Optima localization by vehicle formations imitating the Nelder-Mead simplex algorithm

Shahab Kalantar · Uwe R. Zimmer

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Abstract In this paper, we address the problem of localizing extrema points and iso-contours of ambient environmental fields (specifically, ocean bottom landscape and underwater plumes) using a networked formation of autonomous underwater vehicles. We propose the use of the Nelder-Mead extension to the basic simplex nonlinear optimization algorithm. In these robust gradient-free strategies, decisions are solely made based on field values measured by the individual vehicles, while measurements are fused and actions decided according to the algorithm. A main goal of this paper is to trigger interest in direct search methods as pertains to this type of robotic problem.

Keywords Distributed control · Swarm · Formation · Localization · Nelder-Mead · Simplex

1 Introduction

This paper deals with navigation strategies for formations of autonomous underwater vehicles for the purpose of collectively localizing optima or iso-contours of an ambient underwater field (such as salinity or heat) or bottom terrain. This problem has been of increasing interest in the past few years. Such robotic systems can potentially have many useful applications. Locating deepest or highest points on a natural

landscape, locating heat sources, and finding boundaries of a pollutant plume, are promising candidates.

Development in this area closely mimics that of function optimization theory, where optima of an arbitrary function are sought. Here, though, the environmental field plays the role of the function. The problem is usually considered in two dimensions. Some fields are intrinsically two dimensional (for example, bottom terrain). For three-dimensional phenomena (usually the result of some diffusion process), their projection on a horizontal plane is considered. Robots move constrained to this plane and sample the field.

Previous approaches: Mathematically speaking, if the field is smooth, the local gradient is the only information needed by a single robot to ascend or descend on the field. Guided by the gradient, the vehicle would always end up in a local optimum, depending on the case. The gradient is the main ingredient of a *first-order* approximation of the field. As such, the reached local optima may not be global ones. The method can be made more sophisticated by taking into account more terms of the Taylor series expansion which contain higher-order derivatives of the field (such as the Hessian). Derivative-based methods are the backbone of traditional optimization theory. Naturally enough, some robotics researchers have been prompted to use these techniques in applications where an environmental field plays the role of an objective function. The basic idea is to model the field around a local optimum q_0 by the quadratic (*second order*) approximation

$$\begin{aligned} F(q) &\approx \hat{F}(g) \\ &= \hat{c} + \hat{g}^T (q - q_0) + (1/2)(q - q_0)^T \hat{H} (q - q_0) + \varepsilon \end{aligned} \quad (1)$$

where $\hat{g}$ is an estimate of the gradient $\nabla F(q_0)$, $\hat{H}$ is an estimate of the Hessian $\nabla^2 F(q_0)$, $\hat{c}$ is an estimate of $F(q_0)$,

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S. Kalantar (✉) · U.R. Zimmer
College of Engineering and Computer Science, Australian
National University, Canberra, ACT 0200, Australia
e-mail: shahab.kalantar@rsise.anu.edu.au

U.R. Zimmer
e-mail: uwe.zimmer@ieee.org

and ε represents higher-order terms (assumed negligible). If a first-order approximation is deemed sufficient, a single robot, capable of estimating the gradient on its own, can use the control rule $\dot{q}(t) = -\hat{g}$. If the Hessian can also be estimated, the control rule would be $\dot{q}(t) = -\hat{H}^{-1}\hat{g}$ (see Robinet 2004). In practice, a single robot should visit a number of points, sample them and then employ some technique to estimate the gradient and/or the Hessian (see Pang et al. 2003 for an example). The parameters of the model are computed as functions of geometric relationships between sample points. In a multi-robot system, this process can be accelerated. In Byrne et al. (2003), robots in an aggregate home in on a source using least squares methods for estimating parameters of a quadratic model. In Ögren et al. (2002), triangular formations (using finite difference for gradient estimation) and square-shaped formations (using centred finite differences) are discussed. In Ögren et al. (2004), more general formations are considered using least squares methods for estimating the gradient. To reduce estimation error in methods based on first-order approximations, the shape of the formation (i.e., the degrees of freedom in a multi-robot system) has to be adjusted (Zhang and Leonard 2005; Ögren et al. 2002, 2004). Expressions for optimal inter-robot distances involve entries of the Hessian. The basic idea is to compute formation parameters by minimizing the statistical functional $E[(x - \hat{x})^T(x - \hat{x})]$ where $x = (F(q_0), \nabla F(q_0))$ and $\hat{x} = (\hat{c}, \hat{g})$. Additionally, history of measurements and an iterative estimation scheme (such as the Kalman filter) can be used to improve estimation (Ögren et al. 2004).

As opposed to gradient-based methods, *zero-order* methods do not rely on the estimation of derivatives of the objective function. These methods can roughly be classified as *derivative-free* methods which approximate the objective function without using Taylor series expansions and *direct search* methods which only require the *relative ranks* of a countable set of function values (for unconstrained optimization). There is a lot of confusion in the relevant literature about this nomenclature. The above definition of a direct search is taken from Lewis et al. (2000). Examples of derivative-free methods include *trust-region* methods which use linear or quadratic models, assumed to be valid in a region around the current iterate. Optima of the local model is chosen as the next iterate. Examples of direct search methods include the simplex method, the Nelder-Mead modified simplex method, and pattern search methods. Unlike gradient-based methods, in which the current solution is updated by a *differential inclusion* (thus moving continuously), the current solution (iterate) in a zero-order method jumps from one iteration to the next. In a formation employing a zero-order method, one robot in the aggregate represents the current iterate and some of the robots visit a special pattern of positions. A comparison of values of the field at these positions determines one of the positions already occupied or visited by a robot as the next iterate. Gradient-free

methods are used when the objective function is too noisy and it is meaningless to even talk about gradients. This is the main characteristic of natural fields. Direct search techniques fell out of favour in the optimization community for decades because they were based on seemingly ad-hoc rules. Only recently, convergence results have been discovered for them, putting them back in favour again (Kolda et al. 2003; McKinnon 1998; Lagarias et al. 1998; Wright 1996; Conn et al. 1997). As early as 1996, the authors of (Burian et al. 1996) propose the use of the simplex method as one which is especially suited to underwater applications. In Silva et al. (2004), de Sousa et al. (2005, 2006), and Speranzon et al. (2004), formation coordination strategies based on the simplest form of simplex search are proposed. In Kalantar and Zimmer (2007a, 2007b), the simple simplex method has been extended to incorporate the capability to traverse iso-contours. The strength of the simplex approach stems from the fact that only relative values are used and not the exact ones.

Proposed approach: In this paper, we take this a step further by considering the modified versions of the simplex search which is superior to the basic simplex strategy. However, our aim in this paper is not to propose particular strategies but rather to emphasize the general underlying structure of zero order methods and arrive at a general framework that can be used for modelling and coordinating the class of aggregates which employ these methods. This paper is a first step towards this goal. Zero-order methods are very robust and, in most cases, converge very quickly to a vicinity of optima. However, they are not generally suitable for fine tuning. For this purpose, some researchers have proposed combining the two main strategies and switch to a Newton-type algorithm when close enough to optima. We do not pursue this possibility here. Refer to Kolda et al. (2003) for detailed exposition of recent trends in this area.

The proposed strategy is based on the Nelder-Mead version of the simplex optimization method. In this gradient-free method, decisions are solely made based on field values measured by the individual vehicles, while measurements are fused according to the algorithm. Unlike the basic simplex method, Nelder-Mead algorithm acts aggressively, trying to explore longer distances if there is any chance of improvement. We make several modifications. Some have already been introduced in the optimization literature. Simplex gradients are used to avoid immature stagnation. Constraints are enforced to prevent the formation from getting too much deformed or getting too small. The α -constrained method is used to constrain the formation to certain areas and avoid obstacles. Several other relevant modifications are discussed, as well convergence results. Some issues particular to implementation on robots in the real world, as well as globalization of the search, are elaborated on. The simplex algorithm is a discrete process. As such, hybrid automata

Fig. 1 Vehicles and networks,
(a) Serafina. (b) Three-vehicle
formation immersed in a field
(top view)

(a)

(b)

can be employed as appropriate tools for modelling and controller design. The hybrid state automaton introduced here plays the role of the virtual formation controller. Of particular interest here is that unlike most robotic formation applications, those which implement direct search methods cannot be rigid (Eren 2004) as the formation itself becomes part of the search algorithm and thus call for a more general strategy for formation control.

Physical setups: The strategies discussed here is not targeted towards any specific vehicle. Any underwater vehicle with the following set of generic capabilities could be a candidate:

1. Communication with peer robots in the network. This capability is crucial to synchronization of actions. Long wave radio is a potential means.
2. Measurement of range and bearing to other robots. A synchronized combination of optical and ultra-sound sensor modules can be used for this purpose.
3. Global orientation sensing (using a compass module). This is used for calculating the heading of a robot.
4. Ambient water flow sensing for keeping station.
5. Depth sensing (using pressure sensors). We assume that the vehicles move on a horizontal plane parallel to the surface of the water.
6. Field sensing. The type of sensor is application specific. Examples include temperature and salinity sensors, and sonar for underwater landscape.
7. GPS sensing when resurfacing.

Figure 1 shows a Serafina robot and a network consisting of three Serafinas (see <http://users.rsise.anu.edu.au/~serafina/> for more detail). While moving on the plane, robots can be controlled to go to desired positions expressed relative to

positions and headings of other reference robots. The low-level control system is composed of two sub-controllers: (1) the *horizontal controller* produces torques for the horizontal thrusters for moving on a plane, and (2) the *vertical controller* produces torques for vertical thrusters for stabilization on the desired plane of motion. In this paper, we will not concern ourselves with any of the above low-level issues as we focus here on planning.

Paper organization: We begin, in Sect. 2, by stating the basic Nelder-Mead simplex algorithm, along with introducing the relevant notations and definitions. Following that, in Sect. 3, we will some convergence properties of the basic algorithm. Section 4 is devoted to a short account of numerous modifications of and improvements to the basic version which have been reported in the literature. The shape constraint and necessary modifications are discussed in Sect. 5. The modified algorithm is stated in Sect. 6. In Sect. 7, actual implementation on robotic platforms is discussed. Finally, simulation results are presented in Sect. 8 to demonstrate the algorithm.

