Shape Differentiability of Lagrangians and Application to Overdetermined Problems

Victor A. Kovtunenko and Kohji Ohtsuka

Abstract A class of geometry-dependent Lagrangians is investigated in a functional analysis framework with respect to the property of shape differentiability. General results are presented due to Delfour–Zolésio who adopted to shape optimization an abstract theorem of Correa–Seeger on the directional differentiability. A crucial point concerns the bijective property of function spaces as well as their feasible sets that must be preserved under a kinematic flow of geometry. The shape differentiability result is applied to overdetermined free-boundary and inverse problems expressed by least-square solutions. The theory is supported by explicit formulas obtained for calculation of the shape derivative.

Key words: shape derivative, Lagrangian, Correa–Seeger theorem, Delfour–Zolésio theorem, state-constrained shape optimization, free-boundary, inverse problem

1 Introduction

In this work we establish the shape differentiability of Lagrangians expressed by solutions of saddle-point problems stated over geometry-dependent function spaces. As examples, overdetermined problems of free-boundary and inverse types in the form of least-square minimization subject to state constraints are considered.

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Our motivation came from applications of shape and topology optimization methods to variational problems in mechanics and other engineering sciences, see [15, 27]. Especially aimed at fracture and earthquakes, the variational concept of nonlinear crack problems subject to non-penetration was developed in [10, 11, 12, 13] and other works by the authors. Widely used here Griffith fracture criterion implies the shape derivative of the strain energy with respect to a crack perturbation, which was calculated e.g. in [14, 19] for rectilinear cracks. For the related J-integrals and generalized J-integrals we refer to [2, 24, 25]. Based on the velocity method, see e.g. [9], an explicit formula of the shape derivative is provided by the bijection property of feasible sets which, however, fails for curvilinear cracks. This drawback was remedied in [22, 26] by a Gamma-type convergence, and in [16, 17] based on a Lagrangian setting of the perturbation problem.

The minimization problems subject to unilateral constraints can be reset equivalently as saddle-point problems using Lagrangian formalism. Within this concept, in [20] the Stokes problem, and in [6] the Brinkman problem subject to the divergence-free constraint were analyzed with respect to its shape differentiability, provided by the bijection property of function spaces under mixed Dirichlet–Neumann boundary conditions, and by a counter-example of non-bijection under no-slip conditions. In the present work we get a shape derivative for the least-square minimization subject to state-constraints which approximates overdetermined boundary value problems. Examples are the Bernoulli free-boundary problem, see e.g. [8, 23], and the inverse problem of parameter identification from boundary measurements, see [1, 3, 7, 18, 21].

In a functional analysis framework, in Section 2 we recall the Correa–Seeger theorem on directional differentiability [4], the Delfour–Zolésio theorem on differentiability with respect to a parameter [5, Chapter 10, Theorem 5.1], and in Section 3 we establish the shape differentiability of geometry-dependent Lagrangians under the bijection property of underlying function spaces and feasible sets. An application to the state-constrained shape optimization is given in Section 4.

2 Directional differentiability of Lagrangians

In a locally convex space O, Hausdorff topological spaces V and $H^\star$ with nonempty subsets $K \subseteq V$ and $K^\star \subseteq H^\star$, we consider an abstract *Lagrangian function*

$$\mathscr{L}(\phi, w, p):\ O \times V \times H^\star \mapsto \overline{\mathbb{R}} \tag{1}$$

obeying optimal values $l_\phi, l^\phi \in \overline{\mathbb{R}}$ such that

$$l_\phi := \sup_{p \in K^\star} \inf_{w \in K} \mathscr{L}(\phi, w, p) \leq \inf_{w \in K} \sup_{p \in K^\star} \mathscr{L}(\phi, w, p) =: l^\phi. \tag{2}$$

For given $\phi, d \in O$, the *solution sets* corresponding to (2) are determined by

$$K_\phi = \{u \in K |\ \sup_{p\in K^\star} \mathscr{L}(\phi,u,p) = l^\phi\}, \quad K^\star_\phi = \{\lambda \in K^\star |\ \inf_{w\in K} \mathscr{L}(\phi,w,\lambda) = l_\phi\} \quad (3)$$

yielding multi-valued functions by the mean of

$$\mathbb{R}_+ \rightrightarrows K,\ s \rightrightarrows K_{\phi+sd}, \quad \mathbb{R}_+ \rightrightarrows K^\star,\ s \rightrightarrows K^\star_{\phi+sd}. \quad (4)$$

Assume that there exists $\delta > 0$ such that the following properties are fulfilled:

(P0) $K_{\phi+sd}$ and $K^\star_{\phi+sd}$ are *sequentially semi-continuous* at 0, that is, for every convergent sequence $s_k \to 0^+$ as $k \to \infty$ there exists an accumulation point

$$u_\phi \in K_\phi, \quad \lambda_\phi \in K^\star_\phi \quad (5)$$

and a sequence $(u_{\phi+s_kd}, \lambda_{\phi+s_kd})$ accumulating at (u_ϕ, λ_ϕ) such that for all $k \in \mathbb{N}$ sufficiently large

$$u_{\phi+s_kd} \in K_{\phi+s_kd}, \quad \lambda_{\phi+s_kd} \in K^\star_{\phi+s_kd}; \quad (6)$$

(P1) for every $(w,p) \in K \times K^\star$, the function $\mathbb{R}_+ \mapsto \overline{\mathbb{R}}$, $s \mapsto \mathscr{L}(\phi+sd,w,p)$ is finite and continuous in $[0,\delta)$;

(P2) for all $u \in K_\phi$ the function

$$\mathbb{R}_+ \times K^\star \mapsto \overline{\mathbb{R}}, \quad (s,p) \mapsto \liminf_{\tau\to 0^+} \frac{\mathscr{L}(\phi+(s+\tau)d,u,p) - \mathscr{L}(\phi+sd,u,p)}{\tau} \quad (7)$$

is finite and upper semicontinuous in $\{0\} \times K^\star_\phi$; for all $\lambda \in K^\star_\phi$ the function

$$\mathbb{R}_+ \times K \mapsto \overline{\mathbb{R}}, \quad (s,w) \mapsto \limsup_{\tau\to 0^+} \frac{\mathscr{L}(\phi+(s+\tau)d,w,\lambda) - \mathscr{L}(\phi+sd,w,\lambda)}{\tau} \quad (8)$$

is finite and lower semicontinuous in $\{0\} \times K_\phi$;

(P3) the *saddle-point property* $l_{\phi+sd} = l^{\phi+sd}$ holds for all $s \in [0,\delta)$.

