Methods for reliable topology changes for perimeter regularized geometric inverse problems

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Abstract

This paper is devoted to the incorporation of topological derivative like expansions of first and second order in volume and perimeter into level set methods for perimeter regularized geometric inverse problems.

Based on these expansions we provide a steepest descent type and a Newton-type algorithm to force topology changes in level set methods.

Numerous numerical examples are provided that show the strong and also the weak points of these estimates.

Keywords: Geometric Inverse Problems, Perimeter Regularization, Topological Gradients.

AMS Subject Classification: 35R30, 49Q10, 74B05, 65J20

1 Introduction

Identification of unknown geometries via minimizing appropriate objective functionals is challenging task, appearing in various applications ranging from topology optimization (cf. Bendsøe & Sigmund [11]) over image processing (see cf. Tsai & Osher [41]) to inverse problems (cf. Burger & Osher [18]). During the last years it got very common to use level set methods (cf. Osher & Fedkiw [35], Litman, Lesselier & Santosa [32]) with velocities dependent on shape derivatives (cf. Delfour & Zolésio [20]) to solve such problems. For several optimization problems, these level set methods were successfully applied to compute optimal geometries without a-priori knowledge of the number of connected components (cf. Burger [13, 15], Dorn, Miller & Rapport [21], Hintermüller & Ring [29], Ito, Kunisch & Li [30], Santosa et al. [32, 36, 37]).

Level set methods are gradient like methods that allow a simple and flexible geometry representation and evolution. The evolution of the geometry happens just locally, i.e. just the boundary of the geometry is evolved. Hence topological changes like splitting and merging can occur during the "time" evolution. However, due to their local nature they might easily get stuck in local minima and one can construct examples where this is indeed the case. This

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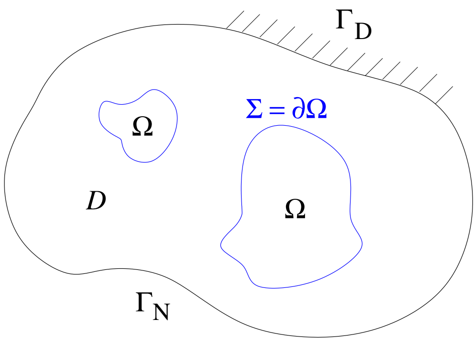
was also observed practically (cf ALLAIRE, JOUVE & TOADER [4, 5] BURGER, HACKL & RING [16]).

Recently a new concept, called topological derivatives (cf. ESCHENAUER, SCHUMACHER ET AL. [22, 23], SOKOLOWSKI & ŻOCHOWSKI [38, 39]) appeared, where one considers the variation of an objective function with respect to the introduction of infinitesimally small holes at a certain point. The topological derivative then indicates whether it is favorable to introduce a hole at this point or not. Already the definition of the topological derivative suggests an algorithm that was successfully applied to several problems (cf. AMSTUTZ ET AL. [7, 8, 9], GUILLAUME & IDRIS [25], GUZINA & BONNET [26], MASMOUDI ET AL. [9, 33]). Also algorithms just based on topological derivatives may stuck in local minima, mainly due to their "disability" to reduce the number of connected components.

Hence several authors (cf. ALLAIRE, GOURNAY, JOUVE & TOADER [3], BURGER, HACKL & RING [16], HINTERMÜLLER [28]) tried successfully to combine classical level set methods with the concept of topological derivatives. Their are basically two ideas how to combine these methods. In one method an additional source term, that depends on the topological derivative, is added to level set methods such that the level set methods allow not just local changes, i.e. evolution of the boundary, but also global changes, due to the of the whole domain defined source term. The other method simply restarts the level set evolution after some fixed time (or due to "clever" chosen stopping criteria), where the initial value is determined via the topological derivative and the last time step. The rational behind these methods is to fulfill the combined necessary optimality condition for shape and topological derivatives (see SOKOLOWSKI & ŻOCHOWSKI [40]).

Nonetheless there are still some problems. First, in geometric inverse problems one usually uses perimeter regularization, which is not topological differentiable at all. Second, topological derivatives sometimes provide only a very rough information, especially do they not provide information about a reliable size and shape of the topology change such that the objective function decreases, when performing this topology change.

By means of a geometric inverse problem we develop an algorithm based on classical level set methods and topological derivatives such that, first, we can deal with perimeter regularizations, second, that topology changes are forced such that the objective function (with perimeter) decreases and the decrease can be estimated from above by the minimum of another, "simpler" minimization problem. In more detail we do a Taylor expansion of the objective function in the volume and the perimeter of the topology change. The expansion up to the first order term in volume, provides us with the topological derivative and together with the remainder, which is of higher order in volume, we get a reliability estimate like for descent methods in the functional analytic framework. Minimizing the first order estimate plus remainder provides a topology change which guarantees a descent in the objective function (with perimeter), where the descent is estimated from above by the minimum of this minimization problem. Likewise for Newton-Trust-region methods, we provide an expansion up to the second order in volume plus remainder of higher order, that provides an estimate whose minimizer is again a topology change with guaranteed descent. As for Newton methods, the calculation of this minimizer is more expensive but provides "close" at the solution, very reliable estimates. The difference of the first and the second order minimization problem is mainly due to an additional partial differential equation as constraint, for the second order problem, that depends on the topology change itself.



The geometric inverse problem we investigate in the following consists of, identifying a compact set $\Omega \in \mathcal{K}(\mathcal{D})$ from measurements $\hat{u}$, with an L_2-error bound, provided on Γ_M, where $\Gamma_M \subset \mathcal{D}$ is either a domain or $\Gamma_M \subset \Gamma_N$. The map of the geometry Ω to the measurements u on Γ_M is defined via the partial differential equation

$$\begin{aligned} -\Delta u + c_\Omega\, u &= f && \text{in } \mathcal{D} \\ \tfrac{\partial u}{\partial n} &= h && \text{on } \Gamma_N \\ u &= g && \text{on } \Gamma_D\,, \end{aligned} \tag{1.1}$$

where $c_\Omega = \underline{c} + (\overline{c} - \underline{c})\chi_\Omega$ and χ_Ω is the characteristic function of Ω.

For a stable identification of the set Ω one usually minimizes the perimeter regularized least squares functional

$$J_\alpha(\Omega) = \frac{1}{2} \int\limits_{\Gamma_M} |u - \hat{u}|^2\, ds + \alpha |\partial\Omega|\,, \tag{1.2}$$

where α acts as regularization parameter and is chosen in dependence of the noise level of the measurements $\hat{u}$. The regularization property of the perimeter and the choice of the parameter α will not be dealt with in this paper (cf. Ben Ameur, Burger & Hackl [10] for a detailed analysis), but only the appearance of the perimeter in the minimization functional will be in the focus in the following, since it prevents the application of known approaches based on topological derivatives.

Notation: We denote with $L^p(\Omega)$ functions on Ω whose p-th power is integrable, with $W^{k,p}(\Omega)$ the Sobolev space of k-times differentiable functions whose derivatives are in $L^p(\Omega)$. Furthermore we abbreviate the Hilbert-space $W^{k,2}(\Omega)$ by $H^k(\Omega)$ and by $H^1_{D,0}(\mathcal{D}) \subset H^1(\mathcal{D}$ the function space with boundary values zero at the boundary $\Gamma_D \subset \partial\mathcal{D}$. Finally we often use the notation $\preceq$ which means $\leq$ up to a constant that does not depend on the important properties.

The paper is organized as follows: In Section 2 we provide the shape and the topological derivative for the objective function (1.2). Then, based on the proof of the topological derivative we provide in Section 3 the first order and also second order expansion of the objective function in volume and perimeter. The first and second order expansions allow to construct steepest descent respectively Newton-type iterations to force topology changes. Hints about the numerical implementation of level set methods and the incorporated steepest descent respectively Newton-type iteration to force topological changes are provided in Section 4. By means of some numerical examples we show in Section 5 the applicability and performance of the, in this paper, suggested methods and finally draw the conclusion in Section 6.

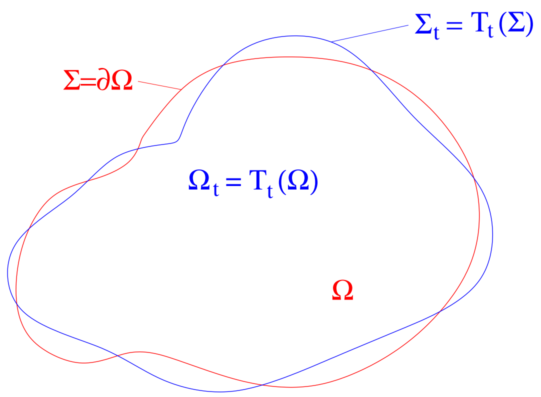
2 Shape- and topological- derivatives

In this section we recall two different notions of shape (geometry) perturbations and consider the sensitivity of the objective function (1.2) with respect to these perturbations. The first perturbation is a pure boundary perturbation by moving a shape (geometry) in a velocity field V. This notion results into the concept of shape derivatives. For a comprehensive introduction to this topic we refer to DELFOUR & ZOLÉSIO [20]. The second perturbation changes the topology of the shape (geometry) by introducing a fixed additional shape with varying size and position. The sensitivity of the objective function (1.2) with respect to the size of the newly introduced shape results into the notion of topological derivatives which were first introduced by ESCHENAUER, SCHUMACHER ET AL. [22, 23] in the context of topology optimization and made mathematically rigorous by SOKOLOWSKI & ŻOCHOWSKI ET AL. [38, 39].

In the following we briefly introduce the notion of shape derivatives where we just state the well-known result about the shape derivative of the objective function (1.2), while we derive the result on the topological derivative of the objective function (1.2) in more detail. The reason for the detailed proof is that it provides an argument which allow estimates of the variation of the objective functional (1.2) in volume and perimeter of the shape (geometry) perturbation.

2.1 Shape derivatives

Shape derivatives for geometric problems allow to characterize extrema and yield directions of steepest descent for appropriate objective functionals, like the *Gateaux-* and *Fréchet derivative* in a functional analytic framework.



The basic idea is to define a perturbation of a domain Ω (piecewise C^2) via the time evolution of the domain in a vector field $V : \mathbb{R}^N \to \mathbb{R}^N$, where V fulfills

$$\begin{aligned} &\exists\, \tau > 0\, \forall\, x \in \mathbb{R}^d : V(.,x) \in C([0,\tau],\mathbb{R}^d) \\ &\exists\, L > 0\, \forall\, x,y \in \mathbb{R}^d : \\ &\quad \|V(.,y) - V(.,x)\|_{C([0,\tau],\mathbb{R}^d)} \le L|y-x|\,. \end{aligned} \tag{2.1}$$

That is, one defines the perturbed domain Ω_t by

$$\Omega_t(V) \;=\; T_t(\Omega, V)\,,$$

where $T_t(.,V)$ is the solution map (the flow) of the dynamical system

$$\begin{aligned} \frac{dT_t(x,V)}{dt} &= V(t, T_t(x,V)) \\ T_0(x,V) &= x\,. \end{aligned} \tag{2.2}$$

With this perturbations we are able to define (formally) the shape derivative of a shape functional $J(\Omega)$ as

$$J'(\Omega)[V] \;=\; \frac{d}{dt} J(T_t(\Omega,V))\big|_{t=0}\,.$$

A basic structure theorem (cf. DELFOUR AND ZOLÉSIO [20]) proves that the shape derivative depends only on $V|_{\partial\Omega}$. Furthermore, for smooth shapes, the perturbation vector field V can be decomposed into a normal and a tangential component on $\partial\Omega$, where the tangential component leaves Ω invariant. Hence the shape derivative is independent of the tangential component and we obtain

$$J'(\Omega)[V] = J'(\Omega)[(V.n)n]\,.$$

In the case that the shape functional $J(\Omega)$ is an objective function in a minimization problem a necessary condition for the shape Ω to be optimal is

$$\forall V \,:\, J'(\Omega)[V] \,=\, 0\,.$$

When the shape functional is not zero we can construct a velocity V such that the objective function decreases, which allows the construction of gradient like descent algorithms, like level set methods (see Section 4.1).

