

Optimization under rare chance constraints

Shanyin Tong¹

jointly with: Anirudh Subramanyam² Vishwas Rao³

¹Department of Applied Physics and Applied Mathematics, Columbia University, NY

²Department of Industrial and Manufacturing Engineering, Pennsylvania State University, PA

³Mathematics and Computer Science division, Argonne National Laboratory, IL

March 22, 2024

INFORMS Optimization Society Conference, Houston, TX

Outline

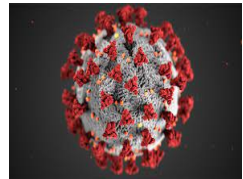
Introduction

Large deviation theory for rare chance constraints

Applications

Conclusion

What are rare events?



Examples:

- ▶ Material failure (bridge/tool/plane stress fractures)
- ▶ Extreme weather (tornadoes, hurricanes, heat waves)
- ▶ Rogue waves, tsunamis, earthquakes
- ▶ Financial sector/bank/company collapse
- ▶ Pandemics

Why study rare events?



Common to all:

- ▶ Rare but high impact/cost/damage

Control and mitigation:

- ▶ Design engineering structures \implies control material failure
- ▶ Design portfolio \implies control risk of investments

Optimization under rare chance constraints

$$\begin{aligned} & \underset{u \in \mathcal{U}}{\text{minimize}} && J(u) \\ & \text{subject to} && \mathbb{P}(F(u, \xi) \geq z) \leq \alpha \quad \text{for some fixed } \alpha \ll 1 \end{aligned}$$

- ▶ $F: \mathcal{U} \times \Xi \rightarrow \mathbb{R}$... parameter-to-observation map, can involve PDEs
- ▶ $J: \mathcal{U} \rightarrow \mathbb{R}$... cost
- ▶ $\Xi \subseteq \mathbb{R}^n$... random space of uncertain parameters ξ with measure \mathcal{P}
- ▶ $\mathcal{U} \subseteq \mathbb{R}^m$... domain for control or decision variable u
- ▶ z ... specified upper bound
- ▶ $\alpha \in (0, 1)$... risk threshold

Challenges for rare chance constraints

Sampling-based methods:

$$\xi^i \stackrel{\text{i.i.d.}}{\sim} \mathcal{P}$$

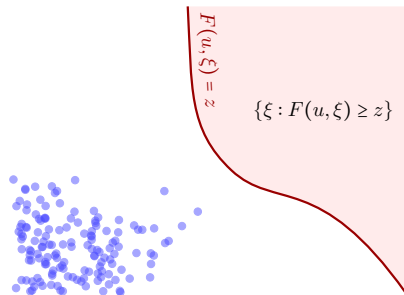
- ▶ Indicator approximation:

$$\mathbb{P}(F(u, \xi) \geq z) \approx \frac{1}{N} \sum_{i=1}^N \mathbb{1}_{[z, \infty)}(F(u, \xi^i))$$

- ▶ Scenario approach:

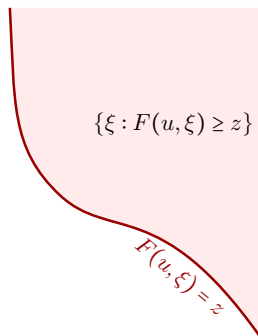
$$F(u, \xi^i) \leq z, \quad i = 1, \dots, N$$

- ▶ Spherical radial decomposition



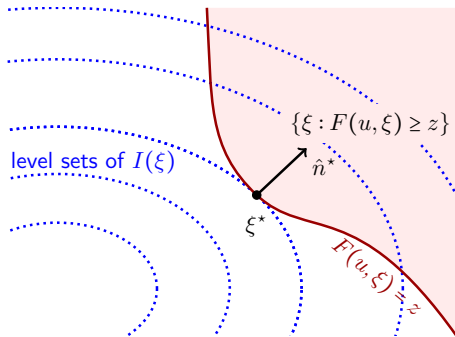
Need $N = O(\alpha^{-1})$ samples, each adds new variables and constraints; intractable for complicated F