Theorem 1 (Correa–Seeger). *If properties (P0)–(P3) hold, then a directional derivative exists, which is characterized by*

$$\begin{aligned}\lim_{s_k\to 0^+} \frac{\mathscr{L}(\phi+s_kd, u_{\phi+s_kd}, \lambda_{\phi+s_kd}) - \mathscr{L}(\phi,u_\phi,\lambda_\phi)}{s_k} &= \sup_{\lambda\in K^\star_\phi} \inf_{u\in K_\phi} \Big(\lim_{s\to 0^+} \frac{\mathscr{L}(\phi+sd,u,\lambda) - \mathscr{L}(\phi,u,\lambda)}{s} \Big) \\ &= \inf_{u\in K_\phi} \sup_{\lambda\in K^\star_\phi} \Big(\lim_{s\to 0^+} \frac{\mathscr{L}(\phi+sd,u,\lambda) - \mathscr{L}(\phi,u,\lambda)}{s} \Big). \quad (9)\end{aligned}$$

Let us now consider the abstract Lagrangian function $\mathscr{L}(t,w,p)$ with a parameter $t_0 < t < t_1$. Using Theorem 1, we have the directional derivative of $\mathscr{L}(t+s, u_{t+s}, \lambda_{t+s})$ with respect to $s \to 0^+$ by setting $O = (t_0,t_1)$, $\phi = t$, $d = 1$, that is $\mathscr{L}(\phi+sd,w,p) = \mathscr{L}(t+s,w,p)$, $l_{\phi+sd} = l_{t+s}$, $l^{\phi+sd} = l^{t+s}$, $K_{\phi+sd} = K_{t+s}$, $K^\star_{\phi+sd} = K^\star_{t+s}$, $u_{\phi+sd} = u_{t+s}$, $\lambda_{\phi+sd} = \lambda_{t+s}$ in (1)–(9). The derivative can be achieved as follows:

Assume that $0 < \delta < t_1 - t$ and $(\mathfrak{T}_V, \mathfrak{T}_{H^\star})$-topology in $V \times H^\star$ exist such that

(H1) for all $s \in [0, \delta)$ the set of saddle-points $\mathfrak{S}(t+s) \subseteq K_{t+s} \times K^\star_{t+s}$ is nonempty:

$$\mathfrak{S}(t+s) := \{(u_{t+s}, \lambda_{t+s}) | \quad l_{t+s} = \mathscr{L}(t, u_{t+s}, \lambda_{t+s}) = l^{t+s}\}; \tag{10}$$

(H2) for all $(u, \lambda) \in \big(\bigcup_{s\in[0,\delta)} K_{t+s} \times K^\star_t\big) \cup \big(K_t \times \bigcup_{s\in[0,\delta)} K^\star_{t+s}\big)$ there exists the *partial derivative* with respect to parameter t:

$$\frac{\partial}{\partial t}\mathscr{L}(t, u, \lambda) = \lim_{s\to 0^+} \frac{\mathscr{L}(t+s,u,\lambda) - \mathscr{L}(t,u,\lambda)}{s} \quad \text{(one-sided);} \tag{11}$$

(H3) as $s \to 0^+$ an accumulation point $u_t \in K_t$ and a sequence $u_{t+s_k} \in K_{t+s_k}$ exist such that

$$u_{t+s_k} \to u_t \quad \text{strongly in } \mathfrak{T}_V\text{-topology} \tag{12}$$

and the lower estimate holds:

$$\liminf_{\tau, s_k \to 0^+} \frac{\partial}{\partial t}\mathscr{L}(t+\tau, u_{t+s_k}, \lambda) \geq \frac{\partial}{\partial t}\mathscr{L}(t, u_t, \lambda) \quad \forall \lambda \in K^\star_t; \tag{13}$$

(H4) as $s \to 0^+$ an accumulation point $\lambda_t \in K^\star_t$ and a sequence $\lambda_{t+s_k} \in K^\star_{t+s_k}$ exist such that

$$\lambda_{t+s_k} \to \lambda_t \quad \text{strongly in } \mathfrak{T}_{H^\star}\text{-topology} \tag{14}$$

and the upper estimate holds:

$$\limsup_{\tau, s_k \to 0^+} \frac{\partial}{\partial t}\mathscr{L}(t+\tau, u, \lambda_{t+s_k}) \leq \frac{\partial}{\partial t}\mathscr{L}(t, u, \lambda_t) \quad \forall u \in K_t. \tag{15}$$

