

GENERATING OPTIMAL CURVES VIA THE C++ STANDARD LIBRARY

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Recent computational breakthroughs in infinite-dimensional optimization have produced explicit, as well as numerically advantageous, gradient formulas. By following the negative gradient trajectories, along so-called steepest descent, the minimizing curve is sought. The C++ standard library supports the assembly of a user-defined type based on the standard cubic splines, and a corresponding operator algebra that is capable of representing all the gradient expressions while preserving the conventional notation. It is crucial that the algebra implements, and is ‘closed’ under, composition with both user-defined and built-in functions, as well as the calculus operations integration and differentiation. Examples illustrate both fixed and free endpoints, and particular attention is paid to the notoriously difficult isoperimetric constraints. In the spirit of ‘component technology’, the implementation uses the ‘boost extension’ of the standard library and adapts efficient legacy code from the book ‘Numerical Recipes in C’. By limiting the choice of numerical methods to the most elementary algorithms, the strength of the gradient formulas is showcased as a general class of problems is successfully attacked using built-in generic algorithms with dynamic memory allocation, as well as object-oriented concepts such as inheritance.

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1. INTRODUCTION

1.1 Background. According to the legend, princess Dido persuaded chieftain Hiarbas to give her “as much land as she could enclose with the hide of a bull.” The cunning Dido cut the hide into thin strips, tied them together to form an extremely long thong that she used to surround a territory in which the city of Carthage was founded (825 or 814 B.C.), see page 2 in [Alekseev et al. 1987]. Dido took advantage of the sea and used the straight shoreline as a border. What is the optimal curve for the thong? Assume one end fixed somewhere along the shoreline. Two things

must be determined, where should the final point of the thong be placed and what shape should the thong have between its endpoints?

1.2 Isoperimetric constraints. This legend offers one of the earliest examples of a problem where the optimal curve is to be determined. Dido's problem illustrates the presence of side conditions since the length of the competing curves is fixed and the endpoints must be on the shoreline. There is of course a limitless collection of problems involving optimal curves subject to side conditions. The purpose of the present paper is to present an implementation that efficiently 'improves' the shape of a given initial curve until the optimal curve is reached. The process is applicable to the general case, and all side conditions are satisfied at each stage. Any side condition that can be expressed as the demand that a certain integral takes on a fixed value is referred to as an isoperimetric constraint. Fixing the length of the competing curves is an example of an isoperimetric constraint. The implementation allows up to two isoperimetric constraints and any combination of fixed or free endpoints. The software is designed to readily extend to cases with more than two isoperimetric constraints, or when a point other than an endpoint is fixed, or if periodic boundary conditions are imposed, or any combination of the above.

1.3 Infinite-dimensional domain with curvature. It is important to recognize that the presence of isoperimetric constraints introduces an essential non-linearity. The objective and the isoperimetric constraints typically involve integrals with integrands depending on derivatives of the function representing the curve. The form of the integrand suggests a choice of a linear function space of sufficiently smooth functions. To increase the likelihood that there is an optimal curve, the selected function space is the least restrictive as far as assumptions on smoothness. The subset of functions that satisfy an isoperimetric constraint inside the selected function space will neither be linear nor flat.

1.4 Inner products. Geometric methods are made accessible once an inner product is defined on the function space. There is some freedom in this choice and the present paper discusses three different inner products. The corresponding so-called Sobolev spaces have the same properties as far as convergence is concerned, but they differ in subtle ways geometrically. The subset of curves satisfying a given isoperimetric constraint is expected to have a well-defined one-dimensional normal space inside the linear space of all curves. The infinite-dimensional linear space of functions perpendicular to this space is the so-called tangent space. Different curves typically correspond to different tangent spaces. The constrained curves form an infinite-dimensional 'level surface' inside the space of all curves. When two isoperimetric constraints are present, it is often the case that the corresponding level surfaces intersect 'transversally' and the normal space to the intersection manifold is two-dimensional. The corresponding orthogonal tangent space is of course still infinite-dimensional.

1.5 Derivatives and gradients. The next step is to compute the so-called Gateaux derivative (or directional derivative) of the non-linear objective and constraint functionals. These derivatives are linear functionals and the Riesz theorem guarantees that there is a function, the gradient, which represents the Gateaux derivative. If the level surfaces are regular and the intersections are transversal, then the gradients of the constraints are in the normal space. It follows that the gradient of the objective can be projected onto the tangent space. There is now a curve, the gradient trajectory, inside the infinite-dimensional manifold with the property that its velocity vector is parallel to the projected gradient. The implementation presented here generates points along the gradient trajectory. These points correspond to ever improving curves that satisfy the constraints of the original problem.

1.6 Motivation. Although the classical problems, such as Dido's, are interesting in their own right, they are not the main motivation behind the development of this code. The real interest is in problems of periodic orbits that require 'floating' boundary conditions constrained to infinite-dimensional manifolds that are not flat. In these problems the solution is not given by some traditional boundary-value problem such as the one related to the Euler-Lagrange equation. As an example consider a distorted sphere E (for Earth). A geodesic on E is a curve x such that if a particle travels along x with constant speed, then its acceleration vector is at all times normal to E . Given a tangent vector v at p in E there is a geodesic emanating from p with initial direction v . This geodesic extends indefinitely producing a curve that winds around E . If the geodesic returns to p and its direction at that instant is v , then it is said to be periodic. In the case of the standard round sphere each geodesic is periodic, and in fact a great circle traversed repeatedly. For a distorted sphere it is not clear that there are any periodic geodesics.

1.7 Recent progress. The work of many mathematicians over several hundred years culminated in the 1990's with the papers [Franks 1992; Bangert 1993; Hingston 1993]. It is now known with certainty that any distorted sphere has an infinite number of geometrically distinct periodic geodesics. Moreover, if $n(L)$ is the number of periodic geodesics of length less than or equal to L , then $n(L)$ grows at least as fast as the prime numbers. It is possible to generalize the notion of geodesics to arbitrary so-called Riemannian manifolds. In this generalized setting the Newtonian evolution of a mechanical system corresponds directly to a geodesic in the appropriate Riemannian manifold. Periodic orbits that are sought in the famous celestial three-body problem thus correspond to periodic geodesics.

