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14. ABSTRACT The focus of this project is about numerical solutions of optimal control problems using the analysis of variance (ANOVA)analysis. The impact of random parameter dependent boundary conditions on the solutions of a class of nonlinear partial differential equations (PDEs) is considered. Because the boundary conditions are random field, the PDE becomes stochastic PDE. The concepts of effective dimensions are used to determine the accuracy of the ANOVA expansions. Demonstrations are given to show that whenever truncated ANOVA expansions of functionals provide accurate approximations, optimizers found through a simple surrogate optimization strategy are also relatively accurate.

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Numerical solutions for optimal control under SPDE constraints

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NUMERICAL SOLUTIONS FOR OPTIMAL CONTROL PROBLEMS UNDER SPDE CONSTRAINTS

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Abstract

In the past 12 months, we have been focusing our effort on three projects: the first one is about numerical solutions of optimal control problems using the analysis of variance (ANOVA)analysis; the second one is error analysis for stochastic partial differential equations with white noise forcing terms and the third one is about efficient Monte Carlo methods using sensitivity derivatives. Numerical approximation for stochastic partial differential equations is the common theme of the three projects.
In the first project, The impact of parameter dependent boundary conditions on the solutions of a class of nonlinear partial differential equations (PDEs) is considered. The concepts of effective dimensions are used to determine the accuracy of the ANOVA expansions. Demonstrations are given to show that whenever truncated ANOVA expansions of functionals provide accurate approximations, optimizers found through a simple surrogate optimization strategy are also relatively accurate. Although most of the results are presented and discussed in the context of surrogate optimization problems, they also apply to other settings such as stochastic ensemble methods and reduced-order modeling for nonlinear PDEs. In the second project, we study finite element numerical methods for class of nonlinear stochastic elliptic partial differential equations as well as stochastic Stokes equation with white noise forcing terms. Error estimates are established. the significance of these error estimates is that they provide a practical guidance to the Monte Carlo simulation. Numerical examples are also presented to examine our theoretical results. In the third project, we continue our research effort on efficient Monte Carlo simulation for stochastic partial differential equations using sensitivity derivatives. We further verified the efficiency of our algorithm by combing sensitivity derivative Monte Carlo method with the quasi-Monte Carlo simulation.

Project I: ANOVA expansions and surrogate optimization problems

Consider a general optimal control problem.

$$\begin{array}{ll} \text{minimize} & \underbrace{\mathcal{J}(u(\vec{\alpha}))}_{\textit{functional}} \\ \text{over} & \underbrace{\vec{\alpha} \in A \subseteq \mathbb{R}^d}_{\textit{admissibility set}} \\ \text{subject to} & \underbrace{F(u; \vec{\alpha}) = 0}_{\textit{nonlinear PDE}} \end{array}$$

When the number of parameters is large and the PDEs as constraints are complicated, this is a large scale computational problem. To reduce the complexity of computation, we proposal to find the numerical solution of the optimal control using the surrogate optimization method. In the surrogate optimization, We first choose N points $\{\vec{\alpha}^{(j)}\}_{j=1}^N$ belonging to admissible set A. Then we solve the N PDE problems

$$F(u^{(j)}; \vec{\alpha}^{(j)}) = 0 \quad j = 1, \ldots, N$$

and calculate the N values $\mathcal{J}_j = \mathcal{J}(u^{(j)})$ $j = 1, \ldots, N$ of the const function. From the set $\{\vec{\alpha}^{(j)}, u^{(j)})\}_{j=1}^N$, we build a surrogate function $\mathcal{J}_{sur}(\vec{\alpha})$ defined over the parameter subset A. The approximation solution of the optimal control problem is then obtained by solving the following surrogate optimization problem.

$$\min_{\vec{\alpha} \in A} \mathcal{J}_{sur}(\vec{\alpha}).$$

In this project, we will choose $\mathcal{J}_{sur}$ as polynomials of the parameters and we will use the ANOVA expansion to determine

- the parameters that can be ignored from the surrogate optimization, and
- the degree of the surrogate polynomial function.

