A model for engaging students in a research experience involving variational techniques, *Mathematica*, and descent methods

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ABSTRACT:

We describe a two-semester numerical methods course that serves as a research experience for undergraduates without requiring external funding or modification of current curriculum. The first semester introduces traditional material and builds a proper set of tools that the students use in the second semester to approach a more research oriented problem. Our vehicle is an engineering problem associated with the hydro-dynamics of keel design which is used to introduce students to constrained optimization via a variation of the traditional isoperimetric problem of finding the curve with fixed endpoints, fixed perimeter, and maximum area.

KEYWORDS: arc-length, isoperimetric, mathematica, optimization, REU, variational

1 Introduction

Research experiences for undergraduates (REU's) are receiving considerable attention as a means to engage students in *doing* mathematics prior to graduation. Regarding the teaching of mathematics, Halmos [4] states, "We all say, we're doing mathematics. And I think what it means, what it should mean for students, is the same thing. I think students should do research, in their subject, at their level." In a review of funded REU's, the National Science Foundation [10] finds, "... (the) program helped uncertain students to clarify their preferences regarding graduate school attendance, field of specialization, and career path; and the program bolstered the certainty of highly interested students about their initial decisions in these areas." Sufficient evidence exists that REU's have a positive impact on students to warrant implementation of such experiences into current curricula. What follows is a model for doing so in a numerical methods course that introduces students to applied research without requiring external support or modifying the current curriculum.

This is accomplished by choosing a research topic or problem and developing a streamlined course that covers the background necessary to bring students to the research level on this specific topic. In order that such a course fit within standard curricula it should mesh with current departmental courses and needs. Thus in our case, the 'necessary background' has significant intersection with a traditional numerical methods course, if being perhaps less exhaustive on certain subjects while adding additional substance to others. The problem we consider in this paper is an engineering problem associated with the hydro-dynamics of keel design. This problem is used as a vehicle to introduce students to constrained optimization via a variation of the traditional isoperimetric problem of finding the curve with fixed endpoints, fixed perimeter, and maximum area. Variational methods, *Mathematica*, and descent methods are all employed in our investigation and exercises are posed throughout the paper to give a small sampling of the type of problems that our students solve and present. The course also gives students a glimpse of the consulting process whereby an engineering problem is given, translated to a mathematical problem, investigated via numerical and theoretical techniques, and then communicated back to the firm. Because of its research nature and content, the course has served as a spring board for several students to pursue directed studies on other applied optimization problems.

2 The Course

We first address the setting in which we have introduced such material. Nicholls State University is an open enrollment university where the mathematics majors have an average ACT under twenty five. The students we serve are typically first generation college students and we nurture them through small classes with a personal touch. The mathematics department offers a five-year BS/MS program that allows undergraduates to take a maximum of six hours of graduate study during their senior year. It is within this dual credit setting that we have had the opportunity to introduce this material at the undergraduate level. We emphasize the value of courses with both an undergraduate and a graduate component. The undergraduates are often the stronger students because they are fresh on the basics, while the graduate students come to the course ready to work. The blend benefits both groups as well as providing a natural funnel for our graduate program by supplying confident undergraduates. The course structure is carefully outlined in [7, p.132-135] and a condensed description follows.

The first semester of this two-semester course is a combination of weekly programming assignments and carefully developed problems that the students work and present at the board. The times I present (perhaps half of total class time) are on the rare occasions when students have nothing to present, when I am providing an overview of material, or when I am addressing how the theory they have developed is to be used in a programming assignment to solve a problem numerically. The theory that is developed during the first semester is carefully selected and streamlined to prepare them for a research project during the second semester. The programming projects that are assigned depend upon the problems that have been presented. The results of these assignments are written up as "industry-quality briefings" and are graded as if I am their supervisor. "Imagine that I must brief my supervisor thirty minutes after you, my employee, hand me your paper. You will get an 'A' for the paper if without prior knowledge of the problem, I can read it, understand it, and am prepared for the briefing." In the beginning of the semester, I write extensive comments designed to improve future projects. While this process is particularly time consuming in the beginning, by mid-semester, students are writing technical reports complete with introduction, problem description, necessary theory, conditions for success, sample computations, solution, validation of solutions, and conclusions. By semester's end, the students have written codes to solve minimization problems, small and large linear systems, and a variety of differential equations. They have worked through a development of the theory associated with inner product spaces, convergence of iterative techniques, and projections. A proof of the Reisz Representation Theorem in finite dimensions is the theoretical capstone of the first semester.

