Probabilistic Constraints in Optimization Problems on Flow Networks

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Structure

Probabilistic Constraints in Optimization Problems

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Optimization problem with a probabilistic constraint

$$\min f(x)$$
$$\text{s.t. } \mathbb{P}(g(x,\xi) \leq 0) \geq \alpha$$

with n-dimensional random variable ξ and $\alpha \in [0,1]$.

How to compute the probability for given x?

Spheric radial decomposition (SRD)

- Consider feasible set $M := \{\xi \in \mathbb{R}^n | g(x,\xi) \leq 0\} \to \mathbb{P}(\xi \in M)$
- Write $\mathbb{P}(\xi \in M)$ as integral over the unit sphere $\mathbb{S}^{n-1}$

Direct approach

- Integration of the probability density function (pdf) of $g(x,\cdot)$
- Estimation of the pdf via kernel density estimation (KDE)

Spheric Radial Decomposition

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Theorem (SRD)

Let $\xi \sim \mathcal{N}(\mu, \Sigma)$ be n-dimensional Gaussian distributed random variable with mean μ and positive definite correlation matrix Σ.
Then, for any Borel measurable subset $M \subset \mathbb{R}^n$ it holds that

$$\mathbb{P}(\xi \in M) = \int_{\mathbb{S}^{n-1}} \mu_\chi \{r \geq 0 | rLw + \mu \in M\} d\mu_\eta(w)$$

where $\mathbb{S}^{n-1}$ is the $(n-1)$-dimensional sphere in $\mathbb{R}^n$, μ_η is the uniform distribution on $\mathbb{S}^{n-1}$, μ_χ denotes the χ-distribution with n degrees of freedom and L is such that $\Sigma = LL^T$.

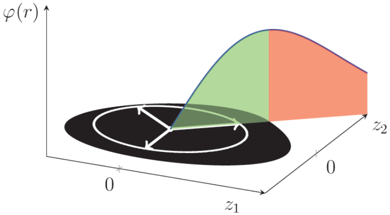
Spheric Radial Decomposition

Theorem: $\mathbb{P}(\xi \in M) = \int_{\mathbb{S}^{n-1}} \mu_\chi\{r \geq 0 | rLw + \mu \in M\} d\mu_\eta(w)$

Algorithm

Let $\xi \sim \mathcal{N}(\mu, \Sigma)$ and L such that $LL^T = \Sigma$.

1. Sample Q points $\{w_1, \dots, w_Q\}$ uniformly distributed on the sphere $\mathbb{S}^{n-1}$.
2. Compute the one-dimensional sets $M_i := \{r \geq 0 | rLw_i + \mu \in M\}$ for $i = 1, \dots, Q$.
3. Set $\mathbb{P}(\xi \in M) \approx (1/Q) \sum_{i=1}^{Q} \mu_\chi(M_i)$



Kernel Density Estimation

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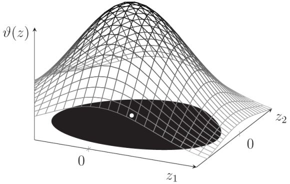
Direct approach: Integration of the probability density function ϱ_g of $g := g(x, \cdot)$

$$\mathbb{P}(g \leq 0) = \int_{-\infty}^{0} \varrho_g(z) dz.$$



Pdf ϱ is in general unknown $\rightarrow$ **KDE** provides approximation $\varrho_{g,N}$

$$\mathbb{P}_N(g \leq 0) = \int_{-\infty}^{0} \varrho_{g,N}(z) dz.$$

Kernel Density Estimation

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Definition (KDE)

- Let y be a n-dimensional real-valued random variable with an absolutely continuous distribution and probability density function ϱ.
- Let $\mathcal{Y} = \{y^{S,1}, \dots, y^{S,N}\}$ be an independent and identically distributed sampling of y.