2 Basic Nelder-Mead algorithm

The Nelder-Mead algorithm (Nelder and Mead 1965) belongs to the class of direct search algorithms which do not require the knowledge of the gradient. It is primarily used for the unconstrained minimization of an objective function f which can be nonconvex, discontinuous or noisy. In the planar case, the problem is defined as

$$\min_{q \in \mathcal{R}^2} f(q). \quad (2)$$

We use the notation $S[q_i, q_2, q_3]$ to represent a planar simplex with respective vertices. The algorithm starts with an

initial simplex $S^{(0)}$, composed of three points (vertices) $q_1^{(0)}$, $q_2^{(0)}$, and $q_3^{(0)}$ in the plane. The simplex is then iteratively changed to generate the sequence $S^{(k)}$ of simplexes. We use the notation $q^{(k)} = (q_1^{(k)}, q_2^{(k)}, q_3^{(k)})^T$ to denote the *positional state* of the algorithm. The change to positions of the vertices of $S^{(k)}$ are made based on the values $f(q_1^{(k)})$, $f(q_2^{(k)})$, and $f(q_3^{(k)})$, which leads to the generation of $S^{(k+1)}$. The algorithm terminates if some function T of the values at the vertices satisfies an inequality of the general form $T(q^{(k)}) \leq \varepsilon$. It is required that $S^{(0)}$ be non-degenerate, i.e., the vectors $q_i^{(k)} - q_j^{(k)}$, $i, j = 1, 2, 3$, $i \neq j$, be linearly independent. The algorithm uses four given numbers δ_r (*reflection coefficient*), δ_2 (*expansion coefficient*), δ_1 (*outside contraction coefficient*), and δ_{-1} (*inside contraction coefficient*), which are required to satisfy the relation

$$-1 < \delta_{-1} < 0 < \delta_1 < \delta_r < \delta_2. \quad (3)$$

Below, we state a formal version of the algorithm.

Algorithm 1 Nelder-Mead Simplex ($S^{(0)}$, f , ε) Set $k = 0$ and go to step 1-1.

Step 1-1 (Sort the vertices)

If $T(S^{(k)}) \leq \varepsilon$, exit. Label the vertices, arbitrarily, as $q_1^{(k)}$, $q_2^{(k)}$ and $q_3^{(k)}$. Sort the vertices of the current simplex $S^{(k)}$ in ascending order of function values, producing a re-labelled version of the vertices

$$q_w^{(k)} = \underset{q_i^{(k)}}{\operatorname{argmin}} \{f(q_i^{(k)})\}, \quad (4)$$

$$q_b^{(k)} = \underset{q_i^{(k)}}{\operatorname{argmax}} \{f(q_i^{(k)})\}, \quad (5)$$

$$q_s^{(k)} = \underset{q_i^{(k)}, q_i^{(k)} \neq q_b^{(k)}}{\operatorname{argmax}} \{f(q_i^{(k)})\}. \quad (6)$$

Thus, we have $f(q_w^{(k)}) \leq f(q_s^{(k)}) \leq f(q_b^{(k)})$. $q_w^{(k)}$, $q_b^{(k)}$, and $q_s^{(k)}$, are called, respectively, the **worst**, the **best**, and the **second (or next) best (or worst)** vertices. Compute the centroid

$$\bar{q}^{(k)} = \frac{1}{2}(q_s^{(k)} + q_b^{(k)}) \quad (7)$$

of

$$S^{(k)} \setminus \{q_w^{(k)}\}. \quad (8)$$

Denote

$$z^{(k)}(\delta_r) = (1 + \delta_r)\bar{q}^{(k)} - \delta q_w^{(k)}, \quad (9)$$

and

$$S_\delta^{(k)} = (S^{(k)} \setminus \{q_w^{(k)}\}) \cup \{z^{(k)}(\delta_r)\} \quad (10)$$

(i.e., $S_\delta^{(k)} = S[q_1^{(k)}, q_2^{(k)}, z^{(k)}(\delta_r)]$).

Step 1-2 (Reflection)

If

$$f(q_b^{(k)}) \leq f(z^{(k)}(\delta_r)) \quad (11)$$

and

$$f(z^{(k)}(\delta_r)) < f(q_s^{(k)}), \quad (12)$$

set $S^{(k+1)} = S_{\delta_r}^{(k)}$ (replace $q_w^{(k)}$ with $z^{(k)}(\delta_r)$) and go to step 1-1.

Step 1-3 (Expansion)

If $f(z^{(k)}(\delta_r)) \geq f(q_b^{(k)})$, go to step 1-4.

If

$$f(z^{(k)}(\delta_r)) < f(q_b^{(k)}) \quad (13)$$

and

$$f(z^{(k)}(\delta_2)) < f(z^{(k)}(\delta_r)), \quad (14)$$

set $S^{(k+1)} = S_{\delta_2}^{(k)}$. Otherwise, set $S^{(k+1)} = S_{\delta_r}^{(k)}$. Go to step 1-1.

Step 1-4 (Outside contraction)

If

$$f(q_s^{(k)}) > f(z^{(k)}(\delta_r)) \quad (15)$$

or

$$f(z^{(k)}(\delta_r)) \geq f(q_w^{(k)}), \quad (16)$$

go to step 1-5.

If

$$f(q_s^{(k)}) \leq f(z^{(k)}(\delta_r)) \quad (17)$$

and

$$f(z^{(k)}(\delta_r)) < f(q_w^{(k)}) \quad (18)$$

and

$$f(z^{(k)}(\delta_1)) < f(q_w^{(k)}), \quad (19)$$

set $S^{(k+1)} = S_{\delta_1}^{(k)}$ and go to step 1-1.

Otherwise, go to step 1-6.

Step 1-5 (Inside contraction)

If $f(z^{(k)}(\delta_r)) < f(q_w^{(k)})$, go to step 1-6.

If

$$f(z^{(k)}(\delta_r)) \geq f(q_w^{(k)}) \quad (20)$$

and

$$f(z^{(k)}(\delta_{-1})) < f(q_w^{(k)}), \quad (21)$$

set $S^{(k+1)} = S_{\delta_{-1}}^{(k)}$ and go to step 1-1.

Otherwise go to step 1-6.

Step 1-6 (Shrink)

Set

$$S^{(k+1)} = q_b^{(k)} + \frac{1}{\xi}(S^{(k)} - q_b^{(k)}) \quad (22)$$

and go to step 1-1.

In the algorithm, $\xi > 0$ determines how much the simplex should reduce in size and is usually taken to be $\xi = 2$. To sort the vertices, any tie-breaking strategy can be used. In essence, the algorithm, just like the original simplex, tries to replace the worst vertex with a new better one. In any case, the average value

$$\overline{f(q^{(k)})} = \frac{1}{3} \sum_{i=1}^3 f(q_i^{(k)}) \quad (23)$$

is decreased. The *value state* of $S^{(k)}$ can either be defined as $f(q_b^{(k)})$ or $\overline{f(q^{(k)})}$. The success of the Nelder-Mead algorithm lies in the fact that it allows *non-isometric* reflections. This same feature also makes this method problematic if certain modifications are not considered, as the next section will show. The values usually used for δ parameters are $\delta_r = 1$, $\delta_2 = 2$, $\delta_1 = 1$, and $\delta_{-1} = -1/2$.

One popular choice for T is

$$T(S^{(k)}) = \left(\frac{1}{3} \sum_{i=1}^3 (f(q_i^{(k)}) - \overline{f(q^{(k)})})^2 \right)^{1/2}. \quad (24)$$

Another choice is simply

$$T(S^{(k)}) = |f(q_w^{(k)}) - f(q_b^{(k)})|. \quad (25)$$

These termination criteria test for *flatness* of the simplex. Other choices will be discussed in the next section. There are other termination criteria which relate to the size of the simplex rather than function values. Among these is *smallness* (Luersen and Le Riche 2004)

$$\max_{v \in \{v_{12}, v_{13}, v_{23}\}} \left(\frac{\langle v, e_x \rangle}{X_+ - X_-} + \frac{\langle v, e_y \rangle}{Y_+ - Y_-} \right) < \varepsilon, \quad (26)$$

where $v_{ij} = q_j^{(k)} - q_i^{(k)}$ denote the *edges* of the simplex, e_x and e_y are unit vectors in the directions of the global coordinate system, and X_+ , X_- , Y_+ and Y_- are some bounds. *Degeneracy* can also be used to determine if the simplex has been stuck in a subspace from which it cannot escape (Luersen and Le Riche 2004). A simplex is degenerate if it is not small but either

$$\frac{\min_{v \in \{v_{12}, v_{13}, v_{23}\}} \|v\|}{\max_{v \in \{v_{12}, v_{13}, v_{23}\}} \|v\|} < \varepsilon \quad (27)$$

or

$$\frac{\det([v_{12}, v_{13}, v_{23}])}{\|v_{12}\| \|v_{13}\| \|v_{23}\|} < \varepsilon. \quad (28)$$

The rationale behind reflection is that the function value decreases along the side of the simplex triangle from $q_w^{(k)}$ to $q_b^{(k)}$. This is also true for the side from $q_w^{(k)}$ to $q_s^{(k)}$. Hence, it is possible that $f(q)$ takes on smaller values at points which lie away from $q_w^{(k)}$ on the opposite side of the *good side* (the line connecting $q_b^{(k)}$ to $q_s^{(k)}$). Figure 2 shows the different operations. The reflection operation is based on this simple observation (Fig. 2(b)). If the reflected point $q_r^{(k)} = z^{(k)}(\delta_r)$ gives indeed a better value, then the direction towards the minimum is correct and it might be the case that if we go even farther (to $q_e^{(k)} = z^{(k)}(\delta_2)$), we get an even better value, which is the reasoning behind the expansion operation (Fig. 2(c)). If the reflection does not provide a better solution, then we should move backwards and try two points which are located on the line connecting $q_w^{(k)}$ and $q_r^{(k)}$. These points are $q_{oc}^{(k)} = z^{(k)}(\delta_1)$ and $q_{ic}^{(k)} = z^{(k)}(\delta_{-1})$ (Fig. 2(d) and Fig. 2(e)). If this also fails, we have no choice but to shrink the simplex towards the best vertex (Fig. 2(f)).

In the literature, it is the convention to set $w = 3$, $s = 2$, and $b = 1$, such that we always have $f(q_1^{(k)}) \leq f(q_2^{(k)}) \leq f(q_3^{(k)})$. We will follow this convention from now on.

3 Properties

Here, we review some of the properties of the basic algorithm. First, we introduce some useful definitions.

