Shape Optimisation with PDE Constraints

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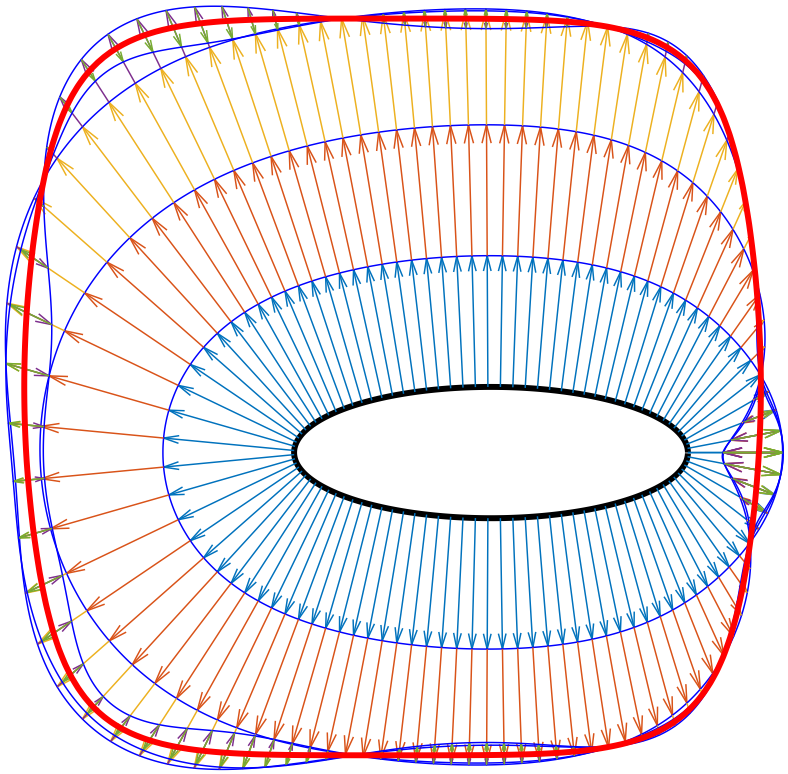


Abstract

Shape optimisation is typically concerned with finding the shape which is optimal in the sense that it minimises a certain cost functional while satisfying given constraints. Often we find that the functional being solved depends on the solution of a PDE constraint.

In this report we briefly discuss unconstrained optimisation methods before introducing the notion of a shape derivative, which will help us to create shape optimisation methods. We then explore a test case that, despite its relative simplicity, exhibits an unexpected behaviour: solving this problem via Newton's method with a *truncated* second shape derivative performs better than using full second order information. We will perform numerical and theoretical investigations using *Chebfun* to try to shed light on this unexpected behaviour.

Contents

1 Unconstrained Optimisation

We first recap on some iterative methods for solving unconstrained optimisation problems. Let $f : \mathbb{R}^n \to \mathbb{R}$ be a function. Suppose we want to find a value x^* such that f is minimal, i.e

$$x^* \in \arg\min_x f(x).$$

We can find such a value by means of an iterative algorithm. That is, given an initial guess $x^{(0)}$ for x^*, we construct a *minimising sequence* $(x^{(k)})$ of points such that

$$f(x^{(k)}) \longrightarrow f(x^*) \quad \text{as } k \to \infty.$$

Often we only require an approximate solution, so we can reduce computational effort by choosing a tolerance $\varepsilon > 0$ such that when $f(x^{(k)}) - f(x^*) \leqslant \varepsilon$, we terminate the algorithm.

1.1 Descent Methods

The minimising sequences we are going to discuss in this section are all of the form

$$x^{(k+1)} = x^{(k)} + t^{(k)}\Delta x^{(k)},$$

where

- $\Delta x^{(k)}$ represents a *search direction* - which direction we travel in to approach x^*,
- $t^{(k)} \geqslant 0$ represents a *step length* - how far we travel along the vector $\Delta x^{(k)}$.

Recall that our aim is to minimise f, so we would like the sequence to have the property

$$f(x^{(k+1)}) < f(x^{(k)}) \tag{1}$$

for all k, unless $x^{(k)}$ is optimal. If f is differentiable, we can Taylor expand up to first-order and write

$$f(x^{(k+1)}) = f(x^{(k)} + t^{(k)}\Delta x^{(k)}) \approx f(x^{(k)}) + t^{(k)}\mathrm{d}f(x^{(k)}, \Delta x^{(k)}),$$

where $\mathrm{d}f$ denotes the *directional derivative*

$$\mathrm{d}f(x, v) := \lim_{t \to 0} \frac{f(x + tv) - f(x)}{t}.$$

Hence, if $x^{(k)}$ is not optimal (so that $t^{(k)} \neq 0$), we can ensure (1) holds up to first-order if

$$\mathrm{d}f(x^{(k)}, \Delta x^{(k)}) < 0. \tag{2}$$

A search direction $\Delta x^{(k)}$ such that (2) holds is called a *descent direction.*

A generic descent method then goes as follows:

Given starting point x
repeat
  (1) Determine *descent direction*, Δx
  (2) Choose *step size*, $t > 0$
  (3) Set $x \leftarrow x + t\Delta x$
until *stopping criterion satisfied*

At the moment this is rather vague. We have a few questions to answer:

- How do we choose the step size?
- What is the descent direction?
- When do we stop the algorithm?

1.2 Line Search

To answer the first question, we discuss two methods of deciding the step size, called *exact line search (ELS)* and *backtracking line search (BLS)*. Here we assume that Δx is a descent direction.

In ELS, we choose t such that f is minimised along the ray $\{x + t\Delta x : t \geqslant 0\}$, i.e

$$t = \arg\min_{s \geqslant 0} f(x + s\Delta x).$$

It may be difficult to find t exactly, so it is generally cost effective to choose a t value such that f is only approximately minimised along the ray. For this reason we may choose to apply BLS, which generates the step size by the following algorithm:

Algorithm 1: Backtracking Line Search

Given descent direction Δx, $\alpha \in (0, 0.5), \beta \in (0, 1)$
$t := 1$
while $f(x + t\Delta x) > f(x) + \alpha t \, \mathrm{d}f(x, \Delta x)$ **do**
  Set $t \leftarrow \beta t$
end

The resulting value of t is chosen as the step size. The line search is called "backtracking" as it starts with unit step size, then reduces it by the factor β until the stopping criterion

$$f(x + t\Delta x) > f(x) + \alpha t \, \mathrm{d}f(x, \Delta x)$$

holds. Since Δx is a descent direction, we have $\mathrm{d}f(x, \Delta x) < 0$, so

$$f(x + t\Delta x) \approx f(x) + t \, \mathrm{d}f(x, \Delta x) < f(x) + \alpha t \, \mathrm{d}f(x, \Delta x)$$

for small enough t, demonstrating that BLS eventually terminates. The choice of parameters α, β has a noticeable but not dramatic effect on convergence (see [1]); ELS can sometimes improve convergence rate but not dramatically. It is generally not worth the computational effort of using ELS.

