Friedrich-Alexander-Universität
Naturwissenschaftliche Fakultät

Probabilistic Constrained Optimization on Flow Networks

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Motivation

Probabilistic Constraints

Consider the optimization problem

$$\min_{x \in \mathcal{X}} \quad f(x)$$
$$\text{s.t.} \quad \mathbb{P}\Big(g(x,\xi) \leq 0 \Big) \geq \alpha$$

with objective function f, constraint g, decision vector x, random variable ξ (with probability distribution and density function) and probability level α.

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How can we evaluate the probability?

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We have

$$\mathbb{P}\big(\, g(x,\xi) \leq 0 \,\big) = \int_{M(x)} \varrho_\xi(z)\, dz,$$

with

$$M(x) = \{\, \omega \in \Omega \mid g(x,\xi(\omega)) \leq 0 \,\}.$$

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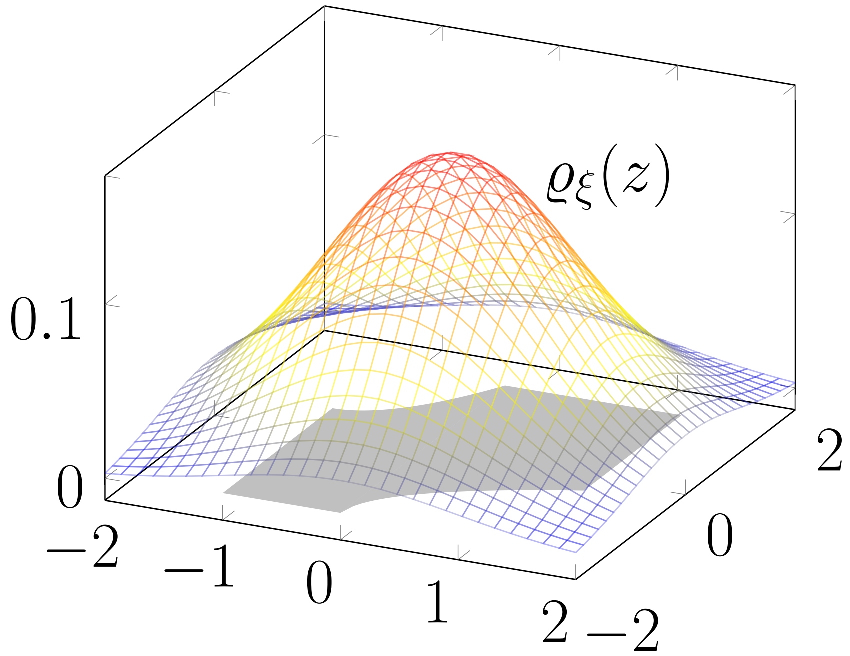
Is there a „better“ way to compute this probability?

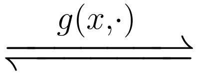
Motivation

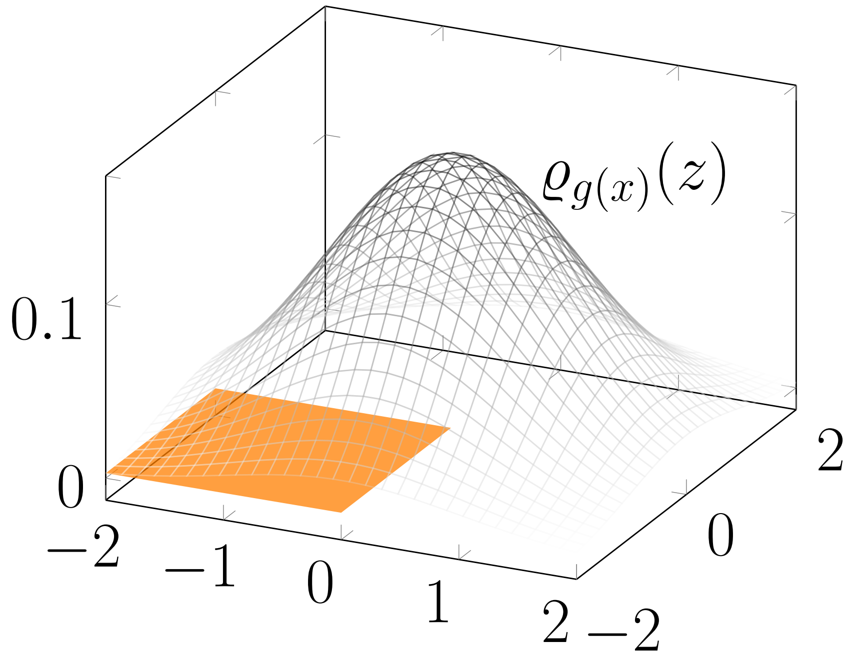
Probabilistic Constraints

Idea: Forward transformation of M along g



(a) Well-known distribution (colored), unknown set of feasible loads (grey)





