Probabilistic Constrained Optimization on Gas Networks

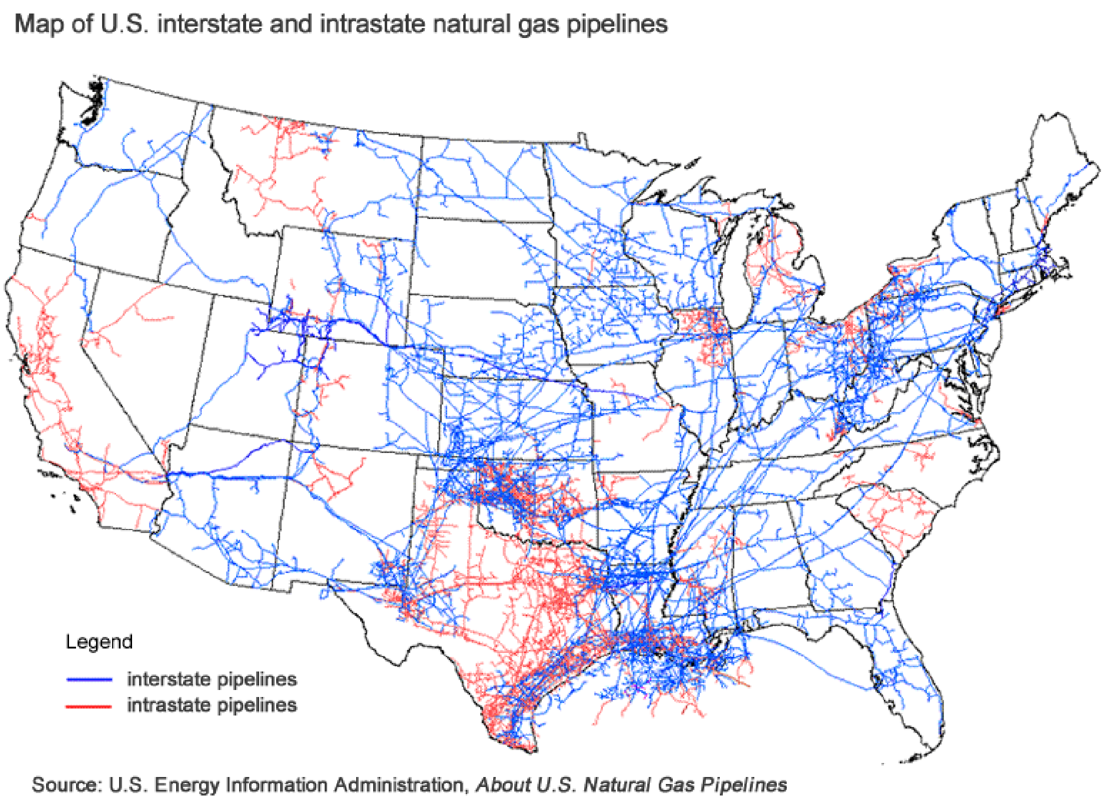
Michael Schuster (FAU), Martin Gugat (FAU), Rüdiger Schultz (UDE)

July 27, ICSP 2023 Davis, CA

Friedrich-Alexander Universität Erlangen-Nürnberg (FAU),
Universität Duisburg-Essen (UDE)

Motivation

Natural Gas Transport



© U.S. Energy Information Administration

© European Hydrogen Backbone

Motivation

Probabilistic Constraints

Consider the optimization problem

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

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

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

with

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

Motivation

Probabilistic Constraints

Consider the optimization problem

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

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

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

with

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

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

Stationary Gas Transport

Mathematical Modelling on Networks

- Consider a connected, directed graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with vertex set $\mathcal{V}$ and set of edges $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$
- We consider the stationary model (ISO4) for ideal gases on every edge $e \in \mathcal{E}$

(ISO4) for ideal gases

$$q_x = 0, \quad p_x = -\frac{c^2 \lambda^F}{2D} \frac{q|q|}{p}$$

solution of (ISO4)

$$q(x) = const., \quad p^2(x) = p(0)^2 - \frac{c^2 \lambda^F}{2D} q|q|\, x$$

Coupling conditions at the nodes:

Conservation of mass

$$\sum_{e \in \mathcal{E}_-(v)} q^e \left(\frac{D^e}{2}\right)^2 \pi = b^v + \sum_{e \in \mathcal{E}_+(v)} q^e \left(\frac{D^e}{2}\right)^2 \pi \quad \forall v \in \mathcal{V} \backslash \mathcal{V}_0.$$

Continuity in pressure

$$p^{e_1}(L^{e_1}) = p^{e_2}(0) \quad \forall e_1 \in \mathcal{E}_-(v),\ e_2 \in \mathcal{E}_+(v).$$

Stationary Gas Transport

Mathematical Modelling on Networks

Boundary Conditions:

Inlet pressure

$$p^e(0) = p_0 \in \mathbb{R}_{\geq 0} \quad \forall e \in \mathcal{E}_+(v_0)$$

Gas outflow

$$q^e(L^e) = b^v \in \mathbb{R}_{\geq 0} \quad \forall e \in \mathcal{E}_-(v)$$

b^v represents the consumers gas demand

- Let $p \in \mathbb{R}^n$ be the vector of pressures at the nodes $v_1, \cdots, v_n$
- We assume box constraints for the pressures at the nodes: $p_i \in [p_i^{\min}, p_i^{\max}]$

Set of feasible loads

$$M := \left\{ b \in \mathbb{R}^n_{\geq 0} \;\middle|\; \begin{array}{l} (p,q) \in \mathbb{R}^n \times \mathbb{R}^n \text{ satisfies:} \\ \bullet \text{ stationary semilinear isothermal Euler equations,} \\ \bullet \text{ inlet pressure and gas outflow,} \\ \bullet \text{ conservation of mass and continuity in pressure,} \\ \bullet \text{ pressure bounds.} \end{array} \right\}$$

[Gugat, Hante, Hirsch-Dick, Leugering, 2015]: *Stationary states in gas networks.* Netw. Heterog. Media, 10(2): 295–320.

Stationary Gas Transport

Gas Networks under Uncertainty

Assume that the consumers gas demand is random in the sense, that there is a random variable

$$\xi_b \sim \mathcal{N}(\mu, \Sigma),$$

on an appropriate probability space. We identify b with the image $\xi_b(\omega)$ for $\omega \in \Omega$.

For a given inlet pressure, can we guarantee, that every consumer receives their demanded gas, s.t. the gas pressure in the network is neither too high nor too low, in at least $\alpha\%$ of all scenarios?

$$\mathbb{P}\big(\, \omega \in \Omega \mid \xi_b(\omega) \in M \,\big) \;\geq\; \alpha$$

Stationary Gas Transport

Gas Networks under Uncertainty

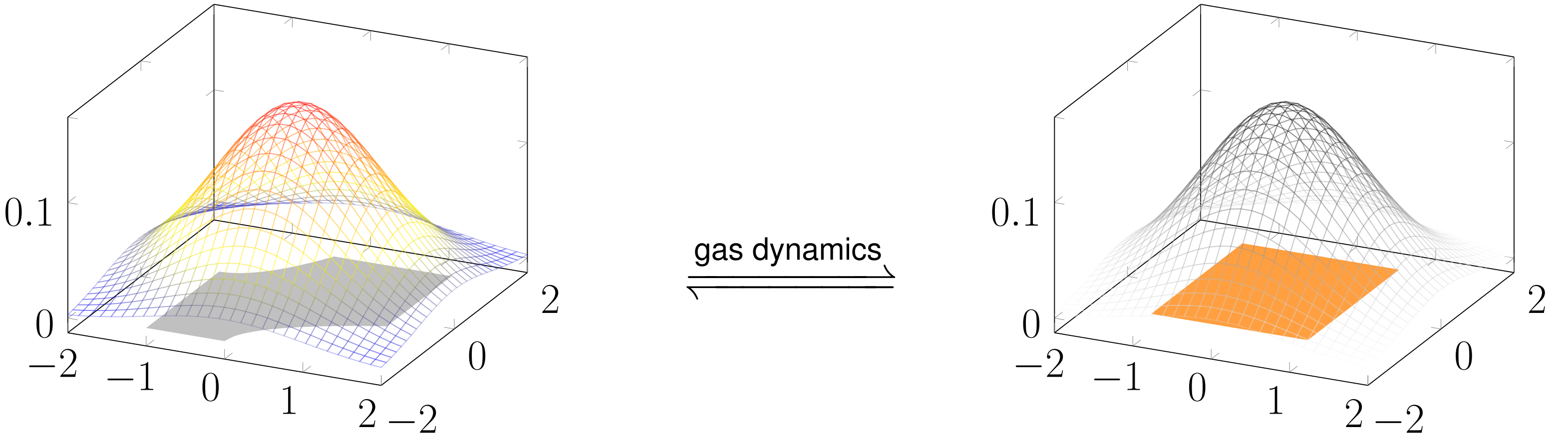
Assume that the consumers gas demand is random in the sense, that there is a random variable