1.3 Steepest Descent

We can find a descent direction by analysing the Taylor expansion of $f(x + \Delta x)$ about x up to first-order. The approximation is

$$f(x + \Delta x) \approx f(x) + \mathrm{d}f(x, \Delta x),$$

so we find the direction of *steepest descent* when we minimise the directional derivative. We define a *normalised steepest descent direction* Δx_{nsd} as a descent direction of unit length that minimises $\mathrm{d}f(x, \Delta x)$, i.e

$$\Delta x_{\mathrm{nsd}} \in \arg\min_{||\Delta x|| = 1} \mathrm{d}f(x, \Delta x)$$

for some norm $||\cdot||$ on $\mathbb{R}^n$.

To piece together the *Steepest Descent* method, it will be useful to introduce the concept of inner products and gradients, particularly when it comes to defining stopping criteria. Let V be a real vector space. An *inner product* $(\cdot,\cdot) : V^2 \to \mathbb{R}$ is a function that satisfies the following properties:

- *Linearity:* $(\alpha u + \beta v, w) = \alpha(u, w) + \beta(v, w) \quad \forall u, v, w \in V,\ \alpha, \beta \in \mathbb{R}$
- *Symmetry:* $(u, v) = (v, u) \quad \forall u, v \in V$
- *Positive definitenesss:* $(u, u) \geqslant 0 \quad \forall u \in V, \quad (u, u) = 0 \iff u = 0.$

It follows from the first two properties that $(\cdot,\cdot)$ is *bilinear*.

We call $\nabla f(x)$ the *gradient* of f at x with respect to an inner product $(\cdot,\cdot)$ if

$$(\nabla f(x), v) = \mathrm{d}f(x, v) \quad \forall v.$$

We occasionally write $\nabla_{(\cdot,\cdot)} f(x)$ to make it clear what the associated inner product is.

Lemma 1.1: If a norm $||\cdot||$ is induced by an inner product $(\cdot,\cdot)$, i.e $||v|| = \sqrt{(v, v)}$, then

$$\Delta x_{\mathrm{nsd}} = -\frac{\nabla f(x)}{||\nabla f(x)||}. \tag{3}$$

Proof: We use the method of Lagrange multipliers. Let

$$L(\Delta x, \lambda) := \mathrm{d}f(x, \Delta x) + \frac{\lambda}{2}(||\Delta x||^2 - 1).$$

Then by definition of Δx_{nsd},

$$\begin{aligned} & \partial_{\Delta x} L(\Delta x_{\mathrm{nsd}}, v) = \mathrm{d}f(x, v) + \lambda(\Delta x_{\mathrm{nsd}}, v) = 0 \quad \forall v \\ \iff \quad & (\lambda \Delta x_{\mathrm{nsd}}, v) = -\mathrm{d}f(x, v) \quad \forall v \\ \iff \quad & \lambda \Delta x_{\mathrm{nsd}} = -\nabla f(x). \end{aligned}$$

Taking norms of both sides, and using the fact that $||\Delta x_{\mathrm{nsd}}|| = 1$, we obtain $|\lambda| = ||\nabla f(x)||$. The result follows, using the fact that Δx_{nsd} is a steepest descent direction.

□

Geometrically speaking, we see that Δx_{nsd} is a step in the unit ball of $||\cdot||$ which extends farthest in the direction of $-\nabla f(x)$. It is more convenient in practice to use an unnormalised descent direction

$$\Delta x_{\mathrm{sd}} := ||\nabla f(x)||_* \Delta x_{\mathrm{nsd}},$$

where $||\cdot||_*$ denotes the *dual norm*

$$||v||_* := \sup_{||x|| \leqslant 1} v^T x.$$

We find that Δx_{sd} is simply the unnormalised version of (3), that is

$$\Delta x_{\mathrm{sd}} = -\nabla_{(\cdot,\cdot)} f(x),$$

and we arrive at the *Steepest Descent* method, which uses Δx_{sd} as a descent direction:

Algorithm 2: Steepest Descent

Given starting point x
repeat
  (1) Set $\Delta x \leftarrow \Delta x_{\mathrm{sd}}$
  (2) Choose t via ELS/BLS
  (3) Set $x \leftarrow x + t\Delta x$
until *stopping criterion satisfied*

To define a stopping criterion, recall that when x^* is optimal we have

$$\mathrm{d}f(x^*, v) = 0 \quad \forall v,$$

so for a sufficiently smooth f, we expect the gradient to be small for $x \approx x^*$. For this reason, we can define a stopping criterion of the form

$$||\nabla f(x)|| \leqslant \varepsilon$$

for some chosen small $\varepsilon > 0$. Most practical uses of Steepest Descent check the stopping criterion after the first step.

1.4 Newton's Method

Which inner product do we use to define Δx_{sd}? An interesting choice, which forms the basis of *Newton's Method*, is to consider the inner product induced by the second derivative

$$\mathrm{d}^2 f(x, u, v) := \lim_{t \to 0} \frac{\mathrm{d}f(x + tv, u) - \mathrm{d}f(x, u)}{t}.$$

If it exists, we can extend our Taylor approximation up to second-order to get

$$f(x + \Delta x) \approx f(x) + \mathrm{d}f(x, \Delta x) + \frac{1}{2}\mathrm{d}^2 f(x, \Delta x, \Delta x) =: g(\Delta x).$$

If $\mathrm{d}^2 f(x, \cdot, \cdot)$ is positive definite then g is *strictly convex**, thus has a unique minimiser Δx_{nt}, called the *Newton step*. Since the second derivative exists, $\mathrm{d}^2 f(x, \cdot, \cdot)$ is also symmetric and linear, hence an inner product. By minimality, the Newton step must satisfy

$$\begin{aligned} & \mathrm{d}g(\Delta x_{\mathrm{nt}}, v) = 0 \quad \forall v \\ \iff \quad & \mathrm{d}f(x, v) + \mathrm{d}^2(x, \Delta x_{\mathrm{nt}}, v) = 0 \quad \forall v \\ \iff \quad & \mathrm{d}^2(x, \Delta x_{\mathrm{nt}}, v) = -\mathrm{d}f(x, v) \quad \forall v \end{aligned}$$

so Δx_{nt} is the negative gradient with respect to the inner product induced by $\mathrm{d}^2 f$, that is,

$$\Delta x_{\mathrm{nt}} = -\nabla_{\mathrm{d}^2 f(x, \cdot, \cdot)} f(x).$$

If f is quadratic, then $f(\Delta x_{\mathrm{nt}}) = g(\Delta x)$ exactly, so $x + \Delta x_{\mathrm{nt}}$ is the *exact* minimiser of f. Hence it should also be a very good estimate for x^* if f is approximately quadratic. Since f is assumed to be twice continuously differentiable, the quadratic model of f is very accurate for x near x^*, so $x + \Delta x_{\mathrm{nt}}$ is a very good estimate for x^*.

Before we introduce *Newton's method*, we will construct a stopping criterion using the directional derivative, as demonstrated in the following lemma:

Lemma 1.2: $\frac{1}{2}\mathrm{d}f(x, \Delta x_{\mathrm{nt}})$ estimates the error $f(x) - f(x^*)$, based on the quadratic approximation of f.

