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# A New Class of Valid Inequalities for Nonlinear Network Design Problems

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**Abstract.** We consider a nonlinear nonconvex network design problem that arises in the extension of natural gas transmission networks. Given is such network with active and passive components, that is, valves, compressors, control valves (active) and pipelines (passive), and a desired amount of flow at certain specified entry and exit nodes of the network. Besides flow conservation constraints in the nodes the flow must fulfill nonlinear nonconvex pressure loss constraints on the arcs subject to potential values (i.e., pressure levels) in both end nodes of each arc. Assume that there does not exist a feasible flow that fulfills all physical constraints and meets the desired entry and exit amounts. Then a natural question is where to extend the network by adding pipes in the most economic way such that this flow becomes feasible. Answering this question is computationally demanding because of the difficult problem structure. We use mixed-integer nonlinear programming techniques that rely on an outer approximation of the overall problem, and a branching on decision variables. We formulate a new class of valid inequalities (or cutting planes) which reduce the overall solution time when added to the formulation. We demonstrate the computational merits of our approach on test instances.

**Keywords:** Network Design; Mixed-Integer Nonlinear Programming; Cutting Planes.

## 1 Introduction

Natural gas is a nontoxic, odorless, transparent, and flammable gas that originates from underground deposits. Today natural gas is mainly used for heating private houses and office buildings, for the generation of electrical power, as fuel for vehicles, and for several reactions in chemical process engineering. The world's joint resources in natural gas are assumed to last for the next 60 to 500 years, if conveyance and consumption remain on the current level. With natural gas around one quarter of the world's energy demand is covered. Since natural gas is the "greenest" energy source among the fossil ones, its market share is estimated to grow to 50% towards the end of this century.

The natural gas must be transported from the deposits to the customers, sometimes over distances of several thousand kilometers. For very long distances (more than 4000km) it is more economic to cool down the gas to  $-160^{\circ}\text{C}$  such that it becomes liquid and to transport it via ships. For shorter distances or for the delivery to the end customers large pipeline systems are used. An existing gas network usually has grown over time. In Germany, it was built by gas supply companies such that it can ensure the transportation of exactly the required amounts of gas to their customers. In the past, the German gas supply companies were gas vendors and gas network operators at the same time: They purchased gas from other suppliers and set up and operated the necessary infrastructure to transport the gas from those suppliers to their customers. In course of the liberalization of the German gas market, these roles and business units were separated by regulatory authorities (see [15] for more details on the regulatory background). Now there are companies whose sole task is the transportation of gas and who operate gas transportation networks for this purpose. Several previously independent networks were aggregated into bigger units. A discrimination free access to these networks has to be granted to everyone. This increase in flexibility for gas vendors and customers requires a higher degree of operational flexibility from the

gas network operators. Although the total amount of transported gas is approximately the same, today's gas networks cannot cope with this. Various congestions show up obstructing the desired flexibility. To overcome these shortcomings a massive investment in the network infrastructure is necessary in the near future. Extension management becomes a crucial issue, since each single investment into a new compressor or a new pipe costs up to several hundreds of million Euros.

A gas network may be extended in several ways to increase the local transportation capacity. It is possible to build new pipes and to extend the capabilities of compressor stations and control valves or to build new ones. A special case of building a new pipe is looping: A *loop* is a pipe that follows an existing one. Loops are to some extent cheaper to build than a new pipe somewhere in the country, because land owner rights are already settled and building permissions are easier to obtain. Hence loop extensions are first-choice, long before a non-loop pipeline is considered. Thus in the computational section we focus on loop extensions, the methods, however, can be applied to any kind of extension by new pipelines. For more details we refer to [13].

Several approaches to improve the topology of a gas network are reported in the literature. Mainly various heuristic and local optimization methods are in use. So far, we are not aware of approaches from the literature that apply global methods to solve network design problems for gas transmission networks. Boyd et al. [5] apply a genetic algorithm to solve a pipe-sizing problem for a network with 25 nodes and 25 pipes, each of which could have one of six possible diameters. Castillo and Gonzalez [7] also apply a genetic algorithm for finding a tree topology solution for a network problem with up to 21 nodes and 20 arcs. In addition to pipes, also compressors can be placed into the network. Mariani et al. [21] describe the design problem of a natural gas pipeline. They present a set of parameters to evaluate the quality of the transportation system. Based on these they evaluate a number of potential configurations to identify the best among them. Osiadacz and Gorecki [24] formulate a network design problem for a given topology as a nonlinear optimization problem, for which they iteratively compute a local optimum. For a given topology the diameter of the pipes is a free design variable. Their method is applied to a network with up to 108 pipes and 83 nodes. De Wolf and Smeers [11] also use a nonlinear formulation and apply a local solver. They distinguish the operational problem (running the network) from the strategical investment problem (extending the network). For a given topology with up to 30 arcs and nodes they can determine (locally) optimized pipe diameters. Bonnans and André [2, 4] consider the optimal design problem of a straight pipeline system, and derive some theoretical properties of an optimal design. In [20] we describe a primal heuristic based on dual information from KKT solutions of the gas network model formulation.

Our contribution in this field is to apply exact optimization methods that can converge to a proven global optimal solution. Our theoretical contribution is the introduction of a new class of valid inequalities that improve the relaxation of the model, and thus have a positive impact on the running time of a branch-and-cut solution algorithm. Our methods were developed in cooperation with Open Grid Europe GmbH (OGE), a large gas transportation company.

The remainder of this article is organized as follows. In Section 2 we introduce the physical background of gas flows and in Section 3 the mathematical background of mixed-integer nonlinear programming. Section 4 presents a mathematical programming model for the simultaneous gas nomination and extension of a given network by selecting from a set of additional loop pipes. For a subproblem of this model to be defined in Section 4.2 we derive valid inequalities in Section 5. These inequalities are extended to a valid cut for the topology optimization problem in Section 6. We show computational results obtained using this procedure in Section 7. Finally we conclude in Section 8 and give some ideas for future research directions.

## 2 Physical and Technical Background of Transmission Networks

We give mathematical descriptions for active and passive elements that are the basic building blocks of the transmission networks we study.

### 2.1 Pipes

The majority of the edges in a transmission network are passive pipes. In a network with node potentials the amount of flow over an edge is determined by the actual node potential values at both ends. Depending on the physical properties of the flow different functional relationships are described in the literature to

approximatively determine the flow value. The fundamental equation we assume for an edge  $e = (v, w)$  is

$$\alpha_e q_e |q_e|^{k_e} = \pi_v - \gamma_e \pi_w. \quad (2.1)$$

Here  $\alpha_e$  and  $k_e$  are constants that subsume all physical properties of the pipe, the flow, and the interactions of the flow with the edge (c.f. Weymouth [31]). The constant  $\gamma_e$  in particular represents the height difference between nodes  $v$  and  $w$ . If some pipelines  $e_1, \dots, e_n$  form a directed cycle, it is assumed that  $\gamma_{e_1} \cdot \dots \cdot \gamma_{e_n} = 1$ . If a cycle is undirected, we assume this constraint holds after reverting some of the arcs, so that this cycle becomes directed. If arc  $(v, w)$  with right-hand side  $\pi_v - \gamma_{(v,w)} \pi_w$  in (2.1) is reverted, then the new right-hand side of arc  $(w, v)$  becomes  $\pi_w - \gamma_{(w,v)}^{-1} \pi_v$ . (Note that the constant on the left-hand side changes from  $\alpha_e$  to  $\alpha_e \cdot \gamma_e^{-1}$ .) Although each edge  $e$  in principle might have a different value for  $k_e$  it is natural to assume that all edges have the same constant. The mathematical theory which we present in the following relies on the fact that  $k_e \in \{0, \text{const}\}$ , with  $\text{const} \in \mathbb{R}_{>0}$ . The variable  $q_e \in \mathbb{R}$  represents the flow, where a positive value is a flow from  $v$  to  $w$ , and a negative value is a flow in the opposite direction from  $w$  to  $v$ . The variables  $\pi_v, \pi_w$  are the node potential values.

**Gas Networks.** The Weymouth equation [31] is an old but still used equation to approximate the flow of gas in long pipelines. It relates the pressure of the gas in the end nodes,  $p_v$  and  $p_w$ , to the flow in the following way:

$$q_e |q_e| = C_e^2 \cdot (p_v^2 - p_w^2),$$

where  $C_e^2$  is computed by the following formula:

$$C_e^2 := 96.074830 \cdot 10^{-15} \frac{d_e^5}{\lambda_e z T L_e \delta},$$

where

$$\frac{1}{\lambda_e} = \left( 2 \log \left( \frac{3.7 d_e}{\varepsilon} \right) \right)^2,$$

with  $L_e$  being the length of the pipe (km),  $d_e$  the inner diameter of the pipe (mm),  $T$  the gas temperature (K),  $\varepsilon$  the absolute roughness of the pipe (mm),  $\delta$  the density of the gas relative to air, and  $z$  the gas compressibility factor [23, 12, 26]. Note that our approach cannot cope with other more accurate pressure loss equations, if  $C_e^2$  is not a constant but a flow- or pressure-dependent variable. After substituting  $\pi_v = p_v^2$  and  $\pi_w = p_w^2$  (for  $\gamma_e = 1$ ) Weymouth's equation takes the form of (2.1). The slightly more general version of Weymouth's equation with  $\gamma_e \neq 1$  (for different heights of the pipe's end nodes) is given in [25].

**Water Networks.** Our mathematical approach is also suited for water networks. The flow of water in pipelines can, for instance, be approximated by the Hazen-Williams equation [18]:

$$\frac{10.67}{C_e^{1.85}} \frac{L_e}{d_e^{4.87}} q_e |q_e|^{0.85} = \rho \cdot g \cdot (h_v - h_w),$$

where  $C_e$  is a dimensionless roughness coefficient (typically ranging between 90 and 150),  $L_e$  is the length (meters),  $d_e$  is the inside diameter (meters),  $\rho$  is the density of the fluid ( $\text{kg}/\text{m}^3$ ),  $g$  is the local acceleration due to gravity ( $\text{m}/\text{s}^2$ ),  $q_e$  is the volumetric flow rate (cubic meters per second), and  $h_v, h_w$  are the geographical heights of nodes  $v$  and  $w$  (Pa). Setting  $\pi_v = h_v$  and  $\pi_w = h_w$  and  $\gamma_e = 1$  the Hazen-Williams equation takes the form of (2.1).

## 2.2 Valves

A valve is installed in the network to separate or join two independent pipes. They allow for a discrete decision, either being open or closed. The spatial dimension of a valve is assumed to be small in comparison to the pipes. Hence in our model the node potential values are identified when the valve is open. If the valve is closed then they are decoupled. Mathematically a valve is an edge  $e = (v, w)$  with the following description:

$$\begin{aligned} x_e = 1 &\Rightarrow \pi_v - \pi_w = 0, \\ x_e = 0 &\Rightarrow q_e = 0, \end{aligned}$$

where  $x_e \in \{0, 1\}$  is a binary decision variable.

### 2.3 Increasing the Node Potential

In transmission networks it is necessary at certain locations to increase the node potential value. For example, in gas networks the pressure is too low after a transport distance of 100-150km. Here compressors are used to increase the pressure level again. For the mathematical description of such active network elements, various models exist in the literature. We follow the approach of De Wolf and Smeers [12], and make use of the following formulation for a pipe  $e = (v, w)$  with a compressor:

$$\alpha_e q_e |q_e|^{k_e} \geq \pi_v - \pi_w, \quad (2.2)$$

which allows a flow larger than the one corresponding to the pressure decrease in the pipe. We rewrite this inequality as equality by introducing a weighted slack variable  $y_e$  as

$$\alpha_e q_e |q_e|^{k_e} + \beta_e y_e = \pi_v - \pi_w \quad (2.3)$$

with constant  $\beta_e \in \mathbb{R}$  and  $\underline{y}_e \leq y_e \leq \bar{y}_e$ . Note that the flow can only go in positive direction through a compressor, hence the lower bound needs to be set accordingly, i.e.,  $q_e \geq 0$ .

### 2.4 Reducing the Node Potential

It can be necessary to reduce the node potential along an edge  $e = (v, w)$  in the network, for example, to protect parts of the network from high potentials. In gas networks, for instance, these are control valves that reduce the gas pressure. A pipe with a control valve  $e = (v, w)$  is inverse to a pipe with a compressor. Hence we need to turn the sense of the inequality (2.2) around:

$$\alpha_e q_e |q_e|^{k_e} \leq \pi_v - \pi_w, \quad (2.4)$$

in order to decrease the pressure in  $w$  more than the flow and the input pressure would actually require. After introducing weighting slack variables  $y_e$  equation (2.4) appears similar to equation (2.3). (The only difference between a compressor and a control valve is either the sign of  $\beta_e$  or the bounds on  $y_e$ .) Note that the flow direction through a control valve is also fixed by setting the lower bound to zero, i.e.,  $q_e \geq 0$ .

## 3 Mathematical Background

In order to obtain proven global optimal solutions we apply linear and nonlinear mixed-integer programming techniques, which we briefly introduce here.

### 3.1 Global Mixed-Integer Nonlinear Programming

We formulate the topology extension problem as mixed-integer nonlinear program (MINLP). Solving optimization problems from this class is theoretically intractable and also known to be computationally difficult in general. By “solving” we mean to compute a feasible solution for a given instance of the problem together with a computational proof of its optimality. Therefore we apply the general framework of a branch-and-cut approach, where the bounds are obtained from relaxations of the original model. To this end, we relax the MINLP first to a mixed-integer linear program (MILP) and then further to a linear program (LP), which is solved efficiently using the simplex algorithm. The so obtained solution value defines a (lower) bound on the optimal value of the original MINLP problem. In case this solution is MINLP feasible, it would be a proven global optimal MINLP solution. However, this rarely happens in practice. Hence we either add cutting planes to strengthen the relaxation, or we decide to branch on a variable. As an example, consider the nonlinear pressure loss constraint (2.1), c.f. Fügenschuh et al. [14]. In the LP relaxation this function is replaced by a polyhedral (linear) outer approximation, which is iteratively refined during the branch-and-cut process by branching on variables (spatial branching), see Figure 3.1. For more details on cutting planes and branch-and-bound for MILP we refer to Nemhauser and Wolsey [22], and for an application of this framework to global mixed-integer nonlinear programming to Smith and Pantelides [27], and Tawarmalani and Sahinidis [28, 29]. Information on the MINLP framework SCIP which we apply is given by Achterberg [1], and in particular on nonlinear aspects of SCIP in Berthold, Heinz, and Vigerske [3].