→ The kernel density estimator $\varrho_N : \mathbb{R}^n \to \mathbb{R}_{\geq 0}$ is defined as

$$\varrho_N(z) = \frac{1}{N \det(H)^{1/2}} \sum_{i=1}^{N} K(H^{\frac{1}{2}}(z - y^{S,i}))$$

with a symmetric positive definite bandwidth matrix $H \in \mathbb{R}^{n \times n}$ and a n-variate density $K : \mathbb{R}^n \to \mathbb{R}_{\geq 0}$ called kernel.

Kernel Density Estimation

KDE: $\varrho_N(z) = \frac{1}{N \det(H)^{1/2}} \sum_{i=1}^{N} K(H^{\frac{1}{2}}(z - y^{S,i}))$

Heuristic Bandwidth Matrix H

Let $\sigma_{N,i}^2$ denotes the sample variance of the i-th variable,

$$H = \left(\frac{4}{(n+2)N}\right)^{\frac{2}{n+4}} \begin{bmatrix} \sigma_{N,1}^2 & & \\ & \ddots & \\ & & \sigma_{N,n}^2 \end{bmatrix}$$

Product Gaussian Kernel

$$K(x) = \prod_{i=1}^{n} \mathcal{K}(x_i) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x_i}{2}\right)$$

Kernel Density Estimation

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L^1-Convergence

$$\|\varrho_N - \varrho\|_{L^1} \xrightarrow{N\to\infty} 0 \quad \mathbb{P} - \text{almost surely}$$

Convergence of $\mathbb{P}_N(g \in D)$

Applying Scheffé's Lemma yields

$$\begin{aligned}|\mathbb{P}(g \in D) - \mathbb{P}_N(g \in D)| &= \left|\int_D \varrho(z)dz - \int_D \varrho_N(z)dz\right| \\ &\leq \frac{1}{2}\|\varrho_N - \varrho\|_{L^1} \xrightarrow{N\to\infty} 0 \quad \mathbb{P} - \text{almost surely}\end{aligned}$$

Stationary Gas Network

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Stationary semi-linear isothermal Euler Equation

$$\partial_x q = 0,$$
$$c^2 \partial_x p = -\frac{\lambda}{2D}(R_s T)^2 \frac{|q|q}{p}$$

- Constant speed of sound c, horizontal pipes, ideal gases ($p = \rho R_s T$)
- Pressure p, gas flow q, friction coefficient λ, specific gas constant R_s, constant temperature T, pipe diameter D

Analytic solution

$$q = \text{const.},$$
$$p(L) = \sqrt{p(0)^2 - \frac{\lambda R_s^2 T^2}{c^2 D} L|q|q},$$

with L be the length of pipe.

Stationary Gas Network

Network modelling

- Tree-structured graph with only one inflow node
- Stationary Euler equation models gas flow through pipes
- Boundary and coupling conditions (conservation of mass and equality of pressure)

Random gas demand

- Sink $v_i \in \mathcal{V}_{out}$ with $|\mathcal{V}_{out}| = n$ and boundary condition $q(v_i) = b_i$
- Gaussian distributed gas demands $b \sim \mathcal{N}(\mu, \Sigma)$ with $\mu \in \mathbb{R}^n_{\geq 0}$ and positive definite covariance matrix $\Sigma \in \mathbb{R}^{n \times n}$
  $\rightarrow$ n-dimensional random vector $p_{out} := (p(v_1), \dots, p(v_n))$, $v_i \in \mathcal{V}_{out}$
- Motivated by the application, μ and Σ are chosen s.t. $\mathbb{P}(b > 0) \approx 1$.

Stationary Gas Network

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- Interested in $\mathbb{P}(p_{out} \in P_{\min}^{\max})$ with $P_{\min}^{\max} = \bigotimes_{i=1}^{n}[p_i^{\min}, p_i^{\max}]$

SRD

- Define set of feasible outflows $M := \left\{b \in \mathbb{R}_{\geq 0}^{n} \middle| p_{out} \in P_{\min}^{\max}\right\}$
  $\rightarrow \mathbb{P}(b \in M) = \mathbb{P}(p_{out} \in P_{\min}^{\max})$

Direct approach - KDE

- Assumption: pressure p_{out} has a continuous distribution with probability density function ϱ_p
- Approximation of the pdf ϱ_p

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Algorithm (SRD)

Let $b \sim \mathcal{N}(\mu, \Sigma)$ and L such that $LL^T = \Sigma$.

