A NEW ALGORITHM FROM SEMI-INFINITE OPTIMIZATION FOR A PROBLEM OF TIME-MINIMAL CONTROL*

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Исследуется алгоритмический подход к задаче управления нагреванием (или охлаждением) однородного шара за минимальное время. Крабс показал [28], что эта задача оптимального управления может быть интерпретирована как задача двухстадийной оптимизации. На первой стадии решается задача минимального по норме управления, а на второй — задача обобщенной полубесконечной оптимизации. Итерационная процедура реализует обе стадии, включая аппроксимацию негладких функций и пошаговое применение метода дискретизации к задаче оптимизации. Для иллюстрации алгоритма наряду с комментированной блок-схемой используются описания различных вариантов, альтернатив и практических приемов.

1. Introduction

This article is devoted to a problem, given by t*ime* m*inimal heating* (or cooling) *of a ball*. In this example of an optimal control problem, we consider questions concerned with problem representation, theoretical and practical solvability and structural frontiers.

The ball B consists of a homogeneous material. Based on a description in the article *Krabs* [28], we study the problem

$$\mathcal{P}^{\mathsf{tm}} \quad \begin{cases} \text{Min } \mathsf{I}(T,u) := T \text{ , such that} & (1)\\ \text{there is a bounded function } \theta : [0,R]\times[0,\infty) \to I\!R, \text{ where} & \\ \theta|(0,R)\times(0,\infty) \text{ is partially differentiable,} & \\ u = \theta(R,\cdot)|[0,T] \text{ is continuous, and} & \\ \theta_t(r,t) = a\Delta\theta(r,t) = \frac{a}{r^2}\frac{\partial}{\partial r}(r^2\theta_r(r,t))((r,t)\in(0,R]\times(0,\infty)), & (2)\\ \theta(r,0) = \theta_0 \quad (r\in[0,R]), & (3)\\ \theta(R,T) = \theta_E, & (4)\\ T \geq 0, & (5)\\ |\sigma_u(R,t)| \leq \sigma^* \quad (t\in[0,T]). & (6) \end{cases}$$

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Here, $\Delta\theta$ represents the Laplacian of θ and R denotes the radius of B. The temperature $\theta(r,t)$ is a function of the radial variable r, where r measures the distance from the center point 0_3 of B, and of the time t. Moreover, we start with an **initial** temperature θ_0 and finish with an intended **target** (end) temperature $\theta_E > \theta_0$ (or $\theta_E < \theta_0$, respectively). Because of this inequality, each time $\widehat{T}$ which is optimal for $\mathcal{P}^{\mathsf{tm}}$, can not be zero (i. e., $\widehat{T} > 0$). The temperature is essentially governed by the heat equation (2), where $a > 0$ describes the coefficient of heat conductivity (see *Myint-U* [32]). This can effectively be realized by the substitution $v(r,t) := r\theta(r,t)$ in (2). We interpret $u_T(\cdot) := u(\cdot) = \theta(R,\cdot)|[0,T]$ as a *control variable* ($T \geq 0$). Now, we are focussing on *partial differential equations* with the following unique solution of the (boundary-value) problem (2) – (4) (see *Krabs* [28]):

$$\left.\begin{array}{rcl} \theta(r,t) & = & 2r \sum\limits_{k=1}^{\infty} \frac{(-1)^{k+1}}{k\pi} \exp(-a(\frac{k\pi}{R})^2 t)\theta_0 \frac{1}{r} \sin(\frac{k\pi}{R} r) \; + \\ & + & \frac{2a}{R} \sum\limits_{k=1}^{\infty} (-1)^{k+1} k\pi \cdot \int\limits_0^t \exp(-a(\frac{k\pi}{R})^2 (t-s))\, u(s)\, ds \; \cdot \frac{1}{r} \sin(\frac{k\pi}{R} r)\,. \end{array}\right\} \tag{7}$$

Furthermore, the function $\sigma_u(r,t)$ denotes some thermal stress tangential to the boundary $\partial\mathsf{B}$ of B ($r = R$). Finally, σ^* is a given upper bound of the stress.

Under suitable physical assumptions, at the boundary the function $\sigma_u = \sigma_u^{\theta_0}$ has the form

$$(\sigma_u(R,t) \;=)\;\; \sigma_u^{\theta_0}(R,t) \;=\; \frac{E\alpha}{1-\mu} \Big(\frac{3}{R^3} \int\limits_0^R \theta(r,t) r^2\, dr \;-\; u(t) \Big). \tag{8}$$

(For more details see *Parkus* [34], where other elementary geometrical bodies are considered.) Here, E is the modulus of elasticity, μ and α are the coefficients of cross-extension and linear heat extension, respectively. By means of (7), (8) represents the thermal stress for $r = R$, that can be evaluated further. Its dependence on the parameter θ_0, indicated in (8), then becomes obvious.

Fig. 1 displays the ball with its distribution of temperatures at some time t.

2. Evaluation of the Problem

2.1. Problem Decomposition

In the article *Krabs* [28], a first interpretation of $\mathcal{P}^{\mathsf{tm}}$ as a problem from **two-stage optimization** is given, based on the representation (7) of the temperature.

On the *lower stage*, for each $T \geq 0$ we consider the one-parameter family $(\mathcal{P}_T^{\mathsf{nm}})_{T\in[0,\infty)}$ of *norm-minimal control problems* on the thermal stress at the boundary, given by

$$\mathcal{P}_T^{\mathsf{nm}} \qquad \left\{ \begin{array}{l} \mathrm{Min}_{u_T} \; ||\sigma_{u_T}^{\theta_0}(R,\cdot)||_{\infty,T}, \\ \\ \text{where } \; u_T \in C([0,T], I\!R) \;\; \text{fulfills} \\ \\ \qquad u_T(T) \;=\; \theta_E. \end{array} \right\} \tag{9}$$

The mapping $||\cdot||_{\infty,T}$ denotes the maximum-norm for continuous functions on $[0,T]$. This problem is called an *approximation problem*. (See *Braess* [3], *Krabs* [27], *Jongen/Jonker/Twilt* [16] for further details.) In *Krabs* [28] we find the following re sult:

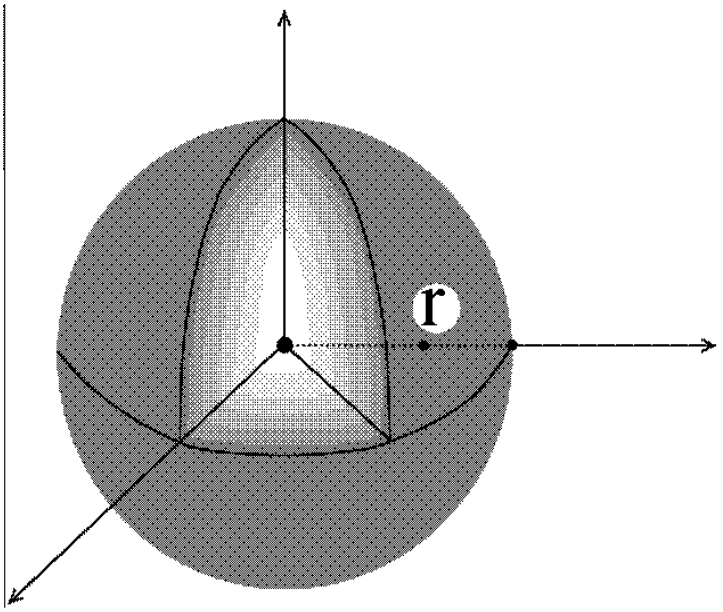

Fig. 1. A ball B consisting of a homogeneous material, and its temperature distribution. Increasing darkness represents increasing temperature.

