FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG

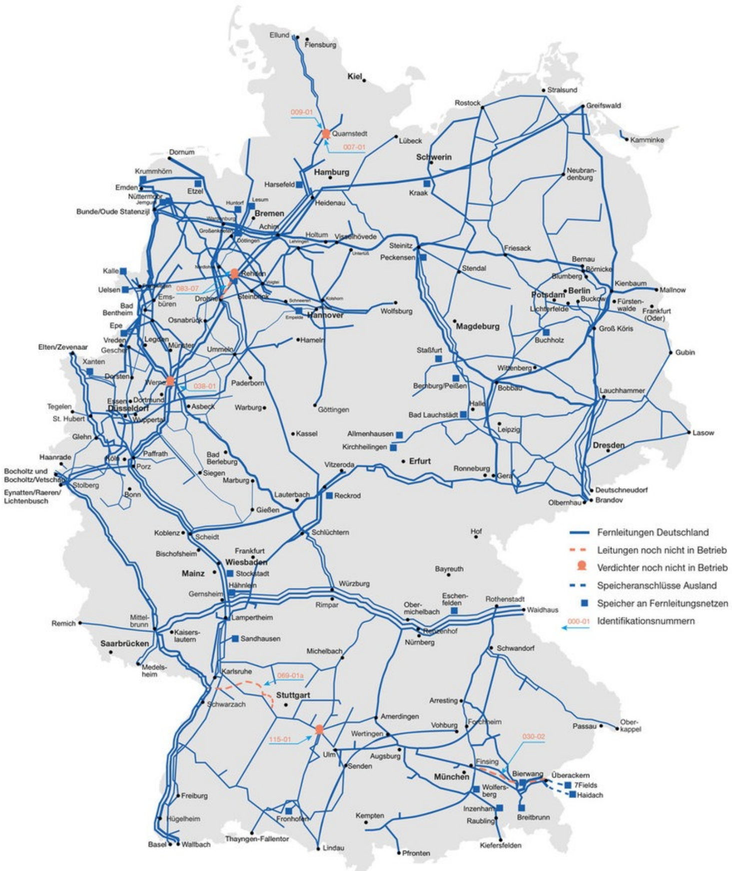
NATURWISSENSCHAFTLICHE
FAKULTÄT

Probabilistic Constrained Optimization on Gas Networks

Michael Schuster, Elisa Strauch, Martin Gugat, Jens Lang
FAU Erlangen-Nürnberg, TU Darmstadt
26.08.2022 - Benasque

CONTINUOUS
OPTIMIZATION

Motivation



©BMWi, Fernleitungsnetzbetreiber

Motivation

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

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

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

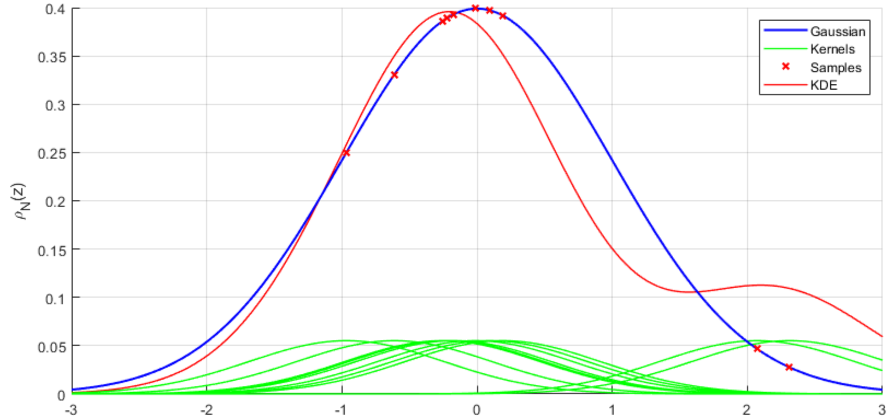
Is there a „better“ way to compute this probability?

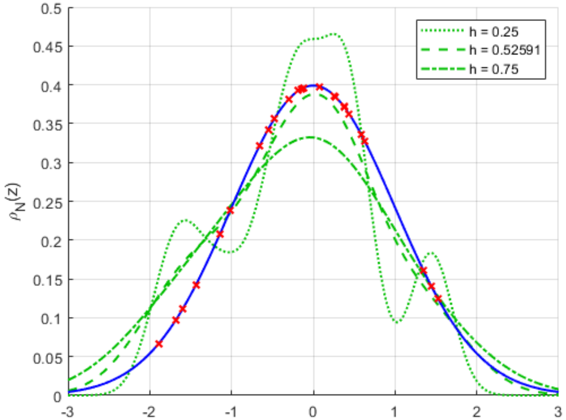
Kernel Density Estimation

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

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





A Stationary Gas Transport Model

- Consider a connected, directed, tree-structured graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with vertex set $\mathcal{V}$ and set of edges $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$
- From the root the graph is numbered using breadth-first search or depth-first search

