Implicit differentiation and constrained local extrema in Giac/Xcas

Luka Marohnić

Email: marohnicluka@gmail.com

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Abstract. In this article, we present an algorithm for finding points of local extrema of a multivariate function under (several) equality constraints, which is implemented in Giac/Xcas computer algebra system. The first seven sections cover the required theoretical background. The technique of implicit differentiation is proposed for solving the problem as an alternative to the classical Lagrange method. For better classification of critical points we consider higher order partial derivative test and show a counter-example to a method proposed in 2013 is discussed. An outline of the algorithm is given in the last section.

Keywords: algorithm, computer algebra, multivariate calculus, Taylor formula, constrained local extrema, Lagrange multipliers, Peano surface

1. Introduction

Generally, the problem of finding local extrema of a multivariate function under equality constraints can be formulated as follows.

The original problem. Let $n,m\in\mathbb{N}$ and let $f:\mathbb{R}^{n+m}\to\mathbb{R}$, $\mathbf{G}:\mathbb{R}^{n+m}\to\mathbb{R}^m$ be differentiable functions. Assuming that the Jacobian matrix of $\mathbf{G}$ has maximal rank, find the points of local extrema of f subject to $\mathbf{G}\equiv\mathbf{0}$.

To formulate the above problem in a more convenient way, let us assume that

$$f(x_1,x_2,\ldots,x_n,y_1,y_2,\ldots,y_m)=f(\mathbf{x},\mathbf{y}),\quad \mathbf{x}=(x_1,\ldots,x_n)\in\mathbb{R}^n,\mathbf{y}=(y_1,\ldots,y_m)\in\mathbb{R}^m, \tag{1}$$

and, denoting $\mathbf{G}=(G_1,G_2,\ldots,G_m)$,

$$G_j(\mathbf{x},\mathbf{y})=0,\quad j=1,2,\ldots,m, \tag{2}$$

such that the last m columns of the Jacobian matrix

$$\mathbf{J}=\mathbf{G}'(\mathbf{x},\mathbf{y})=\left(\begin{array}{cccc|cccc}\frac{\partial G_1}{\partial x_1} & \frac{\partial G_1}{\partial x_2} & \cdots & \frac{\partial G_1}{\partial x_n} & \frac{\partial G_1}{\partial y_1} & \frac{\partial G_1}{\partial y_2} & \cdots & \frac{\partial G_1}{\partial y_m}\\ \frac{\partial G_2}{\partial x_1} & \frac{\partial G_2}{\partial x_2} & \cdots & \frac{\partial G_2}{\partial x_n} & \frac{\partial G_2}{\partial y_1} & \frac{\partial G_2}{\partial y_2} & \cdots & \frac{\partial G_2}{\partial y_m}\\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots\\ \frac{\partial G_m}{\partial x_1} & \frac{\partial G_m}{\partial x_2} & \cdots & \frac{\partial G_m}{\partial x_n} & \frac{\partial G_m}{\partial y_1} & \frac{\partial G_m}{\partial y_2} & \cdots & \frac{\partial G_m}{\partial y_m}\end{array}\right)=\begin{pmatrix}\mathbf{G_x} & \mathbf{G_y}\end{pmatrix} \tag{3}$$

are linearly independent. The problem now reads as follows:

$$\textit{Find the points of local extrema of the function (1) under the constraints (2) with } \det\mathbf{G_y}\neq 0. \tag{4}$$

Note that this formulation may require rearranging the variables of the original problem. Nevertheless, the critical points should always be stored with respect to the original order of variables.

2. Computing the critical points

To solve the problem (4) we use the method proposed in [2] which reduces the given problem to an unconstrained one without using Lagrange multipliers.

Assuming that f and $\mathbf{G}$ are both defined and enough differentiable on an open subset $U\subset\mathbb{R}^{n+m}$, let $S=\{(\mathbf{x},\mathbf{y})\in U:\mathbf{G}(\mathbf{x},\mathbf{y})=0\wedge\det\mathbf{G_y}(\mathbf{x},\mathbf{y})\neq 0\}$ and assume that S is non-empty. Now from the Implicit Function Theorem (see [6], Theorem 6.4.1, pp. 420) follows that for a point $(\mathbf{x}_0,\mathbf{y}_0)\in S$ there exists a neighborhood $X\subset\mathbb{R}^n$ of $\mathbf{x}_0$ and a unique continuously differentiable function $\mathbf{h}:X\to\mathbb{R}^m$ such that $\mathbf{h}(\mathbf{x}_0)=\mathbf{y}_0$ and $V=(X,\mathbf{h}(X))\subset S$. Let $F:X\to\mathbb{R}$ be defined as

$$F(\mathbf{x})=f(\mathbf{x},\mathbf{h}(\mathbf{x})),\quad \mathbf{x}=(x_1,x_2,\ldots,x_n)\in X. \tag{5}$$

Clearly, if

$$\nabla_{\mathbf{x}} F(\mathbf{x}) = \mathbf{0} \tag{6}$$

for some $\mathbf{x} \in X$ then $(\mathbf{x}, \mathbf{h}(\mathbf{x})) \in V$ is a critical point of f subject to (2).

