On the Application of Calculus toward Both Continuous and Discrete Optimization

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1 Introduction

The search for the maximum or minimum of a function is often an essential problem in both pure and applied mathematics; it can be found anywhere from finding the best route to the supermarket to finding the best mix of chemicals for a needed reaction, from maximizing one's crop yield for the year to minimizing the stress on an iron beam used to construct a building. The canonical way of finding the maximum of a function $f : \mathbb{R} \to \mathbb{R}$ has been to find its derivative f' and then locate its roots, but sometimes that derivative is not readily available, and sometimes mitigating circumstances can get in the way of a simple derivative reading as that. This is especially true for more complex systems which cannot be represented as just an equation from $\mathbb{R}$ to $\mathbb{R}$. We will explore two problems and explore their solutions, investigating ways to find maxima and minima of complex systems: one maximizing a complex function along a line, and one minimizing a function from $\mathbb{R}^n$ to $\mathbb{R}$ with very large n.

2 Polya's Angle Maximization Problem

We consider the problem put forth in Polya [2]:

> Given two points and a straight line, all in the same plane, both points on the same side of the line. On the given straight line, find a point from which the segment joining the two given points is seen under the greatest possible angle.

Let A and B be the two points on the same side of the line, and let X be the point of maximum angle on the line ℓ. Polya put forth two solutions of his own in the book, both of which used intuitive yet somewhat informal geometry to find the solution. The first solution considered under which circumstances X would be the only point on ℓ for which $\alpha = \angle AXB$ was unique along the line, and then naming that X the maximum; the second solution was a bit more elegant, considering the locus of all points X' that satisfied $\alpha = \angle AX'B$ for a given α, which happened to be a circle that runs through A and B, and finding the circle that was tangent to ℓ and marking the tangential point as X. Both of these approaches use Polya's intuitive concept of "level curves" to find a solution.

We seek a solution using calculus to verify the intuitive geometrical solution. However, it appears on first inspection that it may not be nearly as simple. We consider the function $\alpha : \mathbb{R} \to \mathbb{R}$, such that $\alpha(x)$ is the measurement $m\angle AXB$, where $X = (x, 0)$. An attempt at a formulation of this function gives us an idea of what we're up against. Let $x_a, y_a, x_b, y_b \in \mathbb{R}$ such that $A = (x_a, y_a)$ and $B = (x_b, y_b)$. Also, let $\mathbf{u} = \overrightarrow{AX}$ and let $\mathbf{v} = \overrightarrow{BX}$. Then, by the definition of the dot product,

$$\mathbf{u} \cdot \mathbf{v} = |\mathbf{u}||\mathbf{v}| \cos \alpha(x)$$

$$\begin{aligned} \alpha(x) &= \cos^{-1}\left(\frac{\mathbf{u} \cdot \mathbf{v}}{|\mathbf{u}||\mathbf{v}|}\right) \\ &= \cos^{-1}\left(\frac{(x - x_a)(x - x_b) + y_a y_b}{\sqrt{(x - x_a)^2 + y_a^2}\sqrt{(x - x_b)^2 + y_b^2}}\right) \end{aligned}$$

This equation is a bit hard to work with, so instead, we choose to work with another function, $\phi(x) = \cos^2 \alpha(x)$. We note that, by the chain rule, $\phi' = -2 \cos \alpha \sin \alpha \cdot \alpha'$, and any instance where α' is zero will also be one where ϕ' is zero.

One more simplification is necessary before we start working on a formulation of the maximum: there still exists a degree of freedom in the system for the points with respect to the line, which could potentially complicate the calculations by introducing an extra variable. To avoid this, we fix the origin such that it lies on the line that runs throgh A and B, and instead of having the four variables x_a, x_b, y_a, and y_b, we reduce the system to three variables x_a, x_b, and λ such that $A = (x_a, x_b)$ and $B = (\lambda x_a, \lambda x_b)$. Note that, since A and B are separate points, $\lambda \neq 1$. We now present the theorem.

Theorem 1 *Let* $A = (x_a, y_a)$ *and let* $B = (\lambda x_a, \lambda y_a)$. *Then the value of* x *that maximizes* $\alpha = \angle AXB$ *with* $X = (x, 0)$ *satisfies*

$$x^2 = \lambda(x_a^2 + y_a^2).$$

There are two proofs of this theorem: one maximizing $\alpha(x)$ along the line ℓ, and the other considering a new function $\beta(x, y)$ over the whole plane and finding a maximum using Lagrange multipliers using the constraint $g(x, y) = y = 0$. Both make use of the above function $\phi(x)$.

