$\rightarrow$ require a large R for long-time integration.

Dynamical Low Rank Approximation

Dynamical Low Rank Approximation

$$u(t, x, \omega) = \sum_{i=1}^{R} U_i(t, x) Y_i(t, \omega)$$

The idea: update both of $\{Y_i\}_{i=1}^R$ and $\{U_i\}_{i=1}^R$
How: Project $\mathcal{F}(u)$ onto the tangent space of manifold of the R-rank function

Note that

- Karhunen–Loève expansion is optimal in this format
(you need to remove the mean term and this optimality is in the sense of mean square)
- Initial Random field should be set as R rank approximation.
- This method was developed in three different fields: matrix differential equations, time-dependent Schrödinger equations, and uncertainty quantification (UQ).

Outline

Setting

- H and V are two separated Hilbert spaces forming a Gelfand triple (V, H, V') e.g. $V = H_0^1(D), H = L^2(D)$
- Final time T
- Probability space $(\Omega, \mathcal{A}, \rho)$

Assume a solution $u_{true} \in L^2(0, T; L^2_\rho(\Omega; V))$ exists with $\dot{u}_{true} \in L^2(0, T; L^2_\rho(\Omega; V'))$ satisfying

$$(\dot{u}_{true)}, v)_{V',V,L^2_\rho} = (\mathcal{F}(u_{true}), v)_{V',V,L^2_\rho} \quad \forall v \in L^2_\rho(\Omega, V)$$

DLRA formulation

There are three equivalent formulations

$$u(t,x,\omega) = \sum_{i=1}^{R} U_i(t,x) Y_i(t,\omega)$$

- Dynamically orthogonal (DO) formulation
  $< U_i(t), U_j(t) >_H = \delta_{i,j}$ and $< \dot{U}_i(t), U_j(t) >_H = 0$
- Dual DO formulation
  $< Y_i(t), Y_j(t) >_{L^2_\rho} = \delta_{i,j}$ and $< \dot{Y}_i(t), Y_j(t) >_{L^2_\rho} = 0$
- Doblue dynamically orthogonal (DDO) formulation

$$u(t,x,\omega) = \sum_{i=1}^{R} S_{i,j}(t) U_i(t,x) Y_j(t,x)$$

$< U_i(t), U_j(t) >_H = < Y_i(t), Y_j(t) >_{L^2_\rho} = \delta_{i,j}$ and
$< \dot{U}_i(t), U_j(t) >_H = < \dot{Y}_i(t), Y_j(t) >_{L^2_\rho} = 0$

Geometric interpretation of DLR

Manifold of R-rank functions (Dual DO formulation)

$$\mathcal{M}_R = \Bigg\{ v \in L^2_\rho(\Omega, V) \mid v = \sum_{i=1}^{R} U_i Y_i = UY^\top,$$

$$\mathbb{E}[Y_i, Y_j] = \delta_{ij}, \forall 1 \leq i, j \leq R, \{U_i\}_{i=1}^{R} \text{ linearly independent } \Bigg\}.$$

$\mathcal{M}_R$ forms an infinite dimensional differential manifold structure

Tangent space at u

The tangent space $\mathcal{T}_u\mathcal{M}_R$ at a point $u = UY^\top \in \mathcal{M}_R$ can be characterized as

$$\mathcal{T}_u\mathcal{M}_R = \Bigg\{ \delta v \in L^2_\rho(\Omega, V) \mid \delta v = \sum_{i=1}^{R} U_i \delta Y_i + \delta U_i Y_i$$

$$\delta U_i \in V, \delta Y_i \in L^2_\rho, \quad \mathbb{E}[\delta Y_i Y_j] = 0, \forall 1 \leq i, j \leq R \Big\}.$$

