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Unique Maximum Likelihood Localization of Nuclear Sources

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***Abstract*— In an earlier paper, [1], we have considered the Maximum Likelihood (ML) localization of a stationary nuclear source using the time of arrival of particles modeled as a Poisson process at a sensing vehicle moving with a constant velocity. In this paper we consider whether the ML location estimate characterized in [1] is unique. Using Morse theory we show that not only is the likelihood function unimodal on either side of the line the sensor moves on (note the source can only be localized uniquely if one knows on which side it resides), but that in fact it has only one critical point in each side and this critical point is the global maximum. These results strongly indicate that gradient ascent maximization will always work. We verify these results with real field data.**

I. Introduction

Localization and tracking of radioactive sources is an area of significant research interest, [1]- [5]. Nuclear materials are difficult to localize as their concentrations and compositions vary greatly. Moreover, they are hidden by shielding material, and immersed in background radiation [6]. While sensors used for their detection [7] are also disparate in nature, in essence they detect by absorbing discrete particles. In this paper as in some others, [1] and [2], we treat this absorption as discrete events modeled as a Poisson process, [8], [9].

We observe that the formulation of the localization problem in [2] involves non-concave expectation maximization and is thus potentially intractable. On the other hand [1] uses Maximum Likelihood (ML) localization, assumes an ideal detector, and ignores timing errors due to the quantum energy-time uncertainty principle, [11]. It assumes that the source is stationary and the detector travels with a known constant velocity. It formulates a likelihood function treating a finite number of arrival times, $t_1, \cdots, t_n$, measured over an infinite horizon, as observations. The maximization of this likelihood function has been shown in [16] to be equivalent to a tractable root locus problem.

Even though the theory in [16] and evidence of simulations in [1] strongly indicate that the *likelihood function is unimodal,* and that in fact it has a solitary critical point, proof of this fact has remained elusive. This paper remedies this lack of proof.

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In particular using an appealing geometrical interpretation of critical points developed in [16], we first prove that the Hessian of the likelihood function is negative definite at every critical point. Then using the powerful machinery of Morse theory, [19]- [24], we prove that this implies that the likelihood function has only one critical point.

Beyond the obvious appeal of unimodality, these results have wide ranging computational implications. The fact that there is only one critical point at which the Hessian is negative definite implies that a gradient ascent algorithm or its variants will converge to the unique maximum. This is so as under mild assumptions, satisfied by the fact that the Hessian is negative definite, gradient ascent must converge to a critical point, [25].

It is noteworthy that though localization from signals like time of arrival (TOA), [17], [18], is very rich, theoretical results for the Poisson arrival model are few and far between. This paper takes a first stride toward establishing such theory.

Section II describes the log likelihood function derived in [1]. Section III proves that the Hessian of the log likelihood function is negative definite at all its critical points. Section IV proves that there is only one critical point, using the pertinent points of Morse theory summarized in the appendix. Section V numerically verifies these results using real data. Section VI is the conclusion. All proofs are omitted due to space constraints.

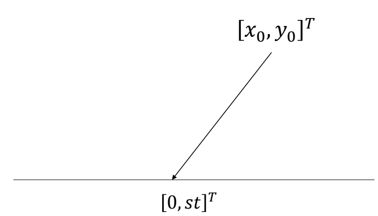

Fig. 1. Ideal detector moving in a straight line with constant velocity.

II. Problem formulation

We assume that the source is at $[x_0, y_0]^T \in \mathbb{R}^2$ and the detector moves at a known constant velocity. Without loss of generality we further assume that as depicted in Figure 1, this trajectory is along the x axis, with velocity $[v, 0]^T$ obeying,

$$v > 0. \tag{II.1}$$

We further assume that the particles arrive at the detector at times governed by an inhomogeneous Poisson process, [15], with mean arrival rate:

$$\lambda(t) = \frac{A_0}{y_0^2 + (x_0 - vt)^2}, \tag{II.2}$$

A_0 being a source strength parameter determined by detector type and the volume, shape and type of the radiation source. This model is obeyed by scintillation devices [14] in isotropic media, but not by directional devices like CZT Compton scattering detectors [13].

