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New Directions in Stochastic Optimisation

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Abstract. Recent work in stochastic programming draws on interaction with Algebraic and Combinatorial Models, Numerical Analysis of PDEs, Risk Analysis, Mathematical Equilibrium, Minimax, and Stochastic Games. For the first time ever, the workshop brought together scholars from these fields to exchange experience and identify promising topics for future research.

Mathematics Subject Classification (2010): 90C15.

Introduction by the Organisers

The workshop *New Directions in Stochastic Optimisation* organized by Jesús De Loera (Davis), Darinka Dentcheva (Hoboken), Georg Ch. Pflug (Vienna) and Rüdiger Schultz (Essen) was well attended by 54 participants with broad geographic representation. By a surprising coincidence, the workshop took place precisely 50 years after the first Oberwolfach Workshop in Operations Research (Organizers: R. Henn (Karlsruhe), H. P. Künzi (Zurich) and H. Schubert (Kiel)).

Topic: Stochastic programming offers mathematically rigorous optimisation models incorporating probabilistic information with uncertain data. Decisions are based exclusively on the information that is available at the moment of taking decisions (nonanticipativity). Depending on when missing information is unveiled and on how this interacts with decision making over time, different principal model setups arise, e.g., one-stage, two-stage, or multi-stage models. Selection and placement (in the objective or the constraints) of the statistical parameters according to which relevant random variables are to be evaluated is another important issue.

This allows to express perceptions such as reliability, risk neutrality, or risk aversion. Finally, the nature of the initial uncertain optimisation problem (linear or nonlinear, with or without integer variables, living in finite or infinite dimension) has crucial impact on the arising stochastic programming model. These aspects lead to a wide variety of stochastic optimization programs as well as to a wide variety of mathematical techniques for their analysis and algorithmic treatment.

Course of the workshop: On the one hand, the workshop reflected the diversity of the involved areas. On the other hand, there was enough overlap among individual expertise to generate new ideas and obtain input from other directions. In particular, the 35 talks together with a brainstorming session on Thursday evening provided the basic ideas for stimulating discussions covering a broad spectrum of topics. We now will discuss some contributions on specific topics.

Numerical Analysis of PDEs: The rapid development of PDE-constrained optimisation is accompanied by approaches to handle uncertainty in appropriate fashion. The approach via stochastic programming aims at finding best possible decisions under data uncertainty. Procedures for reaching optimality in terms of stochastic criteria may incorporate user attitudes such as being risk averse, risk neutral or risk seeking. A related contemporary approach to handling uncertainty, also discussed at the workshop, is uncertainty quantification that looks for "a computational framework for quantifying input and response uncertainties in a manner that facilitates predictions with quantified and reduced uncertainty"[1]. Shape optimization under stochastic loading for elastic materials have been discussed in several talks. Risk neutral and risk averse objective functionals have been investigated and the concept of stochastic dominance constraints was explored. Thereby the expected excess and the excess probability are taken into account, first as objective functional involving the compliance cost of an elastic object under stochastic loading and then as a constraint when comparing a shape with a benchmark shape.

Open problems concern the identification of subclasses allowing for duality and resulting algorithmic shortcuts; exploiting problem similarities for efficient repeated solution of PDE-constrained optimisation problems differing in the realisations of the random data; mathematical foundation and algorithm design of approximation via linearisation of full models, arriving at linear models, development of numerical PDE-solvers taking into account specifics of this problem class.

PDE-constrained optimization under uncertainty has been addressed from further points of view. We mention convergence of projected gradient methods in Hilbert spaces, reduced-order models/incorporating risk functionals /(CVaR) and risk averse optimization; optimal boundary control under uncertain initial data; general characterizations of feasibility, stationarity, optimality, and stability in PDE-constrained optimization.

[1]R.C. Smith: Uncertainty Quantification, SIAM, 2014, page ix.

Shape optimization under uncertainty

Helmut Harbrecht

Introduction. Shape optimization is indispensable for designing and constructing industrial components. Many problems that arise in application, particularly in structural mechanics and in the optimal control of distributed parameter systems, can be formulated as the minimization of functionals which are defined over a class of admissible domains.

Shape optimization problems can be solved by means of gradient based minimization algorithms, which involve the shape functionals' derivative with respect to the domain under consideration. The computation of the shape gradient and the implementation of appropriate numerical optimization algorithms is meanwhile well understood, provided that the state equation's input data are given exactly. In practice, however, input data for numerical simulations in engineering are often not exactly known. One must thus address how to account for uncertain input data in the state equation.

Uncertainty in the state equation might arise from three different sources:

- Uncertainty might arise from geometric entities like a certain part of boundary which has not to be optimized but is prescribed.
- The right-hand side of the state equation might be random.
- The material parameters, entering the partial differential operator, might be not exactly known.

We separately consider these sources of uncertainty and discuss their impact on the shape optimization problem. Especially, we show the well-posedness of the problem formulations and present numerical solution methods.

Shape optimization under geometric uncertainty. Bernoulli's free boundary problem is concerned with finding the exterior (free) boundary Γ of an annular domain $D \subset \mathbb{R}^n$ for a given interior (fixed) boundary Σ such that, besides Dirichlet boundary conditions at both boundaries, also a Neumann boundary condition is satisfied at the exterior boundary. The problem under consideration models for example the growth of anodes in electrochemical processes and can be seen as the prototype of a free boundary problem arising in many applications.