The stationary isothermal Euler equations for ideal gases:

(ISO4)

$$
\begin{aligned}
q_x &= 0, \\
c^2 \rho_x &= -\frac{\lambda^F}{2D} \frac{q|q|}{\rho}.
\end{aligned}
$$

Gugat et al. (2015): *Stationary States in Gas Networks*. Netw. Heterog. Media 10(2): 295–320

Domschke et al. (2021): *Gas Network Modeling: An Overview*. Preprint
https://opus4.kobv.de/opus4-trr154/frontdoor/index/index/docId/411

A Stationary Gas Transport Model

Boundary Conditions:

Inlet pressure

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

Gas outflow

$b_i \in \mathbb{R}_{\geq 0}$ represents the consumers gas demand at node v_i $(i = 1, \cdots, n)$

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

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

A Stationary Gas Transport Model

- 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: $p_i \in \left[p_i^{\min}, p_i^{\max}\right]$

Set of feasible loads

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

A Stationary Gas Transport Model

- 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: $p_i \in \left[p_i^{\min}, p_i^{\max}\right]$

Set of feasible loads

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

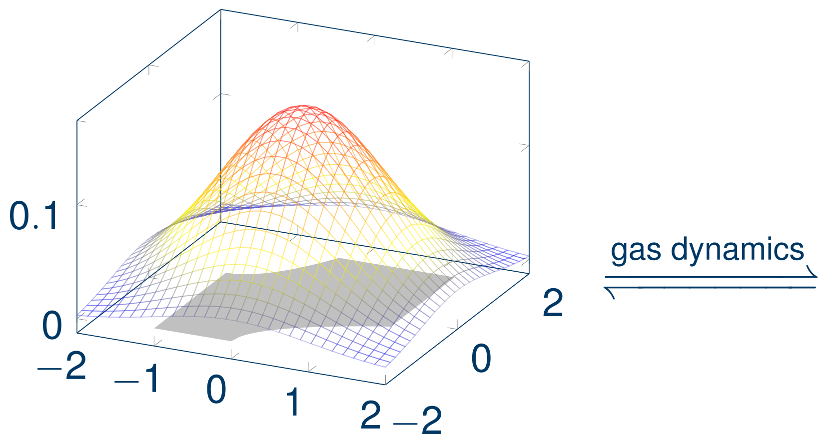
- Assume that the consumers gas demand is random in the sense, that there is a random variable

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

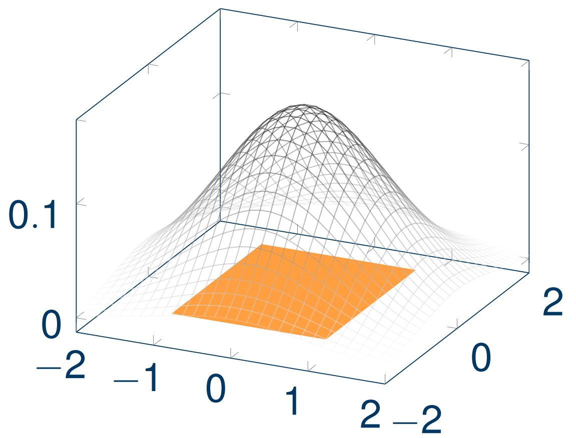
on an appropriate probability space. We identify b with the image $\xi_b(\omega)$ for $\omega \in \Omega$.

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 α% of all scenarios?

A Stationary Gas Transport Model



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



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

Figure: The two different ways to compute the probability for a random load vector to be feasible

see Schuster et al. (2021): *Probabilistic Constrained Optimization on Flow Networks*. Optim. Eng. 2021, `https://doi.org/10.1007/s11081-021-09619-x`.