Overview of large deviation theory-based method



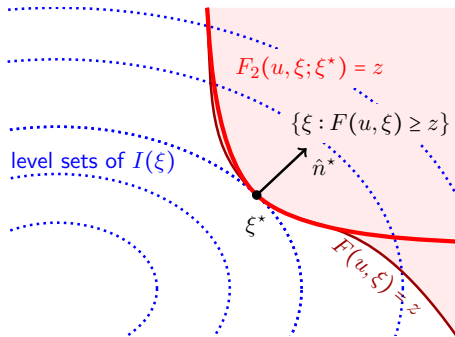
Overview of large deviation theory-based method

1. Find LDT optimizer ξ^*



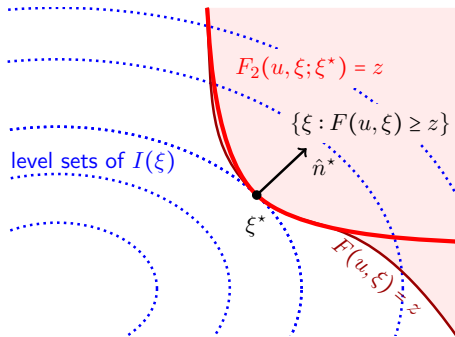
Overview of large deviation theory-based method

1. Find LDT optimizer ξ^*
2. Explicit formula for geometric approx.



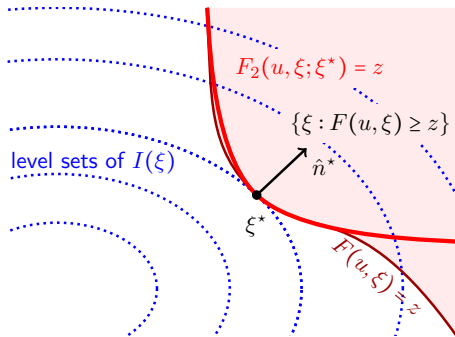
Overview of large deviation theory-based method

1. Find LDT optimizer ξ^*
2. Explicit formula for geometric approx.
3. Bilevel reformulation



Overview of large deviation theory-based method

1. Find LDT optimizer ξ^*
2. Explicit formula for geometric approx.
3. Bilevel reformulation



LDT-based methods:

- ▶ sampling-free
- ▶ insensitive to extremeness
- ▶ work for expensive parameter-to-observation maps
- ▶ solvable by off-the-shelf solvers

Outline

Introduction

Large deviation theory for rare chance constraints

Applications

Conclusion

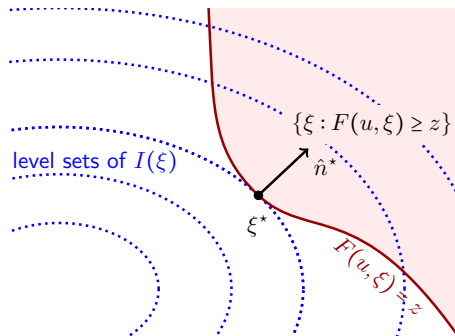
Large deviation theory

$$\mathbb{P}(F(u, \xi) \geq z) \asymp \exp(-I(\xi^*(u, z))) \text{ as } z \rightarrow \infty$$

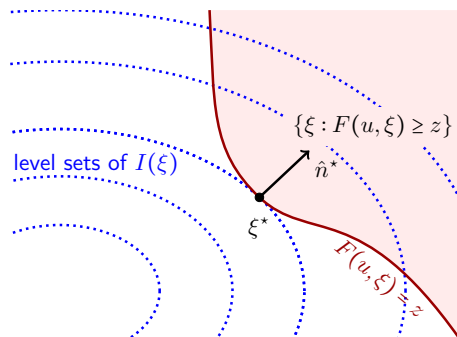
LDT optimizer:

$$\xi^*(u, z) := \underset{\xi \in \Xi}{\operatorname{argmin}} \{I(\xi) : F(u, \xi) \geq z\}$$