Theorem 2 (Delfour–Zolésio). *Under hypotheses (H1)–(H4) there exists a saddle-point (u_t, λ_t) of $\frac{\partial}{\partial t}\mathscr{L}(t, u, \lambda)$ on $K_t \times K^\star_t$ such that*

$$\sup_{\lambda\in K^\star_t} \inf_{u\in K_t} \frac{\partial}{\partial t}\mathscr{L}(t, u, \lambda) = \frac{\partial}{\partial t}\mathscr{L}(t, u_t, \lambda_t) = \inf_{u\in K_t} \sup_{\lambda\in K^\star_t} \frac{\partial}{\partial t}\mathscr{L}(t, u, \lambda) \tag{16}$$

and a derivative with respect to parameter, which is represented by the partial derivative:

$$\lim_{s_k\to 0^+} \frac{\mathscr{L}(t+s_k, u_{t+s_k}, \lambda_{t+s_k}) - \mathscr{L}(t, u_t, \lambda_t)}{s_k} = \frac{\partial}{\partial t}\mathscr{L}(t, u_t, \lambda_t) \quad \textit{(one-sided).} \tag{17}$$

3 Shape differentiability of Lagrangians

In the following we adapt (10)–(17) for the reason of shape differentiability. For the parameter $t \in (t_0, t_1)$ we associate a *reference geometry*

$$t \mapsto \Omega_t \subset \mathbb{R}^d, \quad d \in \mathbb{N} \tag{18}$$

to a *geometry-dependent Lagrangian* over topological spaces $V(\Omega_t)$ and $H^\star(\Omega_t)$:

$$V(\Omega_t) \times H^\star(\Omega_t) \mapsto \mathbb{R}, \quad (w,p) \mapsto \mathscr{L}(w,p;\Omega_t). \tag{19}$$

The corresponding optimal values are defined by

$$l_t := \sup_{p \in K^\star(\Omega_t)} \inf_{w \in K(\Omega_t)} \mathscr{L}(w,p;\Omega_t) \leq \inf_{w \in K(\Omega_t)} \sup_{p \in K^\star(\Omega_t)} \mathscr{L}(w,p;\Omega_t) =: l^t \tag{20}$$

over feasible sets $K(\Omega_t) \subseteq V(\Omega_t)$ and $K^\star(\Omega_t) \subseteq H^\star(\Omega_t)$, the solution sets are

$$\begin{aligned} K_t &= \{u \in K(\Omega_t) | \sup_{p \in K^\star(\Omega_t)} \mathscr{L}(u,p;\Omega_t) = l^t\}, \\ K_t^\star &= \{\lambda \in K^\star(\Omega_t) | \inf_{w \in K(\Omega_t)} \mathscr{L}(w,\lambda;\Omega_t) = l_t\}. \end{aligned} \tag{21}$$

For a small perturbation parameter $s \in (t_0 - t, t_1 - t)$ and the *perturbed geometry* Ω_{t+s} the *perturbed Lagrangian* (19) reads:

$$V(\Omega_{t+s}) \times H^\star(\Omega_{t+s}), \quad (v,\mu) \mapsto \mathscr{L}(v,\mu;\Omega_{t+s}), \tag{22}$$

the *perturbed subsets* $K(\Omega_{t+s}) \subseteq V(\Omega_{t+s})$ and $K^\star(\Omega_{t+s}) \subseteq H^\star(\Omega_{t+s})$, and

$$\begin{aligned} l_{t+s} = &\sup_{\mu \in K^\star(\Omega_{t+s})} \inf_{v \in K(\Omega_{t+s})} \mathscr{L}(v,\mu;\Omega_{t+s}) \\ &\leq \inf_{v \in K(\Omega_{t+s})} \sup_{\mu \in K^\star(\Omega_{t+s})} \mathscr{L}(v,\mu;\Omega_{t+s}) = l^{l+s}. \end{aligned} \tag{23}$$

Definition 1. For *saddle-points* $(u_t, \lambda_t) \in \mathfrak{S}(t) \subseteq K_t \times K_t^\star$ and the *optimal value function* $\ell : (t_0,t_1) \mapsto \overline{\mathbb{R}}$, $\ell(t) = l_t$ written over $\mathfrak{S}(t)$ such that according to (10)

$$\ell(t) = l_t = \mathscr{L}(u_t, \lambda_t; \Omega_t) = l^t, \tag{24}$$

the *shape derivative* of $\mathscr{L}$ is called the following limit (if it exists):

$$\partial_t \mathscr{L}(u_t, \lambda_t; \Omega_t) = \partial \ell(t) := \lim_{s \to 0^+} \tfrac{\ell(t+s) - \ell(t)}{s} \quad \text{(one-sided)}. \tag{25}$$

The principal disadvantage is that Theorem 2 is not applicable to prove the limit in (25) because the function spaces in (19) depend itself on the parameter. By this reason we transform the problem to a fixed geometry. For fixed $t \in (t_0,t_1)$ let

$$[s \mapsto \phi_s], [s \mapsto \phi_s^{-1}] \in C^1([t_0 - t, t_1 - t]; W^{1,\infty}_{\mathrm{loc}}(\mathbb{R}^d;\mathbb{R}^d)) \tag{26}$$

associate the *coordinate transformation* $y = \phi_s(x)$ and its *inverse* $x = \phi_s^{-1}(y)$:

$$(\phi_s^{-1} \circ \phi_s)(x) = x, \quad (\phi_s \circ \phi_s^{-1})(y) = y \tag{27}$$

such that the shape perturbation

$$\Omega_{t+s} = \{y \in \mathbb{R}^d | \quad y = \phi_s(x),\, x \in \Omega_t\} \tag{28}$$

builds the diffeomorphism

$$\phi_s : \Omega_t \mapsto \Omega_{t+s},\, x \mapsto y, \quad \phi_s^{-1} : \Omega_{t+s} \mapsto \Omega_t,\, y \mapsto x. \tag{29}$$