Application of the KDE

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

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

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

kernel density estimator ($h_j^2 := H_{j,j}$)

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

Application of the KDE

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

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

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

Application of the KDE

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

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

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

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

probability via KDE

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

Probabilistic constrained optimization

Example: Probabilistic constrained optimization on GasLib-11

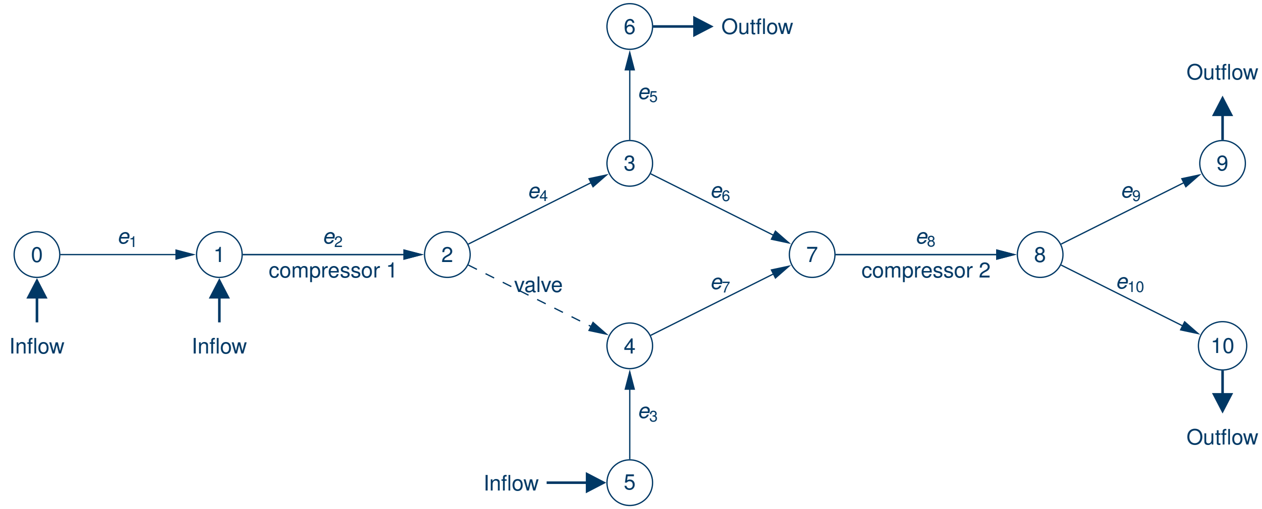


Figure: A scheme of the GasLib-11 (`https://gaslib.zib.de/`)

deterministic optimization

$$\min_{p_{\text{det}}^{\max}} \quad \sum p_{\text{det}}^{\max},$$
$$\text{s.t.} \quad p_i \in [p_i^{\min}, p_{\text{det},i}^{\max}].$$

probabilistic optimization

$$\min_{p_{\text{prob}}^{\max}} \quad \sum p_{\text{prob}}^{\max},$$
$$\text{s.t.} \quad \mathbb{P}\left(p_i \in \left[p_i^{\min}, p_{\text{prob},i}^{\max}\right] \right) \geq 0.75.$$

Probabilistic constrained optimization

p_0	$p^{\min}$	μ	Σ	$p_{\text{det}}^{\max}$	α
$\begin{pmatrix} 60 \\ 58 \\ 60 \end{pmatrix}$	$\begin{pmatrix} 40 \\ 40 \\ 40 \end{pmatrix}$	$\begin{pmatrix} 20 \\ 15 \\ 18 \end{pmatrix}$	$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	$\begin{bmatrix} 46.10 \\ 52.04 \\ 51.08 \end{bmatrix}$	75%

Table: Values for the GasLib-11

$P(b \in M(p_{\text{det}}^{\max}))$	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6	Test 7	Test 8
MC	36.02%	35.66%	35.91%	35.86%	35.34%	35.48%	35.98%	35.90%
KDE	35.72%	35.41%	35.48%	35.39%	34.92%	35.08%	35.75%	35.47%

Table: Probability $\mathbb{P}(b \in M(p_{\text{det}}^{\max}))$ for the optimal deterministic upper pressure bounds

Probabilistic constrained optimization

p_0	p^{min}	μ	Σ	p^{max}_{det}	α
$\begin{pmatrix}60\\58\\60\end{pmatrix}$	$\begin{pmatrix}40\\40\\40\end{pmatrix}$	$\begin{pmatrix}20\\15\\18\end{pmatrix}$	$\begin{pmatrix}2&0&0\\0&2&0\\0&0&2\end{pmatrix}$	$\begin{bmatrix}46.10\\52.04\\51.08\end{bmatrix}$	75%

Table: Values for the GasLib-11

$P(b \in M(p^{max}_{det}))$	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6	Test 7	Test 8
MC	36.02%	35.66%	35.91%	35.86%	35.34%	35.48%	35.98%	35.90%
KDE	35.72%	35.41%	35.48%	35.39%	34.92%	35.08%	35.75%	35.47%

Table: Probability $\mathbb{P}(b \in M(p^{max}_{det}))$ for the optimal deterministic upper pressure bounds