$$\xi_b \sim \mathcal{N}(\mu, \Sigma),$$

on an appropriate probability space. We identify b with the image $\xi_b(\omega)$ for $\omega \in \Omega$.

For a given inlet pressure, can we guarantee, that every consumer receives their demanded gas, s.t. the gas pressure in the network is neither too high nor too low, in at least $\alpha\%$ of all scenarios?

$$\mathbb{P}\big(\ \omega \in \Omega \mid \xi_b(\omega) \in M\ \big) \ \geq\ \alpha$$



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

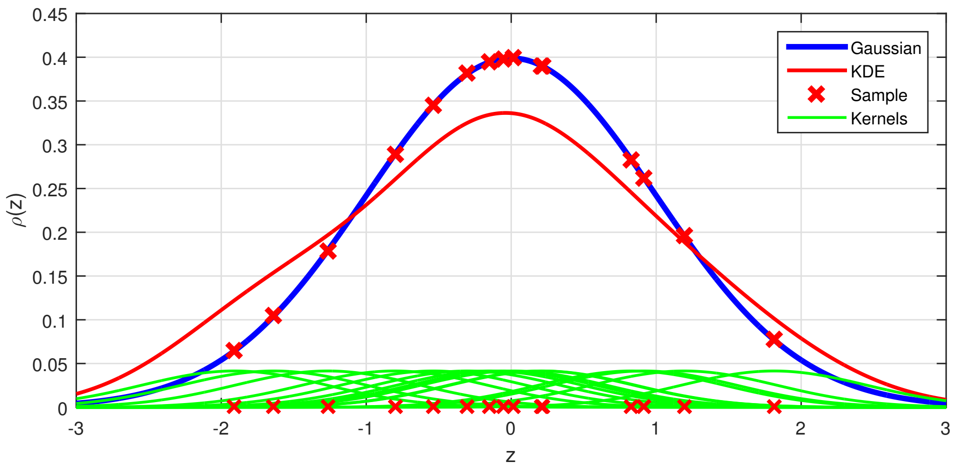
(b) Unknown distribution (grey), well-known set of feasible pressures (orange)