Let us denote $\mathbf{h}(\mathbf{x}) = (h_1(\mathbf{x}), h_2(\mathbf{x}), \ldots, h_m(\mathbf{x}))$. Now from (5), using the chain rule and the total derivative formula [6, Corollary 5.4.4], we obtain

$$\frac{\partial F}{\partial x_i} = \frac{\partial f}{\partial x_i} + \sum_{j=1}^{m} \frac{\partial f}{\partial y_j} \cdot \frac{\partial h_j}{\partial x_i}, \quad i = 1, 2, \ldots, n. \tag{7}$$

Hence, to compute $\frac{\partial F}{\partial x_i}$ for all $i = 1, 2, \ldots, n$ we need to determine the first order partial derivatives (i.e. the Jacobian) of $\mathbf{h}$. From the Implicit Function Theorem we immediately obtain

$$\mathbf{h}' = -\mathbf{G}_{\mathbf{y}}^{-1} \cdot \mathbf{G}_{\mathbf{x}}. \tag{8}$$

However, since we are also interested in computing derivatives of higher order of F, we choose a different approach [2]. Let us define

$$\mathbf{K}(\mathbf{x}) = \mathbf{G}(\mathbf{x}, \mathbf{h}(\mathbf{x})), \quad \mathbf{x} \in X.$$

The function $\mathbf{K} = (K_1, K_2, \ldots, K_m)$ is constant on X, which implies that its partial derivatives vanish in any open subset of X. Hence for all $i = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, m$ we have

$$\frac{\partial K_j}{\partial x_i} = \frac{\partial G_j}{\partial x_i} + \sum_{k=1}^{m} \frac{\partial G_j}{\partial y_k} \cdot \frac{\partial h_k}{\partial x_i} = 0, \tag{9}$$

which implies

$$\sum_{k=1}^{m} \frac{\partial G_j}{\partial y_k} \cdot \frac{\partial h_k}{\partial x_i} = -\frac{\partial G_j}{\partial x_i}. \tag{10}$$

The equations (10) form a linear system of order $n m$ which can be solved by the usual methods to give the derivatives $\frac{\partial h_j}{\partial x_i}$ explicitly for all i, j, which are subsequently substituted into (7), yielding the derivatives $\frac{\partial F}{\partial x_i}$.

Note that partial derivatives of $\mathbf{h}$ and F are obtained as functions in $\mathbb{R}^{n+m}$. Hence it follows from (6) that the solutions to the following system of $n + m$ equations with $n + m$ unknowns [2, Theorem 3.1]

$$\begin{aligned} \frac{\partial F}{\partial x_i}(\mathbf{x}, \mathbf{y}) &= 0, \quad i = 1, 2, \ldots, n, \\ G_j(\mathbf{x}, \mathbf{y}) &= 0, \quad j = 1, 2, \ldots, m \end{aligned}$$

are critical points of f. Note that this method does **not** necessarily find **all** the critical points of f; see the examples below.

Remark 1. To avoid any generality loss in the original problem, critical points are computed separately for each distinct partition of variables into sets $\{x_1, x_2, \ldots, x_n\}$ and $\{y_1, y_2, \ldots, y_m\}$ such that the the matrix $\mathbf{G}_{\mathbf{y}}$ is nonsingular [2], i.e. for all distinct formulations of the problem (4), and the results are collected into a single set (see Example 2). Still, the latter does not necessarily represent the entire set of critical points—there may be points in the domain of f for which $\mathbf{G} = \mathbf{0}$ but some partial derivatives of F are undefined in all instances (see Example 3). In such cases one may consider applying the classical method of LAGRANGE [3] in attempt to find the remaining critical points. Note, however, that both methods may fail (see [4] for an example).

Example 2. To illustrate the importance of Remark 1, we attempt to determine all critical points of the function $f(x, y) = x^2 y^2$ subject to $x^2 + y^2 = 1$. It can be shown that the set of critical points of f is

$$C = \left\{(-1, 0), (1, 0), (0, -1), (0, 1), \left(\tfrac{1}{\sqrt{2}}, \tfrac{1}{\sqrt{2}}\right), \left(-\tfrac{1}{\sqrt{2}}, \tfrac{1}{\sqrt{2}}\right), \left(-\tfrac{1}{\sqrt{2}}, -\tfrac{1}{\sqrt{2}}\right), \left(\tfrac{1}{\sqrt{2}}, -\tfrac{1}{\sqrt{2}}\right)\right\}.$$

The first four are the points of local minima while the last four are the points of local maxima. Also, it is easy to obtain the parametrization of the intersection of the surfaces $z=x^2\,y^2$ and $x^2+y^2=1$, i.e.

