

# On probabilistic capacity maximization in a stationary gas network<sup>†</sup>

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## ABSTRACT

The question for the capacity of a given gas network, i.e., determining the maximal amount of gas that can be transported by a given network, appears as an essential question that network operators and political administrations are regularly faced with. In that context we present a novel mathematical approach in order to assist gas network operators in managing increasing uncertainty with respect to customers gas nominations and in exposing free network capacities while reliability of transmission and supply is taken into account. The approach is based on the rigorous examination of optimization problems with nonlinear probabilistic constraints. As consequence we deal with solving a problem belonging to the class of probabilistic/robust optimization problems, which can be formulated with some joint probabilistic constraint over an infinite system of random inequalities. We will show that the inequality system can be reduced to a finite one in the situation of considering a tree network topology. A detailed study of the problem of maximizing bookable capacities in a stationary gas network is presented that comes up with an algebraic model involving Kirchhoff's first and second laws. The focus will be on both the theoretical and numerical side. The analytical part consists in introducing and validating a generalized version of the known rank two constraint qualification implying the differentiability of the considered capacity problem. The results are important in order to solve the capacity problem numerically, where function and gradient evaluations of the probabilistic constraints are performed by an approach using spheric-radial decomposition applicable for multivariate Gaussian random variables and more general distributions.

## KEYWORDS

Stationary gas networks; booked capacities; probabilistic constraints; constraint qualification; spheric-radial decomposition

## MATHEMATIC SUBJECT CLASSIFICATION (2010)

90B15; 90C15

## 1. Introduction

Recently, in the context of liberalization paradigm, new challenges for the gas network operators appeared. These challenges are consequences of separating the natural gas transmission from production and services. What follows is that network operators are solely responsible for the transportation of gas. On the other hand, gas traders are only needed to specify, by so-called nominations, where they want to inject or extract

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gas (load) at existing entry and exit points of the network. From the operator's point of view, an accurate calculation of transport capacities and the security of supply are the essential components for a reliable gas transport. The so-called *nomination validation* (cf. [12]), i.e., the decision whether the given nominations of entry and exit flows are technically and physically feasible under the available infrastructure, is significantly complicated by the existence of uncertainties due to coverage of future loads. In particular, ensuring security of gas supply to the customers implies the need of quantifying such uncertainties. The actual amount of gas that is transported through the gas net is influenced by volatile prices and by ambient temperatures. The stochastic nature of gas demand that allows to model demand uncertainty by means of stochastic distributions is due to the existence of long term historical data records. We refer to a more in-depth study of nomination validation in [15]. Moreover, robustness of natural gas flows is examined in [6], whereas an explicit characterization of gas flow feasibility under stochastic exit demand is given in [11]. In addition, [10] considers also uncertainty of roughness within pipe segments beside uncertainty of gas demand.

The present paper develops a novel mathematical approach to enable a network operator to both locate and maximize free available network capacities, while keeping a high probability of satisfying some stochastic demand. We consider a passive stationary gas network, which for simplicity will be assumed to be a tree. It is supposed that there exists one entry point coinciding with the root of the tree and supplying a set of exit points with random loads. Exits can nominate their loads only according to given booked capacities. In principle, the network operator has to make sure that all balanced nominations complying with the booked capacities can be satisfied by a feasible flow through the net satisfying given lower and upper pressure bounds at its nodes. Since several nomination patterns may turn out to be highly unlikely, he may content himself with guaranteeing this feasibility only with a certain high probability  $p$ , being aware that rare infeasibilities in the stationary model can be compensated for by appropriate measures in the dispatch mode such as exploiting interruptible contracts (for details see [12]). This probabilistic relaxation of an originally worst-case-type requirement for feasibility, gives the network owner the chance of offering significantly larger bookable capacities. For the given values, it may be the case that the probability of nominations being technically feasible is larger than the value  $p$  desired by the network owner. This degree of freedom can be used then, in order to extend the currently booked capacities by a value which still allows one to keep the desired probability level  $p$  no matter what additional nominations in the extended range have been chosen. The resulting optimization problem will be presented in Sect. 3. The problem turns out to be of a new class of joint probabilistic/robust optimization models that has been introduced in [10] first. A proper substitution of the robust part allows to rewrite the problem of maximizing bookable capacities as a stochastic optimization problem with probabilistic constraints.

The paper is organized as follows. A brief discussion of probabilistic problems is given in the following Sect. 2. After representation of the capacity problem in Sect. 3, the structure and analytical properties of the resulting optimization model are studied in Sect. 4, with a particular focus on the validation of some constraint qualification. What follows is Sect. 5 concerning all computational questions, namely, how to compute function values and gradients of the involved probability function (see below), where the approach of spheric-radial decomposition is applied. The final Sect. 6 concludes the theoretical part by a numerical study that includes solving the capacity problem for a reasonable large sized gas net adapted from real gas transportation networks under Gaussian-like random demand.

## 2. Optimization problems with probabilistic constraints

In this paragraph we shortly want to recall the idea of stochastic optimization problems using probabilistic (or chance) constraints. For a standard reference on probabilistic constraints we refer to the monograph [16] by Prékopa.

Many real world optimization problems with, for example, application to energy, finance, transport and logistics deal with data uncertainty. The optimization models typically come up with systems of inequality constraints of the form

$$g_i(x, z) \geq 0 \quad (i = 1, \dots, k) \quad (1)$$

describing the set of feasible decisions, where  $x \in \mathbb{R}^n$  refers to a control or decision vector,  $z \in \mathbb{R}^m$  is some uncertain parameter and  $g : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^k$  refers to a constraint mapping. Ignoring the uncertainty of the data, for example, when replacing  $z$  by deterministic data in terms of mean values, it would result in optimal decisions that are frequently non-robust, i.e., infeasible with respect to deviations from the mean value. But typically, access to historical observations is given in many situations. Therefore, modelling data uncertainty by a random vector  $\xi$  obeying a certain estimated multivariate distribution turns out to be a preferable alternative. This allows to rewrite (1) as a so-called probabilistic constraint

$$\mathbb{P}(g(x, \xi) \geq 0) \geq p, \quad p \in (0, 1). \quad (2)$$

Here  $\mathbb{P}$  denotes the probability measure of the random data  $\xi$ , i.e.,  $\xi$  is assumed to be given on some probability space  $(\Omega, \mathcal{A}, \mathbb{P})$ . The interpretation of (2) is as follows. Some decision  $x$  is declared to be feasible if and only if the random inequality system (1) is satisfied with at least probability  $p$ . The fixed probability level  $p$  should be chosen reasonable high. By this value we make a trade-off between sufficient robustness of the decision  $x$  and moderate cost. Define

$$\varphi(x) := \mathbb{P}(g(x, \xi) \geq 0)$$

the so-called *probability function*. Then, the optimization problem using the probabilistic constraint (2) can be formulated as a generic optimization problem, in general nonsmooth, of the form

$$\min \{f(x) \mid \varphi(x) \geq p\}, \quad (3)$$

where  $f$  is a cost function mapping from  $\mathbb{R}^n$  to the real numbers. Both analytical and numerical properties of the optimization problem with probabilistic constraints strongly depend on the smoothness properties of the probability function  $\varphi(\cdot)$ . Unfortunately, simple examples show that even if the mapping  $g(\cdot, \cdot)$  in (2) is nice, i.e., particularly smooth, we cannot expect smoothness of the probability function in general. However, under certain regularity assumptions sub-gradients (in the sense of Clarke or Mordukhovich) and even gradients of the probability function might be available [2]. Therefore, the validation of constraint qualifications in the context of gas transportation problems, and, in particular, for the problem of maximizing bookable capacities is considered in Sect. 4.

### 3. The problem of maximizing bookable capacities

In this section, we want to describe the optimization problem of maximizing bookable capacities under uncertain demand that comes up as a highly relevant optimization challenge for network operators. The presented approach of rigorous examination of the underlying optimization problem with nonlinear probabilistic constraints is novel in that context and it focuses on the free capacities on the exit side in a classic entry/exit model. Alongside, in [5] the authors of that article pick up the capacity problem but they do without deeper justification, they rather try to extend the model to the entry side as well. Such extensions do not allow to reduce the mixed probabilistic and robust optimization model to a probabilistic one, in general. Such reductions we will discuss here.

#### 3.1. General formulation as probabilistic/robust problem

As noted in the introduction, we consider a passive and stationary gas network with tree structure. Moreover, we want to assume that the root of the tree refers to a single entry node, labeled by zero, supplying the remaining exit nodes with gas. The exit nodes  $\mathcal{V}$  are labeled by  $1, \dots, |\mathcal{V}|$ . Let  $G = (\mathcal{V}^+, \mathcal{E})$  represent the tree network graph, that is trivially a spanning tree of itself, where  $\mathcal{V}^+$  denotes the set of both exit points and entry. Without loss of generality we direct all edges in  $\mathcal{E}$  away from the root. Using depth-first search, we number the nodes so that all numbers increase along any path from the root to one of the leaves. For  $k, \ell \in \mathcal{V}$ , denote  $k \succeq \ell$  if, in  $G$ , the unique directed path from the root to  $k$  passes through  $\ell$ . The latter path we denote with  $\Pi(k)$ . Moreover, let  $\pi(e)$  denote the head of edge  $e$ , i.e.,  $\pi(e) := \ell$  for  $e = (k, \ell)$ .

According to [11, Corollary 2], a vector of exit loads  $z$  in this configuration is technically feasible, whenever the inequality system

$$\begin{aligned} \min_{k=1, \dots, |\mathcal{V}|} \left\{ (p_k^{\max})^2 + h_k(z) \right\} - (p_0^{\min})^2 &\geq 0 \\ (p_0^{\max})^2 - \max_{k=1, \dots, |\mathcal{V}|} \left\{ (p_k^{\min})^2 + h_k(z) \right\} &\geq 0 \\ \min_{k=1, \dots, |\mathcal{V}|} \left\{ (p_k^{\max})^2 + h_k(z) \right\} - \max_{k=1, \dots, |\mathcal{V}|} \left\{ (p_k^{\min})^2 + h_k(z) \right\} &\geq 0 \end{aligned} \quad (4)$$

is satisfied, where the functions  $h_k(\cdot)$  are given by

$$h_k(z) := \begin{cases} \sum_{e \in \Pi(k)} \phi_e \left( \sum_{t \succeq \pi(e)} z_t \right)^2 & \text{if } k \geq 1, \\ 0 & \text{if } k = 0. \end{cases} \quad (5)$$

Here,  $p_k^{\min}$  and  $p_k^{\max}$  refer to lower and upper pressure limits at the nodes of the gas net. As well as certain positive roughness (or friction) coefficients  $\phi_e$  along edges  $e \in \mathcal{E}$ , they represent fixed network parameters. The interpretation of function  $h_k(\cdot)$  is as follows, it adds for every involved edge of the path  $\Pi(k)$  the square of the overall demand of the corresponding subtree that is supplied by the single edge. By the elimination of minima and maxima, the inequality system (4) can be represented equivalently in

closed form by a number of  $|\mathcal{V}|^2 + |\mathcal{V}|$  constraints of the form

$$g_{k,l}(z) := (p_k^{\max})^2 + h_k(z) - (p_l^{\min})^2 - h_l(z) \geq 0, \quad (6)$$

for all  $k, l = 0, \dots, |\mathcal{V}|$  and  $k \neq l$ . Note, the number of inequalities reduces significantly in the event of considering constant upper and constant lower pressure limits at all nodes. In that case, if  $p_k^{\max} \equiv p^{\max}$  and  $p_k^{\min} \equiv p^{\min}$  for all  $k = 0, \dots, |\mathcal{V}|$ , by eliminating all redundant inequalities from (6), we obtain a system of only  $|\mathcal{V}|$  inequalities

$$(p^{\max})^2 - (p^{\min})^2 - h_k(z) \geq 0, \quad (7)$$

$k = 1, \dots, |\mathcal{V}|$ , to describe technical feasibility in a tree network.