Definition 1

1. $V(S^{(k)})$ denotes the 2×2 matrix of *simplex directions* defined by

$$V(S^{(k)}) = (q_2^{(k)} - q_1^{(k)}, q_3^{(k)} - q_1^{(k)}). \quad (29)$$

For a nondegenerate simplex, $V(S^{(k)})$ is nonsingular.

2. The *outer diameter* of the simplex is defined by

$$\text{diam}_o(S^{(k)}) = \max_{i,j \in \{1,2,3\}} \|q_i^{(k)} - q_j^{(k)}\|. \quad (30)$$

3. The *inner diameter* is defined as

$$\text{diam}_i(S^{(k)}) = \min_{i,j \in \{1,2,3\}} \|q_i^{(k)} - q_j^{(k)}\|. \quad (31)$$

4. The *volume* of a simplex is defined as

$$\text{vol}(S^{(k)}) = \frac{1}{6} \|\det(V(S^{(k)}))\|. \quad (32)$$

Thus, a simplex is nondegenerate if $\text{vol}(S^{(k)}) > 0$.

Fig. 2 Operations of the Nelder-Mead simplex method with vehicles playing the role of simplex vertices. **(a)** Initial simplex. **(b)** Reflection. **(c)** Expansion. **(d)** Inside contraction. **(e)** Outside contraction. **(f)** Shrink

5. If, in a non-shrink step, the coefficient $\tau \in \{\delta_r, \delta_2, \delta_1, \delta_{-1}\}$ is used to generate the next simplex, we call that step of type τ .

Now, we state some properties. See (Lagarias et al. 1998) for proofs and further discussion.

Lemma 1

1. If the initial simplex $S^{(0)}$ is nondegenerate, then so are all the other subsequent simplexes.
2. Following a non-shrink step of type τ ,

$$\text{vol}(S^{(k+1)}) = |\tau| \text{vol}(S^{(k)}). \quad (33)$$

3. Following a shrink step,

$$\text{vol}(S^{(k+1)}) = \frac{1}{\xi^2} \text{vol}(S^{(k)}). \quad (34)$$

4. The Nelder-Mead method is invariant under affine transformation $\phi(q) = Aq + b$, A invertible. When minimizing $f(q)$, starting with simplex $S^{(0)}$, the complete sequence of Nelder-Mead steps and function values is the same as when minimizing the function $\tilde{f}(q) = f(\phi(q))$ with initial simplex $\tilde{S}^{(0)}$ defined by

$$\tilde{S}^{(0)} = \phi^{-1}(S^{(0)}) = A^{-1}(S^{(0)}) - A^{-1}b. \quad (35)$$

5. The sequence $\{f_1^{(k)}\}$ always converges.
6. At every nonshrink iteration, $f_i^{(k+1)} \leq f_i^{(k)}$, $i \in \{1, 2, 3\}$.
7. If there is only a finite number of shrink operations, then each sequence $\{f_i^{(k)}\}$ converges as $k \rightarrow \infty$, $f_i^\infty \leq f_i^{(k)}$, and $f_1^\infty \leq f_2^\infty \leq f_3^\infty$, where $f_i^\infty = \lim_{k \rightarrow \infty} f_i^{(k)}$.
8. If there are only a finite number of nonshrink iterations, then all simplex vertices converge to a single point.
9. If f is strictly convex on $\mathbb{R}^2$ and the algorithm starts with a nondegenerate initial simplex, then no shrink steps will be taken.

The next lemma summarizes some important convergence properties for the planar case for strictly convex functions with bounded level sets. f is strictly convex on $\mathbb{R}^2$ if, for every pair of points q_1 and q_2 , $q_1 \neq q_2$, and every $0 < \lambda < 1$, we have

$$f(\lambda q_1 + (1 + \lambda)q_2) < \lambda f(q_1) + (1 + \lambda)f(q_2). \quad (36)$$

Also, the level set $\Gamma_\mu(f)$ is defined as $\Gamma_\mu(f) = \{q : (f(q) \leq \mu)\}$. f has bounded level sets if $\Gamma_\mu(f)$ is bounded for every μ . A strictly convex function with bounded level sets has a unique minimizer.

Lemma 2 Let f be a strictly convex function on $\mathbb{R}^2$ with bounded level sets, the algorithm starts with a nondegenerate simplex $S^{(0)}$, and $\delta_r = 1$, $\delta_2 = 2$, $\delta_1 = 1/2$, and $\delta_{-1} = -1/2$.

1. $f_1^\infty = f_2^\infty = f_3^\infty$.
2. If the best vertex $q_1^{(k)}$ is constant for all k , then the simplices $S^{(k)}$ converge to $q_1^{(0)}$ as $k \rightarrow \infty$.
3. The simplices $\{S^{(k)}\}$ generated by the algorithm satisfy $\lim_{k \rightarrow \infty} \text{vol}(S^{(k)}) = 0$.
4. We also have $\lim_{k \rightarrow \infty} \text{diam}_o(S^{(k)}) = 0$.

4 Variations

It is well-known that the Nelder-Mead method can stagnate and converge to non-optimal points even for very simple functions. In McKinnon (1998), a family of examples are given for which the algorithm converges to a non-stationary point. To remedy this, many variations of the original algorithm have been proposed. In this section, we discuss some of them as well as other modifications which relate to globalization of the algorithm and those that make the algorithm more suitable for implementation by robotic vehicles. We first give some definitions which will be used.

Definition 2

1. The simplex condition $\kappa(S^{(k)})$ is defined as the l^2 condition number of $V(S^{(k)})$. $\delta(f : S^{(k)})$ denotes the vector of objective function differences

$$\delta(f : S^{(k)}) = (f(q_2^{(k)}) - f(q_1^{(k)}), f(q_3^{(k)}) - f(q_1^{(k)}))^T. \quad (37)$$

2. Oriented lengths of the simplex are defined as

$$\sigma_+(S^{(k)}) = \max_{j \in \{1, 2, 3\}} \|q_1^{(k)} - q_j^{(k)}\|, \quad (38)$$

$$\sigma_-(S^{(k)}) = \min_{j \in \{1, 2, 3\}} \|q_1^{(k)} - q_j^{(k)}\|. \quad (39)$$

We have $\sigma_+(S^{(k)}) \leq \text{diam}_o(S^{(k)}) \leq \sigma_-(S^{(k)})$.

3. Define

$$v(S^{(k)}) = \frac{|\det(V(S^{(k)}))|}{\text{diam}_o(S^{(k)})^2}. \quad (40)$$

$v(S^{(k)}) = 0$ if one of the interior angles of $S^{(k)}$ is zero.

Simplex gradients and sufficient decrease: In Kelley (1999), a very useful variant of the algorithm is proposed which we will adopt here. They based their method on the omission of the shrink step altogether, arguing that it very rarely occurs in practice. They, instead, add an additional step which they call *oriented restart*. It is very similar to the shrink operation but the directions are a function of the simplex gradient.

Definition 3 The simplex gradient $D(f : S^{(k)})$ is defined as

$$D(f : S^{(k)}) = V(S^{(k)})^{-T} \delta(f : S^{(k)}). \quad (41)$$

They consider functions of the form $f(q) = g(q) + \zeta(q)$, where $g(q)$ is a smooth function and $\zeta(q)$ is a low-amplitude perturbation.

Lemma 3

1. Let ∇f be Lipschitz continuous in a neighborhood of $S^{(k)}$ with Lipschitz constant $2K_f$. Then there exists $K > 0$, depending only on K_f , such that

$$\|\nabla f(q_1^{(k)}) - D(f : S^{(k)})\| \leq K\kappa(V(S^{(k)}))\sigma_+(S^{(k)}). \quad (42)$$

2. Suppose $f = g + \zeta$. Let ∇g be Lipschitz continuous in a neighborhood of $S^{(k)}$ with Lipschitz constant $2K_g$. Then there exists $K > 0$, depending only on K_g , such that

$$\begin{aligned} \|\nabla g(q_1^{(k)}) - D(f : S^{(k)})\| \\ \leq K\kappa(V(S^{(k)})) \left(\sigma_+(S^{(k)}) + \frac{\|\zeta\|_{S^{(k)}}}{\sigma_+(S^{(k)})} \right). \end{aligned} \quad (43)$$

Assumption 1

1. $S^{(0)}$ is non-singular.
2. For each k , $\overline{f(q^{(k+1)})} < \overline{f(q^{(k)})}$.

Their method is based on requiring that the $(k+1)$ -th iteration satisfy

$$\overline{f(q^{(k+1)})} - \overline{f(q^{(k)})} < -\alpha \|D(f : S^{(k)})\|^2, \quad (44)$$

where

$$\alpha = \alpha_0 \frac{\sigma_+(S^{(0)})}{\|D(f : S^{(0)})\|} \quad (45)$$

and typically $\alpha_0 = 10^{-4}$.

Theorem 1

1. Let the assumptions Assumption 1, as well as the assumptions of Lemma 3(1) hold true, with the Lipschitz constant K^k bounded. Assume that $\{f(q^{(k)})\}$ is bounded from below. Then, if (44) holds for all but finitely many k and the product $\sigma_+(S^{(k)})\kappa(V(S^{(k)})) \rightarrow 0$, then any accumulation point of the simplices is a critical point of f .
2. Let Assumption 1 hold true, as well as the assumptions of Lemma 3(2), with the Lipschitz constants K_g^k uniformly bounded. Assume that $\{f(q^{(k)})\}$ is bounded from below. Then, if (44) holds for all but finitely many k and if

$$\lim_{k \rightarrow \infty} \kappa(V(S^{(k)})) \left(\sigma_+(S^{(k)}) + \frac{\|\zeta\|_{S^{(k)}}}{\sigma_+(S^{(k)})} \right) = 0, \quad (46)$$

then any accumulation point of the simplices is a critical point of g . Furthermore, $\lim_{k \rightarrow \infty} D(f : S^{(k)}) = 0$.