Proof: The error based on the quadratic approximation is

$$\begin{aligned} f(x) - \inf_y g(y) = \; f(x) - g(\Delta x_{\mathrm{nt}}) &= f(x) - \left(f(x) + \underbrace{\mathrm{d}f(x, \Delta x_{\mathrm{nt}})}_{=0} + \frac{1}{2}\mathrm{d}^2 f(x, \Delta x_{\mathrm{nt}}, \Delta x_{\mathrm{nt}}) \right) \\ &= f(x) - \left(f(x) - \frac{1}{2}\mathrm{d}f(x, \Delta x_{\mathrm{nt}}) \right) \\ &= \frac{1}{2}\mathrm{d}f(x, \Delta x_{\mathrm{nt}}). \end{aligned}$$

□

*A function g is said to be *strictly convex* if the line segment connecting any two distinct points on the surface of g lies strictly above g, except at the endpoints.

We use this as a stopping criterion for Newton's Method, which goes as follows:

Algorithm 3: Newton's Method

Given starting point x, tolerance $\varepsilon > 0$
repeat
  (1) Set $\Delta x \leftarrow \Delta x_{\mathrm{nt}}$
  (2) **Stop** if $\mathrm{d}f(x, \Delta x)/2 \leqslant \varepsilon$
  (3) Choose t via BLS
  (4) Set $x \leftarrow x + t\Delta x$

Observe that this is more or less a general descent method, with the difference that the stopping criterion is checked after computing Δx_{nt}, rather than after updating the value of x.

Newton's Method has many advantages over Steepest Descent. Most importantly it has *quadratic convergence* near x^* [1, page 496] - roughly speaking, this means that the number of correct digits doubles after each iteration. As a result, Newton's Method also scales with the size of the problem: it will perform just as well for a problem in $\mathbb{R}^{10000}$ as it would for problems in $\mathbb{R}^{10}$ say, with only a moderate increase in the number of iterations required.

A pitfall of Newton's Method is the cost of computing Δx_{nt}, which requires solving a system of linear equations. *Quasi-Newton* methods require less cost to form the search direction, sharing some advantages of Newton's Method such as rapid convergence near x^*, but we will not discuss such methods here.

2 Introduction to Shape Optimisation

In the previous section, we had a function $f : \mathbb{R}^n \to \mathbb{R}$ and we used its derivatives to find the points x^* which minimised $f(x)$. What if we were instead given a cost functional $\mathcal{J}[\Omega]$, with the aim of minimising $\mathcal{J}$ over bounded domains (shapes) Ω? We would need a notion of *shape differentiation*.

In this section we define the *shape derivative*. We will ultimately use such derivatives to find a domain Ω^* in a collection of admissible shapes $\mathcal{U}_{\mathrm{ad}}$ which minimises a given cost functional $\mathcal{J}$. For simplicity, we restrict ourselves to functionals of the form

$$\mathcal{J}[\Omega] := \int_\Omega f \,\mathrm{d}x.$$

In the style of Section 1.1, we write

$$\Omega^* \in \operatorname*{arg\,min}_{\Omega \in \mathcal{U}_{\mathrm{ad}}} \mathcal{J}[\Omega].$$

2.1 The Shape Derivative, $\mathrm{d}\mathcal{J}(\Omega, \mathcal{V})$

Let $T : \mathbb{R}^n \to \mathbb{R}^n$ be a sufficiently smooth vector field. Then

$$\mathcal{J}[T(\Omega)] = \int_{T(\Omega)} f \,\mathrm{d}x = \int_\Omega (f \circ T) |\det \mathbf{D}T| \,\mathrm{d}x,$$

where $\mathbf{D}T$ denotes the *Jacobian* of T. Note that $T(\Omega) \neq \Omega$ in general, and similarly $\mathcal{J}[T(\Omega)] \neq \mathcal{J}[\Omega]$.

Furthermore let $\mathcal{V} : \mathbb{R}^n \to \mathbb{R}^n$ be a vector field, and define a duality pairing

$$\left\langle \frac{\mathrm{d}}{\mathrm{d}T} \mathcal{J}[T(\Omega)], \mathcal{V} \right\rangle := \lim_{t \to 0} \frac{\mathcal{J}[(T + t\mathcal{V})(\Omega)] - \mathcal{J}[T(\Omega)]}{t}.$$

We then define the *Eulerian (shape) derivative* of $\mathcal{J}$ in the direction $\mathcal{V}$ as

$$\mathrm{d}\mathcal{J}(\Omega,\mathcal{V}) := \Big\langle \frac{\mathrm{d}}{\mathrm{d}T}\,\mathcal{J}[T(\Omega)],\mathcal{V}\Big\rangle\Big|_{T=I},$$

where I is the identity map $I(\Omega)=\Omega$. Therefore, we can write

$$\begin{aligned}\mathrm{d}\mathcal{J}(\Omega,\mathcal{V}) &= \Big\langle \frac{\mathrm{d}}{\mathrm{d}T}\,\left(\int_\Omega (f\circ T)|\det \mathbf{D}T|\,\mathrm{d}x\right),\mathcal{V}\Big\rangle\Big|_{T=I}\\ &= \int_\Omega \Big\langle \frac{\mathrm{d}}{\mathrm{d}T}((f\circ T)\det \mathbf{D}T),\mathcal{V}\Big\rangle\Big|_{T=I}\mathrm{d}x. \qquad (4)\end{aligned}$$

Ideally we want $\mathrm{d}\mathcal{J}$ to exist for all $\mathcal{V}$, so we say that $\mathcal{J}$ is *shape differentiable* at Ω if the map

$$\mathcal{V}\mapsto \mathrm{d}\mathcal{J}(\Omega,\mathcal{V})$$

is linear and bounded on $C^1(\mathbb{R}^n,\mathbb{R}^n)$, the set of continuously differentiable maps from $\mathbb{R}^n$ to $\mathbb{R}^n$.

2.2 Computing $\mathrm{d}\mathcal{J}(\Omega,\mathcal{V})$

Generally we do not know T so the shape derivative, in the form we have seen it in so far, is quite difficult to compute. Using (4), we prove two formulae for the shape derivative $\mathrm{d}\mathcal{J}$, which will help us shortly to compute it in practice.