Suppose the observed arrival times $\{t_1, \cdots, t_n\}$ are independent on an interval $[T_1, T_2]$. Noting that there are detectors with such short detection time as 150 ms, [12], [1] assumes that the detector can discern particle counts over vanishingly small intervals. Observe that the assumption of a finite n is entirely reasonable as $\lambda(t)$ in (II.2) quadratically approaches zero with $|t|$. Then [1] and [16] show that as $\lim_{T_1 \to -\infty}$ and $\lim_{T_2 \to \infty}$, the maximization of the likelihood function is equivalent to the maximization of

$$L(A_0, x_0, y_0) = -\frac{\pi A_0}{v|y_0|} + n \log A_0 + \sum_{i=1}^{n} \log\left(\frac{1}{y_0^2 + (x_0 - c_i)^2}\right), \tag{II.3}$$

where

$$c_i = vt_i. \tag{II.4}$$

As v is known estimation of A can be accomplished by estimating

$$\bar{A}_0 = \frac{A_0}{v}$$

In this case (II.5) can be replaced by

$$\begin{aligned} L(\bar{A}_0, x_0, y_0) &= -\frac{\pi \bar{A}_0}{|y_0|} + n \log \bar{A}_0 + n \log v \\ &+ \sum_{i=1}^{n} \log\left(\frac{1}{y_0^2 + (x_0 - c_i)^2}\right). \end{aligned} \tag{II.5}$$

Suppose $A_0 > 0$, x and $y \geq 0$ are the ML estimates of $\bar{A}_0 > 0$, x_0 and $y_0 \geq 0$. Then they satisfy the critical point equations

$$A_0 = \frac{n|y|}{\pi}, \tag{II.6}$$

$$\sum_{i=1}^{n} \frac{x - c_i}{y^2 + (x - c_i)^2} = 0, \tag{II.7}$$

$$\sum_{i=1}^{n} \frac{1}{y^2 + (x - c_i)^2} = \frac{n}{2y^2}. \tag{II.8}$$

As neither the physical context nor these equations can distinguish between $\pm y$ uniqueness, of the solutions to (II.6-II.8) will refer to uniqueness in the half plane

$$A_0 > 0 \text{ and } y \geq 0. \tag{II.9}$$

Also note that because of (II.6) this in turn is equivalent to there being a unique solution to (II.7,II.8) for $y \geq 0$. Unsurprisingly, for $n = 2$, there is no unique solution as two observations cannot be used to uniquely determine three variables. Indeed for $n = 2$ any

$$y^2 = |x - c_1||x - c_2| \tag{II.10}$$

simultaneously satisfies (II.7,II.8). Thus we will focus on $n > 2$.

Finally, we note that as $L(A_0, x, y)$ approaches $-\infty$ as y approaches 0 or ∞ and is finite when $y > 0$ it must have a maximum in the set defined by (II.9). As it is also analytic in this half plane (II.6-II.8) must have at least one solution in (II.9).

III. Properties of the Hessian

We begin with a geometrical interpretation of the critical points obeying (II.7) and (II.8) given in [16].

Lemma 3.1: Consider any simultaneous root (x, y) of (II.7,II.8). Define

$$\theta_i = \arctan\left[\frac{y}{x - c_i}\right]. \tag{III.11}$$

Then the following hold.

$$\sum_{i=1}^{n} \sin 2\theta_i = 0 \text{ and } \sum_{i=1}^{n} \cos 2\theta_i = 0 \tag{III.12}$$

In other words with θ_i the phase of $x - c_i + jy$ one has the appealing equality

$$\sum_{i=1}^{n} e^{j2\theta_i} = 0 \tag{III.13}$$

at a critical point. As depicted in Figure 2 for $n = 3$, the θ_i represent the angle made by the source with the x-axis at each point of detection.

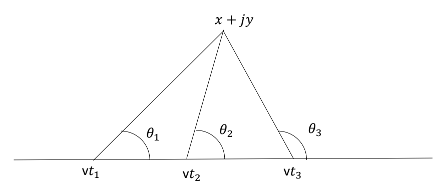

Fig. 2. Depiction of θ_i when $n = 3$.

It is readily seen that for $y \geq 0$ the Hessian of $L(A_0, x, y)$ is given by

$$\begin{bmatrix} -\frac{n}{A_0^2} & 0 & \frac{\pi}{y^2} \\ 0 & -2\sum_{i=1}^{n} \frac{y^2 - (x-c_i)^2}{(y^2 + (x-c_i)^2)^2} & 4y\sum_{i=1}^{n} \frac{x - c_i}{(y^2 + (x-c_i)^2)^2} \\ \frac{\pi}{y^2} & 4y\sum_{i=1}^{n} \frac{x - c_i}{(y^2 + (x-c_i)^2)^2} & -\frac{2\pi A_0}{y^3} - 2\sum_{i=1}^{n} \frac{(x-c_i)^2 - y^2}{(y^2 + (x-c_i)^2)^2} \end{bmatrix}$$