	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6	Test 7	Test 8
p^{max}_{prob}	$\begin{bmatrix}47.51\\53.33\\52.44\end{bmatrix}$	$\begin{bmatrix}47.51\\53.34\\52.45\end{bmatrix}$	$\begin{bmatrix}47.52\\53.33\\52.46\end{bmatrix}$	$\begin{bmatrix}47.52\\53.34\\52.46\end{bmatrix}$	$\begin{bmatrix}47.51\\53.35\\52.46\end{bmatrix}$	$\begin{bmatrix}47.51\\53.35\\52.45\end{bmatrix}$	$\begin{bmatrix}47.53\\53.33\\52.44\end{bmatrix}$	$\begin{bmatrix}47.52\\53.33\\52.46\end{bmatrix}$

Table: Stochastic optimal upper pressure bounds p^{max}_{prob}

Dynamic Gas Transport

The isothermal Euler equations for ideal gases:

(ISO1)

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

Inlet density & Gas outflow

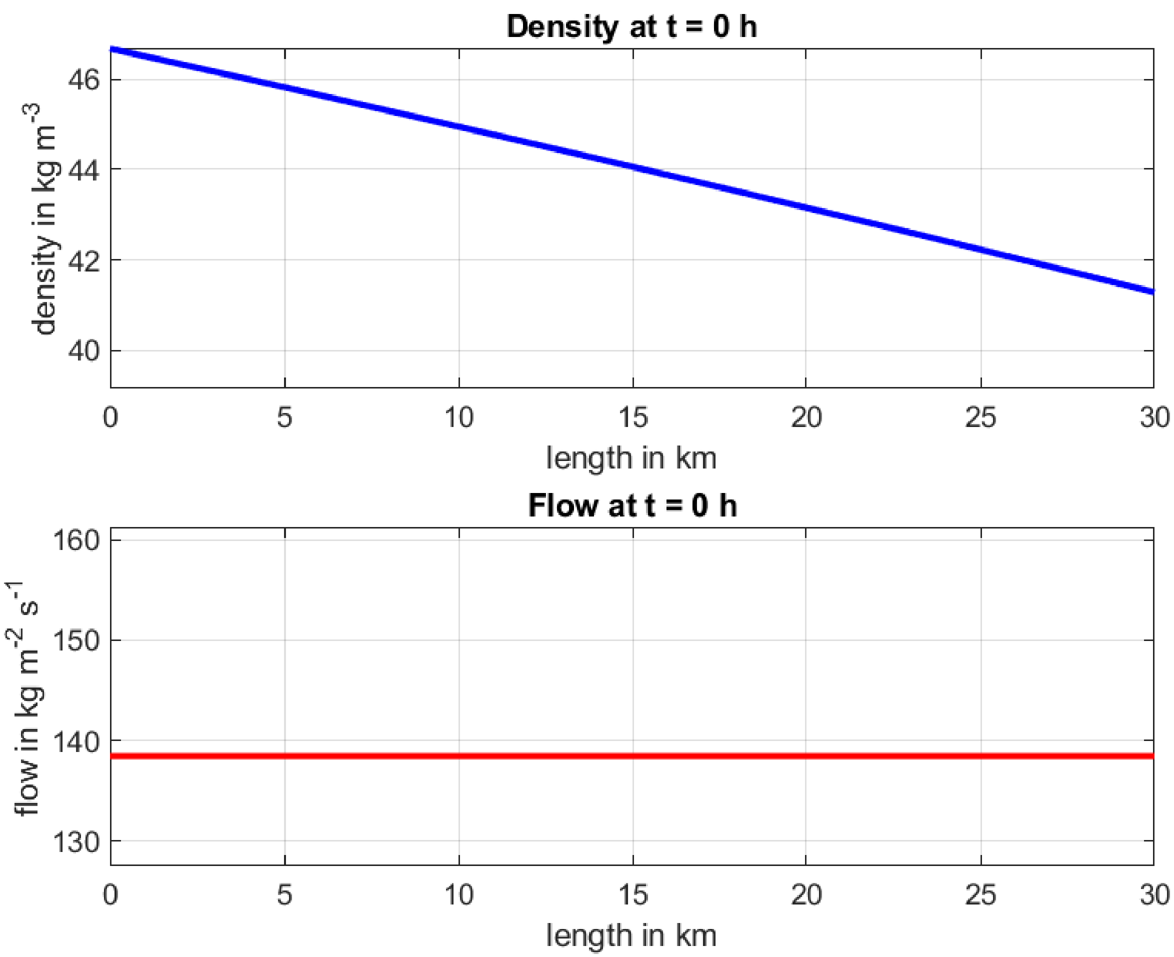
$$\rho(t,0) = \rho_0(t),$$
$$q(t,L) = b(t).$$