Here is a brief description of ANOVA expansion. Let $P = \{1, \dots, p\}$. For any subset of (ordered) coordinate indices $T \subseteq P$, let $|T|$ denote the cardinality of T, $\vec{\alpha}_T \in \mathbb{R}^{|T|}$ denote the $|T|$-vector containing the components of the vector $\vec{\alpha} \in \mathbb{R}^p$ indexed by T, and $A_T^{|T|}$ denote the $|T|$-dimensional unit hypercube which is the projection of the p-dimensional unit hypercube A^p onto the coordinates indexed by T. Then Any function $\mathcal{J}(\vec{\alpha}) \in L^2(A^p)$ may be written as the ANOVA expansion

$$\mathcal{J}(\vec{\alpha}) = \mathcal{J}_0 + \sum_{T \subseteq P} \mathcal{J}_T(\vec{\alpha}_T),$$

where the terms in the expansion are determined recursively by

$$\mathcal{J}_T(\vec{\alpha}_T) = \int_{A^p \setminus A_T^{|T|}} \mathcal{J}(\vec{\alpha})\, d\vec{\alpha}_{P \setminus T} - \sum_{V \subset T} \mathcal{J}_V(\vec{\alpha}_V) - \mathcal{J}_0$$

starting with

$$\mathcal{J}_0 = \int_{A^p} \mathcal{J}(\vec{\alpha})\, d\vec{\alpha}.$$

The following are two of the most important properties for ANOVA expansion.

- The ANOVA terms are mutually orthogonal, i.e.,

$$\int_{A^p} \mathcal{J}_T(\vec{\alpha}_T)\mathcal{J}_V(\vec{\alpha}_V)\, d\vec{\alpha} = 0$$

  whenever one or more of the indices in T and V differ.
- Let T be a subset of P and $\sigma^2(\mathcal{J})$ denote the variance of a function $\mathcal{J}$ then,

$$\sigma^2(\mathcal{J}) = \sum_{|T|>0} \sigma_T^2(\mathcal{J}), \qquad \text{where} \qquad \sigma_T^2(\mathcal{J}) = \int_{A^p} \left(\mathcal{J}_T(\vec{\alpha}_T)\right)^2 d\vec{\alpha}.$$

We will use the concept of effective dimension ([]) to determine the number of parameters and degree of polynomials for the surrogate function.

- The (effective) superposition dimension of $\mathcal{J}(\vec{\alpha})$ is the smallest integer p_s such that

$$\sum_{0<|T|\leq p_s} \sigma_T^2(\mathcal{J}) \geq q\sigma^2(\mathcal{J}).$$

- The (effective) truncation dimension of $\mathcal{J}(\vec{\alpha})$ is the smallest integer p_t such that

$$\sum_{T \subseteq \{1,\dots,p_t\}} \sigma_T^2(\mathcal{J}) \geq q\sigma^2(\mathcal{J}).$$

  Here p is the proportionality close to 1.

If p_t is the truncation dimension, then only the first p_t parameters are needed for the surrogate function. On the other hand, if p_s is the superposition dimension, then we only need to use polynomials with degrees no large than p_s. In [], we prove the approximation property of ANOVA expansion under small perturbation assumption.

To verify our theoretical analysis, we consider the following optimal control problem. The cost functional takes the form

$$\mathcal{J}(u) = \int_\Omega w(u) d\Omega + \eta |\vec{\alpha}|^2$$

where we choose

$$w(u) = (u - \widehat{u})^2 \qquad \text{or} \qquad e^{(u-\widehat{u})} \qquad \text{or} \qquad \sqrt{|u - \widehat{u}|}.$$

The state equation is the following nonlinear elliptic partial differential equation with mixed boundary conditions.

$$\begin{cases} -\Delta u + f(u) = 0 & \text{in } \Omega \\ u = 0 & \text{on } \Gamma_0 \\ u = \sum_{i=1}^{M} \alpha_i \phi_i & \text{on } \Gamma_1 \\ \dfrac{\partial u}{\partial n} = \sum_{i=M+1}^{N} \alpha_i \phi_i & \text{on } \Gamma_2, \end{cases}$$