(b) Unknown distribution (grey), well-known set of feasible pressures (orange)

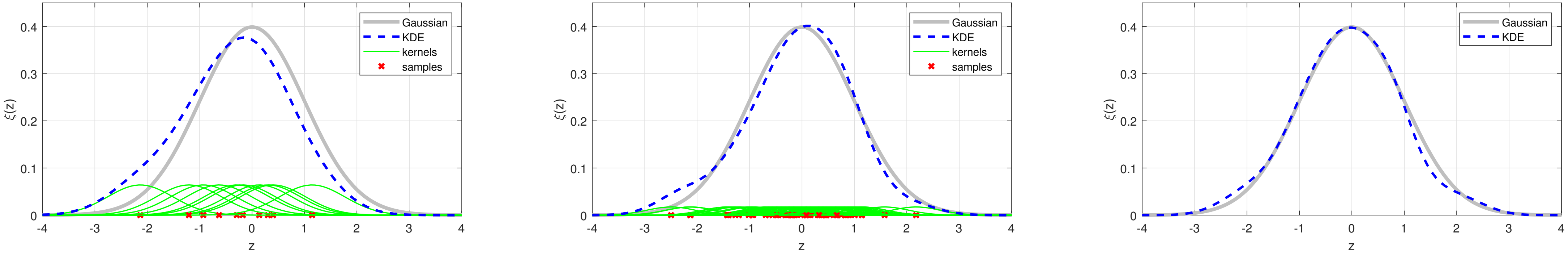
Mathematical Background

Kernel Density Estimation

Definition: Kernel Density Estimator

Let $\mathcal{Y} = \{y_1, \cdots, y_{N_{\text{KDE}}}\} \subseteq \mathbb{R}^n$ be i.i.d. samples of the random variable Y, which has an absolutely continuous distribution function with probability density function ϱ. Let K be a n-dimensional kernel function.
Then the kernel density estimator $\varrho_{N_{\text{KDE}}}$ corresponding to the bandwidth matrix $H \in \mathbb{R}^{n\times n}$ is defined as

$$\varrho_{N_{\text{KDE}}}(z) = \frac{1}{N_{\text{KDE}} \det(H)^{\frac{1}{2}}} \sum_{i=1}^{N_{\text{KDE}}} K\Big(H^{-\frac{1}{2}}(z - y_i)\Big).$$



(a) KDE with 10 samples (b) KDE with 50 samples (c) KDE with 100 samples

A. Gramacki (2018): Nonparametric Kernel Density Estimation and its Computational Aspects. *Springer International Publishing*

Evaluating Probabilities

Application of the KDE

- Let $\mathcal{S} = \{s_1, \cdots, s_{N_{\text{KDE}}}\}$ be independent and identically distributed samples of the random variable ξ.
- Let $\mathcal{G}_{\mathcal{S}}(x) = \{g(x, s_1), \cdots, g(x, s_{N_{\text{KDE}}})\}$ be the corresponding sample of the constraint g (also independent and identically distributed) for $x \in \mathcal{X}$.

Multivariate Gaussian kernel

$$K(z) = \frac{1}{(2\pi)^{\frac{n}{2}}} \exp\left(-\frac{1}{2} \|z\|^2\right)$$

Diagonal bandwidth matrix

$$H_{i,i} = h^2 \left(\Sigma_{N_{\text{KDE}}}\right)_{i,i}$$

$$h = \left(\frac{4}{(n+2) N_{\text{KDE}}}\right)^{\frac{1}{n+4}}$$

$$\varrho_{N_{\text{KDE}}}(z) = \frac{1}{N_{\text{KDE}} \det(H)^{\frac{1}{2}}} \sum_{i=1}^{N_{\text{KDE}}} K\left(H^{-\frac{1}{2}}(z - g(x, s_i))\right)$$

M. Schuster (2021): *Nodal Control and Probabilistic Constrained Optimization using the Example of Gas Networks.* Dissertation, FAU Erlangen-Nürnberg, Germany, 2021. https://opus4.kobv.de/opus4-trr154/frontdoor/index/index/docId/410

M. Schuster, E. Strauch, M. Gugat, J. Lang (2022): *Probabilistic Constrained Optimization on Flow Networks.* Optim. Eng. 23, pp. 1–50.

