On a sequential linear programming approach to finding the smallest circumscribed, largest inscribed, and minimum zone circle or sphere

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Abstract. *Sequential linear programming methods have been successfully used to solve some sphere and circle problems. Indeed, empirical evidence shows that these frequently find the required solutions in one step. An analysis is presented here which attempts to give an explanation of this phenomemon.*

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1. Introduction

Let $\mathbf{x}_i, i = 1, \ldots, m$ be given points in 3 dimensional space. Then of interest here is a sequential linear programming approach to the problems of determining (i) the smallest circumscribed sphere, (ii) the largest inscribed sphere and (iii) the pair of concentric spheres respectively circumscribing and inscribing the points with the smallest difference of radii; such problems arise for example in computational metrology [10]. The last of these problems is often referred to as a minimum zone problem [3], [6], [10], although this terminology is also used for the problem of finding a single approximating sphere [2]. All these problems also arise in 2 dimensions, where circles replace spheres.

For convenience denote the components of $\mathbf{x}_i$ by (x_i, y_i, z_i). Then in mathematical terms, we have to solve the following problems:

Problem MCS

$$\text{minimize } R \text{ subject to}$$

$$(x - x_i)^2 + (y - y_i)^2 + (z - z_i)^2 \leq R^2, \ i = 1, \ldots, m.$$

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Problem MIS

$$\text{maximize } r \text{ subject to}$$
$$(x-x_i)^2+(y-y_i)^2+(z-z_i)^2 \geq r^2,\ i=1,\dots,m,$$
$$(x,y,z) \in \operatorname{conv}\{(x_i,y_i,z_i), i=1,\dots,m\}, \tag{1}$$

where "conv" denotes the convex hull.

Problem MZS

$$\text{minimize } R-r \text{ subject to}$$
$$r^2 \leq (x-x_i)^2+(y-y_i)^2+(z-z_i)^2 \leq R^2,\ i=1,\dots,m.$$

The optimization problems are all performed with respect to the variables (x,y,z) (the unknown centres), and R and/or r (the unknown radii). If the problems involve circles in a plane, then obviously all that changes is that the terms involving z are deleted.

The problem (MIS) needs a constraint like (1) (although there are other possibilities), as otherwise the solution is unbounded. However, the underlying problem involves finding an appropriate local maximum of the problem without (1), and if such a point is sought, then (1) may be ignored. In that case, all the above problems have linear objective functions and quadratic constraints and clearly general nonlinear optimization techniques can be applied. The problems can also be defined in higher dimensions, although computational complexity issues would become increasingly important. Because (MCS) is a convex problem, the global solution will be obtained by any reasonable method for constrained optimization, and for a large value of m, primal-dual interior point methods might be appropriate. Although this problem can be solved in polynomial time, the other problems are not convex, and could have many local solutions. In particular, problem (MIS) is NP-hard. Radius computations of the kind considered here have been studied in some detail; see [4] and the references given there.

The possibility of solving these problems by sequential linear programming techniques has been raised in [7], [8], [9], where it is argued that there are advantages to scientists or engineers who may wish to solve such problems if well known and freely available linear programming routines can be used. Some numerical experiments have shown that this can be effective, with solutions obtained in often just one step. It is the purpose of this note to investigate this phenomenon.

2. Using sequential linear programming

The application of a linearization technique is required to generate an approximate linear programming problem from each of the above 3 problems. Consider first (MCS). Let

$$b_i = -\frac{1}{2}(x_i^2+y_i^2+z_i^2),\ i=1,\dots,m.$$

Then the constraints of (MCS) may be expressed as

$$(\frac{x}{2}-x_i)x+(\frac{y}{2}-y_i)y+(\frac{z}{2}-z_i)z-\frac{1}{2}R^2 \leq b_i,\ i=1,\dots,m.$$

Let approximations $x^{(t)}, y^{(t)}, z^{(t)}$ be given to the coordinates of the centre of the required circle. Then an appropriate linearization is