Item 1: For each $T \geq 0$ the problem $\mathcal{P}_T^{\mathsf{nm}}$ has *precisely one* solution $\hat{u}_T$. ∎

This (unique) solution $\hat{u}_T$ of $\mathcal{P}_T^{\mathsf{nm}}$ $(T \geq 0)$ is

$$\hat{u}_T(t) \;:=\; \tfrac{\theta_E - \overline{y}_T(T)}{\overline{u}_T(T)} \cdot \overline{u}_T(t) + \overline{y}_T(t) \quad (t \in [0,T])\,, \tag{10}$$

where $(\overline{u}_T, \overline{y}_T)$ is the unique solution of the system of integral equations:

$$\left.\begin{array}{rcl} \overline{u}_T(t) \;-\; \int\limits_0^t k(t-s)\overline{u}_T(s)\,ds &=& 1 \\ \overline{y}_T(t) \;-\; \int\limits_0^t k(t-s)\overline{y}_T(s)\,ds &=& \overline{\theta}_0(t) \end{array}\right\} \quad (t \in [0,T])\,. \tag{11}$$

Here, we have

$$k(t) \;:=\; \tfrac{6a}{R^2} \sum_{k=1}^{\infty} \exp(-a(\tfrac{k\pi}{R})^2 t)\,, \tag{12}$$

$$\overline{\theta}_0(t) \;:=\; \tfrac{6}{R^2} \sum_{k=1}^{\infty} \tfrac{1}{(k\pi)^2} \exp(-a(\tfrac{k\pi}{R})^2 t)\,\theta_0\,. \tag{13}$$

The mapping $u_\vee^0(t,T) := \hat{u}_T(t)$ is called a *core of a Kuhn-Tucker function* or, more precisely: a global minimizer function. In the special case $\theta_0 = 0$ and, hence, $\overline{\theta}_0 \equiv 0$, the variable $\overline{y}_T \equiv 0$ is the unique solution of the second equation from system (11). Hence, the representation (10) of $\hat{u}_T$ simplifies and we observe (*Krabs* [28]):

$$\overline{u}_T(t) \;=\; 1 + \int\limits_0^t r(t-s)\,ds \qquad (t \in [0,T])\,, \tag{14}$$

where

$$r(t) \;:=\; \sum_{\kappa=1}^{\infty} k_\kappa(t) \quad (t \in [0,T])\,, \tag{15}$$

$$k_1(t) \;:=\; k(t) \quad (\text{cf. (12)})$$

and

$$k_\kappa(t) \;=\; \int_0^t k_{\kappa-1}(t-s)k(s)\,ds (t \in [0,T],\; \kappa \in I\!N \setminus \{1\}). \tag{16}$$

Tricomi [40] provides more information on the solution theory of integral equations. Related qualitative or numerical aspects can be found in *Gripenberg/Londen/Staffans* [6], *Hackbusch* [9] and *Jörgens* [15]. Concerning the heat equation and methods from the optimal control, we also refer to *Hackbusch* [8]. Moreover, for $\mathcal{P}^{\mathsf{tm}}$ further basic theory can be found in *Krabs* [26], [29].

Inserting the optimal control variables $(u =)\,\hat{u}_T$ into the given problem $\mathcal{P}^{\mathsf{tm}}$ leads to the upper stage, given by the following *generalized semi-infinite ($\mathcal{GSI}$) optimization problem* of class C^0, with $x := T$ and $y := t$:

$$\mathcal{P}_{\mathcal{GSI}}(f,g,v) \qquad \left\{ \begin{array}{l} \text{Min} \quad f(x) := x \quad \text{such that} \\ \qquad \pm\, \sigma_{u_T}^{\sigma_0}(R,y) + \sigma^* \;\geq\; 0 \quad (y \in Y(x)), \\ \qquad x \;\geq\; 0, \\ \text{where} \quad Y(x) \;:=\; [0,x] \quad (x \in I\!R). \end{array} \right\} \tag{17}$$

Here, g, u comprise the three or two continuous inequality constraints on x and y, respectively. A similar way of (partially) representing $\mathcal{P}^{\mathsf{tm}}$ by a *generalized semi-infinite optimization problem* is done in *Kaplan/Tichatschke* [20]. The problem $\mathcal{P}^{\mathsf{tm}}$ is an example of a so-called terminal problem. For a first numerical treatment see the paper *Kaplan/Tichatschke* [21], which also includes a convergence theorem.

From *Krabs* [28] we get the following second item:

Item 2: Under the *parameter constellation*

$$\theta_0 \;=\; 0, \qquad d \;=\; \tfrac{\sigma^*(1-\mu)}{E\alpha} \;<\; |\theta_E|,$$

$\mathcal{P}_{\mathcal{GSI}}(f,g,v)$ has *precisely one* optimal solution $\widehat{T}$. ∎

Then, the pair $(\widehat{T}, \hat{u}_{\widehat{T}})$ is the **unique solution** of the problem $\mathcal{P}^{\mathsf{tm}}$. *Item 2* on $\mathcal{P}_{\mathcal{GSI}}(f,g,v)$ is based on a monotonicity argumentation which ensures that the function

$$\hat{d}(T) \;:=\; |d(T,\theta_E)| - d \quad (T \in [0,\infty)) \tag{18}$$

has a single zero, where

$$d(T,\theta_E) \;:=\; \tfrac{|\theta_E|}{\bar{u}_T(T)}. \tag{19}$$

2.2. Problem Treatment: the Basic Idea

Krabs [28] directs his attention to an approximate solution of the problems $\mathcal{P}_T^{\mathsf{nm}}$ $(T \in [0, \infty))$ of the lower stage. Now, we embed this approximation into an iterative concept of solving $\mathcal{P}^{\mathsf{tm}}$. Remember that our approach can be interpreted as a two-stage optimization problem, where $\mathcal{P}_{\mathcal{GSI}}(f, g, v)$ becomes treated, too. The functional data of this $\mathcal{GSI}$ problem are *continuous*, but they need *not* be differentiable. Hence, in order to apply the approaches from *Weber* [42], [43] or *Pickl, Weber* [35], we must **approximate** continuous data by C^1-differentiable functions. This will be done by means of *approximate problems*, defined by exchanging series (see, e. g., (12) – (13), (15)) by their ν^{th} partial sum $(\nu \in \mathbb{N})$.