Proof using One Dimension We know that the maximum of $\alpha(x)$ will also be the maximum of $\phi(x)$, so we start by finding ϕ'. We simplify the function by making the following substitutions (used here mostly for consistency with the two-dimensional proof):

$$\begin{aligned} a &= x - x_a \\ b &= -y_a \\ c &= x - \lambda x_a \\ d &= -\lambda y_a \end{aligned}$$

Then $\mathbf{u} = (a, b)$, $\mathbf{v} = (c, d)$, and $\mathbf{u} \cdot \mathbf{v} = ac + bd$.

$$\begin{aligned} \phi &= \frac{(\mathbf{u} \cdot \mathbf{v})^2}{|\mathbf{u}|^2 |\mathbf{v}|^2} \\ &= \frac{(ac + bd)^2}{(a^2 + b^2)(c^2 + d^2)} \\ &= 1 - \frac{(ad - bc)^2}{(a^2 + b^2)(c^2 + d^2)} \\ \Rightarrow \phi' &= -\frac{2(ad - bc)(d - b)(a^2 + b^2)(c^2 + d^2) - (ad - bc)^2[2a(c^2 + d^2) + 2c(a^2 + b^2)]}{[(a^2 + b^2)(c^2 + d^2)]^2} \end{aligned}$$

We then solve this expression for $\phi' = 0$.

$$\begin{aligned} 0 &= 2(ad - bc)(d - b)(a^2 + b^2)(c^2 + d^2) - (ad - bc)^2[2a(c^2 + d^2) + 2c(a^2 + b^2)] \\ &= 2(ad - bc)[-(d - b)(a^2 + b^2)(c^2 + d^2) + (ad - bc)[a(c^2 + d^2) + c(a^2 + b^2)]] \\ &= 2(ad - bc)[-(a^2c^2d + a^2d^3 + b^2c^2d + b^2d^3 - a^2bc^2 - a^2bd^2 - b^3c^2 - b^3d^2) \\ &\qquad +(a^2c^2d + a^2d^3 + a^3cd + ab^2cd - abc^3 - abcd^2 - a^2bc^2 - b^3c^2)] \\ &= 2(ad - bc)(ac + bd)(-bc^2 - bd^2 + a^2d + b^2d). \end{aligned}$$

We notice that $ad - bc = |\mathbf{u} \times \mathbf{v}| = 0$ whenever $\alpha = 0$; $\cos^2 \alpha$ always reaches a maximum at this point. We can safely ignore this factor. Also, $ac + bd = \mathbf{u} \cdot \mathbf{v} = 0$ whenever $\alpha = \pi/2$; $\cos^2 \alpha$ also reaches a minimum at this point and we can ignore this factor as well. Therefore, we go on to attempt to solve for x in the factor that has the most promise.

$$\begin{aligned}
0 &= -bc^2 - bd^2 + a^2 d + b^2 d \\
&= -b(c^2 + d^2) + d(a^2 + b^2) \\
&= y_a[(x - \lambda x_a)^2 + \lambda^2 y_a^2] - \lambda y_a[(x - x_a)^2 + y_a^2] \\
&= y_a(x^2 - 2\lambda x x_a + \lambda^2 x_a^2 + \lambda^2 y_a^2 - \lambda x^2 + 2\lambda x x_a - \lambda x_a^2 - \lambda y_a^2) \\
&= y_a(1 - \lambda)(x^2 - \lambda x_a^2 - \lambda y_a^2)
\end{aligned}$$

Since both points A and B are on the same side of ℓ, we can safely assume that A is not actually *on* ℓ, and therefore that $y_a \neq 0$. Also, since A and B are two distinct points, we can also assume that $\lambda \neq 1$, and therefore $1 - \lambda \neq 0$. Thus we arrive at the final statement:

$$\Rightarrow x^2 = \lambda(x_a^2 + y_a^2)$$

This concludes the proof. □

Proof using Two Dimensions Instead of considering the function ϕ of just one variable, we consider the function $\beta(x, y)$ which gives the measurement of the angle $\angle AXB$, where $X = (x, y)$. Let $\psi(x, y) = \cos^2 \beta(x, y)$. Note that $\alpha(x) = \beta(x, 0)$ and $\phi(x) = \psi(x, 0)$.