Problem MCS(t)

$$\text{minimize } R \text{ subject to}$$

$$(\frac{x^{(t)}}{2} - x_i)x + (\frac{y^{(t)}}{2} - y_i)y + (\frac{z^{(t)}}{2} - z_i)z - \frac{1}{2}R^{(t)}R \leq b_i,\ i = 1, \dots, m.$$

Provided that a solution (x, y, z, R) exists, the $(t+1)st$ approximation is given by setting

$$x^{(t+1)} = x;\ y^{(t+1)} = y;\ z^{(t+1)} = z,$$

and defining the new approximation to R by

$$R^{(t+1)} = \sqrt{\max_i\{(x^{(t+1)} - x_i)^2 + (y^{(t+1)} - y_i)^2 + (z^{(t+1)} - z_i)^2\}}.$$

With the assumption that (1) can be ignored, a similar linearization of the problem (MIS) can be obtained. However, an alternative in both cases then arises from a reformulation of the problems as quadratic programming problems. Let

$$u = \frac{1}{2}(R^2 - (x^2 + y^2 + z^2)).$$

Then (MCS) can be rewritten as the quadratic programming problem

Problem MCS′

$$\text{minimize } \frac{1}{2}(x^2 + y^2 + z^2) + u \text{ subject to}$$

$$-x_i x - y_i y - z_i z - u \leq b_i,\ i = 1, \dots, m.$$

Let approximations $x^{(t)}, y^{(t)}, z^{(t)}$ be given to the coordinates of the centre of the required circle, and consider the linear programming problem for unknowns (x, y, z, u):

Problem MCS′(t)

$$\text{minimize } \frac{1}{2}(x^{(t)}x + y^{(t)}y + z^{(t)}z) + u$$

$$\text{subject to } -x_i x - y_i y - z_i z - u \leq b_i,\ i = 1, \dots, m.$$

Provided that a solution (x, y, z, u) exists, the $(t+1)st$ approximation is obtained as for MCS(t).

Similarly defining

$$v = \frac{1}{2}(r^2 - (x^2 + y^2 + z^2)),$$

the problem (MIS) (ignoring (1)) can be rewritten

Problem MIS′

$$\text{maximize } \frac{1}{2}(x^2+y^2+z^2)+v \text{ subject to}$$
$$x_i x + y_i y + z_i z + v \le -b_i,\ i=1,\dots,m.$$

The corresponding linearised problem is

Problem MIS′(t)

$$\text{maximize } \frac{1}{2}(x^{(t)}x+y^{(t)}y+z^{(t)}z)+v$$
$$\text{subject to } x_i x + y_i y + z_i z + v \le -b_i,\ i=1,\dots,m.$$

Provided that a solution (x,y,z,v) exists, the next approximation is given by setting

$$x^{(t+1)}=x;\ y^{(t+1)}=y;\ z^{(t+1)}=z,$$

and defining the new approximation to r by

$$r^{(t+1)}=\sqrt{\min_i\{(x^{(t+1)}-x_i)^2+(y^{(t+1)}-y_i)^2+(z^{(t+1)}-z_i)^2\}}.$$

Finally, consider (MZS). With $b_i, i=1,\dots,m$ defined as before, a suitable linearization is

Problem MZS(t)

$$\text{minimize } \ R-r \ \text{ subject to}$$
$$(\frac{x^{(t)}}{2}-x_i)x+(\frac{y^{(t)}}{2}-y_i)y+(\frac{z^{(t)}}{2}-z_i)z-\frac{1}{2}R^{(t)}R\le b_i,\ i=1,\dots,m,$$
$$-(\frac{x^{(t)}}{2}-x_i)x-(\frac{y^{(t)}}{2}-y_i)y-(\frac{z^{(t)}}{2}-z_i)z+\frac{1}{2}r^{(t)}r\le -b_i,\ i=1,\dots,m.$$

