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Global Optimization: Local Minima and Transition Points

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Abstract. We consider the minimization of smooth functions of the Euclidean space with a finite number of stationary points having moderate asymptotic behavior at infinity. The crucial role of transition points of first order (i.e., saddle points of index 1) is emphasized. It is shown that (generically) any two local minima can be connected via an alternating sequence of local minima and transition points of first order. In particular, the graph with local minima as its nodes and first order transition points representing the edges turns out to be connected (Theorem A). On the other hand, any connected (finite) graph can be realized in the above sense by means of a smooth function of three variables having a minimal number of stationary points (Theorem B).

Key words: Global optimization, Local minima, Saddle points, Transition points of first order

1. Introduction and main results

In this paper we consider the minimization of a C^r function, $f, r \geqslant 2$, on the Euclidean space $\mathbb{R}^n$ with Euclidean norm $||\cdot||$. As a general reference we use [2]. The following asymptotic behavior at infinity (A1) guarantees the existence of global minima.

ASSUMPTION A1: $f(x) \to +\infty$ as $||x|| \to \infty$.

Let $Df(x)$ and $D^2f(x)$ denote the row vector of partial derivatives of f and the Hessian matrix of f evaluated at x, respectively. A point $\bar{x} \in \mathbb{R}^n$ with $Df(\bar{x}) = 0$ is called a stationary (or critical) point. Every local minimum is a stationary point. An additional assumption will be that f has a finite number of critical points (A2) and that every critical point is nondegenerate (A3) (i.e., $D^2f(\bar{x})$ is nonsingular if $Df(\bar{x}) = 0$).

ASSUMPTION A2: The function f has a finite number of critical points.

ASSUMPTION A3: All critical points of f are nondegenerate, that is, $||Df(x)|| + |\det D^2f(x)| > 0$ for all $x \in \mathbb{R}^n$.

We note that assumption A3 is not very restrictive; in fact, it is generic (cf. [2, Chapter 7]).

In order to define general descent and ascent directions we introduce a metric. A Riemannian (or variable) metric $\mathcal{R}$ is defined to be a C^r-mapping, $r \geqslant 1$, from $\mathbb{R}^n$ to the cone of symmetric positive definite (n, n)-matrices. The corresponding gradient $\text{grad}_{\mathcal{R}} f$ is the vector $\mathcal{R}^{-1}(x) \cdot D^T f(x)$, where $D^T f$ is the transpose of Df. In particular, if $\mathcal{R}(x) \equiv I$ ($I =$ identity matrix), then $\text{grad}_{\mathcal{R}} f = \nabla f$. Note that the zero set of $\text{grad}_{\mathcal{R}} f$ is precisely the set of critical points of f. Outside the critical point set of f the vector-$\text{grad}_{\mathcal{R}} f$ ($\text{grad}_{\mathcal{R}} f$) is a direction of descent (ascent) in f. The index of a critical point $\bar{x}$ is defined to be the number of negative eigenvalues of the Hessian $D^2 f(\bar{x})$. Based on assumption A3, local minima are critical points of index 0. It turns out that critical (stationary, saddle-) points of index 1 play a crucial role in global optimization. They are also called transition points of first order (where the order refers to the index). Let $\bar{x} \in \mathbb{R}^n$ be a critical point of index 1. Then, the stable manifold $W^s(\bar{x})$ with respect to the gradient vector field $\text{grad}_{\mathcal{R}} f$ is one-dimensional. Here, $W^s(\bar{x})$ is defined to be the set of initial values for which the solution $x(t)$ of the ODE $\dot{x} = \text{grad}_{\mathcal{R}} f(x)$ has the asymptotic property: $\lim_{t \to \infty} x(t) = \bar{x}$. Concerning the stable manifold $W^s(\bar{x})$ we will make the following mild assumption A4.

ASSUMPTION A4: Let $\bar{x} \in \mathbb{R}^n$ be a critical point of index 1 for f and let $\bar{W}^s(\bar{x})$ be the closure of the stable manifold $W^s(\bar{x})$ corresponding to the gradient field $\text{grad}_{\mathcal{R}} f$. Then, the only critical points in the set $\bar{W}^s(\bar{x}) \backslash \{\bar{x}\}$ are (one or two) local minima.

