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Dual Methods for Nonlinear Best Approximation Problems

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1. INTRODUCTION

Let M be a real linear space equipped with a norm $\|\cdot\|$, and let $f(\mathbf{a})$: $R^n \to M$. We are concerned here with solving the nonlinear best approximation problem:

$$\text{find } \mathbf{a} \in R^n \text{ to minimise } \|f(\mathbf{a})\| \tag{1.1}$$

where $f(\mathbf{a})$ is assumed nonlinear in the components of $\mathbf{a}$. A standard approach to this is to construct a sequence of linear subproblems whose solutions converge to a solution of (1.1): for example, methods based on the Gauss–Newton method for nonlinear least squares problems have been suggested and successfully used in a variety of cases (e.g., [1], [4], [10], [11]). Differences in the numerical performance of this approach have been shown to depend in the first instance on the type of norm being used: for smooth, strictly convex monotonic norms, the rate of convergence is at best first order, unless $\|f\| = 0$; on the other hand, for polyhedral norms in R^m, the rate of convergence can be second order [1], [12]. If appropriate conditions on the problem are not satisfied, then convergence can become intolerably slow, and the method may even fail. An increase in robustness can be achieved by suitable modification of the linear subproblems, resulting, for example, in methods analogous to the Levenberg method for nonlinear least squares [2], [5], [8]; again, however, the rate of convergence can be poor.

The aim of this paper is to give an alternative procedure which may be applied to obtain rapid convergence from an approximation which is reasonably close to a best approximation. The method involves the direct solution of the dual problem of (1.1), formulated as a finite system of nonlinear equations. Assuming the existence of appropriate edrivatives, Newton's method, for example, may then be used. This approach has been proposed

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in some special cases (e.g. [6], [13]); we give here a general treatment, from which particular examples are derived.

The analysis presented here is a local one, and we will restrict attention to problems for which (i) there exists a bounded region $S \subset R^n$ containing a solution (ii) f is sufficiently smooth in S that we can write

$$f(\mathbf{a} + \mathbf{d}) = f(\mathbf{a}) + \ell(\mathbf{d}) + \| \mathbf{d} \|_A^2 \, w(\mathbf{a}, \mathbf{d}), \tag{1.2}$$

with $\| w \| \leqslant W$ in S. Here $\ell(\mathbf{d})$ denotes the linear combination $\sum_{j=1}^{n} d_j g_j(\mathbf{a})$, where g_j is the partial derivative of f with respect to a_j, $j = 1, 2, \ldots, n$, and $\| \cdot \|_A$ is any norm on R^n. For example, (ii) is satisfied if f is a twice continuously differentiable mapping of S into M.

2. Solution of the Dual Problem

Let M^* be the dual space of M, that is the space of continuous linear functionals $v(f)$ defined on M. For convenience, we will write

$$v(f) = \langle f, v \rangle,$$

thus defining the linear functional as an inner product between the elements of M and those of M^*. The dual norm on M^* can then be written

$$\| v \|^* = \sup_{\|f\| \leqslant 1} \langle f, v \rangle.$$

Now let the set $V(f)$ be defined by

$$V(f) = \{ v \in M^* : \| f \| = \langle f, v \rangle, \| v \|^* \leqslant 1 \}, \tag{2.1}$$

which may be interpreted as the set of subgradients of $\| f \|$ at f (Holmes [7]). Then we have the result (see [3] or [14])

THEOREM 2.1. *If* $\mathbf{a}$ *minimises* $\| f \|$, *there exists* $v \in V(f(\mathbf{a}))$ *such that*

$$\langle g_j, v \rangle = 0, \qquad j = 1, 2, \ldots, n.$$

This result motivates the following definition, which generalises a familiar concept in elementary calculus.

DEFINITION 2.1. If $v \in V(f(\mathbf{a}))$ satisfies $\langle g_j, v \rangle = 0$, $j = 1, 2, \ldots, n$, then we say that $\mathbf{a}$ is a *stationary point* of $\| f \|$.

When $f(\mathbf{a})$ is linear in the components of $\mathbf{a}$, then the conditions of Theorem 2.1 are also sufficient for $\mathbf{a}$ to minimise $\| f \|$, as may easily be shown.

This is not the case for general $f(\mathbf{a})$, although algorithms for the nonlinear problem usually attempt to find a point $\mathbf{a}$ satisfying the necessary conditions, and this is the situation here. In order to obtain sufficiency results in the general case, additional second derivative conditions are required. For example, let f satisfy

$$f(\mathbf{a} + \gamma\mathbf{d}) = f(\mathbf{a}) + \gamma\ell(\mathbf{d}) + \tfrac{1}{2}\gamma^2 u(\mathbf{d}) + O(\gamma^3)$$

in a neighborhood of the stationary point, where

$$u(\mathbf{d}) = \sum_{i=1}^{m}\sum_{j=1}^{m} d_i d_j \frac{\partial g_i}{\partial a_j}, \qquad i, j = 1, 2,..., n.$$

Then, we can readily give conditions for all directions at $\mathbf{a}$ to be uphill, in the following sense.