Theorem 2.1: Let $\nabla\cdot\mathcal{V}$ denote the *divergence* of $\mathcal{V}$. Then

$$\mathrm{d}\mathcal{J}(\Omega,\mathcal{V}) = \int_\Omega \nabla f\cdot\mathcal{V} + f\nabla\cdot\mathcal{V}\,\mathrm{d}x.$$

Proof: By the product rule,

$$\mathrm{d}\mathcal{J}(\Omega,\mathcal{V}) = \int_\Omega \left\{\Big\langle \frac{\mathrm{d}}{\mathrm{d}T}(f\circ T),\mathcal{V}\Big\rangle \det\mathbf{D}T + \Big\langle \frac{\mathrm{d}}{\mathrm{d}T}\det\mathbf{D}T,\mathcal{V}\Big\rangle (f\circ T)\right\}\Big|_{T=I}\mathrm{d}x.$$

Considering the first term, we have

$$\Big\langle \frac{\mathrm{d}}{\mathrm{d}T}(f\circ T),\mathcal{V}\Big\rangle = (\nabla f\circ T)\cdot\mathcal{V},$$

hence

$$\Big\langle \frac{\mathrm{d}}{\mathrm{d}T}(f\circ T),\mathcal{V}\Big\rangle \det\mathbf{D}T\Big|_{T=I} = \nabla f\cdot\mathcal{V}.$$

Considering the second term and using Jacobi's formula [2], we have

$$\begin{aligned}\Big\langle \frac{\mathrm{d}}{\mathrm{d}T}\det\mathbf{D}T,\mathcal{V}\Big\rangle &= \lim_{t\to 0}\frac{\det\mathbf{D}(T+t\mathcal{V})-\det\mathbf{D}T}{t}\\ &= \lim_{t\to 0}\frac{\det(\mathbf{D}T+t\mathbf{D}\mathcal{V})-\det\mathbf{D}T}{t}\\ &= \lim_{t\to 0}\frac{(\det\mathbf{D}T + t\,\mathrm{Tr}(\mathrm{adj}(\mathbf{D}T)\mathbf{D}\mathcal{V})+O(t^2))-\det\mathbf{D}T}{t} = \mathrm{Tr}(\mathrm{adj}(\mathbf{D}T)\mathbf{D}\mathcal{V}),\end{aligned}$$

where $\mathrm{Tr}(A),\mathrm{adj}(A)$ denote the *trace* and *adjugate*[†] of A respectively. Hence

$$\Big\langle \frac{\mathrm{d}}{\mathrm{d}T}\det\mathbf{D}T,\mathcal{V}\Big\rangle(f\circ T)\Big|_{T=I} = \mathrm{Tr}(\mathrm{adj}(\mathrm{Id})\mathbf{D}\mathcal{V})f = \mathrm{Tr}(\mathbf{D}\mathcal{V})f = f\nabla\cdot\mathcal{V}$$

[†]For a matrix A, the *adjugate* of A is the transpose of the *cofactor matrix* C, where $c_{ij}=(-1)^{i+j}\det A_{ij}$, and A_{ij} is the matrix A with row i and column j removed. For an invertible matrix, this is simply $\mathrm{adj}A = (\det A)A^{-1}$.

since adj(Id) = Id is the identity matrix, and the result follows. □

Theorem 2.2: The shape derivative is equal to the surface integral

$$\mathrm{d}\mathcal{J}(\Omega, \mathcal{V}) = \int_{\partial\Omega} f(\mathcal{V} \cdot n)\,\mathrm{d}S,$$

where n is the outward pointing unit normal of the boundary $\partial\Omega$.

Proof: Using Theorem 2.1 and the Divergence Theorem,

$$\begin{aligned}\mathrm{d}\mathcal{J}(\Omega, \mathcal{V}) &= \int_{\Omega} \nabla f \cdot \mathcal{V} + f\nabla \cdot \mathcal{V}\,\mathrm{d}x \\ &= \int_{\Omega} \nabla \cdot (f\mathcal{V})\,\mathrm{d}x \\ &= \int_{\partial\Omega} (f\mathcal{V}) \cdot n\,\mathrm{d}S\end{aligned}$$

where the second equality follows from vector calculus. The result follows. □

3 2D Shape Optimisation in MATLAB

We will use Theorem 2.2 to help us develop an efficient shape optimisation method in MATLAB for integrands of the form $f : \mathbb{R}^2 \to \mathbb{R}$. To construct a descent method for shapes, we first need a minimising sequence of shapes, say

$$\Omega^{(k+1)} = T^{(k)}(\Omega^{(k)})$$

for a sequence of smooth vector fields $T^{(k)}$. As mentioned in Section 2.2, the $T^{(k)}$ are generally unknown, certainly when doing computations in MATLAB, so we need to represent the problem in a different manner.

3.1 Descent Methods for Shapes

How could we define the next shape in the sequence in a similar manner to Section 1.1? We could define the shape by its boundary, then *superpose* shape boundaries by taking their parametrisations and summing component-wise. It then makes sense to write

$$\partial\Omega^{(k+1)} = \partial\Omega^{(k)} + t^{(k)}\Delta\partial\Omega^{(k)},$$

where

- $\Delta\partial\Omega^{(k)}$ represents a *(boundary) search direction*,
- $t^{(k)} \geqslant 0$ represents a *step length*.

In MATLAB, we can illustrate this with the help of the *Chebfun* package. For a 2D problem, define the boundary $\partial\Omega$ as being in the complex plane, as the following example demonstrates.

Example 3.1 (Superposition of shape boundaries): Let R_1 be the ellipse

$$R_1 := \left\{ x : \frac{(x_1 - 0.1)^2}{0.6^2} + \frac{(x_2 - 1.2)^2}{1.05^2} \leqslant 1 \right\}.$$

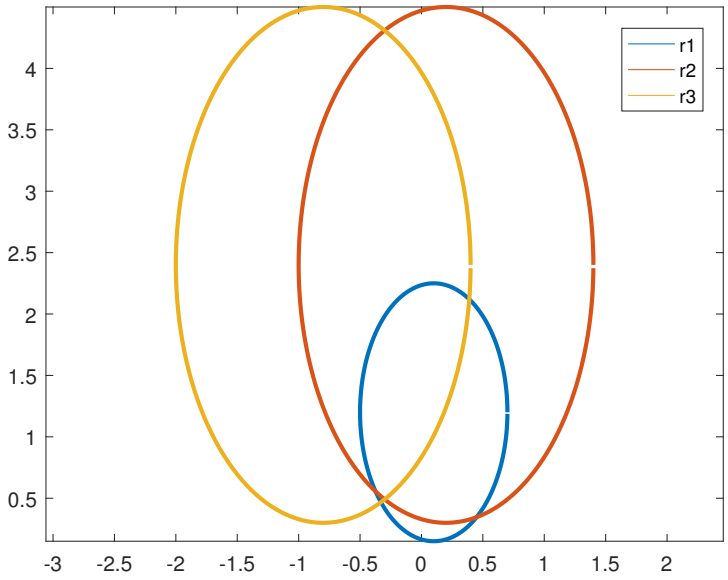
Defining the shape by its boundary in *Chebfun*, we can write the following:

```
r = @(t) [0.1 + 1.2i] + 0.6*cos(t) + 1.05*1i*sin(t);
t = linspace(0,2*pi);
r1 = chebfun(@(t) r(t), [0, 2*pi], 'trig'); %Parametrised boundary
```

Now consider scaling R_1 by a factor of 2, and translating the resulting shape in the negative x_1-direction by 1. Call these shapes R_2 and R_3 respectively. In *Chebfun*, functions are treated as variables and we can simply write the following:

```
r2 = 2*r1; %Scaled boundary
r3 = r2 - [1 + 0i]; %Scaled and translated boundary
```

Finally, we check our intuition by plotting `r1`, `r2` and `r3`:



3.2 Finding a Search Direction

We can find a suitable shape search direction using the gradient definition in Section 1.3. If the shape derivative is linear with respect to $\mathcal{V}$, there is a unique element of $\nabla\mathcal{J} \in L^2(\partial\Omega)$ [3], called the *shape gradient* of $\mathcal{J}$. If $(\cdot,\cdot)_{\partial\Omega}$ is the L^2-inner product on $\partial\Omega$, then

$$\mathrm{d}\mathcal{J}(\Omega,\mathcal{V}) = (\nabla\mathcal{J},\mathcal{V})_{\partial\Omega} := \int_{\partial\Omega} \nabla\mathcal{J}\cdot\mathcal{V}\,\mathrm{d}S.$$

Using Theorem 2.2, we deduce that

$$\nabla\mathcal{J}\big|_{\partial\Omega} = fn.$$

So if we choose our boundary search direction to be the negative gradient

$$\Delta\partial\Omega := -\nabla\mathcal{J}\big|_{\partial\Omega} = -fn,$$

then the shape derivative with search direction $\Delta\partial\Omega$ is

$$\mathrm{d}\mathcal{J}(\Omega,\Delta\partial\Omega) = -\int_{\partial\Omega} f(fn\cdot n)\,\mathrm{d}S = -\int_{\partial\Omega} f^2\,\mathrm{d}S < 0 \tag{5}$$

when $f \neq 0$ on $\partial\Omega$. In line with Section 1.1, we will call any search direction with property (5) a *(boundary) descent direction.*

From (5), we deduce that the shape derivative vanishes when $f = 0$ on $\partial\Omega$. This intuitively makes sense; to minimise $\mathcal{J}$, we want to integrate over the shape $\Omega^* = \{x : f(x) \leqslant 0\}$, with the boundary being the 0-level set of f. Integrating over shapes outside of Ω^* can only increase the value of $\mathcal{J}$.

Example 3.2 (Simple shape optimisation method): Let $f : \mathbb{R}^2 \to \mathbb{R}$ be the function defined by

$$f(x) = x_1^2 + x_2^2 - 1.$$

We know that $\mathcal{J}(\Omega)$ is minimised when integrated over the domain $\Omega = \{x : x_1^2 + x_2^2 \leqslant 1\}$.

We implement a basic shape optimisation method in MATLAB, with initial guess

$$\Omega^{(0)} := \left\{ x : \frac{(x_1 - 0.2)^2}{0.6^2} + \frac{(x_2 - 0.3)^2}{0.2^2} \leqslant 1 \right\},$$

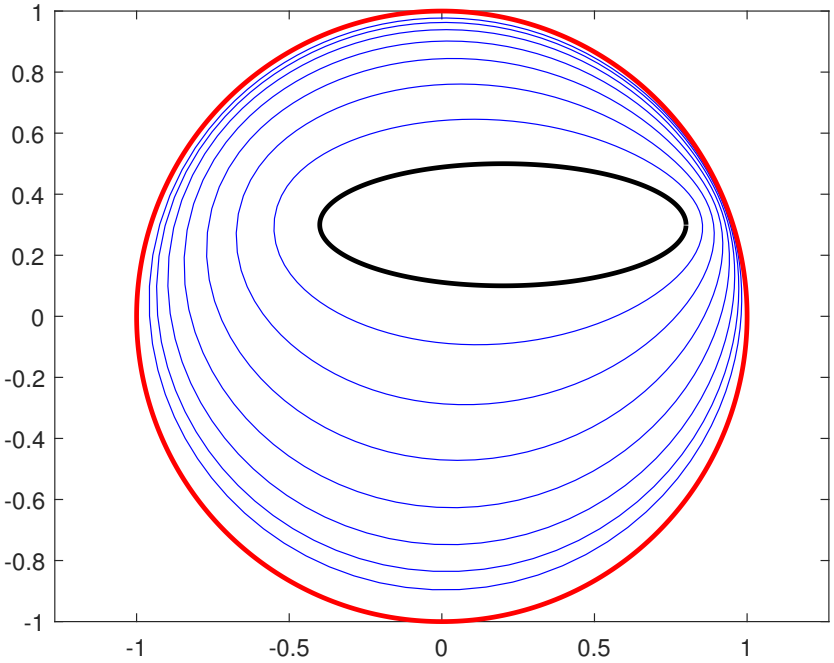
shape search direction $\Delta\partial\Omega = -fn$ and fixed step size $t = 0.2$.

```
g_ = @(t) [0.2+0.3i] + 0.6*cos(t) + 0.2*1i*sin(t);
t = linspace(0,2*pi);
g = chebfun(@(t) g_(t), [0, 2*pi], 'trig'); %Initial boundary
init = plot(g, 'k') %Plot of initial boundary
set(init,'LineWidth',2);

f_ = @(x,y) x.^2 + y.^2 - 1;
f = chebfun2(@(x,y) f_(x,y), [-5 5 -5 5]); %Integrand, f
hold on

for k=1:7
    dg = diff(g); n_ = -1i*dg; n = n_./abs(n_); %Unit normal to boundary
    fn = n.*f(real(g), imag(g));
    g = g - 0.2*fn; %Updated boundary
    plot(real(g(t)), imag(g(t)), 'b')
end

exact = fimplicit(f_, 'r');
set(exact,'LineWidth',2);
axis equal
```



The above figure shows the first 7 iterations $\partial\Omega^{(k)}$ in blue, together with the initial shape boundary $\partial\Omega^{(0)}$ in black and the optimum shape boundary $\partial\Omega^*$ in red.

3.3 Line Search for Shapes

In the previous example we fixed the step size t, but we could try to implement a line search-like method to reduce the number of iterations. In an ideal world, we could use an ELS-like method: choosing t such that $\mathcal{J}$ is minimised along the ray $\{\Omega + t\Delta\Omega : t \geqslant 0\}$, i.e

$$t = \arg\min_{s \geqslant 0} \mathcal{J}(\Omega + s\Delta\Omega).$$

Here we write $\Omega + t\Delta\Omega$ to mean the shape with boundary $\partial\Omega + t\Delta\partial\Omega$.

In Section 1.2 it was difficult to find t exactly; to find t practically we will need to consider a BLS-like algorithm. We will then observe the improvements (if any) on our shape optimisation method. *BLS for Shapes* goes as follows:

Algorithm 4: Backtracking Line Search for Shapes

Given shape descent direction $\Delta\partial\Omega$, $\alpha \in (0, 0.5), \beta \in (0, 1)$
$t := 1$
while $\mathcal{J}(\Omega + t\Delta\Omega) > \mathcal{J}(\Omega) + \alpha t \, \mathrm{d}\mathcal{J}(\Omega, \Delta\partial\Omega)$ **do**
  Set $t \leftarrow \beta t$
end

We can compute the functionals $\mathcal{J}(\Omega)$, $\mathcal{J}(\Omega + t\Delta\Omega)$ and shape derivatives $\mathrm{d}\mathcal{J}(\Omega, \mathcal{V})$ with the *Chebfun* functions `integral2` and `integral`. Conveniently, $\mathcal{J}$ is calculated using the shape boundary. We could then replace the `for` loop in the MATLAB code from Example 3.2 with a `while` loop involving BLS for Shapes. Below is an example of the modified method with $\alpha = 0.1$ and $\beta = 0.7$ say:

```
J = @(f,g) integral2(f,g); %Cost functional, J(\Omega)
dJ = @(f,g,V) integral(f.*dot(V,n),g); %Shape derivative, dJ(\Omega,V)

hold on
tol = 0.05;
iteration = 0;

while abs(dJ(f,g,fn)) ≥ tol

    iteration  = iteration + 1

    dg = diff(g); n_ = -1i*dg; n = n_./abs(n_); %Unit normal to boundary
    fn = n.*f(real(g), imag(g));

    % BLS for shapes; step size algorithm
        alpha = 0.1; beta = 0.7; s = 1;
        while J(f,g-s*fn) > J(f,g) + alpha*s*dJ(f,g,-fn);
              s = beta*s;
        end

    step = s

    g = g - s*fn; %Updated boundary
    plot(real(g(t)), imag(g(t)), 'b')

end
```

We use `iteration` and `step` to track how many iterations the algorithm takes, and what step size is used at each iteration.