1.8 Current research. To the best of the author's knowledge, nobody has successfully implemented an algorithm capable of generating general periodic geodesics. One difficulty is the fact that there is no guarantee that through a given point p with given direction v there is a periodic geodesic. It follows that the implementation must handle 'floating constraints' where p and v are allowed to vary keeping endpoints in agreement as in $x(0) = x(1) = p$ and $x'(0) = x'(1) = v$. This has

turned out to be a considerable challenge. A second source of difficulty is the trivial fundamental group of the sphere. Although it is possible to find two distinct periodic geodesics in a torus by shrinking a pair of suitable closed curves, this approach will not work in a sphere. A third difficulty is the available freedom in the parameterization of the curve. Moreover, for periodic orbits there is also a rotation that leaves the curve invariant. The methodology of projected gradients combined with steepest descent adapts very well to these circumstances. Since the steepest descent takes place along a curved infinite-dimensional manifold, Newton's method is not available as an alternative.

1.9 Notation. Let X be a space of curves and consider functions $F : X \rightarrow \mathbb{R}$. The concern of this paper is the search for $\hat{x} \in X$ with the property that $F(\hat{x}) \leq F(x)$ for all $x \in X$. The examples are drawn from the Calculus of Variations, so the space X is some subset of sufficiently smooth functions defined on the closed interval $[0,1]$. Let $\dot{x} = dx/dt$ be the derivative and define

$$F(x) = \int_0^1 f(t, x(t), \dot{x}(t)) dt,$$

where $f : \mathbb{R}^3 \rightarrow \mathbb{R}$ is a given function. It is often assumed that the endpoints are fixed so that $x(0) = x_0$ and $x(1) = x_1$ for some specified $x_0, x_1 \in \mathbb{R}$. To expose potential candidates for \hat{x} the conventional approach utilizes the Euler-Lagrange equation

$$\frac{d}{dt} \frac{\partial f}{\partial \dot{x}}(t, x(t), \dot{x}(t)) = \frac{\partial f}{\partial x}(t, x(t), \dot{x}(t)).$$

Here $\partial f / \partial x$ represents the partial derivative of f with respect to its second variable, and $\partial f / \partial \dot{x}$ the partial derivative with respect to its third variable. This ordinary differential equation together with the prescribed boundary conditions is an example of the classical boundary value problem. The basic numerical method for this typically nonlinear problem is the so-called 'shooting method' [Conte et al. 1980; Burden et al. 1985; Flowers 1995]. For a more comprehensive overview, including the finite element method, consult the books [Prenter 1975; Glowinski 1984, Nocedal et al. 1999]. The endpoint constraints cause next to no harm since the corresponding domain of functions is at worst a translated linear space. In contrast, suppose $X = G^{-1}(0)$ for some functional $G : H \rightarrow \mathbb{R}$ of the form

$$G(x) = \int_0^1 g(t, x(t), \dot{x}(t)) dt,$$

defined on some suitable Hilbert space H , and with $g : \mathbb{R}^3 \rightarrow \mathbb{R}$ a given function. Typically, the domain X is not 'flat', which leads to considerable complications. In the classical theory, Lagrange multipliers are introduced to deal with this kind of 'isoperimetric constraint'. Algorithms, such as the shooting method, are not designed to deal with unknown parameters like the multipliers. Line-searches are not expected to yield points in X . Alternative methods must be developed and the present paper explores one promising approach.

1.10 Purpose and design issues. The paper presents the implementation of a general-purpose algorithm designed to at least handle all the standard problems in the elementary Calculus of Variations. The algorithm takes advantage of recent computational breakthroughs in infinite dimensional calculus [Linnér 2000]. There are now ‘explicit’ and ‘numerically friendly’ gradient formulas in terms of a certain Euler operator and the ‘Work’ functional. Flexibility in the choice of inner product in the Hilbert space is also permitted. Perhaps surprisingly, only very elementary numerical methods are sufficient as building blocks as the algorithm is assembled. The gradient formulas involve a mix of integrals, derivatives, compositions with special functions, and the usual algebraic operations. The gradient formulas are somewhat complicated and each isoperimetric constraint introduces its own gradient. The presence of endpoint constraints changes the gradient formulas and so does a change of the inner product in the function space. Given this multitude of different formulas, it is obviously desirable that all mathematical expressions are represented by code that mimics the original expressions and thus facilitating error-free translations. The pursuit of the infinite time limit along the negative gradient trajectories necessitates very efficient code.

1.11 Programming language. The adoption of a C++ standard in 1997 [Stroustrup 1997] and its incorporation of most parts of the Standard Template Library [Stepanov-Lee 1995] makes C++ a very attractive choice. The code is easily ported and concerns about computational speed are at the core of the design of the STL. Specifically, the C++ standard library supports a flexible representation of the functions in the infinite-dimensional space using dynamic memory allocation. The C++ `operator` feature is essential to preserve standard mathematical notation. Object-oriented ‘inheritance’ combine with the ‘boost extension’ [<http://www.boost.org>; Josuttis 1999] to supply the necessary algebra with minimal coding. It is shown how both built-in functions and user-defined functions can be represented as function objects capable of proper interaction with the discrete representation of the target functions. By demanding that all operations return an object of the same type, a computationally ‘closed’ framework is created. The gradient formulas are readily expressed in this framework, and steepest descent algorithms are easy to implement. The target functions are represented by cubic splines and implemented by modernizing and extending code in *Numerical Recipes in C* [Press et al. 1992].

1.12 Fundamental difficulty. Recall that the steepest descent is the flow along the trajectories of the negative gradient vector field. In all but the simplest cases this flow is not known explicitly. All numerical algorithms will suffer from an irreversible loss of information at the start of the descent in the infinite dimensional case. The initial point is a curve that can only be represented by a finite number of points. The flow subsequently acts on the discrete representation and this severely limits the number of applicable numerical tools during the descent. To deal with this difficulty, curves and gradients are here represented as instances of a C++ `class S` (S for spline) with the following capabilities. S is derived from the ‘boost extension’ to give it all the usual algebraic operations. In addition, S has integral and derivative member functions that produce

objects of class `S`. `S` has a `friend` `FunctionObject` to permit composition with library functions and user-defined functions. The ability to compose with functions and still have an object of class `S` is crucial when expressing the gradients. `S` has a `Show()` method that displays the values at all the sample points, and a `Save()` method to save the points and the values in a file.

1.13 Organization. Section 2 introduces eight examples in increasing order of difficulty. The following table indicates if the corresponding solutions are known explicitly, implicitly or in terms of special functions:

example number	1	2	3	4	5	6	7	8
isoperimetric constraints	0	0	0	0	0	1	1	2
number of free ends	0	0	0	0	1	0	1	2
trivial explicit solution	✓	✓	✓					
implicit/special functions		✓		✓	✓	?	?	✓

Each example is illustrated by computer graphics. The two question marks indicate that the author is unaware of any rigorous derivation of these solutions in either implicit form or in terms of special functions. To use the implementation the user supplies a file where the types of constraints are indicated. For each functional the integrand and its partial derivatives must be coded, and an initial curve that satisfies all the constraints is coded as well. The gradient formulas are introduced in Section 3, and there is also a brief discussion of the influence of the choice of metric on the steepest descent in the space of curves. Section 3 shows how to deal with isoperimetric constraints. Finally, the spline class `S` is presented in Section 4 together with parts needed from the boost library along with extensions to the Numerical Recipes in C. Section 5 gives a reference to the complete software package and also a few remarks about the testing under UNIX and Windows.