To calculate the shape derivative of the objective functional J_α (1.2) we need the shape derivative of domain, respectively boundary integrals and the solution of the partial differential equation (1.1). These derivatives are well known in the literature (cf. Delfour & Zolésio [20] for shape derivatives of domain and boundary integrals and Hettlich & Rundell [27] for shape derivative of equation (1.1)) and we just state them in the following theorems.

Theorem 2.1 (Shape derivative domain & boundary integrals)**.** *Let Ω be a open, bounded measurable domain of class C^2 with boundary $\Sigma = \partial\Omega$, $V \in C^0\big([0,\tau], C^1_{\text{loc}}(\mathbb{R}^d,\mathbb{R}^d)\big)$ fulfill* (2.1) *and $\varphi \in C\big(0,\tau, W^1_{\text{loc}}(\mathbb{R}^d) \cap C^1(0,\tau,H^2_{\text{loc}}(\mathbb{R}^d))\big)$, then the semi-derivative of the shape functionals*

$$J_D(\Omega_t) \,:=\, \int\limits_{T_t(\Omega,V)} \varphi(t)\,dx \qquad J_B(\Sigma_t) \,:=\, \int\limits_{T_t(\Sigma,V)} \varphi(t)\,ds(t)$$

at $t = 0$ are given by

$$\begin{aligned} J'_D(\Omega)[V(0)] &= \int\limits_{\Omega} \varphi'(0)\,dx + \int\limits_{\Sigma} \varphi(0)V(0).n\,dx \\ J'_B(\Gamma)[V(0)] &= \int\limits_{\Sigma} \varphi'(0) + \Big(\frac{\partial\varphi(0)}{\partial n} + \kappa\varphi(0)\Big)V(0).n\,ds\,, \end{aligned}$$

where κ is the mean curvature

Theorem 2.2. *Let Ω be a domain with C^1 boundary and the velocity field V be as in the previous theorem. Then the solution u of equation* (1.1) *is shape differentiable and its shape derivative is characterized by the unique solution $u' = u'0[V(0)]$ to the transmission problem*

$$\begin{array}{lll} -\Delta u' + c_\Omega\, u' = 0 & & \text{in } \Omega \cup \mathcal{D} \setminus \overline{\Omega} \\ \left[\!\left[\dfrac{\partial u'}{\partial n}\right]\!\right] & = -\left[\!\left[c_\Omega\right]\!\right] V(0).n & \text{on } \partial\Omega \\ \left[\!\left[u'\right]\!\right] & = 0 & \text{on } \partial\Omega \\ \dfrac{\partial u'}{\partial n} & = 0 & \text{on } \Gamma_N \\ u' & = 0 & \text{on } \Gamma_D\,, \end{array} \tag{2.3}$$

where $[\![\,.\,]\!]$ denotes the jump across the interface $\partial\Omega$.

Summing up, the shape derivative of the objective functional J_α (1.2) becomes

$$J'_\alpha(\Omega)[V(0)] \,=\, \int\limits_{\Gamma_M} u'[V(0)](u-\hat{u})\,ds + \alpha \int\limits_{\partial\Omega} \kappa V(0).n\,ds\,.$$

We can simplify this shape derivative when we introduce the adjoint state w defined by

$$\begin{array}{lll} -\Delta w + c_\Omega\, w = -\chi_{\Gamma_M}(u-\hat{u}) & & \text{in } \mathcal{D} \\ \frac{\partial w}{\partial n} \qquad\quad = -\chi_{\Gamma_M}(u-\hat{u}) & & \text{on } \Gamma_N \\ w \qquad\qquad = 0 & & \text{on } \Gamma_D\,. \end{array} \tag{2.4}$$

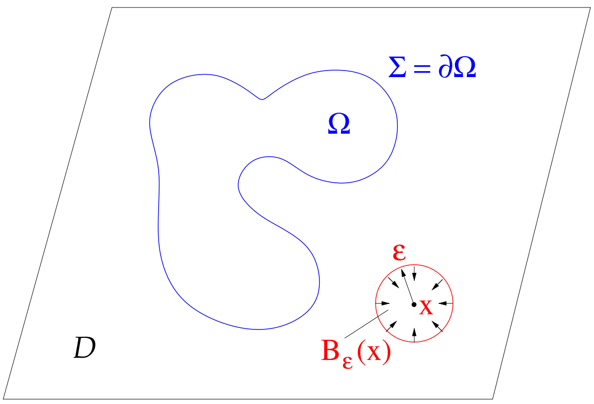
The shape derivative of the objective function $J_\alpha(\Omega)$ finally gets

$$J'_\alpha(\Omega)[V(0)] \;=\; \int_{\partial\Omega} (uw + \alpha\kappa) V(0).n\, ds\,. \tag{2.5}$$

First note that we just solve two partial differential equations, namely (1.1), (2.4) to calculate the full shape derivative. Second, the first order necessary condition for optimal shapes Ω requires $\forall V \,:\, J'_\alpha(\Omega)[V(0)] = 0$, hence $(uw+\alpha\kappa) = 0$ and if this is not the case we can construct a velocity such that $J'_\alpha(\Omega)[V(0)] < 0$. For example take $V = -(uw+\alpha\kappa)n$, but other choices are possible (see Burger [14]).

2.2 Topological derivatives

Opposed to the *shape derivative* where one considers the variation of a shape the *topological derivative* aims for variations of the topology.



The basic idea of the *topological derivative* is to add a small ball with center x and radius ϵ to the domain Ω and consider the variation of the objective functional $J(\Omega \cup B_\epsilon(x))$ with respect to the radius of this sphere (different shapes than balls are possible and might result into different values of the derivatives).

Definition 2.3 (Topological Derivative)**.** Let $J : \Omega \subset \mathbb{R}^d \to \mathbb{R}$ be a objective function. Then the *topological derivative* is defined as the limit (if it exists)

$$d_\tau J(x) \;:=\; \lim_{\epsilon\to 0^+} \frac{J(\Omega \cup B_\epsilon(x)) - J(\Omega)}{|B_\epsilon(x)|} \tag{2.6}$$

A negative *topological derivative* $d_\tau J(x) < 0$ indicates that it might be reasonable to add an infinitely small sphere at the point x to reduce the objective function. Hence it is an indicator that allows to force topology changes.

Instead of adding material it is also possible to subtract material i.e. take the “set-minus” instead of the “union” in (2.6). We will use both notions without mentioning it.

Remark 1. In practice, topology changes forced by the topological derivative are neither spherical nor infinitesimally small. Hence a descent in the objective function is not guaranteed any more. Nonetheless the practical experience by most authors, using the topological derivative as an indicator to force topology changes, are rather positive.

First of all consider the topological derivative of the perimeter $|\partial\Omega|$. From the definition we get

$$d_\tau|\partial\Omega| \;=\; \lim_{\epsilon\to 0}\frac{|\partial B_\epsilon(x)|}{|B_\epsilon(x)|} \;\simeq\; \lim_{\epsilon\to 0}\frac{\epsilon^{d-1}}{\epsilon^d} \;=\; \infty\,.$$

Hence the perimeter is not topologically differentiable. In practical applications one usually neglects this fact and calculates the topological derivative of the objective function without perimeter, i.e. for $J_0(\Omega)$. The topological derivative of $J_0(\Omega)$ is already well known (see Amstutz [6]). Nonetheless we provide a detailed proof, that is based on Hölder estimates, Sobolev embeddings (cf. Adams [1]) and regularity results for elliptic partial differential equations (cf. Giaquinta [24]). Parts of the proof will play a crucial role in the rest of the paper. Let us first state Sobolev's embedding theorem and the interior regularity result for elliptic partial differential equations:

Theorem 2.4 (Sobolev embedding)**.** *Let Ω be a domain having the cone property in $\mathbb{R}^n$. Let $j,n\in\mathbb{N}_0$ and $p\in[1,\infty[$. Then, if*

$n>mp$**:** $W^{j+m,p}(\Omega)\to W^{j,q}(\Omega)$ *for* $p\le q\le\frac{np}{n-mp}$,

$n=mp$**:** $W^{j+m,p}(\Omega)\to W^{j,q}(\Omega)$ *for* $p\le q<\infty$,

$n<mp$**:** $W^{j+m,p}(\Omega)\to C^j_B(\Omega)$

In the following arguments we will, for 2-dimensions, often meet the case $n=mp$ which would require a case study. This is a little bit tedious, hence we are sloppy at this point and keep in mind that we need to adapt the final results to this case.

Theorem 2.5 (Interior regularity)**.** *Let u be the weak solution to the linear elliptic equation*

$$-D_i\big(A_{ij}D_ju\big) \;=\; f-D_if_i\,,$$

where $A_{ij}\in C^{0,1}(\mathcal{D})$ is elliptic, $f\in L^2(\mathcal{D})$ and $F=(f_i)\in H^1(\mathcal{D},\mathbb{R}^n)$, then $u\in H^2_{\mathrm{loc}}(\mathcal{D})$ and even more,

$$\|u\|^2_{H^2([\mathcal{D}]^{-\epsilon})} \;\le\; C(n)\big(\|f\|^2_{L^2(\mathcal{D})}+\|DF\|^2_{L^2(\mathcal{D})}+\frac{1}{\epsilon^2}\|\nabla u\|^2_{L^2(\mathcal{D})}\big) \tag{2.7}$$

where $[\mathcal{D}]^{-\epsilon} \;:=\; \mathrm{cl}\big(\mathrm{int}\{x\in\mathcal{D}\,|\,\mathrm{dist}(x,\partial\mathcal{D})\;\ge\;\epsilon\}\big)\,.$

We will need the interior regularity result quite often, especially estimate (2.7). To keep writing shorter we denote above estimate a little bit sloppy by

$$\|u\|^2_{H^2_{\mathrm{loc}}(\mathcal{D})} \;\preceq\; \|f\|^2_{L^2(\mathcal{D})}+\|DF\|^2_{L^2(\mathcal{D})}+\|\nabla u\|^2_{L^2(\mathcal{D})}\big)$$

but keep always in mind that this estimate depends on the distance to the boundary $\partial\mathcal{D}$.