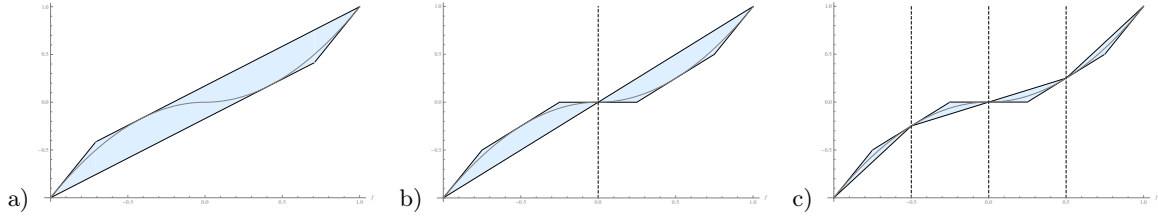


Fig. 3.1: a) Polyhedral outer approximation of  $q_e \mapsto \alpha_e q_e |q_e|$ , b) initial spatial branching on zero, c) further spatial branching.

### 3.2 Nonlinear Programming

In addition to the simplex algorithm for linear programs we use nonlinear solvers on nodes of the branch-and-bound tree. Actually we apply the solver IPOPT from Wächter and Biegler [30]. It applies a primal-dual interior point (or barrier) method with a filter line-search method. One of the central underlying methods in nonlinear programming, which is part of IPOPT and which we also apply directly in our solution approach, are the Karush-Kuhn-Tucker (KKT) conditions. Under certain additional assumptions they provide necessary conditions for a (local) optimum. For a nonlinear optimization problem of the form  $\min\{f(x) : g_i(x) \leq 0, h_j(x) = 0, x \in \mathbb{R}^n\}$ , where  $f$  is the objective function,  $g_i$  ( $i = 1, \dots, m$ ) are continuously differentiable inequality constraint functions and  $h_j$  ( $j = 1, \dots, \ell$ ) are continuously differentiable equality constraint functions, the KKT system reads as follows

$$\nabla f(x^*) + \sum_{i=1}^m \lambda_i \nabla g_i(x^*) + \sum_{j=1}^{\ell} \mu_j \nabla h_j(x^*) = 0, \quad (3.1a)$$

$$g_i(x^*) \leq 0, \quad \forall i = 1, \dots, m, \quad (3.1b)$$

$$h_j(x^*) = 0, \quad \forall j = 1, \dots, \ell, \quad (3.1c)$$

$$\lambda_i \geq 0, \quad \forall i = 1, \dots, m, \quad (3.1d)$$

$$\lambda_i g_i(x^*) = 0, \quad \forall i = 1, \dots, m, \quad (3.1e)$$

where  $x^*$  is a local minimum, and  $\lambda_i$  ( $i = 1, \dots, m$ ),  $\mu_j$  ( $j = 1, \dots, \ell$ ) are constants (called KKT multipliers). The existence of these constants is guaranteed if  $x^*$  satisfies some regularity conditions (to be discussed later). In the special case of  $m = 0$ , i.e., no inequality constraints exist, the KKT multipliers are also called Lagrange multipliers. For more details we refer to Conn, Gould, and Toint [8].

## 4 Topology Optimization of Transmission Networks

In the following we describe a mixed-integer nonlinear model for the extension problem in a transmission network. Our model integrates two features: if the set of potential extensions is empty, it can be used to determine if a configuration of all active elements is possible such that all physical, technical, and contractual constraints are fulfilled. For a non-empty set of potential extensions it can be used to find a subset of extensions having minimal cost and allowing a feasible flow. To this end, the model must be solved numerically with a solving technique that has the potential to give a certificate for optimality, or to prove that no solution exists. The details of our solution technique will be subject of the following sections.

### 4.1 The Model

We use the following notation for sets. A transmission network is modeled by a directed graph  $G = (V, E)$  where  $V$  denotes the set of nodes and  $E \subseteq V \times V$  the set of arcs. We define an extended set of arcs  $E_X \subseteq V \times V \times \mathbb{N}_0$  where each arc  $(v, w, i) \in E_X$  represents the arc  $e = (v, w) \in V \times V$  together with index  $i$ .

This set  $E_X$  contains all “original” arcs from  $E$  with index 1, that is,  $(e, 1) \in E_X$  for all  $e \in E$ . Arcs  $e \in E$  that represent preexisting valves are *additionally* represented by the arc  $(e, 0) \in E_X$  (to indicate the status that the valve is closed). For valves we set  $\alpha_{e,1} = \beta_{e,1} = 0$ .

Furthermore, set  $E_X$  contains potential new network elements (pipes, valves, compressors, or control valves), where a new element can in principle be built between any pair of existing nodes  $v, w \in V, v \neq w$ . A potential extension between nodes  $v$  and  $w$  is represented by at least two arcs:  $(v, w, 0)$  (to indicate in the model below that the element is not erected) and  $(v, w, i)$  for  $i \in \{2, 3, \dots\}$  (to indicate that different design parameters can be selected for the new element).

By  $G_X := (V, E_X)$  we denote the transmission network together with its potential extensions. Note that  $G_X$  is a graph with multiple parallel arcs, i.e., a multigraph.

We assume the following data to be given as parameters. For each node  $v \in V$  we have lower and upper bounds on the node potential,  $\underline{\pi}_v, \bar{\pi}_v \in \mathbb{R}$  with  $\underline{\pi}_v \leq \bar{\pi}_v$ . For each arc  $(e, i) \in E_X$  we have lower and upper bounds on the flow,  $\underline{q}_{e,i}, \bar{q}_{e,i} \in \mathbb{R}$  with  $\underline{q}_{e,i} \leq \bar{q}_{e,i}$ . For each node  $v \in V$  the value  $s_v \in \mathbb{R}$  denotes the amount of flow that is either led into the network (for  $s_v > 0$ ), or taken out of the network (for  $s_v < 0$ ). A node with  $s_v > 0$  is also called source or entry node, and nodes with  $s_v < 0$  are sinks or exit nodes. All other nodes with  $s_v = 0$  are inner or transmission nodes. Vector  $s$  is also called *nomination*. In order not to pose a problem that is trivially infeasible, only those nominations are allowed that have matching entry and exit flows, that is,

$$\sum_{v \in V} s_v = 0. \quad (4.1)$$

Such nominations are said to be *balanced*. For each arc  $(e, i) \in E_X$  we have a transmission coefficient  $\alpha_{e,i} \in \mathbb{R}_+$ , bounds on the weighted slack variable  $\underline{y}_{e,i}, \bar{y}_{e,i} \in \mathbb{R}$  with  $\underline{y}_{e,i} \leq \bar{y}_{e,i}$ , a scaling factor  $\beta_{e,i}$  for the range coefficient, a coefficient  $\gamma_e \in \mathbb{R} \setminus \{0\}$ , and a cost coefficient  $c_{e,i} \in \mathbb{R}_+$ . Note that  $c_{e,1} = 0$  for all existing arcs  $e \in E$  and  $c_{e,0} = 0$  for every preexisting valve  $e$ .

Let us introduce the following variables. The flow on arc  $(e, i) \in E_X, i \neq 0$  is denoted by  $q_{e,i} \in \mathbb{R}$ , where a positive value means the flow is heading in the same direction as the arc, and a negative value indicates the opposite direction. The potential value of a vertex  $v \in V$  is given by  $\pi_v \in \mathbb{R}$ . For example, in a gas transmission network this variable refers to the squared pressure in this node. The variable  $y_{e,i} \in \mathbb{Z}$  specifies that additive component of the pressure loss term in (2.3). For passive pipelines this variable is fixed to zero, whereas for active elements it defines the operating range. We remark that we define this as being an integer variable (and not a continuous, real valued variable). Because of this discretization, the cuts we derive in the following will become classical linear inequalities. For a continuous variable, these cuts would be nonlinear in  $\beta_{e,i} y_{e,i}$ , hence we would no longer be able to apply a linear programming based branch-and-cut approach.

We introduce a binary decision variable  $x_{e,i} \in \{0, 1\}$  for each arc  $(e, i) \in E_X$ , where  $x_{e,i} = 1$  represents the decision that arc  $(e, i)$  is used (i.e., a necessary condition for a non-zero flow).

In Figure 4.1 we show a small example network to demonstrate our notation. In the left part 4.1a, the original network  $(V, E)$  is shown. In the middle part 4.1b of the figure, the arc flow and node potential variables are shown. The right part 4.1c of the figure shows the decision variables  $x$ . Simple arcs, such as  $(2, 1), (5, 1), (6, 1)$  which correspond to the original arcs 2, 5 and 6 represent passive pipelines of the network. In particular, these pipelines do not carry active elements (such as valves), and are also not extendible via loops, i.e., by adding parallel pipes. A pipe with a valve is shown in arc pair  $(4, 0), (4, 1)$ . Note that there is **no** flow variable  $q_{4,0}$ . Such arc pair could also represent a control valve or a compressor station, depending on the actual definition of the parameters  $k_e$  and  $\beta_{e,i}$  for arc  $(e, i)$ . Multiple arcs such as  $(1, 1), (1, 2)$  and  $(3, 1), (3, 2), (3, 3)$  represent each a passive pipeline (which is  $(1, 1)$  and  $(3, 1)$ , respectively), together with one or two possible loop extensions, respectively.

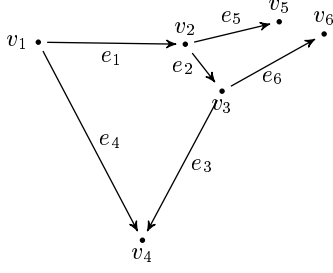
The following nonlinear non-convex mixed-integer program with indicator constraints is called topology optimization problem:

$$\min \sum_{(e,i) \in E_X} c_{e,i} x_{e,i} \quad \text{s. t.} \quad (4.2a)$$

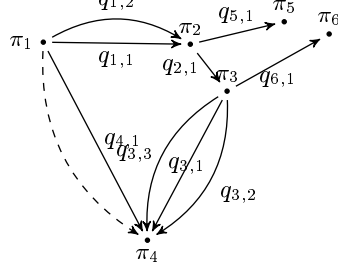
$$x_{e,i} = 1 \Rightarrow \alpha_{e,i} q_{e,i} |q_{e,i}|^{k_e} + \beta_{e,i} y_{e,i} - (\pi_v - \gamma_e \pi_w) = 0 \quad \forall (e, i) \in E_X, i \neq 0, \quad (4.2b)$$

$$x_{e,i} = 0 \Rightarrow q_{e,i} = 0 \quad \forall (e, i) \in E_X, i \neq 0, \quad (4.2c)$$

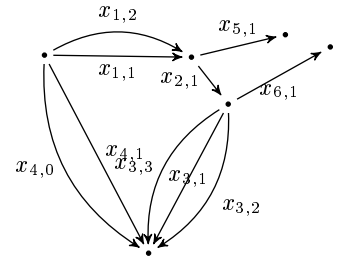




(a) Original network.



(b) Arc flow and node potential variables.



(c) Discrete (switching) variables.

Fig. 4.1: Example for a network.

$$x_{e,i} = 0 \Rightarrow y_{e,i} = 0 \quad \forall (e,i) \in E_X, i \neq 0, \quad (4.2d)$$

$$\sum_{i:(v,w,i) \in E_X} x_{e,i} = 1 \quad \forall e \in E, \quad (4.2e)$$

$$\sum_{\substack{w, i: (v,w,i) \in E_X \\ i \neq 0}} q_{v,w,i} - \sum_{\substack{w, i: (w,v,i) \in E_X \\ i \neq 0}} q_{w,v,i} = s_v \quad \forall v \in V, \quad (4.2f)$$

$$\pi_v \leq \bar{\pi}_v \quad \forall v \in V, \quad (4.2g)$$

$$\pi_v \geq \underline{\pi}_v \quad \forall v \in V, \quad (4.2h)$$

$$q_{e,i} \leq \bar{q}_{e,i} \quad \forall (e,i) \in E_X, i \neq 0, \quad (4.2i)$$

$$q_{e,i} \geq \underline{q}_{e,i} \quad \forall (e,i) \in E_X, i \neq 0, \quad (4.2j)$$

$$x_{e,i} = 1 \Rightarrow y_{e,i} \leq \bar{y}_{e,i} \quad \forall (e,i) \in E_X, i \neq 0, \quad (4.2k)$$

$$x_{e,i} = 1 \Rightarrow y_{e,i} \geq \underline{y}_{e,i} \quad \forall (e,i) \in E_X, i \neq 0, \quad (4.2l)$$

$$x_{e,i} \leq 1 \quad \forall (e,i) \in E_X, \quad (4.2m)$$

$$x_{e,i} \geq 0 \quad \forall (e,i) \in E_X, \quad (4.2n)$$

$$q_{e,i} \in \mathbb{R} \quad \forall (e,i) \in E_X, i \neq 0, \quad (4.2o)$$

$$y_{e,i} \in \mathbb{Z} \quad \forall (e,i) \in E_X, i \neq 0, \quad (4.2p)$$

$$x_{e,i} \in \mathbb{Z} \quad \forall (e,i) \in E_X. \quad (4.2q)$$

The objective function (4.2a) calculates the extension costs for those new pipes that are actually built. The indicator constraints (4.2b) are switching on only those pressure-flow coupling constraints for potential arcs that are actually built. The indicator constraints (4.2c) forbid flow on those arcs that are not used, that is, they are either not built or switched off by a closed valve. These indicator constraints are handled by our numerical solver SCIP by a special purpose constraint handler. Hence it is not necessary to reformulate by, for example, big- $M$ -constraints and further binary variables. Exactly one pressure loss constraint (4.2b) must be selected which is guaranteed by constraints (4.2e). Note that if  $(v,w) \in E$ , that is, nodes  $v$  and  $w$  are already connected in the original network, then the selection of an extension will automatically switch off (or overwrite) the existing connection. If  $e \in E$  is a valve, then the closed mode ( $x_{e,0} = 1$ ) implies ( $x_{e,1} = 0$ ) and zero flow is ensured by constraint (4.2c). The node flow conservation constraints (also called Kirchhoff's constraints) are defined in (4.2f). Constraints (4.2g) – (4.2n) define the trivial bounds on the variables, and constraints (4.2o) – (4.2q) specify the continuous or discrete range of the variables.

For a given nomination  $s$ , the topology optimization problem (4.2) is to find a cost optimal selection of pipe capacities for the transmission of the specific flow  $s$  in the transmission network  $G_X$ . Otherwise, if this transport is not possible for any selection of pipe capacities, the nomination is infeasible.