Provided a solution (x,y,z,R,r) exists, the next approximation is given by

$$x^{(t+1)}=x;\ y^{(t+1)}=y;\ z^{(t+1)}=z,$$

with the new approximations to R and r given by

$$R^{(t+1)}=\sqrt{\max_i\{(x^{(t+1)}-x_i)^2+(y^{(t+1)}-y_i)^2+(z^{(t+1)}-z_i)^2\}},$$

$$r^{(t+1)}=\sqrt{\min_i\{(x^{(t+1)}-x_i)^2+(y^{(t+1)}-y_i)^2+(z^{(t+1)}-z_i)^2\}}.$$

Sequential linear programming is a longstanding technique in nonlinear optimization [5], [11], and a particular form has been used before for (MIS) [1]. As here, the additional constraint (1) is formally included, although it is assumed that it is automatically satisfied at points of interest. The underlying problem is essentially a combinatorial one of identifying the correct or optimal "active set" where equality holds in the constraints. Note that the solution to each linearized subproblem will, because of the way $R^{(t+1)}$ and/or $r^{(t+1)}$ is defined, also define an active set for the original problems.

We do not address convergence properties of the sequence here, although some attention is given to this aspect in [1] and [11]. We start from the empirical fact [7] [8], [9] that in all the above cases, when the starting point is given by taking the average values of the data points,

$$(x^{(0)}, y^{(0)}, z^{(0)}) = (\frac{\sum_{i=1}^m x_i}{m}, \frac{\sum_{i=1}^m y_i}{m}, \frac{\sum_{i=1}^m z_i}{m}),$$

only one iteration is often required to get the desired solution; in other words, only one linear programming solution is actually needed. We consider in the next section the circumstances under which this can happen.

3. Finding Kuhn-Tucker points in one step

Consider first the problem (MCS). Because this is a convex problem, the Kuhn-Tucker conditions are necessary and sufficient for a solution. Let (x, y, z) be a solution with I the set of indices where equality holds in the constraints, ie.

$$(x - x_i)^2 + (y - y_i)^2 + (z - z_i)^2 = R^2,\ i \in I.$$

Then the Kuhn-Tucker conditions tell us that there exist $\lambda_i \geq 0, i \in I$ such that

$$2R \sum_{i \in I} \lambda_i = 1,$$

$$\sum_{i \in I} \lambda_i (x - x_i) = 0,$$

$$\sum_{i \in I} \lambda_i (y - y_i) = 0,$$

$$\sum_{i \in I} \lambda_i (z - z_i) = 0.$$

Thus $\sum_{i \in I} \lambda_i = \frac{1}{2R}$, or

$$\sum_{i \in I} \lambda_i' = 1,$$

where

$$\lambda_i' = 2R\lambda_i,\ i \in I.$$

Thus

$$(x, y, z) \in \text{conv}\{(x_i, y_i, z_i),\ i \in I\}. \tag{2}$$

Now consider the problem (MCS(t)). Necessary and sufficient conditions for a solution (x, y, z) are that this is feasible and there exists an index set $I^{(t)}$ such that constraint equality holds and $\lambda_i \geq 0, i \in I^{(t)}$ with

$$\sum_{i \in I^{(t)}} \lambda_i = \frac{2}{R^{(t)}},$$

$$\frac{x^{(t)}}{2}\sum_{i\in I^{(t)}}\lambda_i=\sum_{i\in I^{(t)}}\lambda_i x_i,$$
$$\frac{y^{(t)}}{2}\sum_{i\in I^{(t)}}\lambda_i=\sum_{i\in I^{(t)}}\lambda_i y_i,$$
$$\frac{z^{(t)}}{2}\sum_{i\in I^{(t)}}\lambda_i=\sum_{i\in I^{(t)}}\lambda_i z_i,$$

or equivalently such that

$$\frac{1}{2}(x^{(t)},y^{(t)},z^{(t)})\in \operatorname{conv}\{(x_i,y_i,z_i),\ i\in I^{(t)}\}. \tag{3}$$

Note that if

$$\frac{1}{2}(x^{(t)},y^{(t)},z^{(t)})\notin \operatorname{conv}\{(x_i,y_i,z_i),i=1,\dots,m\},$$

then there is no solution to (MCS(t)), in fact the solution is unbounded.