With regard to maximizing bookable capacities, we assume that a nomination vector on the exit side is given as the sum of two vectors  $\xi$  and  $y$ . Here,  $\xi$  is some random demand  $\xi \geq 0$  that describes the nomination behavior of former customers and that satisfies already existing booking contracts. The second vector  $y \in [0, x]$  corresponds to additional nominations due to available free capacities, where the components  $x_k$  of  $x$  are extra booking limits, say for new customers at the exit nodes  $k$ ,  $k = 1, \dots, |\mathcal{V}|$ . The motivation for modeling  $\xi$  as a random vector is due to the fact that a sufficient large data basis for load nominations according to former booked capacities may be given, which would allow one to approximate a multivariate distribution of  $\xi$  (see [12]). While this stochastic information enables the network owner to relax the technical feasibility of exit nominations in a probabilistic sense, nothing is known in contrast about the future nomination pattern of the new customer, so that one has to be prepared principally for every possible nomination  $y \in [0, x]$ . This constellation leads the network owner to define a capacity extension  $x$  as feasible, whenever the constraint

$$\mathbb{P}(g_{k,l}(\xi + y) \geq 0 \quad \forall y \in [0, x] \quad \forall k, l = 0, \dots, |\mathcal{V}|) \geq p \quad (8)$$

is satisfied with that  $x$ . The meaning of this constraint is as follows. The capacity extension  $x$  is feasible if and only if, with probability larger than  $p \in [0, 1)$ , the sum  $\xi + y$  of the original random nomination vector and of a new nomination vector can be technically realized for every such new nomination vector in the limits  $[0, x]$ . By its structure, (8) is a probabilistic constraint, but it is a nonstandard one in that it contains a robust (worst case) ingredient which makes the given random inequality system an infinite one. As mentioned in the introduction, such joint probabilistic/robust constraints have been considered first in the context of gas networks in [10].

By regulatory law, the network owner is obligated to maximize the capacity which can be booked. This leads him to the consideration of the following optimization problem

$$\text{maximize } c^T x \quad \text{subject to (8),} \quad (9)$$

where  $c$  is a weighted preference vector for capacity maximization, for example,  $c = (1, \dots, 1)^T$  in the case of no preferences among exit nodes.

### ***3.2. Reformulation of the problem with probabilistic constraints only***

In order to apply theory and methodology of optimization problems with probabilistic (chance) constraints, it might be essential to reduce the infinite system of constraints

in (8) to a finite one. To this end we make use of the equivalence

$$g_{k,l}(z+y) \geq 0 \quad \forall y \in [0, x] \quad \Leftrightarrow \quad \min_{y \in [0, x]} g_{k,l}(z+y) \geq 0, \quad (10)$$

where  $k, l = 0, \dots, |\mathcal{V}|$  and  $k \neq l$ . Let

$$\tilde{g}_{k,l}(x, z) := \min_{y \in [0, x]} g_{k,l}(z+y), \quad k, l = 0, \dots, |\mathcal{V}|, \quad (11)$$

be the minimum function depending on both  $x$  and  $z$ . An explicit representation of the minimum function  $\tilde{g}_{k,l}(x, z)$  can be obtained by taking a closer look to the constraint functions  $g_{k,l}(\cdot)$ . Inserting equation (5) into formula (6) leads to

$$\begin{aligned} g_{k,l}(z) &= (p_k^{\max})^2 + h_k(z) - (p_l^{\min})^2 - h_l(z) \\ &= (p_k^{\max})^2 + \sum_{e \in \Pi(k) \setminus \Pi(l)} \phi_e \left( \sum_{t \geq \pi(e)} z_t \right)^2 \\ &\quad - (p_l^{\min})^2 - \sum_{e \in \Pi(l) \setminus \Pi(k)} \phi_e \left( \sum_{t \geq \pi(e)} z_t \right)^2. \end{aligned} \quad (12)$$

Note that the latter equation appears after cancellation of some summands in  $h_k(z)$  and  $h_l(z)$ . The minimum of (11) is observed by using formula (12) after replacing  $z$  by  $z+y$ . In particular, we have

$$\begin{aligned} \tilde{g}_{k,l}(x, z) &= \min_{y \in [0, x]} g_{k,l}(z+y) \\ &= \min_{y \in [0, x]} \left\{ (p_k^{\max})^2 + \sum_{e \in \Pi(k) \setminus \Pi(l)} \phi_e \left( \sum_{t \geq \pi(e)} (z_t + y_t) \right)^2 \right. \\ &\quad \left. - (p_l^{\min})^2 - \sum_{e \in \Pi(l) \setminus \Pi(k)} \phi_e \left( \sum_{t \geq \pi(e)} (z_t + y_t) \right)^2 \right\} \\ &= (p_k^{\max})^2 + \sum_{e \in \Pi(k) \setminus \Pi(l)} \phi_e \left( \sum_{t \geq \pi(e)} z_t \right)^2 \\ &\quad - (p_l^{\min})^2 - \sum_{e \in \Pi(l) \setminus \Pi(k)} \phi_e \left( \sum_{t \geq \pi(e)} (z_t + x_t) \right)^2, \end{aligned} \quad (13)$$

where  $k, l = 0, \dots, |\mathcal{V}|$  and  $k \neq l$ . The above minimization can be separated due to the fact that the vertices of the involved subtrees generated by the subpaths  $\Pi(k) \setminus \Pi(l)$  and  $\Pi(l) \setminus \Pi(k)$  are disjoint (see also Figure 1). Therefore, the optimization problem of maximizing bookable capacities turns into a classical probabilistic problem with a finite number of probabilistic constraints. The reformulation of (9) reads

$$\begin{aligned} &\text{maximize } c^T x \quad \text{subject to} \\ &\mathbb{P}(\tilde{g}_{k,l}(x, \xi) \geq 0 \quad \forall k, l = 0, \dots, |\mathcal{V}|) \geq p, \end{aligned} \quad (14)$$

where for all  $k, l = 0, \dots, |\mathcal{V}|$  with  $k \neq l$  the constraint mappings  $\tilde{g}_{k,l}(\cdot, \cdot)$  are obtained by the explicit representation given in (13).

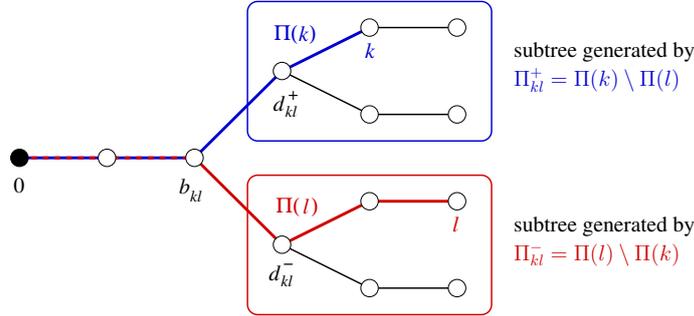
#### 4. The validation of constraint qualifications

The analytical properties of an optimization problem strongly depend on whether it satisfies certain regularity conditions which are given by different types of constraint qualifications. We follow the approach of considering the rank 2 constraint qualification (R2CQ) (cf. [2]) as a sufficient criterion for differentiability of the probability function of the probabilistic constraints.

To discuss the constraint qualification for the constraint mappings in the context of gas transmission we start with the general inequality system  $g_{k,l}(z)$  in (12) for  $k, l = 0, \dots, |\mathcal{V}|$  and  $k \neq l$ . To simplify the representation we are going to introduce the following definitions and notations (see Figure 1).

**Definition 4.1.** For some given pair of nodes  $k, l \in \mathcal{V}$  define

- (i)  $\Pi_{kl}^+ := \Pi(k) \setminus \Pi(l)$  and  $\Pi_{kl}^- := \Pi(l) \setminus \Pi(k)$  the *disjunctive subpaths* with respect to  $\Pi(k)$  and  $\Pi(l)$ ,
- (ii)  $b_{kl} := \begin{cases} \max \{ \pi(e) \mid e \in \Pi(k) \cap \Pi(l) \}, & \text{if } \Pi(k) \cap \Pi(l) \neq \emptyset, \\ 0, & \text{otherwise,} \end{cases}$  the *bifurcation node* of paths  $\Pi(k)$  and  $\Pi(l)$ ,
- (iii)  $d_{kl}^+ := \min \{ \pi(e) \mid e \in \Pi_{kl}^+ \}$  and  $d_{kl}^- := \min \{ \pi(e) \mid e \in \Pi_{kl}^- \}$  the *first direction nodes* for nonempty subpaths  $\Pi_{kl}^+$  and  $\Pi_{kl}^-$ , respectively.



**Figure 1.** Illustration of subpaths and nodes specified by Definition 4.1 for an example.

In order to check constraint qualification (R2QC), we pairwise have to compare gradients of active constraints. The following Lemma displays an analytical representation allowing to compute gradients of the constraint mappings.

**Lemma 4.2.** For the constraint mappings  $g_{k,l}(\cdot)$  in (6) we obtain that

$$[\nabla_z g_{k,l}(z)]_i = \begin{cases} \sum_{e \in \Pi_{kl}^+ \cap \Pi(i)} 2\phi_e \sum_{t \geq \pi(e)} z_t, & \text{if } \Pi_{kl}^+ \cap \Pi(i) \neq \emptyset, \\ - \sum_{e \in \Pi_{kl}^- \cap \Pi(i)} 2\phi_e \sum_{t \geq \pi(e)} z_t, & \text{if } \Pi_{kl}^- \cap \Pi(i) \neq \emptyset, \\ 0, & \text{otherwise,} \end{cases} \quad (15)$$

for all  $k, l = 0, \dots, |\mathcal{V}|$  with  $k \neq l$ , for all  $i = 1, \dots, |\mathcal{V}|$ , and, any  $z$ .

**Proof.** Because the subtrees generated by the paths  $\Pi_{kl}^+$  and  $\Pi_{kl}^-$  are disjoint, for any fixed  $k, l$  with  $k \neq l$  and arbitrary  $i \in \mathcal{V}$  we observe that  $i$  does not belong to any of these subtrees or it belongs exactly to one of them. In the first case from (12) we observe that  $g_{k,l}(z)$  does not depend on  $z_i$  at all, thus, the  $i$ th component of the gradient vanishes. Now, assuming that  $i$  belongs to the subtree either generated by  $\Pi_{kl}^+$  or  $\Pi_{kl}^-$ . Due to uniqueness of paths between two nodes in a tree, for any  $e \in \mathcal{E}$  node  $i$  is contained in the subtree generated by  $e$  (i.e.  $i \succeq \pi(e)$ ) if and only if  $e \in \Pi(i)$ . Hence, from (12) we observe that

$$[\nabla_z g_{k,l}(z)]_i = \sum_{e \in \Pi_{kl}^+ \cap \Pi(i)} 2\phi_e \sum_{t \succeq \pi(e)} z_t - \sum_{e \in \Pi_{kl}^- \cap \Pi(i)} 2\phi_e \sum_{t \succeq \pi(e)} z_t$$

for any  $z$ . But  $\Pi(i)$  can only intersect one of the two sub-paths  $\Pi_{kl}^+$  or  $\Pi_{kl}^-$  at a time. Thus, for any fixed  $i, k, l$  gradient formula (15) is a consequence of the above equation.  $\square$

Another structural result is given by the following observation for active constraints.