Using the method of Lagrange multipliers, we let our constraint be $g(x, y) = y = 0$, since X eventually has to be on the line ℓ. Then, for some $\gamma \in \mathbb{R}$, $\nabla\psi(x, y) = \gamma\nabla g(x, y)$. Clearly $\nabla g = (0, 1)$ for all x and y, so $(\psi_x, \psi_y) = (0, \gamma)$. The two conditions we must satisfy are $\psi_x = 0$ and $y = 0$. Noting that

$$\frac{\partial\psi}{\partial x}(x, 0) = \frac{d\phi}{dx}(x),$$

we can follow the same process as in the first proof to show that

$$x^2 = \lambda(x_a^2 + x_b^2).$$

This concludes the proof. □

3 Maximization of Quadratic Functions in a Box and the Obstacle Problem

The obstacle problem is one of the problems used in Friedlander [1] to present the new algorithm for minimizing quadratic functions from $\mathbb{R}^n$ to $\mathbb{R}$ with box constraints, where quadratic function means one which can be represented in the form $\frac{1}{2}x^T Hx + b^T x + c$, where $H \in \mathbb{R}^{n\times n}$, $b \in \mathbb{R}^n$, $c \in \mathbb{R}$, and H is symmetric and positive semidefinite. While the results of the tests were given in that paper, the manner in which the actual equation was arrived at was not fully explored in that paper. Here we will discuss the formulation of that equation, as well as our own results testing the algorithm.

The problem's objective is to find the equilibrium of a membrane draped over an obstacle, doing so by minimizing the membrane's potential energy. The original obstacle problem consisted of minimizing a function $q : C^1 \to \mathbb{R}$ where

$$q(v) = \frac{1}{2}\int_D |\nabla v|^2 \; \partial D - \int_D fv \; \partial D, \qquad \ell \leq v \leq u$$

where $D \subset \mathbb{R}^2$ is the domain over which the membrane is stretched, $v : \mathbb{R} \to \mathbb{R}$ is the function representing the height of the membrane at a given point in D, $\ell, u \in \mathbb{R}^2 \to \mathbb{R}$ are the lower and upper limit functions for v, and $f : D \to \mathbb{R}$ is the function representing gravity acting on the membrane, usually constant. (In our calculations, it is fixed at -1.) Outside D, v is fixed at ℓ.

The original problem is not too favorable as far as analysis is concerned, being an infinite-dimensional minimization problem; however, by rasterizing D, we convert the problem to an mn-dimensional one, where m and n are the number of rows and columns, respectively, of the grid. For our problem, we only consider a square D, such that $m = n$, and we will always refer to this quantity as n.

Let h be the interval between rows or between columns of the D-grid. Then let z_{ij} be the point in the ith column and jth row of the grid. If $z_{11} = (x_1, y_1)$, then $z_{ij} = (x_1 + h(i-1), y_1 + h(j-1))$. Let $N_k = \{1, 2, \ldots, k\}$, and let A^2 be the Cartesian square of a set A. Let $Z = N_n^2$. We will also be considering points z_{ij} such that $(i,j) \notin Z$, i.e., points with indices 0 or $n+1$. Let $v \in \mathbb{R}^{n\times n}$ be the matrix such that v_{ij} is the height of the membrane at z_{ij}, and let ℓ and u be the lower and upper limit matrices such that, for all $(i,j) \notin Z$, $\ell_{ij} \leq v_{ij} \leq u_{ij}$. (Similarly, for $(i,j) \notin Z$, $v_{ij} = \ell_{ij}$.)

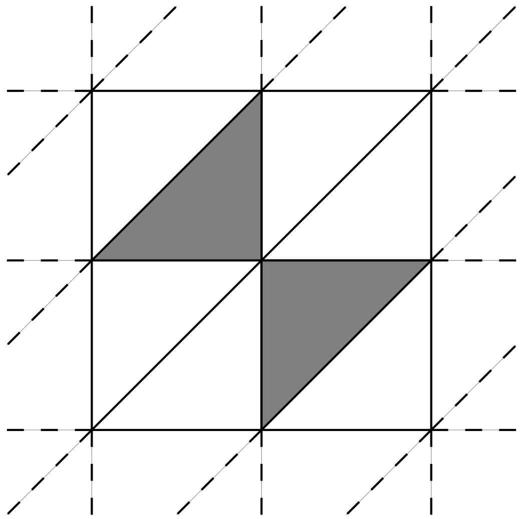

Figure 1: The tesselation of the plane used for estimating $\int_D |\nabla v|^2 \, \partial D$.