At the beginning of the second semester, they are well suited to handle elementary research projects in the area of numerical differential equations and this semester is devoted to a research problem such as the one described in this paper. With the more complex subjects, I describe the material, assigning problems for presentation that yield an understanding of the fundamental mathematics behind the project. The programming assignments are fewer, but more lengthy, and utilize as subroutines the codes they wrote during the first semester.

The course is constructed to meet the following goals for both a numerical methods course and an undergraduate research experience. A significant amount of non-trivial mathematics is introduced and students prove much of this on their own. Students develop both oral and written communication skills via presentation in class and written briefings. Students are introduced to both classical mathematics and modern computational approaches. Lastly, some of the mathematics addressed is *not* part of the traditional undergraduate curriculum so that the students leave with an understanding of an area of mathematical research that other faculty and prospective employers may not be familiar with. This last feature is especially important as it gives the students an edge when they seek out graduate programs or industrial employment.

3 Grading, A Day in Class, and Content

Each student's grade is the average of three grades: the average of all programming assignments (briefings), the average of the midterm and final, and the presentation grade. The programming is done outside of class and students may write in the language of their choice. I have seen solutions in BASIC, C, C++, Excel, FORTRAN, Java, Maple, Mathematica, and Pascal. The midterm and final are basic review of the definitions and theorems, implementation of algorithms, and verification of criteria for success of the algorithms. The presentation grade is subjective and depends on discussions in class, the number of presentations, and the quality of presentations. To make this a pleasant experience, every time they present at the board, regardless of whether they have a complete solution or not, they get positive credit toward that portion of the grade. When a student makes a mistake, they may choose to fix it on the fly, to take it home and present it next time, or to turn to the class for help. I am flexible and yield to the preference of the student at the board. Students with the least number of presentations are chosen first when multiple solutions are offered. Presentations are shaky and time consuming at the beginning of the semester, but improve rapidly to the point that later presentations rival that of any instructor. Some problems in the sequence are as elementary as computing by hand Eigenvalues for a matrix that they will later write a code to find. Other problems are as advanced as proving a case of the Cauchy-Schwartz-Bunakowski theorem. The range in the level of difficulty of the problems assures that every student can present and that every student will have some problem that challenges him.

The atmosphere in the classroom is very important and I strive to create an atmosphere of questions, discussion, and problem posing by the students. Students openly make suggestions and comments regarding my notes, correcting mistakes(!), suggesting additional problems on a given topic, or seeking additional information on the subject. As an example, we are often working with finite dimensional vector spaces that have as their counter part function spaces and we often discuss this relationship. Thus, we might discuss how the standard dot product is the finite dimensional representation of the inner product defined by the integral of the product of two functions. A student with some extra analysis under his belt might even offer a proof that this does indeed define an inner product. While I don't hold them responsible for such notions and certainly don't treat function spaces with anything close to rigor, I do try to give them an idea of where this mathematics fits into a larger picture. On occasion, the students will get some relief as a detailed mathematical discussion may postpone a programming assignment. In these cases, the students feel they have pulled the wool over the professor's eyes and may even try to have more mathematical discussions to delay future programming assignments or presentations. Of course, I am happy to be the object of their clever tactics since the discussions are where students may pose interesting problems or may get a better feel for the subject.

Each day in the classroom follows the same format. Students first present and discuss the problems they have solved since the previous class. They may choose to work together as long as they let me know that the work they are presenting is joint work. The problems come from my own notes (rough, always changing, and available upon request) and from the text [1]. We start the first semester with fairly straightforward material such as the bisection method or the golden search in an effort to build confidence in presentations and to begin developing the writing skills. If on a given day we exhaust all the problems students have solved, then after the presentations I will comment on the next topics and problems from the notes to assure that we will have material to present at the next class period. If there are outstanding problems ready for presentation at the next class meeting, I will discuss the next weekly programming assignment. Starting on very elementary material gives time for the students to hone (relearn?) their programming skills and to develop their own style of writing up the results. There will be adequate difficult material as the semester progresses. It is my goal to instill in them a sense of security at the beginning in order that I may have their confidence and may push them harder toward the end. This is not a linear learning model where material is covered at an equal pace throughout the two semesters – we start slow, build their confidence in presentation, programming, and writing and then drive them faster at the end. Because the course is one that is (most likely) different in structure from previous courses, it is important to build this trust in the beginning.

The material discussed in the remainder of the paper is material from the latter half of the second semester after students have already mastered a reasonable amount of mathematics and numerical methods. The list in the next paragraph was prepared by a student asking me if she had missed anything in preparing for the comprehensive final at the end of the second semester. While the list is surely not complete, it does give a flavor of where we start during the first semester (the bisection method) and where we end during the second semester (differencing for classic partial differential equations). Depending on the class strength, I freely omit or minimize certain topics to be sure there is sufficient time to address a research problem such as the one in this paper.