$$\begin{cases} x=\cos t, \\ y=\sin t, \\ z=\frac{1}{4}\sin^2 2t, \end{cases} \qquad t\in[-\pi,\pi],$$

which allows the local extrema to be easily visualized in Giac using the `plotparam` command (see Figure 1). To find the critical points using the the proposed method, we first formulate the problem such that x is the free and y the dependent variable. Therefore, $\mathbf{J}=(\,\mathbf{G}_x\ \ \mathbf{G}_y\,)=(\,2\,x,\ 2\,y)$ which together with (8) implies

$$\frac{\mathrm{d}h}{\mathrm{d}x}=-\frac{x}{y}.$$

Now from (7) we have

$$\frac{\mathrm{d}J}{\mathrm{d}x}=\frac{\partial f}{\partial x}+\frac{\partial f}{\partial y}\cdot\frac{\mathrm{d}h}{\mathrm{d}x}=2\,x\,y^2-2\,x^2\,y\cdot\frac{x}{y}=2\,x\,y^2-2\,x^3=2\,x\,(y^2-x^2).$$

Solving the system of equations $2\,x\,(y^2-x^2)=0$ and $x^2+y^2=1$ using the command `solve` in Giac [5], we obtain only the last six critical points from C; the first two, $(-1,0)$ and $(1,0)$, obviously do not satisfy the first equation because $\frac{\mathrm{d}h}{\mathrm{d}x}$ is not defined when $y=0$. However, there is an alternative interpretation of the given problem, where y is the free and x the dependent variable. In that case we have $\frac{\mathrm{d}h}{\mathrm{d}x}=-\frac{y}{x}$ and $\frac{\mathrm{d}J}{\mathrm{d}y}=2\,y\,(x^2-y^2)$. Solving the system $2\,y\,(x^2-y^2)=0$ and $x^2+y^2=1$, we also get six critical points but this time the solution contains $(-1,0)$ and $(1,0)$, while $(0,-1)$ and $(0,1)$ are missing (since now $\frac{\mathrm{d}h}{\mathrm{d}x}$ is not defined when $x=0$). We conclude that it is necessary to consider both formulations to obtain the complete set of critical points.

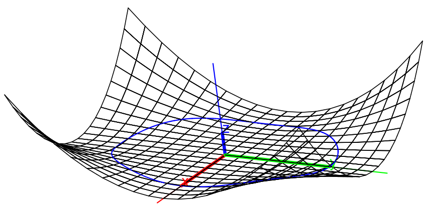

Figure 1. $f(x,y)=x^2\,y^2$ above the unit circle S^1

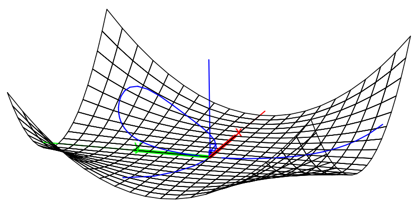

Figure 2. $f(x,y)=x^2\,y^2$ above the folium of Descartes

Example 3. We search for local extrema of the function $f(x,y)=x^2\,y^2$ on the folium of Descartes defined by $g(x,y)\equiv x^3+y^3-3\,x\,y=0$ (see Figure 2). Let y be the dependent variable. Now we have

$$\mathbf{J}=(\,\mathbf{G}_x\ \ \mathbf{G}_y\,)=\left(\,3\,x^2-3\,y,\ 3\,y^2-3\,x\right),$$

hence $\frac{\mathrm{d}h}{\mathrm{d}x}=-\frac{x^2-y}{y^2-x}$ and $\frac{\mathrm{d}F}{\mathrm{d}x}=\frac{\partial f}{\partial x}+\frac{\partial f}{\partial y}\cdot\frac{\mathrm{d}h}{\mathrm{d}x}=2\,x\,y^2-2\,x^2\,y\,\frac{x^2-y}{y^2-x}=\frac{2\,x^4\,y-2\,x\,y^4}{x-y^2}$. The derivative $\frac{\mathrm{d}F}{\mathrm{d}x}$ is not defined at origin $(0,0)$, but it is easy to show that $(0,0)$ is the point of local minimum of f subject to $g(x,y)=0$. If we declare x to be the dependent variable, we obtain a similar situation; therefore, since the above method detects only the local maximum at $\mathbf{c}_1=\left(\frac{3}{2},\frac{3}{2}\right)$, the critical point $(0,0)$ and its classification must be obtained by some other means. We apply the method of Lagrange [3] and define the corresponding Lagrange function $\mathcal{L}$ by

$$\mathcal{L}(x,y,\lambda)=f(x,y)-\lambda\,g(x,y),$$

where λ is the Lagrange multiplier. The system of equations $\nabla\mathcal{L}(x,y,\lambda)=\mathbf{0}$, $g(x,y)=0$ for critical points is solved by using the commands `grad` and `solve` in Giac [5]. We obtain exactly two distinct solutions: $\mathbf{c}_1$ for $\lambda=3$ and $\mathbf{c}_2=(0,0)$ for any $\lambda\in\mathbb{R}$. Note that classifying $\mathbf{c}_2$ must be done with respect to $\mathcal{L}$ (see Section 4).

3. Computing the partial derivatives of higher order

The next step is to classify critical points. At this point, higher derivatives of F are needed. To compute these, the derivatives of $\mathbf{h}$ of the same order are required. We assume that f and $\mathbf{G}$ are both C^n functions for a large enough n.