Initial condition

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

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

A Dynamic Gas Transport Model



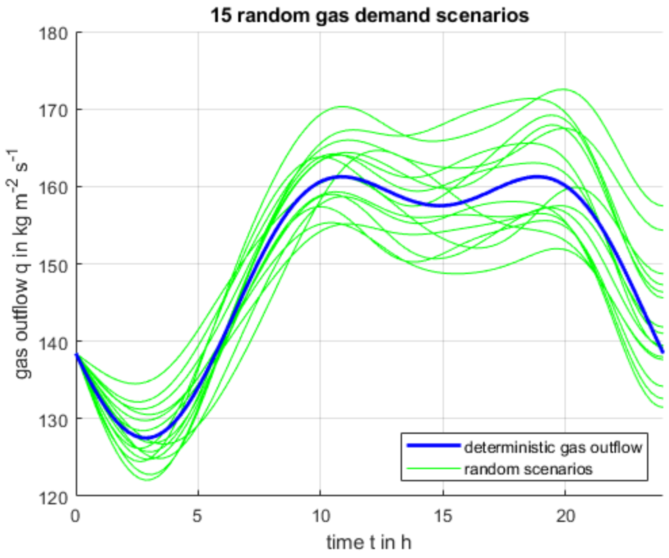
Time dependent Uncertainty

- 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

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



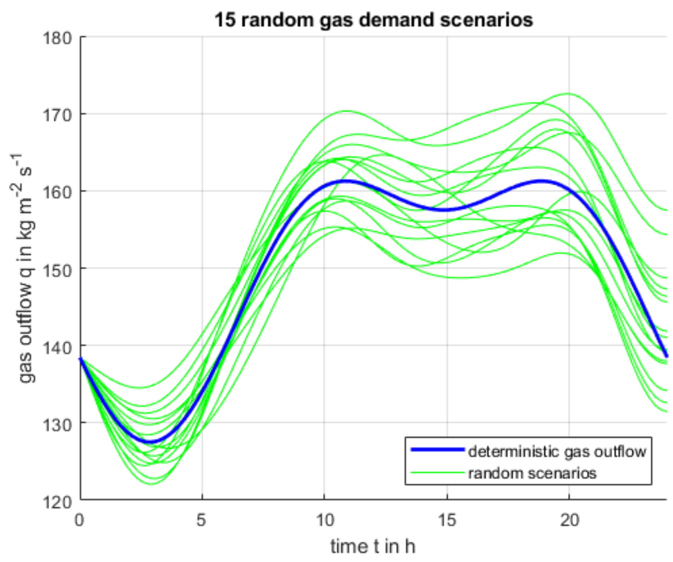
Time dependent Uncertainty

- 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 $t \in [0, T]$."

Application of KDE

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

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

kernel density estimator for bandwidths $h^{\min}$ and $h^{\min}$

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

Probabilistic Constrained Optimization

Example: Probabilistic constrained optimization on a single edge

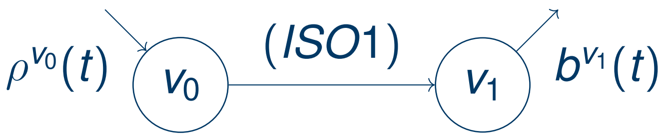


Figure: Dynamic setting on a single edge

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

Table: Values for the dynamic example

deterministic optimization

$$\min_{\rho_{\text{det}}^{\max}} \quad \rho_{\text{det}}^{\max},$$
$$\text{s.t.} \quad \rho(t,L) \in [\rho^{\min}, \rho_{\text{det}}^{\max}].$$
$$\Rightarrow \quad \rho_{\text{det}}^{*,\max} = 42.15\ kg/m^3$$

probabilistic optimization

$$\min_{\rho_{\text{prob}}^{\max}} \quad \rho_{\text{prob}}^{\max},$$
$$\text{s.t.} \quad \mathbb{P}\left(\rho(t,L) \in \left[\rho^{\min}, \rho_{\text{prob}}^{\max}\right] \ \forall t \in [0,T] \right) \geq 0.9.$$
$$\Rightarrow \quad \rho_{\text{prob}}^{*,\max} = 42.49\ kg/m^3$$

References

- A. Gramacki: *Nonparametric Kernel Density Estimation and its Computational Aspects.* Springer International Publishing, 2018
- M. Schuster, E. Strauch, M. Gugat, J. Lang: *Probabilistic Constrained Optimization on Flow Networks.* Optim. Eng. 23, 1–50, 2022
- 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`