Topics: bisection method, strictly unimodal, convex, concave, golden search,

Figure 1 - Keel Bulb

gradients, relative maxima and minima in several dimensions, directional derivatives, Euclidean steepest descent, vector spaces, inner products, norms, normed spaces, inner product spaces, equivalent norms, spectral radius of a matrix, positive definite, eigenvalues, Gaussian elimination, Jacobi's method, Gauss-Seidel, diagonally dominant, one-to-one and onto, subspace of a vector space, projections, Euler's method, Taylors's method, Runge-Kutta, Sobolev descent for differential equations, Lagrange interpolation, divided differences, cubic splines, numerical integration, Crank-Nicolson, Rayleigh-Ritz, divided differences and the heat equation.

4 The Problem

The problem we investigated during the second semester last year came from an engineering firm and arose from the hydro-dynamic properties of keel design. The firm desired to design a bulb for a keel (see *Figure 1*) with specific properties for the two-dimensional cross-sectional shapes obtained by slicing the keel perpendicular to the length of the boat. Now, we restrict our attention to one cross-sectional piece. For that piece, the firm will assign an area, A, and we are to discern the shape for that cross section satisfying the following criteria:

i. the area is A,

ii. the width of the shape is twice the height, and

iii. the perimeter of the shape is minimal.

The firm would then apply our technique to multiple cross-sections and build the bulb. This example is representative of how problems from industry are often stated; clearly it is a mathematical problem, but no function is stated, no equation given. Our first goal is to reduce the two-dimensional problem to a mathematical statement that is tractable and whose solution is relevant to the original problem once solved. The following statement was our suggestion to the firm for a first cut at solving the problem.

Problem 1 *Given an area A, find a continuously differentiable function f defined on the closed interval $[0,1]$ satisfying $f(0) = 1/2, f(1) = 0$, and having minimal arc length.*

Suppose $A = 1/4$. Then the line, $l(x) = -\frac{1}{2}x + \frac{1}{2}$, satisfies *Problem* 1. For an arbitrary area, A, we would not expect a linear solution, although our curve would lie in the first quadrant. We would then construct the desired cross section

Figure 2 - Reflections

(see *Figure 2*) by first reflecting the curve about the y-axis to obtain a function defined on all of $[-1, 1]$. Then we would reflect this extended curve (defined on $[-1, 1]$) about the x-axis. This would result in the desired cross section with area, $4A$, width that was twice its height, and minimal perimeter. The students see what we do as applied mathematicians; we mold a vague problem into a context that we are familiar with, has a solution that can be readily discovered, and is of value to the poser of the question. We have molded the applied problem into a mathematical one that will be the basis of the students' research experience and will be studied via classical and modern mathematical methods.

5 Theoretical Considerations

Consider first our notation. By $\mathbf{C^2}$ we mean the class of twice continuously differentiable functions on $[0, 1]$, that is, the set of all functions f with domain

$[0, 1]$ such that each of f, f', and f'' are defined and continuous on $[0, 1]$. By an **operator** we mean a function whose domain is C^2 (or $C^2 \times C^2$) and whose range is some subset of the set of all functions defined on $[0, 1]$. By a **functional** we mean any function whose range is a subset of $\Re$, the real numbers.

The problem described is referred to as a **constrained optimization** problem and such problems arise frequently in applied fields. It is an *optimization* problem because we seek a function whose arc length is minimal, hence we seek an *optimal* value for the functional, $I(u) = \int_0^1 \sqrt{1 + u'^2}\, du$. It is *constrained* by the equation $J(u) = \int_0^1 u\ du = A$, specifying the area, and by the boundary conditions, $u(0) = 1/2$ and $u(1) = 0$.

Such problems are often addressed using variational methods [2, p.117-127], [13, p.118]. We first cover some background so that we may apply a theorem in this field. Given an operator, L, which has u and u' as its independent variables, for example $L(u, u') = u^3 + (u')^2$, the Euler equation [3, p.185] associated with L is the ordinary differential equation given by $\frac{\partial}{\partial x}(L_{u'}) - L_u = 0$ where L_u and $L_{u'}$ denote the partial of L with respect to u and u' respectively. For our example: $L_u(u, u') = 3u^2$, $L_{u'}(u, u') = 2u'$, and $\frac{\partial}{\partial x}(L_{u'}) = 2u''$. Thus, the Euler equation associated with L is the second-order, nonlinear, ordinary differential equation, $2u'' - 3u^2 = 0$. Here we state the result needed to solve our problem.