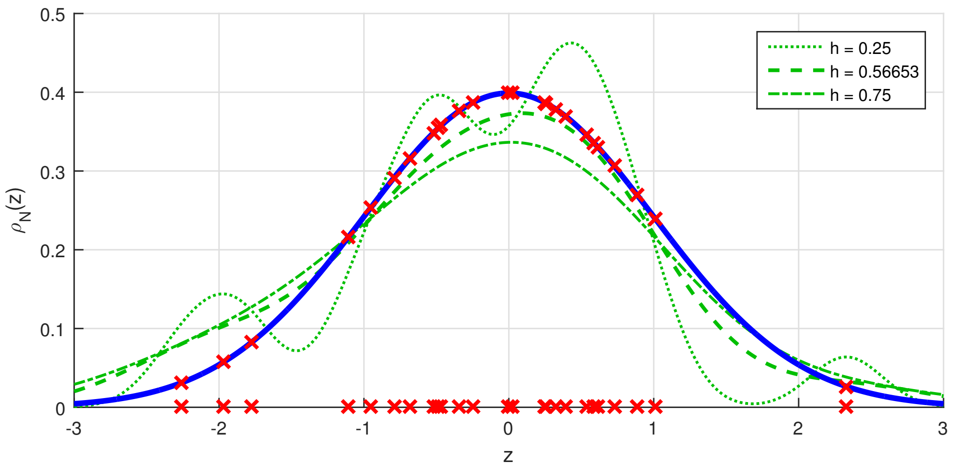
Kernel Density Estimation

Definition: Kernel Density Estimator

Let $\mathcal{Y} = \{y_1, \cdots, y_N\} \subseteq \mathbb{R}^n$ 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 kernel function.
Then the kernel density estimator ϱ_N corresponding to the bandwidth $h \in (0, \infty)$ is defined as

$$\varrho_N(z) = \frac{1}{Nh} \sum_{i=1}^{N} K\left(\frac{z - y_i}{h}\right).$$





[Gramacki 2018]: Nonparametric Kernel Density Estimation and its Computational Aspects. *Springer International Publishing*

Stationary Gas Transport

Application of Kernel Density Estimation

- Let $\mathcal{B} = \{ b^{S,1}, \cdots, b^{S,N_{\mathsf{KDE}}} \} \subseteq \mathbb{R}^n_{\geq 0}$ be independent and identically distributed samples of the random variable ξ_b
- Let $\mathcal{P}_{\mathcal{B}} = \{ p(b^{S,1}), \cdots, p(b^{S,N_{\mathsf{KDE}}}) \} \subseteq \mathbb{R}^n$ be the corresponding pressures at the nodes (also independent and identically distributed)

Gaussian kernel

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

bandwidth matrix

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

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

kernel density estimator

$$\varrho_{p,N_{\mathsf{KDE}}}(z) = \frac{1}{N_{\mathsf{KDE}} \det \sqrt{H_{j,j}}} \sum_{i=1}^{N_{\mathsf{KDE}}} \prod_{j=1}^{n} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{z_j - p_j(b^{S,i})}{\sqrt{H_{j,j}}}\right)^2\right)$$

[Schuster, Strauch, Gugat, Lang, 2022]: *Probabilistic Constrained Optimization on Flow Networks.* Optim. Eng. 23: 1–50

Stationary Gas Transport

Application of Kernel Density Estimation

$$\begin{aligned}
\mathbb{P}_{N_{\mathsf{KDE}}}(p \in P_{\min}^{\max}) &= \int_{P_{\min}^{\max}} \varrho_{p,N_{\mathsf{KDE}}}(z)\, dz \\
&= \int_{P_{\min}^{\max}} \frac{1}{N_{\mathsf{KDE}} \prod_{j=1}^{n} h_j} \sum_{i=1}^{N_{\mathsf{KDE}}} \prod_{j=1}^{n} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2} \left(\frac{z_j - p_j(b^{S,i})}{h_j} \right)^2 \right) dz \\
&= \frac{1}{N_{\mathsf{KDE}} \prod_{j=1}^{n} h_j} \sum_{i=1}^{N_{\mathsf{KDE}}} \prod_{j=1}^{n} \int_{p_j^{\min}}^{p_j^{\max}} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2} \left(\frac{z_j - p_j(b^{S,i})}{h_j} \right)^2 \right) dz_j
\end{aligned}$$

Stationary Gas Transport

Application of Kernel Density Estimation

$$\mathbb{P}_{N_{\mathsf{KDE}}}(p \in P_{\min}^{\max}) = \int_{P_{\min}^{\max}} \varrho_{p,N_{\mathsf{KDE}}}(z)\; dz$$

$$= \int_{P_{\min}^{\max}} \frac{1}{N_{\mathsf{KDE}} \prod_{j=1}^{n} h_j} \sum_{i=1}^{N_{\mathsf{KDE}}} \prod_{j=1}^{n} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{z_j - p_j(b^{S,i})}{h_j}\right)^2\right)\; dz$$

$$= \frac{1}{N_{\mathsf{KDE}} \prod_{j=1}^{n} h_j} \sum_{i=1}^{N_{\mathsf{KDE}}} \prod_{j=1}^{n} \int_{p_j^{\min}}^{p_j^{\max}} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{z_j - p_j(b^{S,i})}{h_j}\right)^2\right)\; dz_j$$