It is proposed in Kelley (1999) that whenever (44) fails but $\overline{f(q^{(k+1)})} - \overline{f(q^{(k)})} < 0$, an oriented restart should be carried out by replacing the vertices with new $\tilde{q}_1 = q_1$, $\tilde{q}_2 = \tilde{q}_1 + \beta_1 e_1$, $\tilde{q}_3 = \tilde{q}_1 + \beta_2 e_2$, where e_1 and e_2 are unit coordinate vectors and

$$\begin{aligned} \beta_l &= \frac{1}{2} \sigma_-(S^{(k)}) \text{sign}(\langle D(f : S^{(k)}), e_l \rangle), \\ &\text{if } \langle D(f : S^{(k)}), e_l \rangle \neq 0, \end{aligned} \quad (47)$$

and

$$\beta_l = \frac{1}{2} \sigma_-(S^{(k)}), \quad \text{if } \langle D(f : S^{(k)}), e_l \rangle = 0, \quad (48)$$

where $l \in \{1, 2\}$. More compactly,

$$\beta_l = \frac{1}{2} \sigma_-(S^{(k)}) \eta(\text{sign}(\langle D(f : S^{(k)}), e_l \rangle)), \quad (49)$$

where $\eta(u) = \text{sign}(u)$ if $u \neq 0$ and $\eta(u) = 1$ otherwise. The diameter of the new simplex is $\sigma_-(S^{(k)})/\sqrt{2}$. The new simplex has orthogonal edges and is a difference approximation to the steepest descent step from the current best point. To quote (Kelley 1999), this re-orientation is intended to compensate for a certain kind of stagnation in which the best vertex remains unchanged throughout the iteration and the simplices converge to that point. It is argued that, although the simplex gradient may not be a very good approximation of the true gradient, it contains enough information to determine an orthant to locate the new simplex. Note that only the sign is used. After several oriented restarts in a row, the algorithm should terminate. Refer to Kelley (1999) for a more detailed discussion and simulations.

Constrained optimization: The original Nelder-Mead algorithm, as well as the variants above, are all unconstrained. Here, we would like to optimize $f(q)$ subject to the constraint $g(q) \leq 0$ which defines a *feasible region* Ω^s inside the *search space*, which, in our case is $\mathcal{R}^2$. The constraints are used to ensure that the simplex formation does not escape a certain region of exploration and also to avoid obstacles. Figure 3 shows a boundary γ past which the formation should not go. The constraint can be defined as

$$g(q) = \|Q(q, \gamma) - q\| - D, \quad (50)$$

where $Q(q, \gamma)$ denotes the closest point on the boundary to q and D indicates a safe distance away from the boundary. In the case of a simplex formation, q can be the position of any of the vertices or the centre of mass. The region defined by $g(q) \leq 0$ is the *safe region*, while $0 < g(q) \leq D/2$ defines the *critical region* Ω^c . The region defined by $g(q) > D/2$ is the *unsafe region* Ω^u . Many methods have been

Fig. 3 Constraints. Boundary is the black line. Φ_1 , $\Phi_{1/2}$, and Φ_0 represent, respectively, isocontours $g(q) = D$, $g(q) = D/2$, and $g(q) = 0$

proposed to transform an unconstrained optimization algorithm into a constrained one. *Barrier methods* add barrier terms to the objective function which grow to infinity as the point approaches the boundary of the constrained domain. *Penalty methods* add penalty terms to the objective function. Here, we adopt the version of the α -constrained method proposed in Takahama and Sakai (2005). In this paper, the *satisfaction level* of a constraint for a point q is defined by $\mu_g(q) = 1$ if $g(q) \leq 0$ and $0 \leq \mu_g(q) < 1$, otherwise. More specifically, we can define $\mu_g(q) = 1 - 2g(q)/D$, whenever $0 \leq g(q) \leq D/2$.

They also define the α -level comparison as an order relation on the set composed of pairs $(f(q), \mu_g(q))$. The idea is that if the satisfaction level of a point is less than 1, the point should be considered infeasible and its value should be low no matter what the function value $f(q)$ is. This makes $\mu_g(q)$ precede $f(q)$, as satisfying the constraint is more important than minimization. Given the pairs $(f(q_1), \mu_g(q_1))$ and $(f(q_2), \mu_g(q_2))$, then, for any $0 \leq \alpha \leq 1$, the α -level comparisons $\leq_\alpha$ and $<_\alpha$ are defined as follows:

1. $(f(q_1), \mu_g(q_1)) <_\alpha (f(q_2), \mu_g(q_2))$ if and only if $f(q_1) < f(q_2)$, when $\mu_g(q_1), \mu_g(q_2) \geq \alpha$ or $\mu_g(q_1) = \mu_g(q_2)$, or $\mu_g(q_1) > \mu_g(q_2)$, otherwise.
2. $(f(q_1), \mu_g(q_1)) \leq_\alpha (f(q_2), \mu_g(q_2))$ if and only if $f(q_1) \leq f(q_2)$, when $\mu_g(q_1), \mu_g(q_2) \geq \alpha$ or $\mu_g(q_1) = \mu_g(q_2)$, or $\mu_g(q_1) > \mu_g(q_2)$, otherwise.

$\leq_0$ and $<_0$ are ordinary comparisons. $\leq_1$ and $<_1$ correspond to lexicographic order. Denote by (P) the unconstrained minimization problem, by $(P_{\leq_\alpha})$ the version of (P) based on α -level comparisons, and by (P^α) the minimization problem subject to $\mu_g(q) \geq \alpha$. The following results are proved in Takahama and Sakai (2005).

Theorem 2

1. If an optimal solution (P^1) of exists, any optimal solution of $(P_{\leq_\alpha})$ is an optimal solution of (P^α) .
2. If an optimal solution of (P) exists, any optimal solution of $(P_{\leq_1})$ is an optimal solution of (P) .
3. Let $\{\alpha_n\}$ be a strictly increasing nonnegative sequence converging to 1. Let $f(q)$ and $\mu_g(q)$ be continuous functions of q . Assume that an optimal solution $\tilde{q}$ of (P^1) exists and an optimal solution $\tilde{q}_n$ of $(P_{\leq_{\alpha_n}})$ exists for any α_n . Then, every accumulation point of the sequence $\{\tilde{q}_n\}$ is an optimal solution of (P^1) .

To transform a simplex method into a constrained one, we simply replace every $f(q_1) \leq f(q_2)$ with $(f(q_1), \mu_g(q_1)) \leq_\alpha (f(q_2), \mu_g(q_2))$. The strict inequality is similarly changed. The value of α is normally kept at 1 but in some situations (e.g., when the feasible region is small), $\alpha(0)$ is chosen less than 1 and its value is increased to 1 by a control law such as $\alpha(t) = (1 - \beta)\alpha(t - 1) + \beta$, where $0 < \beta < 1$ (see Takahama and Sakai 2005).

Golden rule and weighted average: In Nazareth and Tseng (2002), it is argued that the values usually chosen for the coefficients are heuristic and instead propose to set $\delta_r = \rho^{\log_\rho(2)}$, $\delta_2 = \rho^2$, $\delta_1 = \rho$, $\delta_{-1} = \rho^{-1}$, and $\xi = \rho^2$, where $\rho = (\sqrt{5} + 1)/2$. These selections are derived from a reinterpretation of univariate golden-section direct search. They prove that with these choices, in the one dimensional case, if f is strictly unimodal on $\mathfrak{R}$, then, either $\{\text{diam}_o(S^{(k)})\} \rightarrow \infty$ and f has no minimizer, or $\{\text{diam}_o(S^{(k)})\} \rightarrow 0$ linearly and $\{q^{(k)}\}$ converges to the unique minimizer of f .

Moreover, the centroid and the average value of the simplex are computed as weighted averages by choosing $\theta_1 \in (0, 1)$ and setting

$$\bar{q}^{(k)} = \mu_2 q_2^{(k)} + \mu_1 q_1^{(k)}, \quad (51)$$

$$\bar{f}(q^{(k)}) = \mu_2 f(q_2^{(k)}) + \mu_1 f(q_1^{(k)}), \quad (52)$$

where

$$\mu_i = (1 - \theta_1) \frac{f(q_3^{(k)}) - f(q_i^{(k)})}{\sum_{j \in \{1, 2\}} (f(q_3^{(k)}) - f(q_j^{(k)}))} + \frac{\theta_1}{2}, \quad (53)$$

$i \in \{1, 2\}$, provided $f(q_1^{(k)}) \neq f(q_3^{(k)})$. $\theta_1 = 1$ then corresponds to $\mu_i = 1/2$.

Fortified descent and degeneracy safeguards: In Nazareth and Tseng (2002), a convergent version of the basic algorithm is proposed. To do this, they propose certain safeguards. They employ *fortified descent* which is stronger than strict descent and maintain the interior angles of the simplex $S^{(k)}$ bounded away from zero (which is equivalent to bounding $v(S^k)$ away from zero). In their modified algorithm, a $\theta_2 \in (0, v(S^{(k)})]$ and any continuous functions $\sigma : \mathfrak{R}^+ \rightarrow \mathfrak{R}^+$ and $\beta : \mathfrak{R}^+ \rightarrow \mathfrak{R}^+$ are chosen with

the property that $\lim_{t \rightarrow 0}(\sigma(t)/t) = \lim_{t \rightarrow 0}(\beta(t))/t = 0$ and $\inf_{t \geq a} \sigma(t) > 0$ for all $a > 0$. In their modified algorithm, the inequalities in steps 2–5 are replaced with those that involve the term $\sigma(\text{diam}_o(S^{(k)}))$. Also, the condition $v(S_{\delta_2}^{(k)}) \geq \theta_2$ appears in steps 3–5. They then prove that if f is continuously differentiable and quasi-convex on $\mathbb{R}^2$, is uniformly continuous on the level set $\Gamma_{\min_{q \in S(0)} f(q)}(f)$, and if $\inf_{q \in \mathbb{R}^2} f(q) > -\infty$, then $\{\text{diam}_o(S^{(k)})\} \rightarrow 0$, and every cluster point of $\{q^{(k)}\}$ is a stationary point of f , where $\{S^{(k)}, q^{(k)}\}$ is the sequence generated by the modified algorithm.

Note that θ_1 , $\sigma(t)$ and $\beta(t)$ can be selected in such a way that the fortified descent is only slightly stronger than strict descent. From a practical point of view, there is not much difference between the two. Fortified descent is only used to assure convergence. The second modification, though, can be very crucial for avoiding degenerate simplexes. We will take up this idea later on to derive a constrained version of the algorithm.