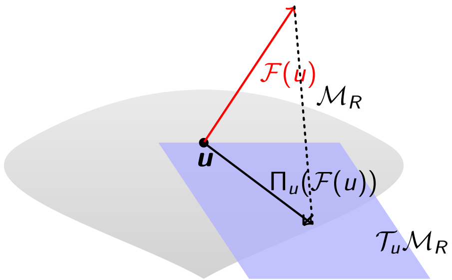
Evolution equation

$$\dot{u} = \Pi_u(\mathcal{F}(u))$$

where Π_u is orthogonal projection on the tangent space at u

Manifold and Tangent Space Projection

$$\dot{u} = \Pi_u(\mathcal{F}(u))$$



DLRA equation

$$\begin{aligned}\dot{u} &= \Pi_u(\mathcal{F}(u)) \\ &= \mathcal{P}_{\mathcal{Y}}[\mathcal{F}(u)] + \mathcal{P}_{\mathcal{Y}}^{\perp}[\mathcal{P}_{\mathcal{U}}[\mathcal{F}(u)]]\end{aligned}$$

- $\{U_i\}_{i=1}^R, \{Y_i\}_{i=1}^R$ are updated while satisfying the following system of equations:

$$\begin{array}{ll} < \dot{U}_j, v >_{V'V} = < \mathbb{E}\left[\mathcal{F}(u) Y_j\right], v >_{V',V} & \forall v \in V, j = 1, \ldots, R \\ \dot{Y}_j = \sum_{i=1}^R \left(M^{-1}\right)_{j,i} \mathcal{P}_{\mathcal{Y}}^{\perp}[< \mathcal{F}(u), U_i >_{V'V}] & \text{in } L^2_\rho, j = 1, \ldots, R \end{array}$$

  - Mass matrix: $M_{i,j} = < U_i, U_j >_{L^2(D)}$
  - Projector on orthogonal complement of $\mathcal{Y}$: $\mathcal{P}_{\mathcal{Y}}^{\perp}[v] = v - \sum_{i=1}^R \mathbb{E}[v Y_i] Y_i$
- For the solution of the equations above,the following variational formulation is hold.

$$< u - \Pi_u(\mathcal{F}(u), v >_{V',V,L^2_\rho} = 0 \quad \forall v \in L^2_\rho(\Omega, V)$$

Discretization

Stochastic discretization:

- Sample points: $\{\omega_k\}_{k=1}^{N_c} \subset \Omega$ with $N_c < \infty$
- Positive weights: $\{\lambda_k\}_{k=1}^{N_c}, \lambda_k > 0, \sum_{k=1}^{N_c} \lambda_k = 1$
- The discrete probability measure: $\hat{\rho} := \sum_{k=1}^{N_c} \lambda_k \delta_{\omega_k}$
- The discrete probability space: $\left(\hat{\Omega} = \{\omega_k\}_{k=1}^{N_c}, 2^{\hat{\Omega}}, \hat{\rho}\right)$

$\rightarrow$ random variables are represented as $\mathbb{R}^{N_c}$ vectors

Space discretization:

- A finite dimensional space: $V_h \subset V$, $|V_h| = N_h$
- Piecewise linear finite elements: $P1$

Time discretization:

- Discretized time: $0 = t_0 < t_1 < \cdots < t_N = T$
- Time step: $\triangle t := t_{n+1} - t_n$

Goal: approximate the solution $u^n \in V_h \otimes \ell^2(N_c) \quad \forall n = 0, \ldots, N.$
effectively!

Fully discretized scheme

1. Compute the deterministic basis $\left\{ \tilde{U}_j^{n+1} \right\}_{j=1,\cdots,R}$

$$\left\langle \frac{\tilde{U}_j^{n+1} - U_j^n}{\Delta t}, v_h \right\rangle_{L^2(D)} - \left\langle \mathbb{E}\left[\mathcal{F}\left(u^n, u^{n+1}\right) Y_j^n \right], v_h \right\rangle_{L^2(D)} = 0, \quad \forall v_h \in V_h.$$