## 4.2 Outline of Our Method

We give an outline of our method here. The details are given in the following sections. In order to solve the topology optimization problem above we apply a standard branch-and-cut approach, where the subproblems at the nodes of the branching tree are solved by linear or nonlinear programming methods. The numerical solver SCIP takes control of the decisions which variable to select for branching, which cut to add, and in which order the open problems (nodes of the branching tree) are selected. For the reader's convenience, we give a brief outline of this procedure below. If the reader is familiar with the method, the remainder of this paragraph can be skipped.

Initially, at the root node of the tree, we consider the linear relaxation of (4.2). This relaxation is obtained by relaxing all binary decision variables (for active elements and for topology extension measures) to their continuous counterparts, and by replacing the nonlinear pressure-flow coupling constraints (4.2b) by initially coarse outer linear approximations. The relaxation is solved by Dantzig's simplex algorithm, and further cutting planes are added by standard routines of the solver (such as Gomory cuts, mixed-integer rounding cuts, and others). Further cuts are also generated by the constraint handler for the nonlinear constraints, if necessary, to strengthen the outer approximation in the convex parts of the nonlinear function.

When no further cuts are added, the root LP solution is usually neither integral nor fulfilling the nonlinearities. We then start branching on  $x$  and  $y$ , that is, we select a fractional variable which is required to be binary or integral, and split the problem into two subproblems: in the one we fix it to the next integer value lower than the LP solution of the variable, and in the other we fix it to the next upper integer value. In this way we obtain two linear subproblems out of one. It is important to remark that we only branch on discrete variables such that no spatial branching is performed. These subproblems are further strengthened by standard integrality cuts and by outer approximation cuts. At this point, also the new cuts presented in this article are invoked and (globally) added to the model. The subproblems are all linear programs, and thus can still be solved by the simplex algorithm. This way of branching creates a tree of subproblems, where the leaves are in generally still not feasible solutions for the initial problem (4.2) as the nonlinearities might not be fulfilled.

## 5 Inequalities for a Leaf Problem

When solving problem (4.2) within a branch-and-cut framework, the solver will iteratively branch on binary and integer decision variables, as well as spatial branching on continuous variables. After some number of subsequent branches, all integer and binary variables are fixed. We consider such a node. Since all discrete decisions are settled, also  $y_{e,i}$  is fixed to some integer value. We set  $\tilde{\beta}_{e,i} := \beta_{e,i} y_{e,i}$ . Throughout this section,  $E'$  contains all arcs where the flow is not fixed to zero, i.e.,  $E' = \{(e, i) \in E_X \mid x_{e,i} = 1\}$ . Note that for each family of arc  $(e, i)$ , exactly one  $i$  is chosen. Hence as an abbreviation we omit the subscript  $i$  and simply write as abbreviation  $q_e$  instead of  $q_{e,i}$ . As further abbreviations we set  $\delta^+(v) := \{(v, w) \in E'\}$  and  $\delta^-(v) := \{(w, v) \in E'\}$  for  $v \in V$ . The remaining problem, which might still be infeasible with respect to the nonlinear constraints, then is the following:

$$\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e - (\pi_v - \gamma_e \pi_w) = 0 \quad \forall e = (v, w) \in E', \quad (5.1a)$$

$$\sum_{e \in \delta^+(v)} q_e - \sum_{e \in \delta^-(v)} q_e = s_v \quad \forall v \in V, \quad (5.1b)$$

$$\pi_v \leq \bar{\pi}_v \quad \forall v \in V, \quad (5.1c)$$

$$\pi_v \geq \underline{\pi}_v \quad \forall v \in V, \quad (5.1d)$$

$$q_e \leq \bar{q}_e \quad \forall e \in E', \quad (5.1e)$$

$$q_e \geq \underline{q}_e \quad \forall e \in E', \quad (5.1f)$$

$$\pi_v \in \mathbb{R} \quad \forall v \in V, \quad (5.1g)$$

$$q_e \in \mathbb{R} \quad \forall e \in E'. \quad (5.1h)$$

This problem (5.1) will be referred to as *leaf problem* in the following. We define a relaxation of the leaf problem (5.1), called *domain relaxation problem*, as follows:

$$\min \sum_{v \in V} \Delta_v + \sum_{e \in E'} \Delta_e \quad \text{s. t.}$$

$$\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e - (\pi_v - \gamma_e \pi_w) = 0 \quad \forall e = (v, w) \in E', \quad (5.2a)$$

$$\sum_{e \in \delta^+(v)} q_e - \sum_{e \in \delta^-(v)} q_e = s_v \quad \forall v \in V, \quad (5.2b)$$

$$\pi_v - \Delta_v \leq \bar{\pi}_v \quad \forall v \in V, \quad (5.2c)$$

$$\pi_v + \Delta_v \geq \underline{\pi}_v \quad \forall v \in V, \quad (5.2d)$$

$$q_e - \Delta_e \leq \bar{q}_e \quad \forall e \in E', \quad (5.2e)$$

$$q_e + \Delta_e \geq \underline{q}_e \quad \forall e \in E', \quad (5.2f)$$

$$\pi_v \in \mathbb{R} \quad \forall v \in V, \quad (5.2g)$$

$$q_e \in \mathbb{R} \quad \forall e \in E', \quad (5.2h)$$

$$\Delta_v \in \mathbb{R}_+ \quad \forall v \in V, \quad (5.2i)$$

$$\Delta_e \in \mathbb{R}_+ \quad \forall e \in E'. \quad (5.2j)$$

In the following we describe how to obtain a valid inequality for our leaf problem (5.1) from a KKT point of the domain relaxation problem (5.2). We write  $\Phi_e(q_e) := \alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e$  and define the Lagrangian of problem (5.2) as

$$\begin{aligned} L(q, \pi, \Delta, \mu, \lambda) &= \sum_{v \in V} \Delta_v + \sum_{e \in E'} \Delta_e \\ &+ \sum_{e=(v,w) \in E'} \mu_e (\Phi_e(q_e) - (\pi_v - \gamma_e \pi_w)) \\ &+ \sum_{v \in V} \mu_v \left( s_v - \sum_{e \in \delta^+(v)} q_e + \sum_{e \in \delta^-(v)} q_e \right) \\ &+ \sum_{v \in V} (\lambda_v^+ (\pi_v - \Delta_v - \bar{\pi}_v) + \lambda_v^- (\underline{\pi}_v - \pi_v - \Delta_v)) \\ &+ \sum_{e \in E'} (\lambda_e^+ (q_e - \Delta_e - \bar{q}_e) + \lambda_e^- (\underline{q}_e - q_e - \Delta_e)) \\ &- \sum_{v \in V} \lambda_v \Delta_v - \sum_{e \in E'} \lambda_e \Delta_e. \end{aligned}$$

For a local optimum of a nonlinear problem it is shown by Boyd and Vandenberghe [6] that there exist values for these dual variables fulfilling the KKT conditions. From these KKT conditions we derive the following constraints, c.f. equation system (3.1):

$$\frac{\partial L}{\partial q_e} : \quad \mu_e (\nabla_{q_e} \Phi_e(q_e)) + \lambda_e^+ - \lambda_e^- = \mu_v - \mu_w \quad \forall e = (v, w) \in E', \quad (5.3a)$$

$$\frac{\partial L}{\partial \pi_v} : \quad \sum_{e \in \delta^+(v)} \mu_e - \sum_{e \in \delta^-(v)} \mu_e \gamma_e = \lambda_v^+ - \lambda_v^- \quad \forall v \in V, \quad (5.3b)$$

$$\frac{\partial L}{\partial \Delta_v} : \quad \lambda_v^+ + \lambda_v^- + \lambda_v = 1 \quad \forall v \in V, \quad (5.3c)$$

$$\frac{\partial L}{\partial \Delta_e} : \quad \lambda_e^+ + \lambda_e^- + \lambda_e = 1 \quad \forall e \in E'. \quad (5.3d)$$

From this we conclude:

$$\pi_v < \bar{\pi}_v \Rightarrow \lambda_v^+ = 0, \quad \pi_v = \bar{\pi}_v \Rightarrow 0 \leq \lambda_v^+ \leq 1, \quad \pi_v > \bar{\pi}_v \Rightarrow \lambda_v^+ = 1 \quad \forall v \in V, \quad (5.4a)$$

$$\pi_v > \underline{\pi}_v \Rightarrow \lambda_v^- = 0, \quad \pi_v = \underline{\pi}_v \Rightarrow 0 \leq \lambda_v^- \leq 1, \quad \pi_v < \underline{\pi}_v \Rightarrow \lambda_v^- = 1 \quad \forall v \in V, \quad (5.4b)$$

$$q_e < \bar{q}_e \Rightarrow \lambda_e^+ = 0, \quad q_e = \bar{q}_e \Rightarrow 0 \leq \lambda_e^+ \leq 1, \quad q_e > \bar{q}_e \Rightarrow \lambda_e^+ = 1 \quad \forall e \in E', \quad (5.4c)$$

$$q_e > \underline{q}_e \Rightarrow \lambda_e^- = 0, \quad q_e = \underline{q}_e \Rightarrow 0 \leq \lambda_e^- \leq 1, \quad q_e < \underline{q}_e \Rightarrow \lambda_e^- = 1 \quad \forall e \in E'. \quad (5.4d)$$

Constraint (5.3b) is the basis for the inequalities that we derive in this section. Therefore we give the following definition:

**Definition 1.** Every vector  $(\mu, \lambda) = (\mu_v, \mu_e, \lambda_v^+, \lambda_v^-, \lambda_e^+, \lambda_e^-)_{v \in V, e \in E}$ , such that  $\mu_v, \mu_e \in \mathbb{R}$  and  $\lambda_v^+, \lambda_v^-, \lambda_e^+, \lambda_e^- \in \mathbb{R}_{\geq 0}$ , which fulfills the constraints

$$\sum_{e \in E} \mu_e - \sum_{e \in E} \gamma_e \mu_e = \lambda_v^+ - \lambda_v^- \quad \forall v \in V, \quad (5.5)$$

is called **dual transmission flow**. This dual transmission flow is always a flow in the original network  $(V, E)$ .

### 5.1 A Nonlinear Inequality

In the next two lemmas we will give two different inequalities for a leaf problem. The first one is derived from a dual transmission flow.

**Lemma 1.** If the leaf problem (5.1) is feasible, then for any dual transmission flow  $(\mu, \lambda)$  with  $\mu_e = 0$  for all arcs  $e \notin E'$ , the inequality

$$\sum_{e \in E'} \mu_e (\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e) \leq \sum_{v \in V} (\lambda_v^+ \bar{\pi}_v - \lambda_v^- \underline{\pi}_v)$$

is valid.

Proof: We multiply equation (5.2a) by  $\mu_e$  and sum over all  $e \in E'$  to obtain

$$\sum_{e \in E'} \mu_e (\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e) = \sum_{e=(v,w) \in E'} \mu_e (\pi_v - \gamma_e \pi_w).$$

We rewrite the right-hand side by changing the order of summation and obtain

$$\sum_{e=(v,w) \in E'} \mu_e (\pi_v - \gamma_e \pi_w) = \sum_{v \in V} \pi_v \left( \sum_{e \in \delta_{E'}^+(v)} \mu_e - \sum_{e \in \delta_{E'}^-(v)} \gamma_e \mu_e \right).$$

Note that all arcs in  $e \in E \setminus E'$  have  $\mu_e = 0$ , hence they can be added:

$$\sum_{v \in V} \pi_v \left( \sum_{e \in \delta_{E'}^+(v)} \mu_e - \sum_{e \in \delta_{E'}^-(v)} \gamma_e \mu_e \right) = \sum_{v \in V} \pi_v \left( \sum_{e \in \delta_E^+(v)} \mu_e - \sum_{e \in \delta_E^-(v)} \gamma_e \mu_e \right).$$

We use equation (5.5) in Definition 1 of a dual transmission flow and obtain

$$\sum_{v \in V} \pi_v \left( \sum_{e \in \delta_E^+(v)} \mu_e - \sum_{e \in \delta_E^-(v)} \gamma_e \mu_e \right) = \sum_{v \in V} \pi_v (\lambda_v^+ - \lambda_v^-).$$

We estimate the right-hand side as follows:

$$\sum_{v \in V} \pi_v (\lambda_v^+ - \lambda_v^-) \leq \sum_{v \in V} (\lambda_v^+ \bar{\pi}_v - \lambda_v^- \underline{\pi}_v).$$

Putting these reformulations together we derive

$$\sum_{e \in E'} \mu_e (\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e) \leq \sum_{v \in V} (\lambda_v^+ \bar{\pi}_v - \lambda_v^- \underline{\pi}_v).$$

□

Before we go on with the next lemma, we give some definitions. We assume that a root node  $r \in V$  is selected, and further that each node  $v \in V$  is reachable from  $r$  on a directed path. Note that this property of the graph is obtained by reorienting some arcs if necessary. Denote by  $P_r(v)$  a path from  $r$  to  $v$ . Then we define  $\gamma_{r,v} := \prod_{e \in P_r(v)} \gamma_e$ . This definition is independent from the actual path  $P_r(v)$ , because on a cycle the product of  $\gamma_e$  equals 1 (c.f. Section 2.1). Using this value  $\gamma_{r,v}$  we define

$$\pi'_v(\pi) := \gamma_{r,v} \pi_v$$

It follows from elementary calculations that

$$\pi'_v(\pi) - \pi'_w(\pi) = \gamma_{r,v} (\pi_v - \gamma_e \pi_w) \quad (5.6)$$

holds for each arc  $e = (v, w) \in E'$ . As a trivial consequence we obtain lower and upper bounds of  $\pi'_v(\pi)$  by  $\underline{\pi}'_v := \pi'_v(\underline{\pi})$  and  $\bar{\pi}'_v := \pi'_v(\bar{\pi})$  respectively.

Let  $q$  be a network flow in  $(V, E)$ . In the next lemma and the ongoing section we will consider this flow as a network flow in  $(V, E')$  by setting  $q_{e,i} := q_e$  for every arc  $(e, i) \in E'$ .