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Diagonal bandwidth matrix

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$$h = \left(\frac{4}{(n+2)N_{\mathsf{KDE}}}\right)^{\frac{1}{n+4}}$$

$$\begin{aligned}\varrho_{N_{\mathsf{KDE}}}(z) &= \frac{1}{N_{\mathsf{KDE}}\det(H)^{\frac{1}{2}}} \sum_{i=1}^{N_{\mathsf{KDE}}} K\left(H^{-\frac{1}{2}}(z - g(x, s_i))\right) \\ &= \frac{1}{N_{\mathsf{KDE}}\det(H)^{\frac{1}{2}}} \sum_{i=1}^{N_{\mathsf{KDE}}} \prod_{j=1}^{n} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{z_j - g_j(x, s_i)}{\sqrt{H_{j,j}}}\right)^2\right)\end{aligned}$$

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Evaluating Probabilities

Application of the KDE

$$\mathbb{P}_{N_{\text{KDE}}}\big(\, g(x,\xi) \le 0 \,\big) = \int_{(-\infty,0]^n} \varrho_{N_{\text{KDE}}}(z)\, dz$$
$$= \int_{(-\infty,0]^n} \frac{1}{N_{\text{KDE}} \det(H)^{\frac{1}{2}}} \sum_{i=1}^{N_{\text{KDE}}} \prod_{j=1}^{n} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2} \left(\frac{z_j - g_j(x, s_i)}{\sqrt{H_{j,j}}} \right)^2 \right) dz$$
$$= \frac{1}{N_{\text{KDE}} \det(H)^{\frac{1}{2}}} \sum_{i=1}^{N_{\text{KDE}}} \prod_{j=1}^{n} \int_{-\infty}^{0} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2} \left(\frac{z_j - g_j(x, s_i)}{\sqrt{H_{j,j}}} \right)^2 \right) dz_j$$

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Gauss error function: $\mathsf{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp\big(-t^2\big)\; dt$

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probability via KDE

$$\mathbb{P}_{N_{\mathsf{KDE}}}\big(\, g(x,\xi) \le 0 \,\big) = \frac{1}{N_{\mathsf{KDE}} 2^n} \sum_{i=1}^{N_{\mathsf{KDE}}} \prod_{j=1}^{n} \left[1 - \mathrm{erf}\left(\frac{g_j(x,s_i)}{\sqrt{2\, H_{j,j}}}\right)\right]$$

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Probabilistic Constrained Optimization

Application of the KDE

We consider the following probabilistic constrained optimization problem and its approximation:

$$(P_\infty) \quad \begin{cases} \min\limits_{x \in \mathcal{X}} & f(x) \\ \text{s.t.} & \mathbb{P}\big(\, g(x,\xi) \leq 0 \,\big) \geq \alpha \end{cases} \qquad (P_{N_{\text{KDE}}}) \quad \begin{cases} \min\limits_{x \in \mathcal{X}} & f(x) \\ \text{s.t.} & \mathbb{P}_{N_{\text{KDE}}}\big(\, g(x,\xi) \leq 0 \,\big) \geq \alpha \end{cases}$$

We assume, that both problems have at least one solution.

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Theorem 1

Let x^* be a solution of (P_∞) with $\mathbb{P}\big(\, g(x^*,\xi) \leq 0 \,\big) > \alpha$. Then there exists ${N_{\text{KDE}}}^*$ sufficiently large, s.t. x^* is also a solution of $(P_{N_{\text{KDE}}})$ for all $N_{\text{KDE}} > N^*$ $\mathbb{P}$-almost surely.

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Theorem 2

If the KDE $\mathbb{P}$-almost surely uniformly converges for every $x \in \mathcal{X}$, and if $(x^*_{N_{\text{KDE}}})_{N_{\text{KDE}}\geq 1}$ is a convergent sequence of solutions of $(P_{N_{\text{KDE}}})$, then its limit x^* is $\mathbb{P}$-almost surely a solution of (P_∞).

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Theorem 3

If x^* is a unique solution of (P_∞) and if $f(x) - f(x^*) < \varepsilon$ only in an area around x^*, then there $\mathbb{P}$-almost surely exists a convergent sequence of solutions of $(P_{N_{\text{KDE}}})$.