2. Compute the stochastic basis $\left\{ \tilde{Y}_j^{n+1} \right\}_{j=1,\cdots,R}$

$$\frac{\tilde{Y}_j^{n+1} - Y_j^n}{\Delta t} \tilde{M}^{n+1} - \mathcal{P}_{\mathcal{Y}}^{\perp}[< \mathcal{F}\left(u^n, u^{n+1}\right), \tilde{U}_j^{n+1} >_{L^2(D)}] = 0,$$

3. Reorthonormalize the stochastic basis

$$\sum_{j=1}^{R} Y_j^{n+1} U_j^{n+1} = \sum_{j=1}^{R} \tilde{Y}_j^{n+1} \tilde{U}_j^{n+1}, \quad \mathbb{E}[Y^{n+1^\top} Y^{n+1}] = \mathrm{Id}.$$

This scheme coincides with projector-splitting scheme when it is full-rank.

Outline

Initial Assignment

Assumption

- Inital random field $u_0(x, \omega) \in L^2(\Omega) \otimes L^2(D)$ is given explicitly
- We can sample from it(each realization will be deterministic function)
- $u_0(x, \omega)$ admits Karhunen-Loève expansion (SVD representation)

Goal

$$u_0(x, \omega) \approx \sum_{i=1}^{R} U_i^0(x) Y_i^0(\omega)$$

- KL expansion(SVD representation) is the best approximatin in this format

Karhunen-Loève expansion(SVD representation)

- Covariance bilinear form: $\mathrm{Cov_u} : L^2(D) \times L^2(D) \to \mathbb{R}$
  $\mathrm{Cov_u}(h, k) = \mathbb{E}[< h, u(\omega) >_{L^2(D)} < k, u(\omega) >_{L^2(D)}]$
- Covariance operator $\mathrm{C_u} : L^2(D) \to L^2(D)$
  $< \mathrm{C_u}\, h, k >_{L^2(D)} = \mathrm{Cov_u}(h, k)$

Diagonalize Covariance operator $\to$ hard to compute ...

Karhunen-Loève expansion(SVD representation)

- Covariance bilinear form: $\mathrm{Cov_u} : L^2(D) \times L^2(D) \to \mathbb{R}$
  $\mathrm{Cov_u}(h, k) = \mathbb{E}[< h, u(\omega) >_{L^2(D)} < k, u(\omega) >_{L^2(D)}]$
- Covariance operator $\mathrm{C_u} : L^2(D) \to L^2(D)$
  $< \mathrm{C_u}\, h, k >_{L^2(D)} = \mathrm{Cov_u}(h, k)$

Diagonalize Covariance operator $\to$ hard to compute ...

- Bilinear form: $\mathbb{F}_u : L^2(\Omega) \times L^2(\Omega) \to \mathbb{R}$
  $\mathbb{F}_u(h, k) =< \mathbb{E}[hu(x)], \mathbb{E}[ku(x)] >_{L^2(D)}$
- Operator $F_u : L^2(\Omega) \to L^2(\Omega)$
  $\mathbb{E}[F_u hk] = \mathbb{F}_u(h, k)$

Diagonalize Operator F_u $\to$ In our setting of discretization, this operator is just a $N_c \times N_c$ matrix !!!

Matrix-like interpretation

Basis functions of finite element space:

$$\Phi = [\varphi_1, \ldots, \varphi_{N_h}] \qquad \varphi_i \in V_h$$

Coefficient matrix for each realization:

$$U = \begin{bmatrix} u_1(\omega_1) & \ldots & u_1(\omega_{N_c}) \\ \vdots & \ddots & \vdots \\ u_{N_h}(\omega_1) & \ldots & u_{N_h}(\omega_{N_c}) \end{bmatrix} \in \mathbb{R}^{N_h \times N_c}$$

Random field can be represented as:

$$[u_h(\omega_1), \ldots, u_h(\omega_{N_c})] = \left[\sum_{i=1}^{N_h} u_i(\omega_1)\varphi_i, \ldots, \sum_{i=1}^{N_h} u_i(\omega_{N_c})\varphi_i \right] = \Phi U$$