3.4 Steepest Descent for Shapes

The MATLAB code above bears close resemblance to the Steepest Descent algorithm we saw in Section 1.3. We could formally write the corresponding algorithm for shapes as follows:

Algorithm 5: Steepest Descent for Shapes

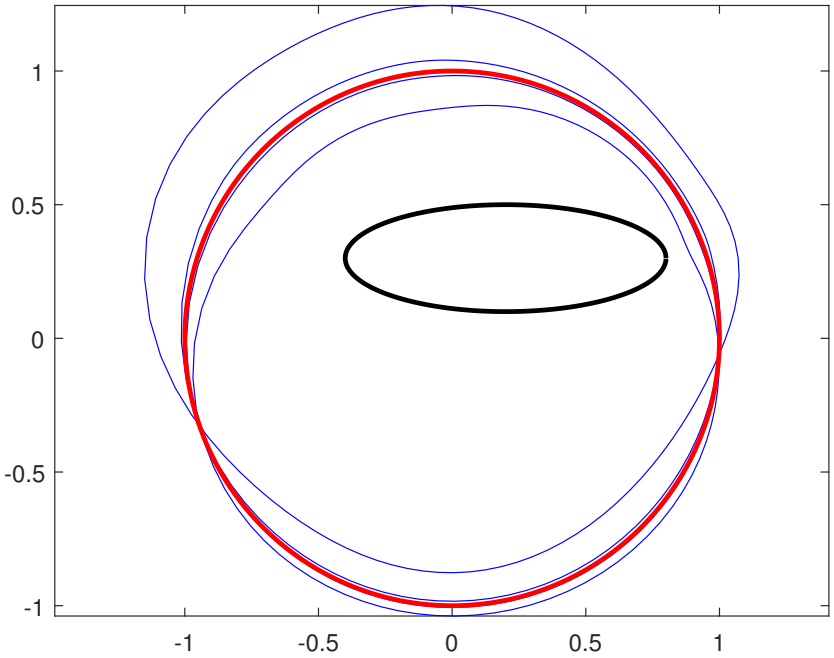
Given starting shape Ω
repeat
  (1) Set $\Delta\partial\Omega \leftarrow -fn$
  (2) Choose t via BLS for Shapes
  (3) Set $\partial\Omega \leftarrow \partial\Omega + t\Delta\partial\Omega$
until *stopping criterion satisfied*

Here we could use a stopping criterion of the form $|\mathrm{d}\mathcal{J}(\Omega, \Delta\partial\Omega)| < \varepsilon$ for a given tolerance $\varepsilon > 0$, which was used in the MATLAB code.

Example 3.3 (Steepest Descent with BLS for Shapes): Running the above code with integrand

$$f(x) = x_1^2 + x_2^2 - 1$$

outputs `iteration` $= 4$ with step sizes 1, 0.7, 0.7, 0.7 respectively, and the following figure:



Though the first iteration shoots outside the level set, we achieve an extremely good approximation when the algorithm terminates after only 4 iterations. The first iteration uses step size 1 - if we chose the initial step size for BLS to be such that the iteration stays within the level set, say $t = 0.5$, the algorithm terminates in just a fraction of the time.

However, after comparing the two descent methods for solving Example 3.2 using `tic` and `toc`, we find that the non-BLS method takes 0.635179 seconds, compared to the BLS method's 19.108205 seconds[‡]. While BLS for Shapes does generally help to reduce the number of iterations required, the effort of computing $\mathcal{J}$ and $\mathrm{d}\mathcal{J}$ makes the Steepest Descent algorithm a lot slower, and for our purposes, impractical. We will revert to using a (small) fixed step size in our method.

[‡]Computed on a Toshiba Satellite P50-C-18L with Intel Core i7.

4 Complications in Shape Optimisation Methods

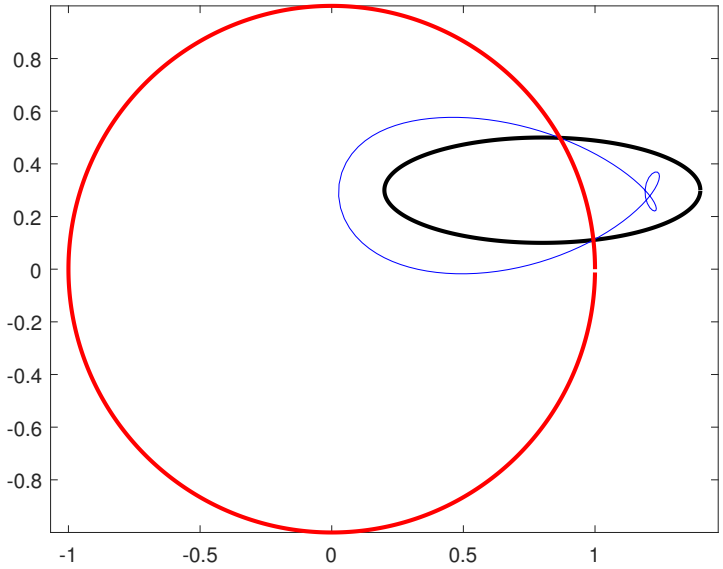
Recall that the optimum shape boundary is the set of points such that f vanishes. If the initial shape boundary intersects the optimum boundary, then at the intersection points we have

$$\Delta\partial\Omega = -fn = 0,$$

so each boundary iteration will always include those points as $\partial\Omega^{(k+1)} = \partial\Omega^{(k)}$ there. This can be problematic - suppose we instead took the initial boundary in Example 3.2 to be