Assumption A4 is mild in the sense that it can be realized by means of a slight C^1-perturbation of the Riemannian metric $\mathcal{R}$. or a slight C^2-perturbation of f near $\bar{x}$.

For a given pair $(f, \mathcal{R})$ satisfying A1–A4 we define the following graph $\Gamma = \Gamma(f, \mathcal{R})$. The nodes of Γ are represented by the local minima of f. Its edges are represented by means of the stable manifolds W^s (with respect to $\text{grad}_{\mathcal{R}} f$) corresponding to the critical points of index 1 for f. Note that an edge might connect two different nodes, but it also might be a loop.

The connectedness of the graph $\Gamma(f, \mathcal{R})$ is of fundamental importance. In fact, if $\Gamma(f, \mathcal{R})$ is connected, then it is possible to connect any two local minimizers by means of a finite sequence min $\to$ 1-order $\to$ min $\to$ 1-order $\to \cdots \to$ min, where 1-order stands for a transition point of first order (i.e., critical point of index 1).

THEOREM A. *Under the assumptions* A1–A4 *the graph* $\Gamma(f, \mathcal{R})$ *is connected.*

REMARK. A version of Theorem A for compact manifolds without boundary was proven in [1]. The case of manifolds with boundary and adaptive metrics is discussed in [3]. In [1, 2] the so called 0-1-0 graph is introduced. Its correspondence with the graph $\Gamma(f, \mathcal{R})$ is as follows: Replace each edge in $\Gamma(f, \mathcal{R})$ (= stable manifold at a critical point of index 1, say $\bar{x}$) by means of a sequence edge-node-edge, where the node is represented by the critical point $\bar{x}$.

Theorem A gives rise to the question what kind of connected graphs may appear as graphs of the type $\Gamma(f, \mathcal{R})$. This is answered by Theorem B.

THEOREM B. *Every connected (finite) graph* Γ *can be realized in* $\mathbb{R}^n$, $n \geqslant 3$, *as a graph of the type* $\Gamma(f, \mathcal{R})$, *where* $(f, \mathcal{R})$ *satisfies the assumptions* A1–A4.

In particular, let $|\Gamma|$ denote the number of nodes of Γ and let v be the cyclomatic number of Γ. We will realize $\Gamma(f, \mathcal{R})$ with a smooth function of three variables which coincides with the quadratic function $(x_1, x_2, x_3) \mapsto x_1^2 + x_2^2 + x_3^2$ outside a compact set, with $\mathcal{R}(x) \equiv I$. The function f will have $|\Gamma|$ local minima, $|\Gamma| + v - 1$ critical points of index 1, v critical points of index 2 and no other critical points.

2. On the special role of first order transition points; proof of Theorem A

The proof of Theorem A is based on ideas from Morse Theory (cf. [2, 4]). In particular, connectivity arguments play the basic role (cf. [1, 2, Theorem 8.4.4]). Let us firstly draw some conclusions from the assumptions A1–A4. With f^a we denote the lower level set $\{x \in \mathbb{R}^n | f(x) \leqslant a\}$. The proofs of the next two lemmas are straightforward.

LEMMA 2.1. *Assumption* A1 *implies that* f^a *is compact for all all* $a \in R$. *Let* C_f *denote the critical point set of* f.

LEMMA 2.2. *If* $a \in \{f(x) | x \in C_f\}$, *then* f^a *is empty or a manifold with boundary.*

For manifolds (with boundary) the concepts connectedness and path connectedness coincide. Therefore, in the sequel we only use the word connectedness.

LEMMA 2.3. *Let* $\bar{c} = \max\{f(x) | x \in C_f\}$. *For* $a > \bar{c}$ *the lower level set* f^a *is connected.*

Proof. For $b > a > \bar{c}$ the sets f^a and f^b are homeomorphic.