and at a critical point, it is evident using (II.6) that this becomes the alternative expression for the Hessian $H(x, y)$ that equals:

$$\begin{bmatrix} -\frac{\pi^2}{ny^2} & 0 & \frac{\pi}{y^2} \\ 0 & -2\sum_{i=1}^{n} \frac{y^2 - (x-c_i)^2}{(y^2 + (x-c_i)^2)^2} & 4y\sum_{i=1}^{n} \frac{x - c_i}{(y^2 + (x-c_i)^2)^2} \\ \frac{\pi}{y^2} & 4y\sum_{i=1}^{n} \frac{x - c_i}{(y^2 + (x-c_i)^2)^2} & -\frac{2n}{y^2} - 2\sum_{i=1}^{n} \frac{(x-c_i)^2 - y^2}{(y^2 + (x-c_i)^2)^2} \end{bmatrix}.$$

We next provide a Lemma that simplifies the proof of negative definiteness of $H(x, y)$ at critical points.

Lemma 3.2: With $y \geq 0$, at any solution of (II.6-II.8), the matrix in (III.14) is negative definite iff the matrix below is negative definite:

$$G(x,y) = \begin{bmatrix} -2\sum_{i=1}^n \frac{y^2-(x-c_i)^2}{(y^2+(x-c_i)^2)^2} & 4y\sum_{i=1}^n \frac{x-c_i}{(y^2+(x-c_i)^2)^2} \\ 4y\sum_{i=1}^n \frac{x-c_i}{(y^2+(x-c_i)^2)^2} & -4\sum_{i=1}^n \frac{(x-c_i)^2}{(y^2+(x-c_i)^2)^2} \end{bmatrix}. \tag{III.14}$$

We next focus on $G(x,y)$ and prove that it must be at least negative semidefinite at a critical point. To this end the lemma below exploits (III.12) to relate $G(x,y)$ to the θ_i define in Lemma 3.1.

Lemma 3.3: With θ_i defined in Lemma 3.1, suppose (III.12) holds. Then $G(x,y)$ in (III.14) can be expressed as:

$$y^2G(x,y) = -\sum_{i=1}^n \begin{bmatrix} \cos 2\theta_i \\ \sin 2\theta_i \end{bmatrix} \begin{bmatrix} \cos 2\theta_i & \sin 2\theta_i \end{bmatrix}. \tag{III.15}$$

Thus indeed at all critical points the Hessian is negative semidefinite. Let us now consider the $n=2$ case. Observe that at a critical point, by multiplying both sides of (II.7) by y we obtain

$$\sin 2\theta_1 = -\sin 2\theta_2. \tag{III.16}$$

From (II.8) we get

$$\sin^2\theta_1 + \sin^2\theta_2 = 1$$

i.e.

$$\cos^2\theta_1 = \sin^2\theta_2 \text{ and } \cos^2\theta_2 = \sin^2\theta_1. \tag{III.17}$$

As $\theta_i \in (0,\pi)$ and the θ_i are distinct both cannot be $\pi/2$. Without loss of generality assume $\theta_1 \neq \pi/2$. Further $\theta_2 \notin \{0,\pi\}$. Then from (III.16) and (III.17) we obtain:

$$\frac{2\sin\theta_1\cos\theta_1}{\cos^2\theta_1} = -\frac{2\sin\theta_2\cos\theta_2}{\sin^2\theta_2}$$

i.e. $\tan\theta_1\tan\theta_2 = -1$. Then as

$$|\tan\theta_1 - \tan\theta_1| = \left|\frac{\tan\theta_1 - \tan\theta_2}{1+\tan\theta_1\tan\theta_2}\right| = \infty$$

we obtain $|\theta_1 - \theta_2| = \frac{\pi}{2}$. As $|2\theta_1 - 2\theta_2| = \pi$, $[\cos 2\theta_1, \sin 2\theta_1] = -[\cos 2\theta_2, \sin 2\theta_2]$. In particular this means that $H(x,y)$ is singular at critical points. This totally accords with our observation that for $n=2$ there is a continuum of points that form critical points of $L(A,x,y)$.

We now prove that in fact for $n>2$, $H(x,y)$ is negative definite at every critical point.

Theorem 3.1: Suppose the c_i in (II.4) are distinct and $n>2$. Then for all A,x,y that satisfy (II.6-II.8), the Hessian of $L(A,x,y)$ in (II.5) is negative definite.