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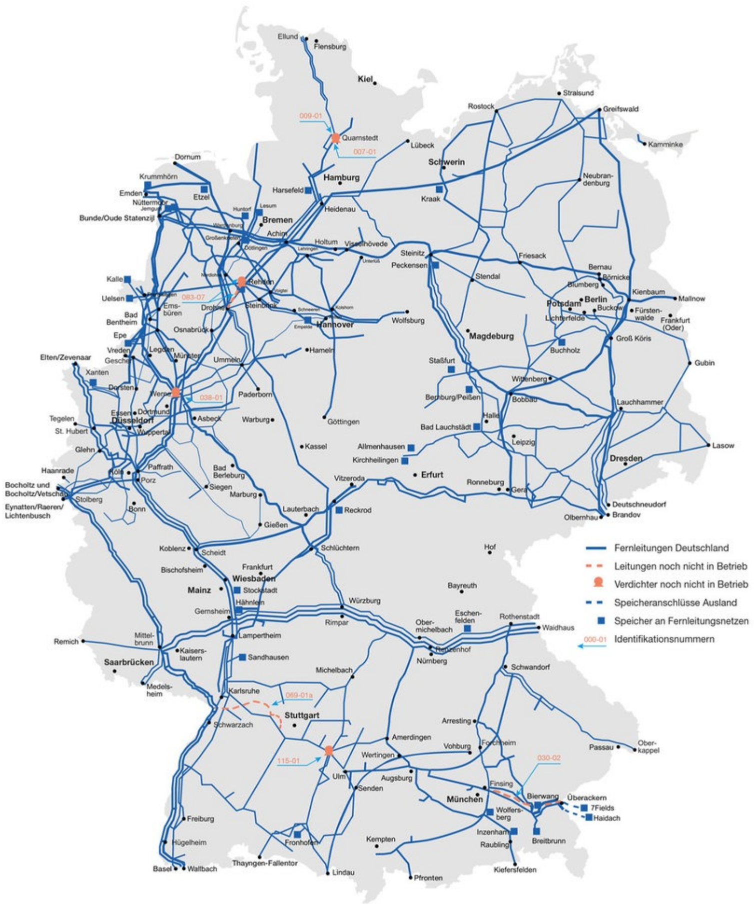
Application to Gas Flow in Pipelines

Motivation



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Application to Gas Flow in Pipelines

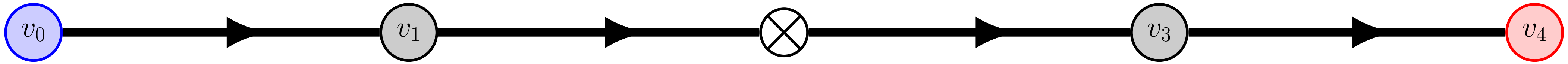
Gas Network Modelling

p	gas pressure	v	gas velocity	g	gravitational constant
ρ	gas density	λ/D	pipe friction	α	pipe slope

Isothermal Euler Equations

$$\rho_t + (\rho v)_x = 0$$

$$(\rho v)_t + \left(p + \rho v^2\right)_x = -\frac{\lambda}{2D}\rho v|v| - g\rho\sin(\alpha)$$



Source: Inlet Pressure

$$p(t) = p_0(t)$$

Compressor Station

$$\frac{p_{\text{out}}(t)}{p_{\text{in}}(t)} = u(t)$$

Sink: Gas Outflow

$$(\rho v)(t) = b(t)$$

Coupling Conditions

Conservation of Mass: $\sum(\rho v)_{\text{in}}(t) = \sum(\rho v)_{\text{out}}(t)$, Continuity in Pressure: $p_{\text{in}} = p_{\text{out}}$

Application to Gas Flow in Pipelines

The Isothermal Euler Equations

The isothermal Euler equations for ideal gases:

(ISO)

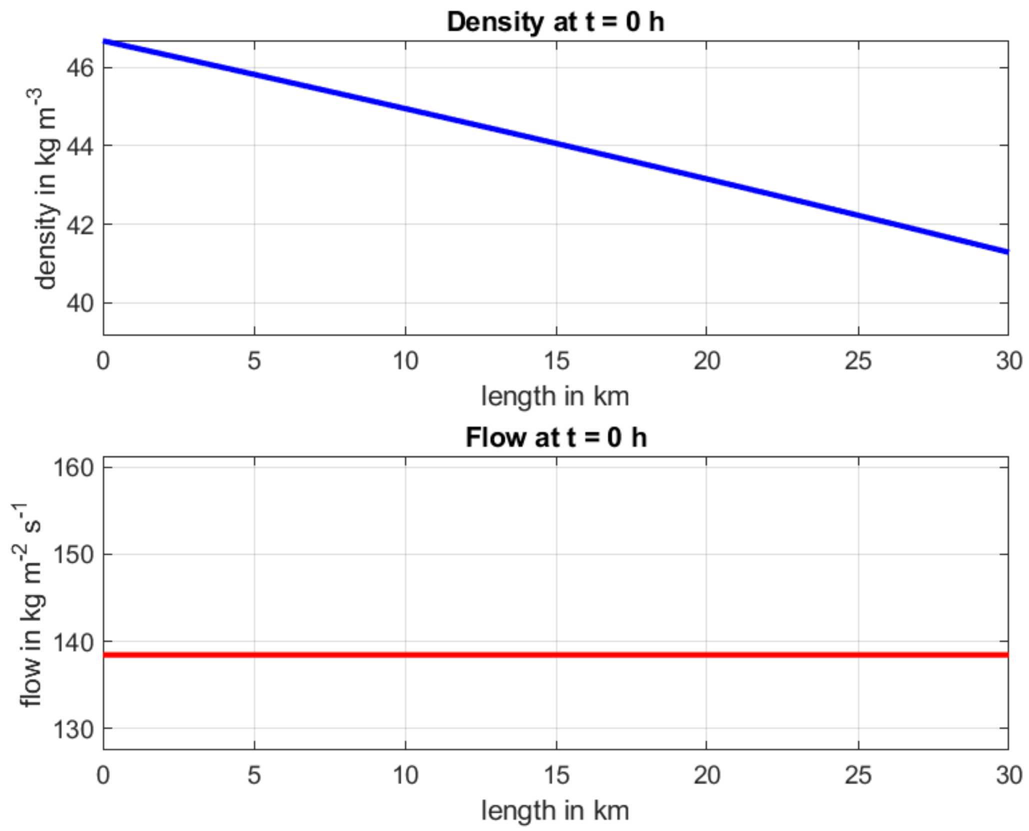
$$\rho_t + q_x = 0,$$
$$q_t + \left(c^2 p + \frac{q^2}{\rho}\right)_x = -\frac{\lambda^F}{2D}\frac{q|q|}{\rho}.$$