We shall consider the situation that the interior boundary is random, i.e., it is $\Sigma = \Sigma(\omega)$ with an additional parameter $\omega \in \Omega$. Such an assumption arises when treating tolerances in fabrication processes or when the interior boundary is only known by measurements which typically contain errors. We are thus looking for a tuple $\big(D(\omega), u(\omega)\big)$ such that there holds

$$\begin{aligned} \Delta u(\omega) &= 0 && \text{in } D(\omega), \\ u(\omega) &= 1 && \text{on } \Sigma(\omega), \\ -\frac{\partial u}{\partial \mathbf{n}}(\omega) &= g,\ u(\omega) = 0 && \text{on } \Gamma(\omega). \end{aligned} \tag{1}$$

The questions which have to be addressed are the following:

(1) What is a suitable model for the domain $D(\omega)$? Is the problem well-posed in the sense of $D(\omega)$ being almost surely well-defined?
(2) How to define the expectation of a random domain? The main difficulty to deal with here is that the space of domains is not linear.
(3) How to compute the solution to the random free boundary problem numerically?

We provide the theoretical background that ensures the well-posedness of the problem under consideration and describe two different frameworks to define the expectation and the deviation of the resulting annular domain. The first approach is based on the Vorob'ev expectation, which can be defined for arbitrary sets. The second approach is based on a particular parametrization. We compare these approaches by analytical computations for circular interior domains and by numerical experiments for more general geometric configurations. For the numerical approximation of the domain's expectation and deviation, we propose a sampling method like the (quasi-) Monte Carlo quadrature. Then, each particular realization Σ_i of the interior boundary leads to an exterior boundary Γ_i via the solution of Bernoulli's free boundary problem. It is computed by solving the shape optimization problem

$$J(D_i) = \int_{D_i} \left\{ \|\nabla u_i\|^2 + g^2 \right\} \mathrm{d}\mathbf{x} \to \min$$
$$\text{subject to} \quad \Delta u_i = 0 \text{ in } D_i, \quad u_i = 1 \text{ on } \Sigma_i, \quad u_i = 0 \text{ on } \Gamma_i.$$

Shape optimization in case of random diffusion. We consider again Bernoulli's free boundary problem (1), but now the situation that the material contained in the domain D is not perfectly homogeneous. Hence, we arrive at the following random free boundary problem: seek the free boundary Γ, such that

$$\begin{aligned} \operatorname{div}\big(\alpha(\omega)\nabla u(\omega)\big) &= 0 && \text{in } D,\\ u(\omega) &= 1 && \text{on } \Sigma,\\ -\alpha(\omega)\frac{\partial u}{\partial \mathbf{n}}(\omega) = g,\ u(\omega) &= 0 && \text{on } \Gamma, \end{aligned} \tag{2}$$

holds for almost all $\omega \in \Omega$. Since we intend to model a uniformly elliptic random perturbation of the Laplace operator, the random diffusion is assumed to satisfy

$$0 < \alpha_{\min} \le \alpha(\omega) \le \alpha_{\max} < \infty$$

almost everywhere in D.

For solving the random free boundary problem (2), we first show that the minimizer of the shape optimization problem

$$\begin{aligned} J(D,\omega) = \int_D \left\{ \alpha(\omega)\|\nabla u(\omega)\|^2 + \frac{g^2}{\alpha(\omega)} \right\} \mathrm{d}\mathbf{x} \to \min \\ \text{subject to} \quad \operatorname{div}\big(\alpha(\omega)\nabla u(\omega)\big) = 0 \text{ in } D, \quad u(\omega) = 1 \text{ on } \Sigma, \quad u(\omega) = 0 \text{ on } \Gamma \end{aligned} \tag{3}$$

solves the free boundary problem (2) for each particular $\omega \in \Omega$. This is done by deriving the Hadamard representation of the associated shape gradient and proving that the necessary optimality condition imposes the desired Neumann boundary condition.

Therefore, since the random diffusion induces a random state and thus a random shape functional, we are going to minimize the ensemble average $\mathbb{E}\big[J(D,\omega)\big]$ of the random shape functional. Note that this shape optimization problem is well-posed since we are minimizing a continuous energy functional.

Shape optimization in case of random right-hand sides. We shall next consider shape optimization problems where the right-hand side in the state equation is random. Then, the state is random, but depends *linearly* on the randomness. In this situation, the expectation and variance of a quadratic objective can be reformulated as deterministic expressions by exploiting the state's moments. This leads to cheap, deterministic algorithms to minimize such objectives.

Consider, for example, Bernoulli's free boundary problem in case of random Dirichlet data at the interior boundary:

$$\begin{aligned} \Delta u(\omega) &= 0 && \text{in } D,\\ u(\omega) &= f(\omega) && \text{on } \Sigma,\\ -\frac{\partial u}{\partial \mathbf{n}}(\omega) &= g,\ u(\omega) = 0 && \text{on } \Gamma. \end{aligned} \tag{4}$$

We show that the random shape optimization problem

$$\begin{gathered} \mathbb{E}[J(D,\omega)] = \mathbb{E}\bigg[\int_D \big\{\|\nabla u(\omega)\|^2 + g^2\big\}\,\mathrm{d}\mathbf{x}\bigg] \to \min\\ \text{subject to}\quad \Delta u(\omega) = 0 \text{ in } D,\quad u(\omega) = f(\omega) \text{ on } \Sigma,\quad u(\omega) = 0 \text{ on } \Gamma \end{gathered} \tag{5}$$

can be reformulated into the deterministic shape optimization problem

$$\mathbb{E}[J(D,\omega)] = \int_D \left\{\left(\|(\nabla\otimes\nabla)\operatorname{Cor}[u](\mathbf{x},\mathbf{y})\|\Big|_{\mathbf{y}=\mathbf{x}}\right)^2 + g^2\right\}\mathrm{d}\mathbf{x} \to \min,$$

where $\operatorname{Cor}[u](\mathbf{x},\mathbf{y})$ denotes the two-point correlation of random state $u(\omega)$ given by (5).

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