Theorem 2 *[12], [13, p.318] If each of F and G are operators then necessary* *conditions for* C^2 *solutions to problems of the form*

$$\begin{aligned}&\textit{Minimize } I(u) = \textstyle\int_a^b F(u)\,du\\&\textit{subject to } J(u) = \textstyle\int_a^b G(u)\,du = A = \textit{constant}\\&\textit{and } u(a) = \alpha, u(b) = \beta\end{aligned} \tag{1}$$

may be found by solving the Euler equation associated with $L = F + \lambda G$ *where* λ *is an unknown constant to be determined from the constraints.*

If $\lambda \in \Re,\ F(u) = \sqrt{1 + (u')^2},\ G(u) = u$, and $L(u) = F(u) + \lambda G(u)$ for all $u \in C^2$ then our problem satisfies the hypothesis of the theorem and we need only solve the Euler equation associated with L to determine necessary conditions for a C^2 solution.

Exercise 3 *Compute the Euler equation associated with* $L = F + \lambda G$ *where* $F(u) = \sqrt{1 + (u')^2}$, $G(u) = u$, $a = 0$, $b = 1$, $\alpha = \frac{1}{2}$, *and* $\beta = 0$ *to obtain,*

$$\frac{u''}{(1 + (u')^2)^{3/2}} = -\lambda. \tag{2}$$

The expression on the left side of the equal sign represents the curvature of the function u, [15, p.582-586]. The next exercise shows that the only functions with constant curvature are lines and portions of circles.

Exercise 4 *Show that any* C^2 *function satisfying Equation 2 must be either a line or a portion of a circle. Hint: Consider the substitution* $u'(\theta) = tan(\theta)$.

These two exercises indicate that any C^2 solutions will be a line or a portion of a circle. As shown earlier, $A = 1/4$, results in a linear solution (or a diamond for the entire cross-section after reflection about both axes). For $A < 1/4$, solutions will be concave up and such solutions are undesirable when hydro-dynamics are considered, so we restrict our attention to the case $A > 1/4$.

One of the features we desire in our REU is an exposure to both the classical mathematics and the use of modern computational techniques. Having addressed some classical theory, in the next section we turn to *Mathematica* for aid in finding solutions based on this classical theory.

6 Circular Solutions for $A > \frac{1}{4}$

For circular solutions, we may write down a system of three equations that determine the solution. Assuming the circle has center (a, b) and radius r, the equation of the circle will be $(x-a)^2 + (y-b)^2 = r^2$ and applying the boundary conditions and area constraint we have,

$$\begin{aligned} &a^2 + (\tfrac{1}{2} - b)^2 = r^2, \\ &(1-a)^2 + b^2 = r^2, \text{ and} \\ &\textstyle\int_0^1 \sqrt{r^2 - (x-a)^2}\, dx + b = A. \end{aligned} \tag{3}$$

At first glance, these equations look innocent enough; there are three equations and three unknowns, a, b, and r. Unfortunately, the last is an integral equation and thus it is not clear how to solve these equations in closed form or even if they have a unique solution.

Exercise 5 *By eliminating b and r, reduce these three equations to one equation*

Figure 3 - Circular Solutions for $A \approx .53$ and $A = 1$

in a yielding,

$$\int_0^1 \sqrt{\frac{5}{16}(5 - 16a + 16a^2) - (x-a)^2}\, dx + (2a - \frac{3}{4}) - A = 0. \tag{4}$$

Solving this equation would allow us to recover b, r, and thus the solution. When we ask our students how they will solve such an equation, each points to their TI's, HP's, or laptops. Hence, this is exactly what we do. But first, we assign the next exercise which indicates existence of a solution for $A > \frac{1}{4}$.

Exercise 6 *Let $f(a) = \int_0^1 \sqrt{\frac{5}{16}(5 - 16a + 16a^2) - (x-a)^2}\, dx + (2a - \frac{3}{4})$. Graph f using Mathematica to see that f is monotonically increasing, $\lim_{a \to -\infty} f(a) = \frac{1}{4}$, and $\lim_{a \to \infty} f(a) = \infty$, thus implying that we have a unique solution for values of $A > \frac{1}{4}$.*

The code in the Appendix (written by a student) takes a given area, A, locates a root of *Equation 4*, recovers b, recovers r, and plots the circle with radius r centered at (a, b). *Figure 3* shows the results from this code for $A \approx .53$ and $A = 1$. From these solutions, we observe two limitations to our methodology.