Another obstacle consists in the fact that, here, it is hard to verify or falsify boundedness and EMFCQ for $M_{\mathcal{GSI}}[g]$. So, little structural or topological knowledge exists about the latter set. If, however, the functional approximations lead to set approximations of $M_{\mathcal{GSI}}[g]$ of *topological manifold* character, then we could **combine** such a process (approximation) with our **iteration procedure** from *Weber* [42] (or [43]). By this stepwise and levelwise process, $\mathcal{P}^{\mathsf{tm}}$ becomes described closer and closer.

Based on a presentation of an iterative concept, we are going to discuss these opportunities of a stepwise (perturbational) approximation. For that purpose we choose the concept of (equidistant) **discretization**, which extends from the $\mathcal{GSI}$ *Approach I* of *Weber* [42] (or [43]) to the whole two-stage problem with its two variables x and y. For a better understanding, we give a short description of that approach (see also *Weber* [44]).

2.3. A General Iteration Concept and Its Foundations

$\mathcal{GSI}$ problems have the following form:

$$\mathcal{P}_{\mathcal{GSI}}(f, h, g, u, v) \qquad \begin{cases} \text{Minimize} \quad f(x) \ \text{ on } \ M_{\mathcal{GSI}}[h, g], \quad \text{where} \\ \\ M_{\mathcal{GSI}}[h, g] \ := \ \{\, x \in \mathbb{R}^n \mid \ h_i(x) = 0 \ \ (i \in I), \\ \\ \qquad\qquad\qquad\qquad g(x, y) \geq 0 \ \ (y \in Y(x))\,\}. \end{cases}$$

The semi-infinite character comes from the perhaps infinite number of elements of $Y = Y(x)$, while the generalized character is due to the x-dependence of $Y(\cdot)$. These latter index sets are supposed to be feasible sets in the sense of f initely constrained $(\mathcal{F})$ optimization, i. e.:

$$Y(x) \ = \ M_{\mathcal{F}}[u(x, \cdot), v(x, \cdot)] := \{\, y \in \mathbb{R}^q \mid u_k(x, y) = 0 \ (k \in K), \ v_\ell(x, y) \geq 0 \ (\ell \in L)\} \qquad (x \in \mathbb{R}^n).$$

Let $h = (h_i)_{i \in I}$, $u = (u_k)_{k \in K}$ and $v = (v_\ell)_{\ell \in L}$ comprise $h_i : \mathbb{R}^n \to \mathbb{R}$, $i \in I := \{1, \ldots, m\}$, $u_k : \mathbb{R}^n \times \mathbb{R}^q \to \mathbb{R}$, $k \in K := \{1, \ldots, r\}$, and $v_\ell : \mathbb{R}^n \times \mathbb{R}^q \to \mathbb{R}$, $\ell \in L := \{1, \ldots, s\}$, respectively. We assume that $f : \mathbb{R}^n \to \mathbb{R}$, $g : \mathbb{R}^n \times \mathbb{R}^q \to \mathbb{R}$, $h_i \, (i \in I)$, $u_k \, (k \in K)$ and $v_\ell \, (\ell \in L)$ are continuously differentiable. We locally focus our attention by referring to a given open, bounded set $\mathcal{U}^0 \subseteq \mathbb{R}^n$. Here, we make the following assumptions on the lower stage (of y):

Assumption $\mathbf{A}_{\mathcal{U}^0}$: $\cup_{x \in \overline{\mathcal{U}^0}} Y(x)$ is *bounded* (hence, by continuity, compact).

In *generalized* semi-infinite optimization, the feasible set need not be closed. However, the following assumption guarantees closedness.

Assumption $\mathbf{B}_{\mathcal{U}^0}$: For all $x \in \overline{\mathcal{U}^0}$, the **linear independence constraint qualification (LICQ)** is fulfilled for $M_{\mathcal{F}}[u(x, \cdot), v(x, \cdot)]$. This means, that the family of vectors

$$D_y u_k(\overline{x},\overline{y}),\ k\in K,\quad D_y v_\ell(\overline{x},\overline{y}),\ \ell\in L_0(\overline{x},\overline{y}),$$

is linearly independent, where $L_0(\overline{x},\overline{y}) := \{\,\ell\in L \mid v_\ell(\overline{x},\overline{y}) = 0\,\}$ consists of active indices.

By means of some differential topology (*Hirsch* [12], *Jongen/Jonker/Twilt* [17]), these assumptions permit local linearization of $Y(x)$ $(x\in\overline{\mathcal{U}^0})$ by finitely many C^1-diffeomor phisms $\phi_x^j : \mathcal{V}^j \to S^j$ $(j\in J)$ in such a way that the images Z^j are *x-independent* squares (in hyperplanes). Herewith, $\mathcal{P}_{\mathcal{GSI}}(f,h,g,u,v)$ becomes represented (in $\overline{\mathcal{U}^0}$) by an **ordinary** *semi-infinite* optimization problem $\mathcal{P}_{\mathcal{OSI}}(f,h,g^0,u^0,v^0)$ with feasible set $M_{\mathcal{OSI}}[h,g^0]\cap\overline{\mathcal{U}^0} = M_{\mathcal{GSI}}[h,g]\cap\overline{\mathcal{U}^0}$. (For details see *Weber* [41], [43].)

We also need a constraint qualification on the upper stage (of x):

Definition. Let a point $\overline{x}\in M_{\mathcal{GSI}}[h,g]$ be given. We say that the **extended Mangasarian-Fromovitz constraint qualification (EMFCQ)** is fulfilled at $\overline{x}$, if the following conditions $EMF_{1,2}$ are satisfied:

EMF$_1$. The family of vectors $Dh_i(\overline{x})$, $i\in I$, is linearly independent.

EMF$_2$. There exists an "*EMF-vector*" $\zeta\in\mathbb{R}^n$ such that

$$Dh_i(\overline{x})\,\zeta = 0 \quad \text{for all } i\in I,$$

$$D_x g_j^0(\overline{x},z)\,\zeta > 0 \quad \text{for all } z\in\mathbb{R}^q,\ j\in J,\ \text{with } (\phi_{\overline{x}}^j)^{-1}(z)\in Y_0(\overline{x}),$$

where $Y_0(\overline{x}) := \{\,y\in Y(\overline{x}) \mid g(\overline{x},y) = 0\,\}$ consists of *active* indices. **EMFCQ** is said to be fulfilled for $M_{\mathcal{GSI}}[h,g]$ on $\overline{\mathcal{U}^0}$, if EMFCQ is fulfilled for all $x\in M_{\mathcal{GSI}}[h,g]\cap\overline{\mathcal{U}^0}$.