**Lemma 4.3.** *Let  $k, l$  with  $k \neq l$  and  $z \geq 0$  be given such that  $g_{k,l}(z) = 0$ . If  $p_k^{\max} > p_l^{\min}$  then it holds*

$$a) \quad \Pi_{kl}^- \neq \emptyset, \quad b) \quad d_{kl}^- \neq 0, \quad c) \quad [\nabla_z g_{k,l}(z)]_{d_{kl}^-} < 0.$$

**Proof.** Due to the assumption  $p_k^{\max} > p_l^{\min}$ , and, due to  $g_{k,l}(\cdot)$  is active constraint in  $z$ , by (12) we obtain that path  $\Pi_{kl}^-$  is nonempty and  $z_t > 0$  for some  $t \succeq d_{kl}^-$ . In particular, we have  $d_{kl}^- \neq 0$  (see Definition 4.1 (iii) above). Moreover, the path  $\Pi(d_{kl}^-)$  intersects the nonempty path  $\Pi_{kl}^-$  by the arc  $(b_{kl}, d_{kl}^-) \in \mathcal{E}$ , and, by applying Lemma 4.2 we conclude with  $z \geq 0$  that

$$[\nabla_z g_{k,l}(z)]_{d_{kl}^-} = - \sum_{e \in \Pi_{kl}^- \cap \Pi(d_{kl}^-)} 2\phi_e \sum_{t \succeq \pi(e)} z_t = -2\phi_{(b_{kl}, d_{kl}^-)} \sum_{t \succeq d_{kl}^-} z_t < 0,$$

where  $b_{kl}$  is the bifurcation node w.r.t.  $\Pi(k)$  and  $\Pi(l)$  (see Definition 4.1 (ii)).  $\square$

The following structural result focuses on the relation between the constraints (6) describing feasibility of gas flows in general and the ones involved in the capacity problem (13).

**Definition 4.4.** For any  $k, l \in \mathcal{V}$  ( $k \neq l$ ) and  $x \geq 0$  we define a mapping  $\varphi_{k,l} : \mathbb{R}^{\mathcal{V}} \rightarrow \mathbb{R}^{\mathcal{V}}$  by

$$[\varphi_{k,l}(x)]_t := \begin{cases} x_t, & \text{if } t \succeq d_{kl}^-, \\ 0, & \text{otherwise,} \end{cases} \quad \forall t \in \mathcal{V}.$$

The functionals  $\varphi_{k,l}(\cdot)$  represent the solution mappings for the generalized constraints in the capacity problem, as shown next.

**Lemma 4.5.** *For any  $k, l \in \mathcal{V}$  ( $k \neq l$ ) and any  $x, z \geq 0$  we have*

$$\min_{y \in [0, x]} g_{k,l}(z + y) = g_{k,l}(z + \varphi_{k,l}(x)).$$

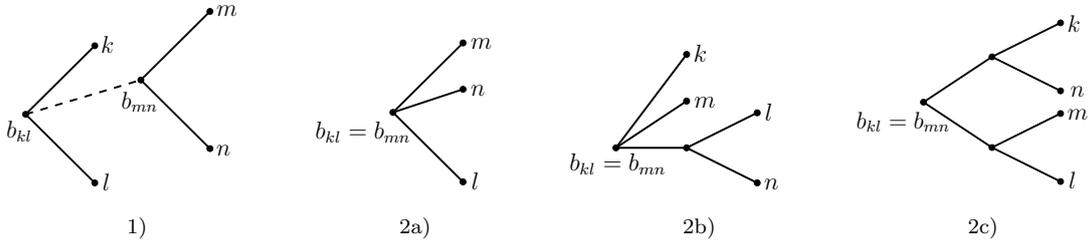
**Proof.** The result is a direct consequence of formula (13).  $\square$

Now we are prepared to state the first main result concerning the constraint mapping involved by the problem of maximizing bookable capacities in a stationary gas transport network, in order to derive constraint qualifications for this type of problem.

**Theorem 4.6.** For given  $x \geq 0$ ,  $z \geq 0$  define  $\alpha := \varphi_{k,l}(x)$ ,  $\beta = \varphi_{m,n}(x)$ ,  $k \neq l$  and  $m \neq n$ . If it holds  $g_{k,l}(z + \alpha) = g_{m,n}(z + \beta) = 0$  and if  $p_s^{\max} > p_t^{\min}$  for all  $s, t \in \mathcal{V}^+$ , then we have that (at least) one of the following statements is satisfied:

- (1) The gradients  $\nabla_z g_{k,l}(z + \alpha)$  and  $\nabla_z g_{m,n}(z + \beta)$  are linearly independent.
- (2) It exist indices  $i, j \in \mathcal{V}$  with  $z_i = z_j = 0$  and  $i \neq j$ .
- (3) There is redundancy, i.e.,  $g_{k,l}(z) \geq g_{m,n}(z)$  or  $g_{m,n}(z) \geq g_{k,l}(z)$  for all  $z \geq 0$ .

**Proof.** We want to prove the statement by a case study with respect to the bifurcation nodes observed from the paths with respect to the index pairs  $(k, l)$  and  $(m, n)$ , respectively. Figure 2 shows pictograms of the cases considered in the following.



**Figure 2.** Pictograms for the case study in order to prove Theorem 4.6.

1) Case  $b_{kl} \neq b_{mn}$ :

If the bifurcation nodes do not coincide, at least one of the relations  $b_{kl} \neq b_{mn}$  or  $b_{mn} \neq b_{kl}$  must be satisfied. Without loss of generality we assume  $b_{kl} \neq b_{mn}$ . We consider the negative path  $\Pi_{kl}^-$  and its first direction node  $d_{kl}^-$ . Clearly, that node can now either be the bifurcation node  $b_{mn}$  itself, or it is even not involved in the paths  $\Pi_{mn}^+$  and  $\Pi_{mn}^-$ . However, in both cases it follows that we have

$$\Pi_{mn}^+ \cap \Pi(d_{kl}^-) = \emptyset \quad \text{and} \quad \Pi_{mn}^- \cap \Pi(d_{kl}^-) = \emptyset.$$

Thus, due to (15) we obtain

$$[\nabla_z g_{m,n}(z + \beta)]_{d_{kl}^-} = 0.$$

On the other hand, due to the assumptions  $g_{kl}(z + \alpha) = 0$ ,  $g_{mn}(z + \beta) = 0$  and  $p_k^{\max} > p_l^{\min}$ , by Lemma 4.3 we have that

$$[\nabla_z g_{k,l}(z + \alpha)]_{d_{kl}^-} < 0 \quad \text{and} \quad [\nabla_z g_{m,n}(z + \beta)]_{d_{mn}^-} < 0.$$

Thus, the gradients  $\nabla_z g_{k,l}(z + \alpha)$  and  $\nabla_z g_{m,n}(z + \beta)$  are linearly independent.

2) Case  $b_{kl} = b_{mn}$ :

In case the bifurcation nodes are identical, we first want to consider the event that

$$\text{a) } \Pi_{kl}^- \cap (\Pi_{mn}^+ \cup \Pi_{mn}^-) = \emptyset \quad \text{or} \quad \Pi_{mn}^- \cap (\Pi_{kl}^+ \cup \Pi_{kl}^-) = \emptyset:$$

Assuming the first expression, completely analog to 1) it follows that

$$[\nabla_z g_{m,n}(z + \beta)]_{d_{kl}^-} = 0, \quad [\nabla_z g_{k,l}(z + \alpha)]_{d_{kl}^-} < 0 \quad \text{and} \quad [\nabla_z g_{m,n}(z + \beta)]_{d_{mn}^-} < 0,$$

which implies linear independence of the considered gradients. Clearly, the same result we obtain for the second expression just by interchanging the role of  $\alpha, \beta$  and indices  $(k, l), (m, n)$ . The next case we want to consider is

b)  $\Pi_{kl}^- \cap \Pi_{mn}^- \neq \emptyset$ :

Because the bifurcation nodes are identical, we observe  $d_{kl}^- = d_{mn}^-$ . Note that  $(b_{kl}, d_{kl}^-) \in \Pi_{kl}^- \cap \Pi_{mn}^-$  here, and thus, due to formula (15) we further obtain

$$[\nabla_z g_{k,l}(z + \alpha)]_{d_{kl}^-} = [\nabla_z g_{m,n}(z + \beta)]_{d_{kl}^-} = -2\phi_{(b_{kl}, d_{kl}^-)} \sum_{t \succeq d_{kl}^-} (z_t + x_t) < 0,$$

because  $\alpha_t = \beta_t = x_t$  for all  $t \succeq d_{kl}^-$  (see Definition 4.4). It follows that the gradients are co-linear, if and only if, all their components coincide. Let us assume co-linearity. In that case, by (15) again, on the one hand we have

$$0 = [\nabla_z g_{k,l}(z + \alpha) - \nabla_z g_{m,n}(z + \beta)]_k = 2 \sum_{e \in \Pi_{kl}^+ \setminus \Pi_{mn}^+} \phi_e \sum_{t \succeq \pi(e)} z_t, \quad (16)$$

$$0 = [\nabla_z g_{k,l}(z + \alpha) - \nabla_z g_{m,n}(z + \beta)]_m = -2 \sum_{e \in \Pi_{mn}^+ \setminus \Pi_{kl}^+} \phi_e \sum_{t \succeq \pi(e)} z_t. \quad (17)$$

(16) can be derived from (15) using the observations

$$\begin{aligned} \Pi_{kl}^+ \cap \Pi(k) &= \Pi_{kl}^+, & \Pi_{kl}^- \cap \Pi(k) &= \emptyset, & \Pi_{mn}^- \cap \Pi(k) &= \emptyset, \\ \Pi_{mn}^+ \cap \Pi(k) &= \Pi_{mn}^+ \cap (\Pi(k) \setminus \Pi(n)) = \Pi_{mn}^+ \cap (\Pi(k) \setminus \Pi(l)) = \Pi_{mn}^+ \cap \Pi_{kl}^+. \end{aligned}$$

Interchanging the role of  $(k, l)$  and  $(m, n)$  results in (17). On the other hand, by similar arguments, we obtain that

$$0 = [\nabla_z g_{k,l}(z + \alpha) - \nabla_z g_{m,n}(z + \beta)]_l = -2 \sum_{e \in \Pi_{kl}^- \setminus \Pi_{mn}^-} \phi_e \sum_{t \succeq \pi(e)} (z_t + x_t), \quad (18)$$

$$0 = [\nabla_z g_{k,l}(z + \alpha) - \nabla_z g_{m,n}(z + \beta)]_n = 2 \sum_{e \in \Pi_{mn}^- \setminus \Pi_{kl}^-} \phi_e \sum_{t \succeq \pi(e)} (z_t + x_t). \quad (19)$$

What follows is, in all cases two indices  $i, j \in \{k, l, m, n\}$  with  $z_i = z_j = 0$  and  $i \neq j$  can be identified, unless  $k = m$  and  $l \succ n$  ( $n \succ l$ ), or,  $l = n$  and  $k \succ m$  ( $m \succ k$ ), respectively. The latter exception appears if three of the above sums vanish due to cancellation of paths. However, if we assume  $k = m$  and  $l \succ n$  (the other cases are analog) we might compute the difference of the active constraints. By using (12) we obtain that

$$0 = g_{k,l}(z + \alpha) - g_{m,n}(z + \beta) = -(p_l^{\min})^2 + (p_n^{\min})^2 - \sum_{e \in \Pi_{kl}^- \setminus \Pi_{mn}^-} \phi_e \left( \sum_{t \succeq \pi(e)} (z_t + x_t) \right)^2.$$