Globalization: The simplex method is a local optimization strategy. As such, it quickly converges to a local minimum. A number of strategies have been proposed to make this algorithm a global search method. One promising method has been proposed in Luersen et al. (2004). The basic idea is to restart the search from a new initial position when a local search finishes. In our case, a local search is considered finished if it has reached a flat area or it cannot get smaller for more fine tuning. A list of past initial points Φ is maintained. Let $q_I^{(i)}$, $i = 0, \dots, M-1$ represent the initial points from which the simplex has already done a local search. The probability of selecting $q_I^{(i)}$ again for restart can be modelled by the Gaussian

$$p_i(q) = \frac{1}{2\pi\sigma^2} e^{-\frac{1}{2\sigma^2} \|q - q_I^{(i)}\|^2}. \quad (54)$$

The probability of sampling a past initial point is then given by

$$p(q, \Phi) = \frac{1}{M} \sum_{i=0}^{M-1} p_i(q). \quad (55)$$

The normalized probability is

$$\tilde{p}(q, \Phi) = \frac{p(q)}{\int_{\Omega} p(q) d\Omega}. \quad (56)$$

We want the probability of sampling an already used initial point to approach zero and thus the probability density of sampling a new initial position can be given by

$$\phi(q, \Phi) = \frac{H - \tilde{p}(q)}{\int_{\Omega} (H - \tilde{p}(q)) d\Omega}, \quad (57)$$

where $H = \max_{q \in \Omega} \tilde{p}(q, \Phi)$. In practice, we can select the new position by the formula $q_I^{(M)} = \arg\min_{q \in \Omega} \phi(q, \Phi)$.

5 Shape-constrained version

As is apparent from the foregoing discussions, the Nelder-Mead can sometimes get very elongated in one direction, making the simplex degenerate. This is a key to its failure in many cases. Moreover, when applying an algorithm such as the Nelder-Mead simplex method to robotic formations, one always has to provide for safeguards against violation of important geometric constraints, most notably the ones imposed on minimum and maximum distances between vehicles participating in the task. The algorithm, as stated above, clearly has the potential to violate the angle constraints and it always violates the distance constraint, if it is going to converge at all. In this section, we present a variant which takes care of these constraints. Except for the safeguard for nondegeneracy, no constraint is normally put on distances between nodes for the simple reason that doing this will prevent the simplex from converging (upon successful convergence, the diameter of the simplex tends to zero). In our application, this does not present a problem. If the simplex gets smaller than some bound, it means that either we are near a local minimizer or else the simplex is going to stagnate. Localizing exactly a minimizer is not needed in the real world application that we are addressing here. Our main goal, by considering the Nelder-Mead method, is to get as close as possible to a certain feature (source or isocline) as fast (and as aggressively) as possible. The idea here is to check if a new point is within desirable bounds and if not project it unto the bound (Fig. 4). The bounds we are interested in are

$$D_l \leq \text{diam}_i(S^{(k)}), \quad (58)$$

$$\text{diam}_o(S^{(k)}) \leq D_u, \quad (59)$$

$$v(S^{(k)}) \leq v_u. \quad (60)$$

Assume that $S^{(k)}$ satisfies these bounds. Instead of the original $\delta \in \{\delta_r, \delta_2, \delta_1, \delta_{-1}\}$, we apply a constrained value $\chi(\delta_i)$. We have $\delta_r = \chi(\delta_r)$, as reflection does not change the shape of the simplex. For the expansion operation, we set

$$\chi(\delta_2) = \min\{\arg\min_{\delta} (v(S_{\delta_2}^{(k)}) - v_u), \delta_2\},$$

$$\arg\min_{\delta} (\text{diam}_o(S_{\delta_2}^{(k)}) - v_u), \delta_2\}. \quad (61)$$

For the outside and inside contractions, we set, respectively,

$$\chi(\delta_1) = \max\{\arg\max_{\delta} (v(S_{\delta_1}^{(k)}) - v_u),$$

$$\arg\max_{\delta} (\text{diam}_o(S_{\delta_1}^{(k)}) - v_u), \delta_1\}, \quad (62)$$

and

$$\chi(\delta_{-1}) = \min\{\arg\min_{\delta} (v(S_{\delta_{-1}}^{(k)}) - v_u),$$

$$\arg\min_{\delta} (\text{diam}_o(S_{\delta_{-1}}^{(k)}) - v_u), \delta_{-1}\}. \quad (63)$$

Fig. 4 Constraining generated points to lie within the desired bounds. The computed points $z^{(k)}(\delta)$ are checked and, if necessary, are modified to $z^{(k)}(\chi(\delta))$. Likewise, β_l is modified to $\chi(\beta_l)$

It is obvious that $\delta_r \leq \chi(\delta_2) \leq \delta_2$, $\delta_1 \leq \chi(\delta_1) \leq \delta_r$, and $0 \leq \chi(\delta_{-1}) \leq \delta_{-1}$. Although the above optimization problems can be solved by simple line search, we prefer to make things simpler by replacing the above constraints with equivalent but more manageable and straightforward ones. For any simplex, we require that, for every q_i and q_j , $i \neq j$, $i, j \in \{1, 2, 3\}$, we have $D_l \leq \|q_i - q_j\| \leq D_u$, and that, for every two edges e_{ij} and e_{ik} , attached to q_i , we have $\varphi_l \leq \varphi(q_i, q_j, q_k) \leq \varphi_u$, where

$$\varphi(q_i, q_j, q_k) = \arccos\left(\frac{\langle (q_j - q_i), (q_k - q_i) \rangle}{\|q_j - q_i\| \|q_k - q_i\|}\right). \quad (64)$$

We denote the distance constraints by $C_{D_l}(q_i, q_j)$ and $C_{D_u}(q_i, q_j)$. The angle constraints are denoted by $C_{\varphi_l}(q_i, q_j, q_k)$ and $C_{\varphi_u}(q_i, q_j, q_k)$. Not all the constraints can be violated by all of the operations. Reflection, as was mentioned, does not violate any constraints. Expansion can only violate the maximum distance constraints $C_{D_u}(q_1^{(k)}, z^{(k)}(\delta_2))$, and $C_{D_u}(q_2^{(k)}, z^{(k)}(\delta_2))$, the minimum angle constraint $C_{\varphi_l}(z^{(k)}(\delta_2), q_1^{(k)}, q_2^{(k)})$, and the maximum angle constraints $C_{\varphi_u}(q_1^{(k)}, q_2^{(k)}, z^{(k)}(\delta_2))$, and $C_{\varphi_u}(q_2^{(k)}, q_1^{(k)}, z^{(k)}(\delta_2))$.

Outside contraction can potentially violate the minimum distance constraints $C_{D_l}(q_1^{(k)}, z^{(k)}(\delta_1))$, and $C_{D_l}(q_2^{(k)}, z^{(k)}(\delta_1))$, the minimum angle constraints $C_{\varphi_l}(q_1^{(k)}, q_2^{(k)}, z^{(k)}(\delta_1))$, and $C_{\varphi_l}(q_2^{(k)}, q_1^{(k)}, z^{(k)}(\delta_1))$, and the maximum angle constraint $C_{\varphi_u}(z^{(k)}(\delta_1), q_1^{(k)}, q_2^{(k)})$.

Likewise, inside contraction can violate the same constraints as outside contraction. We only consider and check for a subset of these constraints. For expansion, we consider $C_{D_u}(q_i^{(k)}, z^{(k)}(\delta_2))$, $i \in \{1, 2\}$, and $C_{\varphi_l}(z^{(k)}(\delta_2), q_1^{(k)}, q_2^{(k)})$. For outside and inside contractions, we check for $C_{D_l}(q_i^{(k)},$

$z^{(k)}(\delta_j))$, $j \in \{1, -1\}$, and $C_{\varphi_l}(q_i^{(k)}, q_k^{(k)}, z^{(k)}(\delta_j))$, $k \in \{1, 2\}$, $k \neq i$.

From the definition of $z^{(k)}(\delta)$, we have

$$z^{(k)}(\delta) - \bar{q}^{(k)} = \delta(\bar{q}^{(k)} - q_w^{(k)}), \quad (65)$$

or

$$\begin{aligned} \|z^{(k)}(\delta) - \bar{q}^{(k)}\| &= \frac{\|z^{(k)}(\delta) - \bar{q}^{(k)}\|}{\|z^{(k)}(\delta) - \bar{q}^{(k)}\|} \\ &= \delta \|\bar{q}^{(k)} - q_w^{(k)}\| \frac{\|\bar{q}^{(k)} - q_w^{(k)}\|}{\|\bar{q}^{(k)} - q_w^{(k)}\|} \end{aligned} \quad (66)$$

which implies that

$$\|z^{(k)}(\delta) - \bar{q}^{(k)}\| = \delta \|\bar{q}^{(k)} - q_w^{(k)}\|. \quad (67)$$

Letting $\Delta^{(k)}(\delta) = \|z^{(k)}(\delta) - \bar{q}^{(k)}\|$, we have

$$\delta = \frac{\Delta^{(k)}(\delta)}{\|\bar{q}^{(k)} - q_w^{(k)}\|}. \quad (68)$$

For the distance constraint we have

$$\begin{aligned} D^2 &= \|q_i^{(k)} - \bar{q}^{(k)}\|^2 + \Delta_i^{(k)}(D)^2 \\ &\quad - 2\Delta_i^{(k)}(D)\|q_i^{(k)} - \bar{q}^{(k)}\| \cos(\varphi(\bar{q}^{(k)}, q_i^{(k)}, \zeta^{(k)})), \end{aligned} \quad (69)$$

where $i \in \{1, 2\}$, $\Delta_i^{(k)}(D)$ corresponds to a δ for which $\|z^{(k)}(\delta) - q_i^{(k)}\| = D$, and

$$\zeta^{(k)} = \bar{q}^{(k)} + \mu \frac{\bar{q}^{(k)} - q_w^{(k)}}{\|\bar{q}^{(k)} - q_w^{(k)}\|}. \quad (70)$$

Fig. 5 Calculations for the distance constraint. **(a)** Upper bound for the distance when expansion is being attempted. **(b)** Lower bound for distance when contracting outside or inside

μ is equal to $\text{sign}(\delta)$. Of course, we are trying to compute δ , so we put $\mu = 1$ for expansion and outside contraction and we put $\mu = -1$ for inside contraction. Solving for $\Delta_i^{(k)}(D)$, we get

$$\Delta_i^{(k)}(D) = \|q_i^{(k)} - \bar{q}^{(k)}\| \cos(\varphi_i^{(k)}) + (\|q_i^{(k)} - \bar{q}^{(k)}\|^2 (\cos(\varphi_i^{(k)})^2 - 1) + D^2)^{1/2} \quad (71)$$

where $\varphi_i^{(k)} = \varphi(\bar{q}^{(k)}, q_i^{(k)}, \zeta^{(k)})$. Here $D \in \{D_l, D_u\}$. Now,

$$\delta_i^{(k)}(D) = \frac{\Delta_i^{(k)}(D)}{\|\bar{q}^{(k)} - q_w^{(k)}\|} \quad (72)$$

is the expression for the δ which places the new vertex on the boundary of the distance constraint. See Fig. 5 for an illustration of the introduced variables. If the real solution of the second order equation does not exist, the simplex is already outside the safe region.