Inlet density & Gas outflow

$$\rho(t,0) = \rho_0(t),$$
$$q(t,L) = b(t).$$

Initial condition

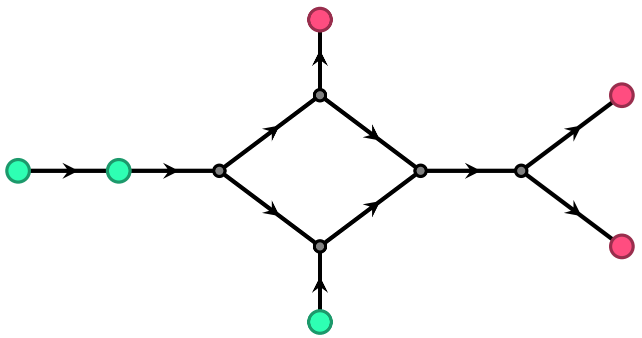
$$\rho(0,x) = \rho_{\text{ini}}(x),$$
$$q(0,x) = q_{ini}(x).$$



Gugat and Ulbrich (2018): *Lipschitz solutions of initial boundary value problems for balance laws.* Math. Models Methods Appl. Sci., 28(5): 921–951

Application to Gas Flow in Pipelines

Stationary Gas Networks



p_0	$p^{\min}$	outflow ξ	covariance	α
$\begin{pmatrix}60\\58\\60\end{pmatrix}$	$\begin{pmatrix}40\\40\\40\end{pmatrix}$	$\begin{pmatrix}20\\15\\18\end{pmatrix}$	$\begin{pmatrix}2&0&0\\0&2&0\\0&0&2\end{pmatrix}$	75%

Deterministic optimization

$$\min_{p^{\text{max}}_{\text{det}}} \sum p^{\text{max}}_{\text{det}}, \quad \text{s.t.} \quad \text{Gas Network Model}, \quad p_i \in [p_i^{\text{min}}, p^{\text{max}}_{\text{det},i}] \quad \Rightarrow \quad p^{\text{max}}_{\text{det}} = \begin{pmatrix}46.10\\52.04\\51.08\end{pmatrix}$$

Probabilistic optimization

$$\min_{p^{\text{max}}_{\text{prob}}} \sum p^{\text{max}}_{\text{prob}}, \quad \text{s.t.} \quad \text{Gas Network Model}, \quad \mathbb{P}\left(p_i \in [p_i^{\text{min}}, p^{\text{max}}_{\text{prob},i}] \right) \geq 0.75. \quad \Rightarrow \quad p^{\text{max}}_{\text{prob}} = \begin{pmatrix}47.52\\53.34\\52.45\end{pmatrix}$$

How good is the optimal deterministic solution in the probabilistic setting?