**Lemma 2.** *If the leaf problem (5.1) is feasible, then for any  $q^*$  being a primal flow in  $E$ , and any slack values  $\Delta_v^\pm \geq 0$  for each node  $v \in V$  such that the flow conservation*

$$\sum_{e \in \delta_{E'}^+(v)} q_e^* - \sum_{e \in \delta_{E'}^-(v)} q_e^* - (\Delta_v^+ - \Delta_v^-) = s_v,$$

*is fulfilled, then the inequality*

$$\sum_{e=(v,w) \in E'} \gamma_{r,v} (q_e - q_e^*) (\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e) \leq \sum_{v \in V} (\Delta_v^- \bar{\pi}'_v - \Delta_v^+ \underline{\pi}'_v)$$

*is valid.*

Proof: We note that  $q_e$  for all  $e \in E'$  is a feasible flow from the sources to the sinks in the network, i.e.,

$$\sum_{e \in \delta_{E'}^+(v)} q_e - \sum_{e \in \delta_{E'}^-(v)} q_e = s_v$$

for all nodes  $v \in V$ . From this we derive

$$\sum_{e \in \delta_{E'}^+(v)} (q_e - q_e^*) - \sum_{e \in \delta_{E'}^-(v)} (q_e - q_e^*) = \Delta_v^- - \Delta_v^+$$

for all nodes  $v \in V$ . We multiply each side by  $\pi'_v(\pi)$ , take the sum over all nodes  $v \in V$  and obtain:

$$\sum_{e=(v,w) \in E'} (q_e - q_e^*) (\pi'_v(\pi) - \pi'_w(\pi)) = \sum_{v \in V} \pi'_v(\pi) (\Delta_v^- - \Delta_v^+) \leq \sum_{v \in V} (\bar{\pi}'_v \Delta_v^- - \underline{\pi}'_v \Delta_v^+).$$

The last estimation is obtained by taking the lower and upper bounds on  $\pi'_v(\pi)$  into account. We use this estimation to obtain from (5.1a) and (5.6)

$$\sum_{e=(v,w) \in E'} \gamma_{r,v} (q_e - q_e^*) (\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e) = \sum_{e=(v,w) \in E'} (q_e - q_e^*) \gamma_{r,v} (\pi_v - \gamma_e \pi_w)$$

$$= \sum_{e=(v,w) \in E'} (q_e - q_e^*)(\pi'_v(\pi) - \pi'_w(\pi)) \leq \sum_{v \in V} (\bar{\pi}'_v \Delta_v^- - \underline{\pi}'_v \Delta_v^+).$$

□

Now we consider a linear combination of both inequalities from the previous two Lemmas:

**Corollary 1.** *Assume that the leaf problem (5.1) is feasible. Let  $(\mu, \lambda)$  be dual transmission flow with  $\mu_e = 0$  for all arcs  $e \notin E'$ . Let  $q^*$  be a primal flow in  $E$ , and let  $\Delta_v^\pm \geq 0$  be slack values for each node  $v \in V$  such that the flow conservation*

$$\sum_{e \in \delta_{E'}^+(v)} q_e^* - \sum_{e \in \delta_{E'}^-(v)} q_e^* - (\Delta_v^+ - \Delta_v^-) = s_v,$$

is fulfilled. Then for any  $\zeta \in [0, 1]$  the inequality

$$\begin{aligned} & \sum_{e=(v,w) \in E'} (\zeta \gamma_{r,v} (q_e - q_e^*) + (1 - \zeta) \mu_e) (\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e) \\ & \leq \zeta \sum_{v \in V} (\Delta_v^- \bar{\pi}'_v - \Delta_v^+ \underline{\pi}'_v) + (1 - \zeta) \sum_{v \in V} (\lambda_v^+ \bar{\pi}_v - \lambda_v^- \underline{\pi}_v) \end{aligned} \quad (5.7)$$

is valid.

Proof: The inequality is a linear combination of the inequalities from Lemma 1 and Lemma 2. □

## 5.2 A Linear Inequality for the Leaf Problem

So far we derived in Corollary 1 a nonlinear inequality which is valid for a leaf problem. In principle, it would be possible to add this inequality to the MINLP model formulation of (4.2), and let the solver SCIP do the work (adding cuts and spatial branching). Nevertheless, in the following, we describe how to derive a linear inequality that can also be used in our linear programming based branch-and-cut framework. Our proposed method has the advantage that we can use this inequality not only locally (for the subtree), but derive a globally valid cut (for the entire tree) in the next Section 5.3.

We will derive a certain linear underestimator for the left-hand side of inequality (5.7) in Corollary 1. This left-hand side is a sum of functions in  $q_e$  for arcs  $e \in E'$ . We consider each of these functions separately and give a linear underestimator. This underestimator will be a function of the following form

$$q_e \mapsto \text{const} + \zeta \gamma_{r,v} (\pi_v^* - \gamma_e \pi_w^*) q_e + (1 - \zeta) (\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-) q_e.$$

for an arc  $e = (v, w) \in E'$ . Using this underestimator, inequality (5.7) rewrites as follows:

**Lemma 3.** *Assume that the leaf problem (5.1) is feasible. Let  $(\mu, \lambda)$  be dual transmission flow with  $\mu_e = 0$  for all arcs  $e \notin E'$ . Let  $q^*$  be a primal flow in  $E$ , and let  $\Delta_v^\pm \geq 0$  be slack values for each node  $v \in V$  such that the flow conservation*

$$\sum_{e \in \delta_{E'}^+(v)} q_e^* - \sum_{e \in \delta_{E'}^-(v)} q_e^* - (\Delta_v^+ - \Delta_v^-) = s_v$$

is fulfilled for each node  $v \in V$ . Furthermore, let  $\pi^*$  be a vector of potential values for each node  $v \in V$  and let  $\zeta \in [0, 1]$ . Then there exists a constant  $\tau_e = \tau_e(\zeta, \alpha_e, \tilde{\beta}_e, q^*, \pi^*, \mu, \lambda)$  for  $e \in E'$  such that the inequality

$$\begin{aligned} & \sum_{e \in E'} \tau_e \leq \zeta \left( \sum_{v \in V} (\Delta_v^- \bar{\pi}'_v - \Delta_v^+ \underline{\pi}'_v) - \sum_{v \in V} s_v \pi'_v(\pi^*) \right) \\ & + (1 - \zeta) \left( \sum_{v \in V} (\lambda_v^+ \bar{\pi}_v - \lambda_v^- \underline{\pi}_v) + \sum_{e \in E'} (\lambda_e^+ \bar{q}_e - \lambda_e^- \underline{q}_e) - \sum_{v \in V} s_v \mu_v \right) \end{aligned} \quad (5.8)$$

is valid.

We remark that the unfixed variables in the leaf problem are flow variables  $q$  and node potentials  $\pi$ . These variables are not contained in inequality (5.8). Thus inequality (5.8) is constant on both sides, left- and right-hand side. If the inequality is violated, the leaf problem is infeasible.

Proof: We define the constant  $\tau_e = \tau_e(\zeta, \alpha_e, \tilde{\beta}_e, q^*, \pi^*, \mu, \lambda)$  for each arc  $e = (v, w) \in E'$  as follows:

$$\begin{aligned} \tau_e(\zeta, \alpha_e, \tilde{\beta}_e, q^*, \pi^*, \mu, \lambda) := & \min_{\underline{q}_e \leq q_e \leq \bar{q}_e} \{ (\zeta \gamma_{r,v}(q_e - q_e^*) + (1 - \zeta)\mu_e) (\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e) \\ & - \zeta \gamma_{r,v}(\pi_v^* - \gamma_e \pi_w^*) q_e - (1 - \zeta)(\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-) q_e \}. \end{aligned}$$

We consider inequality (5.7) of Corollary 1. By the definition of  $\tau_e$  we obtain the underestimator for each summand on the left-hand side as

$$\begin{aligned} & (\zeta \gamma_{r,v}(q_e - q_e^*) + (1 - \zeta)\mu_e) (\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e) \\ \geq & \tau_e + \zeta \gamma_{r,v}(\pi_v^* - \gamma_e \pi_w^*) q_e + (1 - \zeta)(\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-) q_e. \end{aligned}$$

We rewrite the underestimator. Each primal solution  $q$  fulfills the flow conservation constraint

$$\sum_{e \in \delta_{E'}^+(v)} q_e - \sum_{e \in \delta_{E'}^-(v)} q_e = s_v.$$

Multiplying this equation with  $\pi'_v(\pi^*)$  and summing over the nodes  $v \in V$  we obtain

$$\zeta \sum_{e=(v,w) \in E'} (\pi'_v(\pi^*) - \pi'_w(\pi^*)) q_e = \zeta \sum_{v \in V} s_v \pi'_v(\pi^*) \quad (5.9)$$

and multiplying it with  $\mu_v$  and summing over the nodes  $v \in V$  we derive

$$(1 - \zeta) \sum_{e=(v,w) \in E'} (\mu_v - \mu_w) q_e = (1 - \zeta) \sum_{v \in V} s_v \mu_v. \quad (5.10)$$

Using the reformulations (5.6), (5.9), (5.10) we obtain

$$\sum_{e=(v,w) \in E'} (\zeta \gamma_{r,v}(q_e - q_e^*) + (1 - \zeta)\mu_e) (\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e) \quad (5.11a)$$

$$\geq \sum_{e \in E'} \tau_e + \zeta \sum_{v \in V} s_v \pi'_v(\pi^*) + (1 - \zeta) \sum_{v \in V} s_v \mu_v - (1 - \zeta) \sum_{e \in E'} (\lambda_e^+ - \lambda_e^-) q_e. \quad (5.11b)$$

We apply inequality (5.7) of Corollary 1 to the left-hand side (5.11a) in order to obtain an upper estimation. Then we use the lower and upper bounds on  $q_e$  to obtain

$$(1 - \zeta) \sum_{e \in E'} (\lambda_e^+ - \lambda_e^-) q_e \leq (1 - \zeta) \sum_{e \in E'} (\lambda_e^+ \bar{q}_e - \lambda_e^- \underline{q}_e),$$

which gives a lower estimation for the right-hand side (5.11b). Putting these two estimations together yields inequality (5.8).  $\square$

### 5.3 Feasibility Characterization for a Leaf Problem by a Linear Inequality

So far we derived an inequality (5.8) that does not contain the free variables of the leaf problem. The question that now arises is how to choose the parameter  $\zeta \in [0, 1]$  in order to obtain an inequality that represents the infeasibility of the leaf problem, i.e., we want to get an inequality that is violated if and only if the leaf problem is infeasible. First we show, that the inequality (5.8) is violated for a KKT point of the domain relaxation (5.2) for a suitable choice of  $\zeta$ .

In the sequel we will speak of *deriving a dual transmission flow* in  $(V, E)$  from a KKT point of the relaxation (5.2). This means that we consider a KKT point  $(q^*, \pi^*, \Delta^*, \mu^*, \lambda^*)$  of (5.2). Then the dual variables fulfill the dual flow conservation

$$\sum_{e \in \delta_{E'}^+(v)} \mu_e^* - \sum_{e \in \delta_{E'}^-(v)} \mu_e^* \gamma_e = \lambda_v^{+*} - \lambda_v^{-*}$$

for all nodes  $v \in V$ . We obtain a dual transmission flow  $(\mu, \lambda)$  in  $(V, E)$  by setting  $\mu_v := \mu_v^*$  and  $\lambda_v^\pm := \lambda_v^{\pm*}$  for each node  $v \in V$  and  $\mu_e := \mu_e^*, \lambda_e^\pm := \lambda_e^{\pm*}$  if  $e \in E'$  and  $\mu_e := 0, \lambda_e^\pm := 0$  otherwise for each arc  $e \in E \setminus E'$ .

**Lemma 4.** *Consider a KKT point  $(q^*, \pi^*, \Delta^*, \mu^*, \lambda^*)$  of the domain relaxation (5.2). We derive a dual transmission flow  $(\mu, \lambda)$  with  $\mu_e = 0$  for all arcs  $e \notin E'$ . Assume that there exists a  $\zeta \in [0, 1[$  such that the minimum of the function*

$$\begin{aligned} q_e \mapsto & (\zeta \gamma_{r,v}(q_e - q_e^*) + (1 - \zeta)\mu_e)(\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e) \\ & - \zeta \gamma_{r,v}(\pi_v^* - \gamma_e \pi_w^*) q_e - (1 - \zeta)(\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-) q_e \end{aligned}$$

is attained for  $q_e^*$  for each arc  $e = (v, w) \in E'$ . Then for this value of  $\zeta$ , there exists  $\tau_e$  for each arc  $e \in E'$  such that inequality (5.8) is violated if and only if  $(q^*, \pi^*)$  is not feasible for the leaf problem (5.1). The violation (i.e., the absolute difference of the left-hand and the right-hand side of the inequality) equals  $(1 - \zeta)$  times the optimal objective value of the relaxation (5.2).