Theorem 1. *Let (x,y,z) solve (MCS), with I the set of constraint indices where equality is attained, and let*

$$\frac{1}{2}(x^{(t)},y^{(t)},z^{(t)})\in \operatorname{conv}\{(x_i,y_i,z_i).\ i\in I\}. \tag{4}$$

Then (x,y,z) solves (MCS(t)).

Proof. By definition

$$(x-x_i)^2+(y-y_i)^2+(z-z_i)^2\le R^2,\ i=1,\dots,m.$$

Thus for all i,

$$\begin{aligned}(x^{(t)}x-2x_ix+x_i^2)&+(y^{(t)}y-2y_iy+y_i^2)+(z^{(t)}z-2z_iz+z_i^2)\\ &\le R^2+x(x^{(t)}-x)+y(y^{(t)}-y)+z(z^{(t)}-z),\end{aligned}$$

with equality for $i\in I$, where we have used the fact that for every i,

$$\begin{aligned}&(x^{(t)}x-2x_ix+x_i^2)+(y^{(t)}y-2y_iy+y_i^2)+(z^{(t)}z-2z_iz+z_i^2)\\ &=(x-x_i)^2+(y-y_i)^2+(z-z_i)^2+x(x^{(t)}-x)+y(y^{(t)}-y)+z(z^{(t)}-z).\end{aligned} \tag{5}$$

Define R' by

$$\begin{aligned}R'&=\max_i\frac{1}{R^{(t)}}\{(x^{(t)}x-2x_ix+x_i^2)+(y^{(t)}y-2y_iy+y_i^2)+(z^{(t)}z-2z_iz+z_i^2)\}\\ &=\frac{1}{R^{(t)}}\{R^2+x(x^{(t)}-x)+y(y^{(t)}-y)+z(z^{(t)}-z)\},\quad i\in I.\end{aligned}$$

Therefore (x,y,z,R') is feasible for (MCS(t)) and also

$$(x^{(t)}x-2x_ix+x_i^2)+(y^{(t)}y-2y_iy+y_i^2)+(z^{(t)}z-2z_iz+z_i^2)=R^{(t)}R',\quad i\in I.$$

In other words, (MCS) and MCS(t) have the same active sets I at (x, y, z), and so (4) implies (3) and the result follows. $\square$

Corollary 1. *If (4) is satisfied, and if (MCS(t)) has a unique solution, then (MSC) is solved in one linear programming step.*

Now consider (MCS) in the form (MCS′). The Kuhn-Tucker conditions are again necessary and sufficient for a solution. Let (x, y, z) be a solution with I the set of indices where equality holds in the constraints, ie.

$$-x_i x - y_i y - z_i z - u = b_i, \quad i \in I.$$

Then the Kuhn-Tucker conditions are again given by (2). Now consider the problem (MCS′(t)). Arguing exactly as before, necessary and sufficient conditions for (x, y, z) to be a solution are that there exists a set of constraint indices $I^{(t)}$ with equality holding and feasibility with respect to the other constraints such that

$$\frac{1}{2}(x^{(t)}, y^{(t)}, z^{(t)}) \in \mathrm{conv}\{(x_i, y_i, z_i), i \in I^{(t)}\}. \tag{6}$$

Theorem 2. *Let (x, y, z) solve (MCS′), with I the set of constraint indices where equality is attained and let*

$$\frac{1}{2}(x^{(t)}, y^{(t)}, z^{(t)}) \in \mathrm{conv}\{(x_i, y_i, z_i), i \in I\}. \tag{7}$$

Then (x, y, z) solves (MCS′(t)).