$$\mathbb{P}\left(b \in M(p^{\text{max}}_{\text{det}}) \right) \approx 35.4\%$$

https://gaslib.zib.de/

Application to Gas Flow in Pipelines

Time Dependent Uncertainty

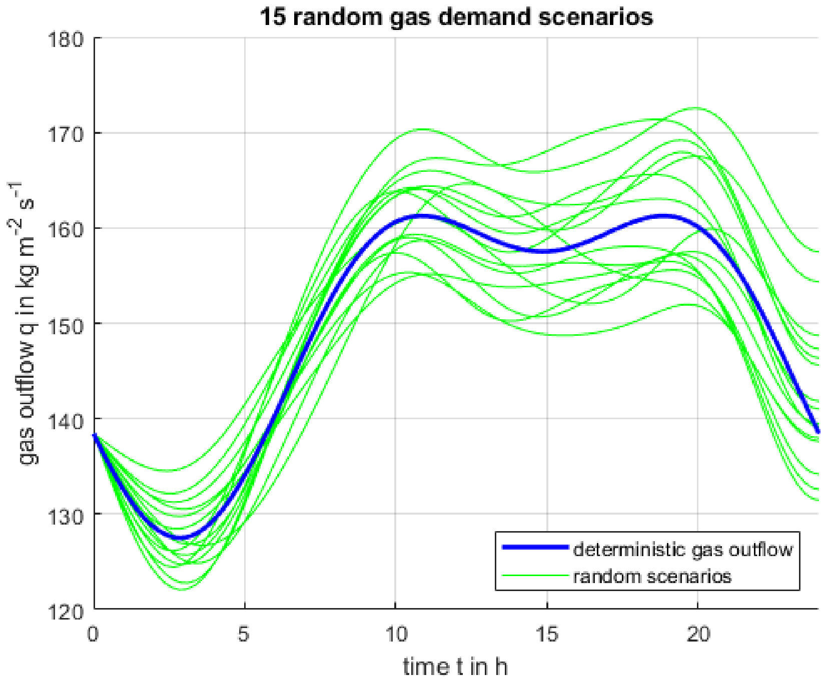
Random Boundary Functions

- Write a function f as Fourier series

$$f(t) = \sum_{m=0}^{\infty} a_m^0(f)\,\psi_m(t)$$

- For random variables $\xi_m \sim \mathcal{N}(1,\sigma)$ define

$$f^{\omega}(t) = \sum_{m=0}^{\infty} \xi_m(\omega)\,a_m^0(f)\,\psi_m(t)$$



Application to Gas Flow in Pipelines

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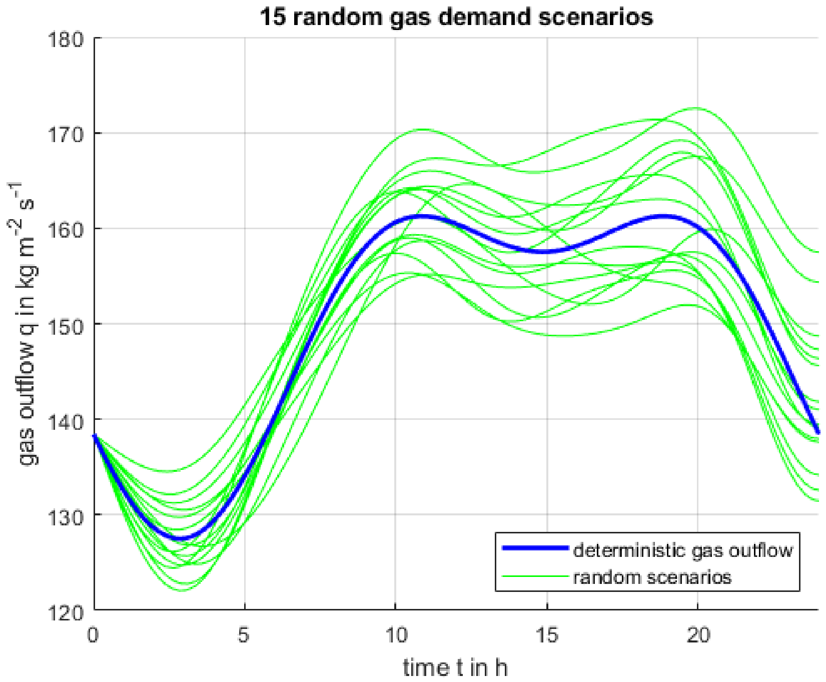

Time dependent probabilistic constraint

$$\mathbb{P}(\ f^\omega \in M(t) \quad \forall t \in [0, T]\ )\ \geq\ \alpha$$

„We want to guarantee that a percentage α of all possible random scenarios is feasible in every point in time $t \in [0, T]$."

Application to Gas Flow in Pipelines

Dynamic Probabilistic Constraints

- Let $\mathcal{B} = \{ \, b^{S,1}(t), \cdots, b^{S,N_{\text{KDE}}}(t) \, \}$ be independent and identically distributed random boundary functions
- There exists a solution $\rho \in C(0,T;L^2(0,L))$, i.e. the densities are continuous in time
- Let $\mathcal{P}_{\mathcal{B}} = \{ \, \rho(t;b^{S,1}), \cdots, \rho(t;b^{S,N_{\text{KDE}}}) \, \}$ be the corresponding densities at the end of the pipe

$$\mathbb{P}\left(\, \rho(t,L) \in \left[\rho^{\text{min}}, \rho^{\text{max}}\right] \quad \forall t \in [0,T] \, \right) \quad = \quad \mathbb{P}\begin{pmatrix} \min\limits_{t\in[0,T]} \rho(t,L) \in \left[\rho^{\text{min}}, \rho^{\text{max}}\right] \\ \max\limits_{t\in[0,T]} \rho(t,L) \in \left[\rho^{\text{min}}, \rho^{\text{max}}\right] \end{pmatrix}$$