*Proof:* First we recall the definition of  $\tau_e = \tau_e(\zeta, \alpha_e, \tilde{\beta}_e, q^*, \pi^*, \mu, \lambda)$  from Lemma 3. If the minimum of the function

$$\begin{aligned} q_e \mapsto & (\zeta \gamma_{r,v}(q_e - q_e^*) + (1 - \zeta)\mu_e)(\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e) \\ & - \zeta \gamma_{r,v}(\pi_v^* - \gamma_e \pi_w^*) q_e - (1 - \zeta)(\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-) q_e \end{aligned}$$

is attained at  $q_e^*$ , then  $\sum_{e \in E'} \tau_e$  rewrites as follows:

$$\begin{aligned} \sum_{e \in E'} \tau_e &= \sum_{e=(v,w) \in E'} ((1 - \zeta)\mu_e(\alpha_e q_e^* |q_e^*|^{k_e} + \tilde{\beta}_e) - \zeta \gamma_{r,v}(\pi_v^* - \gamma_e \pi_w^*) q_e^*) \\ &\quad - \sum_{e=(v,w) \in E'} (1 - \zeta)(\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-) q_e^* \\ &= (1 - \zeta) \sum_{e \in E'} \mu_e(\alpha_e q_e^* |q_e^*|^{k_e} + \tilde{\beta}_e) - \zeta \sum_{v \in V} s_v \pi_v'(\pi^*) \\ &\quad - (1 - \zeta) \sum_{v \in V} s_v \mu_v + (1 - \zeta) \sum_{e \in E'} (\lambda_e^+ - \lambda_e^-) q_e^*. \end{aligned} \tag{5.12}$$

Since  $q_e^*$  realizes the nomination, we derive from

$$\sum_{e \in \delta_{E'}^+(v)} q_e^* - \sum_{e \in \delta_{E'}^-(v)} q_e^* - (\Delta_v^+ - \Delta_v^-) = s_v$$

for each node  $v \in V$ , that the slack variables are zero,  $\Delta_v^+ = \Delta_v^- = 0$ . Then inequality (5.8) reduces to

$$\begin{aligned} \sum_{e \in E'} \tau_e &\leq -\zeta \sum_{v \in V} s_v \pi_v'(\pi^*) \\ &\quad + (1 - \zeta) \left( \sum_{v \in V} (\lambda_v^+ \bar{\pi}_v - \lambda_v^- \underline{\pi}_v) + \sum_{e \in E'} (\lambda_e^+ \bar{q}_e - \lambda_e^- \underline{q}_e) - \sum_{v \in V} s_v \mu_v \right). \end{aligned} \tag{5.13}$$

Combining (5.12) with (5.13) results in

$$\begin{aligned} & (1 - \zeta) \sum_{e \in E'} \mu_e(\alpha_e q_e^* |q_e^*|^{k_e} + \tilde{\beta}_e) + (1 - \zeta) \sum_{e \in E'} (\lambda_e^+ - \lambda_e^-) q_e^* \\ & \leq (1 - \zeta) \sum_{v \in V} (\lambda_v^+ \bar{\pi}_v - \lambda_v^- \underline{\pi}_v) + (1 - \zeta) \sum_{e \in E'} (\lambda_e^+ \bar{q}_e - \lambda_e^- \underline{q}_e). \end{aligned} \tag{5.14}$$

To show that this inequality is violated if and only if  $(q^*, \pi^*)$  is infeasible for the leaf problem we proceed as follows. From the proof of Lemma 1 we obtain the equality

$$\sum_{e \in E'} \mu_e(\alpha_e q_e^* |q_e^*|^{k_e} + \tilde{\beta}_e) = \sum_{v \in V} (\lambda_v^+ - \lambda_v^-) \pi_v^*.$$



Constraints (5.4a) and (5.4b) are fulfilled by the dual variables. Thus it holds that  $\lambda_v^+ > 0$  if  $\pi_v \geq \bar{\pi}_v$  and  $\lambda_v^- > 0$  if  $\pi_v \leq \underline{\pi}_v$ . This implies

$$0 \leq \sum_{v \in V} (\lambda_v^+ - \lambda_v^-) \pi_v^* - \sum_{v \in V} (\lambda_v^+ \bar{\pi}_v - \lambda_v^- \underline{\pi}_v) = \sum_{v \in V} (\lambda_v^+ + \lambda_v^-) \Delta_v^*.$$

The right-hand side is strictly positive, if at least one node potential value  $\pi_v$  violates its bounds. Similarly the constraints (5.4c) and (5.4d) imply that  $\lambda_e^+ \geq 0$  if  $q_e \geq \bar{q}_e$  and  $\lambda_e^- \geq 0$  if  $q_e \leq \underline{q}_e$ . We obtain the inequality

$$0 \leq \sum_{e \in E'} (\lambda_e^+ - \lambda_e^-) q_e^* - \sum_{e \in E'} (\lambda_e^+ \bar{q}_e - \lambda_e^- \underline{q}_e) = \sum_{e \in E'} (\lambda_e^+ + \lambda_e^-) \Delta_e^*$$

which is strict, if at least one flow variable  $q_e$  violates its bounds. Thus (5.14) rewrites as

$$(1 - \zeta) \left( \sum_{v \in V} (\lambda_v^+ + \lambda_v^-) \Delta_v^* + \sum_{e \in E'} (\lambda_e^+ + \lambda_e^-) \Delta_e^* \right) \leq 0.$$

Now it follows from (5.4) that  $\lambda_v^+ + \lambda_v^- = 1$  if  $\Delta_v^* > 0$  and  $\lambda_e^+ + \lambda_e^- = 1$  if  $\Delta_e^* > 0$ . Thus we rewrite (5.14) as

$$(1 - \zeta) \left( \sum_{v \in V} \Delta_v^* + \sum_{e \in E'} \Delta_e^* \right) \leq 0.$$

It is violated if and only if the primal solution  $(q^*, \pi^*)$  is not feasible to the leaf problem (5.1). As (5.14) is a reformulation of (5.8), (5.8) is violated if and only if the primal solution  $(q^*, \pi^*)$  is not feasible to the leaf problem (5.1). This proves the Lemma.  $\square$

**Lemma 5.** *Let  $(q^*, \pi^*, \Delta^*, \mu^*, \lambda^*)$  be a KKT point of the relaxation (5.2). We derive a dual transmission flow  $(\mu, \lambda)$  with  $\mu_e := 0$  for all arcs  $e \notin E'$ . Let  $e = (v, w) \in E'$ . Select  $\zeta \in [0, 1]$  such that*

1. *if  $\mu_e q_e^* > 0$ , then  $\zeta \gamma_{r,v} |q_e^*| > (1 - \zeta) |\mu_e|$ ,*
2. *if  $\mu_e q_e^* < 0$ , then  $(1 - \zeta) |\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-| < \zeta \gamma_{r,v} |\pi_v^* - \gamma_e \pi_w^* - \tilde{\beta}_e|$ ,*
3. *if  $\mu_e q_e^* = 0$ , then  $(1 - \zeta) \mu_e = 0$ .*

*Then the minimum of the function*

$$\begin{aligned} q_e \mapsto & (\zeta \gamma_{r,v} (q_e - q_e^*) + (1 - \zeta) \mu_e) (\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e) \\ & - \zeta \gamma_{r,v} (\pi_v^* - \gamma_e \pi_w^*) q_e - (1 - \zeta) (\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-) q_e \end{aligned} \quad (5.15)$$

*is attained in  $q_e^*$ .*

**Proof:** We consider an arc  $e = (v, w) \in E'$  and write the derivative of function (5.15) as

$$\begin{aligned} q_e \mapsto & \zeta \gamma_{r,v} (k_e + 2) \alpha_e q_e |q_e|^{k_e} + \zeta \gamma_{r,v} \tilde{\beta}_e - (\zeta \gamma_{r,v} q_e^* - (1 - \zeta) \mu_e) (k_e + 1) \alpha_e |q_e|^{k_e} \\ & - \zeta \gamma_{r,v} (\pi_v^* - \gamma_e \pi_w^*) - (1 - \zeta) (\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-). \end{aligned}$$

We set  $q_e = q_e^*$  and obtain

$$\begin{aligned} & \gamma_{r,v} (\zeta (k_e + 2) \alpha_e q_e^* |q_e^*|^{k_e} - \zeta (k_e + 1) q_e^* \alpha_e |q_e^*|^{k_e} + \zeta \tilde{\beta}_e - \zeta (\pi_v^* - \gamma_e \pi_w^*)) \\ & + (1 - \zeta) \mu_e (k_e + 1) \alpha_e |q_e^*|^{k_e} - (1 - \zeta) (\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-) \\ = & \gamma_{r,v} (\zeta (\alpha_e q_e^* |q_e^*|^{k_e} + \tilde{\beta}_e) - \zeta (\pi_v^* - \gamma_e \pi_w^*)) + (1 - \zeta) \mu_e (k_e + 1) \alpha_e |q_e^*|^{k_e} - (1 - \zeta) (\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-) \\ & = 0 + 0. \end{aligned}$$

This implies, that function (5.15) has an extreme point for  $q_e = q_e^*$ . The question is, whether this point is a global minimum for the choice of  $\zeta$ . In the case that  $\alpha_e = 0$  it follows from (5.2a) and (5.3a) that function (5.15) is constant. This implies that  $q_e^*$  is a global minimum. To prove that the point is a global minimum for the case  $\alpha_e > 0$  we assume w.l.o.g. the arc  $e$  to be oriented such that  $\mu_e \geq 0$ . We write function (5.15) as  $f(q_e) - g(q_e)$  where  $f$  and  $g$  are defined by

$$f : q_e \mapsto (\zeta \gamma_{r,v} q_e + (1 - \zeta) \mu_e - \zeta \gamma_{r,v} q_e^*) \alpha_e q_e |q_e|^{k_e} + ((1 - \zeta) \mu_e - \zeta q_e^*) \tilde{\beta}_e$$

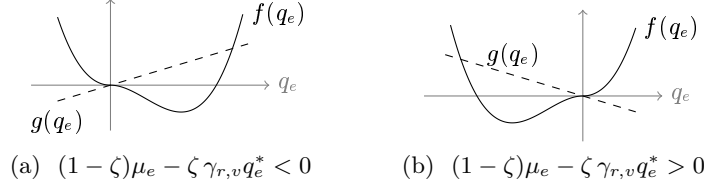


Fig. 5.1: Visualization of the functions  $f(q_e)$  and  $g(q_e)$  defined in the proof of Lemma 5 for different values of  $(1 - \zeta)\mu_e - \zeta \gamma_{r,v} q_e^*$  and  $\alpha_e > 0$ .

and

$$g : q_e \mapsto \zeta \gamma_{r,v} (\pi_v^* - \gamma_e \pi_w^* - \tilde{\beta}_e) q_e + (1 - \zeta) (\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-) q_e.$$

Figure 5.1 shows a visualization of these two functions.

Now we analyze the cases  $q_e^* \neq 0$  and  $q_e^* = 0$  consecutively. First we concentrate on  $q_e^* \neq 0$ . The first function  $f$  is quasi-convex by the choice of  $\zeta$  which we show as follows: If  $q_e^* > 0$ , the function  $f$  has its global minimum at some  $q_e > 0$ , as  $(1 - \zeta)\mu_e - \zeta \gamma_{r,v} q_e^* < 0$  holds if either  $\mu_e = 0$  or, if  $\mu_e > 0$ , by assumption 1 of the lemma. If  $q_e^* < 0$ , the function  $f$  has its global minimum at some  $q_e < 0$ , because of  $(1 - \zeta)\mu_e - \zeta \gamma_{r,v} q_e^* > 0$ , which follows from  $\mu_e \geq 0$ .

The second function  $g$  is linear. The definition of  $\zeta$  implies that  $g$  has positive slope in the case  $q_e^* > 0$  and negative slope in the case  $q_e^* < 0$ . This follows from  $\text{sign}(q_e^*) = \text{sign}(\pi_v^* - \pi_w^* - \tilde{\beta}_e)$  and assumption 2 of the lemma for the case  $\mu_e > 0$ . For the case  $\mu_e = 0$  it follows from  $0 = \text{sign}(\mu_e) = \text{sign}(\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-)$  and  $\text{sign}(q_e^*) = \text{sign}(\pi_v^* - \pi_w^* - \tilde{\beta}_e)$ .

The previous observations guarantee that function (5.15) has only one local optimum if  $\mu_e q_e^* \neq 0$  and  $\alpha_e > 0$ . This implies that the extreme point  $q_e^*$  is global.

Now we turn to the case  $q_e^* = 0$ . This implies  $\mu_e q_e^* = 0$  and we have  $(1 - \zeta)\mu_e = 0$  by assumption 3 of the lemma. It follows that function (5.15) is a convex function. We note that this function is constant if  $\zeta = 0$ . Because of the convexity the extreme point  $q_e = q_e^*$  is a global minimum.  $\square$

**Corollary 2.** *Let  $(q^*, \pi^*, \Delta^*, \mu^*, \lambda^*)$  be a KKT point of the relaxation (5.2). We derive a dual transmission flow  $(\mu, \lambda)$  with  $\mu_e := 0$  for all arcs  $e \notin E'$ . Let  $\zeta \in [0, 1[$  such that*

1. *if  $\mu_e q_e^* > 0$  then  $\zeta \gamma_{r,v} |q_e^*| > (1 - \zeta) |\mu_e|$ ,*
2. *if  $\mu_e q_e^* < 0$  then  $(1 - \zeta) |\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-| < \zeta \gamma_{r,v} |\pi_v^* - \gamma_e \pi_w^* - \tilde{\beta}_e|$ ,*
3. *if  $\mu_e q_e^* = 0$  then  $(1 - \zeta) \mu_e = 0$*

*holds for each arc  $e = (v, w) \in E'$ . Then there exists a constant  $\tau_e$  for each arc  $e \in E'$  such that the inequality*

$$\begin{aligned} \sum_{e \in E'} \tau_e \leq & -\zeta \sum_{v \in V} s_v \pi'_v(\pi^*) \\ & + (1 - \zeta) \left( \sum_{v \in V} (\lambda_v^+ \bar{\pi}'_v - \lambda_v^- \underline{\pi}'_v) + \sum_{e \in E'} (\lambda_e^+ \bar{q}_e - \lambda_e^- \underline{q}_e) - \sum_{v \in V} s_v \mu_v \right) \end{aligned} \quad (5.16)$$

*is violated if and only if  $(q^*, \pi^*)$  is not feasible for the leaf problem (5.1). The violation is greater than or equal to  $(1 - \zeta)$  times the optimal objective value of the relaxation (5.2).*

Proof: First we write the flow conservation with  $\Delta_v^\pm := 0$  as

$$\sum_{e \in \delta_{E'}^+(v)} q_e^* - \sum_{e \in \delta_{E'}^-(v)} q_e^* - (\Delta_v^+ - \Delta_v^-) = s_v$$

for each node  $v \in V$ . Next we define the constant  $\tau_e = \tau_e(\zeta, \alpha_e, \tilde{\beta}_e, q^*, \pi^*, \mu, \lambda)$  for each arc  $e = (v, w) \in E'$  as follows:

$$\begin{aligned} \tau_e := \min_{\underline{q}_e \leq q_e \leq \bar{q}_e} \{ & (\zeta \gamma_{r,v} (q_e - q_e^*) + (1 - \zeta) \mu_e) (\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e) \\ & - \zeta \gamma_{r,v} (\pi_v^* - \gamma_e \pi_w^*) q_e - (1 - \zeta) (\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-) q_e \}. \end{aligned}$$

Then it follows from Lemma 3 that inequality (5.16) is valid for the leaf problem. By Lemma 5 the value  $\zeta$  is chosen such that the global minimum of the function

$$q_e \mapsto (\zeta \gamma_{r,v}(q_e - q_e^*) + (1 - \zeta)\mu_e) (\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e) - \zeta \gamma_{r,v}(\pi_v^* - \gamma_e \pi_w^*) q_e - (1 - \zeta)(\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-) q_e$$

is attained in  $q_e^*$ . We set

$$\tau'_e := \min_{q_e \in \mathbb{R}} \left\{ (\zeta \gamma_{r,v}(q_e - q_e^*) + (1 - \zeta)\mu_e) (\alpha_e q_e |q_e|^{k_e} + \tilde{\beta}_e) - \zeta \gamma_{r,v}(\pi_v^* - \gamma_e \pi_w^*) q_e - (1 - \zeta)(\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-) q_e \right\}.$$

Then it follows from  $\tau'_e \leq \tau_e$  for all arcs  $e \in E'$  that the inequality

$$\begin{aligned} \sum_{e \in E'} \tau'_e &\leq -\zeta \sum_{v \in V} s_v \pi'_v(\pi^*) \\ &+ (1 - \zeta) \left( \sum_{v \in V} (\lambda_v^+ \bar{\pi}_v - \lambda_v^- \underline{\pi}_v) + \sum_{e \in E'} (\lambda_e^+ \bar{q}_e - \lambda_e^- \underline{q}_e) - \sum_{v \in V} s_v \mu_v \right) \end{aligned}$$

is valid for the leaf problem. The violation is equal to the optimal objective value of the relaxation (5.2) by Lemma 4. Now it follows from  $\tau'_e \leq \tau_e$  that the violation of (5.16) is greater than or equal to the optimal objective value of the relaxation (5.2).  $\square$

## 6 A Capacity Inequality for the Topology Optimization Problem

We derive a capacity inequality for the topology optimization problem by lifting inequality (5.8) which is valid for a certain leaf problem.