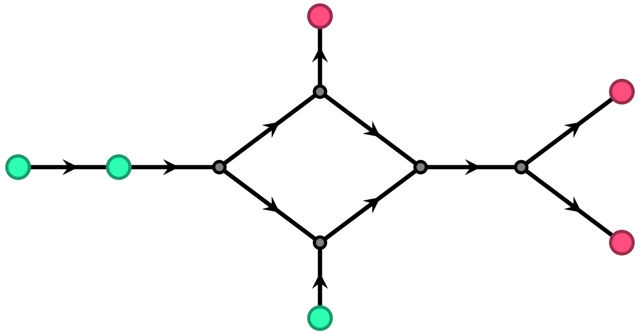
Gauss error function: $\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp\left(-t^2\right)\; dt$

probability via KDE

$$\mathbb{P}_{N_{\mathsf{KDE}}}(p \in P_{\min}^{\max}) = \frac{1}{N_{\mathsf{KDE}} 2^n} \sum_{i=1}^{N_{\mathsf{KDE}}} \prod_{j=1}^{n} \left[\operatorname{erf}\left(\frac{p^{\max} - p_j(b^{S,i})}{\sqrt{2}\, h_j}\right) - \operatorname{erf}\left(\frac{p^{\min} - p_j(b^{S,i})}{\sqrt{2}\, h_j}\right)\right]$$

Stationary Gas Transport

A Numerical Example



p_0	$p^{\min}$	outflow	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

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

Probabilistic optimization

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

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

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

https://gaslib.zib.de/

Dynamic Gas Transport

The Isothermal Euler Equations

The isothermal Euler equations for ideal gases:

(ISO)

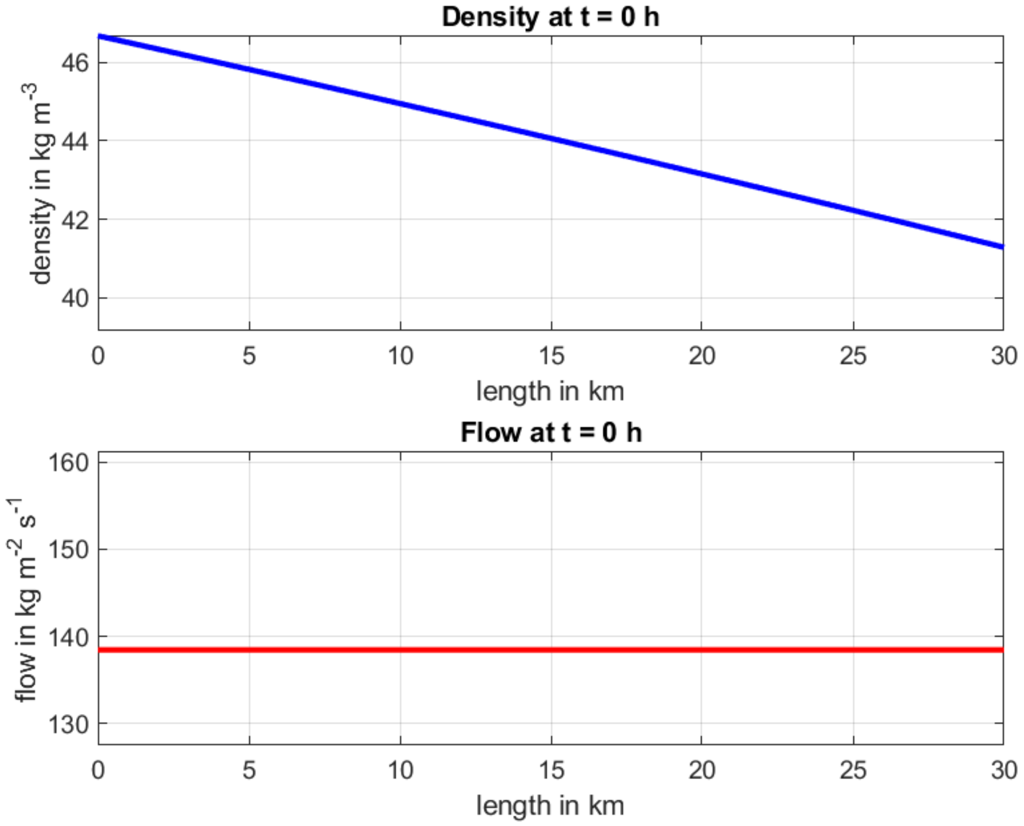
$$\rho_t + q_x = 0,$$
$$q_t + \left(c^2 p + \frac{q^2}{\rho}\right)_x = -\frac{\lambda^F}{2D}\frac{q|q|}{\rho}.$$