DEFINITION 2.2. Let $\| \mathbf{d} \|_A = 1$. Then $\mathbf{d}$ is *uphill* at $\mathbf{a}$ if, for all $\gamma > 0$ sufficiently small,

$$\| f(\mathbf{a} + \gamma\mathbf{d}) \| > \| f(\mathbf{a}) \|.$$

THEOREM 2.2. *Let* $v \in V(f(\mathbf{a}))$ *satisfy*

$$\langle g_j , v \rangle = 0, \qquad j = 1, 2,..., n$$
$$\langle u(\mathbf{d}), v \rangle > 0, \qquad \forall \mathbf{d} \in R^n, \qquad \mathbf{d} \neq 0.$$

Then all directions at $\mathbf{a}$ *are uphill.*

Proof. Let v satisfy the above conditions, and $\| \mathbf{d} \|_A = 1$. Then

$$\begin{aligned} \| f(\mathbf{a} + \gamma\mathbf{d}) \| &\geqslant \langle f(\mathbf{a} + \gamma\mathbf{d}), v \rangle \\ &= \| f(\mathbf{a}) \| + \tfrac{1}{2}\gamma^2 \langle u(\mathbf{d}), v \rangle + O(\gamma^3) \\ &> \| f(\mathbf{a}) \| \end{aligned}$$

for $\gamma > 0$ sufficiently small.

Based on Definition 2.1, the *dual problem* to that defined by (1.1) may be stated as

$$\text{find } \mathbf{a} \in R^n, \quad v \in V(f(\mathbf{a})) \text{ such that } \langle g_j , v \rangle = 0, \qquad j = 1, 2,..., n.$$

Now any point in a convex set in R^n can be expressed as a convex combination of at most $(n + 1)$ extreme points of the set. Thus, there exist $t \leqslant n + 1$

"extreme elements" $v_1, v_2, \ldots, v_t \in V(f(\mathbf{a}))$ such that the above problem may be considered as one in R^{n+t}:

$$\begin{aligned} &\text{find } \mathbf{a} \in R^n,\ \boldsymbol{\lambda} \in R^t \text{ such that} \\ &\sum_{i=1}^{t} \lambda_i \langle g_j, v_i \rangle = 0, \qquad j = 1, 2, \ldots, n \\ &\langle f, v_i \rangle = \|f\|, \ i = 1, 2, \ldots, t \\ &\boldsymbol{\lambda}^T \mathbf{e} = 1 \\ &\lambda_i \geqslant 0, \qquad i = 1, 2, \ldots, t, \end{aligned} \tag{2.2}$$

where $\mathbf{e}$ is a vector each component of which is unity. In many cases the form of the extreme elements is known, or can be given in a way which does not introduce additional degrees of freedom, and so we have essentially $(n + t + 1)$ nonlinear equations, and t inequalities, for the $(n + t + 1)$ unknowns $\mathbf{a}$, $\boldsymbol{\lambda}$ and $\|f\|$. Assuming a good approximation to the stationary point (so that in particular t is known) then the inequalities may safely be ignored, and the stationary point obtained by direct solution of the nonlinear system. We now consider some special cases, where the system of equations to be solved has a simple form by virtue of the structure of the set V, or of its extreme elements.

3. Smooth, Strictly Convex, Monotonic Norms in R^m

For norms of this class, there exists a unique vector $\mathbf{v} \in V(\mathbf{f}(\mathbf{a}))$ given by

$$\mathbf{v} = U\mathbf{f}$$

where U is a diagonal $m \times m$ matrix with (i, i) element u_i such that

$$u_i > 0, \qquad f_i \neq 0; \qquad u_i = 0, \qquad f_i = 0.$$

For example, for the L_p norms, $1 < p < \infty$,

$$u_i = |f_i|^{p-2} \|\mathbf{f}\|^{1-p}, \qquad f_i \neq 0.$$

The dual problem is then:

$$\text{find } \mathbf{a} \in R^n \text{ to satisfy } \mathbf{f}^T U A = 0,$$

where A is the $m \times n$ matrix $\nabla\mathbf{f}(\mathbf{a})$ of partial derivatives of $\mathbf{f}$ with respect to the components of $\mathbf{a}$. If U is a continuously differentiable function of $\mathbf{f}$, then second derivative methods may be applied. This holds, for example,

in the case of L_p norms if $p = 2$ or $p \geqslant 3$. When $p = 2$, the problem is a familiar one, and, for example, Gill and Murray [5] show how Newton-type methods can be implemented in a stable manner via sequences of linear least squares calculations.