- ▶ $I(\cdot)$: rate function
- ▶ depends only on distribution of ξ
- ▶ Legendre transform of cumulant generating fct
- ▶ Gaussian $\xi \sim \mathcal{N}(\mu, \Sigma)$: $I(\xi) = \frac{1}{2} \|\xi - \mu\|_{\Sigma^{-1}}^2$



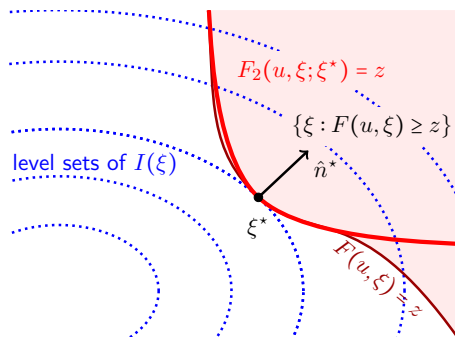
Geometric approximation of rare event probability



Geometric approximation of rare event probability

Geometric approx: measure bounded by second-order Taylor expansion

$$\mathbb{P}(F(u, \xi) \geq z) \approx P_2(u, z, \xi^*) = \mathcal{P}(\{\xi \in \Xi : F_2(u, \xi; \xi^*) \geq z\})$$



Geometric approximation of rare event probability

Geometric approx: measure bounded by second-order Taylor expansion

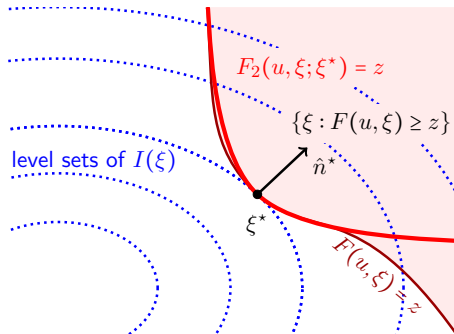
$$\mathbb{P}(F(u, \xi) \geq z) \approx P_2(u, z, \xi^*) = \mathcal{P}(\{\xi \in \Xi : F_2(u, \xi; \xi^*) \geq z\})$$

- ▶ **Gaussian mixture model**

$$\xi \sim \sum_{i=1}^M w_i \mathcal{N}(\mu_i, \Sigma_i), \quad \sum_{i=1}^M w_i = 1$$

- ▶ Explicit algebraic formula
- ▶ Only require local derivative info
- ▶ Universal approximation

$$P_2(u, z, \xi^*) = \sum_{i=1}^M w_i \Phi(-\|\tilde{\xi}_i - \mu_i\|_{\Sigma_i^{-1}}) \det_{\perp \tilde{n}_i} \left(\mathbf{I}_n - \frac{\|\tilde{\xi}_i - \mu_i\|_{\Sigma_i^{-1}}}{\|\Sigma_i^{\frac{1}{2}} \nabla_{\xi} F_2(u, \tilde{\xi}_i; \xi^*)\|} \Sigma_i^{\frac{1}{2}} \nabla_{\xi}^2 F(u, \xi^*) \Sigma_i^{\frac{1}{2}} \right)^{-\frac{1}{2}}$$



Bilevel Reformulation

Optimization under rare chance constraints

$$\begin{aligned} & \underset{u \in \mathcal{U}}{\text{minimize}} && J(u) \\ & \text{subject to} && \mathbb{P}(F(u, \xi) \geq z) \leq \alpha \quad \text{for some fixed } \alpha \ll 1 \end{aligned}$$