We proceed by obtaining second order derivatives of $\mathbf{K}$ by differentiating the equations (9). It follows

$$\begin{aligned}\frac{\partial^2 K_p}{\partial x_i\,\partial x_j} &= \frac{\partial^2 G_p}{\partial x_i\,\partial x_j} + \sum_{q=1}^m \frac{\partial^2 G_p}{\partial x_i\,\partial y_q}\cdot\frac{\partial h_q}{\partial x_j} + \\ &\quad + \sum_{k=1}^m \left(\left(\frac{\partial^2 G_p}{\partial x_j\,\partial y_k} + \sum_{q=1}^m \frac{\partial^2 G_p}{\partial y_q\,\partial y_k}\cdot\frac{\partial h_q}{\partial x_j}\right)\cdot\frac{\partial h_k}{\partial x_i} + \frac{\partial G_p}{\partial y_k}\cdot\frac{\partial^2 h_k}{\partial x_i\,\partial x_j}\right) \\ &= \frac{\partial^2 G_p}{\partial x_i\,\partial x_j} + \sum_{q=1}^m \left(\frac{\partial^2 G_p}{\partial x_i\,\partial y_q}\cdot\frac{\partial h_q}{\partial x_j} + \frac{\partial^2 G_p}{\partial x_j\,\partial y_k}\cdot\frac{\partial h_k}{\partial x_i}\right) + \\ &\quad + \sum_{k=1}^m \frac{\partial h_k}{\partial x_i}\sum_{q=1}^m \frac{\partial^2 G_p}{\partial y_q\,\partial y_k}\cdot\frac{\partial h_q}{\partial x_j} + \sum_{k=1}^m \frac{\partial G_p}{\partial y_k}\cdot\frac{\partial^2 h_k}{\partial x_i\,\partial x_j} = 0,\end{aligned}$$

which implies

$$\sum_{k=1}^m \frac{\partial G_j}{\partial y_k}\cdot\frac{\partial^2 h_k}{\partial x_i\,\partial x_j} = -\frac{\partial^2 G_p}{\partial x_i\,\partial x_j} - \sum_{q=1}^m \left(\frac{\partial^2 G_p}{\partial x_i\,\partial y_q}\cdot\frac{\partial h_q}{\partial x_j} + \frac{\partial^2 G_p}{\partial x_j\,\partial y_q}\cdot\frac{\partial h_k}{\partial x_i}\right) - \sum_{k=1}^m \frac{\partial h_k}{\partial x_i}\sum_{q=1}^m \frac{\partial^2 G_p}{\partial y_q\,\partial y_k}\cdot\frac{\partial h_q}{\partial x_j} \tag{11}$$

for all $i, j = 1, 2, \ldots, n$ and $p = 1, 2, \ldots, m$. Substituting the first order derivatives $\mathbf{h}$ obtained by solving the system (10) in the equations (11) yields the linear system of order $n^2 m$ with the second order partial derivatives of $\mathbf{h}$ as unknowns. (The order of the system can be reduced to $\frac{1}{2} m n (n+1)$ since from the SCHWARZ' theorem we have $\frac{\partial^2}{\partial x_i\,\partial x_j} = \frac{\partial^2}{\partial x_j\,\partial x_i}$ for all $i \neq j$). When these are computed, the formula

$$\frac{\partial^2 F}{\partial x_i\,\partial x_j} = \frac{\partial^2 f}{\partial x_i\,\partial x_j} + \sum_{q=1}^m \left(\frac{\partial^2 f}{\partial x_i\,\partial y_q}\cdot\frac{\partial h_q}{\partial x_j} + \frac{\partial^2 f}{\partial x_j\,\partial y_q}\cdot\frac{\partial h_k}{\partial x_i}\right) + \sum_{k=1}^m \frac{\partial h_k}{\partial x_i}\sum_{q=1}^m \frac{\partial^2 f}{\partial y_q\,\partial y_k}\cdot\frac{\partial h_q}{\partial x_j} + \sum_{k=1}^m \frac{\partial f}{\partial y_k}\cdot\frac{\partial^2 h_k}{\partial x_i\,\partial x_j},$$

obtained by differentiating the i-th equation in (7) with respect to x_j, yields the second order partial derivatives of F for all $i, j = 1, 2, \ldots, n$.

We may now proceed inductively to compute the derivatives of the third order, fourth order and so on, until reaching derivatives of the required degree (see [2] for practical examples). This method is used by the `implicitdiff` command in Giac [5].

4. The second order partial derivative test

To classify the critical points of F we use the second order partial derivative test. According to [2, Theorem 3.2], we look at the set E of distinct eigenvalues $e_1, e_2, \ldots, e_k$ of the $n \times n$ Hessian matrix

$$\operatorname{Hess}(F) := \left[\frac{\partial^2 F}{\partial x_i\,\partial x_j}\right]_{1 \leqslant i,j \leqslant n}$$

at the critical point $\mathbf{c} = (\mathbf{x}_0, \mathbf{y}_0) \in \mathbb{R}^{n+m}$. There are four possibilities:

1. if $e > 0$ for all $e \in E$ (i.e. if the Hessian is positive definite), then $\mathbf{c}$ is a local minimum,
2. if $e < 0$ for all $e \in E$ (i.e. if the Hessian is negative definite), then $\mathbf{c}$ is a local maximum,
3. if $0 \notin E$ and there exist $e_i, e_j \in E$ such that $e_i\, e_j < 0$, then $\mathbf{c}$ is a saddle point,
4. if $0 \in E$, the test is inconclusive.