Note that $\|u\|_{H^1(\mathcal{D})}$ is usually the solution to some boundary value problem and can be estimated by

$$\|u\|_{H^1(\mathcal{D})} \;\preceq\; \|f\|_{L^2(\mathcal{D})}+\|F\|_{L^2(\mathcal{D})}+\|g\|_{H^{\frac{1}{2}}(\Gamma_D)}+\|h\|_{H^{-\frac{1}{2}}(\Gamma_N)}\,,$$

where the constant in above estimate depends just on the ellipticity of A_{ij} and geometric properties of $\mathcal{D}$, Γ_D. Furthermore note that with additional smoothness assumptions on $\partial\mathcal{D}$, regularity and compatibility conditions of the boundary conditions the interior regularity can be extended to a regularity everywhere, i.e. instead of $H^2([\mathcal{D}]^{-\epsilon})$ we get an estimate of above type for $H^2(\mathcal{D})$ where the constant depends just on $C(n,\mathcal{D})$.

Finally, before we calculate the topological derivative, let us recall the direct (1.1) and adjoint (2.4) partial differential equation, but in their weak form.

Direct problem:

$$\langle \nabla u, \nabla v\rangle + \langle c_\Omega u, v\rangle \;=\; \langle f, v\rangle \qquad \forall\, v \in H^1_{0,D}(\mathcal{D}) \tag{2.8}$$

Adjoint problem:

$$\langle \nabla v, \nabla w\rangle + \langle c_\Omega v, w\rangle \;=\; -D_u J(\Omega)[v] \qquad \forall\, v \in H^1_{0,D}(\mathcal{D}) \tag{2.9}$$

In the following we will often use the topologically perturbed domain $\tilde{\Omega}$ and the corresponding solution $\tilde{u}$ of (1.1). Furthermore note that due to the interior regularity result we have:

$$\begin{aligned}\|u\|_{H^2_{\text{loc}(\mathcal{D})}} &\preceq \|f\|_{L^2(\mathcal{D})} + \|g\|_{H^{\frac{1}{2}}(\Gamma_D)} + \|h\|_{H^{-\frac{1}{2}}(\Gamma_N)}\\ \|w\|_{H^2_{\text{loc}(\mathcal{D})}} &\preceq \|u-\hat{u}\|_{L^2(\Gamma_M)}\end{aligned}$$

Proposition 2.6. *For every point $x \in \operatorname{int}\mathcal{D}$ the topological derivative of the shape function J_0 (1.2) is given by*

$$d_\mathcal{T} J_0(\Omega)(x) \;=\; -2(\chi_\Omega - \frac{1}{2})(\overline{c} - \underline{c})u(x)w(x)\,.$$

Proof. Let $\tilde{\Omega}$, $\Omega \subset \operatorname{int}\mathcal{D}$ be arbitrary domains with positive Lebesgue measure and consider a Taylor expansion of the objective function J_0 with respect to the state u.

$$J_0(\tilde{\Omega}) - J_0(\Omega) \;=\; D_u J_0(\Omega)[\tilde{u}-u] + D_u^2 J_0(\Omega)[\tilde{u}-u]^2 + \mathcal{O}(\|\tilde{u}-u\|^3_{H^1(\mathcal{D})})\,.$$

In our case we have a quadratic functional, hence the remainder term vanishes. In the following we deal with every term of the expansion separately.

$\|\tilde{u}-u\|_{H^1(\mathcal{D})} \simeq |\tilde{\Omega}\Delta\Omega|^{\frac{n+2}{2n}}$**:** We subtract the two determining partial differential equations for u respectively $\tilde{u}$ and rearrange the terms to get

$$\langle \nabla(\tilde{u}-u), \nabla v\rangle + \langle c_{\tilde{\Omega}}(\tilde{u}-u), v\rangle \;=\; -\langle (c_{\tilde{\Omega}} - c_\Omega)u, v\rangle \;\preceq\; |\overline{c}-\underline{c}|\|u\|_{L^{\frac{2n}{n+2}}(\tilde{\Omega}\Delta\Omega)}\|v\|_{H^1(\mathcal{D})}$$

$D_u^2 J_0(\Omega)[\tilde{u}-u]^2 \simeq |\tilde{\Omega}\Delta\Omega|^2$**:** First note that $D_u^2 J_0(\Omega)[\tilde{u}-u]^2 = \frac{1}{2}\|\tilde{u}-u\|^2_{L^2(\Gamma_M)}$. Next, let s be the solution to a modified adjoint problem

$$\langle \nabla v, \nabla s\rangle + \langle c_\Omega v, s\rangle \;=\; -D_u^2 J_0(\Omega)[\tilde{u}-u][v] \qquad \forall\, v \in H^1_{0,D}(\mathcal{D})\,.$$

The interior regularity result also applies to s, i.e $\|s\|^2_{H^2_{\text{loc}}(\mathcal{D})} \preceq D_u^2[\tilde{u}-u]^2$ and we get $\|s\|_{H^2_{\text{loc}(\mathcal{D})}} \preceq \|\tilde{u}-u\|_{L^2(\Gamma_M)}$. Hence we obtain from a standard technique

$$\begin{aligned} D_u^2 J_0(\Omega)[\tilde{u}-u]^2 &= -\langle \nabla(\tilde{u}-u), s\rangle - \langle c_\Omega(\tilde{u}-u), s\rangle \;=\; \langle (c_{\tilde{\Omega}} - c_\Omega)\tilde{u}, s\rangle\\ &\preceq |\overline{c}-\underline{c}|\big(|\tilde{\Omega}\Delta\Omega|^{\frac{n+2}{2n}}\|\tilde{u}-u\|_{H^1(\mathcal{D})} + \|u\|_{L^1(\tilde{\Omega}\Delta\Omega)}\big)\|s\|_{H^2_{\text{loc}}(\mathcal{D})}\,.\end{aligned}$$

$DJ_0(\Omega)[\tilde u - u] \,=\, \langle (c_{\tilde\Omega} - c_\Omega)u, w\rangle + \mathcal{O}\big(|\tilde\Omega\Delta\Omega|^{\frac{n+2}{n}}\big)$: Finally we estimate the linear term in the Taylor expansion:

$$\begin{aligned} DJ_0(\Omega)[\tilde u - u] \;&=\; -\langle \nabla(\tilde u - u), \nabla w\rangle - \langle c_\Omega(\tilde u - u), w\rangle \;=\; \langle (c_{\tilde\Omega} - c_\Omega)\tilde u, w\rangle \\ &=\; \langle (c_{\tilde\Omega} - c_\Omega)u, w\rangle + \langle (c_{\tilde\Omega} - c_\Omega)(\tilde u - u), w\rangle \\ &\leq\; \langle (c_{\tilde\Omega} - c_\Omega)u, w\rangle + \mathcal{O}\big(|\overline{c} - \underline{c}|\|\tilde u - u\|_{H^1(\mathcal{D})}\|w\|_{L^{\frac{2n}{n+2}}(\tilde\Omega\Delta\Omega)}\big) \end{aligned}$$

Summing up all the estimates we get

$$J_0(\tilde\Omega) - J_0(\Omega) \;\leq\; \langle (c_{\tilde\Omega} - c_\Omega)u, w\rangle + \mathcal{O}\big(|\tilde\Omega\Delta\Omega|^{\frac{n+2}{n}}\big)\,.$$

Now set $\tilde\Omega \;=\; B_\epsilon(x) \cup \Omega$ and perform the limit according to the definition of the topological derivative. The limit exists due to the Lebesgue differentiation theorem (cf. Giaquinta [24]) and the fact that $u,\, w \in C_{\mathrm{loc}}(\mathcal{D})$. □

Like the shape derivative (2.5), the topological derivative depends on the solution u of (1.1) and the adjoint w (2.4) only, which is standard for adjoint methods. Moreover, both derivatives seem to be the same, which is not true in general, but holds, up to a constant, for surprisingly many cases.

3 Topological expansions up to the first and second order

While we developed two different notions of derivatives in the last section, where the shape derivative fitted quite well into a functional analytic framework and allowed the development of steepest descent type and even Newton-type algorithms which is not true for the topological derivatives because it is just an indicator, we develop in this section estimates for topology changes, that again allow to construct steepest descent type and even Newton-type steps. The estimates for the objective function $J_\alpha(\Omega)$, we develop in the following, are accurate in the first respectively second order in volume and perimeter of the topology change. Hence we phrase them first and second order topological expansion. These expansions correspond very well to functional analytic ideas where one expands objective functionals $J(x)$, where $x \in X$ is an element of some normed function space X equipped with the norm $\|\,.\,\|_X$, up to first and second order, i.e.

First order expansion: $J(\tilde x) - J(x) \;\leq\; \partial_x J(x)[\tilde x - x] + c\|\tilde x - x\|_X^{1+\beta}$

Second order expansion: $J(\tilde x) - J(x) \;\leq\; \partial_x J(x)[\tilde x - x] + \partial_x^2 J(x)[\tilde x - x]^2 + c\|\tilde x - x\|_X^{2+\beta}$

where $\beta \,>\, 0$. Minimizing the right hand side of above estimates, in $\tilde x$, result into steepest descent type steps for the first order expansion and Newton-type steps for the second order expansion.

In the following we develop similar estimates where we replace the function space elements $x, \tilde x$ by geometric objects $\Omega, \tilde\Omega$, which are not elements of function spaces, and the norm $\|\tilde x - x\|_X$ by the volume $|\tilde\Omega\Delta\Omega|$ and the perimeter $|\partial(\tilde\Omega\Delta\Omega)|$.

3.1 First order topological expansion

A closer look at the proof of the topological derivative (Proposition 2.6) shows that we already have an estimate of a topology change in the objective function $J_\alpha(\Omega)$ (1.2) up to the first order namely

$$J_\alpha(\tilde{\Omega}) - J_\alpha(\Omega) \;\leq\; \langle (c_{\tilde{\Omega}} - c_\Omega)u, w\rangle + \alpha|\partial(\tilde{\Omega}\Delta\Omega)| + \mathcal{O}\big(|\tilde{\Omega}\Delta\Omega|^{\frac{n+2}{2}}\big)\,. \tag{3.1}$$

Our aim is to minimize the objective function $J_\alpha(\Omega)$ (1.2) with respect to the geometry Ω. Hence, when we already have an initial guess Ω_k we can "improve" it and calculate a new geometry Ω_{k+1} such that we reduce the objective function $J_\alpha(\Omega_k)$, when we solve the minimization problem

$$\Omega_{k+1} \;=\; \operatorname*{argmin}_{\Omega\in\mathcal{K}(\mathcal{D})} \langle (c_\Omega - c_{\Omega_k})u, w\rangle + \alpha|\partial(\Omega\Delta\Omega_k)| + c\big(|\Omega\Delta\Omega_k|^{\frac{n+2}{2}}\big)\,, \tag{3.2}$$

where only c is an unknown constant arising from the embedding and regularity results. In principle the constant c can be estimated from above, but algorithmically it seems favorable to perform a trust region approach and vary c until the predicted decrease of the objective function $J_\alpha(\Omega)$ is close to the actual decrease.

In principle above argument would already suggest an steepest descent type algorithm to solve the original minimization problem of $J_\alpha(\Omega)$, but we are more interested to use just one step of this algorithm in level set methods to force systematically reliable topology changes such that the objective function $J_\alpha(\Omega)$ decreases.

Any way, we first have to prove that the minimization problem (3.2) has a solution, not necessarily unique.

Proposition 3.1. *Minimization problem* (3.2) *has a solution in the class of sets with finite perimeter* $\mathcal{K}(\mathcal{D})$.