In fact, note that $f^{-1}([a, b])$ is compact and does not contain critical points. The desired homeomorphism can be realized by means of integrating the C^1 vector field $||Df||^{-2} \cdot D^T f$. Integrating the latter vector field over the time $b - a$, the level $f = a$ is moved into the level $f = b$, inducing a homeomorphism between f^a and f^b. In particular, there is a one-to-one correspondence between the (connected) components of f^a and those of f^b. Now, let $a > \bar{c}$ and suppose that f^a is not connected. Then, as a compact manifold (with boundary), f^a consists of a finite number of connected components. Choose a point in each component; the latter points are contained in some ball $B = \{x \in \mathbb{R}^n \mid ||x|| \leqslant r\}$. It follows that the set $f^a \cup B$ is connected. With $b = \max\{f(x) | x \in B\}$ we have $b > a$. To each (connected) component of f^b corresponds precisely one component of f^a. This, however, cannot be the case since f^b contains the connected set $f^a \cup B$. $\square$

Next, we recall the role of critical points of index k with respect to the topology of lower level sets. As in the proof of Lemma 2.3 we see: If $b > a$ and $f^{-1}([a, b])$ does not contain critical points, then f^a and f^b are homeomorphic. Consequently, in this case the lower level sets f^a and f^b are the same from a topological point of view. In particular we have $\#(f^a) = \#(f^b)$, where # stands for the number of connected components. Now, suppose that $\bar{x} \in \mathbb{R}^n$ is a critical point of index k, $a < f(\bar{x}) < b$ and that x is the only critical point in $f^{-1}([a, b])$. Then, f^b has the homotopy type of f^a with a k-cell (= k-dimensional ball) attached (along its boundary) (cf. [2, Theorem 2.8.5]). If $k = 0$ (local minimum case), this means that $\#(f^b) = \#(f^a) + 1$. Now, let $k = 1$ (transition point of first order). A 1-cell is a topological copy of the interval [0, 1]. The crucial point is that the boundary of [0, 1] consists of two components $\{0\}$ and $\{1\}$. When attaching a 1-cell there are precisely two possibilities (P1), (P2):

(P1): The two boundary points are attached at two different components of f^a. In this case we have $\#(f^b) = \#(f^a) - 1$. Such a critical point of index 1 is called a decomposition point. In fact, as the function value decreases from b to a, one component splits up (decomposes) into two components.

(P2): The two boundary points are attached to the same component of f^a. In this case, we have $\#(f^b) = \#(f^a)$.

If $k > 1$ (transition points of higher order), the boundary of a k-cell is a sphere S^{k-1} which is connected. Attaching a k-cell to f^a means that the boundary S^{k-1} is mapped continuously to the set f^a. Since the image of a connected set under a continuous mapping is connected, we see that the number of connected components does not change in this case, hence we have $\#(f^b) = \#(f^a)$.

Altogether we have:

$$\#(f^b) = \#(f^a) + 1 \quad \text{iff } \bar{x} \text{ is a local minimum}$$
$$\#(f^b) = \#(f^a) - 1 \quad \text{iff } \bar{x} \text{ is a decomposition point}$$

In all other cases: $\#(f^b) = \#(f^a)$.

Now we are ready to prove Theorem A.

Proof of Theorem A. Let $(f, \mathcal{R})$ satisfy the assumptions A1–A4. Set $C_f = \{\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_p\}$. In case that some of the values $f(\bar{x}_i)$ coincide, we locally perturb f (in the C^2-sense) by adding (locally) suitable small constants to the values $f(\bar{x}_i)$, $i = 1, \ldots, p$. For small perturbations the resulting graph will be isomorphic to $\Gamma(f, \mathcal{R})$. Therefore, we assume in the rest of the proof that the critical values, $f(\bar{x}_i)$, $i = 1, \ldots, p$, are pairwise different. Set $m = \min\{f(x) | x \in C_f\}$, $M = \max\{f(\bar{x}) | x \in C_f\}$. Now let us monotonically increase the functional value, starting at a value $a < m$ and ending up at a value $b > M$. In between we mark the changes in the number of components of the corresponding lower level sets. Note that $\#(f^a) = 0$ (since $f^a = \emptyset$) and that $\#(f^b) = 1$ (since f^b is connected; see Lemma 2.3). Between a and b there is only a change in # at local minima ($\# := \# + 1$) and at decomposition points ($\# := \# - 1$). It follows in particular, that the number of decomposition points is one less than the number of local minima. As in the proof of Theorem 8.4.4 in [2] it follows that the subgraph $\widetilde{\Gamma}(f, \mathcal{R})$ is connected. Here, $\widetilde{\Gamma}(f, \mathcal{R})$ is obtained from $\Gamma(f, \mathcal{R})$ by deleting the edges corresponding to the stable manifolds of those critical points of index 1 which are not decomposition points. But then, $\Gamma(f, \mathcal{R})$ is connected as well. In fact, $\widetilde{\Gamma}(f, \mathcal{R})$ is a spanning tree for $\Gamma(f, \mathcal{R})$. $\square$