Matrix-like interpretation

KL expansion is essentially SVD of $\Phi U \in V_h \otimes \ell^2(N_c)$.
$U' \in R \times N_h$ and $Y' \in R \times N_c$

$$\Phi U = \Phi U'^T \Sigma Y'$$

Here,we define $(\Phi^T\Phi)_{i,j} = <\varphi_i, \varphi_j>_{L^2(D)}$, $(Y'Y'^T)_{i,j} = \frac{1}{N_c}\sum_{k=1}^{N_c} y'^i_k y'^j_k$

$$U'\Phi^T\Phi U^T = I_R$$
$$Y'Y'^T = I_R$$

Covariance operator C_u is essentially
$\Phi U U^T \Phi^T = \Phi U'^T \Sigma^2 U' \Phi^T \in V_h \otimes V_h$ hard to compute...
Operator F is essentially
$U^T \Phi^T \Phi U = Y'^T \Sigma^2 Y' \in \mathbb{R}^{N_c \times N_c}$ Computable !!!

Outline

Stability result(Continuous)

- $\mathcal{F}(u) = f - \mathcal{L}(u)$ with $\mathcal{L}$ linear elliptic. And assume that $\mathcal{L}$ can be decomposed as $\mathcal{L} = \mathcal{L}_{det} + \mathcal{L}_{stoch}$
- $C_{\mathcal{L}}, C_p > 0$ are coercivity and continuous embedding constant

$$
\begin{aligned}
&|u_{\text{true}}(T)\|^2_{H,L^2_p} + C_{\mathcal{L}} \int_0^T \|u_{\text{true}}(t)\|^2_{V,L^2_p}\, dt \\
&\leq \|u_{\text{true}}(0)\|^2_{H,L^2_p} + \frac{C_p^2}{C_{\mathcal{L}}} \|f\|^2_{L^2_p(0,T;L^2_p(\Omega;H))}
\end{aligned}
$$

The same equation holds for DLRA answer

Stability result(Discrete)

- Implicit scheme $\mathcal{F}(u_{n+1}, u_n) = f - \mathcal{L}(u_{n+1})$

$$\|u_h^N\|^2_{H,L^2_p} + \Delta t C_L \sum_{n=0}^{N-1} \|u_h^{n+1}\|^2_{V,L^2_p} \leq \|u_h^0\|^2_{H,L^2_p} + \Delta t \frac{C_p^2}{C_L} \sum_{n=0}^{N-1} \|f(t_{n+1})\|^2_{H,L^2_p}$$

- Explicit scheme $\mathcal{F}(u_{n+1}, u_n) = f - \mathcal{L}(u_n)$
  Under CFL condition $\frac{\Delta t}{h^2} \leq C$,

$$\|u_h^N\|^2_{H,L^2_p} + \Delta t C_L (1-\kappa) \sum_{n=0}^{N-1} \|u_h^{n+1}\|^2_{V,L^2_p} \leq \|u_h^0\|^2_{H,L^2_p} + \frac{\Delta t C_p^2}{C_L} \sum_{n=0}^{N-1} \|f(t_n)\|^2_{H,L^2_p}$$

- Semi-implicit scheme $\mathcal{F}(u_{n+1}, u_n) = f - \mathcal{L}_{stoch}(u_{n+1}) - -\mathcal{L}_{det}(u_n)$ Under CFL condition $\frac{\Delta t}{h^2} \leq C$,

$$\|u_h^N\|^2_{H,L^2_p} + \Delta t C_L (1-\kappa) \sum_{n=0}^{N-1} \|u_h^{n+1}\|^2_{V,L^2_p} \leq \|u_h^0\|^2_{H,L^2_p} + \frac{\Delta t C_p^2}{C_L} \sum_{n=0}^{N-1} \|f(t_n, t_{n+1})\|^2_{H,L^2_p}$$