First, depending on the area, A, such solutions may, upon reflection, generate a cross section with cusps at $(0, \pm\frac{1}{2})$ and $(\pm 1, 0)$ which have undesirable hydrodynamic characteristics. Second, as we generate circular solutions for varying values of A, there is a value for the area, call it A^*, such that the circle generated for this value of A will have a vertical tangent at $(1, 0)$. In *Exercise* 7 we will see that $A^* \approx .53$. For $A > A^*$ any circle generated in this manner will intersect the line $x = 1$ twice. Thus, for values of $A \geq A^*$ the circles generated by applying Theorem 2 in this manner are either not differentiable on the interval or are not functions, and thus they are not solutions to the original problem.

At this point in the class, students have generated solutions for a wide range of inputs A, using various technologies and codes they have written. Upon reflection some solutions are almost smooth, having horizontal tangents at $(0, \frac{1}{2})$, and thus have 'nice' reflections – some are not. We discuss these solutions and ask if they satisfy the original problem in spirit. Are the problems with the solution serious? Do we need to reassess our original translation of the applied problem? These considerations lead us to add the constraint of a horizontal tangent at $(0, \frac{1}{2})$. That is, we need $y'(0) = 0$ for physically admissible solutions. To eliminate concave up solutions and vertical tangents at $(1, 0)$, we also restrict our attention to $\frac{1}{4} < A < A^*$. The last problem in this section enables us to compute the value of A^*, the value of A for which the circular solution has a vertical tangent at $(1, 0)$.

Exercise 7 *Show that when the (circular) solution has a vertical tangent at*

$(1,0)$*, the center of the circle must be the intersection of the x-axis and the line* $y = 2x - \frac{3}{4}$*. Use this information to see that* $A^* = \frac{25}{256}\pi + \frac{3}{32} + \frac{25}{128}Arcsin(\frac{3}{5}) \approx .53$*.*

Students now have seen a classical approach to the problem implemented using *Mathematica.* Because we cannot address the additional constraint with this theory, we turn to a numerical treatment of the problem and add numerical methods to the research experience.

7 Numerical Considerations for Non-circular Solutions ($\frac{1}{4} < A < A^*$)

The numerical capstone of the first semester was the ability to approximate solutions to differential equations via steepest descent in Euclidean spaces, while the theoretical capstone was the Reisz Representation Theorem for finite dimensional spaces relating inner-products and linear functionals. Both results are necessary to build the algorithms developed in the second semester. This duality between the numerical and theoretical is an important point of education for the students. So often, we hear students who 'don't like the theory, only the applied mathematics.' Here, students have seen the need for pure mathematics in order to solve applied problems, allowing an opportunity for us to stress the need for deep mathematical understanding of the pure mathematics in order to be effective applied mathematicians. The capstone of the second semester is the implementation of the algorithm to solve this 'real-world' problem and utilizes both the theory and the numerical methods developed during the first semester including: Golden search, successive-over-relaxation, differentiation techniques, integration techniques, and descent algorithms.

While there are many optimization techniques capable of solving our problem, Sobolev descent is chosen as it is especially forgiving when one encounters large derivatives such as are likely to occur at the right boundary in this problem. Thorough introductory information on steepest descent and optimization may be found in [1, p.568], [5], [11], or [14]. The material that follows is introduced to and presented by the students in the classroom as described in the earlier sections. While the notation may at first glance appear overwhelming, mathematically, all that is required is an understanding (in finite dimensions) of gradients, inner products, norms, projections, and linear operators, making this an ideal transition between the typical sophomore linear algebra course and the typical first course in functional analysis. This is a key feature in choosing a project – that one can start with materials students have previous experience with and build on that success.

Fix n to be the number of equal subdivisions of the interval $[0, 1]$ and $\delta = 1/n$ to be the width of these divisions. Let $(\Re^{n+1}, \langle \cdot, \cdot \rangle)$ represent Euclidean space where $\langle \cdot, \cdot \rangle$ is the usual dot product and $\mathbf{x} \in \Re^{n+1}$ is denoted by $\mathbf{x} = (x_1, \ldots, x_{n+1})$. We consider $\mathbf{x}$ as the set of values of a function f over a set of points in $[0, 1]$. Thus, $x_i = f(\frac{i-1}{n})$ for $i = 1, 2, \ldots, n + 1$.

Define discrete versions of the identity and derivative operators, $D_0,\, D_1 : \Re^{n+1} \to \Re^n$, where

$$D_0(\mathbf{x}) = \begin{pmatrix} \frac{x_1+x_2}{2} \\ \vdots \\ \frac{x_n+x_{n+1}}{2} \end{pmatrix} \quad \text{and} \quad D_1(\mathbf{x}) = \begin{pmatrix} \frac{x_2-x_1}{\delta} \\ \vdots \\ \frac{x_{n+1}-x_n}{\delta} \end{pmatrix}.$$

Then $D_0(\mathbf{x})$ is a sequence of approximations to the value of f at the n midpoints of the intervals in the partition of $[0, 1]$ and $D_1(\mathbf{x})$ is an approximation to the derivative of f at those same points.