Inlet density & Gas outflow

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

Initial condition

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



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

Dynamic Gas Transport

Time Dependent Uncertainty

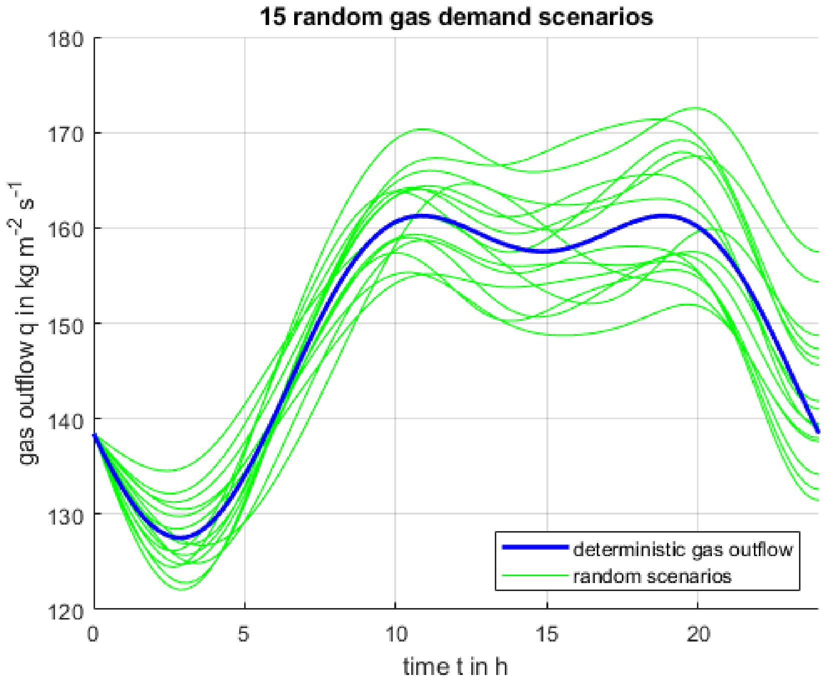
Random Boundary Functions

- 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

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



Dynamic Gas Transport

Time Dependent Uncertainty

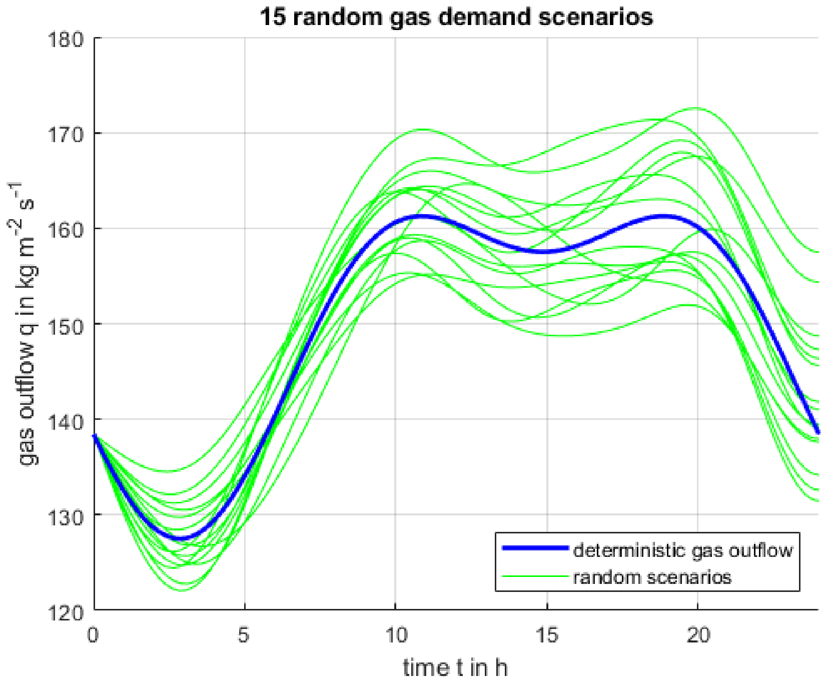
Random Boundary Functions

- 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

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



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 $t \in [0, T]$.“

Dynamic Gas Transport

Application of Kernel Density Estimation

- Let $\mathcal{B} = \{\, b^{S,1}(t), \cdots, b^{S,N_{\mathsf{KDE}}}(t) \,\}$ be independent and identically distributed random boundary functions
- Let $\mathcal{P}_{\mathcal{B}} = \{\, \rho(t; b^{S,1}), \cdots, \rho(t; b^{S,N_{\mathsf{KDE}}}) \,\}$ be the corresponding densities at the end of the pipe

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

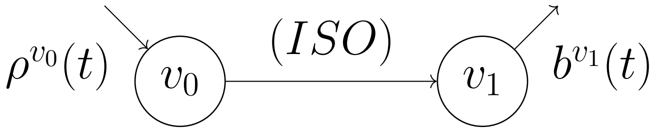
- Let $\left\{ \begin{bmatrix} \underline{\rho}(b_1) := \min\limits_{t\in[0,T]} \rho(t; b^{S,1}) \\ \overline{\rho}(b_1) := \max\limits_{t\in[0,T]} \rho(t; b^{S,1}) \end{bmatrix}, \cdots, \begin{bmatrix} \underline{\rho}(b_{N_{\mathsf{KDE}}}) := \min\limits_{t\in[0,T]} \rho(t; b^{S,N_{\mathsf{KDE}}}) \\ \overline{\rho}(b_{N_{\mathsf{KDE}}}) := \max\limits_{t\in[0,T]} \rho(t; b^{S,N_{\mathsf{KDE}}}) \end{bmatrix} \right\} \subseteq \mathbb{R}^2$ be a sample of the minimal and maximal densities in $[0,T]$