Thus indeed for $n>2$, the Hessian of $L(A,x,y)$ is negative definite at every critical point. In the next section we invoke Morse theory to show that this not only means that $L(A,x,y)$ is unimodal, but that it in fact has precisely one critical point in the half plane defined by (II.9).

IV. Unimodality of $L(A,x,y)$

For technical convenience we will convert the maximization in $\mathbb{R}^3$ to an equivalent problem in $\mathbb{R}^2$. To this end observe that as (II.6) holds at critical points of $L(A,x,y)$, for $y \geq 0$, the maximization of $L(A,x,y)$ is equivalent to the maximization of

$$\begin{aligned} J(x,y) &= L(A,x,y)|_{A=\frac{ny}{\pi}} = -n + n\log\frac{n}{\pi} + n\log v \\ &+ n\log y + \sum_{i=1}^n \log\frac{1}{y^2+(x-c_i)^2}, \end{aligned} \tag{IV.18}$$

with A determined by (II.6). In particular

(A) $J(x,y)$ has the same number of critical points in the domain $y \geq 0$ as does $L(A,x,y)$ in the domain (II.9).

(B) The nature of the critical points of $J(x,y)$ in $y \geq 0$ and $L(A,x,y)$ in (II.9), are the same.

Indeed the lemma below confirms (A).

Lemma 4.1: The number of critical points of the utility function $L(A,x,y)$ in (II.5) in the domain (II.9) equals the number of critical points as $J(x,y)$ in (IV.18) in the domain $y \geq 0$.

Proof: The gradient of $J(x,y)$ is given by

$$\nabla J(x,y) = \begin{bmatrix} -2\sum_{i=1}^n \frac{x-c_i}{y^2+(x-c_i)^2} \\ \frac{n}{y} - 2\sum_{i=1}^n \frac{y}{y^2+(x-c_i)^2} \end{bmatrix}. \tag{IV.19}$$

Thus the critical points of $J(x,y)$ satisfy (II.7,II.8). Observe from (II.6) that if a critical point of $L(A,x,y)$ satisfies $y>0$ then it also satisfies $A>0$. Further, $y \neq 0$ at every critical point of both $L(A,x,y)$ and $J(x,y)$. The result follows from the fact that there are as many solutions to (II.6-II.8) in (II.9) as there are of (II.7,II.8) for $y \geq 0$. ■

The next lemma also confirms that the Hessian of $J(x,y)$ is negative definite at each of its critical points.

Lemma 4.2: Under the conditions of Theorem 3.1, for $n>2$, the Hessian of $J(x,y)$ is negative definite at every critical point of $J(x,y)$ in the domain $y \geq 0$.

Proof: The Hessian of $J(x,y)$ is given by

$$\begin{bmatrix} -2\sum_{i=1}^n \frac{y^2-(x-c_i)^2}{(y^2+(x-c_i)^2)^2} & 4y\sum_{i=1}^n \frac{x-c_i}{(y^2+(x-c_i)^2)^2} \\ 4y\sum_{i=1}^n \frac{x-c_i}{(y^2+(x-c_i)^2)^2} & -\frac{2n}{y^2} - 2\sum_{i=1}^n \frac{(x-c_i)^2-y^2}{(y^2+(x-c_i)^2)^2} \end{bmatrix} \tag{IV.20}$$

and is the bottom 2×2 principal submatrix of $H(x,y)$ in (III.14). The result follows from Theorem 3.1. ■

Then the main theorem below is proved by invoking Morse theory whose pertinent points have been presented in the appendix to prove the main result in Theorem 4.1 below. The salient point of the appendix is the following. Suppose a convex domain $\mathscr{D} \subset \mathbb{R}^2$ has a boundary which at each point can be locally described by $g=0$, where g is a smooth function. Suppose a smooth function $f(\cdot): \mathscr{D} \to \mathbb{R}$ has a positive definite Hessian at every critical point in $\mathscr{D}$ and obeys Assumption A.1. Then $f(\cdot)$ has only one critical point in $\mathscr{D}$ which is a minimum.

Theorem 4.1: Under the conditions of Theorem 3.1, for $n>2$, $L(A,x,y)$ has precisely one critical point in (II.9). Further this critical point is the only maximum in (II.9).