4. Polyhedral Norms

Let $M = R^m$, and consider the consistent set of linear inequalities

$$B\mathbf{f} \leqslant \mathbf{e}$$

where $\mathbf{f} \in R^m$, and B is an $N \times m$ matrix. Then if

(i) $C = \{\mathbf{f}: B\mathbf{f} \leqslant \mathbf{e}\}$ is bounded and has a nonvoid interior,

(ii) $\mathbf{f} \in C$ iff $-\mathbf{f} \in C$

the polyhedral norm of $\mathbf{f}$ specified by B is defined by

$$\|\mathbf{f}\| = \min\{\nu: B\mathbf{f} \leqslant \nu\mathbf{e}\}.$$

Let

$$\rho_i(B)\mathbf{f} = \|\mathbf{f}\|, \qquad i \in I_B$$

where $\rho_i(B)$ denotes the ith row of B. Then we have

$$V(f(\mathbf{a})) = \operatorname{conv}\{\rho_i(B)^T, i \in I_B\}.$$

Thus $\mathbf{v} \in V(\mathbf{f}(\mathbf{a}))$ iff

$$\mathbf{v} = \sum_{i \in I_B} \lambda_i \rho_i(B)^T, \qquad \lambda_i \geqslant 0, \qquad i \in I_B,$$
$$\boldsymbol{\lambda}^T\mathbf{e} = 1,$$

where I_B may be restricted to a maximum of $(n + 1)$ elements. The system of equations corresponding to (2.2) is thus

$$\sum_{i \in I_B} \lambda_i \rho_i(B)\, A = 0$$
$$\rho_i(B)\,\mathbf{f} = \|\mathbf{f}\| \qquad i \in I_B$$
$$\lambda_i \geqslant 0 \qquad i \in I_B$$
$$\boldsymbol{\lambda}^T\mathbf{e} = 1,$$

where A again defines the $m \times n$ matrix $\nabla\mathbf{f}(\mathbf{a})$. For this class of problems, Anderson and Osborne [2] give an algorithm of Levenberg type for which the assumptions here are appropriate for a basic convergence result. Thus

a good approximation to a solution of the above system may be obtained, and, in particular, an appropriate set I_B identified. If a linear programming method is used to solve the linear subproblems, then a good approximation to $\boldsymbol{\lambda}$ is also available [2].

An important example of a polyhedral norm is the L_∞ norm, for which B is the $2m \times m$ matrix $\begin{bmatrix} I \\ -I \end{bmatrix}$, with I the $m \times m$ unit matrix. The nonlinear system can be written in the form

$$\begin{aligned} f_{\sigma_i} - \theta_i \| \mathbf{f} \| &= 0 \qquad i = 1, 2, \ldots, t \\ \boldsymbol{\mu}^T A^\sigma &= 0 \\ 1 - \boldsymbol{\mu}^T \boldsymbol{\theta} &= 0 \\ \mu_i \theta_i &\geqslant 0, \qquad i = 1, 2, \ldots, t, \end{aligned}$$

where $I_B = \{\sigma_1, \sigma_2, \ldots, \sigma_t\}$, A^σ is the $t \times n$ submatrix of A with ith row $\rho_{\sigma_i}(A)$, and $\boldsymbol{\theta}$ is a vector of elements $+1$ or -1. Newton's method can be applied to this system provided that the matrix

$$H = \begin{bmatrix} C & A^{\sigma T} & \mathbf{0} \\ A^\sigma & 0 & -\boldsymbol{\theta} \\ \mathbf{0}^T & -\boldsymbol{\theta}^T & 0 \end{bmatrix}$$

is nonsingular, where $C = \sum_{i=1}^{t} \mu_i G_{\sigma_i}$ with G_i the Hessian matrix of f_i, $i = 1, 2, \ldots, m$.