For example, given a *stationary velocity* $\Lambda(x) \in W^{1,\infty}_{\rm loc}(\mathbb{R}^d;\mathbb{R}^d)$ establishes the flow (26) determined by the solution of the autonomous ODE system:

$$\begin{cases} \frac{d}{ds}\phi_s = \Lambda(\phi_s),\ s \neq 0, \\ \phi_s = x,\ s = 0, \end{cases} \quad \begin{cases} \frac{d}{ds}\phi_s^{-1} = -\Lambda(\phi_s^{-1}),\ s \neq 0, \\ \phi_s^{-1} = y,\ s = 0 \end{cases} \tag{30}$$

and forms a semigroup of transformations. Generally, the *kinematic velocity* is time-dependent $\Lambda \in C([t_0,t_1];W^{1,\infty}_{\rm loc}(\mathbb{R}^d;\mathbb{R}^d))$ defined from (26) as

$$\Lambda(t+s,y) := \tfrac{d}{ds}\phi_s(\phi_s^{-1}(y)). \tag{31}$$

Assume that

(A0) the map $[(v,\mu) \mapsto (v\circ\phi_s, \mu\circ\phi_s)]$ is bijective between the function spaces

$$V(\Omega_{t+s}) \mapsto V(\Omega_t), \quad H^\star(\Omega_{t+s}) \mapsto H^\star(\Omega_t) \tag{32}$$

and between the feasible sets

$$K(\Omega_{t+s}) \mapsto K(\Omega_t), \quad K^\star(\Omega_{t+s}) \mapsto K^\star(\Omega_t). \tag{33}$$

The assumption (32) determines well the *transformed perturbed Lagrangian*:

$$(t_0-t, t_1-t) \times V(\Omega_t) \times H^\star(\Omega_t), \quad (s,w,p) \mapsto \tilde{\mathscr{L}}(s,w,p;\Omega_t) \tag{34}$$

in such a way that for arbitrary $(v,\mu) \in V(\Omega_{t+s}) \times H^\star(\Omega_{t+s})$ it holds

$$\tilde{\mathscr{L}}(s, v\circ\phi_s, \mu\circ\phi_s;\Omega_t) = \mathscr{L}(v,\mu;\Omega_{t+s}). \tag{35}$$

We note that (33) may fail for feasible sets involving integral and gradient operators which are generally not preserved under a velocity-induced geometry flow.

Let us put for $s \in (t_0-t, t_1-t)$ the optimal values for $\tilde{\mathscr{L}}$:

$$\tilde{l}_{t+s} := \sup_{p\in K^\star(\Omega_t)} \inf_{w\in K(\Omega_t)} \tilde{\mathscr{L}}(s,w,p;\Omega_t) \le \inf_{w\in K(\Omega_t)} \sup_{p\in K^\star(\Omega_t)} \tilde{\mathscr{L}}(s,w,p;\Omega_t) =: \tilde{l}^{t+s} \tag{36}$$

and the corresponding solution sets

$$\begin{aligned} \tilde{K}_{t+s} &= \{u \in K(\Omega_t) | \sup_{p\in K^\star(\Omega_t)} \tilde{\mathscr{L}}(s,u,p;\Omega_t) = \tilde{l}^{t+s}\}, \\ \tilde{K}^\star_{t+s} &= \{\lambda \in K^\star(\Omega_t) | \inf_{w\in K(\Omega_t)} \tilde{\mathscr{L}}(s,w,\lambda;\Omega_t) = \tilde{l}_{t+s}\}. \end{aligned} \tag{37}$$

Definition 2. For saddle-points $(\tilde{u}_{t+s}, \tilde{\lambda}_{t+s}) \in \tilde{\mathfrak{S}}(t+s) \subseteq \tilde{K}_{t+s} \times \tilde{K}^\star_{t+s}$ from the set

$$\tilde{\mathfrak{S}}(t+s) := \{(\tilde{u}_{t+s}, \tilde{\lambda}_{t+s}) | \quad \tilde{l}_{t+s} = \tilde{\mathscr{L}}(s, \tilde{u}_{t+s}, \tilde{\lambda}_{t+s}; \Omega_t) = \tilde{l}^{t+s}\} \tag{38}$$

and the *optimal value function* $\tilde{\ell} : (t_0 - t, t_1 - t) \mapsto \overline{\mathbb{R}}$, $\tilde{\ell}(s;t) = \tilde{l}_{t+s}$ written over $\tilde{\mathfrak{S}}(t+s)$ according to (36), the *shape derivative* of $\tilde{\mathscr{L}}$ is called the following limit (if it exists):

$$\partial_s \tilde{\ell}(0;t) := \lim_{s \to 0^+} \tfrac{\tilde{\ell}(s;t) - \tilde{\ell}(0;t)}{s} \quad \text{(one-sided).} \tag{39}$$

Now Theorem 2 is applicable to prove the limit in (39), when we reformulate the hypotheses (H1)–(H4) as follows. For fixed $t \in (t_0, t_1)$ we assume that there exist $\delta \in (0, t_1 - t)$ and $(\mathfrak{T}_V, \mathfrak{T}_{H^\star})$-topology such that

(A1) for all $s \in [0, \delta)$ the set of saddle-points $\tilde{\mathfrak{S}}(t+s)$ given in (38) is nonempty;
(A2) for all $(u, \lambda) \in \big(\bigcup_{s \in [0,\delta)} \tilde{K}_{t+s} \times \tilde{K}^\star_t\big) \cup \big(\tilde{K}_t \times \bigcup_{s \in [0,\delta)} \tilde{K}^\star_{t+s}\big)$ and $\tau \in [0, \delta)$ there exists the *partial derivative* at $s = \tau$:

$$\tfrac{\partial}{\partial s} \tilde{\mathscr{L}}(\tau, u, \lambda; \Omega_t) := \lim_{s \to 0^+} \tfrac{\tilde{\mathscr{L}}(\tau+s, u, \lambda; \Omega_t) - \tilde{\mathscr{L}}(\tau, u, \lambda; \Omega_t)}{s} \quad \text{(one-sided);} \tag{40}$$