Proof. First note that the minimization problem (3.2) in the class of sets with finite perimeter is equivalent to

$$\min_{p\in \mathrm{BV}(\mathcal{D},\{0,1\})} -2(\overline{c}-\underline{c})\langle(\chi_{\Omega_k} - \frac{1}{2})pu, w\rangle + \alpha|p|_{\mathrm{BV}} + c\big(|p|^{\frac{n+2}{2}}_{L^1(\mathcal{D})}\big)\,.$$

Due to the perimeter regularization term a minimizing sequence (p_n) is uniformly bounded in BV. Hence it has a BV weak-* limit p which is, due to the compact embedding of $\mathrm{BV}\hookrightarrow L^1$, also the strong limit in L^1. Finally, the lower semi-continuity of $|\,.\,|_{\mathrm{BV}}$ in the functions of bounded variation $\mathrm{BV}(\mathcal{D})$ guarantees that p is a solution to the minimization problem and hence $\Omega_{k+1} = \big(\Omega_k \setminus \{\chi_{\Omega_k}p = 1\}\big) \cup \{(1-\chi_{\Omega_k})p = 1\}$ is a minimizer to (3.2). $\square$

Note that the minimizer might be Ω_k itself, i.e. no topology change is favorable to generate a guaranteed descent in the objective function $J_\alpha(\Omega)$. This happens when the perimeter term dominates the first order term, i.e. when the topology changes get too small or when the topology is already the optimum to $J_\alpha(\Omega)$.

Remark 2. Algorithmically it might be even better to take the refined estimate, that comes from an accurate collection of the remainder terms in the proof of Theorem 2.6.

$$\begin{aligned} J_\alpha(\tilde{\Omega}) - J_\alpha(\Omega) \;\leq\; & \langle (c_{\tilde{\Omega}} - c_\Omega)u, w\rangle + \alpha|\partial(\tilde{\Omega}\Delta\Omega)| \\ & + \mathcal{O}\Big(|\overline{c}-\underline{c}|^2\|u\|_{L^{\frac{2n}{n+2}}(\tilde{\Omega}\Delta\Omega)}\big(\|u\|_{L^{\frac{2n}{n+2}}(\tilde{\Omega}\Delta\Omega)}|\tilde{\Omega}\Delta\Omega|^{\frac{n-2}{n}} + \|w\|_{L^{\frac{2n}{n+2}}(\tilde{\Omega}\Delta\Omega)}\big)\Big) \end{aligned}$$

3.2 Second order topological expansion

As for the topological derivative we start with a Taylor expansion of the objective function $J_0(\Omega)$ with respect to the state variable, but this time we perform a expansion up to the second order in volume. For this sake we have to introduce a linearization of the partial differential equation (1.1).

Linearized problem:

$$\begin{aligned} -\Delta u^{\mathrm{lin}} + c_\Omega u^{\mathrm{lin}} &= -(c_{\tilde\Omega} - c_\Omega)u && \text{in } \mathcal{D} \\ \frac{\partial u^{\mathrm{lin}}}{\partial n} &= 0 && \text{on } \Gamma_N \\ u^{\mathrm{lin}} &= 0 && \text{on } \Gamma_D \end{aligned}$$

We will need the weak form of the linearized problem, which is given by

$$\langle \nabla u^{\mathrm{lin}}, \nabla v\rangle + \langle c_\Omega u^{\mathrm{lin}}, v\rangle \;=\; -\langle (c_{\tilde\Omega} - c_\Omega)u, v\rangle \qquad \forall\, v \in H^1_{0,D}(\mathcal{D}) \tag{3.3}$$

Hence the refined Taylor expansion for the gets.

$$\begin{aligned} J(\tilde\Omega) - J(\Omega) \;=\;& D_u J(\Omega)[\tilde u - u] + \tfrac{1}{2} D_u^2 J(\Omega)[u^{\mathrm{lin}}]^2 \\ & + D_u^2 J(\Omega)[\tilde u - u - u^{\mathrm{lin}}][u^{\mathrm{lin}}] + \tfrac{1}{2} D_u^2 J(\Omega)[\tilde u - u - u^{\mathrm{lin}}]^2 + \mathcal{O}\big(\|\tilde u - u\|^3_{H^1(\mathcal{D})}\big) \end{aligned}$$

Again we estimate the higher order terms in the second row and reformulate the terms in the first row to obtain.

$\|u^{\mathbf{lin}}\|_{H^1(\mathcal{D})} \preceq |\tilde\Omega \Delta \Omega|^{\frac{n+2}{2n}}$**:**

$$\langle a\nabla u^{\mathrm{lin}}, \nabla v\rangle + \langle c_\Omega u^{\mathrm{lin}}, v\rangle \;=\; -\langle (c_{\tilde\Omega} - c_\Omega)u, v\rangle \;\preceq\; \|u\|_{L^{\frac{2n}{n+2}}(\tilde\Omega\Delta\Omega)} \|v\|_{H^1(\mathcal{D})}$$

$\|\tilde u - u - u^{\mathbf{lin}}\|_{H^1(\mathcal{D})} \preceq |\tilde\Omega \Delta \Omega|^{\frac{n+6}{2n}}$**:**

$$\begin{aligned} \langle a\nabla(\tilde u - u - u^{\mathrm{lin}}), \nabla v\rangle + \langle c_\Omega(\tilde u - u - u^{\mathrm{lin}}), v\rangle \;&=\; -\langle (c_{\tilde\Omega} - c_\Omega)(\tilde u - u), v\rangle \\ \preceq |\tilde\Omega\Delta\Omega|^{\frac{2}{n}} \|\tilde u - u\|_{H^1(\mathcal{D})} \|v\|_{H^1(\mathcal{D})} \;&\preceq\; |\tilde\Omega\Delta\Omega|^{\frac{2}{n}} \|u\|_{L^{\frac{2n}{n+2}}(\tilde\Omega\Delta\Omega)} \|v\|_{H^1(\mathcal{D})} \end{aligned}$$

$DJ(\Omega)[\tilde u - u] \;=\; \langle (c_{\tilde\Omega} - c_\Omega)(u + u^{\mathbf{lin}}), w\rangle + \mathcal{O}\big(|\tilde\Omega\Delta\Omega|^{\frac{n+4}{n}}\big)$**:**

$$\begin{aligned} DJ(\Omega)[\tilde u - u] \;&=\; -\langle a\nabla(\tilde u - u), \nabla w\rangle - \langle c_\Omega(\tilde u - u), w\rangle \;=\; \langle (c_{\tilde\Omega} - c_\Omega)\tilde u, w\rangle \\ &=\; \langle (c_{\tilde\Omega} - c_\Omega)(u + u^{\mathrm{lin}}), w\rangle + \langle (c_{\tilde\Omega} - c_\Omega)(\tilde u - u - u^{\mathrm{lin}}), w\rangle \\ &\preceq\; \langle (c_{\tilde\Omega} - c_\Omega)(u + u^{\mathrm{lin}}), w\rangle + \|w\|_{L^{\frac{2n}{n+2}}(\tilde\Omega\Delta\Omega)} \|\tilde u - u - u^{\mathrm{lin}}\|_{H^1(\mathcal{D})} \\ &\preceq\; \langle (c_{\tilde\Omega} - c_\Omega)(u + u^{\mathrm{lin}}), w\rangle + |\tilde\Omega\Delta\Omega|^{\frac{2}{n}} \|u\|_{L^{\frac{2n}{n+2}}(\tilde\Omega\Delta\Omega)} \|w\|_{L^{\frac{2n}{n+2}}(\tilde\Omega\Delta\Omega)} \end{aligned}$$

When we sum up the different contributions we end up in the second order topological expansion

$$J_\alpha(\tilde\Omega) - J_\alpha(\Omega) \;\leq\; \langle (c_{\tilde\Omega} - c_\Omega)(u + u^{\mathrm{lin}}), w\rangle + \frac{1}{2} D_u^2 J(\Omega)[u^{\mathrm{lin}}]^2 + \alpha|\partial(\tilde\Omega\Delta\Omega)| + \mathcal{O}\big(|\tilde\Omega\Delta\Omega|^{\frac{n+4}{n}}\big)\,. \tag{3.4}$$

In contrast to the first order topological expansion (3.1) the second order expansion is a partial differential equation constraint problem. Again, like for optimization problems in function spaces, we can "improve" an initial geometry Ω_k, such that the objective function $J_\alpha(\Omega)$ decreases, when we solve the partial differential equation constraint minimization problem

$$\Omega_{k+1} = \underset{u^{\text{lin}} \text{ solves } (3.3), \Omega \in \mathcal{K}(\mathcal{D})}{\operatorname{argmin}} \langle (c_\Omega - c_{\Omega_k})(u + u^{\text{lin}}), w \rangle + \frac{1}{2} D_u^2 J_\alpha(\Omega_k)[u^{\text{lin}}]^2 + \alpha |\partial(\Omega \Delta \Omega_k)| \quad (3.5)$$

The constraint minimization problem is similar to Newton-type step. Later we will use the solution to the minimization problem to force a topology change in level set methods. But before we have to proof that this constraint minimization problem has a solution.

Proposition 3.2. *The partial differential equation constraint minimization problem* (3.5) *has a solution in the class of sets with finite perimeter* $\mathcal{K}(\mathcal{D})$.

Proof. The partial differential equation constraint minimization problem (3.5) in the class of sets with finite perimeter is equivalent to

$$\min_{u^{\text{lin}} \text{ solves } (3.3), p \in \text{BV}(\mathcal{D}, \{0,1\})} -2(\overline{c} - \underline{c}) \langle (\chi_{\Omega_k} - \frac{1}{2}) p (u + u^{\text{lin}}), w \rangle + \frac{1}{2} D_u^2 J_\alpha(\Omega_k)[u^{\text{lin}}]^2 + \alpha |p|_{\text{BV}} .$$

The minimization problem is bounded from below because u^{lin} is uniformly bounded in H^1. Hence we can take a minimizing sequence (p_n) which is due to the perimeter regularization term bounded from above in BV. The minimizing sequence converges weak-* in BV to p and due to the compact embedding BV $\hookrightarrow L^1$, also strong in L^1. Furthermore the to p_n corresponding solution u_n^{lin} (3.3) converges even strongly in H^1. This strong convergence and the lower semi-continuity of the perimeter in the function space BV guarantees that p is a minimizer and hence $\Omega_{k+1} = \big(\Omega_k \setminus \{\chi_{\Omega_k} p = 1\}\big) \cup \{(1 - \chi_{\Omega_k}) p = 1\}$ is a minimizer of (3.5). ☐

In principle, minimization problem (3.5) is as difficult as the original problem but first we do not need to solve it too accurately. It is enough to correct the first order solution. Second, it might be much easier to construct efficient solvers for problems with "linear" (in the shape) partial differential equation constraints. For example in imaging it is possible to reformulate problems in $\text{BV}(\{0,1\})$ to problems in $\text{BV}([0,1])$ (cf. Burger & Hintermüller [17]). Furthermore there is a well developed theory for BV-regularization for linear problems (cf. Osher et al. [34]). Third, it is possible to solve the second order estimate problem with phase-field methods (for an introduction cf. Alberti [2]) and it is probably easier to prove Γ-convergence for the minimization problem (3.5) than for the original one.