Bilevel Reformulation

Optimization under rare chance constraints

$$\begin{aligned} & \underset{u \in \mathcal{U}}{\text{minimize}} && J(u) \\ & \text{subject to} && \mathbb{P}(F(u, \xi) \geq z) \leq \alpha \quad \text{for some fixed } \alpha \ll 1 \end{aligned}$$

Bilevel opt: Approximate rare event probability with LDT estimates

$$\begin{aligned} & \underset{u \in \mathcal{U}}{\text{minimize}} && J(u) \\ & \text{subject to} && P_2(u, z, \xi^*) \leq \alpha, \quad \xi^* \in \underset{\xi \in \Xi}{\operatorname{argmin}} \{I(\xi) : F(u, \xi) \geq z\} \end{aligned}$$

Bilevel Reformulation

Optimization under rare chance constraints

$$\begin{aligned} & \underset{u \in \mathcal{U}}{\text{minimize}} && J(u) \\ & \text{subject to} && \mathbb{P}(F(u, \xi) \geq z) \leq \alpha \quad \text{for some fixed } \alpha \ll 1 \end{aligned}$$

Bilevel opt: Approximate rare event probability with LDT estimates

$$\begin{aligned} & \underset{u \in \mathcal{U}}{\text{minimize}} && J(u) \\ & \text{subject to} && P_2(u, z, \xi^*) \leq \alpha, \quad \xi^* \in \underset{\xi \in \Xi}{\operatorname{argmin}} \{I(\xi) : F(u, \xi) \geq z\} \end{aligned}$$

Single-level opt: Replace lower-level with first-order optimality conditions

$$\begin{aligned} & \underset{u \in \mathcal{U}, \xi^* \in \Xi, \lambda \in \mathbb{R}_+}{\text{minimize}} && J(u) \\ & \text{subject to} && P_2(u, z, \xi^*) \leq \alpha, \quad F(u, \xi^*) = z, \quad \nabla I(\xi^*) = \lambda \nabla_{\xi} F(u, \xi^*) \end{aligned}$$

Bilevel Reformulation

Optimization under rare chance constraints

$$\begin{aligned} & \underset{u \in \mathcal{U}}{\text{minimize}} && J(u) \\ & \text{subject to} && \mathbb{P}(F(u, \xi) \geq z) \leq \alpha \quad \text{for some fixed } \alpha \ll 1 \end{aligned}$$

Bilevel opt: Approximate rare event probability with LDT estimates

$$\begin{aligned} & \underset{u \in \mathcal{U}}{\text{minimize}} && J(u) \\ & \text{subject to} && P_2(u, z, \xi^*) \leq \alpha, \quad \xi^* \in \underset{\xi \in \Xi}{\operatorname{argmin}} \{I(\xi) : F(u, \xi) \geq z\} \end{aligned}$$

Single-level opt: Replace lower-level with first-order optimality conditions

$$\begin{aligned} & \underset{u \in \mathcal{U}, \xi^* \in \Xi, \lambda \in \mathbb{R}_+}{\text{minimize}} && J(u) && \text{solvable by off-the-shelf solvers, e.g. Ipopt} \\ & \text{subject to} && P_2(u, z, \xi^*) \leq \alpha, && F(u, \xi^*) = z, \quad \nabla I(\xi^*) = \lambda \nabla_{\xi} F(u, \xi^*) \end{aligned}$$

Outline

Introduction

Large deviation theory for rare chance constraints

Applications

Conclusion

Short column design

Find width and height $u = [w, h]$ to minimize area wh of rectangular cross section, avoiding material failure with probability $1 - \alpha$, with uncertain material parameter $\xi = [\xi_F, \xi_M, \xi_Y]$

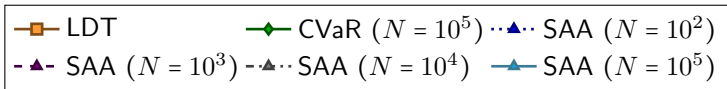
$$\begin{aligned} & \underset{u=[w,h] \in \mathbb{R}^2}{\text{minimize}} && wh \\ & \text{subject to} && L_w \leq w \leq U_w, \\ & && L_h \leq h \leq U_h, \\ & && \mathbb{P}(F(u, \xi) \geq 1) \leq \alpha, \quad \text{for fixed } \alpha \ll 1 \end{aligned}$$