Exercise 8 *Write a matrix representation for each of D_0 and D_1.*

We define a subset, called a perturbation space, of $\Re^{n+1}$ by

$$\Re_0^{n+1} = \{\mathbf{x} \in \Re^{n+1} : x_1 = x_{n+1} = 0, \text{ and } \sum_2^n x_i = 0\}.$$

This subspace is the collection of vectors representing functions that are zero on the boundaries (endpoints of $[0, 1]$) and have integral zero over this interval.

Exercise 9 *Show that our perturbation space is a subspace of $\Re^{n+1}$.*

Let π_e denote the orthogonal projection of $\Re^{n+1}$ onto $\Re_0^{n+1}$. That is, π_e is the function from $\Re^{n+1}$ to $\Re_0^{n+1}$ so that $\|\pi_e\mathbf{x} - \mathbf{x}\| \le \|\mathbf{z} - \mathbf{x}\|$ for all $\mathbf{z} \in R^m$ where $\|\mathbf{x}\| = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle}$.

Exercise 10 *Let $\mathbf{u} \in \Re^{n+1}$ and compute $\pi_e(\mathbf{u})$ (the projection of $\mathbf{u}$ onto $\Re_0^{n+1}$) by defining $\psi(\mathbf{x}) = \frac{1}{2}\|\mathbf{x} - \mathbf{u}\|^2$ and minimizing ψ over $\Re^{n+1}$ via Lagrange multipliers.*

Because our goal is to determine a function of minimal arc length, recall that the arc-length of a differentiable function f on $[a, b]$ may be computed via $\int_a^b \sqrt{1 + (f'(x))^2}\, dx$. Thus, we define a functional ϕ on our vector space $\Re^{n+1}$ that represents the discrete version of this integral. We then minimize this functional ϕ over all vectors in our subspace. Define the functional to be minimized as the discrete version of the arc length integral,

$$\phi(\mathbf{x}) = \delta \sum_{i=1}^{n} \sqrt{1 + \left((D_1(x))_i\right)^2}. \tag{5}$$

Exercise 11 *Compute $\nabla\phi$, the gradient of ϕ; that is, compute $\dfrac{\partial \phi}{\partial x_i}$ for $i =$* $1, 2, \ldots, n+1$.

We are now prepared to describe the descent process based on the Euclidean inner product that is used to find an approximate minimum of ϕ as defined in *Equation* 5. Choose an initial estimate for the solution, $\mathbf{x}^0$, satisfying the boundary conditions. The process is to generate a sequence of points, typically called successive approximations, that converge to a point at which ϕ attains a relative minimum. If there were no boundary conditions, then the sequence would be generated by setting $\mathbf{x}^{k+1} = \mathbf{x}^k - h_k \nabla\phi(\mathbf{x}^k)$ for $k = 0, 1, 2, \ldots$ where $\nabla\phi$ was computed in *Exercise* 11 and the step size, h_k, is chosen either by experimentation (try .01 or .001) or optimally at each step. Since we seek a zero of ϕ, h_k is 'optimal' means that h_k is the value of h so that $g(h) = \phi\big(\mathbf{x} - h\nabla\phi(\mathbf{x})\big)$ is minimized over $h > 0$. We would stop when the norm of the difference between two successive approximations is less than some input

Figure 4 - Solutions from Sobolev Descent

tolerance. Because of our integral and endpoint constraints on the interval $[0,1]$, this process must be refined slightly. The sequence must be generated by setting $\mathbf{x}^{k+1} = \mathbf{x}^k - h_k \pi_e \nabla\phi(\mathbf{x}^k)$ for $k = 0, 1, 2, \ldots$ where π_e was computed in *Exercise* 10. Projecting the gradient onto the subspace via π_e assures us that when we subtract $h_k \pi_e \nabla\phi(\mathbf{x}^k)$ from $\mathbf{x}^k$, our new approximation $\mathbf{x}^{k+1}$ still satisfies the constraints. Now we see why the subspace is called a *perturbation* space, it is the collection of elements by which we perturb each previous estimate.