Proof. Since the constraints for both problems are identical, obviously (x, y, z) is feasible in (MCS′(t)). Further we can choose $I^{(t)} = I$. Thus (7) implies (6) and so (x, y, z) solves (MCS′(t)). $\square$

Corollary 2. *If (7) is satisfied, and if (MCS′(t)) has a unique solution, then (MSC′) is solved in one linear programming step.*

Exactly the same analysis can be carried out for (MIS) and (MIS′) except that the conditions (2) are only **necessary** for a solution. The results are stated only for (MIS).

Theorem 3. *Let (x, y, z) solve (MIS), with I the set of constraint indices where equality is attained and let (7) hold. Then (x, y, z) solves (MIS(t)).*

Corollary 3. *If (7) is satisfied, and if (MIS(t)) has a unique solution, then (MIS) is solved in one linear programming step.*

Corollary 4. *If (7) is satisfied for any index set I defined by a Kuhn-Tucker point of (MIS), and if (MIS(t)) has a unique solution, then Kuhn-Tucker conditions for (MIS) are satisfied in one linear programming step.*

We turn next to the problem (MZS). Assume that the solution is non-degenerate, in the sense that at the solution $R > r > 0$. Then if equality holds in one of the first set of constraints, it cannot hold in the corresponding constraint of the other. Thus for a solution, in addition to feasibility, from the Kuhn-Tucker conditions there are two sets where equality holds, say I^R and I^r, **mutually exclusive**, and non-negative multipliers $\lambda_i, i \in I^R$, and $\gamma_i, i \in I^r$ such that

$$\sum_{i \in I^R} \lambda_i (x - x_i) = \sum_{i \in I^r} \gamma_i (x - x_i),$$

$$\sum_{i\in I^R}\lambda_i(y-y_i)=\sum_{i\in I^r}\gamma_i(y-y_i),$$

$$\sum_{i\in I^R}\lambda_i(z-z_i)=\sum_{i\in I^r}\gamma_i(z-z_i),$$

$$1-2R\sum_{i\in I^R}\lambda_i=0,$$

$$-1+2r\sum_{i\in I^r}\gamma_i=0.$$

Thus

$$\sum_{i\in I^R}\lambda_i+\sum_{i\in I^r}\gamma_i=\frac{1}{2R}+\frac{1}{2r},\quad \text{or}\quad \sum_{i\in I^R}\lambda_i'+\sum_{i\in I^r}\gamma_i'=1,$$

where

$$\lambda_i'=\lambda_i(\frac{1}{2R}+\frac{1}{2r})^{-1},\ i\in I^R\quad\text{and}\quad \gamma_i'=\gamma_i(\frac{1}{2R}+\frac{1}{2r})^{-1},\ i\in I^r.$$

Further,

$$x(\frac{1}{2R}-\frac{1}{2r})=\sum_{i\in I^R}\lambda_i x_i-\sum_{i\in I^r}\gamma_i x_i,$$

and similarly for y, z, so that

$$x(\frac{1}{2R}-\frac{1}{2r})=(\frac{1}{2R}+\frac{1}{2r})(\sum_{i\in I^R}\lambda_i' x_i-\sum_{i\in I^r}\gamma_i' x_i),$$

and similarly for y, z. Thus

$$\frac{r-R}{r+R}(x,y,z)\in\operatorname{conv}\{(x_i,y_i,z_i),i\in I^R,(-x_i,-y_i,-z_i),i\in I^r\}. \tag{8}$$

Now consider problem (MZS(t)). Arguing in the same way shows that necessary (and sufficient) conditions for a solution are feasibility and (mutually exclusive) sets I^{Rt}, I^{rt} such that

$$\frac{r^{(t)}-R^{(t)}}{2(r^{(t)}+R^{(t)})}(x^{(t)},y^{(t)},z^{(t)})\in\operatorname{conv}\{(x_i,y_i,z_i),i\in I^{Rt},\ (-x_i-y_i,-z_i)\in I^{rt}\}. \tag{9}$$