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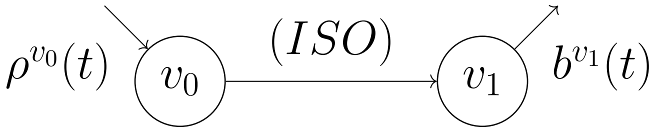
$\Rightarrow$ The sample $\left\{ \begin{bmatrix} \underline{\rho}(b_1) := \min\limits_{t\in[0,T]} \rho(t;b^{S,1}) \\ \overline{\rho}(b_1) := \max\limits_{t\in[0,T]} \rho(t;b^{S,1}) \end{bmatrix}, \cdots, \begin{bmatrix} \underline{\rho}(b_{N_{\text{KDE}}}) := \min\limits_{t\in[0,T]} \rho(t;b^{S,N_{\text{KDE}}}) \\ \overline{\rho}(b_{N_{\text{KDE}}}) := \max\limits_{t\in[0,T]} \rho(t;b^{S,N_{\text{KDE}}}) \end{bmatrix} \right\} \subseteq \mathbb{R}^{2n}$

is a sample of random numbers and we can apply the KDE-approach as introduced before.

Application to Gas Flow in Pipelines

Dynamic Probabilistic Constraints



$\rho_0(t)$	$\rho^{\min}$	c	λ^F	D	L	T	α
46.75 kg/m^3	34 kg/m^3	343 m/s	0.1	0.5 m	30 km	24 h	90%

Deterministic Optimization

$$\min_{\rho_{\text{det}}^{\text{max}}} \quad \rho_{\text{det}}^{\text{max}},$$

s.t. Isothermal Euler Equations,

$$\rho(t,L) \in [\rho^{\text{min}}, \rho_{\text{det}}^{\text{max}}]$$

$$\Rightarrow \quad \rho_{\text{det}}^{*,\text{max}} = 42.15\ kg/m^3$$

Probabilistic Optimization

$$\min_{\rho_{\text{prob}}^{\text{max}}} \quad \rho_{\text{prob}}^{\text{max}},$$

s.t. Isothermal Euler Equations

$$\mathbb{P}\left(\rho(t,L) \in \left[\rho^{\text{min}}, \rho_{\text{prob}}^{\text{max}}\right] \ \forall t \in [0,T]\right) \geq 0.9.$$

$$\Rightarrow \quad \rho_{\text{prob}}^{*,\text{max}} = 42.49\ kg/m^3$$

How good is the optimal deterministic solution in the probabilistic setting?

$$\mathbb{P}\left(b(t) \in M(t; p_{\text{det}}^{\max}) \quad \forall t \in [0,T] \right) \approx 50\%$$

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Probabilistic Robustness

Let bounds for the pressures $0 < p_{\min} < p_{\max}$ be given at every node. For $\varepsilon > 0$ consider the optimal control problem

$$\min_{u(t)} \quad f(u, q)$$

s.t.

$\rho_t + (\rho v)_x = 0$ $(\rho v)_t + \left(p + \rho v^2\right)_x = -\frac{\lambda}{2D}\rho v\lvert v\rvert - g\rho\sin(\alpha)$	on every edge	Gas Network Model
$p(t) = p_0(t)$	on every source node	
$(\rho v)(t) = b(t)$	on every sink node	
$\sum(\rho v)_{\text{in}}(t) = \sum(\rho v)_{\text{out}}(t)$ $p_{\text{in}} = p_{\text{out}}$	on every inner node	
$\frac{p_{\text{out}}(t)}{p_{\text{in}}(t)} = u(t)$	for every compressor	
$p(t) \in \left[\, p_{\min} + \varepsilon,\ p_{\max} - \varepsilon \,\right] \quad \forall t \in [0, T]$	on every node	State Constraint