Thus indeed $L(A,x,y)$ has precisely one critical point, the global maximum, in (II.9). Observe that with $v=1$, $y>0$

$$\nabla L(A,x,y) = \begin{bmatrix} -\frac{\pi}{y}+\frac{n}{A} \\ -2\sum_{i=1}^{n}\frac{x-c_i}{y^2+(x-c_i)^2} \\ \frac{\pi A}{y^2}-2\sum_{i=1}^{n}\frac{y}{y^2+(x-c_i)^2} \end{bmatrix}. \qquad \text{(IV.21)}$$

Then the gradient ascent algorithm

$$\begin{bmatrix} \dot{\hat{A}} \\ \dot{\hat{x}} \\ \dot{\hat{y}} \end{bmatrix} = \nabla L(A,x,y)|_{(A,x,y)=(\hat{A},\hat{x},\hat{y})} \qquad \text{(IV.22)}$$

initialized with $\hat{y}(0)>0$ $\hat{A}(0)>0$ and augmented with projection will converge to the only critical point, the global maximum, in (II.9).

V. Numerical Results

We now present some numerical results to illustrate our analysis.

Figure 3 shows the likelihood function $L(A_0,x,y)$ in the neighborhood of the true source location (x_0,y_0) with simulated random arrival times. It is clear from this figure that in the range of x,y shown in this plot, the unique local maximum is close to the true source location. The figure also shows the evolution of estimates of the source location over iterations of a fixed-point algorithm described in [1]. While no theoretical guarantees are available for this fixed-point algorithms, our results in this paper show that a gradient search will converge to the maximum likelihood estimate, and we can see from Fig. 3 that the fixed-point estimates appear to follow the gradient of the likelihood function.

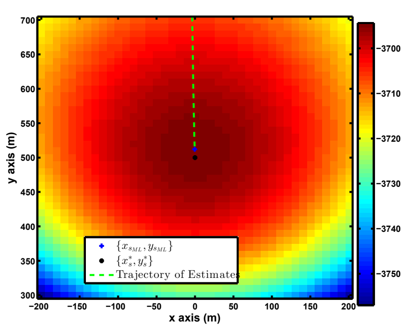

Fig. 3. Heatmap of the likelihood function.

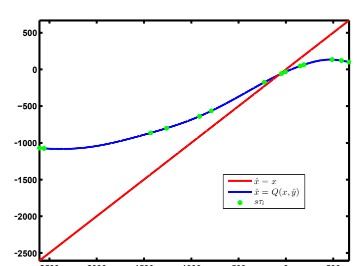

Fig. 4. Illustrating the uniqueness of the x coordinate solution to the critical equation.

Figure 4 shows the function

$$Q(x) \doteq \frac{\sum_i vt_i\alpha(x,y_0,t_i)}{\sum_i \alpha(x,y_0,t_i)}$$

where

$$\alpha(x,y,t) \doteq \frac{1}{y^2+(x-vt)^2}.$$

Note that the critical point equations (II.6) defining the maximum likelihood estimate satisfies $Q(x)=x$. This plot visually illustrates the uniqueness of the solution to the critical equation for the x coordinate.

Figure 5 shows 10 time-series of *actual* measured radiation intensity as a function of position from a sensor moving with a constant speed of approximately 1 m/s for a period of 512 seconds. The same figure also shows estimates of the source location obtained using the fixed-point algorithm described in [1]. Although the ground truth source location is unknown, we can see that the estimates from the different time-series are consistent with each other in the sense of being clustered close to their mean value as we would expect from observations of the same source.

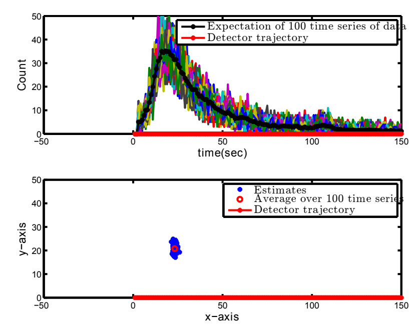

Fig. 5. Source location estimates with noisy radiation measurements.

VI. Conclusion

We have considered the maximum likelihood estimation of a static radiation source from measurements of the time of arrival of particles at a sensor moving with a constant velocity. Under mild assumptions a previous reference [1] formulated a likelihood function. Simulations in [1] strongly suggest that the likelihood function is unimodal, on either side of the line on which the detector travels.

In this paper we leverage Morse theory to prove unimodality. This opens up the prospect of localization through gradient ascent as well as a number of directions of future research: Can we localize when the detector traverses on nonlinear trajectories? Will that improve the quality of detection? Can we use gradient ascent to track a relatively slowly moving source? These directions are being jointly pursued at ANU and Iowa.