Note that, if we use method of LAGRANGE to find some critical points (as suggested in Remark 1 regarding some special cases), in order to apply the second derivative test we have to compute the Hessian of the Lagrange function $\mathcal{L}$, which is a $(n + 2\,m) \times (n + 2\,m)$ matrix

$$H_{\mathcal{L}}(\boldsymbol{\lambda}, \mathbf{x}) = \begin{pmatrix} \mathbf{0} & -\mathbf{J} \\ -\mathbf{J}^T & H_{\mathcal{L}}(\mathbf{x}) \end{pmatrix},$$

called the *bordered Hessian*[1], where $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \ldots, \lambda_m)$ are the Lagrange multipliers, $\mathbf{x} \in \mathbb{R}^{n+m}$, $\mathbf{J} = \mathbf{G}'$ and $H_{\mathcal{L}}(\mathbf{x})$ is the $(n+m) \times (n+m)$ Hessian of $\mathcal{L}$ with multipliers treated as constants.

To perform the second partial derivative test in this case, one needs to examine the signs s_{2m+1}, $s_{2m+2}, \ldots, s_{n+2m}$ of the last n principal minors of $H_{\mathcal{L}}(\boldsymbol{\lambda}_0, \mathbf{x}_0)$ for every critical point $(\boldsymbol{\lambda}_0, \mathbf{x}_0)$ of $\mathcal{L}$ (the k-th principal minor is the intersection of the first k rows and columns):

1. if $s_k = (-1)^{k-m}$ for all $0 < k - 2m \leqslant n$, then $\mathbf{x}_0$ is a point of local maximum,
2. if $s_k = (-1)^m$ for all $0 < k - 2m \leqslant n$, then $\mathbf{x}_0$ is a point of local minimum,
3. if $s_k \neq 0$ for all $0 < k - 2m \leqslant n$ but the sequence of signs does not fit neither of the above two patterns, then $\mathbf{x}_0$ is a saddle point,
4. if $s_k = 0$ for some $0 < k - 2m \leqslant n$, the test is inconclusive.

5. Critical point classification by using higher order derivatives

If the second partial derivative test is inconclusive for some critical point $\mathbf{x}_0$ of the function F, we can use higher order derivatives in attempt to classify it. Firstly we define a certain family of multivariate polynomials which exhibits certain useful properties.

Definition 4. *A polynomial* $\mathbf{p}: \mathbb{R}^n \to \mathbb{R}$ *is* homogeneous *if* $\mathbf{p}(t\,\mathbf{x}) = t^d\,\mathbf{p}(\mathbf{x})$ *for every* $\mathbf{x} \in \mathbb{R}^n$ *and* $t \in \mathbb{R}$*, where* $d = \deg \mathbf{p}$.

Obviously, if $\mathbf{p}$ is a homogeneous polynomial, then $\mathbf{p}(\mathbf{x}) = 0$ if and only if $\mathbf{x} = \mathbf{0}$. Furthermore, we introduce the following types of homogeneous polynomials.

Definition 5. *Homogeneous polynomial* $\mathbf{p}$ *is* positive semidefinite *resp.* negative semidefinite *if* $\mathbf{p}(\mathbf{x}) \geqslant 0$ *resp.* $\mathbf{p}(\mathbf{x}) \leqslant 0$ *for all* $\mathbf{x} \in \mathbb{R}^n$*. If* $\mathbf{p}(\mathbf{x}) > 0$ *resp.* $\mathbf{p}(\mathbf{x}) < 0$ *for all* $\mathbf{x} \in \mathbb{R}^n \setminus \{\mathbf{0}\}$*, then* $\mathbf{p}$ *is* positive definite *resp.* negative definite.

A practical method for determining whether a homogeneous polynomial $\mathbf{p}$ is positive resp. negative (semi)definite is given in Section 6.

The technique of implicit differentiation of F presented in Section 3 allows us, assuming that f and $\mathbf{G}$ are $k+1$ times differentiable for $k \geqslant 2$, to apply the Taylor formula [6, Theorem 5.4.8] for F at the point $\mathbf{x}_0$. We obtain

$$F(\mathbf{x}) - F(\mathbf{x}_0) = \sum_{r=1}^{k} \frac{1}{r!} \left(D_{\mathbf{x}_0}^{(r)} F\right)(\mathbf{x} - \mathbf{x}_0) + \frac{1}{(k+1)!} \left(d_{\boldsymbol{\xi}}^{(k+1)} F\right)(\mathbf{x} - \mathbf{x}_0), \tag{12}$$

where the point $\boldsymbol{\xi} \notin \{\mathbf{x}, \mathbf{x}_0\}$ lies somewhere on the line segment connecting $\mathbf{x}$ and $\mathbf{x}_0$ and $D_{\mathbf{x}_0}^{(r)} F$ is defined by

$$\left(D_{\mathbf{x}_0}^{(r)} F\right)(\mathbf{x}) = \sum_{\mathbf{r}} \frac{r!}{r_1!\, r_2! \cdots r_n!} \cdot \frac{\partial^r J}{\partial x_1^{r_1}\, \partial x_2^{r_2} \cdots \partial x_n^{r_n}}(\mathbf{x}_0) \cdot x_1^{r_1}\, x_2^{r_2} \cdots x_n^{r_n}, \tag{13}$$

where $\sum_{\mathbf{r}}$ indicates the summation over all n-tuples $\mathbf{r} = (r_1, r_2, \ldots, r_n)$ of nonnegative integers such that $r_1 + r_2 + \cdots + r_n = r$. By definition, $D_{\mathbf{x}_0}^{(r)} F$ is a homogeneous polynomial of degree k.