3. Proof of Theorem B

In this section we show the main steps in the proof of Theorem B. Let Γ be a connected graph with $|\Gamma|$ nodes and cyclomatic number v. The Riemannian metric $\mathcal{R}$ will be fixed by putting $\mathcal{R}(x) = I$. Set $F(x_1, x_2, x_3) = x_1^2 + x_2^2 + x_3^2$. We will construct a smooth function f of three variables with $\Gamma(f, \mathcal{R})$ isomorphic to Γ. The function f coincides with F outside a ball $B(r)$, where $B(r) = \{x \in \mathbb{R}^3 \mid ||x|| \leqslant r\}$. Its critical point set consists precisely of $|\Gamma|$ local minima, $|\Gamma| + v - 1$ critical points of index 1 and v critical points of index 2.

We note that an example in higher dimensions, say in dimension $n > 3$, will be provided by the function $f(x_1, x_2, x_3) + \sum_{i=4}^{n} x_i^2$.

The function f will be constructed step by step by deforming the initial function F in a suitable way. In fact, in each step a pair of critical points $(\bar{x}, \bar{y})$ of indices (0, 1) and (1, 2), respectively, is inserted. During this process we have to avoid knots in stable manifolds corresponding to critical points of index 1 (see [2, Figure 1.6.5] for such a situation).

The desired pairs of critical points will be inserted by plugging in (slightly deformed) copies of the functions $\varphi(u_1) + u_2^2 + u_3^2$ and $\psi(u_1, u_2) + u_3^2$, where φ and ψ are shaped as in Figure 1.

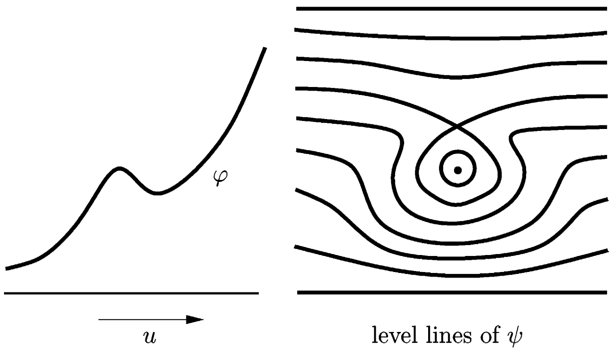

Figure 1. The functions φ and ψ.

Note that the function φ in Figure 1 has one local minimum and one local maximum. Consequently, the function $\varphi(u_1) + u_2^2 + u_3^2$ has one local minimum and one critical point of index 1 (both nondegenerate).

The function ψ in Figure 1 has precisely one saddle point and one local maximum. Hence, the function $\psi(u_1, u_2) + u_3^2$ has one critical point of index 1 and one critical point of index 2 (both nondegenerate).

For the global construction we choose a spanning tree T of the graph Γ. Suppose that a proper subtree $\widetilde{T}$ of T is already established. We show how to insert an additional pair (node $\bar{x}$, edge $\bar{e}$) where the edge $\bar{e}$ connects a given node $\widetilde{x}$ of $\widetilde{T}$ with the node $\bar{x}$.