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A.1. Background on Morse Theory

Morse theory deals with results concerning the nature of critical points on manifolds, see e.g. [19], [20]. [21].

Let M be a smooth m-dimensional manifold and let $f : \mathscr{M} \to \mathbb{R}$ be a smooth function defined on $\mathscr{M}$. A critical point of f is a point at which the gradient of f is zero. The function f is said to be a Morse function if the Hessian is nonsingular at every critical point (equivalently, each critical point is nondegenerate). In any particular coordinate basis, the Hessian is an $m \times m$ matrix, and the number of its negative eigenvalues (which is invariant with the coordinate basis) is termed the index of the critical point. A critical point of index 0 is thus a minimum of f and a critical point of index m is a maximum.

Any manifold $\mathscr{M}$ has associated with it an integer number called its Euler characteristic $\chi(\mathscr{M})$, which is a particular topological invariant. All manifolds that can be smoothly contracted to a point, e.g. *any convex set* in $\mathbb{R}^2$ and $\mathbb{R}^3$, have $\chi(\mathscr{M}) = 1$. A key and basic result of the theory is the following:

Theorem A.1: Let $\mathscr{M}$ be a smooth compact m-dimensional manifold and $f : M \to \mathbb{R}$ a Morse function. Let $n_i(\mathscr{M})$ denote the number of critical points of f with index i. Then there holds

$$\sum_{i=1}^{m} (-1)^i n_i(\mathscr{M}) = \chi(\mathscr{M}) \quad \text{(A.1)}$$

In the above theorem, the terminology regarding $\mathscr{M}$ is taken to imply that any neighborhood in $\mathscr{M}$ can be defined by a set of simultaneous equalities, but not equalities together with some adjoined inequalities or inequalities alone. (It may be that the same equalities and inequalities apply globally in $\mathscr{M}$, but this is not necessary.) Thus $\mathscr{M}$ could be a sphere S^2 in $\mathbb{R}^3$, defined by $x^2 + y^2 + z^2 = 1$, but it cannot be the open ball defined by $x^2 + y^2 + z^2 < 1$, or the closed ball $x^2 + y^2 + z^2 \leq 1$. To treat such cases, one works with the concept of a "manifold-with-boundary", see [19], [21]. A manifold-with-boundary is a concept which accords with intuition, but there are additional technical requirements.

The concept may have been first treated in [22], and though generalizations have since been obtained, see e.g. [21], it is easiest in this paper to work with the ideas and requirements of [22] as they are simpler.

The manifolds in question are connected bounded open domains in $\mathbb{R}^m$ with the property that at each point p_0 on the boundary, the boundary can be locally described by an equation of the form $g = 0$ where g is a smooth function. In particular, in two-dimensional space, one could have an axis-parallel rectangle with rounded corners (to provide the smoothness).

In addition to the properties of the manifold $\mathscr{M}$ itself, the function f is more tightly constrained than simply being a Morse function. In particular, we require that

Assumption A.1: 1) f has no critical points on the boundary.

2) the gradient of f points outwards from the boundary, i.e. its inner product with the outward normal to the boundary is positive.

In [22], these conditions are termed "boundary conditions β". They are presented as a development of "boundary conditions α", which require that f be constant on the boundary.

The relevant result, a straightforward generalization of Theorem A.1, is

Theorem A.2: Let $\mathscr{M}$ be a smooth bounded m-dimensional manifold-with-boundary, such that at each point p_0 on the boundary, the boundary can be locally described by an equation of the form $g = 0$ for some smooth g. Suppose further that $f : M \to \mathbb{R}$ is a Morse function smoothly extendable to include a domain including the boundary of $\mathscr{M}$, and satisfying Assumption A.1. Let $n_i(\mathscr{M})$ denote the number of critical points of f in $\mathscr{M}$ with index i. Then (A.1) holds.

This then allows statement of the following theorem, obtained by introducing special knowledge concerning the number of critical points associated with each index. Results such as the following have been used before, see e.g. [23] and [24].

Theorem A.3: Let $\mathscr{M}$ be a smooth bounded m-dimensional manifold-with-boundary, contractible to a point, and such that at each point p_0 on the boundary, the boundary can be locally described by an equation of the form $g = 0$ for some smooth g. Suppose further that $f : \mathscr{M} \to \mathbb{R}$ is a Morse function smoothly extendable to include a domain including the boundary of M, and satisfying Assumption A.1. Suppose that every critical point of f in $\mathscr{M}$ is a minimum. Then f has a single minimum and in fact a single critical point in $\mathscr{M}$.