**Theorem 1.** *Let  $(\mu, \lambda)$  be a dual transmission flow. Let  $\pi^*$  be a vector of potential values for each node  $v \in V$  and  $q^*$  be a vector of flow values for each arc  $e \in E$ . Furthermore let slack values  $\Delta_v^\pm \geq 0$  be given for each node  $v \in V$  such that the flow conservation*

$$\sum_{e \in \delta_E^+(v)} q_e^* - \sum_{e \in \delta_E^-(v)} q_e^* - (\Delta_v^+ - \Delta_v^-) = s_v$$

is fulfilled for each node  $v \in V$ . There exist constants  $\tau_{e,i} = \tau_{e,i}(y_{e,i})$  for each arc  $(e, i) \in E_X, i \neq 0$  such that the inequality in  $x, y$

$$\begin{aligned} &\sum_{\substack{(e,i) \in E_X \\ i \neq 0}} x_{e,i} \tau_{e,i}(y_{e,i}) \leq \\ &\zeta \left( \sum_{v \in V} (\Delta_v^- \bar{\pi}'_v - \Delta_v^+ \underline{\pi}'_v) - \sum_{v \in V} s_v \pi'_v(\pi^*) \right) \\ &+ (1 - \zeta) \left( \sum_{v \in V} (\lambda_v^+ \bar{\pi}_v - \lambda_v^- \underline{\pi}_v) + \sum_{\substack{(e,i) \in E_X \\ i \neq 0}} x_{e,i} (\lambda_e^+ \bar{q}_{e,i} - \lambda_e^- \underline{q}_{e,i}) - \sum_{v \in V} s_v \mu_v \right) \tag{6.1} \\ &\quad + \zeta \sum_{e=(v,w) \in E} x_{e,0} \max \{ q_e^* (\bar{\pi}'_v - \underline{\pi}'_w), q_e^* (\underline{\pi}'_w - \bar{\pi}'_v) \} \\ &\quad + (1 - \zeta) \sum_{e=(v,w) \in E} x_{e,0} \max \{ \mu_e (\bar{\pi}_v - \underline{\pi}_w), \mu_e (\bar{\pi}_w - \underline{\pi}_v) \} \end{aligned}$$

is valid for the topology optimization problem (4.2).

Proof: We are going to apply Lemma 3 that yields a valid inequality for a leaf problem corresponding to the arc set  $E'$ . We write  $E' = E'(x)$  depending on the active configuration  $x$  by  $E'(x) := \{(e, i) \in E_X \mid x_{e,i} = 1\}$ . In order to apply Lemma 3 we define  $\Delta$  variables in dependence of  $E'(x)$  by considering the following equality which is valid for each active configuration  $x$ :

$$\sum_{e \in \delta_E^+(v)} x_{e,0} q_e^* - \sum_{e \in \delta_E^-(v)} x_{e,0} q_e^* + \sum_{e \in \delta_{E'(x)}^+(v)} q_e^* - \sum_{e \in \delta_{E'(x)}^-(v)} q_e^* - (\Delta_v^+ - \Delta_v^-) = s_v.$$

We define variables  $\tilde{\Delta}_v^+(x) \geq 0$  and  $\tilde{\Delta}_v^-(x) \geq 0$  where at least one of both values equals zero by

$$\tilde{\Delta}_v^-(x) - \tilde{\Delta}_v^+(x) := \sum_{e \in \delta_E^+(v)} x_{e,0} q_e^* - \sum_{e \in \delta_E^-(v)} x_{e,0} q_e^*.$$

From this we obtain

$$\sum_{e \in \delta_{E'(x)}^+(v)} q_e^* - \sum_{e \in \delta_{E'(x)}^-(v)} q_e^* - (\tilde{\Delta}_v^+(x) + \Delta_v^+) + (\tilde{\Delta}_v^-(x) + \Delta_v^-) = s_v \quad (6.2)$$

for every node  $v \in V$ . We proceed analogously for  $\mu$  in order to obtain a dual transmission flow for  $E'(x)$ . For each active configuration  $x$  it holds

$$\sum_{e \in \delta_E^+(v)} x_{e,0} \mu_e - \sum_{e \in \delta_E^-(v)} x_{e,0} \mu_e + \sum_{e \in \delta_{E'(x)}^+(v)} \mu_e - \sum_{e \in \delta_{E'(x)}^-(v)} \mu_e = \lambda_v^+ - \lambda_v^-$$

for every node  $v \in V$ . We define variables  $\tilde{\lambda}_v^+(x) \geq 0$  and  $\tilde{\lambda}_v^-(x) \geq 0$  with at least one of both values being equal to zero by

$$\tilde{\lambda}_v^-(x) - \tilde{\lambda}_v^+(x) := \sum_{e \in \delta_E^+(v)} x_{e,0} \mu_e - \sum_{e \in \delta_E^-(v)} x_{e,0} \mu_e$$

and obtain

$$\sum_{e \in \delta_{E'(x)}^+(v)} \mu_e - \sum_{e \in \delta_{E'(x)}^-(v)} \mu_e = (\tilde{\lambda}_v^+(x) + \lambda_v^+) - (\tilde{\lambda}_v^-(x) - \lambda_v^-). \quad (6.3)$$

Now equation (6.2) and (6.3) allow to write inequality (5.8) for each active configuration  $x$  as

$$\begin{aligned} & \sum_{e \in E'(x)} \tau_e \leq \\ & \zeta \left( \sum_{v \in V} ((\Delta_v^- + \tilde{\Delta}_v^-(x)) \bar{\pi}'_v - (\Delta_v^+ + \tilde{\Delta}_v^+(x)) \underline{\pi}'_v) - \sum_{v \in V} s_v \pi'_v(\pi^*) \right) \\ & + (1 - \zeta) \left( \sum_{v \in V} ((\lambda_v^+ + \tilde{\lambda}_v^+(x)) \bar{\pi}_v - (\lambda_v^- + \tilde{\lambda}_v^-(x)) \underline{\pi}_v) \right) \\ & + (1 - \zeta) \left( \sum_{e \in E'(x)} (\lambda_e^+ \bar{q}_e - \lambda_e^- \underline{q}_e) - \sum_{v \in V} s_v \mu_v \right). \end{aligned}$$

We replace

$$\sum_{e \in E'(x)} \tau_e = \sum_{\substack{e \in E_X \\ i \neq 0}} x_{e,i} \tau_{e,i},$$

and take the definition of the constant  $\tau_{e,i} = \tau_{e,i}(\zeta, \alpha_{e,i}, \beta_{e,i} y_{e,i}, q^*, \pi^*, \mu, \lambda)$  for each arc  $(e, i) = (v, w, i) \in E_X, i \neq 0$  as follows:

$$\tau_{e,i}(y_{e,i}) := \min_{q_e \leq q_e \leq \bar{q}_e} \{ (\zeta \gamma_{r,v}(q_{e,i} - q_e^*) + (1 - \zeta) \mu_e) (\alpha_{e,i} q_{e,i} |q_{e,i}|^{k_e} + \beta_{e,i} y_{e,i}) \}$$

$$-\zeta \gamma_{r,v}(\pi_v^* - \gamma_e \pi_w^*) q_{e,i} - (1 - \zeta)(\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-) q_{e,i} \}.$$

Furthermore we write

$$\sum_{e \in E'(x)} (\lambda_e^+ \bar{q}_e - \lambda_e^- \underline{q}_e) = \sum_{\substack{(e,i) \in E_X \\ i \neq 0}} x_{e,i} (\lambda_e^+ \bar{q}_{e,i} - \lambda_e^- \underline{q}_{e,i}).$$

We proceed by deriving an estimation for the right-hand side using the previous definitions for  $\tilde{\Delta}_v^+(x)$  and  $\tilde{\Delta}_v^-(x)$  by setting

$$\tilde{\pi}_v := \begin{cases} \bar{\pi}'_v & \text{if } \tilde{\Delta}_v^-(x) - \tilde{\Delta}_v^+(x) \geq 0, \\ \underline{\pi}'_v & \text{else.} \end{cases}$$

Then we obtain

$$\begin{aligned} \sum_{v \in V} (\tilde{\Delta}_v^-(x) \bar{\pi}'_v - \tilde{\Delta}_v^+(x) \underline{\pi}'_v) &= \sum_{v \in V} (\tilde{\Delta}_v^-(x) - \tilde{\Delta}_v^+(x)) \tilde{\pi}_v = \\ \sum_{e=(v,w) \in E} x_{e,0} q_e^* (\tilde{\pi}_v - \tilde{\pi}_w) &\leq \sum_{e=(v,w) \in E} x_{e,0} \max \{q_e^* (\bar{\pi}'_v - \underline{\pi}'_w), q_e^* (\underline{\pi}'_w - \bar{\pi}'_v)\}. \end{aligned}$$

Similarly, using the definition of  $\lambda_v^+(x)$  and  $\lambda_v^-(x)$  we derive the estimation

$$\sum_{v \in V} (\tilde{\lambda}_v^+(x) \bar{\pi}_v - \tilde{\lambda}_v^-(x) \underline{\pi}_v) \leq \sum_{e=(v,w) \in E} x_{e,0} \max \{\mu_e (\bar{\pi}_v - \underline{\pi}_w), \mu_e (\underline{\pi}_w - \bar{\pi}_v)\}.$$

□

**Theorem 2.** Let  $(\mu, \lambda)$  be derived from a KKT point  $(q^*, \pi^*, \Delta^*, \mu^*, \lambda^*)$  of the relaxation (5.2) for arc set  $E'$ . Let  $\zeta \in [0, 1[$  be minimal such that

1. if  $\mu_e q_e^* > 0$  then  $\zeta \gamma_{r,v} |q_e^*| > (1 - \zeta) |\mu_e|$ ,
2. if  $\mu_e q_e^* < 0$  then  $(1 - \zeta) |\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-| < \zeta \gamma_{r,v} |\pi_v^* - \gamma_e \pi_w^* - \tilde{\beta}_e|$ ,
3. if  $\mu_e q_e^* = 0$  then  $(1 - \zeta) \mu_e = 0$ ,

holds for each arc  $e = (v, w) \in E'$ . Then there exist constants  $\tau_{e,i} = \tau_{e,i}(y_{e,i})$  for each arc  $(e, i) \in E_X, i \neq 0$  such that the inequality in  $x$  and  $y$

$$\begin{aligned} \sum_{\substack{(e,i) \in E_X \\ i \neq 0}} x_{e,i} \tau_{e,i}(y_{e,i}) &\leq -\zeta \sum_{v \in V} s_v \pi'_v(\pi^*) \\ + (1 - \zeta) &\left( \sum_{v \in V} (\lambda_v^+ \bar{\pi}_v - \lambda_v^- \underline{\pi}_v) + \sum_{\substack{(e,i) \in E_X \\ i \neq 0}} x_{e,i} (\lambda_e^+ \bar{q}_{e,i} - \lambda_e^- \underline{q}_{e,i}) - \sum_{v \in V} s_v \mu_v \right) \\ &+ \zeta \sum_{e=(v,w) \in E'} x_{e,0} \max \{q_e^* (\bar{\pi}_v - \underline{\pi}_w), q_e^* (\underline{\pi}_w - \bar{\pi}_v)\} \\ &+ (1 - \zeta) \sum_{e=(v,w) \in E} x_{e,0} \max \{\mu_e (\bar{\pi}_v - \underline{\pi}_w), \mu_e (\underline{\pi}_w - \bar{\pi}_v)\} \end{aligned} \quad (6.4)$$

is valid for the topology optimization problem (4.2). This inequality cuts off the leaf problem corresponding to the arc set  $E'$  if it is infeasible. For the corresponding decision vector  $x, y$  the violation of inequality (6.4) is greater than or equal to  $(1 - \zeta)$  times the optimal objective value of the leaf problem's relaxation.

Proof: We define  $q_e^* := 0$  for all arcs  $e \in E \setminus E'$  and obtain

$$\sum_{e \in \delta_E^+(v)} q_e^* - \sum_{e \in \delta_E^-(v)} q_e^* = s_v.$$

Hence  $\Delta_v^+ = \Delta_v^- = 0$  for all  $v \in V$ , and thus the validity of (6.4) as a globally valid inequality for (4.2) follows from Theorem 1.

If  $x$  and  $y$  are the binary and integer values, respectively, that correspond to the leaf problem of the relaxation (5.2) for arc set  $E'$ , then (6.4) can be rewritten as (5.16). Now the theorem follows from the special choice of  $\zeta$  (which is the same as in Corollary 2).  $\square$

Let us visualize  $\tau_{e,i}$  for an arc  $e = (v, w) \in E$ . The value of  $\tau_{e,i}$  depends on  $\alpha_{e,i}$ . Thus we consider  $\tau_{e,i}$  as a function  $\tau(\alpha)$  defined by

$$\begin{aligned} \tau(\alpha) := \min_{q \in \mathbb{R}} \{ & (\zeta \gamma_{r,v}(q - q_e^*) + (1 - \zeta)\mu_e) \alpha |q|^{k_e} \\ & - \zeta \gamma_{r,v}(\pi_v^* - \gamma_e \pi_w^*) q - (1 - \zeta)(\mu_v - \mu_w - \lambda_e^+ + \lambda_e^-) q \}. \end{aligned}$$

A visualization of this function is shown in Figure 6.1. From this image we conclude, that either increasing or decreasing the diameter of a pipe reduces the violation of inequality (6.4) of the previous Theorem 2.