1. Sample Q points $\{w_1, \dots, w_Q\}$ uniformly distributed on the sphere $\mathbb{S}^{n-1}$.
2. Compute the one-dimensional sets $M_i := \{r \geq 0 | rLw_i + \mu \in M\}$ for $i = 1, \dots, Q$.
   $\longrightarrow$ Using analytic solution we get a representation of M_i as union of disjoint intervals $M_i = \bigcup_{j=1}^{t} [\underline{a}_j, \overline{a}_j]$
3. Set $\mathbb{P}(b \in M) \approx Q^{-1} \sum_{i=1}^{Q} \mu_\chi(M_i)$
   $\longrightarrow \mu_\chi(M_i) = \sum_{j=1}^{t} \mathcal{F}_\chi(\overline{a}_j) - \mathcal{F}_\chi(\underline{a}_j)$ with χ-distribution function $\mathcal{F}_\chi$

Stationary Gas Network

Kernel Density Estimator

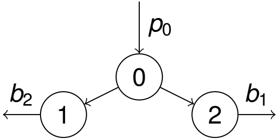
Algorithm (KDE)

1. Generate N independent and identically distributed (iid) samples $b^{S,i}$ of random outflow $b \sim \mathcal{N}(\mu, \Sigma)$
2. For every sample $b^{S,i}$ compute pressure $p_{out}(b^{S,i})$
3. Compute the kernel density estimator $\varrho_{p,N}$ for iid samples $p_{out}(b^{S,i})$ $\rightarrow$ Approximation of the exact pdf ϱ_p
4. Compute

$$\mathbb{P}(p_{out} \in P_{\text{min}}^{\text{max}}) \approx \int_{P_{\text{min}}^{\text{max}}} \varrho_{p,N}(z) dz = \frac{1}{N \prod_{j=1}^{n} h_j} \sum_{i=1}^{N} \prod_{j=1}^{n} \int_{p_j^{\text{min}}}^{p_j^{\text{max}}} \mathcal{K}\left(\frac{z_j - p_{out}(b^{S,i})}{h_j}\right) dz_j$$

Stationary Gas Network

Illustrative Example - Minimal Tree-Structured Graph



p_0	p^{min}	p^{max}	μ	Σ
60	$\begin{pmatrix} 40 \\ 30 \end{pmatrix}$	$\begin{pmatrix} 60 \\ 50 \end{pmatrix}$	$\begin{pmatrix} 4 \\ 4 \end{pmatrix}$	$\begin{pmatrix} 0.25 & 0 \\ 0 & 0.25 \end{pmatrix}$

10^5 Gaussian distributed samples for KDE, 10^4 uniform distributed samples of sphere $\mathbb{S}^1$ for SRD

	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6	Test 7
MC	75.07%	75.15%	75.22%	75.08%	74.88%	75.02%	74.99%
KDE	74.75%	74.84%	74.89%	74.78%	74.55%	74.76%	74.67%
SRD	74.95%						

Contamination flow in water network

For $(t, x) \in [0, T] \times [0, L]$ and constants $d < 0$, $m \leq 0$, we consider the deterministic scalar linear PDE with initial condition and boundary condition

$$\begin{aligned} \partial_t r(t, x) + d\partial_x r(t, x) &= mr(t, x), \\ r(0, x) &= r_0(x), \\ r(t, L) &= b(t). \end{aligned}$$

- Concentration r of the contamination
- Water gets polluted: $b(t) \geq 0$; water gets cleaned: $b(t) < 0$

Dynamic Flow Network

Time dependent random boundary data $b(t) \rightarrow$ representation as Fourier series

- boundary function $b_D \in L^2([0, T])$

$$b_D(t) = \sum_{m=0}^{\infty} a_m^0 \psi_m(t).$$

with

$$a_m^0 := \int_0^T b_D(t)\psi_m(t)dt, \quad \psi_m(t) := \frac{\sqrt{2}}{\sqrt{T}} \sin\left(\left(\frac{\pi}{2} + m\pi\right)\frac{t}{T}\right),$$