Due to (18) the last terms need to equal zero, hence, we have  $(p_l^{\min})^2 = (p_n^{\min})^2$ . But, as consequence of that observation from (12) it follows with  $m = k$  that

$$g_{m,n}(z) \geq g_{k,l}(z) \quad \forall z \geq 0,$$

and, hence, inequality  $g_{m,n}$  is redundant. Finally, it remains to show the claim of the theorem for the case

c)  $\Pi_{kl}^- \cap \Pi_{mn}^+ \neq \emptyset$  and  $\Pi_{kl}^+ \cap \Pi_{mn}^- \neq \emptyset$ :

In this case, first of all, we define non-negative numbers

$$\begin{aligned} a &:= 2\Phi_{(b_{kl}, d_{kl}^+)} \sum_{t \succeq d_{kl}^+} z_t \geq 0, & c &:= 2\Phi_{(b_{kl}, d_{kl}^+)} \sum_{t \succeq d_{kl}^+} x_t \geq 0, \\ b &:= 2\Phi_{(b_{kl}, d_{kl}^-)} \sum_{t \succeq d_{kl}^-} z_t \geq 0, & d &:= 2\Phi_{(b_{kl}, d_{kl}^-)} \sum_{t \succeq d_{kl}^-} x_t \geq 0. \end{aligned}$$

Assuming c) the numbers are well-defined. Moreover, we observe  $d_{kl}^+ = d_{mn}^-$  and  $d_{kl}^- = d_{mn}^+$ . By (15) combined with Definition 4.4 it is easy to show that

$$\begin{aligned} [\nabla_z g_{k,l}(z + \alpha)]_{d_{kl}^+} &= a, & [\nabla_z g_{m,n}(z + \beta)]_{d_{kl}^+} &= -a - c, \\ [\nabla_z g_{k,l}(z + \alpha)]_{d_{kl}^-} &= -b - d, & [\nabla_z g_{m,n}(z + \beta)]_{d_{kl}^-} &= b. \end{aligned} \quad (20)$$

Now, a sufficient condition for gradients  $\nabla_z g_{k,l}(z + \alpha)$  and  $\nabla_z g_{m,n}(z + \beta)$  being linearly independent is

$$0 \neq \det \begin{pmatrix} a & -a - c \\ -b - d & b \end{pmatrix} = c(b + d) + ad = d(a + c) + bc.$$

Because Lemma 4.3 implies that  $a + c > 0$  and  $b + d > 0$ , the determinant is nonzero if  $c > 0$  or  $d > 0$ . It remains to show linear independence even for the event that  $c = d = 0$ , where the above determinant is zero. Due to the definitions of  $c$  and  $d$  this case implies  $x_t = 0$  for all  $t \succeq d_{kl}^+ = d_{mn}^-$  as well as  $x_t = 0$  for all  $t \succeq d_{kl}^-$ . Moreover, from (20) we see that for  $c = d = 0$  the gradients are independent if there exist some component  $t_0 \in \mathcal{V}$  such that  $[\nabla_z g_{k,l}(z + \alpha)]_{t_0} + [\nabla_z g_{m,n}(z + \beta)]_{t_0} \neq 0$ . To this end we compute the sum of the constraints  $g_{k,l}(z + \alpha)$  and  $g_{m,n}(z + \beta)$  which, by using (12) and the assumption that the constraints are active, results in

$$\begin{aligned} 0 &= (p_k^{\max})^2 + (p_m^{\max})^2 - (p_l^{\min})^2 - (p_n^{\min})^2 \\ &+ \sum_{e \in \Pi_{kl}^+ \setminus \Pi_{mn}^-} \phi_e \left( \sum_{t \succeq \pi(e)} z_t \right)^2 + \sum_{e \in \Pi_{mn}^+ \setminus \Pi_{kl}^-} \phi_e \left( \sum_{t \succeq \pi(e)} z_t \right)^2 \\ &- \sum_{e \in \Pi_{kl}^- \setminus \Pi_{mn}^+} \phi_e \left( \sum_{t \succeq \pi(e)} z_t \right)^2 - \sum_{e \in \Pi_{mn}^- \setminus \Pi_{kl}^+} \phi_e \left( \sum_{t \succeq \pi(e)} z_t \right)^2. \end{aligned}$$

Note, joint paths disappear by canceling out here, due to the fact that  $x_t = 0$  along

the involved paths. In particular, it follows that

$$\sum_{e \in \Pi_{kl}^- \setminus \Pi_{mn}^+} \phi_e \left( \sum_{t \geq \pi(e)} z_t \right)^2 + \sum_{e \in \Pi_{mn}^- \setminus \Pi_{kl}^+} \phi_e \left( \sum_{t \geq \pi(e)} z_t \right)^2 > 0, \quad (21)$$

i.e., there exists  $\hat{e}$  with  $\hat{e} \in \Pi_{kl}^- \setminus \Pi_{mn}^+$  or  $\hat{e} \in \Pi_{mn}^- \setminus \Pi_{kl}^+$ , respectively, and  $\hat{t}$  with  $\hat{t} \geq t_0 := \pi(\hat{e})$  such that  $z_{\hat{t}} > 0$ . However, in both cases with (15) we conclude that

$$| [\nabla_z g_{k,l}(z)]_{t_0} + [\nabla_z g_{m,n}(z)]_{t_0} | \geq 2\phi_{\hat{e}} \sum_{t \geq t_0} z_t \geq 2\phi_{\hat{e}} z_{\hat{t}} > 0.$$

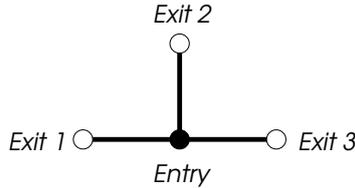
Thus, in case c) the gradients of the constraints are always linearly independent.

In any cases we have proven that either two active constraints have linearly independent gradients, or there exist at least two distinct indices  $i, j$  with  $z_i = z_j = 0$ , or one of the two active constraints is redundant at all.  $\square$

In fact, property 3 of Theorem 4.6 does not appear if we remove all redundant inequalities from the inequality system  $g(z) \geq 0$  first. However, contained redundant inequalities do not affect the feasibility set and the analytical properties of the probability function. Of a somewhat different nature are conditions 1 and 2 of Theorem 4.6. As we will show later on, both conditions are sufficient for the the existence of gradients of the probability function.

The following example shows that beside generic property 1 even property 2 of Theorem 4.6 has to be taken into account when considering gas nets. In particular, the example shows that the rank 2 condition may be violated in special instances. Recall that we have  $\nabla_z \tilde{g}_{kl}(x, z) = \nabla_z g_{kl}(z + \varphi(x))$ .

**Example 4.7.** We consider a gas net consisting of one entry and three exit nodes as displayed in Figure 3. From the system of feasibility constraints  $\tilde{g}_{k,l}(\cdot, \cdot)$  in (11) we



**Figure 3.** Small gas net example containing 3 pipes as well as 1 entry and 3 exit nodes.

select just  $\tilde{g}_{1,3}(\cdot, \cdot)$  and  $\tilde{g}_{2,3}(\cdot, \cdot)$ . For any  $x \in \mathbb{R}^3$  with  $x \geq 0$ , according to (13), we have for  $z \in \mathbb{R}^3$

$$\begin{aligned} \tilde{g}_{1,3}(x, z) &= (p_1^{\max})^2 - (p_3^{\min})^2 + \phi_{(0,1)} z_1^2 - \phi_{(0,3)} (z_3 + x_3)^2 \geq 0, \\ \tilde{g}_{2,3}(x, z) &= (p_2^{\max})^2 - (p_3^{\min})^2 + \phi_{(0,2)} z_2^2 - \phi_{(0,3)} (z_3 + x_3)^2 \geq 0. \end{aligned}$$

As gradients we obtain

$$\nabla_z \tilde{g}_{1,3}(x, z) = \begin{pmatrix} 2\phi_{(0,1)} z_1 \\ 0 \\ -2\phi_{(0,3)} (z_3 + x_3) \end{pmatrix}, \quad \nabla_z \tilde{g}_{2,3}(x, z) = \begin{pmatrix} 0 \\ 2\phi_{(0,2)} z_2 \\ -2\phi_{(0,3)} (z_3 + x_3) \end{pmatrix}.$$

We see that the gradients above are co-linear if both  $z_1$  and  $z_2$  are zero. Moreover, chose for example  $p_1^{\max} = p_2^{\max}$  and define (for some given  $x \geq 0$  with sufficient large  $x_3$ )  $z^* := (((p_1^{\max})^2 - (p_3^{\min})^2)/\phi_{(0,3)})^{1/2} - x_3$ . Then, we observe that on the one hand, both constraints are active, i.e. we have  $g_{1,3}(x, (0, 0, z^*)) = g_{2,3}(x, (0, 0, z^*)) = 0$ , on the other hand, the gradients are co-linear. Thus, in this example the rank 2 condition is violated at  $z = (0, 0, z^*)$ . But, two components  $z_1$  and  $z_2$  turn out to be zero (cf. Theorem 4.6).

Before proving the next result, we are going to simplify the notation. With respect to the formulation of the problem of maximizing bookable capacities (14) let

$$\mathcal{J} := \{j = (k, l) \mid k, l = 1, \dots, |\mathcal{V}|; k \neq l\}$$

be the index set of the feasibility constraints. We make use of the notation  $\tilde{g}_j(\cdot, \cdot) \equiv \tilde{g}_{k,l}(\cdot, \cdot)$  for  $j \in \mathcal{J}$  and  $j = (k, l)$ . Moreover, let  $\mathcal{J}^* \subseteq \mathcal{J}$  be the index set of all nonredundant constraints (cf. Theorem 4.6, item (3)). With this notation and with  $\tilde{g}_{kl}(x, z) = g_{kl}(z + \varphi(x))$ , Theorem 4.6 implies the following Corollary.

**Corollary 4.8.** *For given  $x, z \geq 0$  and  $i, j \in \mathcal{J}^*$  let be  $\tilde{g}_i(x, z) = \tilde{g}_j(x, z) = 0$  and  $i \neq j$ , where  $\tilde{g}(\cdot, \cdot)$  is given by (13). Under the assumptions of Theorem 4.6, i.e., if  $p_s^{\max} > p_t^{\min}$  for all  $s, t \in \mathcal{V}^+$ , then one of the following statements is satisfied:*

- (1) *The gradient vectors  $\nabla_z \tilde{g}_i(x, z)$  and  $\nabla_z \tilde{g}_j(x, z)$  are linearly independent.*
- (2) *It exist indices  $k, l \in \mathcal{V}$  with  $z_k = z_l = 0$  and  $k \neq l$ .*

The derived constraint qualification for the considered feasibility constraints turns out to be sufficient to guarantee differentiability of the involved probability function, as we will show in the following. To this end, we first state the following Lemma.