We choose $q = 0.99$ in the superposition dimension and derive, after computation that,

$$p_s = \begin{cases} 1 & \text{if } w(u) = e^{(u-\widehat{u})} & \text{and} & f(u) = u^2 & \text{or} & \sqrt{|u|} \\ 3 & \text{if } w(u) = \sqrt{|u - \widehat{u}|} & \text{and} & f(u) = e^u & \text{or} & \sqrt{|u|} \\ 4 & \text{if } w(u) = \sqrt{|u - \widehat{u}|} & \text{and} & f(u) = u^2 & & \\ 2 & \text{otherwise} & & & & \end{cases}$$

The above results indicate that the effective dimensions depend on the smoothness of the cost functionals. In all cases we use quadratic polynomials as surrogate functions and the errors for optimal controls are listed in Table 1. Here MC is the Monte Carlo sampling, LHS the Latin hypercube sampling and CVT Centroid Voronoi tessellation sampling. Our numerical results confirm that When the effective dimensions are two or less, the quadratic surrogate optimization provides accurate numerical solution for the optimal controls.

Talbe 1: Errors of optimal controls with surrogate optimizations

sampling method	$w(u) = (u - \widehat{u})^2$			$w(u) = \|u - \widehat{u}\|^{1/2}$		
	$f(u)$			$f(u)$		
	u^2	e^u	$\|u\|^{1/2}$	u^2	e^u	$\|u\|^{1/2}$
MC	0.036	0.018	0.086	0.556	0.566	0.574
LHS	0.021	0.012	0.035	0.378	0.427	0.380
CVT	0.067	0.026	0.069	0.436	0.433	0.436

Project II: Finite element approximation for Stochastic Stokes equation
In this project, we consider the stochastic Stokes equation with a white noise forcing term which describes the motion of an incompressible viscous fluid.

$$\begin{aligned} -\nu \Delta u + \nabla p &= f + \dot{W}, \quad \text{in } \Omega, \\ \text{div} u &= 0, \quad \text{in } \Omega, \\ u &= 0, \quad \text{on } \partial\Omega \end{aligned} \tag{0.1}$$

where Ω is a bounded convex domain in R^2 with piecewise continuous boundary, $u : \Omega \to R^2$ is the velocity of the fluid flow, p is the pressure, $f \in L^2(\Omega)$ and $\dot{W} = (\dot{W}^1, \dot{W}^2)$ is the white noise such that

$$E(\dot{W}^j(x)\dot{W}^j(x')) = \delta(x - x'), \quad x,\ x' \in \Omega, \quad j = 1, 2$$

where δ denotes the usual Delta δ function and E the expectation. Assume that G and D are the Green's functions for the Stokes equation corresponding to u and p, respectively. We define the weak solution of (0.1) as follows.

$$u(x) = \int_\Omega G(x,y)f(y)dy + \int_\Omega G(x,y)dW(y) \tag{0.2}$$

and

$$p(x) = \nabla \int_\Omega D(x,y)f(y)dy + \nabla \int_\Omega D(x,y)dW(y) \tag{0.3}$$

where the stochastic integral is defined in Ito's sense. The noise term occurs, for example, when the fluid's temperature affects the flow of the fluid but is omitted in the equation because of insufficient knowledge of the boundary data for the temperature.

We define an approximate solution of (0.1) by discretizing the white noise $\dot{W}$. First we introduce a discretization for the white noise. Let $\{\mathcal{T}_h\}$ be a family of triangulations of $\overline{\Omega}$ (see [?] for the requirements on $\{\mathcal{T}_h\}$), where $h \in (0,1)$ is the meshsize. We assume the family is quasiuniform, i.e., there exist positive constants ρ_1 and ρ_2 such that

$$\rho_1 h \le R_T^{\mathrm{inr}} < R_T^{\mathrm{cir}} \le \rho_2 h, \quad \forall\, T \in \mathcal{T}_h, \quad \forall\, 0 < h < 1, \tag{0.4}$$