Finally, I like to take this opportunity to thank the three referees and the editor for proposing a series of concrete improvements to the original manuscript.

2. EXAMPLES

2.1 Minimizing length. The first example involves the familiar length functional given by

$$F(x) = \int_0^1 \sqrt{1 + \dot{x}^2(t)} dt.$$

This simple example is useful as an introduction since the solution is known to be the straight line-segment connecting the two endpoints. Assume $x(0) = 0$ and $x(1) = 2$. To get a good illustration of steepest descent, let the initial curve be given by $x_0(t) = 2t^6$. The initial curve is coded by supplying the underlined part in:

```
double initial(double t){return 2.0*std::pow(t,6);}
```

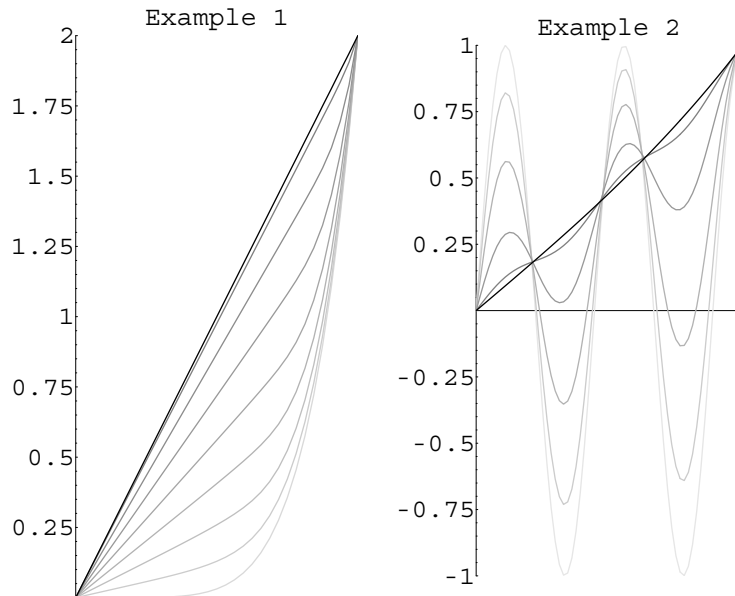
The convention is that reserved words in C++ are in **boldface**. Names from the C++ standard library or the boost extension are in *italic*. All other names are in regular type. This way it is clear at a glance which of the names must be remembered and which names are invented. The code corresponding to the initial curve is omitted in the subsequent examples. Next, the user supplies the function f and the partial derivatives $\partial f / \partial x = f_x$, $\partial f / \partial \dot{x} = f_{\dot{x}}$. Here is the code:

```
f = Sqrt(1.0 + xDot*xDot);  fx = 0.0*x;  fxDot = xDot/Sqrt(1.0 + xDot*xDot);
```

(It is possible to modify the code so that these calculations can be performed discretely by ‘other programs’. If this is the case the actual data points of x and $x\text{Dot}$ must be exposed through some additional interface.) The names x , $x\text{Dot}$ correspond to objects of class S . The S -algebra creates S objects from expressions like $1.0 + x\text{Dot}*x\text{Dot}$, and $0.0*x$. Observe that 0.0 by itself is not an S -object, so the compiler will not accept $fx = 0.0$. The decision to prohibit this assignment supports type safety. All the standard functions are already converted to function objects as in

```
FunctionObject Sqrt(std::sqrt);
```

Each picture shows curves at increasing times along the descent. The negative gradient trajectories extend indefinitely and there is an exponential slowing as the limit is approached. To increase the flow-time interval between stored curves there is a user-supplied constant that can be used to exponentially increase the time separation between each save. To simplify the interpretation, curves are plotted with a lighter gray that darkens as the flow time increases. Only the solution is plotted in black.



2.2 Euler-Lagrange. The second example involves the functional

$$F(x) = \int_0^1 x^2(t) + \dot{x}^2(t) dt.$$

Assume that $x(0) = 0$ and $x(1) = 1$. It is tempting to believe that the solution is given by a straight line since making x smaller necessarily increases \dot{x} and conversely. To get a nice illustration the steepest descent is applied to the initial curve $x_0(t) = \sin(9\pi t/2)$. The minimizing curve is not a straight line. This time the code is:

```
f = x*x + xDot*xDot;  fx = 2.0*x;  fxDot = 2.0*xDot;
```

The functional is the square of a standard norm in the Hilbert space of functions with the integral of the square of the derivative finite. It is possible to show that there is a function of minimal norm in the space of functions satisfying the boundary condition. The classical theory proves that the Euler-Lagrange equation must be satisfied at the minimum provided the solution is sufficiently differentiable. In the current example the Euler-Lagrange equation simplifies to $\ddot{x} = x$. The general solution is a linear combination of the hyperbolic functions \sinh and \cosh . The only solution that satisfies the boundary conditions is $x(t) = \sinh(t)/\sinh(1)$, which agrees with the solution generated by the implemented algorithm.

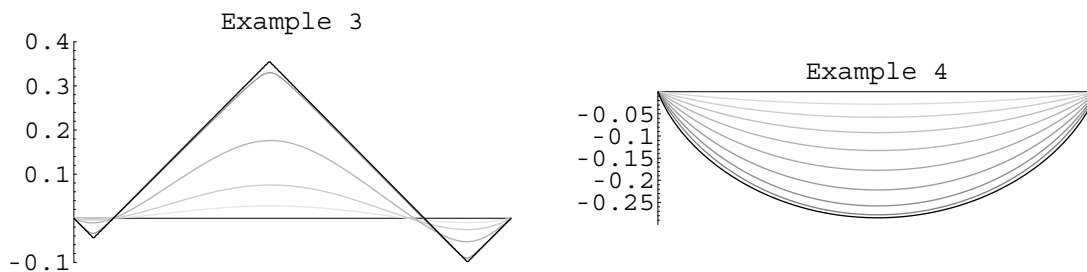
2.3 Less smoothness. The third example illustrates a steepest descent flow towards a curve with discontinuous derivative. The functional is given by

$$F(x) = \int_0^1 (1 - \dot{x}^2(t))^2 dt.$$

Observe that $F(x) \geq 0$, and a curve with derivative ± 1 yields equality. Assume $x(0) = x(1) = 0$, with initial curve $x_0(t) = t(t - 1/11)(t - 13/17)(t - 1)$.