The following three theorems underline the importance of *EMFCQ* for establishing that $M_{\mathcal{GSI}}[h,g,u,v] := M_{\mathcal{GSI}}[h,g]$ is a topological manifold with boundary, it behaves continuous, but also stable under perturbations of the defining functional data. With these perturbations we remain inside of suitable open neighbourhoods of (h,g,u,v) in the sense of the *strong* or *Whitney topology* C_S^1 that takes into account asymptotic effects. Concerning the Lipschitzian condition of local linearizability (by Lipschitzian charts), upper and lower semi-continuity, continuity (in the Hausdorff-metric), transversality (absense of tangentiality) and topological stability (in the sense of homeomorphy) see *Berge* [2] and *Weber* [43].

Manifold Theorem (*Weber* [43]). Let EMFCQ be fulfilled in $\overline{\mathcal{U}^0}$ for $M_{\mathcal{GSI}}[h,g]$. Then there is an open neighbourhood $\mathcal{W}\subseteq\mathbb{R}^n$ of $\overline{\mathcal{U}^0}$ such that $M_{\mathcal{GSI}}[h,g]\cap\mathcal{W}$ is a *Lipschitzian manifold (with boundary)* of the *dimension* $n-m$.

Continuity Theorem (*Weber* [42], [43]). Let EMFCQ be fulfilled in $\overline{\mathcal{U}^0}$ for $M_{\mathcal{GSI}}[h,g]$. Moreover, let the closure $\overline{\mathcal{W}}\subseteq\mathbb{R}^n$ of some open set $\mathcal{W}\subseteq\mathcal{U}^0$ be representable as a feasible set from finitely constrained optimization which fulfills *LICQ*, and let the intersection of its boundary $\partial\mathcal{W}$ with $M_{\mathcal{GSI}}[h,g]$ be transversal. Then, there is an open C_S^1-neighbourhood $\mathcal{O}\subseteq(C^1(\mathbb{R}^n,\mathbb{R}))^m\times C^1(\mathbb{R}^{n+q},\mathbb{R})\times(C^1(\mathbb{R}^{n+q},\mathbb{R}))^r\times(C^1(\mathbb{R}^{n+q},\mathbb{R}))^s$ of (h,g,u,v) such that $\mathsf{M}^{\mathcal{W}} : (\tilde{h},\tilde{g},\tilde{u},\tilde{v})\mapsto M_{\mathcal{GSI}}[\tilde{h},\tilde{g},\ \tilde{u},\tilde{v}]\cap\overline{\mathcal{W}}$, is *upper* and *lower semi-continuous* at all $(\tilde{h},\tilde{g},\tilde{u},\tilde{v})\in\mathcal{O}$.

If, moreover, $\mathcal{W}$ is bounded, then $\mathcal{O}$ can be chosen so that $\mathcal{O}$ is mapped to $\mathcal{P}_c(\mathbb{R}^n)$ by M and M is *continuous*.

Stability Theorem (*Weber* [42], [43]). The feasible set $M_{\mathcal{GSI}}[h,g]$ is *topologically stable, if and only if EMFCQ* is fulfilled for $M_{\mathcal{GSI}}[h,g]$.

In Approach I of *Weber* [42], [43] we *discretize* the x-independent squares Z^j of inequality constraints. Here, we take a regular grid, such that any two neighbouring points of the finitely

many grid points $z^{\sigma,\nu}$ are equidistant (in each step $\nu \in \mathbb{N}$). Making the underlying grid finer and finer, we arrive at a sequence of *finitely constrained* problems $\mathcal{P}_{\mathcal{F}}(f,h,g^{0,\nu})$ ($\nu \in \mathbb{N}$) which are easier to treat and have global minimizers $\hat{x}^{\nu}$. Using *Continuity Theorem* and *Stability Theorem*, we see that there exists a subsequence $(\hat{x}^{\nu_\kappa})_{\kappa\in\mathbb{N}}$ converging towards a global minimizer $\hat{x}$ of our given problem. (For more details and further approaches cf. *Weber* [43].)

2.4. Problem Treatment: an Explanation

Let us come back to the treatment of $\mathcal{P}^{\mathsf{tm}}$, interpreted as a two-stage problem. For our approach, first numerical experience is done by *Jathe/Pickl/Weber* [14] using *Mathematica* (cf. *Kaufmann* [24]). The computation bases on given (fixed) parameters $a, R, \alpha, \mu, \sigma^*$, θ_0, θ_E, and more technical (auxiliary) parameters of initialization and termination. These auxiliary parameters are ν^0, ν^1, and ν^E (being sufficiently large, $\nu^0 < \nu^1 < \nu^E$), $m_{\nu^0-1}, c^0, \ell^0, s^0, \epsilon^0, \epsilon^E$, and d (defined in the way of *Item 2*). Herewith, we have initialized the essence of a corresponding "*commented flow diagram*".

After the following basic considerations, we continue to present and explain the *flow diagram* below.

We also can weaken the full discretization by means of referring to nondiscretized (here: differentiable) approximate functions on the upper stage. If we rigorously simplified the model functions, then this weakening would become a preferable alternative. For example, then we could apply the nonlinear optimization subroutine *Find Minimum* of *Mathematica* on Lagrange (penalty) functions or, alternatively, a quasi-Newton method for finding a zero of its gradient (later on, see also (33)).

Let us come back to the preparation of our *flow diagram*. If we do not know whether $M_{\mathcal{GSI}}[g]$ is bounded, we introduce an upper bound $T_\nu^{m_\nu-1} > 0$ of $(x =)\, T$ in each step ν, where $m_\nu = 4^{\nu-\nu^0}\nu^0 + 1$ and $T_\nu^{m_\nu-1} = 2^{\nu-\nu^0}\nu^0$. Let $\nu \in \mathbb{N}$ be already chosen appropriately large, say $\nu \geq \nu^0$ with respect to some $\nu^0 \in \{4k \,|\, k \in \mathbb{N}\}$ being divisible by 4. In other words, we remain in the T-interval $[0, T_\nu^{m_\nu-1}]$ (or, to make a numerical differentiation later on: in a bit larger interval $[T_\nu^{-1}, T_\nu^{m_\nu}]$). This set becomes discretized and then, based on the grid points $T = T_\nu^\ell$ ($\ell \in \{-1, \ldots, m_\nu\}$), the $(y =)\, t$-interval $Y(T) = [0,T]$ becomes analogously discretized, too. Here, we are in a standard situation with natural coordinate transformation $\phi_x : y \mapsto z$, where $y = zT$, $z \in [0,1]$. Turning from step ν to step $\nu+1$, the considered T-interval reaches a double size and a double finess of discretization.