**Lemma 4.9.** *For any fixed  $x \geq 0$  we define*

$$S_j(x) := \{z \in \mathbb{R}^{|\mathcal{V}|} \mid \tilde{g}_j(x, z) = 0, \tilde{g}_\ell(x, z) \geq 0 \forall \ell \in \mathcal{J}^*\} \quad j \in \mathcal{J}^* .$$

*Then it holds for all  $i \neq j$*

$$\text{mes}_{|\mathcal{V}|-1}(S_i(x) \cap S_j(x)) = 0,$$

*where  $\text{mes}_{|\mathcal{V}|-1}(\cdot)$  denotes the surface Lebesgue measure in  $\mathbb{R}^{|\mathcal{V}|}$ .*

**Proof.** Due to Corollary 4.8 the intersection of the two active sets decomposes into two subsets  $A$  and  $B$  such that  $A \cup B = S_i(x) \cap S_j(x)$  with the property that, first,  $z \in A$  implies that  $\text{rank} \{\nabla_z \tilde{g}_i(x, z), \nabla_z \tilde{g}_j(x, z)\} = 2$ , secondly,  $z \in B$  implies that there exist zero components  $z_k = z_l = 0$  ( $k \neq l$ ). It is evidently sufficient to show  $\text{mes}_{|\mathcal{V}|-1}(A) = 0$  and  $\text{mes}_{|\mathcal{V}|-1}(B) = 0$ .

Given  $x$ , for any  $i \neq j$  we define a mapping  $F(\cdot)$  such that

$$F(z) := \begin{pmatrix} \tilde{g}_i(x, z) \\ \tilde{g}_j(x, z) \end{pmatrix} \in \mathbb{R}^2, \quad z \in \mathbb{R}^{|\mathcal{V}|}.$$

Hence,  $F(\cdot)$  is continuously differentiable, and, for arbitrary  $\bar{z} \in A$  we obtain  $F(\bar{z}) = 0$ . Moreover, due to the linear independence of the gradients, the Jacobian matrix  $D_F$  has rank 2 in  $\bar{z}$ . Thus, there exist indices  $k, l$  ( $k \neq l$ ) such that the according Jacobian

sub-matrix is invertible. Without loss of generality let's assume  $k = 1$  and  $l = 2$ . By the Implicit Function Theorem the equation  $F(z) = 0$  can be resolved in a neighbourhood  $U_{\bar{z}}$  of  $\bar{z}$  equivalently as

$$z_1 = f_1(z_3, \dots, z_{|\mathcal{V}|}) \quad \text{and} \quad z_2 = f_2(z_3, \dots, z_{|\mathcal{V}|}) \quad \forall (z_3, \dots, z_{|\mathcal{V}|}) \in V_{\bar{z}}, \quad (22)$$

where  $f_1, f_2 : V_{\bar{z}} \rightarrow \mathbb{R}$  are continuous differentiable functions and  $V_{\bar{z}}$  is a well-defined neighbourhood of  $(\bar{z}_3, \dots, \bar{z}_{|\mathcal{V}|})$ . Moreover, the mapping  $X : \mathbb{R} \times V_{\bar{z}} \rightarrow \mathbb{R}^{|\mathcal{V}|}$  given by

$$X(t, z_3, \dots, z_{|\mathcal{V}|}) := (f_1(z_3, \dots, z_{|\mathcal{V}|}) + t, f_2(z_3, \dots, z_{|\mathcal{V}|}) + t, z_3, \dots, z_{|\mathcal{V}|})$$

defines a parametrization of some surface  $S$  in  $\mathbb{R}^{|\mathcal{V}|}$ . Clearly, the set  $\{z \in U_{\bar{z}} \mid F(z) = 0\}$  is a subset of the surface  $S$  and due to (22) we observe that

$$X^{-1}(\{z \in U_{\bar{z}} \mid F(z) = 0\}) = \{0\} \times V_{\bar{z}} \quad \text{and} \quad \lambda_{|\mathcal{V}|-1}(\{0\} \times V_{\bar{z}}) = 0,$$

where  $\lambda_{|\mathcal{V}|-1}$  is the Lebesgue measure in space  $\mathbb{R}^{|\mathcal{V}|-1}$ . In particular, for the according surface measure we obtain that  $\text{mes}_{|\mathcal{V}|-1}(\{z \in U_{\bar{z}} \mid F(z) = 0\})$  is zero. On the other hand, the union of the family of open sets  $\{U_{\bar{z}_n}\}_{\bar{z}_n \in A}$  covers  $A$ . Because  $\mathbb{R}^{|\mathcal{V}|}$  is separable, a countable selection  $(\bar{z}_n)_{n \in \mathbb{N}}$  in  $A$  exists, where we obtain

$$A = \bigcup_{n \in \mathbb{N}} U_{\bar{z}_n} \cap A.$$

Due to the fact that  $\text{mes}_{|\mathcal{V}|-1}(U_{\bar{z}_n} \cap A) = 0$  ( $n \in \mathbb{N}$ ), we found a union of countable many subsets of  $S$  having surface measure zero that covers  $A$ . Therefore, from [14, Proposition 4.32] we conclude that  $\text{mes}_{|\mathcal{V}|-1}(A) = 0$ .

It remains to show that  $B$  has surface measure zero. But, subset  $B$  is included in the finite union of linear subspaces  $U_{kl} := \{z \in \mathbb{R}^{|\mathcal{V}|} \mid z_k = 0, z_l = 0\}$ ,  $k \neq l$ , of co-dimension 2 ( $k, l = 1, \dots, |\mathcal{V}|$ ). As a consequence, as well as subset  $A$ , also subset  $B$  has surface measure zero. This completes the proof.  $\square$

Note that Lemma 4.9 does not make use of the special structure of the constraints of the capacity problem and also remains valid in a more general context. It just requires a finite systems of continuously differentiable inequalities, where the claim of Corollary 4.8 is satisfied. The property, having surface measure zero of the intersection with respect to two active constraints, turns out to be the essential property when asking for differentiability of the probability function, as shown in [13]. Hence, with Lemma 4.9 we are prepared for the main result of this section, the differentiability of the capacity problem.

**Theorem 4.10.** *Let  $\bar{x} \geq 0$  be given such that  $\tilde{g}_j(\bar{x}, 0) > 0$  for all  $j \in \mathcal{J}$ . Then, the probability function  $\varphi(x) := \mathbb{P}_{\xi \geq 0}(\tilde{g}_j(x, \xi) \geq 0, j \in \mathcal{J})$  of the problem of maximizing bookable capacities (14) is differentiable on some neighbourhood  $U$  of  $\bar{x}$ , if the distribution  $\mathbb{P}$  of the random vector  $\xi$  has a continuous and bounded density on  $\mathbb{R}^{|\mathcal{V}|}$ , and if  $p_s^{\max} > p_t^{\min}$  for all  $s, t \in \mathcal{V}^+$ .*

**Proof.** To prove the result of the Theorem we want to apply a general result regarding differentiability of probability functions in [13]. To this end, we first discuss the gradients of the constraints  $\tilde{g}_j(x, \cdot)$ . The special structure of the constraints allows to

derive the following property. With the notation of Definition 4.1 and by applying Lemma 4.2 it is easy to show that for any  $j \in \mathcal{J}$  the equation  $\tilde{g}_j(\bar{x}, \bar{z}) = 0$  implies that

$$\|\nabla_z \tilde{g}_j(\bar{x}, \bar{z})\| \geq |[\nabla_z \tilde{g}_j(\bar{x}, \bar{z})]_{d_j^-}| \geq 2\phi^{\min} \left( \frac{\Delta p}{|\mathcal{V}|\phi^{\max}} \right)^{\frac{1}{2}} =: \gamma,$$

where  $\phi^{\max} := \max\{\phi_e | e \in \mathcal{E}\}$ ,  $\phi^{\min} := \min\{\phi_e | e \in \mathcal{E}\}$  denote maximal and minimal roughness coefficients, respectively, and  $\Delta p := \min\{(p_k^{\max})^2 - (p_l^{\min})^2 | k, l \in \mathcal{V}^+\}$  denotes the minimal quadratic pressure difference. As consequence, due to continuity, we observe that

$$\|\nabla_z \tilde{g}_j(x, z)\| \geq \frac{\gamma}{2} > 0$$

on some neighbourhood  $U$  of  $\bar{x}$  and  $V$  of  $\bar{z}$  for any  $j \in \mathcal{J}$ . Secondly, we state that

$$\mathbb{P}_{\xi \geq 0}(\tilde{g}_j(x, \xi) \geq 0, j \in \mathcal{J}) \equiv \mathbb{P}(\tilde{g}_j(x, \xi) \geq 0, j \in \mathcal{J}; \xi_k \geq 0, k \in \mathcal{V})$$

and mention that the additional inequalities  $\xi_k \geq 0$  ( $k \in \mathcal{V}$ ) are compatible with the constraint  $\tilde{g}(x, \xi) \geq 0$  in the sense that they do not destroy the recent properties. In particular, assuming  $\xi_k = 0$  and  $\tilde{g}_j(\bar{x}, \xi) = 0$  implies that there exists some  $l \neq k$  with  $\xi_l \neq 0$  (due to assumption  $\tilde{g}_j(\bar{x}, 0) > 0$ ). Hence, the gradients to these active constraints are linearly independent. Moreover, the additional non-negative constraints themselves satisfy the constraint qualifications of Corollary 4.8. Note that the norm of their gradients each equals one, no matter what  $\xi$ . As consequence, we apply Lemma 4.9 for the total system of inequalities, and, all requirements of [13, Theorem 2.4] are satisfied. We conclude that the probability function  $\varphi(x)$  is differentiable for all  $x \in U$ .  $\square$

We want to complete this section by discussing Example 4.7 again. Therefore, we illustrate the constraint qualifications of Corollary 4.8 and the resulting surface measure condition for the intersection of the boundary of both involved constraints for a special instance. By setting quadratic pressure differences and roughness coefficients equal to 1, for the constraints in Example 4.7 we obtain for any  $x, z \in \mathbb{R}^3$

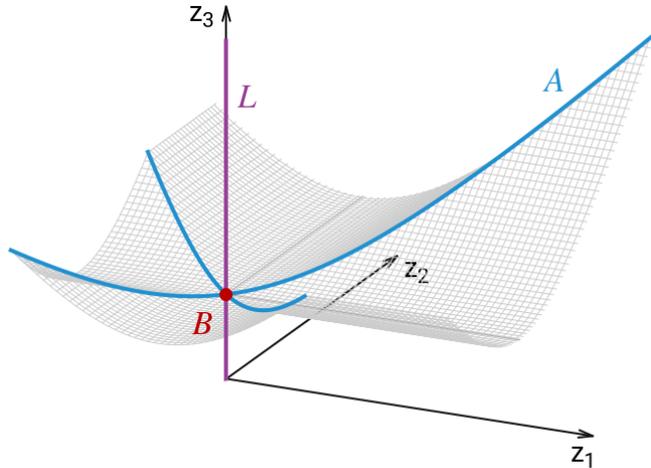
$$\begin{aligned} g_1(x, z) &= 1 + z_1^2 - (z_3 + x_3)^2 \geq 0, \\ g_2(x, z) &= 1 + z_2^2 - (z_3 + x_3)^2 \geq 0. \end{aligned}$$

Moreover, for the  $x$  variable we select  $\bar{x} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ . Then, for the gradients with respect to  $z$  we observe the two vectors

$$\nabla_z g_1(\bar{x}, z) = \begin{pmatrix} 2z_1 \\ 0 \\ -2z_3 - 1 \end{pmatrix}, \quad \nabla_z g_2(\bar{x}, z) = \begin{pmatrix} 0 \\ 2z_2 \\ -2z_3 - 1 \end{pmatrix}.$$

The intersection  $S = S_1(\bar{x}) \cap S_2(\bar{x})$  of surfaces  $S_1(\bar{x}) = \{z | g_1(\bar{x}, z) = 0, g_2(\bar{x}, z) \geq 0\}$  and  $S_2(\bar{x}) = \{z | g_2(\bar{x}, z) = 0, g_1(\bar{x}, z) \geq 0\}$  decomposes into the two subsets: The regularity set  $A = \{z \in S | \text{rank 2 condition satisfied}\}$  and the set of singularities  $B = \{z \in S | \text{rank 2 condition violated}\}$ . In that example, for the singularity set we obtain the singleton  $B = \{(0, 0, \frac{1}{2})\}$ . But note, this set is included in the linear subspace  $L = \{z \in \mathbb{R}^3 | z_1 = 0; z_2 = 0\}$  of co-dimension 2 (cf. Proof of Lemma 4.9).