We estimate the integral of the gradient over D by dividing D up into triangles, two for every square cell (see Figure 3) and finding the gradient of the linear function that passes through the three corners of the triangle. We consider two classes of triangle: the "lower-left" triangles, which consist of three points of the form z_{ij}, $z_{i+1,j}$, and $z_{i,j+1}$; and the "upper-right" triangles, which consist of three points of the form , $z_{i+1,j}$, $z_{i,j+1}$, and $z_{i+1,j+1}$. We notice that, for any given point z_{ij}, there are two triangles that have that point at its right corner: the triangle through z_{ij}, $z_{i+1,j}$, and $z_{i,j+1}$ (a "lower-left" triangle), and the triangle through z_{ij}, $z_{i-1,j}$, and $z_{i,j-1}$ (an "upper-right" triangle). We examine the linear function f_ℓ that runs through the first three points:

$$f_\ell(x, y) = ax + by + c \qquad \nabla f_\ell = (a, b)$$

$$\begin{aligned} v_{ij} &= a(x_1 + h(i-1)) + b(y_1 + h(j-1)) + c \\ v_{i+1,j} &= a(x_1 + hi) + b(y_1 + h(j-1)) + c \\ v_{i,j+1} &= a(x_1 + h(i-1)) + b(y_1 + hj) + c \end{aligned}$$

$$a = \frac{v_{i+1,j} - v_{ij}}{h} \qquad b = \frac{v_{i,j+1} - v_{ij}}{h}$$

$$|\nabla f_\ell|^2 = a^2 + b^2 = \frac{(v_{i+1,j} - v_{ij})^2 + (v_{i,j+1} - v_{ij})^2}{h^2}$$

We perform a similar derivation to find

$$|\nabla f_u|^2 = \frac{(v_{i-1,j} - v_{ij})^2 + (v_{i,j-1} - v_{ij})^2}{h^2}$$

Since the area of the projection of each triangle onto D is $\frac{1}{2}h^2$, we can estimate $|\nabla v|^2\ \partial D$ as $\frac{1}{2}h^2|\nabla f_\ell|^2 + \frac{1}{2}h^2|\nabla f_u|^2) = \frac{1}{2}[(v_{i+1,j} - v_{ij})^2 + (v_{i,j+1} - v_{ij})^2 + (v_{i-1,j} - v_{ij})^2 + (v_{i,j-1} - v_{ij})^2]$.

Along the same lines, if $f = c$ where c is a constant, then we can estimate $f\ \partial D$ as $ch^2 v_{ij}$. Then the discrete formula becomes

$$q(v) = \frac{1}{4} \sum_{(i,j)\in Z} q_{ij}(v) - ch^2 \sum_{(i,j)\in Z} v_{ij},$$

where

$$q_{ij}(v) = (v_{i+1,j} - v_{ij})^2 + (v_{i,j+1} - v_{ij})^2 + (v_{i-1,j} - v_{ij})^2 + (v_{i,j-1} - v_{ij})^2.$$

This system can be represented as a quadratic system; the only thing that remains to be seen as how. We choose to employ a transformation $p : N_n^2 \to N_{n^2}$ such that $p(i,j) = (i-1)n + j$. Notice that $p^{-1}(i) = (\lfloor \frac{i-1}{n} \rfloor + 1, [(i-1) \bmod n] + 1)$, and thus p is a bijection between $\{1, 2, \ldots, n\} \times \{1, 2, \ldots, n\}$. We can then refer to the indices of H and b by the points in N_n^2 that they represent.

Let H be the matrix such that

$$H_{p(i_1,j_1),p(i_2,j_2)} = \begin{cases} 4 & \text{if } (i_1, j_1) = (i_2, j_2) \\ -1 & \text{if } (i_1, j_1) \text{ is adjacent to } (i_2, j_2) \\ 0 & \text{otherwise} \end{cases}$$

and let b be the vector such that

$$b'_{p(i,j)} = -ch^2$$

$$b''_{p(i,j)} = \begin{cases} -2v_{0,j} & \text{if } i = 1 \\ -2v_{n+1,j} & \text{if } i = n \\ 0 & \text{otherwise} \end{cases}$$

$$b'''_{p(i,j)} = \begin{cases} -2v_{i,0} & \text{if } j = 1 \\ -2v_{i,n+1} & \text{if } j = n \\ 0 & \text{otherwise} \end{cases}$$

$$b = b' + b'' + b'''$$

With H and b, we now have a quadratic function $q(v) = \frac{1}{2}v^T Hv + b^T v + c$ for some constant c. The value of c doesn't matter in this particular case, since the minimizer will be the same for any $c \in \mathbb{R}$. Note that $\nabla q(v) = Hv + b$. Given these functions, we can now attempt to minimize them using the algorithm given in Friedlander [1], using ℓ and u as the box.

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