The left graph in *Figure 4* shows an initial function satisfying the boundary conditions on the interval of interest requested by the firm which was not $[0,1]$ but on a slightly larger interval. The right graph in *Figure 4* shows the approximate solution obtained via Sobolev descent. While Euclidean descent will generate results similar to these, the process will be slow to yield accurate results. The development of *preconditioning* techniques such as Sobolev descent offer considerable improvements in both efficiency and accuracy over Euclidean descent methods, and are highly versatile for incorporating constraints. We offer a brief description of the technique used to provide the numerical approximation in *Figure 4* as this is the portion of the research experience that is completely new to the students and utilizes the theoretical capstone of the first semester.

Just as the students presented examples of vector spaces, inner products, and positive-definite matrices during the first semester, they are now showing in class that each of the newly defined candidates are norms or inner products. They will also show that the perturbation spaces we need are subspaces and will be responsible for finding the projections onto the subspaces and verifying that they are projections. Some of these problems require creativity, and others are consequences of the tools they built during the first semester for determining conditions for a matrix to be positive-definite or conditions for a function to be a projection. While these materials are introduced to and developed by the students, the analysis of the efficiencies and convergence of the techniques are not treated. Students write codes to implement both Euclidean and Sobolev descent for the necessary equations. We would like to introduce a more general theory of preconditioning and convergence analysis, but time constraints prevent this. Furthermore, we feel that the "hands on" experience from coding has more value than analyzing the efficiencies of a method they have not implemented. A treatment of Sobolev descent for systems of ordinary differential equations may be found in [6, p.67-72], [9, p.187-195], and [8, p.19-32]. The first listed papers present the technique in detail, demonstrate the efficiency of the method and provide convergence results. The last paper includes examples and exercises targeted toward undergraduates in a way that develops the linear algebra associated with the projections, subspaces, and inner products.

The difference between Sobolev and Euclidean descent is conceptually simple. The Euclidean inner product or dot product is given by

$$\mathbf{u} \cdot \mathbf{v} =< \mathbf{u}, \mathbf{v} >= \sum_{i=1}^{n+1} u_i v_i$$

and a slight variation could be written in terms of our previously defined operators as

$$\begin{aligned} \langle \mathbf{u}, \mathbf{v} \rangle_e &= \langle D_0(\mathbf{u}), D_0(\mathbf{v}) \rangle \\ &= \sum_{k=1}^{n} \left(\frac{u_{k+1} + u_k}{2} \right) \left(\frac{v_{k+1} + v_k}{2} \right). \end{aligned} \tag{6}$$

To consider Sobolev descent, we define a new function,

$$\langle \mathbf{u}, \mathbf{v} \rangle_s = \langle D_0(\mathbf{u}), D_0(\mathbf{v}) \rangle + \langle D_1(\mathbf{u}), D_1(\mathbf{v}) \rangle =$$

$$\sum_{k=1}^{n} \left(\frac{u_{k+1} + u_k}{2} \right) \left(\frac{v_{k+1} + v_k}{2} \right) + \left(\frac{u_{k+1} - u_k}{\delta} \right) \left(\frac{v_{k+1} - v_k}{\delta} \right). \tag{7}$$

Exercise 12 *Prove that the function* $\langle \cdot, \cdot \rangle_s : \Re^{n+1} \times \Re^{n+1} \to \Re$ *in Equation 7 is indeed an inner product.*

Observe that this new inner product takes the derivative of the functions into consideration, providing a bit of intuition as to why Sobolev descent outperforms Euclidean descent in problems where the differential operator appears in the functional to be optimized.

Let $(\Re^{n+1}, \langle \cdot, \cdot \rangle_s)$ denote our Sobolev space and let π_s denote the orthogonal projection of $\Re^{n+1}$ onto $\Re_0^{n+1}$ under the Sobolev inner product. Thus $\pi_s(\mathbf{u})$

would be the unique nearest point to $\mathbf{u}$ in $\Re_0^{n+1}$ where 'nearest' is determined by the Sobolev inner product defined in *Equation* 7. To define the Sobolev gradient we must invoke the capstone of the first semester, the Riesz Representation Theorem in finite dimensions.

Theorem 13 *Riesz Representation Theorem: If V is a finite dimensional inner product space and l is a linear functional on V then there exists a unique element,* $z \in V$, *such that* $l(v) = \langle z, v \rangle$ *for all* $v \in V$.