From elastic-plastic constitutive law

$$F(u, \xi) := \frac{4\xi_M}{wh^2 \exp(\xi_Y)} + \frac{\xi_F^2}{w^2h^2 \exp(2\xi_Y)}$$

Short column design

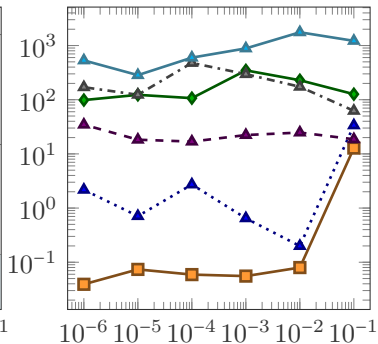
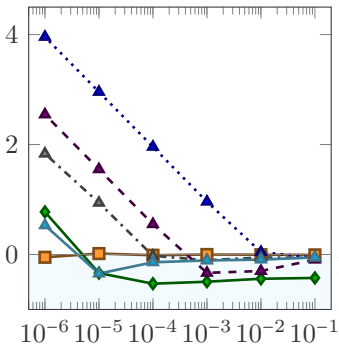
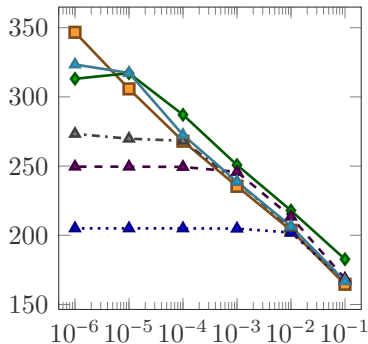
Compare LDT-based methods with sampling-based methods (SAA, CVaR)



Optimal area wh [m^2]

$\log_{10} \mathbb{P}(F(u^*, \xi) \geq 1) - \log_{10} \alpha$

Time [sec]



Optimal PDE boundary control

Control temperature at boundary Γ_c as close to 0 as possible, while ensuring average temperature in Ω_0 bounded by z with high probability

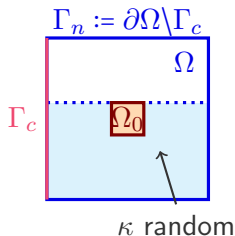
$$\begin{aligned} & \underset{u}{\text{minimize}} && \frac{1}{2} \int_{\Gamma_c} u^2(x) dx, \\ & \text{subject to} && \mathbb{P}(F(u, \xi) \geq z) \leq \alpha \end{aligned}$$

$$F(u, \xi) := \frac{1}{|\Omega_0|} \int_{\Omega_0} y(x; u, \xi) dx$$

$y(x; u, \xi)$ is solution of 2D steady-state advection-diffusion equation

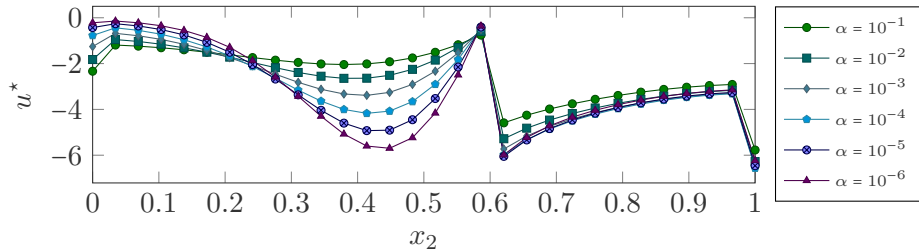
$$\begin{aligned} -\nabla \cdot (\kappa(x, \xi) \nabla y(x)) + w(x) \cdot \nabla y(x) &= f(x, \xi), & x \in \Omega, \\ (\kappa(x, \xi) \nabla y(x)) \cdot n(x) &= \frac{1}{\epsilon_0} (u(x) - y(x)), & \text{on } \Gamma_c, \\ (\kappa(x, \xi) \nabla y(x)) \cdot n(x) &= 0, & \text{on } \Gamma_n. \end{aligned}$$