(A3) as $s \to 0^+$ an accumulation point $\tilde{u}_t \in \tilde{K}_t$ and a sequence $\tilde{u}_{t+s_k} \in \tilde{K}_{t+s_k}$ exist such that

$$\tilde{u}_{t+s_k} \to \tilde{u}_t \quad \text{strongly in } \mathfrak{T}_V\text{-topology} \tag{41}$$

and the lower estimate holds:

$$\liminf_{\tau, s_k \to 0^+} \tfrac{\partial}{\partial s} \tilde{\mathscr{L}}(\tau, \tilde{u}_{t+s_k}, \lambda; \Omega_t) \geq \tfrac{\partial}{\partial s} \tilde{\mathscr{L}}(0, \tilde{u}_t, \lambda; \Omega_t) \quad \forall \lambda \in \tilde{K}^\star_t; \tag{42}$$

(A4) as $s \to 0^+$ an accumulation point $\tilde{\lambda}_t \in \tilde{K}^\star_t$ and a sequence $\tilde{\lambda}_{t+s_k} \in \tilde{K}^\star_{t+s_k}$ exist such that

$$\tilde{\lambda}_{t+s_k} \to \tilde{\lambda}_t \quad \text{strongly in } \mathfrak{T}_{H^\star}\text{-topology} \tag{43}$$

and the upper estimate holds:

$$\limsup_{\tau, s_k \to 0^+} \tfrac{\partial}{\partial s} \tilde{\mathscr{L}}(\tau, u, \tilde{\lambda}_{t+s_k}; \Omega_t) \leq \tfrac{\partial}{\partial s} \tilde{\mathscr{L}}(0, u, \tilde{\lambda}_t; \Omega_t) \quad \forall u \in \tilde{K}_t. \tag{44}$$

Then Theorem 2 follows the main theorem on shape differentiability of Lagrangians.

Theorem 3. *Under assumptions (A1)–(A4) there exists a saddle-point* $(\tilde{u}_t, \tilde{\lambda}_t)$ *of* $\frac{\partial}{\partial s} \tilde{\mathscr{L}}(0, u, \lambda; \Omega_t)$ *on* $\tilde{K}_t \times \tilde{K}^\star_t$ *such that*

$$\sup_{\lambda \in \tilde{K}^\star_t} \inf_{u \in \tilde{K}_t} \tfrac{\partial}{\partial s} \tilde{\mathscr{L}}(0, u, \lambda; \Omega_t) = \tfrac{\partial}{\partial s} \tilde{\mathscr{L}}(0, \tilde{u}_t, \tilde{\lambda}_t; \Omega_t) = \inf_{u \in \tilde{K}_t} \sup_{\lambda \in \tilde{K}^\star_t} \tfrac{\partial}{\partial s} \tilde{\mathscr{L}}(0, u, \lambda; \Omega_t) \tag{45}$$

and the shape derivative (39) *is represented by the partial derivative:*

$$\partial_s \tilde{\ell}(0;t) = \tfrac{\partial}{\partial s} \tilde{\mathscr{L}}(0, \tilde{u}_t, \tilde{\lambda}_t; \Omega_t) \quad \textit{(one-sided).} \tag{46}$$

Under the assumption (A0) the shape derivatives defined in (25) *and* (39) *coincide:*

$$\partial_t \mathscr{L}(u_t, \lambda_t; \Omega_t) = \partial_s \tilde{\ell}(0;t). \tag{47}$$

4 Application to state-constrained shape optimization

As application of Theorem 3 we consider a least-square minimization subject to state-constraint which approximates overdetermined boundary value problems.

Let a reference domain Ω_t be contained in the hold-all domain $D \subset \mathbb{R}^d$, the velocity $\Lambda(t,x) \in C([t_0,t_1]; W^{1,\infty}(D;\mathbb{R}^d))$ be zero at ∂D. We assume that the boundary $\partial\Omega_t$ is Lipschitz-continuous with the outward unit normal vector n^t and consists of disjoint parts Γ_t^{D}, Γ_t^{N}, Γ_t^{O}. For given $g(x), z(x) \in H^2(D;\mathbb{R})$ we start with the *overdetermined problem*: find a domain $\Omega_t \subset D$ and a function $u_t(x) \in H^1(\Omega_t;\mathbb{R})$ satisfying

$$\begin{aligned} &\text{the Laplace equation:} && -\Delta u_t = 0 && \text{in } \Omega_t, && (48)\\ &\text{the Dirichlet condition:} && u_t = 0 && \text{on } \Gamma_t^{\mathrm{D}}, && (49)\\ &\text{the Neumann condition:} && \tfrac{\partial}{\partial n^t} u_t = g && \text{on } \Gamma_t^{\mathrm{N}}, && (50)\\ &\text{overdetermined conditions:} && \tfrac{\partial}{\partial n^t} u_t = g, \quad u_t = z && \text{on } \Gamma_t^{\mathrm{O}}. && (51) \end{aligned}$$

In particular, prescribing both data g, z and varying Γ_t^{O} describes the *Bernoulli free-boundary problem*. The *inverse identification problem* corresponds to prescribed data g and observed z at fixed Γ_t^{O}. In general, all parts Γ_t^{D}, Γ_t^{N}, Γ_t^{O} can be varied.