However, we have that  $A \cup B = S$ . Figure 4 shows the surfaces  $S_1$  and  $S_2$  of the active sets, obtained from the two inequalities, as well as the intersection curve  $S$  represented by the subsets  $A$  and  $B$ . As shown in Lemma 4.9, it turns out that the 2-dimensional surface measure of  $S$  is zero. Indeed, we obtain  $\text{mes}_2(S) = 0$ .



**Figure 4.** Boundary of the feasibility region obtained for the special instance (above) of Example 4.7.

## 5. Algorithmic approach

In this section we want to provide an algorithmic solution for the problem of maximizing bookable capacities. In the previous sections we have shown that the capacity problem under weak conditions to the distribution of the random exit demand is differentiable with respect to the probabilistic constraint. Therefore, in principle any algorithm of nonlinear optimization that uses derivative information could be applied in order to solve the problem numerically. However, an efficient numerical solution is linked to an efficient computation of the involved probability function values and its gradients.

Returning to the capacity problem (14), for any fixed decision  $x$  the set of feasible nominations is given by

$$M_x := \left\{ \xi \in \mathbb{R}^{|\mathcal{V}|} \mid \tilde{g}_{k,l}(x, \xi) \geq 0; k, l = 0, \dots, |\mathcal{V}| \right\}, \quad (23)$$

where  $\tilde{g}_{k,l}(\cdot, \cdot)$  taken from (13). Thus, the set  $M_x$  is described explicitly and we might use the finite inequality system in (23) in order to test the feasibility of simulated outcomes of the random demand  $\xi$  according to the given continuous distribution. Taking the averaged number of feasible simulations would provide the Monte Carlo estimation for the desired probability  $\mathbb{P}(\xi \in M_x)$ . One drawback carried out in [11] is that the application of Monte Carlo may cause comparatively large variance for the obtained probability estimation. But, even more harmful in the context of solving an optimization problem is the fact that Monte Carlo simulation does not provide any information about the sensitivity of the probability with respect to changes of  $x$ . For this reason, an alternative approach is to make use of the so-called *spheric-radial decomposition* of Gaussian random vectors.

In general, given a random vector  $\xi(\omega)$  on some probability space  $(\Omega, \mathcal{A}, \mathbb{P})$  the computation of the probability

$$\mathbb{P}\{\omega \in \Omega \mid \xi(\omega) \in M_x\} \quad (24)$$

is correlated to resolving a potentially high dimensional multiple integral (depending on the number of exits). A particular situation to carry out this computation under Gaussian distribution occurs for polyhedral sets. Under this assumption in [9] an algorithmic approach is presented in order to compute Gaussian probabilities efficiently. Unfortunately, in our setting the feasible set  $M_x$  can not be expected to be polyhedral, not even convex. Therefore, an efficient computation in a more general setup is required as we will discuss next.

### 5.1. Spheric-radial decomposition under Gaussian distribution

We propose here the so-called spheric-radial decomposition of a Gaussian distribution (e.g., [7]). By this approach a significantly reduce of variance while estimating (24) can be expected compared to crude sampling. Additionally, the proposed method offers the possibility of an efficient approximation of gradients with respect to the optimization parameter  $x$ . To consider Gaussian or more general Gaussian-like distribution in context of gas transmission comes up in natural way. Even if the main variation of exit load data is temperature driven, certain temperature classes of sufficient large temperature range (usually 2K) can be identified such that considerable random variation remains within each temperature class. By this way the exit demand may be characterized by a finite family of multivariate distributions covering the given set of exit points according to different temperature intervals (for more details see [12, Chapter 13]). As stated in the same reference [12, Table 13.3], these distributions are most likely to be Gaussian (possibly truncated) or lognormal. We are going to sketch the usage of the spheric-radial decomposition method by the assumption of a underlying multivariate Gaussian distribution for  $\xi$ . As shown in Sec. 6 later on, the methodology can easily adapted without much effort to a more realistic setting, like truncated Gaussian distribution. The following result is well-known.

**Theorem 5.1** (spheric-radial decomposition). *Let  $\xi \sim \mathcal{N}(\mu, \Sigma)$  be some  $m$ -dimensional Gaussian distribution with mean vector  $\mu$  and covariance matrix  $\Sigma$ . Then, for any Borel measurable subset  $M \subseteq \mathbb{R}^m$  it holds that*

$$\mathbb{P}(\xi \in M) = \int_{\mathbb{S}^{m-1}} \mu_\chi \{r \geq 0 \mid rLv + \mu \in M\} d\mu_\eta(v),$$

where  $\mathbb{S}^{m-1}$  is the  $(m-1)$ -dimensional sphere in  $\mathbb{R}^m$ ,  $\mu_\eta$  is the uniform distribution on  $\mathbb{S}^{m-1}$ ,  $\mu_\chi$  denotes the  $\chi$ -distribution with  $m$  degrees of freedom and  $L$  is such that  $\Sigma = LL^T$  (e.g., Cholesky decomposition).

In order to evaluate the integrand in the spheric integral above, for any fixed direction  $v \in \mathbb{S}^{m-1}$  one has to compute the  $\chi$ -probability of the one-dimensional set

$$\{r \geq 0 \mid (rLv + \mu) \in M\}.$$

Since we are interested in the probability of the set  $M_x$ , this amounts by (23) to

characterizing the set

$$\{r \geq 0 \mid \tilde{g}_{k,l}(x, rLv + \mu) \geq 0; k, l = 0, \dots, |\mathcal{V}|\} \quad (v \in \mathbb{S}^{|\mathcal{V}|-1}). \quad (25)$$

Using the idea of spheric-radial decomposition presented in Theorem 5.1, we propose the following algorithm for computing the probability  $\mathbb{P}(\xi \in M_x)$  for a fixed value  $x$ . The conceptual form of the algorithm can be found in [11, Algorithm 4]. Here, we proceed with the reformulation specifically for optimization problems with probabilistic constraints in [10, Algorithm 3.1].

**Algorithm 1** (Function evaluation). *Let be  $x \geq 0$ ,  $\xi \sim \mathcal{N}(\mu, \Sigma)$  and  $L$  such that  $\Sigma = LL^T$ :*

- (1) *Sample  $N$  points  $\{v^1, v^2, \dots, v^N\}$  uniformly distributed on the sphere  $\mathbb{S}^{|\mathcal{V}|-1}$ .*
- (2)  *$i := 0; S := 0$ .*
- (3)  *$i := i + 1$ . Find the zero's of the one-dimensional function (in  $r$  for  $x$  fixed)*

$$\theta_x^i(r) := \min_{k,l=0,\dots,|\mathcal{V}|} \tilde{g}_{k,l}(x, rLv^i + \mu)$$

*with  $\tilde{g}_{k,l}(\cdot, \cdot)$  defined in (13), and, represent the set  $M_x^i := \{r \geq 0 \mid \theta_x^i(r) \geq 0\}$  corresponding to (25) as a disjoint union of intervals:  $M_x^i = \cup_{j=1}^i [\alpha_j(x), \beta_j(x)]$ , where  $\alpha_j(x), \beta_j(x)$  are the zero's obtained before and ordered appropriately.*

- (4) *Compute the  $\chi$ -probability of  $M_x^i$  according to*

$$\mu_\chi(M_x^i) = \sum_j F_\chi(\beta_j(x)) - F_\chi(\alpha_j(x)), \quad (26)$$

*where  $F_\chi$  refers to the cumulative distribution function of the one-dimensional  $\chi$ -distribution with  $|\mathcal{V}|$  degrees of freedom. Put  $S := S + \mu_\chi(M_x^i)$ .*

- (5) *Continue, if  $i < N$ , with step 3.*
- (6) *Finally, set  $\mathbb{P}(\xi \in M_x) := S/N$ .*

It is obvious that the above algorithm only provides an approximation to the spheric integral in Theorem 5.1. The integral is replaced by a finite sum based on samples for the unique sphere and representing the average value of the integrand. Nevertheless, the accuracy of approximation can be controlled by the sampling size  $N$  that should be chosen reasonably large compared to the problem dimension  $|\mathcal{V}|$  (the number of exit nodes). Computation of the zero's of the one-dimensional function  $\theta_x^i(r)$  (step 3 of the algorithm) can be done analytically. As disclosed in formula (13) the constraint mappings  $\tilde{g}_{k,l}(\cdot, \cdot)$  provide a particular quadratic structure such that  $\theta_x^i(r)$ ,  $i = 1, \dots, N$ , turn out to be piecewise quadratic functions as well.

Another remark concerns the sampling scheme on the unique sphere. As it is comprehensible that the uniform distribution on the sphere  $\mathbb{S}^{|\mathcal{V}|-1}$  can be represented as the distribution of  $\eta/\|\eta\|$  (here  $\|\cdot\|$  is the Euclidean norm), where  $\eta$  has a standard Gaussian distribution in  $\mathbb{R}^{|\mathcal{V}|}$ , a simple way to sample points  $v^i$  on the sphere as in step 1 of Algorithm 1 is as follows. Sample independently a number of  $|\mathcal{V}|$  values  $w_j$  of the one-dimensional standard normal distribution, and, putting  $v^i := w/\|w\|$  for  $w := (w_1, \dots, w_{|\mathcal{V}|})$ . Even if standard random generators for sampling of the normal distribution could be used, a better choice would be the application of Quasi-Monte Carlo sampling. Such sampling is based on deterministic low discrepancy sequences

and it provides a relevant improvement in the precision of the result, as observed in [11], where Monte Carlo as well as Quasi-Monte Carlo sampling is studied for the problem of nomination validation in gas networks.

## 5.2. Computing gradients of the probability function

As well as the function evaluations also gradient computations in view of the probabilistic constraints within the capacity problem are needed in order to solve the problem efficiently. The above spheric-radial decomposition approach has the advantage that in many situations derivatives with respect to involved parameters can be computed without additional effort by using nearly the same approximation scheme. As shown in [1,2], gradients can be represented as spheric integrals as well, just with different integrands. The basis for computing derivatives is the gradient formula for the probability function

$$\varphi(x) := \mathbb{P}(g(x, \xi) \geq 0)$$

(see Sect. 2) formulated in [2, Theorem 4.1]. Under some regularity assumptions for the constraint mapping  $g(\cdot, \cdot)$  including differentiability in both and convexity in the second argument we have the following representation. If  $g(x, \mu) \geq 0$ , in the Gaussian case  $\xi \sim \mathcal{N}(\mu, \Sigma)$  and with the notation of Theorem 5.1, the gradient of  $\varphi(\cdot)$  is of the form

$$\nabla \varphi(x) = \int_{\substack{v \in \mathbb{S}^{m-1} \\ \#J(x,v)=1}} \frac{\chi(\rho(x, v))}{\langle \nabla_{\xi} g_{j(v)}(x, \rho(x, v)Lv + \mu), Lv \rangle} \nabla_x g_{j(v)}(x, \rho(x, v)Lv + \mu) d\mu_{\eta}(v), \quad (27)$$

where  $\chi$  denotes the density of the  $\chi$ -distribution,  $\rho(x, v) := \max\{r \geq 0 \mid g(x, rLv + \mu) \geq 0\}$  and  $J(x, v) := \{j \in \{1, \dots, k\} \mid g_j(x, \rho(x, v)Lv + \mu) = 0\}$ . Moreover, the index  $j(v)$  is the unique index  $j \in \{1, \dots, k\}$  satisfying  $g_j(x, \rho(x, v)Lv + \mu) = 0$ . Unfortunately, as mentioned before the property of convexity with respect to the capacity problem will not be satisfied in general. Anyway, we are going to use the gradient formula (27) as pattern for an algorithmic computation of the gradient similar to Algorithm 1. One reason for doing so is that we consider bounded feasibility sets  $M_x$  only, i.e., the above convexity condition is quite strong just to ensure that the radius function  $\rho(x, v)$  is well-defined for any radial  $v \in \mathbb{S}^{m-1}$ . Therefore, the convexity condition could be replaced by the much weaker requirement of starshapeness with respect to the feasibility set in order to achieve the same gradient formula. Even though starshapeness of feasibility sets is hardly to verify, nevertheless, it is a reasonable condition in the context of gas transportation networks.