Now we can state the higher derivative test. Assume that $D_{\mathbf{x}_0}^{(r)} F = 0$ for $r = 1, 2, \ldots, k-1$ and $\mathbf{p}_k := D_{\mathbf{x}_0}^{(k)} F \neq 0$. According to [6, Theorem 5.4.10], the critical point $\mathbf{x}_0$ of F—and hence also the critical point $(\mathbf{x}_0, \mathbf{h}(\mathbf{x}_0))$ of f—is a

1. saddle point if $\mathbf{p}_k$ is indefinite (in particular, this is the case when k is odd),
2. local minimum if $\mathbf{p}_k$ is positive definite,
3. local maximum if $\mathbf{p}_k$ is negative definite.

The test is inconclusive when $\mathbf{p}_k$ is semidefinite but not positive nor negative definite. However, if $\mathbf{p}_k$ is positive semidefinite resp. negative semidefinite there is still a possibility that $\mathbf{x}_0$ is a point of local minimum resp. local maximum of F. This information is reported by our algorithm.

1. See here for the details on bordered Hessian.

The classification of a nontrivial homogeneous polynomial $\mathbf{p}:\mathbb{R}^n\to\mathbb{R}$ in terms of Definition 5 can be significantly simplified by using the fact, stated in [2, Lemma 6.3], that the image of the restriction of $\mathbf{p}$ to the $(n-1)$-sphere S^{n-1} is a segment $[a,b]\in\mathbb{R}$ such that $\mathbf{p}$ is

1. positive semidefinite resp. positive definite if and only if $0=a<b$ resp. $0<a<b$,
2. negative semidefinite resp. negative definite if and only if $a<b=0$ resp. $a<b<0$.

These results are used in our algorithm when applying the higher derivative test. The proof is straightforward and relies on the fact that, by Definition 4, for $\mathbf{x}\in\mathbb{R}^n\setminus\{\mathbf{0}\}$ we have

$$\mathbf{p}(\mathbf{x})=\mathbf{p}\left(\frac{\|\mathbf{x}\|}{\|\mathbf{x}\|}\,\mathbf{x}\right)=\|\mathbf{x}\|^d\,\mathbf{p}\left(\frac{1}{\|\mathbf{x}\|}\,\mathbf{x}\right),$$

where $d=\deg\mathbf{p}$. Note that $\frac{1}{\|\mathbf{x}\|}\,\mathbf{x}\in S^{n-1}$, hence the image of $\mathbf{p}$ is completely determined by the image of the restriction $\mathbf{p}|_{S^{n-1}}$ (except for $\mathbf{x}=\mathbf{0}$, but recall that $\mathbf{p}(\mathbf{0})=0$ always holds).

6. On the difficulty of classifying critical points correctly

[2, Theorem 6.5] was proposed as an alternative, more detailed method for classifying critical points using homogeneous polynomials, supposedly handling the case in which the first non-vanishing polynomial $\mathbf{p}_k$ is semidefinite. However, the claim turns out to be incorrect as shown by the following counter-example: the proposed chain of reasoning leads to a false conclusion when classifying the critical point $(0,0)$ of the function (see Figure 3 and also Fig. 1–2 in [1]) defined by

$$f(x,y)=(2\,x^2-y)\,(y-x^2) \tag{14}$$

and commonly called *Peano surface*. It was devised by GIUSEPPE PEANO to demonstrate the falsity of some of the hitherto accepted criteria for maxima and minima of functions of several variables [1]. The Maclaurin expansion of f is trivial:

$$T_4(x,y)=-y^2+3\,x^2\,y-2\,x^4.$$

According to [2, Theorem 6.5], we find the first non-vanishing homogeneous polynomial. That happens to be $\mathbf{p}_2(x,\,y)=-y^2$. Computing its image on the unit circle S^1, we conclude that $\mathbf{p}_2$ attains the maximal value 0 at points $(-1,0)$ and $(1,0)$, which leads to the case c_5 of [2, Theorem 6.5]. The next homogeneous polynomial which does not vanish on $\mathbf{p}_2^{-1}(0)\cap S^1=\{(-1,0),(1,0)\}$ is $\mathbf{p}_4(x,\,y)=-2\,x^4$, which has negative values on $\mathbf{p}_2^{-1}(0)\cap S^1$. This leads to the case c_{53} which classifies the point $(0,0)$ as being a point of strict local maximum. However, this conclusion coincides with the one often being falsely "deduced" in the past. The truth is that $(0,0)$ is a saddle point since it is the only critical point, $f(0,0)=0$ and $f(t,t)\,f\left(t,\frac{3}{2}\,t^2\right)<0$ for all $t<\frac{1}{2}$. This means that the proof of [2, Theorem 6.5] is flawed.