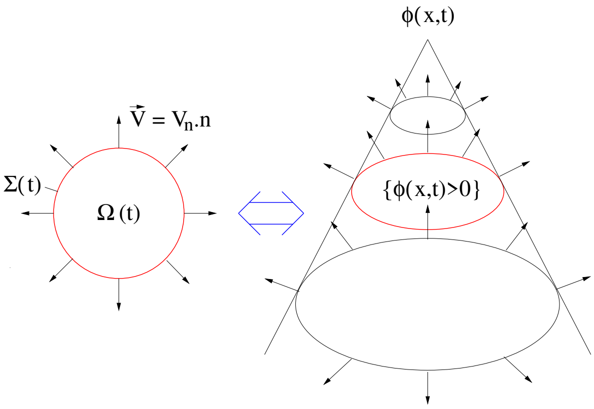
4 Numerical solution

In this section we discuss on one hand how to incorporate the topological steepest descent (3.2) respectively the Newton-type (3.5) step into level set methods and on the other hand how to solve these minimization problems (3.2), (3.5) for the topological steepest descent respectively Newton-type step. Furthermore we describe the setting used for numerical calculations presented in Section 5.

We start with a brief introduction into level set methods. For a detailed exposition about level set methods for the propagation of interfaces refer to Osher & Fedkiw [35]. Next we provide the so called phase I/II method which was already used by several authors (cf. ALLAIRE ET AL. [3], BURGER, HACKL & RING [16], HINTERMÜLLER [28]) to incorporate the topological gradient into level set methods. Finally we describe solution methods to solve the minimization problems (3.2), (3.5).

4.1 Level Set Methods

The main idea of level set methods is to represent an evolving front $\Sigma(t) = \partial\Omega(t)$ as the zero level set of a continuous function, i.e.



$$\Omega(t) = \{x \in \mathcal{D} \mid \phi(x,t) > 0\}$$
$$\Sigma(t) = \{x \in \mathcal{D} \mid \phi(x,t) = 0\}$$

The geometric motion of the level set with normal velocity $\vec{V} = V_n.n$ is given by the Hamilton-Jacobi equation

$$\frac{\partial\phi}{\partial t} - V_n|\nabla\phi| = 0 \qquad \text{in } \mathbb{R}^d \times \mathbb{R}^+ \qquad (4.1)$$

which is the analog to the flow equation (2.2).

As already mentioned in Section 2.1 the crucial point is an appropriate choice of the velocity, such that the objective function $J_\alpha(\Omega)$ (1.2) decreases. This resembles the classical speed method in shape optimization (cf. DELFOUR & ZOLÉSIO [20]), but the weak formulation via the level set method allows for more general evolutions and in particular for topological changes such as splitting or merging of domains.

Let us recall the shape derivative $J'_\alpha(\Omega)[V_n]$ for the objective function $J_\alpha(\Omega)$ (1.2).

$$J'_\alpha(\Omega)[V_n] = \int_{\partial\Omega} \big(uw + \alpha\kappa\big) V_n \, ds$$

The simplest choice for the normal velocity V_n to reduce the objective function (1.2) would be $V_n = -\big(uw + \alpha\kappa\big)$. This choice results into a very regular velocity. Due to BURGER [14] a preconditioned velocity $V_n \in H^{-\frac{1}{2}}(\partial\Omega)$ is more appropriate and results into faster convergence. This $H^{-\frac{1}{2}}$ velocity can be calculated when we solve the subproblem

$$\langle\psi, v\rangle = -\langle uw + \alpha\kappa, \left[\!\left[\frac{\partial v}{\partial n}\right]\!\right]\rangle_{\partial\Omega} \qquad \forall\, v \in H^1_0(\mathcal{D}),$$

and set $V_n = \left[\!\left[\frac{\partial\psi}{\partial n}\right]\!\right]$.

We solve the level set equation (4.1) with a standard fifth order WENO scheme for the spatial and a third order explicit Runga-Kutta scheme for the time discretization (see JIANG, PENG [31]).

4.2 Phase I/II algorithm

In BURGER, HACKL & RING [16] the topological derivatives were incorporated as an extra source term in the level set methods.

$$\frac{\partial\phi}{\partial t} - V_n|\nabla\phi| + \mathcal{S} = 0 \qquad V_n = V_n(J'_\alpha),\ \mathcal{S} = \mathcal{S}(d_\tau J_0)$$

This idea fits very well to the basic idea of topological derivatives because the topological changes usually appear at a very small size (like infinitesimally small balls) and grow (shrink) according to the shape derivatives. An inherent time step control in the level set methods guaranteed that the topological change was such that the objective function decreased. Another method, also suggested in Burger, Hackl & Ring [16] but also in Allaire et al. [3] and Hintermüller [28] is to restart the level set evolution after a fixed time (or due to "clever" criteria) with an initial level set function generated by the last time step plus the topological change due to the topological derivatives. This algorithm was phrased phase I/II algorithm by Hintermüller [28] where phase I corresponds to the algorithm for the topology change and phase II to the "classical" level set evolution. Let us put this into a more mathematical formulation: Let $(T_i)_{i\in\mathbb{N}_0}$ be a series of time steps, either fixed or generated due to a termination criterion in the level set evolution. Set $\phi_{-1}(T_{-1})$ to an initial guess (usually no material or material everywhere), Then the phase I/II algorithm is given by

$$\begin{aligned} &\tfrac{\partial \phi_i}{\partial t} + V_n(J'_\alpha)|\nabla\phi_i| = 0 \\ &\phi_i(t=0) = \mathcal{S}(d_\tau J_0, \phi_{i-1}(T_{i-1}))\,, \end{aligned}$$

where $\mathcal{S}(.,.)$ describes phase I, i.e. the algorithm that forces the topology change. Usually phase I, that depends just on the topological derivative $d_\tau J_0$ might increase the objective function J_α. Only a clever algorithm, like the line search algorithm proposed by Hintermüller [28], guarantees a descent in the objective J_0, also for phase I. An extension of the line search algorithm to problems with perimeter constraints J_α is possible with the methods developed in this paper.

Our main idea was to construct topological changes such that the decrease in the objective functional $J_\alpha(\Omega)$ is guaranteed and even maximal with respect to the first, respectively second order topological expansion. Hence we choose for $\mathcal{S}(J_\alpha, \phi_{i-1}(T_{i-1}))$ the solution-map of the minimization problem (3.2) respectively (3.5). In the following we will describe just briefly how to solve these minimization subproblems numerically.

Phase I

We proposed two sub-minimization problems (3.2), (3.5), where the first provides a steepest descent type topology change and the second a Newton-type topology change. Both are different in their numerical treatment.

Steepest descent type topology changes

First recall the associated minimization problem (3.2) whose minimizer provide a steepest descent type topology change.

$$\Omega_{k+1} = \operatorname*{argmin}_{\Omega\in\mathcal{K}(\mathcal{D})} \underbrace{\langle (c_\Omega - c_{\Omega_k})u, w\rangle + \alpha|\partial(\Omega\Delta\Omega_k)| + c|\Omega\Delta\Omega_k|^{\frac{n+2}{2}}}_{=:\mathcal{F}_{\Omega_k}(\Omega)}$$

As soon as the direct problem u (1.1) and the adjoint problem w (2.4) is given, we can solve this minimization problem, without solving further partial differential equations. Furthermore the objective function $\mathcal{F}_{\Omega_k}(\Omega)$ depends just on domain and boundary integrals. Hence we can easily calculate, using Theorem 2.1, its shape derivative

$$\mathcal{F}'_{\Omega_k}(\Omega)[V(0)] = \int\limits_{\partial(\Omega\Delta\Omega_k)} \big(2(\overline{c} - \underline{c})(\chi_{\Omega_k} - \frac{1}{2})uw + c\frac{n+2}{2}|\tilde{\Omega}\Delta\Omega|^{\frac{n}{2}} + \alpha\kappa\big)V(0).n\,ds\,.$$

This allows us to use level set methods to solve above minimization problem, using the velocity

$$V_n \;=\; -\big((\overline{c}-\underline{c})(\chi_{\Omega_k}-\frac{1}{2})uw + c\frac{n+2}{2}|\tilde{\Omega}\Delta\Omega|^{\frac{n}{2}} + \alpha\kappa\big)\,.$$

As an initial guess we solve either the above minimization problem with $\alpha = 0$ which results into finding the level sets

$$2(\overline{c}-\underline{c})(\chi_{\Omega_k}-\frac{1}{2})uw\big|_{\partial(\tilde{\Omega}\Delta\Omega)} + c\frac{n+2}{n}|\tilde{\Omega}\Delta\Omega|^{\frac{n}{2}} \;=\; 0\,,$$

and can be solved by bisection, or we start with the classical guess

$$\Omega\setminus\big\{\chi_\Omega d_\tau J_0 \;\le\; p\min(\chi_\Omega d_\tau J_0,0)\big\}\cup\big\{(1-\chi_\Omega)d_\tau J_0 \;\le\; p\min((1-\chi_\Omega)d_\tau J_0,0)\big\}\,,$$

with $p\in[0,1]$.

Newton-type topology changes

Again we first recall the minimization problem, whose minimizer results in Newton-type topology changes.

$$\Omega_{k+1} \;=\; \underset{u' \text{ solves (3.3)},\Omega\in\mathcal{K}(\mathcal{D})}{\operatorname{argmin}} \underbrace{\langle (c_\Omega - c_{\Omega_k})(u+u'),w\rangle + \frac{1}{2}D_u^2 J_\alpha(\Omega)[u']^2 + \alpha|\partial(\Omega\Delta\Omega_k)|}_{=:\mathcal{G}_{\Omega_k}(\Omega)}$$

This minimization problem has a partial differential equation as constraint. Hence it is as difficult to treat as the original minimization problem of the objective functional $J_\alpha(\Omega)$ (1.2) and allows also the same tools. So one way to solve above minimization problem is to calculate its shape derivative, chose an appropriate velocity and apply level set methods. We do not follow this approach her. Instead we use a phase field approach which is based on the equivalent formulation of above minimization problem in the space $\mathrm{BV}(\mathcal{D},\{0,1\})$, that we already met in the proof of Proposition 3.2. In the phase-field approach the minimization problem, formulated in $\mathrm{BV}(\mathcal{D},\{0,1\})$, is relaxed, in the framework of Γ-convergence (cf. Braides [12]) to a Hilbert-space problem, namely:

$$\begin{aligned} p_{k+1} \;=\; \underset{u' \text{ solves (3.3)},\, p\in H_0^1(\mathcal{D})}{\operatorname{argmin}} \quad & 2(\overline{c}-\underline{c})\langle(\tfrac{1}{2}-\chi_{\Omega_k})p(u+u'),w\rangle + \tfrac{1}{2}D_u^2 J_\alpha(\Omega_k)[u']^2 \\ & + \Big(\epsilon\|\nabla p\|^2_{L^2(\mathcal{D})} + \tfrac{\alpha^2}{\epsilon}\int_{\mathcal{D}} W_N(p)\,dx\Big)\,. \end{aligned}$$

$W_N(.)$ is a normalized double well potential with $W_N(0) = W_N(1) = 0$, $W_N(s) > 0 \quad s\in \mathbb{R}\setminus\{0,1\}$ and $2\int_0^1 \sqrt{W_N(s)}\,ds \;=\; 1$.