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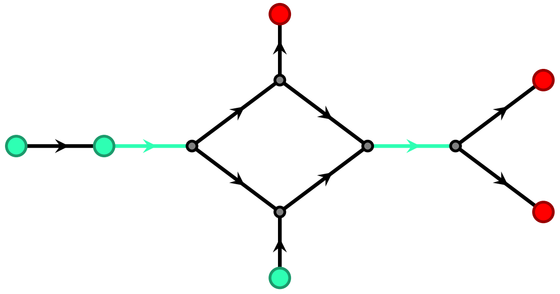
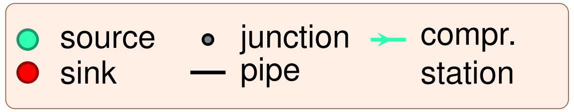
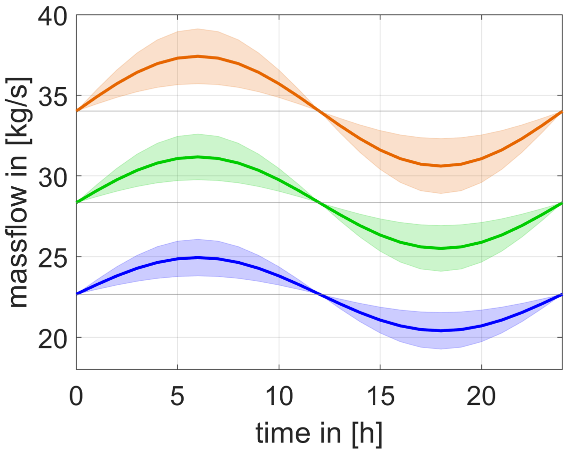
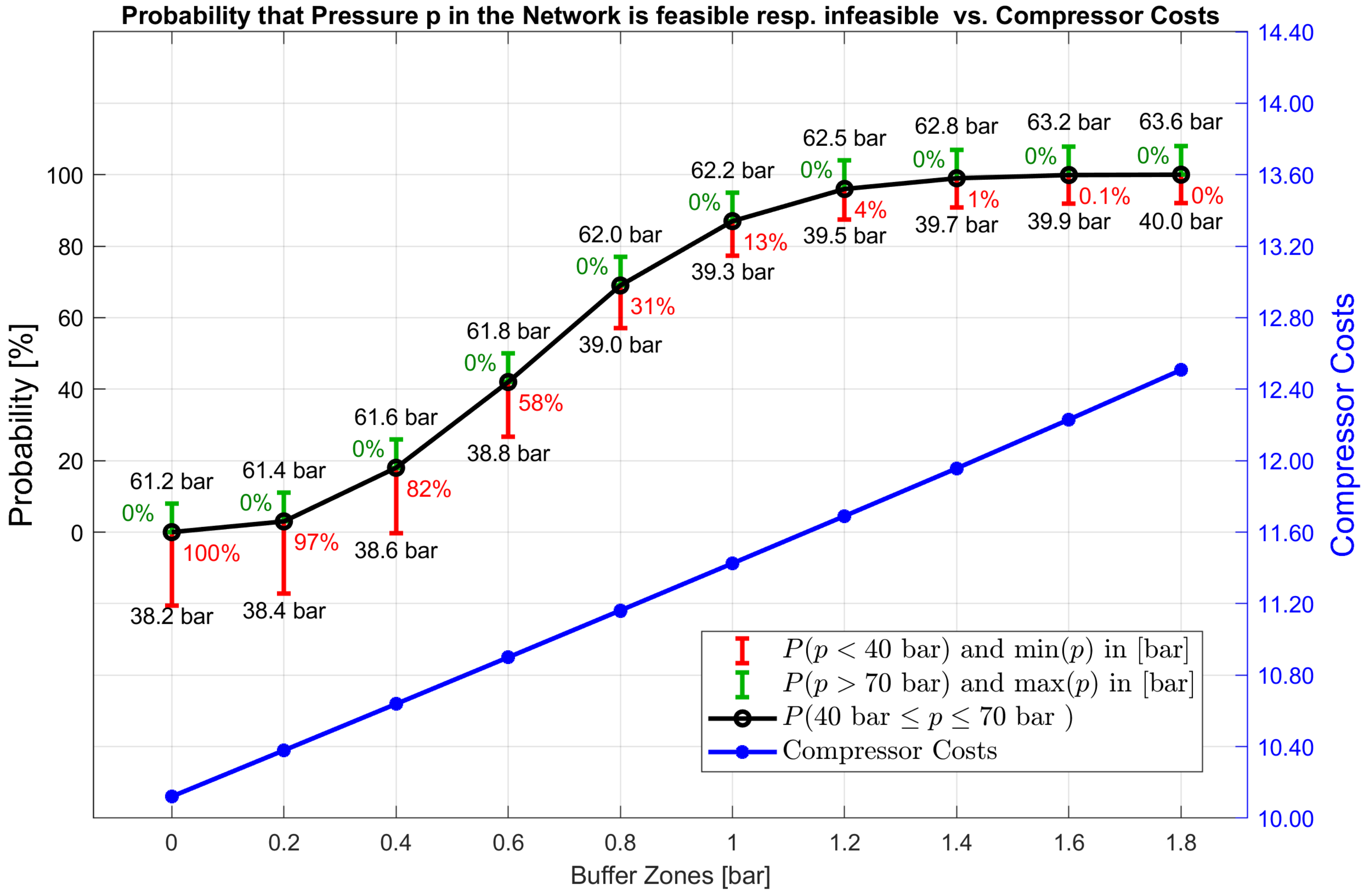
Probabilistic Robustness









Schuster, Wilka, Strauch, Lang, Gugat (2025): *Probabilistic Robustness for Compressor Controls in Transient Pipeline Networks.* Preprint to be submitted soon.

Probabilistic Constrained Optimization

References

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