Because of our discretization, the constraint $T \geq 0$ on the upper stage will be satisfied automatically. For the two other constraint functions g_σ ($\sigma \in \{1, 2\}$) we need not distinguish between index sets $Y^\sigma(T)$, but refer to $Y(T)$ alone. Despite of some nice properties (e. g., the reverse monotonicity behaviour of g_1 and g_2) the special properties from *Weber* [43], Chapters 1 and 3, (e. g., quasi concavity) are hard to verify here.

We shall study the geometry or topology of some approximate set $M_{\mathcal{GSI}}[g^\nu] \cap (-\infty, T_\nu^{m_\nu-1}]$. In the case of a manifold form we conclude EMFCQ for this set by using *Manifold Theorem*.

Using *Krabs* [28] and a convergence argumentation based on strictly monotonical decreasing (invertibility), we easily prove the "approximate version" of *Item 2*. For an illustration see Fig. 2, (a).

Item 3: Under the parameter constellation from *Item 2*, the ν^{th} approximate problem has precisely one optimal solution $\widehat{T}_\nu$ for sufficiently large ν. For $\nu \to \infty$, the sequence of solutions $\widehat{T}_\nu$ tends to the desired (unique) solution $\widehat{T}$ of $\mathcal{P}^{\mathsf{tm}}$. ∎

In the *general* case of a parameter constellation, our iteration also analyzes the strictly monotonical decreasing of a function $T \mapsto \hat{d}_\nu(T)$, which approximates $T \mapsto \hat{d}(T)$. We write in short: $\hat{d}_{\cdot,\nu} := \hat{d}_\nu(\cdot)$; see the illustration in Fig. 2, (*b*), (i) (*Jathe/Pickl/Weber* [14]). Herewith, we study the zero sets of $\hat{d}_{\cdot,\nu}$ and $\hat{d}(\cdot)$. We get a better visualization and qualitative understanding of $M_{\mathcal{GSI}}[g]$ by raising the bound $T_\nu^{m_\nu - 1}$ with the factor 2 step by step.

Altogether, on the other hand, we wish to find (in certain steps) a smaller (sub)interval that contains a solution $\widehat{T}$. Finally, to hope to arrive at an approximate solution $\widehat{T}_\nu \approx \widehat{T}$ of the given problem $\mathcal{P}^{\mathsf{tm}}$ ("$\approx$" stands for *nearby*), where $\widehat{T}_\nu$ lies in the zero set of $\hat{d}_{\cdot,\nu}$. In case of such a successful interval adaption, the doubling of the interval size *stops*.
For the iteration process, we choose a mainly **Lagrangian** *(penalty)* way. This way is presented below, and it also incorporates the (previously described) graphical and numerical evaluations with respect to $\hat{d}_{T,\nu}$.

The intimate relation between t and T ($t \in [0,T]$) motivates a slightly *modified* variant of Approach I (see Alternative (II) below). We have $z_\nu^{\ell,j} := \frac{t_\nu^j}{T_\nu^\ell}$, where $t_\nu^j = T_\nu^j$ ($j \in \{0, \ldots, \ell\}$). Subsequently, we state both versions and indicate two further alternative variants. (Our notational modifications with respect to Subsection 2.3 should not cause misunderstandings.)

Now, we define, calculate and visualize according to the following (commented) "flow diagram". We omit technicalities, e. g., smaller enumerating loops. For more information on the ("discrete") variables in (20) – (25) below, we refer to *Kaiser/Krabs* [19] (cf. also *Tricomi* [40]). In a balanced way we consider both the usual (functional) notation of this work and elements of *Mathematica*. (The causal sequel within the "flow" differs from *Mathematica*.)

Commented flow diagram (fixed parameters being given, alternatives implied):

Mark (A) $\underline{\nu = \nu^0}$ *(initialization)*:

$c_{\nu^0} := 4\,, \quad q_{\nu^0} := 1\,, \quad p_{\nu^0} := 1\,,$
$s_{\nu^0} := s^0 > 0\,, \quad \epsilon_{\nu^0} := \epsilon^0 > 0\,,$ and $\ell_{\nu^0} := \ell^0 \quad$ (e. g., $\ell^0 := \nu^0$)$\,,$
$m_{\nu^0 - 1} := \frac{\nu^0}{4} + 1\,,$
$v^j_{\sigma,\nu^0} := 1 \quad (j \in \{0, \ldots, m_{\nu^0-1} - 1\},\ \sigma \in \{1, 2\})\,.$ **Mark (B)** $\underline{\nu \geq \nu^0}$ *(declarations, recursion and adaptions)*:

$m_\nu := c_\nu \cdot (m_{\nu-1} - 1) + 1,$
$(T =)\ T_\nu^{-1} := -2^{-\nu+\nu^0}, \quad (t =)\ t_\nu^{-1} := -2^{-\nu+\nu^0},$
$(T =)\ T_\nu^{\ell+1} := T_\nu^\ell + 2^{-\nu+\nu^0}, \quad (t =)\ t_\nu^{\ell+1} := t_\nu^\ell + 2^{-\nu+\nu^0} \quad (\ell \in \{-1, \ldots, m_\nu - 1\})\,.$
(Subsequently, we especially refer to these discrete values of T and t.)

$$k_\nu(t) := \tfrac{6a}{R^2} \sum_{k=1}^{\nu} \exp(-a(\tfrac{k\pi}{R})^2 t)\,, \tag{20}$$

$$k_{\nu,1}(t) := k_\nu(t) \quad \text{and} \tag{21a}$$

$$k_{\nu,\kappa}(t) := \int_0^t k_{\nu,\kappa-1}(t-s) k_\nu(s)\, ds \quad (\kappa \in I\!N \setminus \{1\}). \tag{21b}$$