The code is given by:

```
f = (1.0 - xDot*xDot) * (1.0 - xDot*xDot);  fx = 0.0*x;  fxDot = -4.0*xDot*(1.0 - xDot*xDot);
```



2.4 Brachistochrone with fixed endpoints. Consider a particle that glides without friction along a curve in a vertical plane. Assume that the gravitational force is the only cause of the motion. The curve that yields the shortest time to traverse the curve between a pair of given points is known as the brachistochrone with fixed endpoints. Assume the initial point is given by $x(0) = 0$ with gravity acting in the negative direction so that $x(t) \leq 0$. Assume the initial speed is given by $v_0 > 0$. The functional is given by

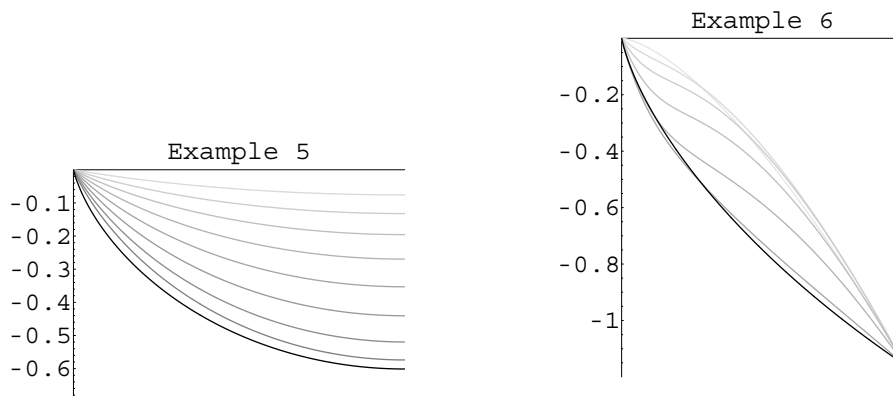
$$F(x) = \int_0^1 \frac{\sqrt{1 + \dot{x}^2(t)}}{\sqrt{v_0^2 - x(t)}} dt.$$

It is often assumed that $v_0 = 0$, but this leads to an unbounded integrand and a number of related technical difficulties. The code is given by:

```
f = Sqrt(1.0 + xDot*xDot)/Sqrt(v0*v0 - x);
fx = 0.5 * Sqrt(1.0 + xDot*xDot)/( Sqrt(v0*v0 - x)*(v0*v0 - x) );
fxDot = xDot/( Sqrt(1.0 + xDot*xDot)*Sqrt(v0*v0 - x) );
```

The initial curve is given by $x_0(t) = 0$ and the initial speed throughout is given by $v_0 = 0.2$ so that $F(x) = 5$ at the start. Observe that the integrand f does not depend on t explicitly. The classical approach takes advantage of this fact and the ‘second’ Euler-Lagrange equation is derived as $f(t, x(t), \dot{x}(t)) - \dot{x}(t) f_x(t, x(t), \dot{x}(t)) = \text{constant}$; [Weinstock 1974; Troutman 1983; Gelfand et al. 2000]. Using the second Euler-Lagrange equation it is possible to express the solution as a parameterized curve $\bar{t} = \bar{t}(\tau)$ and $\bar{x} = \bar{x}(\tau)$. It should be pointed out that neither \bar{t} nor τ corresponds to time. The curve turns out to be a cycloid. It is possible to change the parameter to the arc-length parameter s and get explicit formulas $\bar{t} = \bar{t}(s)$ and $\bar{x} = \bar{x}(s)$ [Dombrowski 1996]. To use the parametric formulas and get the optimal $\hat{x}(t)$ produced by the steepest descent algorithm, it is necessary to solve a transcendental equation. This explains why $\hat{x}(t)$ is never given explicitly in the literature. The graph of the function $\hat{x}(t)$ produced by the algorithm and the trace of the parametric curve $(\bar{t}(\tau), \bar{x}(\tau))$ are the same.

2.5 Brachistochrone with a free endpoint. If it is only required that the curve reaches the vertical line $t = 1$, then the right-hand endpoint is said to be free. Since the Euler-Lagrange equation is a second order equation, its solutions have two constants that must be determined. In the case of a free endpoint a second necessary condition is therefore required. The condition, known as a ‘natural’ boundary condition [Gelfand et al. 2000; Troutman 1983], is in general given by $f_x(1, x(1), \dot{x}(1)) = 0$. In the case of the brachistochrone this simplifies to $\dot{x}(1) = 0$. In the implementation there is no need to change any of the code assuming. All that is needed is the information that the right-hand endpoint is free. This will activate a different set of gradient formulas behind the scenes. In general it is possible to have the left-hand endpoint free or both endpoints free. In any case the corresponding gradient formulas are known and there is no need to change any of the code.



2.6 Length constrained brachistochrone with fixed endpoints. Since it is possible to give a parametric representation in terms of the arc-length parameter, it follows that the length L_0 of the brachistochrone is known. Consider now the following problem. Choose a length L_1 different from L_0 and determine the curve \hat{x} of length L_1 with $F(\hat{x}) \leq F(x)$ for all curves of length L_1 satisfying the boundary conditions. This is an example of an isoperimetric problem. In addition to

$$F(x) = \int_0^1 \frac{\sqrt{1 + \dot{x}^2(t)}}{\sqrt{v_0^2 - x(t)}} dt,$$

there is also the constraint functional

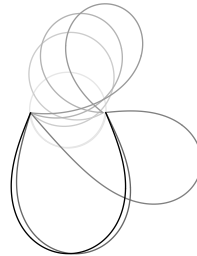
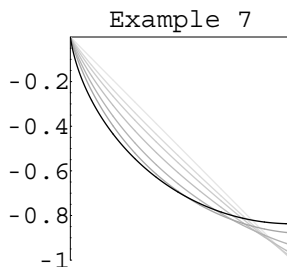
$$G(x) = \int_0^1 \sqrt{1 + \dot{x}^2(t)} dt.$$

Assume that $x(0) = 0$, and let the initial curve be given by $x_0(t) = -\frac{2}{\sqrt{3}}t\sqrt{t}$ so that $x(1) = -\frac{2}{\sqrt{3}}$. The appropriate gradient formulas keep both the endpoints fixed. This particular initial curve is useful since its length is known to be exactly equal to $14/9$. With `f` as before the additional code is given by:

```
g1 = Sqrt(1.0 + xDot*xDot);  g1x = 0.0*x;  g1xDot = xDot/Sqrt(1.0 + xDot*xDot);
```

2.7 Length constrained brachistochrone with a free endpoint. Unlike the case with both endpoints fixed, it is possible to use a straight segment as the initial curve. Let $x_0(t) = -t$ so that the fixed length is given by $\sqrt{2}$. This time the ‘natural’ boundary condition involves a Lagrange multiplier associated with the isoperimetric constraint. It is therefore in general not possible to draw conclusions about the geometry of the optimal curve at the free endpoint. In contrast, the two concerns about the endpoint and the fixed length are kept separate in the implementation. One is resolved by the choice of gradient formula, and the other is handled by the projection onto the proper tangent space.