The double well potential on one hand forces p to approach $\{0,1\}$ when $\epsilon\to 0$, whereas the H^1-seminorm of p requires smooth solutions. More or less, with $\epsilon\to 0$ the H^1-seminorm term forces the solution to switch smoothly form 0 to 1 in an ϵ-region. All together these two terms approximate with $\epsilon\to 0$ the perimeter term. The minimization problem is now posed in a Hilbert-space setting and one can use Richardson or Newton-type methods to solve this problem. For our numerical tests we chose

$$W_N(s) \;=\; \begin{cases} \left(\frac{4}{\pi}\right)^2 s(1-s) & s\in[0,1] \\ \infty & \text{else} \end{cases}\,.$$

and perform a Gauss-Newton algorithm. The implementation should not be discussed further at this point but let us point out some hints how to chose ϵ appropriately.

From the theoretical point of few ϵ should be very small to approximate the original problem best, but numerically there should be a relation that connects $\frac{\epsilon}{\alpha}$ to the mesh-size h. Practical experience led us to set this relation to

$$\frac{\epsilon}{\alpha} = \tau h \qquad \tau \geq 2$$

Furthermore, when one starts the optimization with a very small ϵ, then the double well potential provides a too strict restriction and the algorithm cannot perform topology changes other than merging and splitting. In this case the algorithm behaves more like classical level set methods and therefore it is better to use a level set method, due to its clear, reliable and simple implementation. Hence ϵ should be chosen large at the beginning and get close to the finally chosen ϵ.

5 Numerical results

In this section we compare the classical level set method to the, in this paper, proposed level set method that incorporates steepest descent type (3.2) and Newton-type (3.5) topology changes. We just restrict our attention to problems with more than one connected component, namely to the identification of two ellipses and of an elliptic hole in another ellipse. The two ellipse case we consider for full measurements, i.e. $\Gamma_M = \mathcal{D}$ as well as for boundary measurements, i.e. $\Gamma_M = \Gamma_N$, while we consider the ellipse in ellipse case just for full measurements.

We perform all numerical tests on a fixed domain $\mathcal{D} = [-1, 1]^2$. To avoid inverse crime (cf. Colton & Kress [19, p 133]), we generate the data on a different grid (finer mesh and higher order basis functions) and perturb it with 1% Gaussen noise, measured in the $\|\,.\,\|_{L^2(\Gamma_M)}$ norm. We use 1% noise because we expect the numerical error of our discretization to be of the same magnitude.

To visualize the evolution of the geometry for each algorithm, we present a series of pictures (see Figure 4, 5, 6), starting with the first iteration up to the final solution. The pictures are arranged such that each column represents the evolution for one algorithm, namely the left column represents the classical level set method, the middle column represents the level set method with incorporated steepest descent type topology change and the right column represents the level set method with incorporated Newton-type topology change. Furthermore we provide graphs that show the iteration number versus objective $J_\alpha(\Omega_k)$, L^1-distance $d_{L^1}(\Omega_k, \Omega^{\text{exact}})$ and the Hausdorff-distance $d_H(\Omega_k, \Omega^{\text{exact}})$ of Ω_k to the exact solution Ω^{exact} (see Figure 1, 2, 3). The L^1-distance is defined via

$$d_{L^1}(\Omega, \tilde{\Omega}) := |\Omega \Delta \tilde{\Omega}|\,,$$

and the Hausdorff-distance is defined by

$$d_H(\Omega, \tilde{\Omega}) := \max\Big(\sup_{x\in\Omega} \inf_{y\in\tilde{\Omega}} |x-y|, \sup_{y\in\tilde{\Omega}} \inf_{x\in\Omega} |x-y| \Big)\,.$$

Our theoretic results for the topological derivative (Theorem 2.6) as well as for the steepest descent type (3.2) and the Newton-type (3.5) topology change are just valid inside the domain $\mathcal{D}$ and all constants depend on the distance to the boundary $\partial\mathcal{D}$. To respect this restriction, which can be relaxed in most cases, we restrict our algorithm to the domain $[-0.9, 0.9]^2$, i.e. we solve (3.2), (3.5) just for sets $\Omega \in \mathcal{K}([-0.9, 0.9]^2)$.

Our objective functional $J_\alpha(\Omega)$ incorporates perimeter regularization. To get a proper choice of α in our numerical tests we chose α such that the classical level set method, started at the exact solution (with 1% noisy data), does not iterate away from the exact solution too far. A too large α would not allow to get topology changes in our algorithms and a too small α does not regularize the problem enough.

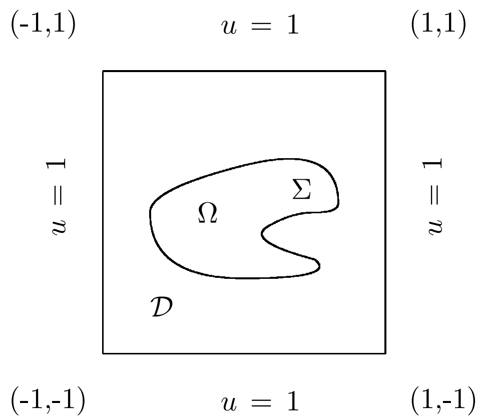
As initial guess we take for all of our test examples a circle with radius $r = 0.7$ and centered at the origin $(0, 0)$ for the classical level set method, while we started with no material for the level set method incorporating steepest descent type respectively Newton-type topological changes.

For the level set method incorporating a steepest descent type topology change we solve (3.2) after every 10^{th} classical level set iterations, while for Newton-type topology changes we solve (3.5) after every 50^{th} classical level set iteration.

5.1 Full measurements $\Gamma_M = \mathcal{D}$

In this section we consider the identification of two ellipses and an ellipse with an elliptic hole from full measurements, i.e. $\Gamma_M = \mathcal{D}$. The full measurement case is mildly ill-posed, something like twice differentiation, and provides a lot of data, such that we can expect good results for all algorithms. Most challenging is probably the ellipse with elliptic hole. For this case we expect that the classical level set method does not perform a topology change.

The partial differential equation (1.1), (2.4) is described by



$$
\begin{array}{lll}
-\Delta u + \chi_\Omega u &= 0 & \text{in } \mathcal{D} \\
u|_{\Gamma_D} &= 1 & \\
\frac{\partial u}{\partial n}|_{\Gamma_N} &= 0 & \\
-\Delta w + \chi_\Omega w &= -(u - \hat{u}) & \text{in } \mathcal{D} \\
w|_{\Gamma_D} &= 0 & \\
\frac{\partial w}{\partial n}|_{\Gamma_N} &= 0 &
\end{array}
$$

Measurements:

$$
\begin{array}{ll}
\hat{u} = u|_{\mathcal{D}} & \text{in } L^2(\mathcal{D}) \\
J_\alpha(\Omega) = \frac{1}{2}\|u - \hat{u}\|^2_{L^2(\mathcal{D})} + \alpha|\partial\Omega| &
\end{array}
$$

Due to the Dirichlet boundary conditions $u = 1$ on $\partial\mathcal{D}$ and the "weak" influence of the material to the solution u, solution u is close to the solution of the system without material $u(\emptyset) = 1$. Hence the linearized problem (3.3) approximates the original problem (1.1) quite good and we can expect that the level set method, incorporating Newton-type topology changes, performs very well and indeed we will see that already the first solution to (3.5) provides a very good initial guess and predicts the correct topology of the desired geometry.

Two ellipses, $\Gamma_M = \mathcal{D}$

We choose $\alpha = 10^{-3}\|\hat{u}\|^2_{L^2(\Gamma_M)} 1\%$ and compare the classical level set method to a level set method incorporating a steepest descent type topology change (3.2) and a level set method incorporating a Newton-type topology change (3.5). As expected all three methods perform very well and approximate the exact geometry quite accurately (see Figure 4 last row).

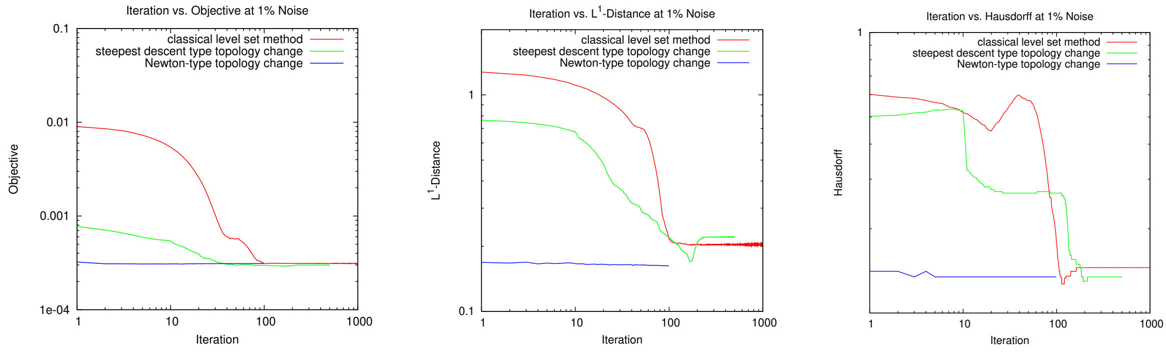
Classical level set method (Figure 4, 1^{st}-column): The classical level set method performs quite well and even performs the necessary topology change, by splitting, to approximate the exact geometry. The number of iterations needed to approach the solution is large but reasonable. The distance to the exact geometry in both, the L^1- and the Hausdorff-metric, is reasonable small see Figure 1.

Steepest descent type topology change (Figure 4, 2^{nd}-column): The level set method incorporating steepest descent type topology changes (3.2), does not predict the correct topology within the first solution to (3.2). It needs a second call (Figure 4, 2^{nd} row, 2^{nd} column) to generate a further topology change. Even when this topology change does not result into a sever decrease in the objective functional (see Figure 1(a), the topological change can be observed in the jump of the Hausdorff-distance of the exact geometry to the current geometry (see Figure 1(c)). Interestingly this topology change adds two new geometries at the right position but does not try to reduce the "wrong" geometry. Further calls of (3.2) does not cause any changes of the geometry. The only topology change that occur, happens during the level set evolution where the above two geometries merge together. Even when the level set method incorporating a steepest descent type topology change almost reaches the minimum of the objective functional $J_\alpha(\Omega)$ before the classical level set method (see Figure 1(a)) it needs more iterations until it stays at the final geometry.

Newton-type topology change (Figure 4, 3^{rd}-column): The level set method incorporating Newton-type topology changes (3.5), already predicts the topology correct within the first solution of (3.5) (see Figure 4 1^{st} row, 3^{rd} column). Also the objective function $J_\alpha(\Omega)$ as well as the L^1- and Hausdorff-distance (see Figure 1) gets very close to its optimum and need just a few correction steps with the classical level set method. This is probably not too unexpected because the linearized problem (3.3) approximates the nonlinear partial differential equation (1.1) very accurate. Even when the number of iterations, to approach to the solution, is very low, note that one solution of (3.5) is more expansive. We solve (3.5) only once and it takes approximately as much time as 33 classical level set iterations, but even than the level set method incorporating Newton-type topology changes is significantly faster than the two other methods.

Ellipse in ellipse, $\Gamma_M = \mathcal{D}$

For the elliptic hole in an ellipse we choose $\alpha = 10^{-3}\|\hat{u}\|^2_{L^2(\Gamma_M)}1\%$ and do the same comparisons as before. This geometry is more challenging and we expect that the classical level set method stucks in a local minima and does not predict the correct geometry, even when the objective function $J_\alpha(\Omega)$ gets close to the optimum, while the power of the other two methods should show up. Again the linearized partial differential equation (3.3) approximates the original partial differential equation (1.1) very good and we can expect that the level set method incorporating Newton-type topology changes perform very well within the first solution of (3.5).