(Here, we apply a standard method from numerical integration; e. g., *Krylov* [31], or the subroutine *Integrate*.) For the following *approximate* definitions (23), (25) (remember (11)), the *index* T may be omitted in the variables $\overline{u}_{T,\nu}(t)$, $\overline{y}_{T,\nu}(t)$, respectively:

$$r_\nu(t) := \sum_{\kappa=1}^{\nu} k_{\nu,\kappa}(t)\,, \tag{22}$$

$$\overline{u}_{T,\nu}(t) := 1 + \int_0^t r_\nu(t-s)\, ds\,, \tag{23}$$

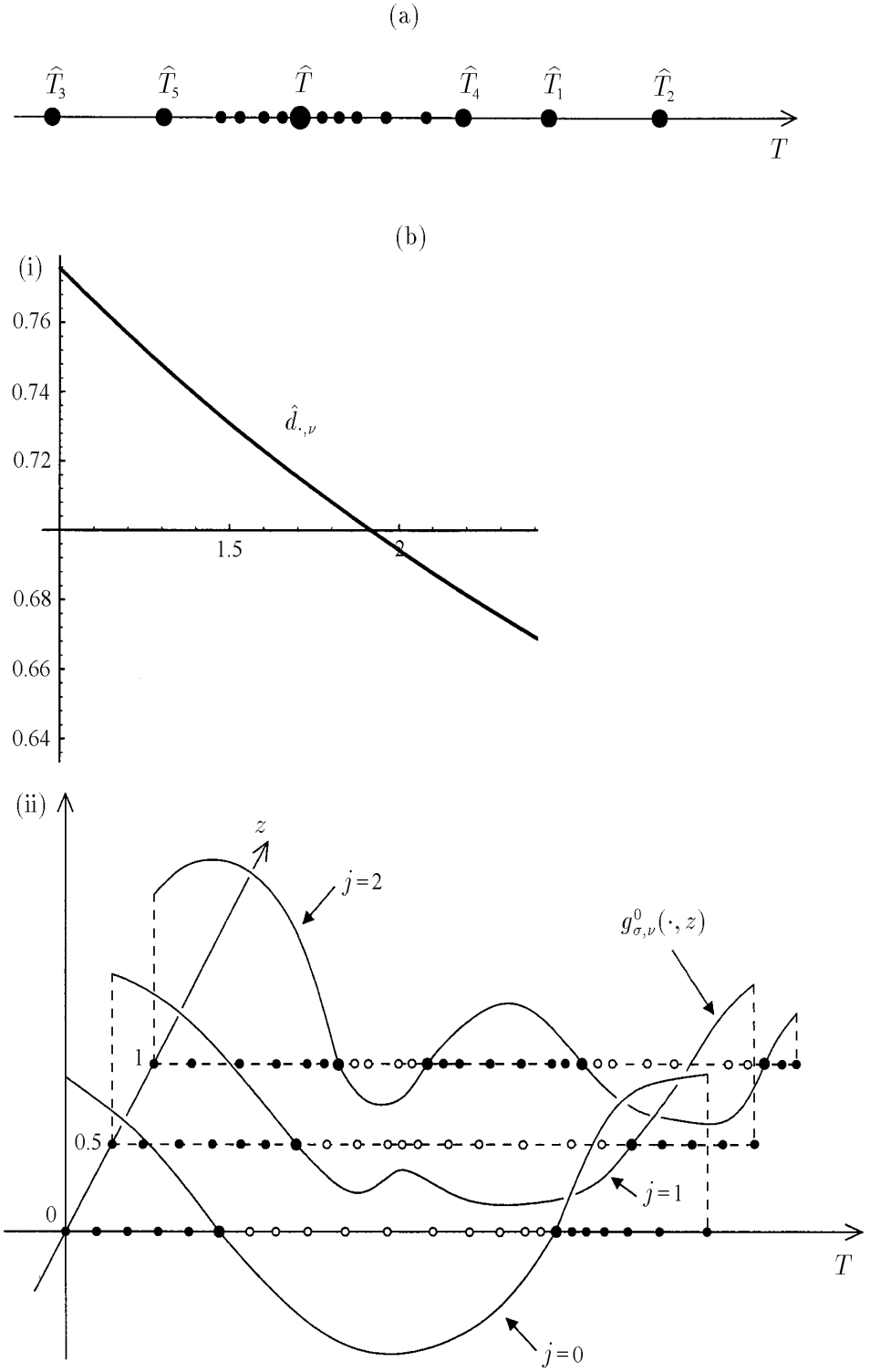

Fig. 2. Iteration procedure for solving $\mathcal{P}^{\mathsf{tm}}$ (visualization, some examples):
(a) Under the parameter constellation from *Item 2*: *Find the unique solution* $\widehat{T}$ *with the help of stepwise minima* $\widehat{T}_\nu$ (see *Item 3*).
(b) General parametrical case:
(i) a function $\hat{d}_{\cdot,\nu}$ (based on a numerical computation from *Jathe/Pickl/Weber* [14]),
(ii) graphs $g^0_{\sigma,\nu}(\cdot,z)$ and zeroes of functions $g^0_{\sigma,\nu}(\cdot,z)-\alpha$.

$$\overline{\theta}_{0,\nu}(t) \;:=\; \tfrac{6}{R^2}\big(\sum_{k=1}^{\nu} \tfrac{1}{(k\pi)^2}\exp(-a(\tfrac{k\pi}{R})^2 t)\big)\theta_0\,, \tag{24}$$

$$\overline{y}_{T,\nu}(t) \;:=\; \overline{\theta}_{0,\nu}(t) + \int_0^t r_\nu(t-s)\overline{\theta}_{0,\nu}(s)\,ds \quad \text{and, finally,} \tag{25}$$

$$d_{T,\nu} \;:=\; \tfrac{|\theta_E - \overline{y}_{T,\nu}(T)|}{\overline{u}_{T,\nu}(T)}\,, \tag{26}$$

$$\hat{d}_{T,\nu} \;:=\; |d_{T,\nu}| \,-\, d\,. \tag{27}$$

Alternative (I): Up to a renumbering, about a quarter of all the points t the values $k_\nu(t)$, $\overline{\theta}_{0,\nu}(t)$ can recursively be determined from $k_{\nu-1}(t)$, $\overline{\theta}_{0,\nu-1}(t)$. Hence, storing suitable variables from the foregoing step, many calculations need not to be performed. Therefore, we put

$$k_{\nu^0-1}(t) := \tfrac{6a}{R^2}\sum_{k=1}^{\nu^0-1}\exp(-a(\tfrac{k\pi}{R})^2 t), \quad \overline{\theta}_{0,\nu^0-1}(t) := \tfrac{6}{R^2}\big(\sum_{k=1}^{\nu^0-1}\tfrac{1}{(k\pi)^2}\exp(-a(\tfrac{k\pi}{R})^2 t)\big)\theta_0,$$
$$k_\nu(t) := k_{\nu-1}(t) + \tfrac{6a}{R^2}\exp(-a(\tfrac{\nu\pi}{R})^2 t), \quad \overline{\theta}_{0,\nu}(t) := \overline{\theta}_{0,\nu-1}(t) + \tfrac{6}{(\nu\pi R)^2}\exp(-a(\tfrac{\nu\pi}{R})^2 t)\theta_0$$
$$(\nu \geq \nu^0). \quad \square$$