Example 8



2.8 Multiple isoperimetric constraints. Another one of the oldest examples in the calculus of variations is the elastic curve. The problem is to minimize the elastic energy of a wire with fixed

endpoints. Since the optimal curve need not be a graph of a function it is reasonable to let the tangent angle represent the curve. It is also convenient to choose a parameter proportional to the arc-length since this circumvents the fixed length constraint. Let $x(t)$ correspond to the tangent angle and plot $t \mapsto \int_0^t (\cos(x(s)), \sin(x(s))) ds$. The elastic energy is proportional to

$$F(x) = \int_0^1 \dot{x}^2(t) dt.$$

To keep the endpoints fixed the following constraints hold

$$G_1(x) = \int_0^1 \cos(x(t)) dt, \quad G_2(x) = \int_0^1 \sin(x(t)) dt.$$

The initial tangent curve is given by $x_0(t) = 3\pi t - \pi/2$. The corresponding curve is a circle and a half. By letting the ends rotate freely, it is possible to reduce the elastic energy dramatically.

```
g1 = Cos(x); g1x = (-1.0)*Sin(x); g1xDot = 0.0*x;
g2 = Sin(x); g2x = Cos(x); g2xDot = 0.0*x;
```

This solution shows the stable configuration of a springy wire held so that the endpoints are fixed but with free tangent directions. There is no bending at the endpoints and hence the second derivative is zero. If, unlike here, the symmetry of reflection is preserved during steepest descent, then the limit curve will not be the minimal energy configuration.

2.9 Convergence criterion and computational speed. In all the examples the limit curve drawn in black corresponds to a curve where the norm of the projected gradient vector field is less than 10^{-6} . The user supplies this value along with other parameters that control the behavior of the algorithm. The number n of cubic splines carried by each S-object is one such important parameter. To measure the speed of the algorithm a method for timing generic algorithms is employed, see Chapter 19 in [Musser et al. 2001].

n	b_0	t_0	f_0	b_1	t_1	f_1	b_2	t_2	f_2
4	0.46	0.27		1.30	0.99		0.53	1.60	
8	0.56	0.36	1.33	1.70	1.33	1.34	0.65	2.14	1.34
16	1.20	0.76	2.13	3.31	2.71	2.04	1.36	4.60	2.14
32	1.66	1.15	1.50	4.88	4.13	1.52	1.84	6.93	1.51
64	2.78	2.01	1.75	8.47	7.40	1.79	3.08	12.3	1.76
128	4.81	3.60	1.79	14.9	13.6	1.84	5.21	22.6	1.83
256	8.85	7.02	1.95	28.6	27.0	1.98	9.52	43.1	1.91
512	16.9	13.4	1.90	55.6	55.6	2.06	18.2	81.8	1.90
1024	33.3	29.2	2.18	111	88.9	1.60	37.0	163	1.99
2048	66.7	58.3	2.00	250	250	2.81	71.4	429	2.63
4096	143	107	1.84	500	500	2.00	143	857	2.00

The results are split as baseline time b_i (preparation of data) and computational time t_i . The values are given in milliseconds and the index i corresponds to the number of isoperimetric

constraints. The timing is for a Sun Ultra 5 running Solaris 7 using GNU g++ version 2.95 compiled with speed optimization. The ratio $f_i \langle n \rangle = t_i \langle n \rangle / t_i \langle \frac{1}{2} \rangle$ is listed and Examples 1, 6, and 8 are tabulated as index 0, 1, and 2 respectively. The next table lists, by example, the step sizes h and the number of steps taken before the norm of the projected gradient vector is zero within the acceptable tolerance of 10^{-6} . All constraints are satisfied to at least three significant digits.

example	1	2	3	4	5	6	7	8
n	32	64	256	128	128	512	512	128
h	0.5	0.1	0.001	0.001	0.001	0.01	0.01	0.01
steps	256	64	16384	20480	40960	4096	8192	512

By combining the information in the two tables one estimates example 6 to take between $4096 \cdot t_1(512)$ and $4096 \cdot (b_1(512) + t_1(512))$ milliseconds. With $b_1(512) = t_1(512) = 55.6$ milliseconds the estimate is 4 to 8 minutes. A stopwatch trial yielded 5 minutes and 40 seconds. It is increasingly difficult to visually distinguish between curves of tolerances less than 10^{-4} , so in practice these times can often be reduced by a factor of four without a loss of geometric insight.

3. GRADIENTS

3.1 Definitions. Given a smooth (sufficiently differentiable) function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, the directional derivatives $Df \langle x \rangle : \mathbb{R}^n \rightarrow \mathbb{R}$ are linear maps represented by the matrices

$$Df \langle x \rangle = \left[\begin{array}{ccc} \frac{\partial f}{\partial x_1} \langle x \rangle & \cdots & \frac{\partial f}{\partial x_n} \langle x \rangle \end{array} \right].$$

The gradient vector field $\nabla f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is given by

$$\nabla f \langle x \rangle = \begin{bmatrix} \frac{\partial f}{\partial x_1} \langle x \rangle \\ \vdots \\ \frac{\partial f}{\partial x_n} \langle x \rangle \end{bmatrix}.$$

Let $\langle \cdot, \cdot \rangle$ represent the standard Euclidean dot product. Given any $v \in \mathbb{R}^n$ the formula for matrix multiplication shows that $Df \langle x \rangle v = \langle \nabla f \langle x \rangle, v \rangle$. This generalizes to the case $F : H \rightarrow \mathbb{R}$, where H is a Hilbert space of curves. Define the *directional derivative* $DF : H \rightarrow \mathbb{R}$ by

$$DF \langle x \rangle v = \lim_{t \rightarrow 0} \frac{F(x + tv) - F \langle x \rangle}{t}.$$

If H is equipped with the inner product $\langle \cdot, \cdot \rangle$, then the gradient ∇F is *defined* by the relationship $DF \langle x \rangle v = \langle \nabla F \langle x \rangle, v \rangle$. The existence and uniqueness of ∇F is the content of the Riesz-Fréchet Theorem [Luenberger 1969]. It is important to recognize that different choices of metrics yield different gradient vector fields.