EXAMPLE. We consider a problem treated in [1], [2] and [8], where $M = R^3$ and

$$\mathbf{f} = \begin{bmatrix} a_1^2 + a_1 a_2 + a_2^2 \\ \sin a_1 \\ \cos a_2 \end{bmatrix}.$$

The difficulty occurring here is typical of the kind which is likely to arise with methods which reach the solution via a sequence of linear subproblems: these problems do not have unique solutions which depend continuously on $\mathbf{a}$. In general terms, this means that satisfactory numerical performance of such methods can only be possible if the nonlinear problem has a solution whose characteristics are consistent with those of the solutions of the linear subproblems. In this particular example, A fails to satisfy the Haar condition at the solution, and $t = 2$, with $\sigma_1 = 1$ and $\sigma_2 = 3$. Taking as initial values $a_1 = 0.45$, $a_2 = -0.9$ (used in [1]), $\mu_1 = 0.35$, $\mu_2 = 0.65$, we obtain after 2 steps of Newton's method the values $a_1 = 0.453296$, $a_2 = -0.906592$, $\| \mathbf{f} \| = 0.616432$ correct to the number of figures shown.

Another example of a polyhedral norm is the L_1 norm. In this case, the

rows of B correspond to the 2^m ways of filling m locations with either $+1$ or -1, and a system of equations corresponding to those given above for the L_∞ norm can readily be derived. However, an equivalent nonlinear system is more conveniently derived in this case as follows. We have

$$V(\mathbf{f}) = \{\mathbf{v}: v_i = \operatorname{sgn}(f_i), f_i \neq 0; \mid v_i \mid \leqslant 1, f_i = 0\}$$

and so if it is assumed that at the solution $\mathbf{f}$ has zero components corresponding to the index set J, the system of equations can immediately be written as

$$f_i(\mathbf{a}) = 0 \qquad i \in J$$

$$\sum_{i \in J} v_i \rho_i(A) + \sum_{i \notin J} \operatorname{sgn}(f_i)\, \rho_i(A) = 0$$

$$\mid v_i \mid \leqslant 1 \qquad i \in J.$$

If J contains d indices $\sigma_1, \sigma_2, \ldots, \sigma_d$, and A^σ now denotes the $d \times n$ matrix with ith row the σ_ith row of A, then a step of Newton's method involves the inversion of the $(n + d) \times (n + d)$ matrix H defined by

$$H = \begin{bmatrix} C & A^{\sigma T} \\ A^\sigma & 0 \end{bmatrix}$$

where $C = \sum_{i=1}^{d} v_{\sigma_i} G_{\sigma_i}$, with G_i defined as before. Sufficient conditions for H to be nonsingular are that C is nonsingular, and A^σ has full rank.

The solution to a full-rank linear L_1 approximation problem in R^m with n unknowns is characterised by the existence of n zero residuals. Thus difficulties with conventional linearisation methods will arise if the nonlinear problem does not have a solution with this property.

EXAMPLE. Let $M = R^3$ and define

$$\mathbf{f} = \begin{bmatrix} a_1^2 + a_2^2 - 1 \\ a_1 a_2 - 0.5 \\ a_1 - \cos a_2 + 0.5 \end{bmatrix}.$$

Here, there is only one zero residual at the solution, with $\sigma_1 = 1$. Taking the initial approximation $a_1 = 0.5$, $a_2 = 0.9$, $v_1 = 0$, 3 steps of Newton's method give the results (correct to 6 decimal places): $a_1 = 0.516\,873$, $a_2 = 0.856\,062$, $v_1 = -0.139\,239$, $\| \mathbf{f} \| = 0.418\,981$.

Finally, we consider the case where $M = C[a, b]$ with the L_∞ norm. This stands in close relationship to the polyhedral norms already considered,

being a generalisation to the case where B can have an infinite number of rows and columns. Here

$$V(f) = \text{conv}\{\text{sgn}(f(x, \mathbf{a}))\, \delta(x) : x \in [a, b],\ |f(x, \mathbf{a})| = \|f\|\}$$

where $\langle f(x, \mathbf{a}), \delta(\xi)\rangle = f(\xi, \mathbf{a})$. The equations corresponding to (2.2) can be written

$$\sum_{i=1}^{t} \lambda_i \theta_i g_j(x_i, \mathbf{a}) = 0 \qquad j = 1, 2, \ldots, n$$

$$f(x_i, \mathbf{a}) = \theta_i \|f\| \qquad i = 1, 2, \ldots, t$$

$$\boldsymbol{\lambda}^T \mathbf{e} = 1$$

$$\lambda_i \geqslant 0, \qquad i = 1, 2, \ldots, t.$$

Assuming that $\boldsymbol{\theta}$ is known, we have $(t + n + 1)$ equations in $(2t + n + 1)$ unknowns. The additional degrees of freedom may, however, be removed by adding the equations

$$f'(x_i, \mathbf{a}) = 0, \qquad x_i \in (a, b)$$

with (if necessary) $x_1 = a$ and /or $x_t = b$, where $'$ denotes differentiation with respect to x. Examples of this approach are given in [13], where the initial approximations are obtained by solving a discrete problem on a subset of $[a, b]$.

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