- For $a_m \sim \mathcal{N}(\mu, \sigma^2)$ consider random boundary data

$$b(t) = \sum_{m=0}^{\infty} a_m a_m^0 \psi_m(t) \qquad \in L^2([0, T]) \quad \mathbb{P}\text{-almost surely}$$

Dynamic Flow Network

Probabilistic Constraints in a Time-Dependent Setting

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What is the probability that the contamination concentration r_1 at the inflow node v_1 meets the bounds $B := [r^{\min}, r^{\max}]$ during the whole time?

- With $M(t) := \{b \in L^2([0, T]; \mathbb{R}^n_{\leq 0}) | r_1(t, b) \in B\}$ we can write

$$\mathbb{P}\left(b \in M(t) \quad \forall t \in [0, T]\right)$$

- Set $\underline{t} := \operatorname{argmin}_{t \in [0,T]} r_1(t), \bar{t} := \operatorname{argmax}_{t \in [0,T]} r_1(t)$

$$\mathbb{P}(b \in M(\underline{t}) \text{ and } b \in M(\bar{t})) \qquad \longrightarrow \text{SRD?}$$

- Minimal and maximal value of $r_1(t)$ in $t \in [0, T]$ meet the bounds B

$$\mathbb{P}\left(\left(\min_{t \in [0,T]} r_1(t), \max_{t \in [0,T]} r_1(t)\right)^T \in B^2\right)$$

Dynamic Flow Network
KDE

Assumption

Random vector $R := (\min_{t\in[0,T]} r_1(t,b), \max_{t\in[0,T]} r_1(t,b))^T$ has an absolutely continuous distribution with pdf ϱ_R

Algorithm KDE

- Generate N iid samples $a_m^{S,i}$ of $a_m \sim \mathcal{N}(\mu,\Sigma)$ for $m = 1, \dots, N_F$
- Compute corresponding sample $b^{S,i}$ of truncated random boundary function b
- For every sample $b^{S,i}$ compute

$$\underline{r_1}^{S,i} := \min_{t\in[0,T]} r_1(t, b^{\mathcal{S},i}), \qquad \overline{r_1}^{S,i} := \max_{t\in[0,T]} r_1(t, b^{\mathcal{S},i}).$$

- Compute KDE $\varrho_{R,N}$ for 2-dim. samples $R^{S,i} = (\underline{r_1}^{S,i}, \overline{r_1}^{S,i})^T$ and approximate

$$\mathbb{P}(R \in [r^{\min}, r^{\max}]^2) \approx \int_{[r^{\min}, r^{\max}]^2} \varrho_{R,N}(z)dz$$

Dynamic Flow Network
Illustrative Example - One Pipe

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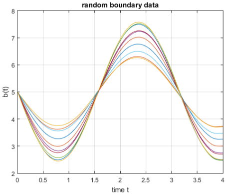
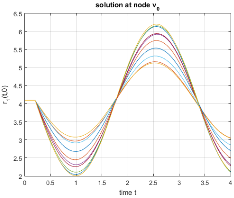
$r^{\min}$	$r^{\max}$	μ	σ	d	m	L	T
2	6	1	0.25	-5	-1	1	4

Further: 101 time discretization points, 30 terms in the Fourier series, sampling of 10^5 boundary functions





	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6	Test 7
MC	74.32%	74.39%	74.22%	74.32%	74.24%	74.33%	74.51%
KDE	74.33%	74.39%	74.21%	74.31%	74.24%	74.32%	74.51%

Conclusion

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- Compare SRD and KDE on a minimal tree-structured graph
- Extend probabilistic constraints to a time dependent setting
- Illustrative example for KDE in dynamic setting

Outlook

- Exact solution unknown $\rightarrow$ Need numerical method for approximation $\rightarrow$ Reduce sampling cost for KDE using adaptive stochastic collocation method
- Analysis of necessary optimality conditions

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