For the minimum angle constraint $C_{\varphi_l}(z^{(k)}(\delta), q_1^{(k)}, q_2^{(k)})$ (Fig. 6), we note that, by the sine law,

$$\Delta_z^{(k)}(\varphi_l) = \|\bar{q}^{(k)} - q_1^{(k)}\| \frac{\sin(\tilde{\gamma}_1^{(k)})}{\sin(\tilde{\varphi}_l)}, \quad (73)$$

where

$$\tilde{\varphi}_l = \frac{\|\bar{q}^{(k)} - q_1^{(k)}\|}{\|q_2^{(k)} - q_1^{(k)}\|} \varphi_l, \quad (74)$$

$$\tilde{\gamma}_1^{(k)} = \pi - (\varphi_1^{(k)} + \tilde{\varphi}_l). \quad (75)$$

The vertex $q_2^{(k)}$ could have alternatively been used. The corresponding δ is thus

$$\delta_z^{(k)}(\varphi_l) = \Delta_z^{(k)}(\varphi_l) / \|\bar{q}^{(k)} - q_w^{(l)}\|. \quad (76)$$

See Fig. 6(a).

Fig. 6 Calculations for the angle constraint. **(a)** Lower bound for the angle when expansion is being attempted. **(b)** Lower bound for angle when contracting outside or inside

For the constraint $C_{\varphi_l}(q_i^{(k)}, q_k^{(k)}, z^{(k)}(\delta_j))$ imposed on outside and inside contraction operations (Fig. 6(b)), we use the formula

$$\Delta_i^{(k)}(\varphi_l) = \|\bar{q}^{(k)} - q_i^{(k)}\| \frac{\sin(\varphi_l)}{\sin(\gamma_i^{(k)})}, \quad (77)$$

where $\gamma_i^{(k)} = \pi - (\varphi_i^{(k)} + \varphi_l)$, and so

$$\delta_i^{(k)}(\varphi_l) = \mu \Delta_i^{(k)}(\varphi_l) / \|\bar{q}^{(k)} - q_w^{(k)}\|. \quad (78)$$

The following lemma sums up the main strategy.

Lemma 4 Define the *simplex shape space* $\Gamma \subseteq \mathfrak{R}^3 \otimes \mathfrak{R}^3$ as the set of all the *consistent tuples*

$$(\|q_1 - q_2\|, \|q_1 - q_3\|, \|q_2 - q_3\|, \varphi(q_1, q_2, q_3), \varphi(q_2, q_1, q_3), \varphi(q_3, q_1, q_2)), \quad (79)$$

denoted $\widehat{S}$. Let

$$\Pi = \prod_{i=1}^3 [D_l, D_u] \otimes \prod_{i=1}^3 [\varphi_l, \varphi_u] \quad (80)$$

be the *constrain hypercube* in Γ . Assume that $\widehat{S}^{(0)} \in \Pi$. If, instead of δ_2 , δ_1 , δ_{-1} , and β_l in the original algorithm, we use, respectively,

$$\chi(\delta_2) = \min\{\delta_1^{(k)}(D_u), \delta_2^{(k)}(D_u), \delta_z^{(k)}(\varphi_l), \delta_1^{(k)}(\varphi_u), \delta_2^{(k)}(\varphi_u), \delta_2\}, \quad (81)$$

$$\chi(\delta_1) = \max\{\delta_1^{(k)}(D_l), \delta_2^{(k)}(D_l), \delta_1^{(k)}(\varphi_l), \delta_2^{(k)}(\varphi_l), \delta_z^{(k)}(\varphi_u), \delta_1\}, \quad (82)$$

$$\chi(\delta_{-1}) = \min\{-\delta_1^{(k)}(D_l), -\delta_2^{(k)}(D_l), -\delta_1^{(k)}(\varphi_l), -\delta_2^{(k)}(\varphi_l), -\delta_z^{(k)}(\varphi_u), \delta_{-1}\}, \quad (83)$$

$$\chi(\beta_l) = \min\{(1/2)\sigma_-(S^{(k)}), D_l\}, \eta(\text{sign}(\langle D(f : S^{(k)}), e_l \rangle)), \quad (84)$$

then we will have $\widehat{S}^{(k)} \in \Pi$, for every $k \geq 0$.

6 The modified algorithm

We can now state the new algorithm. First, let us introduce the special notation we will use throughout the algorithm. We use τ_μ to denote the mode of operation. If $\tau_\mu = 1$, the task is that of minimization and if $\tau_\mu = 2$, we are maximizing. Let $u_1, u_2 \in \mathfrak{R}^2$.

1. We use the notation $f(u_1)[\tau_\mu, <]f(u_2)$ (or, equivalently $f(u_2)[\tau_\mu, >]f(u_1)$) to denote the fact that $f(u_1)$ is *strictly better than* $f(u_2)$. For *minimization*, this is equivalent to $f(u_1) < f(u_2)$, while for *maximization*, it is equal to $f(u_1) > f(u_2)$.
2. We use the notation $f(u_1)[\tau_\mu, \leq]f(u_2)$ (or, equivalently $f(u_2)[\tau_\mu, \geq]f(u_1)$) to denote the fact that $f(u_1)$ is *better than or equal to* $f(u_2)$.
3. We use the notations $(f(u_1), \mu_g(u_1))[\tau_\mu, \leq_\alpha](f(u_2), \mu_g(u_2))$, $(f(u_1), \mu_g(u_1))[\tau_\mu, <_\alpha](f(u_2), \mu_g(u_2))$, $(f(u_1), \mu_g(u_1))[\tau_\mu, \geq_\alpha](f(u_2), \mu_g(u_2))$, and $(f(u_1), \mu_g(u_1))[\tau_\mu, >_\alpha](f(u_2), \mu_g(u_2))$ to convey the fact that α -level comparisons have been used.

n_{or} denotes the number of oriented restarts in a row. Following Conn et al. (1997), we terminate the search after three such restarts. A denotes the initial size of the simplex. The algorithm is composed of two loops. The outer loop generates random initial positions and the inner one iterates the

local search until termination. After a sufficient number of probabilistic restarts, the algorithm terminates.

Algorithm 2 Shape-Constrained Nelder-Mead ($q_I^{(0)}$, f , ε , A).

Set $l = 0$, $\Phi = \{ \}$, and go to step 2-1.

Step 2-1 (Generation of initial point)

Set $n_{or} = 0$. If $l \neq 0$, $\Phi = \Phi \cup \{q_I^{(l-1)}\}$. Set $q_I^{(l)}$ to a sample point drawn from the probability density $\phi(q, \Phi)$. Go to step 2-2.

Step 2-2 (Construction of initial simplex)

Construct the initial simplex by setting (see Haftka and Guerdal 1993)

$$q_1^{(0)} = q_I^{(l)}, \quad (85)$$

$$q_2^{(0)} = q_1^{(0)} + \frac{A}{2\sqrt{2}}(\sqrt{3} + 1)e_1 + \frac{A}{2\sqrt{2}}(\sqrt{3} + 1)e_2, \quad (86)$$

$$q_3^{(0)} = q_1^{(0)} + \frac{A}{2\sqrt{2}}(\sqrt{3} + 1)e_1 + \frac{A}{2\sqrt{2}}(\sqrt{3} + 1)e_2, \quad (87)$$

set $k = 0$ and go to step 2-3.

Step 2-3 (Checking for termination)

The current local search should be terminated if (see Nazareth and Tseng 2002)

$$\left\| \begin{bmatrix} (q_2^{(k)} - q_1^{(k)})^T \\ (q_3^{(k)} - q_1^{(k)})^T \end{bmatrix}^{-1} \begin{bmatrix} f(q_2^{(k)}) - f(q_1^{(k)}) \\ f(q_3^{(k)}) - f(q_1^{(k)}) \end{bmatrix} \right\| \leq \varepsilon. \quad (88)$$

If is continuously differentiable, $v(S^{(k)})$ is bounded away from zero and $\text{diam}(S^{(k)})$ tends to zero, then the above criterion means that $\nabla f(q_1^{(k)}) \approx 0$. If this is true, set $l \leftarrow l + 1$ and go to step 2-1.

Step 2-4 (Oriented restart)

If $k = 0$, go to step 2-5. If

$$(\overline{f(q^{(k)})} - \overline{f(q^{(k-1)})})[\tau_\mu, <] 0 \quad (89)$$

but

$$(\overline{f(q^{(k)})} - \overline{f(q^{(k-1)})})[\tau_\mu, \geq] - \alpha_0 \frac{\sigma_+(S^{(0)})}{\|D(f : S^{(0)})\|} \|D(f : S^{(k-1)})\|^2 \quad (90)$$

then, if $n_{or} = 2$, set $l \leftarrow l + 1$ and go to step 2-1. Otherwise, set $n_{or} \leftarrow n_{or} + 1$, and

$$\tilde{S} = S[q_1^{(k)}, q_1^{(k)} + \Psi(e_1)e_1, q_1^{(k)} + \Psi(e_2)e_2] \quad (91)$$

where

$$\Psi(u) = \frac{1}{2}\sigma_-(S^{(k)})\eta(\text{sign}(\langle D(f : S^{(k)}), u \rangle)). \quad (92)$$

Set $S^{(k)} = \tilde{S}$.

Step 2-5 (Sort the vertices)

Sort and label the vertices according to functional value as $q_w^{(k)}$, $q_s^{(k)}$, and $q_b^{(k)}$ such that

$$(f(q_b^{(k)}), \mu_g(q_b^{(k)}))[\tau_\mu, \leq_{\alpha(t)}](f(q_s^{(k)}), \mu_g(q_s^{(k)})) \\ [\tau_\mu, \leq_{\alpha(t)}](f(q_w^{(k)}), \mu_g(q_w^{(k)})). \quad (93)$$

Step 2-6 (Reflection)

If

$$(f(q_b^{(k)}), \mu_g(q_b^{(k)}))[\tau_\mu, \leq_{\alpha(t)}](f(z^{(k)}(\delta_r)), \mu_g(z^{(k)}(\delta_r))), \quad (94)$$

and

$$(f(z^{(k)}(\delta_r)), \mu_g(z^{(k)}(\delta_r)))[\tau_\mu, <_{\alpha(t)}](f(q_s^{(k)}), \mu_g(q_s^{(k)})), \quad (95)$$

set $S^{(k+1)} = S_{\delta_r}^{(k)}$ and go to step 2-5.