Kernel density estimator for bandwidths h^{min} and h^{min}

$$\varrho_{p,N_{\mathsf{KDE}}}(z) = \frac{1}{N_{\mathsf{KDE}}\; h^{\mathsf{min}}\; h^{\mathsf{max}}} \sum_{i=1}^{N_{\mathsf{KDE}}} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{z-\underline{\rho}(b_i)}{h^{\mathsf{min}}}\right)^2\right) \cdot \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{z-\overline{\rho}(b_i)}{h^{\mathsf{max}}}\right)^2\right)$$

Dynamic Gas Transport

A Numerical Example



$\rho_0(t)$	$\rho^{\min}$	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

$$\min_{\rho^{\max}_{\text{det}}} \quad \rho^{\max}_{\text{det}},$$

$$\text{s.t.} \quad \rho(t,L) \in [\rho^{\min}, \rho^{\max}_{\text{det}}].$$

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

Probabilistic Optimization

$$\min_{\rho^{\max}_{\text{prob}}} \quad \rho^{\max}_{\text{prob}},$$

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

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

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

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

A Dynamic Gas Transport Model

References

- M. Gugat, R. Schultz, M. Schuster: *Convexity and Starshapedness of Feasible Sets in Stationary Flow Networks.* Netw. Heterog. Media 15(2), pp. 171–195, 2020
- M. Schuster: *Nodal Control and Probabilistic Constrained Optimization.* PhD thesis, FAU Erlangen-Nürnberg, Germany, 2021, https://opus4.kobv.de/opus4-trr154/frontdoor/index/index/searchtype/latest/docId/410/start/2/rows/10
- M. Schuster, E. Strauch, M. Gugat, J. Lang: *Probabilistic Constrained Optimization on Flow Networks.* Optim. Eng. 23, 1–50, 2022