However, by applying formula (27) in a more general case we want to adapt Algorithm 1 in order to compute the gradient of the probability function, approximately. Therefore, the zero's  $\alpha_j(x)$ ,  $\beta_j(x)$  of the functional  $\theta_x^i(r)$  in Algorithm 1 play the role of the radius function  $\rho(x, v)$  in (27) for any direction  $v = v^i$ ,  $i = 1, \dots, N$ . By inclusion of the partial derivatives (gradients) of the constraints  $\tilde{g}_{k,l}(\cdot, \cdot)$  we provide the following algorithm.

**Algorithm 2** (Gradient evaluation). *Let be  $x \geq 0$ ,  $\xi \sim \mathcal{N}(\mu, \Sigma)$  and  $L$  such that  $\Sigma = LL^T$ :*

- (1) Sample  $N$  points  $\{v^1, v^2, \dots, v^N\}$  uniformly distributed on the sphere  $\mathbb{S}^{|\mathcal{V}|-1}$ .
- (2)  $i := 0; S' := 0$ .
- (3)  $i := i + 1$ . Find the zero's of the one-dimensional function (in  $r$  for  $x$  fixed)

$$\theta_x^i(r) := \min_{k,l=0,\dots,|\mathcal{V}|} \tilde{g}_{k,l}(x, rLv^i + \mu)$$

with  $\tilde{g}_{k,l}(\cdot, \cdot)$  defined in (13), and, represent the set  $M_x^i := \{r \geq 0 \mid \theta_x^i(r) \geq 0\}$  corresponding to (25) as a disjoint union of intervals:  $M_x^i = \cup_{j=1}^t [\alpha_j(x), \beta_j(x)]$ , where  $\alpha_j(x), \beta_j(x)$  are the zero's obtained before and ordered appropriately.

- (4) To any of the zero's  $\alpha_j(x), \beta_j(x)$  select the active constraints, i.e., assign index mappings  $\tau_\alpha(j), \tau_\beta(j) \in \{0, \dots, |\mathcal{V}|\}^2$  such that

$$\tilde{g}_{\tau_\alpha(j)}(x, \alpha_j(x)Lv + \mu) = 0 \quad \text{and} \quad \tilde{g}_{\tau_\beta(j)}(x, \beta_j(x)Lv + \mu) = 0. \quad (28)$$

Compute the derivative of the  $\chi$ -probability of  $M_x^i$  according to

$$\begin{aligned} D_j^\alpha(x) &= \frac{f_\chi(\alpha_j(x))}{\langle \nabla_\xi g_{\tau_\alpha(j)}(x, \alpha_j(x)Lv^i + \mu), Lv^i \rangle} \nabla_x g_{\tau_\alpha(j)}(x, \alpha_j(x)Lv^i + \mu), \\ D_j^\beta(x) &= \frac{f_\chi(\beta_j(x))}{\langle \nabla_\xi g_{\tau_\beta(j)}(x, \beta_j(x)Lv^i + \mu), Lv^i \rangle} \nabla_x g_{\tau_\beta(j)}(x, \beta_j(x)Lv^i + \mu), \\ \nabla_x (\mu_\chi(M_x^i)) &= \sum_j D_j^\alpha(x) - D_j^\beta(x), \end{aligned} \quad (29)$$

where  $f_\chi$  refers to the probability density function of the one-dimensional  $\chi$ -distribution with  $|\mathcal{V}|$  degrees of freedom. Put  $S' := S' + \nabla_x (\mu_\chi(M_x^i))$ .

- (5) Continue, if  $i < N$ , with step 3.
- (6) Finally, set  $\nabla_x (\mathbb{P}(\xi \in M_x)) := S'/N$ .

Before concluding this section some remarks to the stated Algorithm 1 and 2 are appropriate. The update formula (29) for the derivative of the probability function with respect to the parameter  $x$  in step 4 of Algorithm 2 can be considered as rigorous differentiation of formula (26) for updating the probability within step 4 of Algorithm 1. Since we have

$$\nabla_x (F_\chi(\beta_j(x)) - F_\chi(\alpha_j(x))) = f_\chi(\beta_j(x)) \nabla_x \beta_j(x) - f_\chi(\alpha_j(x)) \nabla_x \alpha_j(x),$$

formula (29) in Algorithm 2 appears when inserting the gradients  $\nabla_x \alpha_j(x)$  and  $\nabla_x \beta_j(x)$  which are obtained by total differentiation of the equations in (28) with respect to  $x$  and resolving them for  $\nabla_x \alpha_j(x)$  and  $\nabla_x \beta_j(x)$ , respectively. Moreover, note that both algorithms are compatible in a sense that, after computing the sampling scheme on the unique sphere, one and the same sample  $v^i$  can be employed in order to update values and gradients of the involved probability function. Also the needed zero's  $\alpha_j(x)$  and  $\beta_j(x)$  are the same here. In general, determining these zero's corresponds to the most expensive parts. On the other hand, due to the analytical representation (13) the partial derivatives of the mappings  $\tilde{g}_{k,l}(\cdot, \cdot)$  can easily be determined analytically (similar to Lemma 4.2). To perform both function end gradient evaluations, almost no additional effort for computing gradients is needed when computing function values and performing Algorithm 1 and 2 simultaneously.

The strategy of computing function values and gradients of the probabilistic constraints of the capacity problem by Algorithms 1 and 2 can be embedded into a simple projected gradient method. Clearly, due to the non-convexity of the model, performing a projected gradient method causes a termination at local minima, in general. Therefore, the accuracy strongly depend on finding reasonable starting points heuristically. However, the practicability of the approach is shown in the next section, where a numerical study related to realistic network data is presented.

## 6. Numerical study

In this section we finally want to test the performance of the presented methodology for solving the problem of maximizing bookable capacities. Clearly, here we use the reformulation in terms of the classical probabilistic constrained optimization problem obtained in (14). In order to solve the underlying non-linear optimization problem we designed a straight forward descent method based on projected gradients. The core of the method consists in local linearizations of the feasibility set and the projection of the negative objective gradient onto these linearizations. Whenever this projection is non-zero a new descent step can be performed which results in a feasible point with improved objective. Because the descent direction could point away from the feasibility set, if necessary, a redirection back to the feasibility set must be performed, where the gradient information of the constraints may be used. The method terminates in a stationary point, where the projected objective gradient is zero.

The described descent method actually aims to solve a minimum problem that can be obtained just by switching the sign of the objective function in (14). All needed to perform this method are function and gradient evaluations for both the objective and constraint function. Function values and derivatives of the objective are computed analytically. Because we do not assume any preferences in the allocation of new capacities, the weight vector in the objective of problem (14) is chosen just as  $c^T = (1, \dots, 1)$ .

For the probabilistic constraint, represented by the probability function, the spherical-radial decomposition is applied. More precisely, Algorithm 1 and Algorithm 2 from the previous section are used in order to compute function values and gradients. Therefore, we employed Quasi-Monte Carlo (QMC) sampling on the bases of Sobol sequences as a special case of low-discrepancy sequences that are included in the category of  $(t, m, d)$ -nets and  $(t, d)$  sequences [8]. A QMC sample of 10 000 scenarios was created according to a standard Gaussian distribution (zero mean and identity covariance matrix). Normalizing each scenario to unit length provides a sample of the uniform distribution on the sphere as required in the simultaneous update of values and gradients of the probability function within Algorithm 1 and 2.

The appropriate choice of model parameters is a crucial step in numerical experiments. In the view of exit load nominations, as already mentioned, [12, Chapter 13] provides a wide study concerning the statistical analysis of gas demand data in real gas networks. The approach is based on analyzing historical data with respect to different temperature classes and in identifying multivariate distributions coming up into consideration. According to the results, random gas demand can often be described by combinations of Gaussian-like multivariate distributions (Gaussian, truncated Gaussian, lognormal). Distribution parameters like mean, standard deviation and correlations can be estimated statistically from historical data, where the network owner may benefit from a long term data record.

### 6.1. *Multivariate Gaussian distribution*

We start our numerical experiences with an example wherein assuming a multivariate Gaussian distributed exit demand as in Theorem 5.1 with parameters (mean  $\mu$ , covariance  $\Sigma$ ) chosen in a way to represent real-life data.

The particular gas net is taken from [4]. The parameters are in fact slightly modified distribution parameters obtained from a real gas network and adapted to an artificial example net containing one entry node, 11 exit nodes and representing a tree. All remaining network parameters, particularly roughness, lower and upper pressure bounds are chosen in range of typical values for existing gas nets.

Results for solving the problem of maximizing bookable capacities (14) for Gaussian distributed exit demand are displayed in Table 1. In addition, Figure 5 visualizes the network topology and the allocated free capacities at the exit nodes for the selected probability levels  $p = 0.90$  and  $p = 0.80$ , respectively. Clearly, a decreasing probability level for technical feasibility of random demand yields an increasing free capacity left in the net.

In Figure 6 we perform a posterior check of the computed solution for the probability level  $p = 0.80$ . By a simulation of 4 sets of exit load situations according to the chosen Gaussian distribution we check the feasibility of the computed solution, i.e., the allocated capacity, against the particular exit demand in the robust sense of (10). Feasibility is displayed by green circles indicating that the computed capacity as solution of (14) could even be increased by upscaling while remaining feasible with respect to the simulated scenario. On the other hand, if the allocated capacity exceeds the possible technical feasibility in the simulated situation, this is displayed by red circles according to a needed downscale of the solution in order to become feasible with respect to the robust condition (10). As seen in Figure 6, three out of four simulated exit demand situations turn out to be feasible whereas in one case the solution do not satisfy the simulated demand. However, when simulating a large set of such scenarios, say 1 000, it would turn out that according to the probability level  $p = 0.80$  approximately 800 are feasible, while 200 are infeasible.

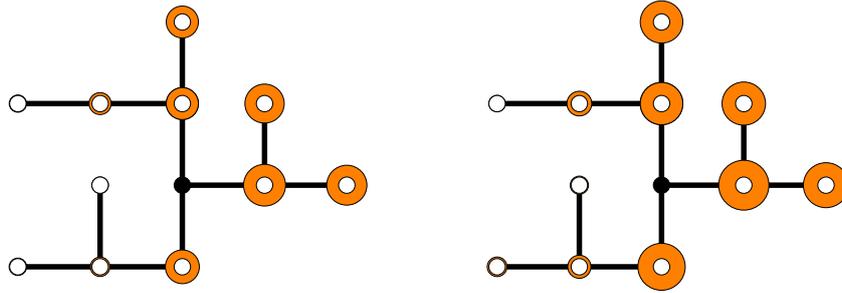
### 6.2. *Extension to more general distributions*

As discussed, according to [12] Gaussian and Gaussian-like distributions are mostly relevant for describing random demand in gas transportation networks. But in fact, the described methodology to treat optimization problems with probabilistic constraints via spheric-radial decomposition can be extended even to more general distributions. In [3] the class of elliptical distributions is considered, where the approach is used for the investigation of probability functions acting on nonlinear systems wherein the random vector can follow an elliptically symmetric distribution. Beside the Gaussian distribution the Student's distribution would be another example for an elliptically symmetric distribution.