(a) Iteration vs. Objective (b) Iteration vs. L^1-Distance (c) Iteration vs. Hausdorff-distance

Figure 1: Two ellipse, $\Gamma_M = \mathcal{D}$: Iteration vs. Objective, L^1-distance, Hausdorff-distance

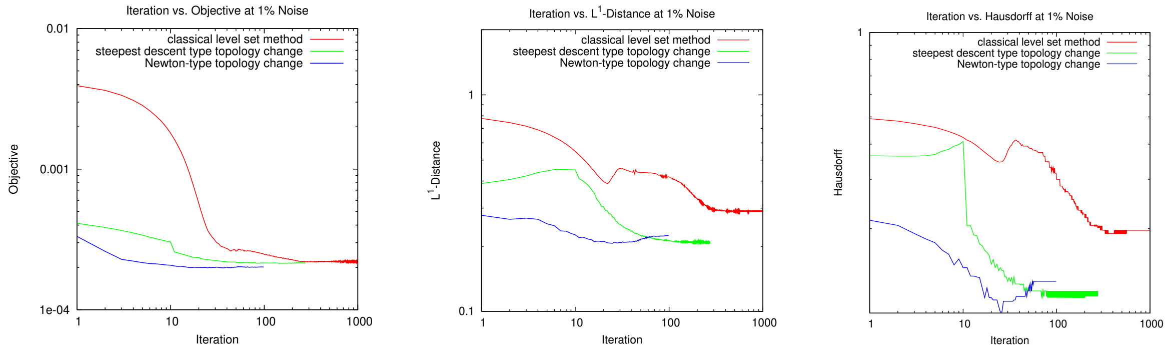
Classical level set method (Figure 5, 1st-column): As expected the classical level set method does not identify the correct topology. Nonetheless the identified geometry does not look to bad (visually) and also the L^1- respectively the Hausdorff-distance (see Figure 2(b), 2(c)) is not too bad. Also the objective function $J_\alpha(\Omega)$ at the solution (see Figure 2(a))is close to the minimum of the problem. The number of iterations is again large, but still reasonable.

Steepest descent type topology change (Figure 5, 2nd-column): As for the two ellipse case the steepest descent type topology change (3.2) does not generate the correct topology within one step but needs two steps (Figure 5, 2nd row, 2nd column). Further solver calls of (3.2) does not force further changes. Hence after the second solution call of (3.2) we evolve the geometry just by the classical level set method. This can also be seen in the Hausdorff-distance (see Figure 2(c)) and this time also in the objective function (see Figure 2(a)) which have a jump at iteration 12. We are at the final solution at approximately 40 level set iterations which makes an equivalent, due to 3 times calling a solver for (3.2), of 50 classical level set iterations in total.

Newton-type topology change (Figure 5, 3rd-column): Again the level set method incorporating Newton-type topology changes (3.5), already predict the topology correct within the first solution of (3.5) (see Figure 5 1st row, 3rd column) but this time the objective function $J_\alpha(\Omega)$ as well as the L^1- and Hausdorff-distance (see Figure 2 are not yet too close to its optimum. Hence we additionally need 20 to 40 classical level set iteration to end at the final solution. Due to just one solution call of (3.5) these 40 iterations plus solving (3.5) once, are equivalent to 76 iteration steps for the classical level set method. In total the level set method incorporating Newton-type topology changes is slightly more expansive than the level set method incorporating steepest descent like topology changes

5.2 Boundary measurements $\Gamma_M = \Gamma_N$

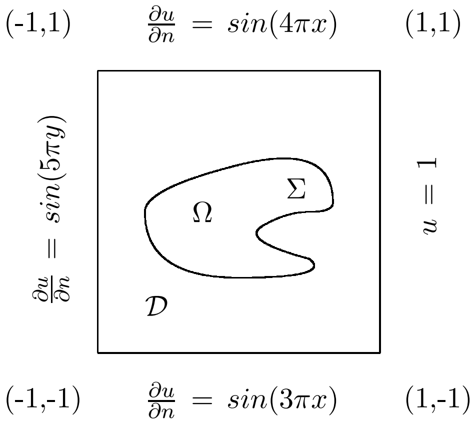
Finally we consider the identification of two ellipses from just one set of boundary measurements, i.e. $\Gamma_M = \Gamma_N$. This case is supposed to be exponentially ill-posed. Exponentially



(a) Iteration vs. Objective (b) Iteration vs. L^1-Distance (c) Iteration vs. Hausdorff-distance

Figure 2: Ellipse in ellipse, $\Gamma_M = \mathcal{D}$: Iteration vs. Objective, L^1-Distance, Hausdorff-distance

ill-posed problems are an extreme challenge to every algorithm and usually one can not expect too good results for it. Especially topology changes are extremely difficult to achieve. We expect that the classical level set method is not able to perform the desired topology change, even when it managed it for the full measurements case. To deal with boundary measurements we have to change slightly our boundary conditions for the partial differential equations (1.1), (2.4), namely



$$\begin{aligned} -\Delta u + \chi_\Omega u &= 0 && \text{in } \mathcal{D} \\ u|_{\Gamma_D} &= 1 \\ \tfrac{\partial u}{\partial n}|_{\Gamma_N} &= h \end{aligned}$$

$$\begin{aligned} -\Delta w + \chi_\Omega w &= 0 && \text{in } \mathcal{D} \\ w|_{\Gamma_D} &= 0 \\ \tfrac{\partial w}{\partial n}|_{\Gamma_N} &= -(u - \hat{u}) \end{aligned}$$

Measurements:

$$\begin{aligned} \hat{u} &= u|_{\Gamma_N} && \text{in } L^2(\Gamma_N) \\ J_\alpha(\Omega) &= \tfrac{1}{2}\|u - \hat{u}\|^2_{L^2(\Gamma_N)} + \alpha|\partial\Omega| \end{aligned}$$

Due to the Neumann boundary conditions the solution u to above system, is not close to the solution $u(\emptyset) = 1$ (solution without material). Hence the linearized partial differential equation (3.3) does not approximate the original problem (1.1) very good (when starting with no material). As a consequence of this the first step of a Newton-type topology change (3.5) shall not perform as good as in the full measurement cases.

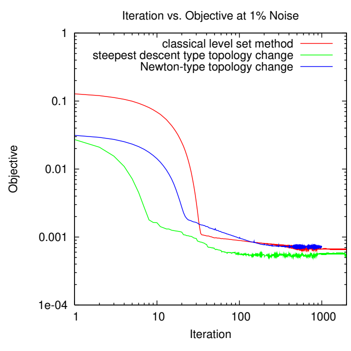
Two ellipse $\Gamma_M = \Gamma_N$

Again we choose $\alpha = 10^{-3}\|\hat{u}\|^2_{L^2(\Gamma_M)} 1\%$ and compare the classical level set method to a level set method incorporating a steepest descent type topology change (3.2) and a level set method incorporating a Newton-type topology change (3.5).

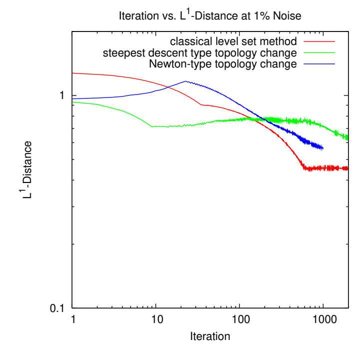
Classical level set method (Figure 6, 1st-column): As expected the classical level set method does not split. Nonetheless the finally identified geometry does not look too bad. The number of iterations needed, til it appraoches its optimum, is very high but this is not uncommon for exponentially ill posed problems. Although we do not get the correct topology, the objective function $J_\alpha(\Omega)$ (see Figure 3(a)) gets close to its minimum.

Steepest descent type topology change (Figure 6, 2nd-column): As before the level set method incorporating steepest descent type topology changes (3.2), does not predict the correct topology within the first solution to (3.2). Even worse, this time the first step seems to be far away and looks intuitively unreasonable. Iterating further and calculating several times the solution to (3.2), the algorithm forces further topology changes, some of them reasonable, some not (see Figure 6, 1st-column). Nonetheless the objective function decreases, as predicted by the theory. After many iterations the algorithm stops with four non-connected components, where two are reasonable and the others are not.

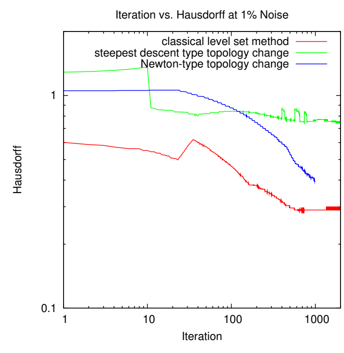
Newton-type topology change (Figure 6, 3rd-column): Finally we consider the level set method incorporating Newton-type topology changes (3.5). Already the first calculation of the solution to (3.5) predicts the correct number of connected components and later solution calls of (3.5) does not force any additional topology changes. As for the steepest descent type topology changes, the first solution to (3.5) does not look too good, but it is enough for the classical level set method to approach the exact solution. For the final result presented in Figure 6 3rd column, 4th row the objective function and also the L^1- and Hausdorff-distance (see Figure 3) would decrease further. Hence, iterating further would still improve the result. Nonetheless we terminated the algorithm, because the number of iteration is already very high and we can already see from Figure 6 3rd-column, that the algorithm behaves better than the two other.



(a) Iteration vs. Objective



(b) Iteration vs. L^1-Distance



(c) Iteration vs. Hausdorff-distance

Figure 3: Two ellipse, $\Gamma_M = \Gamma_N$: Iteration vs. Objective, L^1-distance, Hausdorff-distance

6 Conclusion

In this paper we presented a way to generalize the notion of topological derivatives such that we can also deal with perimeter regularized objective functionals. The generalization allows to formulate sub minimization problems similar to steepest descent type and Newton-type minimization problems, such that a descent in the objective function is guaranteed. This is in contrast to classical topological derivatives where one gets just an indicator where to force topology changes, but the indicator does not guarantee a descent in the objective function.

We incorporated this generalization of topological derivatives into the classical level set method and showed at hand of some examples its applicability. While, in some cases, the classical level set method failed to predict the correct topology, the suggested level set methods with incorporated steepest descent type respectively Newton-type topology changes, succeed to get the correct topology or at least forced topology changes.

The numerical results for the specific example, presented in this paper, were quite promising and an extension to more complicated problems might be of interest.