Step 2-7 (Expansion)

Let

$$B : (f(z^{(k)}(\delta_r)), \mu_g(z^{(k)}(\delta_r))) \\ [\tau_\mu, <_{\alpha(t)}](f(q_b^{(k)}), \mu_g(q_b^{(k)})). \quad (96)$$

If $\bar{B}$, go to step 2-8.

If B and

$$(f(z^{(k)}(\chi(\delta_2))), \mu_g(z^{(k)}(\chi(\delta_2)))) \\ [\tau_\mu, <_{\alpha(t)}](f(z^{(k)}(\delta_r)), \mu_g(z^{(k)}(\delta_r))), \quad (97)$$

set $S^{(k+1)} = S_{\chi(\delta_2)}^{(k)}$. Otherwise, set $S^{(k+1)} = S_{\delta_r}^{(k)}$. Go to step 2-5.

Step 2-8 (Outside contraction)

Let

$$B_1 : (f(q_s^{(k)}), \mu_g(q_s^{(k)})) \\ [\tau_\mu, \leq_{\alpha(t)}](f(z^{(k)}(\delta_r)), \mu_g(z^{(k)}(\delta_r))), \quad (98)$$

and

$$B : (f(z^{(k)}(\delta_r)), \mu_g(z^{(k)}(\delta_r))) \\ [\tau_\mu, <_{\alpha(t)}](f(q_w^{(k)}), \mu_g(q_w^{(k)})). \quad (99)$$

Let $B = B_1 \wedge B_2$.

If $\bar{B}$, go to step 2-9.

If B and

$$(f(z^{(k)}(\chi(\delta_1))), \mu_g(z^{(k)}(\chi(\delta_1)))) \\ [\tau_\mu, <_{\alpha(t)}](f(q_w^{(k)}), \mu_g(q_w^{(k)})), \quad (100)$$

set $S^{(k+1)} = S_{\chi(\delta_1)}^{(k)}$ and go to step 2-5.

Otherwise, set $l \leftarrow l + 1$ and go to step 2-1.

Step 2-9 (Inside contraction)

If $|\chi(\delta_{-1})| \geq \varepsilon$,

$$(f(z^{(k)}(\delta_r)), \mu_g(z^{(k)}(\delta_r))) [\tau_\mu, \geq_{\alpha(t)}] (f(q_w^{(k)}), \mu_g(q_w^{(k)})) \quad (101)$$

and

$$(f(z^{(k)}(\chi(\delta_{-1}))), \mu_g(z^{(k)}(\chi(\delta_{-1})))) [\tau_\mu, <_{\alpha(t)}] (f(q_w^{(k)}), \mu_g(q_w^{(k)})), \quad (102)$$

set $S^{(k+1)} = S_{\chi(\delta_{-1})}^{(k)}$ and go to step 2-5.

Otherwise, set $l \leftarrow l + 1$ and go to step 2-1.

Considering this modified version, a number of explanations are in order:

1. We did not use fortified descent. As was mentioned previously, fortified descent is basically a means to ascertain convergence. Moreover, it can be designed to be very similar to strict descent. If the underlying function is reasonably well-behaving, both versions of the algorithm should behave exactly the same behaviour.
2. As is apparent from the convergence results, in cases where convergence is possible, the size of the simplex should go to zero. The shape-constrained version will stagnate when the size of the simplex can not be made smaller. In such situations, the simplex is very close (in the sense of the scale of the environment with respect to the minimum allowable size) to an optimal point. In practical applications, this is all we need.
3. In step 2-9, we check to see if $|\chi(\delta_{-1})|$ is larger than some value. If this check is not done, the simplex may indefinitely try the reflection step and attempt inside contraction in case of failure only to end up in the same state as before. This indicates stagnation due to size limitations.
4. The convergence results should all hold true for this modified version. Firstly, the globalization strategy has no effect on the performance of local searches. Secondly, the α -constrained comparisons do not change the properties of the algorithm. The only major change is the replacement of the constant coefficients with time-dependent ones. This, too, poses no difficulties since, for the algorithm equipped with oriented restarts, it is only required that the relations (3) hold true and we can choose D_l , D_u and φ_l in such a way that

$$\begin{aligned} -1 < \chi(\delta_{-1}) \leq \delta_{-1} < 0 < \delta_1 \leq \chi(\delta_1) < \delta_r \\ < \chi(\delta_2) \leq \delta_2. \end{aligned} \quad (103)$$

5. No tests for degeneracy is done as the shape constraints make sure that the angles stay away from zero.

7 Implementation by robotic formations

In this section, we proceed to design a robotic system composed of three vehicles which implements the Nelder-Mead simplex method. The robots R_1 , R_2 and R_3 are assumed to be equipped with a compass module, flow meter, range and bearing sensors, as well as specific sensors for the application to measure the field value. It is assumed that the robots can communicate with each other using a fixed schedule. The time-dependent positions of the robots are denoted by $q_1(t)$, $q_2(t)$, and $q_3(t)$. The formation itself is represented by the underlying simplex implicitly defined by the positions of the robots with respect to each other.

The function f is now replaced with the environmental field $F: \mathcal{R}^2 \rightarrow \mathcal{R}$. The robots measure a possibly noisy value for the field which is denoted $\tilde{F}(q(t))$. The field can be the bottom terrain, in which case altimeter sensors can be used. It can alternatively be a concentration. The field can be time-varying, denoted by $F(q, t)$ but it has to satisfy some conditions which will be stated later on.

The formation moves constrained to a plane parallel to the surface of the ocean. The vehicles are modelled as non-holonomic devices on this plane.

If the search region is constrained, sensors should be provided to measure $g(q(t))$. For the case of obstacles, optical or acoustic sensors are usually used. If the feasible region is defined by the operators, dead-reckoning might be sometimes used. If more accuracy is required, then resurfacing of the formation and using GPS is the only choice.

Likewise, when restarts are needed, the formation has to resurface. An alternative to resurfacing might be to employ a fourth vehicle especially designed for global localization purposes.

Assume that at the start of the mission (or the start of a local search), the robots form a nonsingular simplex $S^{(0)}$ and that all the distance and angle bounds are respected. Let $\tilde{F}(q_1(t_0))$, $\tilde{F}(q_2(t_0))$ and $\tilde{F}(q_3(t_0))$ be the measurements at time t_0 . For the moment, let us assume that the robots can keep stationary perfectly such that $q_i(t_0 + T) = q_i(t_0)$, for all $T \geq 0$. We can sort the values and relabel the robots, together with their positions (dropping the time dependence), as R_w , R_s and R_b (correspondingly, $q_w^{(0)}$, $q_s^{(0)}$ and $q_b^{(0)}$), such that

$$\begin{aligned} (\tilde{F}(q_b^{(0)}), \mu_g(q_b^{(0)})) [\tau_\mu, \leq_\alpha] (\tilde{F}(q_s^{(0)}), \mu_g(q_s^{(0)})) \\ [\tau_\mu, \leq_\alpha] (\tilde{F}(q_w^{(0)}), \mu_g(q_w^{(0)})). \end{aligned} \quad (104)$$

To enact operations of the proposed algorithm, some of the robots have to do *exploratory manoeuvres*. In our system, we consider R_b as the pivot robot which is to keep station during an operation. Briefly, the system first *tries* reflection. To do this, R_s goes to $z^{(0)}(\delta_r)$ (while R_w is stationary) and measures the field value at that point. If the try is successful, R_s resumes the new location while R_w goes to $q_s^{(0)}$.

If expansion is promising, $\mathbf{R}_s$ goes to $z^{(0)}(\chi(\delta_2))$ instead. If successful, it remains there, otherwise, it returns back to $z^{(0)}(\delta_r)$. For outside contraction, $\mathbf{R}_s$ goes to $z^{(0)}(\chi(\delta_1))$. For inside contraction, though, $\mathbf{R}_s$ returns back to $q_s^{(0)}$, while $\mathbf{R}_w$ goes to $z^{(0)}(\chi(\delta_{-1}))$. If shrink is allowed, $\mathbf{R}_s$ goes to $r(s)$, where

$$r(u) = q_b^{(0)} + \max \left\{ \frac{1}{\xi} \|q_u^{(0)} - q_b^{(0)}\|, D_l \right\} \cdot \frac{(q_s^{(0)} - q_b^{(0)})}{\|q_u^{(0)} - q_b^{(0)}\|}, \quad (105)$$

while $\mathbf{R}_w$ goes to $r(w)$. In the case of oriented restart, $\mathbf{R}_s$ goes to $q_b^{(0)} + \Psi(e_1)e_1$ or $q_b^{(0)} + \Psi(e_2)e_2$, whichever is closer to $q_s^{(0)}$, and $\mathbf{R}_w$ goes to the other point. This latter operation requires the use of the compass to determine directions of the global principal coordinates. These manoeuvres are depicted in Fig. 8.

Let us now consider a more realistic setting. At the beginning of the mission, the robot $\mathbf{R}_1$ (the choice is arbitrary) is assigned the role of the pivot robot. This means that the other vehicles should adjust their positions with respect to the pivot. The pivot itself should keep station at all times. This role may be given to other robots, as will be explained later. The positions of $\mathbf{R}_2$ and $\mathbf{R}_3$ with respect to $\mathbf{R}_1$ can be represented by the pairs $(D_{21}(t), \theta_{21}(t))$ and $(D_{31}(t), \theta_{31}(t))$, where $D_{i1}(t)$ is the distance measured by the range sensor and $\theta_{i1}(t)$ is the angle measured by the bearing sensor. Let us denote by D_{i1}^d and θ_{i1}^d , the desired distance and bearing. At the beginning of the mission, we put

$$D_{i1}^d = \left(\frac{2A}{\sin(\pi/3)} \right)^{1/2}, \quad (106)$$

$$\theta_{21}^d = 0, \quad \text{and} \quad \theta_{31}^d = \pi/2. \quad (107)$$

Note that this is different from the initialization scheme in the algorithm but has the same effect. They try to keep station in this position by counteracting the flow of the medium until the first synchronization point t_0 . At this time, field measurements are done and the robots are sorted. The role of the pivot is now relegated to $\mathbf{R}_b$. The relative measurements should now be calculated with respect to the new pivot. This is summarized in the following lemma (Fig. 7).