In the function space taking into account the Dirichlet condition (49):

$$V(\Omega_t) = \{ w \in H^1(\Omega_t;\mathbb{R}) | \quad w = 0 \text{ a.e. } \Gamma_t^{\mathrm{D}} \}$$

let the *objective* function $D \times V(\Omega_t) \mapsto \mathbb{R}$, $(\Omega_t, w) \mapsto \mathscr{J}$ approximate the Dirichlet condition in (51) by the least-square misfit:

$$\mathscr{J}(w;\Omega_t) := \frac{1}{2} \int_{\Gamma_t^{\mathrm{O}}} (w - z)^2 \, dx. \tag{52}$$

We consider the *state variational problem* describing relations (48)–(50) and the Neumann condition in (51): for fixed Ω_t there exists unique $u_t \in V(\Omega_t)$ minimizing the *energy* function:

$$\mathscr{E}(u_t;\Omega_t) = \min_{w \in V(\Omega_t)} \mathscr{E}(w;\Omega_t) := \frac{1}{2} \int_{\Omega_t} |\nabla w|^2 \, dx - \int_{\Gamma_t^{\mathrm{N}} \cup \Gamma_t^{\mathrm{O}}} g w \, dS_x, \tag{53}$$

or satisfying the equivalent first-order *optimality condition*:

$$\langle \mathscr{E}_u(u_t;\Omega_t), p \rangle := \int_{\Omega_t} \nabla u_t \cdot \nabla p \, dx - \int_{\Gamma_t^{\mathrm{N}} \cup \Gamma_t^{\mathrm{O}}} g p \, dS_x = 0 \quad \forall p \in V(\Omega_t). \tag{54}$$

The *state-constrained shape optimization problem* implies: find $\Omega_t \subset D$ such that

$$\min_{\Omega_t \in D} \mathscr{J}(w;\Omega_t) \quad \text{subject to } \mathscr{E}_u(w;\Omega_t) = 0. \tag{55}$$

For the *Lagrangian* function $D \times V(\Omega_t) \times V(\Omega_t) \mapsto \mathbb{R}$, $(\Omega_t, w, p) \mapsto \mathscr{L}$ given by

$$\mathscr{L}(w,p;\Omega_t) := \mathscr{J}(w;\Omega_t) - \langle \mathscr{E}_u(w;\Omega_t), p \rangle \tag{56}$$

the corresponding *primal-dual shape optimization* reads: find triple $(\Omega_{t+s}, u_{t+s}, \lambda_{t+s}) \in D \times V(\Omega_{t+s}) \times V(\Omega_{t+s})$ with $s > 0$ such that

$$\mathscr{L}(u_{t+s}, \lambda_{t+s}; \Omega_{t+s}) < \mathscr{L}(u_t, \lambda_t; \Omega_t). \tag{57}$$

The optimality condition for (57) implies that $u_t \in V(\Omega_t)$ solves the primal equation (54), and the dual variable $\lambda_t \in V(\Omega_t)$ solves the *adjoint equation*:

$$\int_{\Omega_t} \nabla w \cdot \nabla \lambda_t \, dx - \int_{\Gamma_t^{\mathrm{O}}} (u_t - z) w \, dS_x = 0 \quad \forall w \in V(\Omega_t) \tag{58}$$

which describes the following boundary-value problem:

$$\text{the Laplace equation:} \quad -\Delta \lambda_t = 0 \quad \text{in } \Omega_t, \tag{59}$$

$$\text{the Dirichlet condition:} \quad \lambda_t = 0 \quad \text{on } \Gamma_t^{\mathrm{D}}, \tag{60}$$

$$\text{the Neumann condition:} \quad \tfrac{\partial}{\partial n^t} \lambda_t = 0 \quad \text{on } \Gamma_t^{\mathrm{N}}, \tag{61}$$

$$\text{the Neumann condition:} \quad \tfrac{\partial}{\partial n^t} \lambda_t = u_t - z \quad \text{on } \Gamma_t^{\mathrm{O}}. \tag{62}$$

The underlying *optimal value function* $\ell : D \mapsto \overline{\mathbb{R}}$,

$$\ell(\Omega_t) := \mathscr{L}(u_t, \lambda_t; \Omega_t) = \mathscr{J}(u_t;\Omega_t) \tag{63}$$

coincides for the Lagrangian $\mathscr{L}$ and for the objective $\mathscr{J}$ since $\mathscr{E}_u(u_t;\Omega_t) = 0$.

We parametrize perturbed domains by the flow $\phi_s : \Omega_t \mapsto \Omega_{t+s}$ according to (26) and choose small $\delta > 0$ such that $\Omega_{t+s} \subset D$ for $s \in [0, \delta)$. By the construction,

(T1) the map $V(\Omega_{t+s}) \mapsto V(\Omega_t), [(v,\mu) \mapsto (v \circ \phi_s, \mu \circ \phi_s)]$ is bijective.

For the *perturbed Lagrangian* $V(\Omega_{t+s}) \times V(\Omega_{t+s}) \mapsto \mathbb{R}$, $(v, \mu) \mapsto \mathscr{L}$,

$$\mathscr{L}(v,\mu;\Omega_{t+s}) := \frac{1}{2} \int_{\Gamma_{t+s}^{\mathrm{O}}} (v - z)^2 \, dS_y - \int_{\Omega_{t+s}} \nabla_y v \cdot \nabla_y \mu \, dy + \int_{\Gamma_{t+s}^{\mathrm{N}} \cup \Gamma_{t+s}^{\mathrm{O}}} g\mu \, dS_y \tag{64}$$

there exists a unique *saddle-point* $(u_{t+s}, \lambda_{t+s}) \in V(\Omega_{t+s}) \times V(\Omega_{t+s})$ such that

$$\mathscr{L}(u_{t+s}, \lambda_{t+s}; \Omega_{t+s}) = \min_{v \in V(\Omega_{t+s})} \max_{\mu \in V(\Omega_{t+s})} \mathscr{L}(v,\mu;\Omega_{t+s}). \tag{65}$$