In the third semester of calculus and again in advanced calculus, students have seen shades of this important result, although perhaps not in this form. They have seen that for a given differentiable function $F : \Re^{n+1} \to \Re$ with $\mathbf{x}$ and $\mathbf{y}$ in the domain of F, the derivative of F at $\mathbf{x}$ in the direction of the unit vector $\mathbf{y}$ may be computed by $F'(\mathbf{x})(\mathbf{y}) = \nabla F(\mathbf{x}) \cdot \mathbf{y} = \langle \nabla F(\mathbf{x}), \mathbf{y} \rangle$. Because for each $\mathbf{u} \in \Re^{n+1}$, $\phi'(\mathbf{u})$ is a linear functional, by the Riesz Representation Theorem, we know that there is a unique element representing this functional and we *define* the **Sobolev gradient** of ϕ at $\mathbf{u}$, denoted $\nabla_s \phi(\mathbf{u})$, to be the unique element in $\Re^{n+1}$ satisfying $\phi'(\mathbf{u})(\mathbf{v}) = \langle \nabla_s \phi(\mathbf{u}), \mathbf{v} \rangle_s$ for all $\mathbf{v}$ in $\Re^{n+1}$. Having defined our new gradient (a non-trivial result which many a mathematician has struggled with), our descent process now parallels Euclidean descent, differing only in the computation of the projection and the gradient.

Choose an initial guess for the solution, $\mathbf{x}^0$, satisfying the boundary conditions. This time we generate a sequence of successive approximations based on following this new gradient that converge to a point at which ϕ is minimized. Again, the approximations are defined by $\mathbf{x}^{k+1} = \mathbf{x}^k - h_k \pi_s \nabla_s \phi(\mathbf{x}^k)$ for $k = 0, 1, 2, \ldots$ where the step size, h_k, is chosen either by experimentation (try .1 or .01) or optimally as described previously. We would stop when the norm of the difference between successive approximations is less than some tolerance.

8 Summary of Mathematical Results

While the cases $A \leq \frac{1}{4}$ and $A > A^*$ did not yield feasible solutions because of the hydrodynamic properties of the reflection, two methods for generating solutions were found to be acceptable. The first was found by varying the area A incrementally between $\frac{1}{4}$ and A^* to determine the value of A that produced the visually "smoothest" bulb after reflection. All my students implement this method both using the *Mathematica* codes that they produce and using descent codes they write. They then compare their results from the two different methods. The second solution was found by applying Sobolev descent and adding the additional constraints that f must have a vertical tangent at $(1, 0)$ and satisfy $f'(0) = 0$ to assure a smooth bulb after reflection. This necessary refinement of the problem is the one that required us to consider optimization techniques over the classical theory with which we began. To date I have not had a student implement both boundary conditions (the vertical tangent is somewhat tricky) but numerous students have made good progress on this problem.

9 Conclusions

Any undergraduate course may serve as a research experience for undergraduates. General features that we have tried to build into all such courses include:

- mesh course syllabus with current departmental requirements,
- start with material that students have experience with and build on what they know,
- address significant classical mathematics,
- address significant modern computational methods (such as *Mathematica*, Maple, or other computer algebra systems),
- assure that materials are appropriate to prepare students for both graduate study or industry employment,
- address some mathematics that is *not* part of a standard undergraduate degree, and
- involve the students in both development of and presentation of the material so that they are truly doing research at their level.

Additional features incorporated into this course included covering a significant number of numerical methods, developing the students' written and oral communication skills, demonstrating the ties between the theoretical and numerical aspects of mathematics, and providing a taste for how mathematicians interface with industry.

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10 Appendix - Mathematica Code

```
Integrate[Sqrt[ 5/16 ( 5 - 16 a + 16 a^2) - (x-a)^2],{x,0,1}];

area = .53;

% The next three lines are just the output of the

% integration above + (2 a  - 3/4)  - area;

f[a_] := 1/32 ( -4 Sqrt[(3-8 a)^2] (-1+a) - 5 ( 5 - 16a + 16a^2) *

ArcTan[ 4 ( -1 + a) / Sqrt[ (3 - 8a)^2]]) + 1/32 ( 4 Sqrt[ (5-8a)^2] a

+ 5 ( 5 - 16a + 16a^2) ArcTan[4a/Sqrt[(5-8a)^2]]) + (2 a  - 3/4) - area;

a=FindRoot[f[x]==0,{x,0}][[1]][[2]]; b= 2 a - 3/4;

r = Sqrt [5/16(5 - 16 a + 16 a^2)];

Print["area=",area]; Print["radius=",r]; Print["center = (",a,",",b,")"];

Show[ Graphics[ {Circle[{a,b},r], Line[{{0,0},{0,1/2}}],

         Line[{{0,0},{1,0}}]} ], AspectRatio -> 1];

% Next lines just make the graphics prettier.

Clear[a,b,r]; a=0.378342735; b=0.00668547; r=0.621693;

Show[ Graphics[ Circle[{a,b},r]

       ] ,AspectRatio -> .8,Axes->True,PlotRange->{{0,1.1},{0,.85}}]
```

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Biographical Sketch

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