Lemma 5 Let $(b, s, w) = \partial(1, 2, 3)$ be any permutation of the ordered triple $(1, 2, 3)$. Then we have

$$D_{sb}^d = \sqrt{(D_{\partial^{-1}(b)1}^d)^2 + (D_{\partial^{-1}(s)1}^d)^2 - 2B_s}, \quad (108)$$

$$B_s = D_{\partial^{-1}(b)1}^d D_{\partial^{-1}(s)1}^d \cos(\varphi_{1,23}), \quad (109)$$

$$D_{wb}^d = \sqrt{(D_{\partial^{-1}(b)1}^d)^2 + (D_{\partial^{-1}(w)1}^d)^2 - 2B_w}, \quad (110)$$

Fig. 7 Relative coordinates for the permutation $(3, 1, 2) = \partial(1, 2, 3)$

$$B_w = D_{\partial^{-1}(b)1}^d D_{\partial^{-1}(w)1}^d \cos(\varphi_{1,23}), \quad (111)$$

$$\theta_{sb}^d = \arccos \left(\frac{v_{sb}}{\|v_{sb}\|} \right), \quad (112)$$

$$\theta_{wb}^d = \arccos \left(\frac{v_{wb}}{\|v_{wb}\|} \right), \quad (113)$$

where

$$\cos(\varphi_{1,23}) = \arccos \left(\left(\begin{pmatrix} \cos(\theta_{21}^d) \\ \sin(\theta_{21}^d) \end{pmatrix} \cdot \begin{pmatrix} \cos(\theta_{31}^d) \\ \sin(\theta_{31}^d) \end{pmatrix} \right) \right), \quad (114)$$

$$v_{wb} = c(\partial^{-1}(b)) D_{\partial^{-1}(w)1}^d \begin{pmatrix} \cos(\theta_{\partial^{-1}(w)1}^d) \\ \sin(\theta_{\partial^{-1}(w)1}^d) \end{pmatrix} + D_{\partial^{-1}(b)1}^d \wedge d \begin{pmatrix} \cos(\theta_{\partial^{-1}(b)1}^d) \\ \sin(\theta_{\partial^{-1}(b)1}^d) \end{pmatrix}, \quad (115)$$

$$v_{sb} = c(\partial^{-1}(b)) D_{\partial^{-1}(s)1}^d \begin{pmatrix} \cos(\theta_{\partial^{-1}(s)1}^d) \\ \sin(\theta_{\partial^{-1}(s)1}^d) \end{pmatrix} + D_{\partial^{-1}(b)1}^d \wedge d \begin{pmatrix} \cos(\theta_{\partial^{-1}(b)1}^d) \\ \sin(\theta_{\partial^{-1}(b)1}^d) \end{pmatrix}. \quad (116)$$

$c(u)$ is -1 if $u \neq 1$ and 1 , otherwise.

By convention, $D_{ii}^d = 0$.

It is easy to verify that for the case of identity permutation, the values do not change. Given range and bearing measurements, relative coordinates of the generated points for various operations with respect to the best vertex can be computed according to the following lemma.

Fig. 8 Exploratory manoeuvres for enactment of the simplex steps. (a) Successful reflection. (b) Successful expansion. (c) Unsuccessful expansion. (d) Successful outside contraction. (e) Inside contraction. (f) Shrinking after unsuccessful outside contraction. (g) Shrinking after unsuccessful inside contraction. (h) Oriented restart

Lemma 6 For every δ , the coordinates of a generated point in terms of range and bearing ($D_{\delta b}^d, \theta_{\delta b}^d$) are given by

$$D_{\delta b}^d = \sqrt{\left(\frac{1}{2}D_{sb}^d\right)^2 + (\delta a)^2 - 2D_{sb}^d|\delta a|\tilde{\vartheta}}, \quad (117)$$

$$\theta_{\delta b}^d = \text{acos}\left(\frac{v_2 \cdot e_1}{\|v_2\|}\right), \quad (118)$$

where

$$a = \sqrt{\left(\frac{1}{2}D_{sb}^d\right)^2 + (D_{wb}^d)^2 - D_{sb}^d D_{wb}^d \tilde{a}}, \quad (119)$$

$$\tilde{a} = \begin{pmatrix} \cos(\theta_{sb}^d) \\ \sin(\theta_{sb}^d) \end{pmatrix} \cdot \begin{pmatrix} \cos(\theta_{wb}^d) \\ \sin(\theta_{wb}^d) \end{pmatrix}, \quad (120)$$

$$v_2 = \frac{1}{2}D_{sb}^d \begin{pmatrix} \cos(\theta_{sb}^d) \\ \sin(\theta_{sb}^d) \end{pmatrix} + \delta a \begin{pmatrix} \cos(\vartheta) \\ \sin(\vartheta) \end{pmatrix}, \quad (121)$$

$$\tilde{\vartheta} = \text{acos}\left(\left| -\begin{pmatrix} \cos(\theta_{sb}^d) \\ \sin(\theta_{sb}^d) \end{pmatrix}, \text{sign}(\delta) \begin{pmatrix} \cos(\vartheta) \\ \sin(\vartheta) \end{pmatrix} \right| \right), \quad (122)$$

$$\vartheta = \text{acos}\left(\frac{v_1 \cdot e_1}{\|v_1\|}\right), \quad (123)$$

$$v_1 = \frac{1}{2}D_{sb}^d \begin{pmatrix} \cos(\theta_{sb}^d) \\ \sin(\theta_{sb}^d) \end{pmatrix} - D_{wb}^d \begin{pmatrix} \cos(\theta_{wb}^d) \\ \sin(\theta_{wb}^d) \end{pmatrix}. \quad (124)$$

Moreover, the centroid is given by $(\frac{1}{2}D_{sb}^d, \theta_{sb}^d)$, and the oriented restart points are given by

$$\begin{aligned} (D_{o1b}^d, \theta_{o1b}^d) \\ = \left(\frac{1}{2}\sigma_-(S^{(k)}), \frac{1}{2}(\pi - \eta(\text{sign}(\langle D(F : S^{(k)}), e_1 \rangle))\pi) \right) \end{aligned} \quad (125)$$

and

$$\begin{aligned} (D_{o2b}^d, \theta_{o2b}^d) \\ = \left(\frac{1}{2}\sigma_-(S^{(k)}), \right. \\ \left. \frac{\pi}{2} + \frac{1}{2}(\pi - \eta(\text{sign}(\langle D(F : S^{(k)}), e_2 \rangle))\pi) \right). \end{aligned} \quad (126)$$

Figure 9 illustrates some of the variables. Each step of the algorithm is executed by determining which of the worst and next best robots should go to which of the desired configurations designed above. Convergence to any of the desired locations signals the start of the next consecutive step. Note that the way we implement the algorithm makes sure that the shape of the simplex does not drift due to inaccuracies in reaching the desired points exactly. This is because

Fig. 11 Plots. **(a)** Inter-robot distances: (solid) $\|q_0 - q_1\|$, (dot) $\|q_0 - q_2\|$, (dash) $\|q_1 - q_2\|$. **(b)** Diameters: (solid) $\text{diam}_i(S)$, (dot) $\text{diam}_o(S)$. **(c)** Field values: (solid) $F(q_0)$, (dot) $F(q_1)$, (dash) $F(q_2)$. **(d)** Angles between edges: (solid) $\varphi_{0,12}$, (dash) $\varphi_{1,02}$, (dot) $\varphi_{2,01}$. **(e)** $\nu(S)$

8 Simulations

In this section, we present a few simulation runs which are supposed to show the behaviour of the modified Nelder-Mead algorithm.

Figure 12(a) shows localization of a local minimum by a formation using only reflection (basic simplex method). Figure 12(b) shows the trace of a formation climbing a noisy field. Figure 12(c) shows a scenario where motion is constrained to a part of the field due to the barrier shown as a line. Figure 12(d) shows the situation where the optimum of the field is located very close to the boundary. The formation goes through two oriented restarts and finally terminates operation as it has to shrink.

Figure 11 shows plots of inter-robot distances, triangle diameters, field values, angles, and finally $\nu(S)$, for a simulation run with $D_l = 50$, $D_u = 200$, and $\varphi_l = \pi/10$.

9 Conclusions and future research

In this paper, we examined the possibility of using the Nelder-Mead extension to the basic simplex method for lo-

calizing optima of natural fields by networks of autonomous robots playing the role of sample points. This problem corresponds to nonlinear function minimization or maximization in optimization theory. The proposed strategy is only one of many direct and/or derivative-free search methods proposed in mathematical literature in the past. Close examination of these methods (when implemented by a robotic network) reveals certain similarities: (1) the robot aggregate is deformable, (2) it moves from one iteration to the next as opposed to continuous motion in rigid formations, (3) in each iterate, some of the robots remain stationary while others carry on exploratory motions to go to sample points in the vicinity of the aggregate, (4) relative values at sampled points are used as a basis for determining the next iterate. It would certainly be worthwhile to look into general frameworks for such *exploratory aggregates* (see Kalantar 2007 for such an attempt). Future research should address: (1) study of faithfulness of a robotic implementation to the original algorithm in the face of uncertainties, (2) the challenge of station keeping in underwater environments, (3) exploring other similar search strategies, (4) designing a general system which can autonomously implement a given

Fig. 12 (a) Basic simplex. (b) Noisy field. (c) Constrained region. (d) Optimum close to barrier; the formation has to shrink

blueprint for a search algorithm, (5) peculiarities of time-varying fields, (6) communication and synchronization issues.

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Shahab Kalantar got his Master's degree in Robotics and Machine Intelligence in 1997 from Tehran University and his Bachelor's in Applied Mathematics in 1991. He received his PhD degree at the Australian National University in 2007. His current research interest is the interaction of deformable formations of autonomous vehicles with environmental fields.

Uwe R. Zimmer is currently a fellow at the Australian National University at the Faculty of Engineering and Information Technology and at the Research School of Information Sciences and Engineering. He received his Dr. rer. nat. degree in 1995 at the University of Kaiserslautern, Germany. Building up an underwater research group in Germany at the former German National Research Center for Information Technology, and setting up a research laboratory for autonomous robust systems in Kyushu, Japan have been the other major activities since then. He is currently the head of the underwater robotics group at the Australian National University. His major research interests are in distributed swarm control and communication with application to real-time and real-world environments.