where R_T^{inr} and R_T^{cir} are the inradius and the circumradius of T. Write

$$\xi_T^j = \frac{1}{\sqrt{|T|}} \int_T 1\, dW^j(x) \quad j = 1, 2$$

for each triangle $T \in \mathcal{T}_h$, where $|T|$ denotes the area of T. It is well-known that $\{\xi_T^j\}_{T\in\mathcal{T}_h}$ is a family of independent identically distributed normal random variables with mean 0 and variance 1 (see [?]). Then the piecewise constant approximation to $\dot{W}^j(x)$ is given by

$$\dot{W}_h^j(x) = \sum_{T\in\mathcal{T}_h} |T|^{-\frac{1}{2}} \xi_T^j \chi_T(x) \tag{0.5}$$

We consider the numerical approximations of (??) using the finite element method. Denote $P_k = P_k(x,y)$ as the set of polynomials of degree k. Let $X := (H_0^1(\Omega))^2$ and $Q := L_0^2(\Omega) = \{q \in L^2(\Omega),\ \int_\Omega q(x)dx = 0\}$. We approximate the velocity on each element T in $\mathcal{T}_h$ by a polynomial of

$$\mathcal{P}(T) = \{P_1 \oplus \mathrm{span}\{\lambda_1, \lambda_2, \lambda_2\}\}^2 \tag{0.6}$$

where λ_j are barycentric coordinates defined as

$$\lambda_j \in P_1 \quad \lambda_j(a_i) = \delta_{ij}, \quad i, j = 1, 2$$

where a_i are the vertices of T. Then we choose the following finite element spaces.

$$X_h = \{v \in C^0(\bar{\Omega})^2;\ \ v|_T \in \mathcal{P}(T), \ \ \forall\, T \in \mathcal{T}_h, \ \ v|_{\partial\Omega} = 0\}, \tag{0.7}$$

$$Q_h = \{q \in C^0(\bar{\Omega})^2;\ \ q|_T \in P_1(T), \ \ \forall\, T \in \mathcal{T}_h\}. \tag{0.8}$$

The finite element solution is to solve the variational equation in the finite element space. Assume that u_h and p_h are the finite element approximations for u and p, respectively. We have the following error estimates.

Theorem 1 *There exists a constant* C *such that*

$$E(\|u - u_h\|^2) \leq C|\ln h|h^{\frac{1}{2}}, \tag{0.9}$$

$$E(\|p - p_h\|_{-1}^2) \leq C|\ln h|h^2.$$

The significance of the errors estimates is that they provide practical guidance for the choice of the number of samples in the Monte Carlo simulation. We have conducted a number of Monte Carlo simulations using our algorithm. Figure 1 and Figure 2 show the expectation and variance of the velocity, respectively.

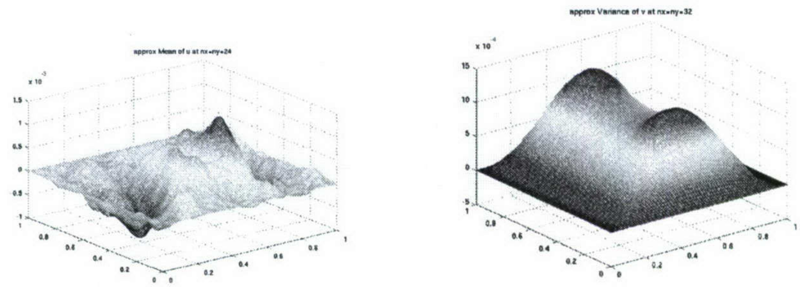

Figure 1 the expectation and variance of velocity

Conclusion and future research

We posed the problem of optimal control and design optimization using the statistical tool ANOVA. Our numerical experiments indicate that ANOVA expansion combined with concept of effective dimension is effective in choosing the surrogate functions for optimal control problems. We have also studied numerical solutions stochastic Stokes equations with white noise forcing terms. Our error analysis shows that the finite element method for stochastic Stokes equations has one order lower convergence rate than deterministic problems. Future research includes ANOVA analysis for optimal control problems with large number of parameters, numerical solutions for time dependent partial differential equations with multiplicative noises.

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