The *transformed perturbed Lagrangian* $[0,\delta) \times V(\Omega_t) \times V(\Omega_t) \mapsto \mathbb{R}$, $(s, w, p) \mapsto \tilde{\mathscr{L}}$

$$\tilde{\mathscr{L}}(s,w,p;\Omega_t) := \frac{1}{2}\int_{\Gamma_t^{\mathrm{O}}} (w - z\circ\phi_s)^2\,\omega_s dS_x$$
$$-\int_{\Omega_t}\big((\nabla\phi_s^{-T}\circ\phi_s)\nabla w\cdot(\nabla\phi_s^{-T}\circ\phi_s)\nabla p\big)\,J_s dx + \int_{\Gamma_t^{\mathrm{N}}\cup\Gamma_t^{\mathrm{O}}} (g\circ\phi_s)p\,\omega_s dS_x, \quad (66)$$

where $J_s := \det(\nabla\phi_s)$ and $\omega_s := |(\nabla\phi_s^{-T}\circ\phi_s)n^t|J_s$, obeys the unique saddle-point

$$(\tilde{u}_{t+s},\tilde{\lambda}_{t+s}) := (u_{t+s}\circ\phi_s, \lambda_{t+s}\circ\phi_s) \in V(\Omega_t)\times V(\Omega_t) \quad (67)$$

solving the transformed minimax problem

$$\tilde{\mathscr{L}}(s,\tilde{u}_{t+s},\tilde{\lambda}_{t+s};\Omega_t) = \min_{w\in V(\Omega_t)}\max_{p\in V(\Omega_t)} \tilde{\mathscr{L}}(s,w,p;\Omega_t). \quad (68)$$

Therefore, the transformed perturbed Lagrangian has the following traits:

(T2) due to (67) the solution sets $\tilde{K}_{t+s} = \{\tilde{u}_{t+s}\}$, $\tilde{K}^{\star}_{t+s} = \{\tilde{\lambda}_{t+s}\}$ are singleton, and the set of saddle-points $\tilde{\mathfrak{S}}(t+s)$ defined in (38) is nonempty for all $s\in[0,\delta)$;

(T3) for all $(w,p)\in V(\Omega_t)\times V(\Omega_t)$ there exists the *partial derivative* at $s=0$:

$$\frac{\partial}{\partial s}\tilde{\mathscr{L}}(0,w,p;\Omega_t) = \int_{\Gamma_t^{\mathrm{O}}}\big(\tfrac{1}{2}(\mathrm{div}_\Gamma\Lambda)(w-z)^2 - (\Lambda\cdot\nabla z)(w-z)\big)\,dS_x$$
$$-\int_{\Omega_t}\big((\mathrm{div}\Lambda)(\nabla w\cdot\nabla p) - \nabla w\cdot((\nabla\Lambda+\nabla\Lambda^\top)\nabla p)\big)\,dx$$
$$+\int_{\Gamma_t^{\mathrm{N}}\cup\Gamma_t^{\mathrm{O}}}\big((\mathrm{div}_\Gamma\Lambda)g + \Lambda\cdot\nabla g\big)p\,dS_x \quad (69)$$

with the velocity $\Lambda(t,x)$, where $\mathrm{div}_\Gamma\Lambda = \mathrm{div}\Lambda - (\nabla\Lambda n^t)\cdot n^t$, and the asymptotic expansion holds:

$$\tilde{\mathscr{L}}(s,w,p;\Omega_t) = \tilde{\mathscr{L}}(0,w,p;\Omega_t) + s\frac{\partial}{\partial s}\tilde{\mathscr{L}}(0,w,p;\Omega_t) + \mathrm{o}(s);$$

(T4) as $s\to 0^+$ there exists a subsequence s_k such that

$$(\tilde{u}_{t+s_k},\tilde{\lambda}_{t+s_k}) \to (u_t,\lambda_t) \quad \text{strongly in } V(\Omega_t)\times V(\Omega_t). \quad (70)$$

Indeed, the representation (69) follows directly from (66) due to the expansions:

$$\nabla\phi_s^{-1}\circ\phi_s = I - s\nabla\Lambda + \mathrm{o}(s), \quad J_s = 1 + s\,\mathrm{div}\Lambda + \mathrm{o}(s), \quad \omega_s = 1 + s\,\mathrm{div}_\Gamma\Lambda + \mathrm{o}(s),$$
$$z\circ\phi_s = z + s\Lambda\cdot\nabla z + \mathrm{o}(s), \quad g\circ\phi_s = g + s\Lambda\cdot\nabla g + \mathrm{o}(s), \quad (71)$$

and the proof of (70) can be found, for example, in [8].

Theorem 4. *For the* parametrized optimal value function $[0,\delta)\mapsto\overline{\mathbb{R}}$, $s\mapsto\tilde{\ell}(s;\Omega_t) := \tilde{\mathscr{L}}(s,\tilde{u}_{s+t},\tilde{\lambda}_{s+t};\Omega_t)$ *there exists the shape derivative represented by*

$$\partial_t\ell(\Omega_t) = \partial_s\tilde{\ell}(0;\Omega_t) = \frac{\partial}{\partial s}\tilde{\mathscr{L}}(0,u_t,\lambda_t;\Omega_t) \quad \textit{(one-sided)}. \quad (72)$$

Proof. Traits (T1)–(T3) yield (A0)–(A2), the partial derivative $\frac{\partial}{\partial s}\tilde{\mathscr{L}}(\tau,u,\lambda;\Omega_t)$ at $s=\tau$ in (A2) is determined by formula (69) with the respective velocity $\Lambda(t+\tau,x)$. The trait (T4) implies the strong convergences (41) and (43), while continuity of the map $(w,p)\mapsto \frac{\partial}{\partial s}\tilde{\mathscr{L}}(0,w,p;\Omega_t)$ in (69) follows (42) and (44) in assumptions (A3) and (A4). □