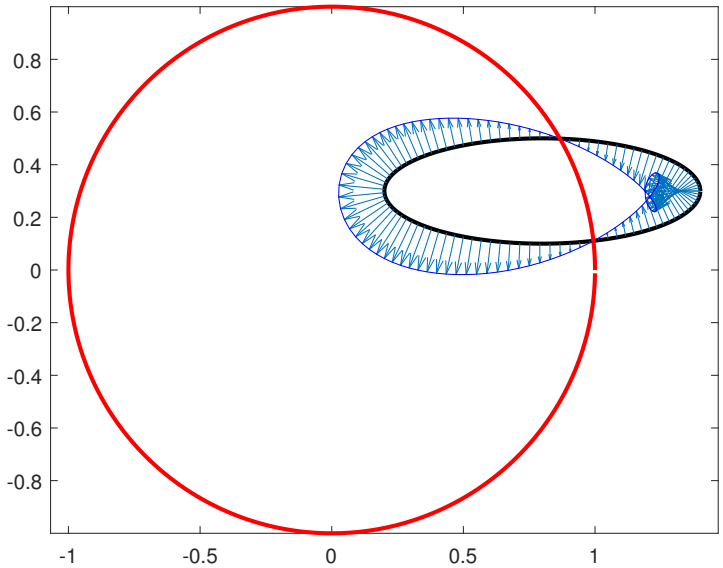
$$\Omega^{(0)} := \left\{ x : \frac{(x_1 - 0.8)^2}{0.6^2} + \frac{(x_2 - 0.3)^2}{0.2^2} \leqslant 1 \right\},$$

which intersects the optimum boundary at two points. The first iteration would look like this:



A complication arises in that the curve is no longer simple. Why does this happen? We can visualise the direction that points of the initial boundary are being transformed to using `quiver`:

```
quiver(real(g(t)), imag(g(t)), -0.2*real(fn(t)), -0.2*imag(fn(t)),0)
```



Points further away from the optimum boundary outside the 0-level set have a greater value of f, so they are being transformed towards the level set with a greater scale factor than closer points. How can we choose $\partial\Omega^{(0)}$ to avoid this scenario?

4.1 Choosing the Initial Boundary

At the cost of some computational time, we can avoid this initial boundary-crossing behaviour by defining the initial boundary to be a small ball around a point at which f is minimised, i.e

$$\Omega^{(0)} := \{x : |x - x^*| \leqslant R\}, \quad x^* \in \arg\min_x f(x)$$

for some chosen radius $R > 0$. We can find such a point in MATLAB either with a descent method (as in Section 1), or using *Chebfun*'s `min2` command. The following code takes $R = 0.1$:

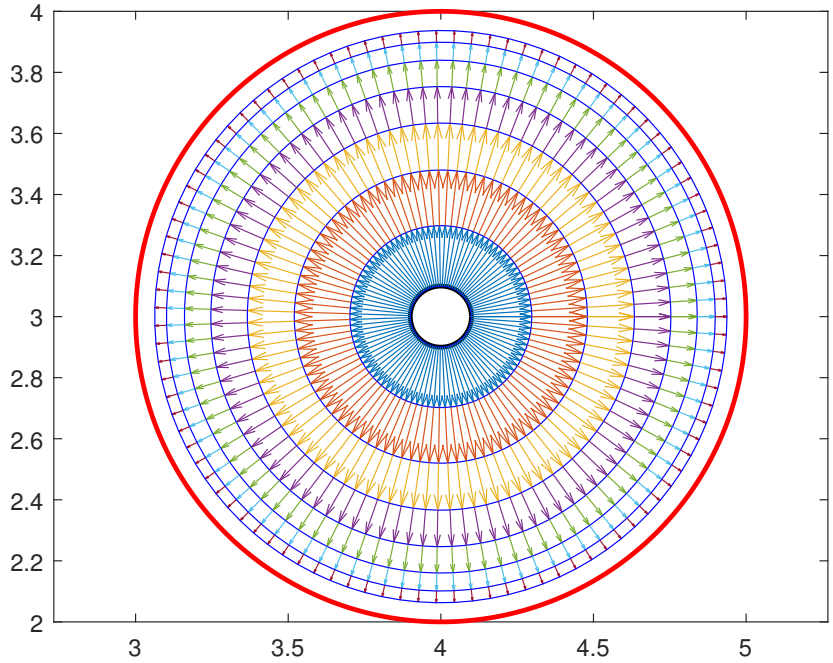
```
[Y,X] = min2(f);
x1 = X(1); x2 = X(2);
r = sqrt(x1.^2+x2.^2);
the = atan2(x2,x1);
R = 0.1;
g_ = @(t) r*(cos(the) + 1i*sin(the)) + R*(cos(t) + 1i*sin(t));
```

Note that in the above, `r*(cos(the)+1i*sin(the))` is a scalar translating the parametrised ball `R*(cos(t)+*1i*sin(t))`, and is not to be confused with the parametrisation itself. We test our new initial boundary technique on some different integrands in the following example.

Example 3.4 (New initial boundary): Let $f : \mathbb{R}^2 \to \mathbb{R}$ be defined by for

$$f(x) = (x_1 - 4)^2 + (x_2 - 3)^2 - 1.$$

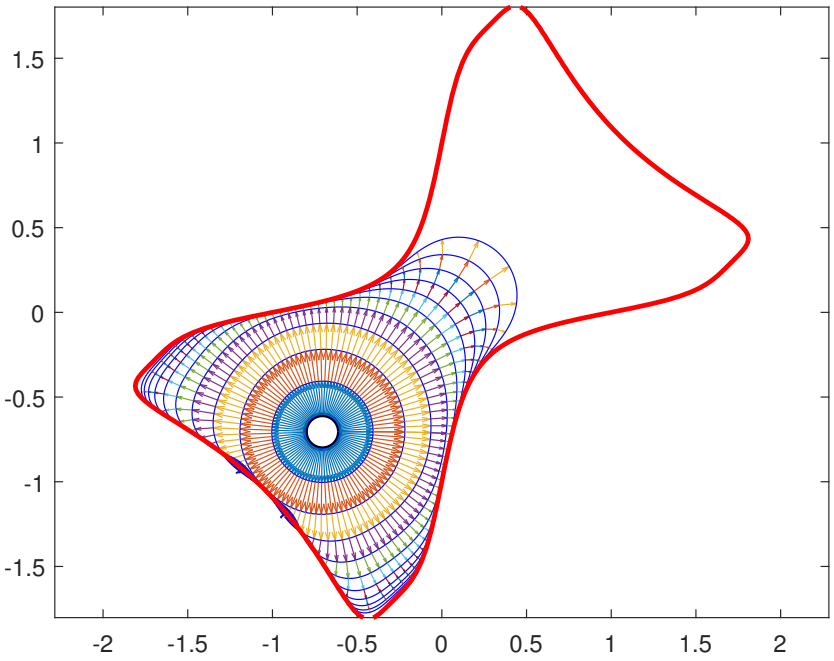
The figure below plots the first 7 iterations of the shape optimisation method, with step size $t = 0.2$.



Using `pause` in the `for` loop allows us to check the speed of each iteration one at a time. In this case, the iterations are computed virtually immediately.