Theorem 4. *Let (x, y, z, R, r) solve (MZS), with R and r attained at $i\in I^R$ and $i\in I^r$, respectively. Let*

$$\frac{r^{(t)}-R^{(t)}}{2(r^{(t)}+R^{(t)})}(x^{(t)},y^{(t)},z^{(t)})\in\operatorname{conv}\{(x_i,y_i,z_i),i\in I^{R},\ (-x_i-y_i,-z_i)\in I^{r}\}. \tag{10}$$

Then x, y, z solves (MZS(t)).

Proof. By definition

$$r^2\le(x-x_i)^2+(y-y_i)^2+(z-z_i)^2\le R^2,\quad i=1,\dots,m.$$

Thus for all i,

$$\begin{aligned} & r^2 + x(x^{(t)} - x) + y(y^{(t)} - y) + z(z^{(t)} - z) \\ \leq\ & (x^{(t)}x - 2x_ix + x_i^2) + (y^{(t)}y - 2y_iy + y_i^2) + (z^{(t)}z - 2z_iz + z_i^2) \\ \leq\ & R^2 + x(x^{(t)} - x) + y(y^{(t)} - y) + z(z^{(t)} - z), \end{aligned}$$

where we have used (5). Define R', r' by

$$R' = \max_i \frac{1}{R(t)}\{(x^{(t)}x - 2x_ix + x_i^2) + (y^{(t)}y - 2y_iy + y_i^2) + (z^{(t)}z - 2z_iz + z_i^2)\}$$

$$= \frac{1}{R(t)}\{R^2 + x(x^{(t)} - x) + y(y^{(t)} - y) + z(z^{(t)} - z)\}, \quad i \in I^R,$$

$$r' = \min_i \frac{1}{r(t)}\{(x^{(t)}x - 2x_ix + x_i^2) + (y^{(t)}y - 2y_iy + y_i^2) + (z^{(t)}z - 2z_iz + z_i^2)\}$$

$$= \frac{1}{r(t)}\{r^2 + x(x^{(t)} - x) + y(y^{(t)} - y) + z(z^{(t)} - z)\}, \quad i \in I^r.$$

Therefore (x, y, z, R', r') is feasible for (MZS(t)), and also

$$(x^{(t)}x - 2x_ix + x_i^2) + (y^{(t)}y - 2y_iy + y_i^2) + (z^{(t)}z - 2z_iz + z_i^2) = R(t)R', \quad i \in I^R,$$

$$(x^{(t)}x - 2x_ix + x_i^2) + (y^{(t)}y - 2y_iy + y_i^2) + (z^{(t)}z - 2z_iz + z_i^2) = r(t)r', \quad i \in I^r.$$

In other words, (MZS) and (MZS(t)) have the same "active sets" $I^R \cup I^r$, and so (10) implies (9) and therefore (x, y, z) solves (MZS(t)). □

Corollary 5. *If (10) holds and if the solution to (MZS(t)) is unique, then (MZS) is solved in one linear programming step.*

Corollary 6. *If (10) is satisfied for any index sets I^R and I^r defined by a Kuhn-Tucker point of (MZS), and if (MZS(t)) has a unique solution, then Kuhn-Tucker conditions for (MZS) are satisfied in one linear programming step.*

4. Concluding remarks

Experiments have been carried out running the sequential linear programming algorithms on the problems considered here for a fixed number of iterations and accepting as solution that which gives the best objective function value, and this can be effective. The process acts as a search procedure over different active sets, and this is a type of strategy which is likely to be particularly useful for non-convex problems.

Of primary interest here, however, has been the fact that such an approach frequently gives a solution (or possibly a Kuhn-Tucker point) in one step. We have given an analysis of the situation which identifies the circumstances under which this happens.

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