Observe that the function f has zero values on two parabolas $y=x^2$ and $y=2\,x^2$ shown in Figure 4. The narrow area enclosed by the parabolas, but not including them, is the open set on which f is strictly positive. But, on the interior of the complement of that set f is strictly negative. It is obvious that the restriction of f to an arbitrary line passing through the origin attains a strict local maximum at $(0,0)$, as demonstrated in Figure 4 for the line $x-y=0$. However, this is not sufficient to claim that $(0,0)$ is a point of local maximum of f on $\mathbb{R}^2$. The rigorous, valid check would be to test the critical point $(0,0)$ with the restriction of f to every smooth curve passing through origin—an impossible mission. Hence there is little hope that [2, Theorem 6.5] could be easily fixed. In general, the Taylor expansion of a multivariate function near a critical point of that function simply does not provide enough data to assert that it is not a saddle point.

7. The algorithm

In this section we outline the algorithm, implemented in Giac as the command `extrema` [5], which attempts to solve the problem (4) using implicit differentiation or the method of LAGRANGE (the former is the default, while the latter may be specified by passing the option `lagrange` to the command `extrema`).

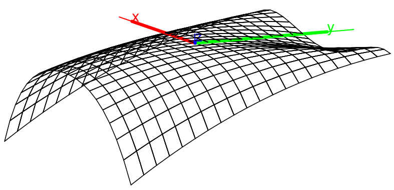

Figure 3. PEANO's function (14)

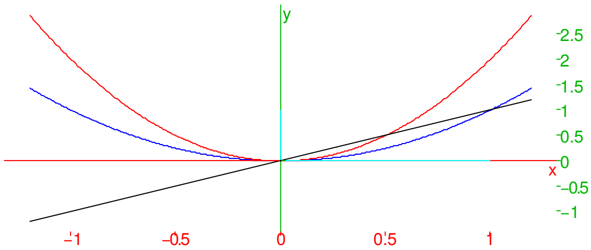

Figure 4. zeros of the PEANO's function

The branch of the algorithm which uses Lagrange multipliers is rather straightforward: after computing critical points, the bordered Hessian is used as the only method of classification. The pseudocode of this branch is given in Algorithm 1.

Algorithm 1
Input: the original constrained local extrema problem 1
Output: a set of (classified) critical points

begin
  $\boldsymbol{\lambda} \leftarrow (\lambda_1, \lambda_2, \ldots, \lambda_m)$, Lagrange multipliers
  $\mathcal{L}(\boldsymbol{\lambda}, \mathbf{x}) \leftarrow f(\mathbf{x}) - \boldsymbol{\lambda} \cdot \mathbf{G}(\mathbf{x})$, the Lagrangian function ($\cdot$ denotes the scalar product)
  solve the system $\nabla \mathcal{L} = \mathbf{0}$, $\mathbf{G} = \mathbf{0}$ to obtain critical points
  label each critical point as unclassified
  $H_{\mathcal{L}} \leftarrow$ the bordered Hessian of $\mathcal{L}$ w.r.t. $\boldsymbol{\lambda}, \mathbf{x}$
  for each critical point $\mathbf{x}_0$ **do**
    for $k = 1, 2, \ldots, n$ **do**
      $M \leftarrow$ the $(2m+k)$-th principal minor of $H_{\mathcal{L}}(\boldsymbol{\lambda}_0, \mathbf{x}_0)$
      $s \leftarrow \operatorname{sgn}(\det M) \in \{-1, 0, 1\}$
      if $s = 0$ **then** label $\mathbf{x}_0$ as unclassified and **break**; **fi**
      if $\mathbf{x}_0$ is labeled with saddle **then continue**; **fi**
      if $s = (-1)^m$ and $\mathbf{x}_0$ is not labeled as strict_max **then**
        label $\mathbf{x}_0$ with strict_min
      else if $s = (-1)^{m+k}$ and $\mathbf{x}_0$ is not labeled as strict_min **then**
        label $\mathbf{x}_0$ as strict_max
      else label $\mathbf{x}_0$ as saddle
      fi
    rof
  rof
end

Here we analyze the branch of the algorithm which uses implicit differentiation. The procedure, given in Algorithm 2, is applied to all distinct formulations of the problem (4) to find as many critical points as possible (see Remark 1). At each instance, critical points are added to the common set and labeled with unclassified. The common set is implemented as a static map with points as keys and labels as values. Unless $L = 1$, an attempt is made to classify critical points: each of them is either a strict local minimum (strict_min), a strict local maximum (strict_max), a saddle point (saddle), a possible (non-strict) local minimum (min?) or a possible (non-strict) local maximum (max?). Also, it may remain unclassified.

The partial derivatives of F are found in succession: the first order derivatives are needed for computing the critical points, but also for obtaining the second order derivatives when applying the Hessian test. If this attempt to classify a critical point fails, the third order derivatives are computed and so on, until the classification succeeds or the limit L is reached. Hence the partial derivatives are always stored once computed.