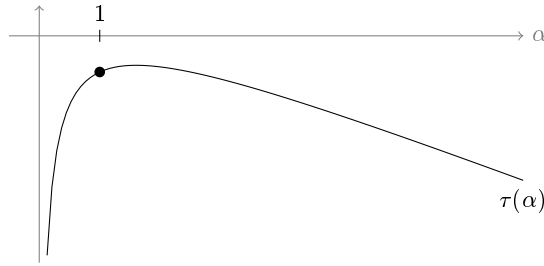


Fig. 6.1: Visualization of  $\tau(\alpha)$  for  $q_e^* = 5, \mu_e = 1, \gamma_e = 1, \pi_v - \pi_w = 25, \mu_v - \mu_w = 10, \lambda_e^+ - \lambda_e^- = 0, k = 1, \zeta = 0.7, \gamma_{r,v} = 1$ . The depicted point corresponds to the original  $\alpha = 1$  of the leaf problem.

We remark that the inequality in Theorem 2 is not a linear inequality yet. In order to add it to the problem as a globally valid cut, it needs to be linearized. To this end, we introduce binary variables  $z_{e,i}^k \in \{0, 1\}$  for  $k \in Z_{e,i} := [y_{e,i}, \bar{y}_{e,i}] \cap \mathbb{Z}$ , and the constraints

$$y_{e,i} = \sum_{k \in Z_{e,i}} k z_{e,i}^k, \quad x_{e,i} = \sum_{k \in Z_{e,i}} z_{e,i}^k.$$

Now we compute  $\tau_{e,i}^k := \tau_{e,i}(k)$  for all  $k \in Z_{e,i}$ , which gives the coefficients in the linear inequality

$$\begin{aligned} & \sum_{\substack{(e,i) \in E_X \\ i \neq 0}} \sum_{k \in Z_{e,i}} z_{e,i}^k \tau_{e,i}^k \leq -\zeta \sum_{v \in V} s_v \pi'_v(\pi^*) \\ & + (1 - \zeta) \left( \sum_{v \in V} (\lambda_v^+ \bar{\pi}_v - \lambda_v^- \underline{\pi}_v) + \sum_{\substack{(e,i) \in E_X \\ i \neq 0}} x_{e,i} (\lambda_e^+ \bar{q}_{e,i} - \lambda_e^- \underline{q}_{e,i}) - \sum_{v \in V} s_v \mu_v \right) \\ & + \zeta \sum_{e=(v,w) \in E'} x_{e,0} \max \{ q_e^* (\bar{\pi}_v - \underline{\pi}_w), q_e^* (\underline{\pi}_w - \bar{\pi}_v) \} \\ & + (1 - \zeta) \sum_{e=(v,w) \in E} x_{e,0} \max \{ \mu_e (\bar{\pi}_v - \underline{\pi}_w), \mu_e (\bar{\pi}_w - \underline{\pi}_v) \}. \end{aligned} \tag{6.5}$$

These globally valid inequalities are added to the problem.

## 7 Computational Results

We consider two different transmission networks with different topologies. Both networks consist of pipelines only and all pipes are modelled with  $\beta_{e,i} = 0$  and  $k_{e,i} = 1$ . The first network **Net1** in Figure 7.1

has 20 nodes and 29 pipelines, which represent the backbone network of the Belgium natural gas network. The data for this network can be found in [16], and results using this network in De Wolf et al. [12, 10]. The second network **Net2** in Figure 7.2 consists of 32 nodes and 37 pipelines. It is an approximation to the German L-gas network in the Rhine-Main-Ruhr area. The data of network **Net2** is publicly available at URL <http://gaslib.zib.de> under the name `gaslib-40`. We generate the cuts described

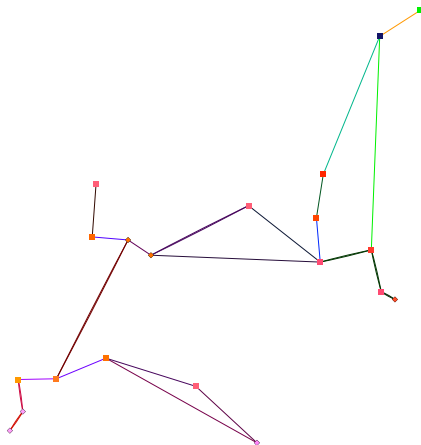


Fig. 7.1: The test network **Net1**. All extensions are parallel arcs (or loops) and thus not visible in the picture.

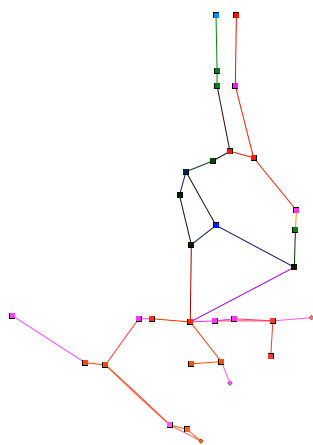


Fig. 7.2: The test network **Net2**. All extensions are parallel arcs (or loops) and thus not visible in the picture.

in Theorem 6.4 as follows. Consider an open subproblem the branching tree, which can be a leaf, or an integer feasible node. Out of this we define a nonlinear optimization problem which has the form of (5.1), where we fix all integer variables to the given values at this node. Since the problem might be nonlinear infeasible, we reformulate the problem and obtain (5.2). Note that this relaxation is always feasible (see [19]). After solving the NLP with a nonlinear solver, one of the following two cases occurs.

In the first case, the NLP has a zero objective function value in the optimal solution. We obtain a primal feasible solution and prune the current node.

In the second case, the NLP might have a positive objective function value in the optimal solution. This means that some slack variables could not become zero. In this case we use the KKT point, i.e.,

primal and dual solution values and derive a cutting plane (6.5) which is valid for the topology optimization problem by Theorem 2. The inequality is stored in and managed by a cut pool of the solver. We continue by spatial branching.

We implemented the cut generation algorithms described in section 6 in C on a cluster of 64bit Intel Xeon X5672 CPUs at 3.20 GHz with 12 MByte cache and 48 GB main memory, running an OpenSuse 12.1 Linux with a gcc 4.6.2 compiler. We used the following software packages: SCIP 3.0.1 as mixed-integer nonlinear branch-and-cut framework (for details on SCIP we refer to [1]), CPLEX 12.1 [9] as linear programming solver, Ipopt 3.10 [30] as nonlinear solver, and Lamatto++ [17] as framework for handling the input data. Hyperthreading and TurboBoost were disabled. In all experiments, we ran only one job per node to avoid random noise in the measured running time that might be caused by cache-misses if multiple processes share common resources. In our initial implementation we added all obtained cuts directly to the branch-and-cut process. In the final implementation we do not add them immediately. Instead we store them in a cut pool, until a predefined number of inequalities is reached (experimentally, a pool size of 40 inequalities turned out to be a good value). Then, we restart the whole branch-and-cut solution process and multiply the cut pool size by 1.5. Additionally, we also restart, if a new primal feasible solution with a better objective function compared to the current best is found. For the restart, only the best feasible solution and the valid inequalities are kept. Now the solver SCIP uses its proprietary routines to further strengthen our cuts (together with all other model inequalities).

Given is a (balanced) flow demand at the entry (source) and exit (sink) nodes of the network. For this given demand, there exists a feasible flow in the network. Now we scale up this demand, that is, we multiply each entry and exit value by the same scalar  $> 1$ . For a certain value (2.0 for instance **net1** and 2.1 for instance **net2**) the instance is not longer feasible, i.e., there is no valid flow that fulfills all model constraints. In order to obtain a feasible flow again, the network topology needs to be extended, for which we introduce a number of loops. For instance **net1** we allow up to 7, ..., 11 loops, and for instance **net2** we allow between 2 and 4 loops, respectively. That is, each original pipeline can be extended by at most this number of pipelines having the same characteristic as the original one.

The computational results are shown in the Tables 1–4. We distinguish between results that were solved to proven global optimality within a given time limit of 12 hours and those that did not. In the latter case an optimality gap remains, that is defined as the ratio between the best upper bound  $u$  (i.e., the objective function value of best feasible solution) and the best lower bound  $\ell$ . That is,  $\text{gap} = \left(\frac{u-\ell}{\ell}\right) \cdot 100\%$ .

The first column of the Tables 1–4 shows the scaling factor of the demand vector. The second column gives the number of loops that can maximally be selected by the topology optimization. We compare the results that are achieved with our cuts (with and without restarts) against the results that are achieved without our cuts. In the latter case, the model is solved using the default settings of the solver SCIP. For each run we report the optimality gap (as defined above). A gap of 0.0% means that the solver was able to find a proven global optimal solution within the time limit of 12 hours. Furthermore we report in column “primal” the objective function value of the best feasible solution, i.e., the building cost for the chosen loop pipes, and in column “dual” the best lower bound. Note that in Table 1 and Table 3 these two columns are merged into one single “primal/dual” column, because both values coincide. In the column “time” we report the CPU time (runtime) in seconds, and column “nodes” shows the number of nodes that were solved during the branch-and-cut process. In the case that we use multiple restarts when adding our cuts, this “node” value refers to the total number of all nodes, summing up the individual restarted solution processes. In the column “#cuts” we report the total number of cuts that were added. The rows in Table 2 and Table 4 are ordered such that we first have those instances that can be solved to global optimality when using our cuts, then those instances where the gap can be reduced when using our cuts, and finally those instances where we do not have a gap (because of no primal feasible solution). Figure 7.3 shows a scatter plot of the runtimes that are achieved without cuts gainst with using our cuts and restarts.

For those instance that were solved to optimality within the time limit, Table 1 and Table 3 show huge reductions of the nodes of the branch-and-bound tree and the runtime when using our cuts and restarts. Practically speaking, an instance is more computationally demanding, the more potential loops are offered and the higher the scaling factor. The runtime and node reduction becomes more significant, the more demanding the instance. Table 2 shows that 5 instances of **net1** that reached the time limit can be solved to proven global optimality when using our inequalities. Table 4 shows that for all instances of **net2** that reached the time limit while at least one primal solution was found, the gap was reduced and much better primal feasible solutions were found.



scale loops	no cuts			with cuts (no restart)			with cuts (restart)							
	gap	primal/dual	time	gap	dual	time	gap	primal/dual	time	nodes	#cuts			
2.0	7	0.0	1500.00	212.07	176615	199.41	144901	435	0.0	1500.00	178.09	37103	81	
2.0	8	0.0	1500.00	113.19	83832	118.62	78936	273	0.0	1500.00	375.97	28436	61	
2.0	9	0.0	1500.00	140.55	100641	151.01	98970	241	0.0	2400.00	332.68	6460	40	
2.0	10	0.0	1500.00	130.05	91718	170.99	90952	468	0.0	1500.00	704.81	24993	61	
2.0	11	0.0	1500.00	132.34	91469	102.79	57992	282	0.0	1500.00	549.83	15434	61	
2.1	7	0.0	1800.00	2127.98	1034782	2979.29	1412698	1791	0.0	1800.00	218.77	72187	192	
2.1	8	0.0	1800.00	859.88	625947	511.23	399210	472	0.0	1800.00	285.13	51743	91	
2.1	9	0.0	1700.00	719.39	444753	732.26	509227	485	0.0	1700.00	740.41	85876	146	
2.1	10	0.0	1700.00	774.49	504599	715.90	476250	605	0.0	1700.00	676.72	54069	91	
2.1	11	0.0	1700.00	728.04	471606	852.27	547297	683	0.0	1700.00	886.80	51291	91	
2.2	7	0.0	2200.00	7069.36	4521738	24096.02	9108228	1364	0.0	2200.00	409.11	136746	136	
2.2	8	0.0	2000.00	3874.54	2274304	3261.68	2237394	1973	0.0	2000.00	377.68	114416	136	
2.2	9	0.0	2000.00	2594.73	1441304	2407.03	1540813	1015	0.0	2000.00	370.33	62605	61	
2.2	10	0.0	2000.00	2919.78	1713374	2074.94	1404573	1240	0.0	2000.00	802.20	235620	136	
2.2	11	0.0	2000.00	2699.99	1494467	3025.57	1817371	1255	0.0	2000.00	1176.24	199786	136	
2.3	9	0.0	2300.00	16496.05	6038279	36419.23	10346133	1570	0.0	2300.00	569.23	177965	109	
2.3	10	0.0	2200.00	5380.25	3104723	11369.54	5531508	1695	0.0	2200.00	914.43	126162	136	
2.3	11	0.0	2200.00	9881.80	4006313	7978.24	3808101	2127	0.0	2200.00	1260.02	225291	204	
2.4	11	0.0	2500.00	41011.36	13944805	1942.82	43200.00	11854344	2221	0.0	2500.00	1374.45	392992	204
2.5	7	0.0	inf	1.01	1	inf	1.17	1	0.0	inf	1.05	1	0	
Average				4893.29	2108263		7018.30	2573244				610.14	104958	

Table 1: Instances for Net1 solved to proven global optimality within the time limit.

scale loops	no cuts					with cuts (no restart)					with cuts (restart)							
	gap	primal	dual	time	nodes	gap	primal	dual	time	nodes	#cuts	gap	primal	dual	time	nodes	#cuts	
2.3	8	18.34	2400.00	2028.03	43200.00	13912926	0.00	2400.00	2400.00	36677.33	15084376	1429	0.0	2400.00	2400.00	692.95	343155	73
2.4	9	39.92	2700.00	1929.71	43200.00	10522647	38.42	2700.00	1950.61	43200.00	12865583	1919	0.0	2700.00	2700.00	1145.60	633067	204
2.4	10	33.4	2600.00	1948.95	43200.00	12099342	32.51	2600.00	1962.13	43200.00	15528615	2274	0.0	2600.00	2600.00	963.62	422751	91
2.5	10	61.29	3100.00	1922.04	43200.02	3805350	46.33	3000.00	2050.17	43200.00	12506089	1608	0.0	3000.00	3000.00	2894.08	1072167	554
2.5	11	47.74	3000.00	2030.65	43200.00	10600042	49.28	3000.00	2009.69	43200.00	11717582	2249	0.0	2900.00	2900.00	2415.01	987747	204
2.3	7	63.16	3100.00	1900.00	43202.97	10801193	76.21	3200.00	1816.01	43200.15	8190038	1351	16.19	3000.00	2581.98	43200.02	2937744	5224
2.4	7	133.77	5900.00	2523.81	43200.00	4451666	118.64	5700.00	2606.96	43200.00	7836839	3076	71.65	5500.00	3204.20	43200.01	11801255	688
2.4	8	67.13	3200.00	1914.71	43200.00	5744040	54.42	3100.00	2007.47	43200.00	10101719	1319	15.66	3100.00	2680.35	43200.01	2629225	5224
2.5	8	131.61	5200.00	2245.16	43200.01	7162185	114.87	4700.00	2187.39	43200.00	10447778	1657	42.82	4700.00	3290.88	43200.0	5507212	2322
2.5	9	86.88	4000.00	2140.45	43200.00	10425831	64.57	3400.00	2066.05	43200.00	9811535	1483	11.04	3300.00	2971.89	43200.03	3156117	4625