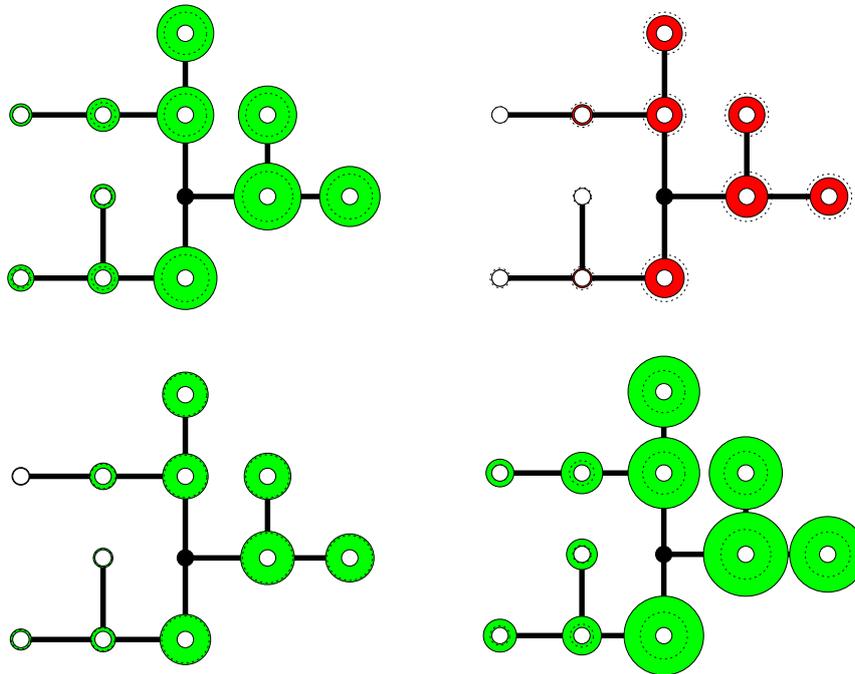
In the context of capacity optimization in a gas transportation network, we want to discuss a slightly more realistic situation, where gas nominations are in fact regulated by contracts between the network owner and the customers. Such contracts usually provide upper limits for the quantity of gas that could be delivered to the customers. Therefore, in the second numerical example for the problem of maximizing bookable capacities we will suppose that the stochastic exit demand vector  $\xi$  follows a truncated

**Table 1.** Results for the gas net example of medium size. Displayed are the obtained free bookable capacities (total sum for all exits) compared to the average of the total gas demand at all exits computed by solving problem (14) for different chosen probability levels and fixed underlying multivariate normal distribution for the exit demand.

Probability	Average demand [kW]	Free capacity [kW]	Descent steps	Computing time [s]
0.95	19 685.93	1 147.73	72	51.14
0.90	19 685.93	2 119.57	104	90.08
0.85	19 685.93	2 692.52	132	126.68
0.80	19 685.93	3 127.60	153	140.95



**Figure 5.** Network topology of a medium sized gas net for the example of Gaussian exit demand. Illustration of the solution of the capacity maximization at exit points for different probability levels  $p = 0.90$  (left) and  $p = 0.80$ . The entry and exit points are displayed in black (entry) and white (exit), respectively. A decreasing probability level allows for a higher allocation of capacities in certain regions of the network highlighted by colored circles of different size.



**Figure 6.** Four simulated exit demand realizations according to the chosen multivariate Gaussian distribution and the respective available free capacity compared to the allocated capacity provided by the numerical solution for the medium network for the probability level  $p = 0.80$ . Feasible and infeasible situations are displayed in green and red, respectively.

multivariate Gaussian distribution

$$\xi \sim \mathcal{TN}(\mu, \Sigma, [0, L]). \quad (30)$$

More precisely, the distribution of  $\xi$  is obtained by truncating a  $|\mathcal{V}|$ -dimensional Gaussian distribution with mean  $\mu$  and covariance matrix  $\Sigma$  to an  $|\mathcal{V}|$ -dimensional rectangle  $[0, L]$  with upper limits  $L_k$  at exit node  $k$ . Therefore, the vector  $L$  represents booking limits given by former contracts. Clearly, the network owner is aiming to extend these limits by the allocation of free network capacities according to the solution of (14).

We want to proceed with the same methodology from Sec. 5, in particular, we want to apply Algorithm 1 and 2 based on spheric-radial decomposition in order to solve the capacity problem (14), but under truncated instead of Gaussian distribution. Therefore, a transformation back to a normal distribution can be discovered as follows. By definition of the truncated normal distribution, (30) is equivalent to the property

$$\mathbb{P}(\xi \in A) = \frac{\mathbb{P}(\tilde{\xi} \in A \cap [0, L])}{\mathbb{P}(\tilde{\xi} \in [0, L])}$$

for all Borel measurable subsets  $A$  of  $\mathbb{R}^{|\mathcal{V}|}$ , and, where  $\tilde{\xi}$  is the associated Gaussian random vector with  $\tilde{\xi} \sim \mathcal{N}(\mu, \Sigma)$ . Hence, in order to determine probabilities under a truncated Gaussian distribution, it is sufficient to be able to determine probabilities under the Gaussian distribution itself. Applying this observation to the probabilistic constraint of the capacity problem, the equivalent representation to the reformulation (14) of the problem of maximizing bookable capacities with truncated Gaussian exit load distribution  $\mathcal{TN}(\mu, \Sigma, [0, L])$  reads

$$\begin{aligned} & \text{maximize } c^T x \quad \text{subject to} \\ & \mathbb{P} \left( \left\{ \begin{array}{ll} \tilde{g}_{k,l}(x, \tilde{\xi}) \geq 0 & (k, l = 0, \dots, \mathcal{V}) \\ \tilde{\xi}_k \geq 0 & (k = 1, \dots, \mathcal{V}) \\ \tilde{\xi}_k \leq L_k & (k = 1, \dots, \mathcal{V}) \end{array} \right\} \right) \geq p \cdot \mathbb{P}(\tilde{\xi} \in [0, L]), \end{aligned} \quad (31)$$

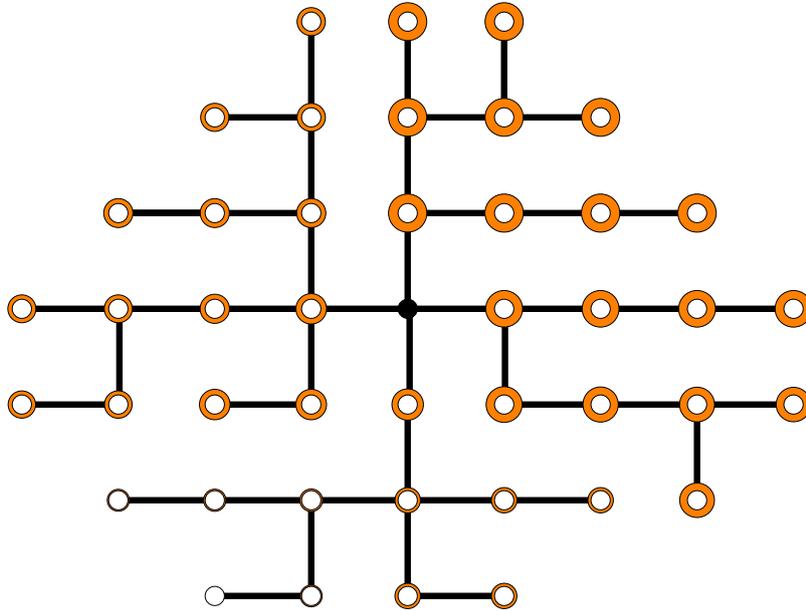
where  $\tilde{\xi} \sim \mathcal{N}(\mu, \Sigma)$  is the Gaussian distribution with mean  $\mu$  and covariance matrix  $\Sigma$  and  $\tilde{g}_{k,l}(\cdot, \cdot) \geq 0$  corresponds to the system of inequalities obtained in (13). Hence, the modified problem formulation (31) arises from (14) only by adding additional box constraints to the system of random inequalities, and, by scaling the given probability accordingly. The probability value  $\mathbb{P}(\tilde{\xi} \in [0, L])$  can easily be computed by the spheric-radial decomposition, or alternatively, by other efficient computation schemes for the probability of rectangles when dealing with multivariate normal distributions [9].

The following numerical results are obtained for a larger example network containing 1 entry and 43 exit nodes. The more realistic sized network could be viewed as a topological extension of the medium size network before. Although this network is academical constructed as well, the network parameters are adapted from real networks in the same way as before. The initial multivariate truncated Gaussian distribution again involves correlations between the exit points. The truncation limits are chosen in a way that one obtains an initial probability level of approximately  $p = 0.98$  for the technical feasibility of the random demand (with no capacity extension). The truncation probability in (31), i.e., the Gaussian probability of the rectangle  $[0, L]$ , turns out to be  $\mathbb{P}(\tilde{\xi} \in [0, L]) = 0.71$ . However, the high initial probability level allows for allocating free capacities when decreasing the prescribed probability as shown

in Table 2. In Figure 7, a visualization of the network topology and the allocated free capacities at the exit nodes for the second example under truncated Gaussian distribution and for a selected probability level of  $p = 0.80$  is given. It turns out that, although no preferences such as certain weights are assigned to the different exit points, the total amount of allocated free capacity is not uniformly distributed at the whole network. In fact, network and distribution specifics play the major role when answering the question of allocating and maximizing free bookable capacities.

**Table 2.** Numerical results for the gas net example of large size. Displayed are the obtained free capacities (total sum for all exits) compared to the average of the total gas demand at all exits computed by solving problem (14) for different chosen probability levels and fixed underlying multivariate truncated normal distribution for the exit demand.

Probability	Average demand [kW]	Free capacity [kW]	Descent steps	Computing time [s]
0.95	28 870.74	727.08	20	212.66
0.90	28 870.74	1 271.07	32	277.58
0.85	28 870.74	1 654.31	53	362.09
0.80	28 870.74	1 941.04	45	363.83



**Figure 7.** Network topology of the large sized network for the example of truncated Gaussian exit demand. Illustration of the solution of the capacity maximization at exit points for the probability level of  $p = 0.80$ . The entry and exit points are displayed as before. The picture shows the allocated free capacities obtained at the particular exit nodes of the network. Quantities are highlighted by colored circles of different size.

## Conclusion

This paper concerns a deep theoretical analysis of a class of optimization problems with probabilistic constraints. The investigation is motivated by an application coming up with optimization in gas transport under uncertainty. Substantial structural questions are answered in that context. But the main theoretical results of this paper allow for application beyond the gas context. A constraint qualification for the differentiability of probability functions has been provided for situations, where the rank

2 condition is violated in some points. Some easily verifiable measure zero condition based on the general result in [13, Theorem 2.4] has been added for such cases. The paper is completed by a numerical study of a highly relevant problem, the maximization of bookable capacities in an entry/exit gas transportation model. The presented methodology and algorithmic provide a pattern for general numerical treatment of problems with probabilistic constraints.

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