The next figure shows 10 iterations with a step size of $t = 0.1$ on a bow tie-shaped integrand

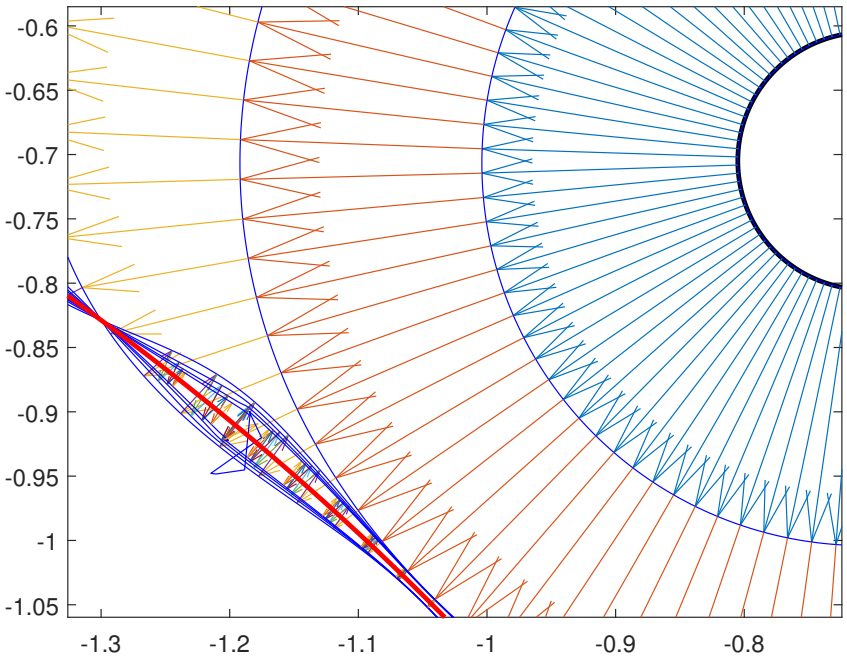
$$f(x) = (x_1 - x_2)^2 + (2x_1x_2 - 1)^4 - 5/2. \tag{6}$$



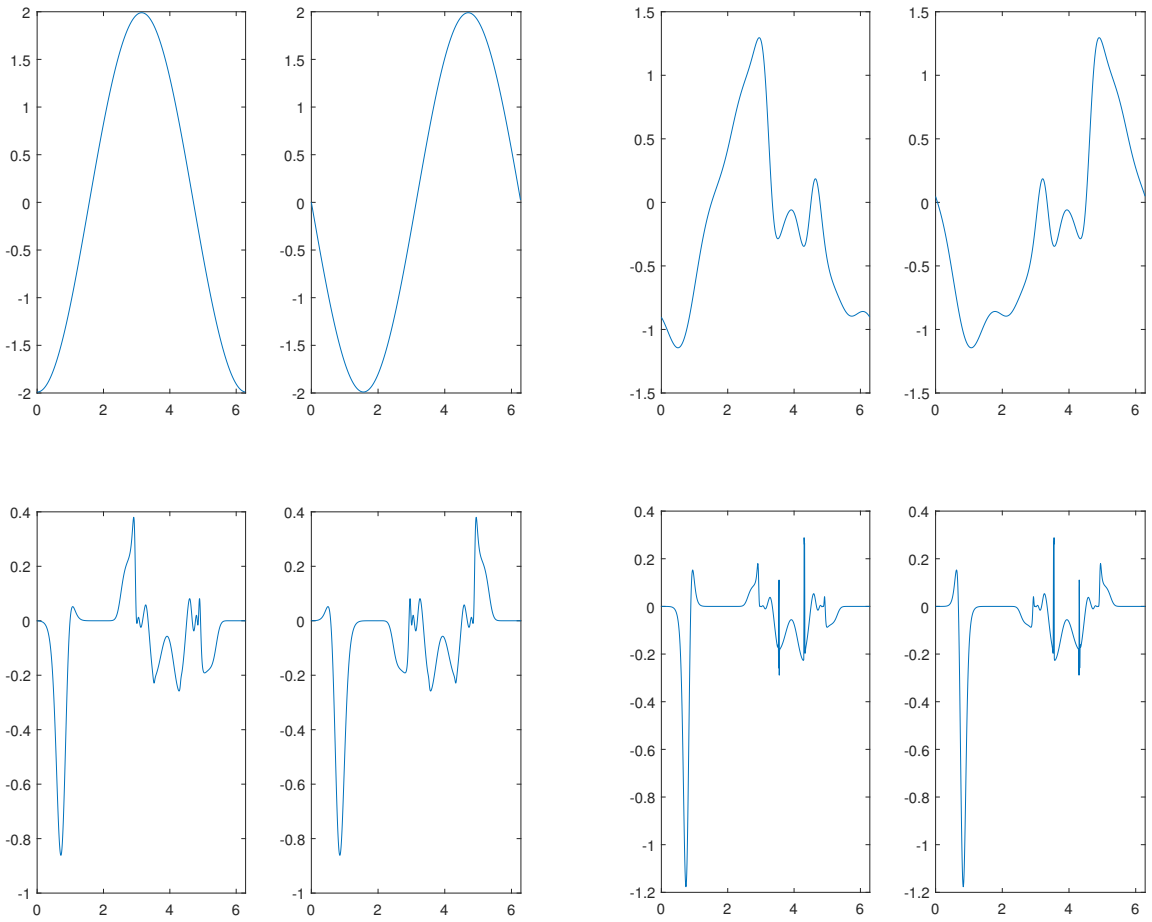
Again using `pause`, we observe that the shape descent method struggles with the latter iterations. At the 10th iteration, we get the message

```
Warning: Composition with @(x)feval(op,feval(f,x)) failed to converge with 65536 points
```

and the shape boundary loses its simple form at the bottom end of the level set:



The update misbehaves only at very small parts of the boundary. Sketching real and imaginary parts of fn using `subplot` gives the following figures:



The figures show subplots for iterations 1, 4, 8 and 10 respectively. In each pair of figures, the real part is plotted on the left, and the imaginary part on the right. Note that the spikes in the real and imaginary parts of fn are appearing at exactly the points where our boundary misbehaves - in an ideal shape optimisation method, we would expect fn to approach 0 for large iterations, without such spikes.

4.2 Reparametrising the Boundary

Recall that we require $\mathcal{V} \to \mathrm{d}\mathcal{J}(\Omega, \mathcal{V})$ to be linear and bounded on $C^1(\mathbb{R}^2, \mathbb{R}^2)$ for $\mathcal{J}$ to be shape differentiable - particularly it must hold for $\mathcal{V} = fn$. We are currently computing boundaries as complex `chebfun`s with a parametrisation $t \in [0, 2\pi]$, but if we reparametrise the boundary as $\gamma(t)$ such that $|\gamma'(t)|$ is small, we will get rid of the spikes and improve the optimisation method. We attempt to create such a γ by reparametrising in terms of arc length.

5 Conclusion

6 Acknowledgements

References

[1] Stephen Boyd and Lieven Vandenberghe. *Convex Optimisation*. Cambridge University Press, 2004. `web.stanford.edu/~boyd/cvxbook/bv_cvxbook.pdf`

[2] Jan R Magnus and Heinz Neudecker. *Matrix Differential Calculus with Applications in Statistics and Econometrics*. Wiley, 1999.

[3] *Shape Optimization*. Wikipedia. `en.wikipedia.org/wiki/Shape_optimization`

[4] Tobin Driscoll, Nicholas Hale and Lloyd Trefethen. *Chebfun Guide*. `chebfun.org/docs/guide/chebfun_guide.pdf`