with random diffusion coefficient $\kappa(x, \xi)$ and random source $f(x, \xi)$



Optimal PDE boundary control

Sampling-based methods are untenable

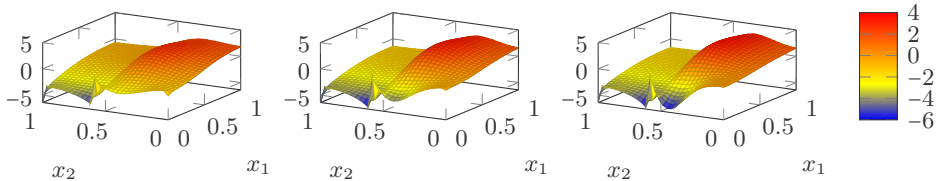


Optimal boundary condition u^* with $z = 1$ for different α using LDT

$\alpha = 10^{-2}$

$\alpha = 10^{-4}$

$\alpha = 10^{-6}$



Temperature y under u^* and ξ^* with $z = 1$ for different α using LDT

Outline

Introduction

Large deviation theory for rare chance constraints

Applications

Conclusion

Main takeaways

- ▶ Large deviation theory for rare chance constraints
- ▶ Explicit algebraic formulations for Gaussian mixture
- ▶ Methods for optimization under rare chance constraints:
 - ▶ sampling-free
 - ▶ solvable by off-the-shelf solvers
 - ▶ insensitive to extremeness
- ▶ Examples on nonlinear and PDE-constrained optimization problems

Main takeaways

- ▶ Large deviation theory for rare chance constraints
- ▶ Explicit algebraic formulations for Gaussian mixture
- ▶ Methods for optimization under rare chance constraints:
 - ▶ sampling-free
 - ▶ solvable by off-the-shelf solvers
 - ▶ insensitive to extremeness
- ▶ Examples on nonlinear and PDE-constrained optimization problems

Future directions

- ▶ Refine asymptotic approx
- ▶ Generalize to more distributions
- ▶ Release some regularity assumptions
- ▶ SunA7 (March 24, 8:30 - 10:00am): Anirudh Subramanyam
Self-Structured Importance Sampling for Chance-Constrained Optimization
- ▶ Improve efficiency for large-scale problems: SDEs/SPDEs (ongoing)

References

- S. Tong, A. Subramanyam, V. Rao. *Optimization under rare chance constraints*.
SIAM Journal on Optimization 32.2 (2022)
<https://epubs.siam.org/doi/abs/10.1137/20M1382490>
<https://arxiv.org/abs/2011.06052>
- ▶ S. Tong, E. Vanden-Eijnden, G. Stadler. *Extreme event probability estimation using PDE-constrained optimization and large deviation theory, with application to tsunamis*. Communications in Applied Mathematics and Computational Science (2021)
 - ▶ S. He, G. Jiang, H. Lam, & M. Fu. Adaptive importance sampling for efficient stochastic root finding and quantile estimation. Operations Research (2023)
 - ▶ Y. Aoues and A. Chateauneu, *Benchmark study of numerical methods for reliability-based design optimization*, Struct. Multidiscipl. Optim. (2010)
 - ▶ J. Luedtke and S. Ahmed. *A sample approximation approach for optimization with probabilistic constraints*, SIAM Journal on Optimization (2008)
 - ▶ A. Nemirovski and A. Shapiro, *Convex approximations of chance constrained programs*, SIAM Journal on Optimization (2007)