Algorithm 2
Input: the constrained local extrema problem (4), limit $L \in \mathbb{N}$
Output: a set of (classified) critical points

```
begin
    compute the first order partial derivatives of F
    solve the system ∇F = 0, G = 0 for critical points, add them to the common set
    label each newly found critical point as unclassified
    if L = 1 then return; fi
    compute the second order partial derivatives of F
    H_F ← the Hessian of F
    for each critical point c = (x_0, y_0) found in this instance labeled unclassified do
        {e_1, e_2, ..., e_k} ← the set of distinct eigenvalues of H_F(c)
        e ← 0
        for i = 1, 2, ..., k do
            if e_i = 0 then label c as unclassified and break
            else if e = 0 then
                e ← e_i
                if e > 0 then label c as strict_min
                else label c as strict_max
                fi
            else if e_i e < 0 then label c as saddle
            fi
        rof
        if c is labeled unclassified then
            for k = 2, 3, ..., L do
                fetch or compute the k-th order partial derivatives of F
                p_k ← the k-th hom. polynomial in the Taylor expansion of F near x_0
                if p_k ≢ 0 then
                    if k is odd then label c as saddle
                    else
                        [a, b] ← p_k(S^{n-1}), the image of p_k|_{S^{n-1}} (a = b is possible)
                        if a < 0 < b then label c as saddle
                        else if a > 0 then label c as strict_min
                        else if b < 0 then label c as strict_max
                        else if a = 0 then label c as min?
                        else if b = 0 then label c as max?
                        fi
                    fi
                    break
                fi
            rof
        fi
    rof
end
```

The implementation of the subroutine for finding the partial derivatives of the implicit functions $h_1, h_2, \ldots, h_m$, which are needed for computing the partial derivatives of J, is realized using the simplest data structures—integer arrays—alongside the linear system solver already available in Giac [5]. It is possible because each term in the equations (10), (11) and the analogous equations for higher order is a product of an integer A, a partial derivative $\frac{\partial^r G_j}{\partial x_1^{r_1} \partial x_2^{r_2} \cdots \partial x_n^{r_n}}$ for some $j \in \{1, 2, \ldots, m\}$ and $r = r_1 + r_2 + \cdots + r_n$, and possibly a number of nonnegative powers of partial derivatives of h_1, $h_2, \ldots, h_j$. Each of these factors, except A, can be represented as an array of nonnegative integers. These arrays together with the number A are gathered into a larger structure representing the entire term. Differentiating these terms symbolically is relatively easy to implement since only three rules of differentiation were used: the total derivative formula (7), the chain rule and the product rule.

The homogeneous polynomial $\mathbf{p}_k$ for $k=2,3,\ldots,L$ is computed using (13). To obtain a and b such that $\mathbf{p}_k(S^{n-1})=[a,b]$ (which is always possible as $\mathbf{p}_k$ is continuous, so it maps the connected compact subset $S^{n-1}\subset\mathbb{R}^n$ to a connected compact subset of $\mathbb{R}$, hence $[a,b]$, note that $a=b$ is allowed), we use the same subroutine utilized by `minimize` and `maximize` commands in Giac [5], which computes the global extrema of a multivariate continuous function on a compact domain by applying Karush-Kuhn-Tucker (KKT) conditions. Because of the polynomial input, solving the system of conditions is straightforward.

In the end, the common set contains all critical points found, paired with their class labels. The local minima and local maxima, which are kept in two separate lists, are returned as the solution to the original problem. The rest of data collected in the classification process is dumped to the log stream to provide useful information about saddle points and possible local extrema. Note that setting L to 1 will force the algorithm to skip the classification process (as the order of partial derivatives that are allowed to be computed is limited by L). In that case, only the set of critical points is returned.

It is recommended to set the limit L of the order of partial derivatives to 10 or lower, as the complexity of the algorithm for computing the partial derivatives of order $k\geqslant 2$ is greater than $O(n^{2k}m^2)$, which is the necessary (but not sufficient) number of operations needed to solve a linear system of order $n^k m$. In Giac, the default limit is set to $L=5$.

CONCLUSION

The algorithm described in this text first reduces the original problem to an unconstrained one. Then, two attempts are made: the first one to find the locations of the critical points and the second one to classify them. Note that both attempts may fail. For example, some functions have infinitely many critical points. On the other hand, in some cases computing partial derivatives of higher order—as seen in PEANO's example discussed in Section 6—may not be enough to determine whether a critical point is indeed a local extremum. Also, since our algorithm performs exact computations, classifying a critical point can only use the data available at that precise point. Inspecting the function behavior in a neighborhood of that point can surely help to determine the classification in special cases, but generally cannot be used: it is not clear how to determine the size of the neighborhood, and it is also difficult to assert that no critical points, undetected by the solver, reside in it; there is also the problem of checking whether f is well-defined in each point of the neighborhood. This alternative might, however, be useful to consider when f and $\mathbf{G}$ are polynomials, as the issues mentioned above do not seem to pose a problem in that case.

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