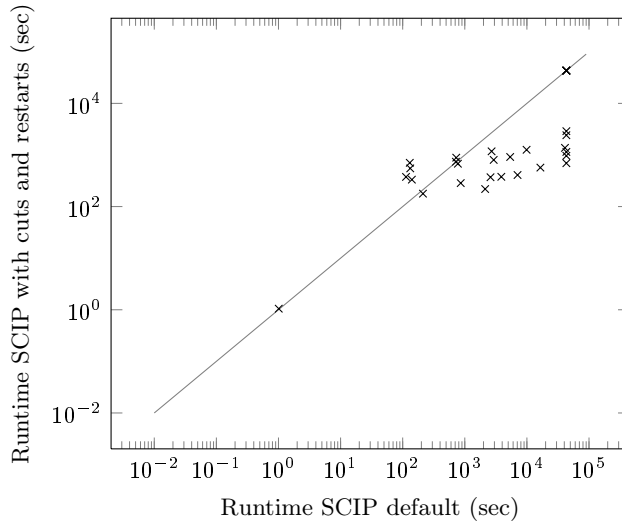
Table 2: Instances for Net1 that reached the time limit of 12 hours (without cuts).

scale loops	no cuts			with cuts (no restart)			with cuts (restart)								
	gap	primal/dual	time	nodes	gap	primal/dual	time	nodes	#cuts	gap	primal/dual	time	nodes	#cuts	
2.0	2	0.0	100.00	2.60	469	0.0	100.00	0.94	15	2	0.0	100.00	0.67	2	1
2.0	3	0.0	100.00	2.96	412	0.0	100.00	2.07	34	9	0.0	100.00	1.54	11	2
2.0	4	0.0	100.00	3.58	527	0.0	100.00	2.44	47	16	0.0	100.00	4.74	65	9
2.1	2	0.0	100.00	1.60	297	0.0	100.00	6.31	216	75	0.0	100.00	0.28	2	1
2.1	3	0.0	100.00	2.37	394	0.0	100.00	2.77	90	26	0.0	100.00	2.71	37	4
2.1	4	0.0	100.00	2.86	342	0.0	100.00	4.23	170	24	0.0	100.00	12.1	178	22
2.2	2	0.0	200.00	2.16	421	0.0	200.00	3.48	121	32	0.0	200.00	8.25	288	24
2.2	3	0.0	200.00	2.93	558	0.0	200.00	7.37	319	57	0.0	200.00	32.71	811	13
2.2	4	0.0	200.00	5.25	993	0.0	200.00	8.59	441	68	0.0	200.00	40.08	1094	41
2.3	2	0.0	200.00	1.71	293	0.0	200.00	11.32	502	126	0.0	200.00	9.14	242	32
2.3	3	0.0	200.00	4.34	1013	0.0	200.00	6.10	444	42	0.0	200.00	38.04	1194	31
2.3	4	0.0	200.00	2.85	313	0.0	200.00	12.42	703	90	0.0	200.00	70.43	1722	18
2.4	2	0.0	300.00	2.98	1108	0.0	300.00	4.84	223	33	0.0	300.00	25.35	1151	25
2.4	3	0.0	300.00	3.91	966	0.0	300.00	11.15	865	92	0.0	300.00	56.79	2338	27
2.4	4	0.0	300.00	5.67	1155	0.0	300.00	22.76	1154	213	0.0	300.00	109.02	3408	104
2.5	2	0.0	400.00	4.47	1620	0.0	400.00	5.05	699	25	0.0	400.00	3.12	152	3
2.5	3	0.0	400.00	4.88	1280	0.0	400.00	6.86	1024	29	0.0	400.00	56.05	2575	26
2.5	4	0.0	400.00	6.54	1751	0.0	400.00	9.66	1374	36	0.0	400.00	71.44	3546	7
2.6	2	0.0	500.00	11.79	6584	0.0	500.00	8.09	1682	54	0.0	500.00	6.03	726	34
2.6	3	0.0	500.00	9.98	5154	0.0	500.00	8.37	2201	35	0.0	500.00	56.35	2494	46
2.6	4	0.0	500.00	5.81	2919	0.0	500.00	9.04	2343	30	0.0	500.00	83.39	4464	26
2.7	2	0.0	700.00	26.60	21115	0.0	700.00	58.83	20406	454	0.0	700.00	37.78	3753	98
2.7	3	0.0	600.00	38.08	28762	0.0	600.00	98.87	33476	782	0.0	600.00	45.85	2988	41
2.7	4	0.0	600.00	52.79	34265	0.0	600.00	20.91	8956	81	0.0	600.00	76.91	8505	41
2.8	2	0.0	800.00	164.18	140745	0.0	800.00	407.46	101838	3853	0.0	800.00	70.43	15359	229
2.8	3	0.0	800.00	252.11	193589	0.0	800.00	167.90	82620	975	0.0	800.00	83.18	8516	113
2.8	4	0.0	800.00	141.97	118166	0.0	800.00	141.33	95989	518	0.0	800.00	81.86	11084	28
2.9	2	0.0	1000.00	895.94	690477	0.0	1000.00	1318.74	589481	5689	0.0	1000.00	183.29	36191	450
2.9	3	0.0	900.00	1190.60	805692	0.0	900.00	1338.20	636547	5423	0.0	900.00	134.94	33161	268
2.9	4	0.0	900.00	1427.94	869203	0.0	900.00	491.28	373578	1194	0.0	900.00	109.55	23000	91
3.0	2	0.0	1300.00	5243.31	4327789	0.0	1300.00	8535.32	4578526	22155	0.0	1300.00	486.45	106213	1166
3.0	3	0.0	1100.00	6380.04	2557433	0.0	1100.00	3725.82	1806564	10288	0.0	1100.00	243.68	75504	355
3.0	4	0.0	1100.00	7994.69	5176313	0.0	1100.00	2734.76	2015023	5254	0.0	1100.00	309.92	87278	357
3.1	4	0.0	1200.00	30775.47	10316726	0.0	1200.00	19133.20	9892773	14742	0.0	1200.00	273.23	124921	306
Average				1605.40	744377			1123.42	595601				81.69	16558	

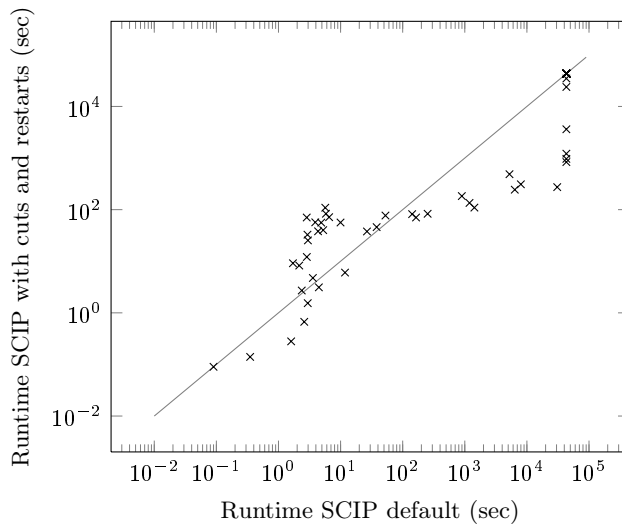
Table 3: Instances for Net2 solved to proven global optimality within the time limit.

scale loops	no cuts					with cuts (no restart)					with cuts (restart)							
	gap	primal	dual	time	nodes	gap	primal	dual	time	nodes	#cuts	gap	primal	dual	time	nodes	#cuts	
3.1	2	53.55	1700.00	1107.11	43200.00	24381440	67.15	1700.00	1017.03	43200.00	17451268	174194	0.0	1700.00	1700.00	34817.21	1134330	14639
3.1	3	57.02	1300.00	827.93	43200.00	7358275	53.03	1300.00	849.47	43200.00	9459329	23136	0.0	1300.00	1300.00	964.83	214025	1548
3.2	3	108.26	1700.00	816.28	43200.00	6878911	64.73	1500.00	910.55	43200.00	11178211	22420	0.0	1500.00	1500.00	836.03	233780	1361
3.2	4	39.05	1400.00	1006.86	43200.00	24473376	66.48	1500.00	901.02	43200.00	22508960	12380	0.0	1400.00	1400.00	1215.38	365577	1032
3.3	4	105.08	1800.00	877.71	43200.00	8842062	71.53	1600.00	932.79	43200.00	20658136	6024	0.0	1600.00	1600.00	3613.06	693711	2035
3.4	4	116.26	2000.00	924.82	43200.01	7219501	96.99	1900.00	964.51	43200.01	21179671	7031	0.0	1800.00	1800.00	23857.71	1613672	5431
3.2	2	125.44	3000.00	1330.70	43200.02	40470382	195.17	3600.00	1219.64	43200.02	21817523	3305	47.14	2500.00	1699.03	43200.06	1268782	9178
3.3	2	400.23	7400.00	1479.30	43200.01	24672027	296.61	5600.00	1411.97	43200.01	26737928	182344	89.79	4300.00	2265.70	43200.01	1086705	17631
3.3	3	125.43	2100.00	931.54	43200.02	90942229	103.04	1900.00	935.75	43200.02	10987939	88689	23.74	1800.00	1454.61	43200.01	1948049	17631
3.4	3	136.64	2600.00	1098.71	43200.00	13464692	107.98	2300.00	1105.89	43200.00	25781066	17990	46.34	2400.00	1639.99	43200.03	1255323	11754
3.5	3	153.76	3000.00	1182.20	43200.01	14580836	142.08	2800.00	1156.63	43200.01	21265189	32038	28.63	2600.00	2021.31	43200.05	1363678	17631
3.5	4	198.02	3000.00	1006.65	43200.00	11273438	132.63	2400.00	1031.69	43200.00	17624328	19996	22.67	2100.00	1711.96	43200.01	1971200	11754
3.6	3	149.98	3200.00	1280.12	43200.01	17477233	226.87	4000.00	1223.74	43200.01	14877739	9742	24.93	3000.00	2401.32	43200.01	1878263	9493
3.6	4	164.76	2800.00	1057.54	43200.01	15527932	161.29	2800.00	1071.60	43200.01	14206830	46080	27.52	2500.00	1960.44	43200.03	2736316	11754
3.7	3	3284.48	5200.00	1352.47	43200.02	13760208	300.34	5200.00	1298.89	43200.02	9677659	10788	31.46	3800.00	2890.57	43200.02	1613400	7836
3.7	4	206.61	3600.00	1174.11	43200.01	17115145	164.17	3100.00	1173.49	43200.01	15885318	25322	42.41	3100.00	2176.83	43200.02	2297454	10899
3.8	3	409.71	7500.00	1471.42	43200.01	10677370	359.69	6600.00	1435.74	43200.01	10756745	12222	53.4	5300.00	3455.03	43200.01	1273240	7836
3.8	4	237.99	4100.00	1213.06	43200.01	14844993	204.6	3800.00	1247.52	43200.01	17622238	17448	48.24	3500.00	2361.06	43200.01	2341599	14010
3.9	4	237.83	4200.00	1243.21	43200.01	12183208	198.08	3900.00	1308.38	43200.01	15001778	11417	38.84	3800.00	2736.98	43200.01	2101490	7836
3.4	2	n/a	n/a	1736.73	43200.02	41286307	n/a	n/a	1653.04	43200.02	29158478	0	n/a	n/a	4280.55	43200.00	983809	0
3.5	2	n/a	n/a	2014.37	43200.01	37965000	n/a	n/a	1831.86	43200.01	23410711	0	n/a	n/a	1831.48	43200.01	2330517	0
3.6	2	n/a	n/a	2400.10	43200.01	29469613	n/a	n/a	2185.59	43200.01	16634483	0	n/a	n/a	2185.47	43200.03	16614547	0
3.7	2	n/a	n/a	3194.06	43200.01	28045959	n/a	n/a	2703.76	43200.01	6096904	0	n/a	n/a	2704.18	43200.0	6110110	0
3.9	3	n/a	n/a	1654.94	43200.01	10211824	n/a	n/a	1588.79	43200.01	10207254	0	n/a	n/a	4576.74	43200.03	1192210	0

Table 4: Instances for Net2 that reached the time limit of 12 hours (without cuts).



(a) Runtime comparison on `net1`.



(b) Runtime comparison on `net2`.

Fig. 7.3: Runtime comparison on instance `net1` and `net2`. Each cross ( $\times$ ) corresponds to a single instance of the test set. Note that multiple crosses are drawn in the upper right corner of the plots that cannot be differed. They represent those instances that ran into the time limit for SCIP without and with using our cuts.

## 8 Conclusions and Outlook

We considered a network design and extension problem for natural gas transmission networks, where the gas flow is not only governed by flow conservation constraints in nodes (as in classical linear network flow problems), but also subject to nonlinear functions depending on node potential values (which represent the gas pressure in the nodes). We gave a model formulation, and applied a standard MINLP solver for its solution. We derived additional valid inequalities for the topology optimization problem. We could demonstrate by numerical experiments on a test set of instances that the separation of these new inequalities leads to significant smaller branch-and-bound trees and thus lower overall running times.

So far, we considered loop extensions only. From a practical point of view these kind of extensions are desired by network operations since they are cheaper than non-loop pipelines. From a computational point of view this restriction limits the amount of potential extensions. When adding all possible pipelines between all node pairs in the network, the model and the combinatorial decisions would be so large that the computations would not finish within a reasonable time limit, even when adding our cuts. Hence new techniques for making a reasonable selection of new pipes are necessary in the first place. To this end, it is necessary to further speed up the computations. Hereto, the methods presented in [19] could be used, instead of solving subproblems of the topology optimization model via linear programming. This is one of our future research directions.

Finally, our method was applied to the case of a single invalid nomination. In practice, however, one has to deal with a whole set of different infeasible nominations, and needs to determine a topology extension that can cope with all of them simultaneously. The extension of our methods to this multi-scenario case is a further area of our current research.

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