3.2 Projected gradients. The presence of constraints invariably leads to spaces of curves that are not linear subspaces. For instance, consider the space of curves with fixed endpoints. Specifically, let H be a Hilbert space of functions defined on $[0,1]$ and let

$$X = \left\{ x \in H \mid x(0) = x_0, x(1) = x_1 \right\}.$$

X is not a linear subspace except when $x_0 = x_1 = 0$. Let $H_0 = \{x \in H \mid x(0) = x(1) = 0\}$ and observe that $X = H_0 + \bar{x}$ where $\bar{x}(t) = x_0 + t(x_1 - x_0)$. X is an example of a translated linear subspace. Suppose $F : H \rightarrow \mathbb{R}$ is smooth and let $\langle \cdot, \cdot \rangle$ be the inner product. The restriction of F to X has a projected gradient $\nabla^\pi F$ that satisfies $\langle \nabla F - \nabla^\pi F, v \rangle = 0$ for all $v \in H_0$. The gradient vector field is the tangential part of the ambient gradient vector field. In the case of isoperimetric constraints, things are more complicated since the tangent space is no longer a single fixed subspace. In either case there is a projected gradient vector field on the tangent bundle of X , i.e., the union of tangent spaces to X . The steepest descent takes place along the trajectory in X such that its velocity is always the negative of the projected gradient.

3.3 From gradient formula to code. Let the inner product be given by

$$\langle w, v \rangle = w(0)v(0) + \int_0^1 \dot{w}(t)\dot{v}(t)dt.$$

Suppose the functional is given by

$$F(x) = \int_0^1 f(t, x(t), \dot{x}(t))dt.$$

Define the Euler operator by

$$E_x^f(t) = \frac{\partial f}{\partial \dot{x}}(t, x(t), \dot{x}(t)) - \int_0^t \frac{\partial f}{\partial x}(s, x(s), \dot{x}(s))ds.$$

In the case of fixed endpoints, the gradient formula is given by [Linnér 2000]

$$\nabla F(x) = \int_0^t E_x^f(s)ds - t \int_0^1 E_x^f(s)ds.$$

The gradient clearly vanishes at both endpoints. Observe that the gradient is a function that can be expressed in terms of x and \dot{x} using operations provided by the class `S`. Assume that x is an `S`-object representing the current curve. The code corresponding to the gradient formula is given by:

```
S Euler;
Euler = fxDot - Integral(fx);
Gradient = Integral(Euler) - Identity*CompleteIntegral(Euler);
```

(Ultimately the definitions of the spline class will be placed in its own `namespace` (`Spline` say) to protect against name clashes, so `S` will be replaced by `Spline::S`, much the same way names from the standard library are prefixed by `std::`). The values of `f`, and the partial derivatives `fx` and `fxDot` are supplied by the user. The coded gradient formula exposes the central idea of the implementation: *Everything representing a point in the infinite-dimensional space must be an S-object.* The `S`-object

Identity has the property that $\text{Identity}(t) = t$ for all t . It is incorrect to replace Identity by a **double t** since this creates a gradient where the t in front of the second integral is the current value of t as the statement is executed.

3.4 Different gradients due to side conditions and choice of inner product. The implementation supports gradient formulas for free endpoints, free left-hand endpoint, free right-hand endpoint, and fixed endpoints. The inner product induces a metric in the space of curves. A change in the metric alters the gradients. The steepest descent trajectory is different. Geometric properties, such as symmetries, are preserved in some metrics but not in others. Observe that, although the gradient depends on the metric, the collection of curves where the gradient vanishes is fixed. There are also differences in the level of smoothness in the gradient formulas as the metric changes. All gradient formulas are expressed in terms of the Euler operator and the Work integral

$$W_x^f = \int_0^1 \frac{\partial f}{\partial x}(t, x(t), \dot{x}(t)) dt.$$

3.5 Examples with fixed endpoints. The most common type of constraints is to fix one or both of the endpoints. Computationally these constraints are easier to deal with than the unconstrained case. This is due to the fact that the explicitly known gradient formulas are simpler in this case. For instance, if both endpoints are fixed, then the corresponding gradients are given by

$$\begin{aligned} \nabla_I^\pi F(x) &= \int_0^t E_x^f(s) ds - t \int_0^1 E_x^f(s) ds \\ \nabla_{II}^\pi F(x) &= \int_0^t E_x^f(s) \cosh(t-s) ds - \frac{\sinh(t)}{\sinh(1)} \int_0^1 E_x^f(s) \cosh(b-s) dt \\ \nabla_{III}^\pi F(x) &= \begin{cases} \int_0^t E_x^f(s) ds - \frac{t}{(1+p)(2-p)-1} \int_0^1 E_x^f(s) ds & 0 \leq t \leq p \\ \int_0^t E_x^f(s) ds - \frac{(1+p)(1+t-p)-1}{(1+p)(2-p)-1} \int_0^1 E_x^f(s) ds & p \leq t \leq 1 \end{cases} \end{aligned}$$

Here the subscript refers to the metric. The superscript indicates that this is the projected gradient. The three metrics are given by

$$\begin{aligned} \langle w, v \rangle_I &= w(0)v(0) + \int_0^1 \dot{w}(t)\dot{v}(t) dt, \\ \langle w, v \rangle_{II} &= \int_0^1 w(t)v(t) dt + \int_0^1 \dot{w}(t)\dot{v}(t) dt, \end{aligned}$$

and

$$\langle w, v \rangle_{III} = w(p)v(p) + \int_0^1 \dot{w}(t)\dot{v}(t) dt.$$

The gradients are given in a form where it is obvious that they vanish at the endpoints. Another

noteworthy property is the absence of the work integral. The third metric is included here to illustrate how, when $0 < p < 1$, the gradient is less smooth than when using either of the first two metrics.

3.6 Examples with free right-hand endpoint. To see examples where the work integral is present, consider the case of a free right-hand endpoint so the projection has changed. The first two metrics yield

$$\nabla_I^{\pi,0} F(x) = \int_0^t E_x^f(s) ds + W_x^f t,$$

and

$$\nabla_{II}^{\pi,0} F(x) = \int_0^t E_x^f(s) \cosh(t-s) ds + \left(W_x^f - \int_0^1 E_x^f(s) \sinh(b-s) ds \right) \frac{\sinh(t)}{\cosh(1)}.$$

It is clear that the gradients vanish at the left-hand endpoint, but not necessarily at the right-hand endpoint. Here a second superscript indicates that only the right-hand endpoint is fixed.