Assuming a piecewise $C^{1,1}$-boundary $\partial\Omega_t$ without singular points such that the saddle-point $(u_t,\lambda_t)\in H^2(\Omega_t;\mathbb{R})\times H^2(\Omega_t;\mathbb{R})$ in Theorem 4, the integration by parts over the domain Ω_t due to (48)–(51) and (59)–(62) yields the expression

$$\int_{\Omega_t}\big((\mathrm{div}\Lambda)(\nabla u_t\cdot\nabla\lambda_t)-\nabla u_t\cdot((\nabla\Lambda+\nabla\Lambda^{\top})\nabla\lambda_t)\big)\,dx$$
$$=\int_{\partial\Omega_t}\Lambda\cdot\big(n^t(\nabla u_t\cdot\nabla\lambda_t)-\nabla u_t\tfrac{\partial\lambda_t}{\partial n^t}-\nabla\lambda_t\tfrac{\partial u_t}{\partial n^t}\big)\,dS_x. \quad (73)$$

At $\partial\Omega_t$ we decompose $\Lambda=\Lambda_\Gamma+n^t(\Lambda\cdot n^t)$ such that $\mathrm{div}_\Gamma\Lambda=\mathrm{div}_\Gamma\Lambda_\Gamma+(\Lambda\cdot n^t)\varkappa_t$ with the curvature $\varkappa_t:=\mathrm{div}_\Gamma n^t$. After integration by parts of the tangential term $\mathrm{div}_\Gamma\Lambda_\Gamma$ with the help of formulas from [28, Section 4.4] it follows

$$\int_{\Gamma_t^i}(\mathrm{div}_\Gamma\Lambda)u\,dS_x=\int_{\Gamma_t^i}\Lambda\cdot\big(n^t(u\varkappa_t+\tfrac{\partial u}{\partial n^t})-\nabla u\big)\,dS_x$$
$$+\int_{\partial\Gamma_t^i}\Lambda\cdot(\tau^t\times n^t)u\,dL_x,\quad i=\mathrm{N},\mathrm{O}, \quad (74)$$

where τ^t is a tangential vector at $\partial\Gamma_t^i$ positive oriented to n^t. Using (73) and (74), from (69) we derive the *Hadamard structure representation*:

$$\tfrac{\partial}{\partial s}\tilde{\mathscr{L}}(0,u_t,\lambda_t;\Omega_t)=\int_{\Gamma_t^{\mathrm{D}}}\Lambda\cdot a^t\,dS_x+\int_{\Gamma_t^{\mathrm{O}}}(\Lambda\cdot n^t)b_t\,dS_x+\int_{\Gamma_t^{\mathrm{N}}}(\Lambda\cdot n^t)c_t\,dS_x$$
$$+\int_{\partial\Gamma_t^{\mathrm{O}}}\Lambda\cdot(\tau^t\times n^t)G_t\,dL_x+\int_{\partial\Gamma_t^{\mathrm{N}}}\Lambda\cdot(\tau^t\times n^t)g\lambda_t\,dL_x \quad (75)$$

over the boundary, with the components

$$a^t:=(\nabla u_t\tfrac{\partial\lambda_t}{\partial n^t}+\nabla\lambda_t\tfrac{\partial u_t}{\partial n^t})-n^t(\nabla u_t\cdot\nabla\lambda_t),\quad b_t:=\varkappa_t G_t+\tfrac{\partial G_t}{\partial n^t}-\nabla u_t\cdot\nabla\lambda_t,$$
$$c_t:=\varkappa_t g\lambda_t+\tfrac{\partial(g\lambda_t)}{\partial n^t}-\nabla u_t\cdot\nabla\lambda_t,\quad G_t:=\tfrac{1}{2}(u_t-z)^2+g\lambda_t. \quad (76)$$

This suggests the strategy for numerical shape optimization as follows:

- For fixed Ω_t set a velocity $\Lambda(x)$ at the parts of the boundary $\partial\Omega_t$ either $\Lambda=0$ or

$$\begin{aligned}
\Lambda &= -a^t \quad \text{on } \Gamma_t^{\rm D},\\
\Lambda \cdot n^t = -b_t \text{ and } \Lambda_\Gamma &= 0 \quad \text{on } \Gamma_t^{\rm O},\\
\Lambda \cdot n^t = -c_t \text{ and } \Lambda_\Gamma &= 0 \quad \text{on } \Gamma_t^{\rm N},\\
\Lambda \cdot (\tau^t \times n^t) &= -G_t \quad \text{on } \partial\Gamma_t^{\rm O},\\
\Lambda \cdot (\tau^t \times n^t) &= -g\lambda_t \quad \text{on } \partial\Gamma_t^{\rm N}
\end{aligned}$$

providing a *descent direction* by the virtue of (76):

$$\frac{\partial}{\partial s}\tilde{\mathscr{L}}(0,u_t,\lambda_t;\Omega_t) = -\int_{\Gamma_t^{\rm N}} |a_t|^2\, dS_x - \int_{\Gamma_t^{\rm D}} b_t^2\, dS_x - \int_{\Gamma_t^{\rm O}} c_t^2\, dS_x - \int_{\partial\Gamma_t^{\rm O}} G_t^2\, dL_x - \int_{\partial\Gamma_t^{\rm N}} (g\lambda_t)^2\, dL_x < 0;$$

- find a domain $\Omega_{t+s} \subset D$ bounded by

$$\partial\Omega_{t+s} = \{y \in \mathbb{R}^d | \quad y = x + s\Lambda(x),\ x \in \partial\Omega_t\} \tag{77}$$

  with a suitable parameter $s > 0$ minimizing the objective $\mathscr{J}(u_{t+s};\Omega_{t+s})$;
- reset $\Omega_t := \Omega_{t+s}$ and iterate.

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