With $\epsilon > 0$ sufficiently small, let $B_\varepsilon(\widetilde{x})$ be the component of the set $\{x | f(\widetilde{x}) \leqslant f(x) \leqslant f(\widetilde{x}) + \varepsilon\}$ which contains $\widetilde{x}$. Let $S_\varepsilon(\widetilde{x})$ denote the boundary of $B_\varepsilon(\widetilde{x})$. On the set $S_\varepsilon(\widetilde{x})$ we choose a point x_s which is not included in the intersection set of $S_\varepsilon(\widetilde{x})$ with all stable manifolds corresponding to critical points of index 1 (constructed so far). Put $c(\widetilde{T}) = \max\{f(x)|x$ is a local minimum or a critical point of index 1 involved in $\widetilde{T}\}$. We suppose that for some value $a > c(\widetilde{T})$ the function f (constructed so far) coincides with F outside the ball $B(\frac{1}{2}\sqrt{a})$. The integral curve of the ODE $\dot{x} = D^T f(x)$ with the chosen point x_s as initial point intersects the level set $F = a$ in exactly one point, say x_s^a. In a neighborhood of the point x_s^a we may plug in a suitable copy of the function $\varphi(u_1) + u_2^2 + u_3^2$ (+constant) such that the stable manifold corresponding to the new critical point of index 1 (say $x_{\bar{e}}$) contains the point x_s. The latter stable manifold represents the edge $\bar{e}$ new local minimum represents the node $\bar{x}$. In this way we obtain a further update of f. The levels of f exceeding the level $f(x_{\bar{e}})$ have to be adapted in such a way that from a certain level b on, the function f coincides with F outside the ball $B(\frac{1}{2}\sqrt{b})$. This roughly explains the realization of the spanning tree T.

Now we proceed realizing the remaining part of the graph Γ. The cyclomatic number of Γ equals v. We successively insert v pairs of critical points of index (1,2). Suppose that we already realized $v' < v$ edges of $\Gamma\backslash T$. We show how to realize an edge $\bar{e}$ in $\Gamma\backslash T$ which has not yet been constructed. The edge $\bar{e}$, might connect two different nodes (local minima) $\widetilde{x}_1$ and $\widetilde{x}_2$, or it is only connected with one node $\widetilde{x}$ (the case of a loop). We start with the case of two different local minima $\widetilde{x}_1$, $\widetilde{x}_2$. As in the discussion before, we choose again) spheres $S_\varepsilon(\widetilde{x}_1)$ and $S_\varepsilon(\widetilde{x}_2)$ around $\widetilde{x}_1$ and $\widetilde{x}_2$, respectively. On $S_\varepsilon(\widetilde{x}_1)$ we choose a point x_s^1 which is not included in the intersection set of $S_\varepsilon(\widetilde{x}_1)$ with all stable manifolds corresponding to critical points of indices 1 and 2 constructed so far. In a similar way we choose a point x_s^2 on $S_\varepsilon(\widetilde{x}_2)$. Put $c = \max\{f(x)|x$ is a local minimum or a critical point of index 1or 2, constructed so far$\}$. We suppose that for some $a > c$ the function f (constructed so far) coincides with F outside the ball $B(\frac{1}{2}\sqrt{a})$. The integral curves of the ODE $\dot{x} = D^T f(x)$ with the points x_s^1 and x_s^2 as initial points, intersect the level $F = a$ in two points, say x_s^{1a} and x_s^{2a}, respectively. A suitable choice of x_s^1 will guarantee that the points x_s^{1a} and x_s^{2a} are not antipodal on the sphere $F = a$. Let G be the unique geodesic on the sphere $F = a$ connecting x_s^{1a} and x_s^{2a}. Along this geodesic we may plug in a suitable copy of the function $\psi(u_1, u_2) + u_3^2$ (+ constant), such that the stable manifold corresponding to the new critical point of index 1 (say $x_{\bar{e}}$) contains both points x_s^1, x_s^2. The latter stable manifold represents the edge $\bar{e}$. Let $\hat{x}$ denote the new critical point of index 2. The levels of f exceeding the level $f(\hat{x})$ have to be adapted in such a way that from a certain level b on, the function f coincides with F outside the ball $B(\frac{1}{2}\sqrt{b})$. This completes the construction step in case that the edge $\bar{e}$ connects two different nodes (local minima). If $\bar{e}$ is a loop connected to the node $\widetilde{x}$ we choose both points x_s^1 and x_s^2, $x_s^1 \neq x_s^2$, on the same sphere $S_\varepsilon(\widetilde{x})$ and we proceed as above. $\square$

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