Outline

Dynamical Low Rank Approximation for Matrix Case

Solving the following matrix differential equation where $A(t) \in \mathbb{R}^{m \times n}, 0 \leq t \leq T$

$$\dot{A} = F(A)$$

- Best R rank approximation is given by

$$X \in \mathcal{M}_{\mathcal{R}} \quad s.t. \quad ||X - A|| = min!$$

- Instead,

$$\dot{Y} \in \mathcal{T}_{\mathcal{Y}}\mathcal{M}_{\mathcal{R}} \quad s.t. \quad ||\dot{Y} - F(Y)|| = min!$$
$$\Leftrightarrow \dot{Y} = \mathcal{P}_{\mathcal{Y}}[F(Y)]$$

where $\mathcal{P}_{\mathcal{Y}}$ is orthogonal projection onto $\mathcal{T}_{\mathcal{Y}}\mathcal{M}_{\mathcal{R}}$

Dynamical Low Rank Approximation for Matrix Case

- None unique decomposition $Y = USV^T$
  where $U \in \mathbb{R}^{m\times r}$and $V \in \mathbb{R}^{n\times r}$ with orthonormal columns ,and $S \in \mathbb{R}^{r\times r}$,
- $\mathcal{P}_{\mathcal{Y}}[Z] = ZVV^T + UU^TZ - UU^TZVV^T$ at $Y = USV^T$
- Gauge condition $U^T\dot{U} = 0$ and $V^T\dot{V} = 0$
- $\dot{Y} = \mathcal{P}_{\mathcal{Y}}[F(Y)]$

From these, we can derive the following updates

$$\dot{U} = (I_m - UU^T)F(Y)VS^{-1}$$
$$\dot{V} = (I_n - VV^T)F(Y)^TUS^{-T}$$
$$\dot{S} = U^TF(Y)V$$

This is not robust when small singular values are involved

Projector-splitting integrator

$$\begin{aligned}\dot{Y} &= \mathcal{P}_{\mathcal{Y}}[F(Y)] \\ &= F(Y)VV^T + UU^T F(Y) - UU^T F(Y)VV^T \\ &= \mathcal{P}_{\mathcal{V}}[F(Y)] + \mathcal{P}_{\mathcal{U}}[F(Y)] - \mathcal{P}_{\mathcal{V}}[\mathcal{P}_{\mathcal{U}}[F(Y)]]\end{aligned}$$

Let $Y_0 = U_0 S_0 V_0^\top \in \mathcal{M}_r$.

1. **K-step: Update** $U_0 \to U_1$, $S_0 \to \hat{S}_1$
   $\dot{K}(t) = F\big(K(t)V_0^\top\big)V_0, \quad K(t_0) = U_0 S_0$
   Integrate to $t = t_1$ and perform a QR factorization $K(t_1) = U_1 \hat{S}_1$.
2. **S-step: Update** $\hat{S}_1 \to \tilde{S}_0$
   $\dot{S}(t) = -U_1^\top F\big(U_1 S(t) V_0^\top\big)V_0, \quad S(t_0) = \hat{S}_1$
   Integrate to $t = t_1$.
3. **L-step: Update** $V_0 \to V_1$, $\tilde{S}_0 \to S_1$
   $\dot{L}(t) = F\big(U_1 L(t)^\top\big)^\top U_1, \quad L(t_0) = V_0 \tilde{S}_0^\top$
   Integrate to $t = t_1$ and perform a QR factorization $L(t_1) = V_1 S_1^\top$.

The approximation is given by $Y_1 = U_1 S_1 V_1^\top \in \mathcal{M}_r$.

Properties of Projector-splitting integrator

Properties:

- No need to calculate the inverse of matrix.
- Robustness in presence of small singular value.
- For R rank matrix $A = USV^t$ with $U^T U$ and $V^T V$ invertible, This approximation is exact.
- This scheme extends to $\dot{A} = F(A)$ by setting $\Delta A := \Delta t F(A_0)$ (but exactness result does not hold).

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Thanks for your attention!