We investigate the qualitative form of the graph of $T \mapsto \hat{d}_{T,\nu}$, especially its monotonicity and, finally, its zeroes. Therefore, Newton's method can be applied (see, e. g., *Jongen/Triesch* [18]). *Krabs* [30] suggests *regula falsi*. Moreover, we *visualize* (plot) the graph in a figure and, concerning monotonicity, we study the corresponding arithmetic mean $\triangle\hat{d}_\nu^\ell$ of the left and right hand side difference quotients at T_ν^ℓ: $\triangle\hat{d}_\nu^\ell := \frac{\hat{d}_{T_\nu^{\ell+1},\nu} - \hat{d}_{T_\nu^{\ell-1},\nu}}{2^{-\nu+\nu_0+1}}$. (One can make a case study based on the nondifferentiable form of $\hat{d}_{\cdot,\nu}$; see (18).) During the investigation, we observe the behaviour of the sequence of zero sets. In particular we look for a limit set, perhaps consisting of the singleton $\widehat{T}$. Furthermore, we define

$$\hat{u}_{T,\nu}(t) \;:=\; \tfrac{\theta_E - \overline{y}_{T,\nu}(T)}{\overline{u}_{T,\nu}(T)} \cdot \overline{u}_{T,\nu}(t) + \overline{y}_{T,\nu}(t) \quad \text{(computation: together with (26))}, \tag{28}$$

$$\sigma_{T,\nu}(t) \;:=\; \tfrac{E\cdot\alpha}{1-\mu} \cdot \Big(\overline{\theta}_{0,\nu}(t) \,-\, \hat{u}_{T,\nu}(t) \,+\, \int_0^t k_\nu(t-s)\cdot\hat{u}_{T,\nu}(s)\,ds\Big)\,, \tag{29}$$

$$g_{1,\nu}(T,t) \;:=\; \sigma_{T,\nu}(t) + \sigma^*, \quad g_{1,\nu}(T,t) \;:=\; -\sigma_{T,\nu}(t) + \sigma^*, \tag{30}$$

$$(z =)\; z_\nu^{\ell,j} \;:=\; \tfrac{t_\nu^j}{T_\nu^\ell} \quad (j \in \{0,\ldots,\ell\}). \tag{31}$$

Soon we shall evaluate functions $g_{\sigma,\nu}^0(T,z) := g_{\sigma,\nu}(T,zT)$ at $T \in \{T_\nu^{-1},\ldots,T_\nu^{m_\nu}\}$ ($\sigma \in \{1,2\}$).

First of all, we *visualize* the graph of $g_{\sigma,\nu}^0(\cdot,z)$ (referring to the numbers z from (31)); moreover, in view of the approximate (bounded) feasible set, we calculate and visualize the zeroes of $g_{\sigma,\nu}^0(\cdot,z) - \alpha$ for, e. g., $\alpha \in \{-10,-9,\ldots,9,10\} \cup \{\pm\frac{1}{2},\pm\frac{1}{4},\pm\frac{1}{8},\pm\frac{1}{16},\pm\frac{1}{32}\}$. An illustration is given in Fig. 2, (*b*), (ii).

If we think that the approximate feasible set describes $M_{\mathcal{GSI}}[g]$ in a sufficiently close way and if $\nu \geq \nu^1$ holds, then we put $c_{\nu+1} := 2$. From this illustration we may (but need not) make a conjecture, whether the properties EMFCQ and boundedness hold for $M_{\mathcal{GSI}}[g] \cap (-\infty, T_\nu^{m_\nu-1}]$.

Otherwise (in the case of no approximation), we put $c_{\nu+1} := c_\nu$.

At certain steps ν, we adapt the iteration procedure. Our decision may on the one hand be based on the insights about $\hat{d}_{T,\nu}$ and $g_{\sigma,\nu}^0$ (for example, we redefine *intervals* with respect to both their size and their fineness of decomposition). On the other hand, we may vary the auxiliary *parameters* (according to $\mathcal{P}^{\mathsf{tm}}$ perhaps also the fixed parameters; cf. mark (*A*)) and

the values p_ν, q_ν, or we can turn to *Alternative (I)*, or to the subsequent *Alternatives (II), (III)*. The variation of the parameters can be interpreted as a further entrance of *parametric programming* or optimal control theory and its methods into this work.

Referring to $T = T_\nu^\ell$, we write shortly:

$$g^0_{\sigma,\nu,\ell,j} := g_{\sigma,\nu}(T, z_\nu^{\ell,j}T) \;\; (= g^0_{\sigma,\nu}(T_\nu^\ell, z_\nu^{\ell,j})) \quad (j \in \{0, \ldots, \ell\}). \tag{32}$$

Alternative (II): In Approach I, we originally discretize analogously with the help of $z_\nu^{\ell,j} := \frac{j-1}{m_\nu - 1}$ $(j \in \{1, \ldots, m_\nu - 1\}$ or, for numerical differentiation, $j \in \{0, m_\nu\})$. As a result we obtain functions $g^{0,\nu}$ in the sense of Subsection 2.3. □

Motivated by *Hestenes* [10], [11], *Powell* [36] (referring to equality constraints) and modified in the sense of *Rockafellar* [37] (referring to inequalities see *Kaiser/Krabs* [19] and *Weber* [43], Remarks 3.1.6), now we mimic a *"discretized"* **Lagrange function**. Namely, in the sense of a *penalty* method, we put:

$$L_\nu^\ell := T_\nu^\ell + \tfrac{1}{4s_\nu} \sum_{\sigma=1}^{2} \sum_{j=0}^{\ell} ((\max\{0, v^j_{\sigma,\nu} - 2\, s_\nu\, g^0_{\sigma,\nu,\ell,j}\})^2 - {v^j_{\sigma,\nu}}^2),$$
$$\ell \in \{0, \ldots, m_\nu - 1\}. \tag{33}$$

By comparing these nonnegative values we select a minimum ℓ_ν, which corresponds to the point $T_\nu^{\ell_\nu}$:

$$\ell_\nu \in \operatorname{Arg\,min}\{L_\nu^\ell \mid \ell \in \{0, \ldots, m_\nu - 1\}\}. \tag{34}$$

Alternative (III): Here, we exploit the information of the inequalities, given by their approximate derivatives. Namely, we put the (arithmetic mean) difference quotient of the smooth function $g^0_{\sigma,\nu}(, z_\nu^{\ell,j})$ at T_ν^ℓ by

$$\triangle g^0_{\sigma,\nu,\ell,j} := \frac{g^0_{\sigma,\nu,\ell+1,j} - g^0_{\sigma,\nu,\ell-1,j}}{2^{-\nu+\nu^0+1}},$$

and then we define

$$\triangle L_\nu^\ell := 1 + \sum_{\sigma=1}^{2} \sum_{j=0}^{\ell} \max\{0, v^j_{\sigma,\nu} - 2 s_\nu g^0_{\sigma,\nu,\ell,j}\} \triangle g^0_{\sigma,\nu,\ell,j} \;\; (\ell \in \{0, \ldots, m_\nu - 1\}).$$