3.7 Isoperimetric Constraints. Recall that the case of fixed endpoints generated translated linear subspaces and the need for an orthogonal projection to compute the gradient vector field. The tangent space to a translated linear subspace is the linear subspace itself. Isoperimetric constraints $G : H \rightarrow \mathbb{R}$ defined in a Hilbert space H are more complicated since they generate tangent spaces that vary from point to point. Since $G(x) = 0$ for each x that satisfies the isoperimetric constraint G , it must be that the directional derivative satisfies $DG(x)v = 0$ for all tangential v , and the familiar $\langle \nabla G(x), v \rangle = 0$ holds. Now consider $F : H \rightarrow \mathbb{R}$ and its gradient vector field. The idea is to introduce a scalar field $\lambda(x)$ and express the tangential component $\nabla^\pi F$ as $\nabla^\pi F(x) = \nabla F(x) - \lambda(x) \nabla G(x)$. The condition $DG(x)v = 0$ leads to

$$\lambda(x) = \frac{DG(x) \nabla F(x)}{DG(x) \nabla G(x)}.$$

For this approach to work it is necessary to assume that $\nabla G(x) \neq 0$ for all x such that $G(x) = c$. This assumption is referred to as *regularity*.

3.8 Multiple isoperimetric constraints. Suppose a finite number of isoperimetric constraints $G_i : H \rightarrow \mathbb{R}$ are invoked. Each x of interest satisfies $G_i(x) = 0$ for $i \in \{1, \dots, n\}$. This time the projected gradient is given by

$$\nabla^\pi F(x) = \nabla F(x) - \sum_{i=1}^n \lambda_i(x) \nabla G_i(x),$$

where each λ_i is a scalar field. The additional difficulty when $n > 1$ is the necessity to solve the linear system

$$\begin{bmatrix} DG_1 \nabla G_1(x) & \cdots & DG_1 \nabla G_n(x) \\ \vdots & \ddots & \vdots \\ DG_n \nabla G_1(x) & \cdots & DG_n \nabla G_n(x) \end{bmatrix} \begin{bmatrix} \lambda_1(x) \\ \vdots \\ \lambda_n(x) \end{bmatrix} = \begin{bmatrix} DG_1 \nabla F(x) \\ \vdots \\ DG_n \nabla F(x) \end{bmatrix}.$$

For this system to have a unique solution it is not enough for each constraint to be regular. It must be assumed that the matrix is invertible at each x such that $G_i(x) = 0$ for all $i \in \{1, \dots, n\}$. Geometrically this corresponds to transversal intersections and the dimension of the space normal to the tangent space is at each point equal to n .

4. IMPLEMENTATION

4.1 The spline class. In this section the code is dissected and the different techniques used in the implementation are highlighted. Objects of the `class S` represent the curves and the gradients. `S` is given by the following `C++` code. Reserved words are in bold. Names from either the standard library or the boost extension are in italic.

```

#include "operators.hpp" //boost extension
#include <vector>
#include <string>
#include <functional>
class FunctionObject; //Forward declaration
class S : private boost::addable<S>, boost::addable<S,double>,
             boost::subtractable<S>, boost::subtractable<S,double>,
             boost::multipliable<S>, boost::multipliable<S,double>,
             boost::dividable<S>, boost::dividable<S,double>
{public: friend FunctionObject;
        S(std::vector<double>, std::vector<double>);
        double operator()(double);
        void Show() const; void Save(const std::string&) const;
        S& operator+=(const S&); S& operator+=(const double&);
        S& operator-=(const S&); S& operator-=(const double&);
        S& operator*=(const S&); S& operator*=(const double&);
        S& operator/=(const S&); S& operator/=(const double&);
        S Integral(double) const; S Derivative() const;
private: std::vector<double> m_p, m_v, m_vdotdot;};

class FunctionObject : public std::unary_function<double,double>
{public: FunctionObject(double (*)(double));
        double operator()(double) const;
        S operator()(const S&) const;
private: double (*m_f)(double);};

```

A reader unfamiliar with `C++` may think of a `S` as an example of a user-defined type like the built-in `double`. Unlike built-in types, a user-defined type must supply functions to control creation and manipulation of its objects. The boost extension to the standard library will leverage these functions and restore some of the functionality available to built-in types. Here the extension uses the eight user-supplied member operators to define almost all the standard algebraic operations. As an example look at the boost extension's `addable` class which permits the compiler to properly interpret the plus in expressions like $x*x + x\text{Dot}*x\text{Dot}$:

```

template<class T>
class addable
{ friend T operator+(T x, const T& y) {return x += y;} };

```

The `class S` has three `private` data members stored as dynamically allocated vectors based on the built-in type `double`. To create an object of `class S` representing a function x , it suffices to supply a discrete set of parameters p_i and the corresponding values $v_i = x(p_i)$. The second derivative of the cubic spline, passing through the points (p_i, v_i) in order, is automatically computed and saved in the third data member. To illustrate this consider how the `Identity` object is created and the initial `x`.

```

//Sample points
double* p;
p = new double[NumberOfCubicPolynomials + 1];
//Uniform sample
for(unsigned int i = 0; i <= NumberOfCubicPolynomials; ++i) p[i] = double(i)/NumberOfCubicPolynomials;
//Initialize a standard vector
const std::vector Points(p,p + NumberOfCubicPolynomials + 1);
//Clean-up
delete[] p;
//Base S-object
S Identity = S(Points,Points);
//FunctionObject created from initial curve
FunctionObject Initial(initial);
//S-object corresponding to initial curve
S x = Initial(Identity);
S xDot = Derivative(x);

```

Armed with its three data members, `S` has member functions to compute objects of `class S` corresponding to the derivative as well as the integral operation. The `S class` is also equipped with an evaluation `operator`. This method calls a cubic spline routine to calculate the value. There is a `friend class FunctionObject` to facilitate composition with functions. Specifically, if `s` is an object of `class S`, then `s(0.3)` returns the value of `s` at 0.3. Moreover, if `f` is an object of the `FunctionObject class`, then `f(s)` is an object of the `S class` so in terms of the composition operation \circ , $f \circ s \langle 0.3 \rangle = f \circ s \langle 0.3 \rangle$.