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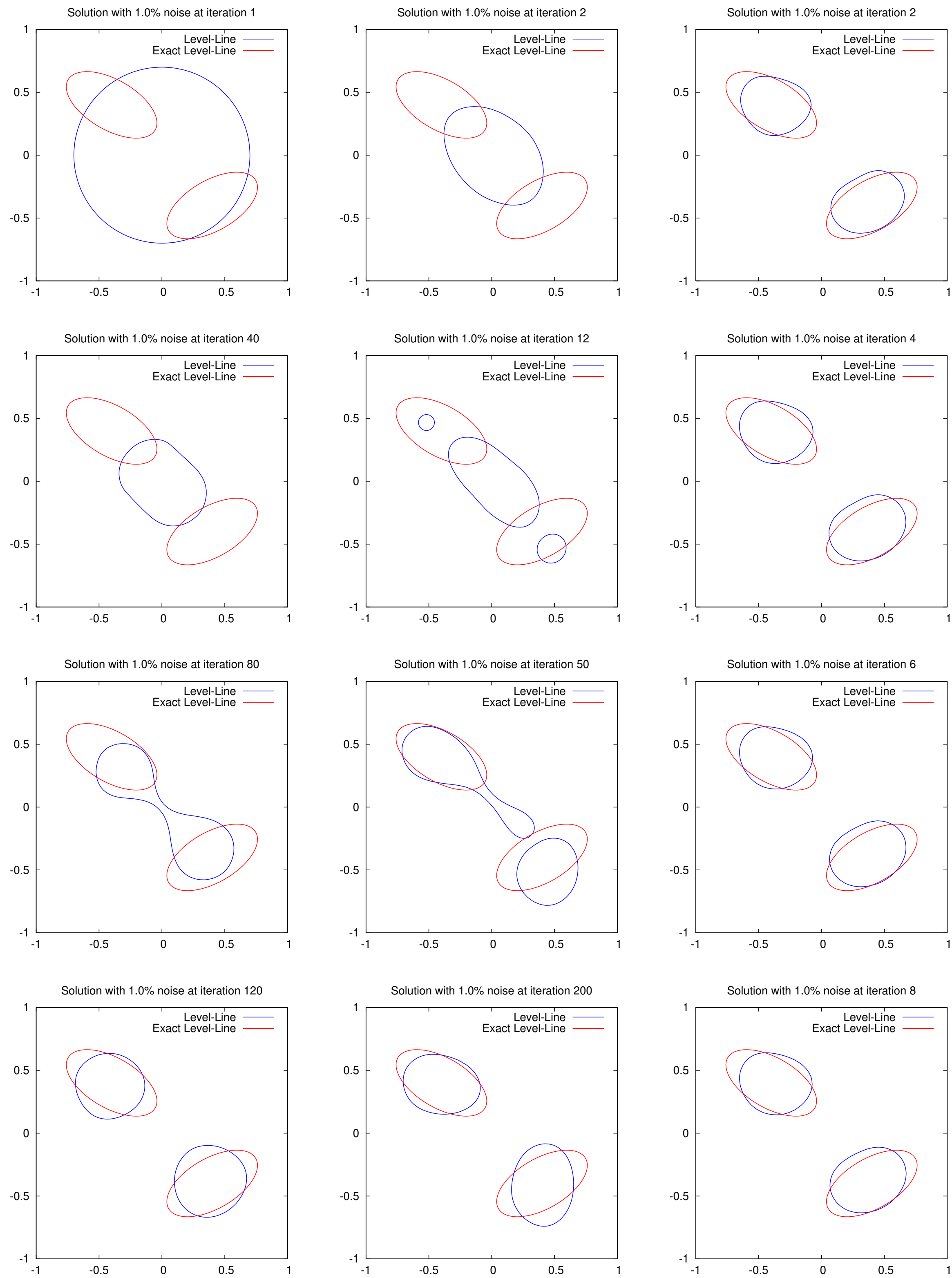
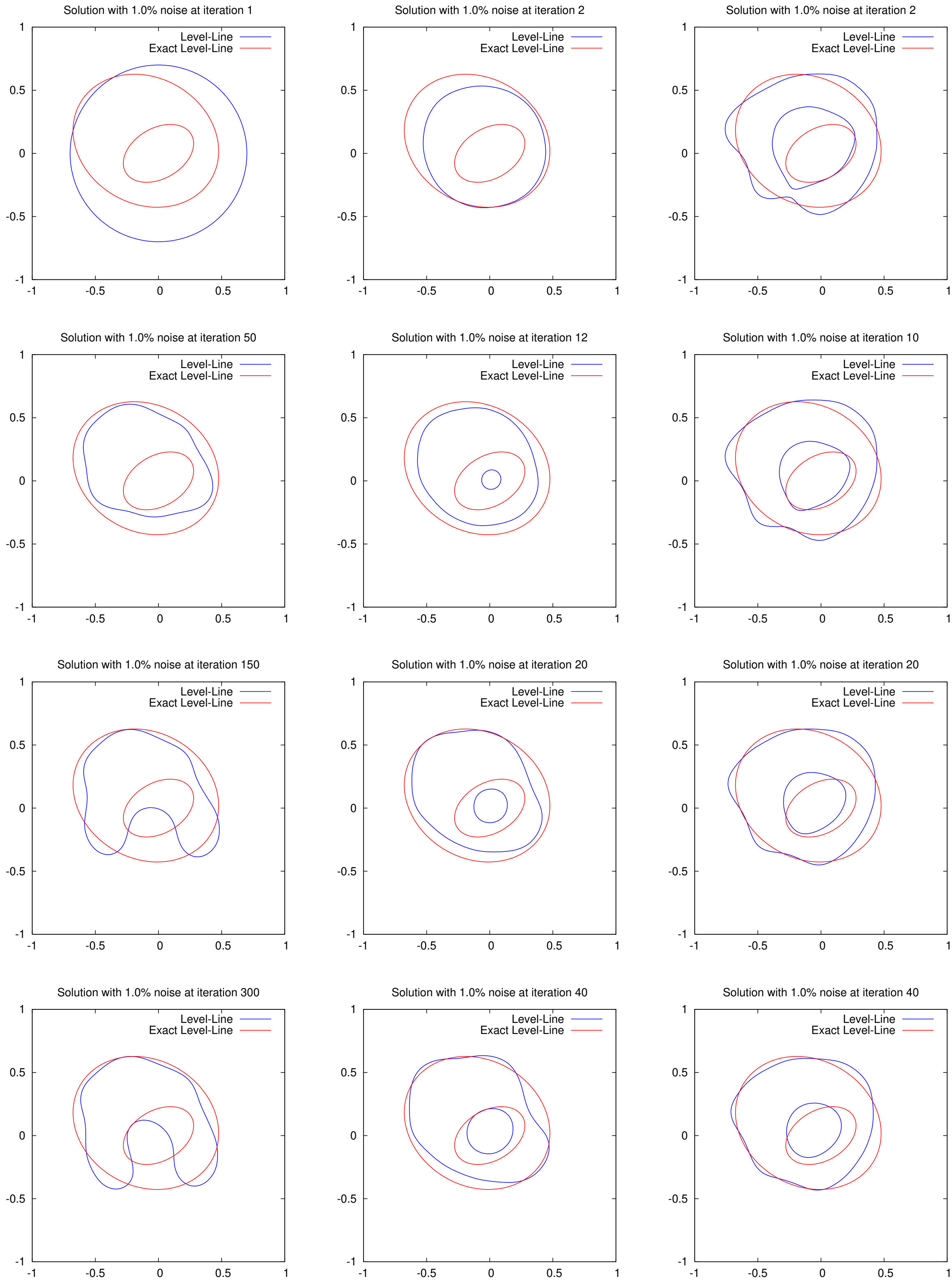


(a) Classical Level Set Methods

(b) Steepest descent like topology changes

(c) Newton-type topology changes

Figure 4: Two ellipse, $\Gamma_M = \mathcal{D}$: Evolution of algorithm

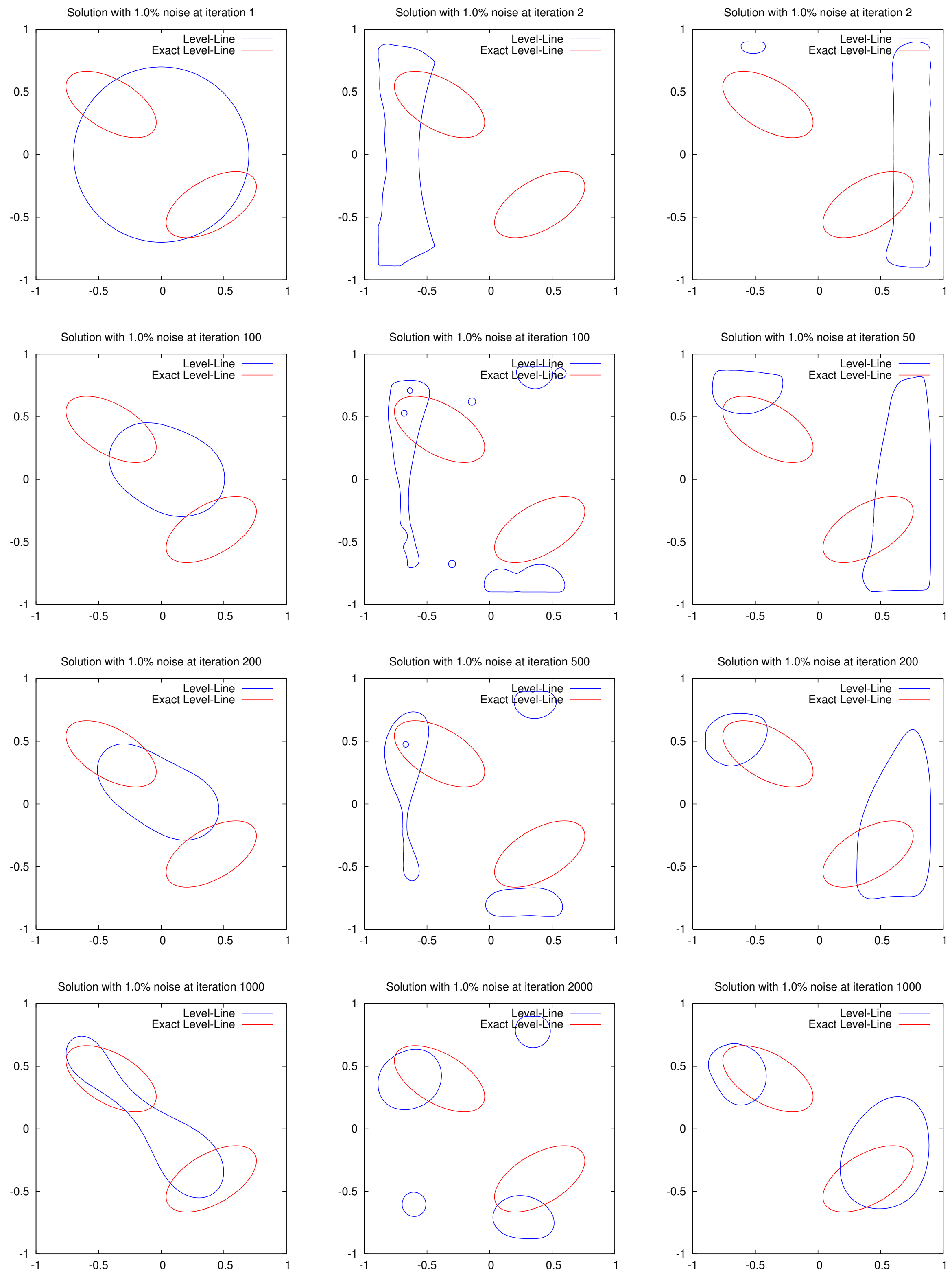


(a) Classical Level Set Methods

(b) Steepest descent like topology changes

(c) Newton-type topology changes

Figure 5: Ellipse in ellipse, $\Gamma_M = \mathcal{D}$: Evolution of algorithm



(a) Classical Level Set Methods

(b) Steepest descent like topology changes

(c) Newton-type topology changes

Figure 6: Two ellipse, $\Gamma_M = \Gamma_N$: Evolution of algorithm