Then we ask whether there is an ℓ satisfying $|\triangle L_\nu^\ell| < \epsilon_\nu$. If this is not the case and $\nu + 1 < \nu^E$, then we may suitably adapt the penalty variable $s_{\nu+1} := \frac{s_\nu}{2^{p_\nu}}$ to the control of convergence: we put "$\nu := \nu + 1$" and go back to the mark (B). Otherwise, we select a minimum $\ell_\nu \in \operatorname{Arg\,min}\{|\triangle L_\nu^\ell| \mid \ell \in \{0, \ldots, m_\nu - 1\}\}$. □

The number $T_\nu^{\ell_\nu}$ is given both as an numerical output and as a point inside a figure (visualization). Of course, this output can be arranged just for a number of iteration steps ν. If $\nu + 1 < \nu^E$ or $|\hat{d}_{T_\nu^{\ell_\nu},\nu}| > \epsilon_\nu$ holds, then we could suitably define $p_{\nu+1}, q_{\nu+1}$ and we put

$$v^j_{\sigma,\nu+1} := \max\{0, v^j_{\sigma,\nu} - 2 s_\nu g^0_{\sigma,\nu,\ell_\nu,j}\}, \tag{35}$$
$$s_{\nu+1} := \tfrac{s_\nu}{2^{p_{\nu+1}}}, \quad \epsilon_{\nu+1} := \tfrac{\epsilon_\nu}{2^{q_{\nu+1}}}, \quad \text{"}\nu := \nu + 1\text{"}; \tag{36}$$

afterwards we return to mark (B). Otherwise, the whole procedure *stops*.

In the case of $|\hat{d}_{T_\nu^{\ell_\nu},\nu}| \leq \epsilon_\nu$, we regard the number $T_\nu^{\ell_\nu}$ (of the last step ν) as a satisfying approximation of the desired minimum $\widehat{T}$. This is an optimistic reservation. (Another approximate candidate could be an expected *lim inf* of all forthcoming values $T_{\tilde{\nu}}^{\ell_{\tilde{\nu}}}$, assuming that the procedure continues running.) $\Diamond$

If, furthermore, in the limit of $\tilde{\nu}$ (imagining $\tilde{\nu} \to \infty$) we suppose EMFCQ and boundedness to hold for $M_{\mathcal{GSI}}[g]$, then the heuristic (optimistic) approximation reservation, made at the termination of our iteration, is supported by the theory of *Approach I*. (Remember the stepwise arising question on the validity of EMFCQ and boundedness, and the iteration procedure of Approach I. This approach was presented in Subsection 2.3, based on the a topological study.) For that purpose, we choose a sufficiently large parameter ν^E. However, in the present Subsection 2.4, our main *Lagrangian (penalty) approach* also evaluates the $\mathcal{F}$ optimization problems which result from Approach I with its discretization on the lower stage. For more information on the corresponding numerical obstacles in $\mathcal{F}$ optimization see *Spellucci* [39]. We also remember the reflection under *absence* of a discretized upper stage, where different subroutines may be applied on the (less complex) $\mathcal{GSI}$ optimization problem.
Another opportunity for insights is established by the additional (parallel) approach from the values $\hat{d}_{T,\tilde{\nu}}$ $(\tilde{\nu} \geq \nu^0)$. In the case of the parameter constellation from *Item 2*, we indeed have an existence and convergence theory (see *Item 3*).

2.5. Further Evaluations

Until now, we studied the structure and numerical treatment of our control problem $\mathcal{P}^{\mathsf{tm}}$. **Existence** and **convergence results** were stated (*Items 1 – 3*) and a (commented) **flow diagram** was presented. Moreover, we expoited relations to *generalized semi-infinite optimization* and discussed *alternatives* and *obstacles*. Further difficulties will be noted below. For an illustration and a numerical evaluation see Fig. 2, and for further information cf. *Weber* [43].

From foregoing reflections we learn that in such a concrete problem there may be obstacles (*frontiers*) in applying iteration procedures, resulting from lacking structural knowledge of the feasible set $M_{\mathcal{GSI}}[g]$ (here $I = \emptyset$). In our iteration procedure, given above in the flow diagram, a great algorithmical effort (a lot of operations) has to be performed in order to overcome these **structural frontiers**. Errors can happen in the course of the procedure by accumulation of roundings (*sensitivity*).

However, we also remember the treatments, or *adaptions*, stated above in Alternatives (I) – (III), by studying the mappings $T \mapsto \hat{d}_{T,\nu}$, $T \mapsto g^0_{\sigma,\nu}(T,z)$ and by varying auxiliary parameters and variables. For our present concrete, but structurally complex problem, some further **practical treatments** from $\mathcal{GSI}$ optimization may turn out to be helpful again.

Namely, in order to get an idea how $M_{\mathcal{GSI}}[g]$ looks like and whether EMFCQ is fulfilled, we can utilize (vectors of) *pseudo-random numbers* (*Eichenauer-Herrmann* [4]). Hereby, we obtain more information on structures of *(in)feasibility*. We also mention *Karger* [22], [23] on *randomization* in graph (or matroid) optimization problems. In a forthcoming article, we return to pseudo-random numbers from the viewpoint of *random graphs* which admit insights being related to the Morse theory (see also *Weber* [43]). Concerning the *diagnosing of infeasibilies* we refer to *Aggarwal/Ahuja/Hao/Orlin* [1] on certain discrete optimization problems. (For the continuous case see *Kearfott* [25].) Furthermore, we refer to methods from *reverse engineering* (*Elsässer* [5], *Hoschek/Dankwort* [13]), *image restoration* (*Noll* [33]), *discrete tomography* (*Gritzmann*

[7]) and *discrete topology* (*Rozvany* [38]). These methods approximately describe or visualize a manifold or a structure based on discrete data.

In this way we have widened our scope from continuous problems of invertibility and reconstruction in optimal control and $\mathcal{GSI}$ optimization (*Weber* [43]) to *discrete* inverse problems.

3. Conclusion

In this article, we presented, analyzed and algorithmically treated an optimal control problem from time-minimal heating (or cooling). First systematical analysis and evaluation was done by Krabs. Our research additionally utilized an approach from generalized semi-infinite optimization, and we discussed the wide field of alternative methods, structural obstacles and related mathematical techniques. Hereby, we finally took into consideration stochastic and discrete features and methods.

Treating the heating problem in terms of a general model is very hard, such that rigorous utilization of the topological, geometrical or intrinsic combinatorial character of the specialized real-world problem is undispensable.

In the sense of these reflections, our heating problem remains an interesting subject of future reserach from both the theoretical and numerical viewpoint.

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