4.2 Cubic splines. The cubic spline routines are based on the code given in *Numerical Recipes in C* [Press et al. 1992]. The main difference is the use of *vectors* from the standard library rather than the built-in arrays. This renders the use of memory allocation routines in the Recipes obsolete. The calling interface is simplified since there is no need to pass the dimension of the vectors to each routine. To this end, the implementation uses the `size()` member function from `<vector>`. In addition, the implementation supplies two extensions to the cubic spline recipes. The first computes the value of the derivative of the spline. The second computes the value of the

integral with a supplied initial value to facilitate piecewise integration. To retain notational compatibility with the code in the recipes, this part of the code uses indices and array notation.

```

double SplineDerivativeValue(std::vector<double>& x, std::vector<double>& y,
                             std::vector<double>& yDotDot, double t)
{int klo=0, khi = x.size() - 1,k;
while( khi-klo > 1 )
    {k=(khi+klo) >> 1;
      if(x[k] > t) khi=k; else klo=k;}
double h,a,b;
h = x[khi]-x[klo];
a = (x[khi]-t)/h;
b = (t-x[klo])/h;
return (y[khi]-y[klo])/h + ((1.0 - 3.0*a*a)*yDotDot[klo] + (3.0*b*b - 1.0)*yDotDot[khi])*h/6.0;}

double SplineIntegralValue(std::vector<double>& x, std::vector<double>& y,
                            std::vector<double>& yDotDot, double t)
{int klo=0, khi = x.size() - 1, k;
while( khi-klo > 1 )
    {k=(khi+klo) >> 1;
      if(x[k] >= t) khi=k;else klo=k;}
double h,a,b;
h = x[khi]-x[klo];
a = (x[khi]-t)/h;
b = (t-x[klo])/h;
return (b*b*y[khi] + (1.0 - a*a)*y[klo])*h/2.0 +
        ((2.0*a*a - a*a*a*a - 1.0)*yDotDot[klo] + (b*b*b*b - 2.0*b*b)*yDotDot[khi])*h*h/24.0;}

```

The Spline routine in the recipes updates the second derivative vector. The derivative and integral S member functions are given by the following code.

```

S S::Derivative() const
{S New(*this), Old(*this);
 std::vector<double>::const_iterator pIterator = Old.m_p.begin();
 std::vector<double>::iterator vIterator = New.m_v.begin();
while( pIterator != Old.m_p.end() )
    *vIterator++ = SplineDerivativeValue(Old.m_p,Old.m_v,Old.m_vdotdot,*pIterator++);
Spline(New.m_p,New.m_v,New.m_vdotdot);
return New;}

S S::Integral(double InitialValue) const
{S New(*this), Old(*this);
 std::vector<double>::const_iterator pIterator = Old.m_p.begin();
 std::vector<double>::iterator vIterator = New.m_v.begin();
*vIterator++ = InitialValue;
++pIterator;
while( pIterator != Old.m_p.end() )
    *vIterator++ = SplineIntegralValue(Old.m_p,Old.m_v,Old.m_vdotdot,*pIterator++);
std::partial_sum(New.m_v.begin(),New.m_v.end(),New.m_v.begin());

```

```
Spline(New.m_p,New.m_v,New.m_vdotdot);
return New;}
```

Note how the standard library's generic algorithm `std::partial_sum` in `<numeric>` is very helpful here. It is interesting to compare the index-free coding style of the last two functions and the pre-standard-template-library style of the Recipes code. The C++ standards committee exhibited considerable leadership when it decided to incorporate most of the standard template library [Stepanov et al. 1995] into the standard library. To further conform to standard mathematical notation it is useful to define four global functions.

```
S operator-(const double& x, const S& y) {return (-1.0)*(y-x);}
S Integral(const S& x){return x.Integral(0.0);}
double CompleteIntegral(const S& x){return x.Integral(0.0)(1.0);}
S Derivative(const S& x){return x.Derivative();}
```

In what follows the cubic splines are shielded from the rest of the implementation, and any collection that provides the same functionality could take the place of the cubic splines.

4.3 FunctionObject. The implementation of composition in the `FunctionObject` class is given by the following code.

```
double FunctionObject::operator()(double t) const {return m_f(t);}
S FunctionObject::operator()(const S& x) const
{S result(x);
std::transform(x.m_v.begin(),x.m_v.end(),result.m_v.begin(),*this);
Spline(result.m_p, result.m_v, result.m_vdotdot);
return result;}
```

A `FunctionObject` is equipped with one 'evaluation operator' and one 'composition operator'. The composition operator uses the evaluation operator through self-reference inside the generic algorithm `std::transform`. The abstraction built-in to the standard template library is here paying great dividend.

4.4 Steepest descent. The most basic way of implementing steepest descent is with the help of Euler's method. The curve is represented by an object `x` of class `S` and the gradient at `x` by the `S`-object `Gradient`. The initial curve is represented by the `S`-object `x0`. The step size is given by a `double h`.

```
S x = x0, xDot, Gradient;
xDot = Derivative(x); //Start of the Euler step
ProjectedGradient = ...
x -= h*ProjectedGradient; //End of the Euler step
```

The value of the functional is lower at this new `x` compared to `x0`. To lower the value further, repeat the Euler step.

5. CONCLUSIONS.

About a decade ago, while working on implementations of infinite-dimensional problems, it became clear to the author that it is necessary to bridge the notational gap between the mathematical formulas and the corresponding computer code. Back then, the coding of sophisticated mathematical formulas and the demand for performance yielded very frail and difficult to extend programs. The emergence of \mathbf{C}^{++} and the standard template library has changed all of this. As this article demonstrates, it is now possible to write code where the notational gap between the mathematical formulas and the computer code has all but disappeared. Significantly, this does not come with severe, or even noticeable, performance degradation. Moreover, the code here is easily extended to cover more than two isoperimetric constraints, or more than one metric. It is also designed to be user-friendly in the sense that next to no knowledge of \mathbf{C}^{++} is required to add code for new examples. All that is needed is a straightforward translation of the mathematical expressions corresponding to the integrand of each functional involved and its partial derivatives. The complete software package is available for download at:

<http://www.math.niu.edu/~alinner/Software/CoV00/>

Testing has been done in UNIX Solaris 7 and Windows 98 Second edition using GNU g++ version 2.95 and Borland C++ Builder 4.0, respectively. One reasonable approach to improve the performance of the software is to combine the Euler step with Adams-Bashforth's method and invoke higher order formulas as soon as enough points are calculated. As seen in Section 2.9, the subsequent freedom to aggressively increase the step size is desirable. In the context of 'critical curves at infinity' this feature is essential. Examples of this, using a completely different implementation, are given in [Linnér 2001]. The current implementation avoids all but the most basic numerical methods to showcase the strengths of the underlying gradient formulas as well as the power of \mathbf{C}^{++} and the standard library.

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