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MGDA II: A direct method for calculating a descent direction common to several criteria

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Abstract: This report is a sequel of the publications [1] [3] [2]. We consider the multiobjective optimization problem of the simultaneous minimization of n ($n \geq 2$) criteria, $\{J_i(Y)\}_{(i=1,\dots,n)}$, assumed to be smooth real-valued functions of the design vector $Y \in \Omega \subset \mathbb{R}^N$ ($n \leq N$) where Ω is the (open) admissible domain of \mathbb{R}^N over which these functions admit gradients. Given a design point $Y^0 \in \Omega$ that is not Pareto-stationary, we introduce the gradients $\{J'_i\}_{(i=1,\dots,n)}$ at $Y = Y^0$, and assume them to be linearly independent. We also consider the possible “scaling factors”, $\{S_i\}_{(i=1,\dots,n)}$ ($S_i > 0, \forall i$), as specified appropriate normalization constants for the gradients. Then we show that the Gram-Schmidt orthogonalization process, if conducted with a particular calibration of the normalization, yields a new set of orthogonal vectors $\{u_i\}_{(i=1,\dots,n)}$ spanning the same subspace as the original gradients; additionally, the minimum-norm element of the convex hull corresponding to this new family, ω , is calculated explicitly, and the Fréchet derivatives of the criteria in the direction of ω are all equal and positive. This direct process simplifies the implementation of the previously-defined *Multiple-Gradient Descent Algorithm (MGDA)*.

Key-words: multiobjective optimization, descent direction, convex hull, Gram-Schmidt orthogonalization process

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MGDA II: Une méthode directe de calcul de direction de descente de plusieurs critères

Résumé : Ce rapport est une suite des publications [1] [3] [2]. On considère le problème d'optimisation multiobjectif dans lequel on cherche à minimiser n ($n \geq 2$) critères, $\{J_i(Y)\}_{(i=1,\dots,n)}$, supposés fonctions régulières d'un vecteur de conception $Y \in \Omega \subset \mathbb{R}^N$ ($n \leq N$) où Ω est le domaine (ouvert) admissible, partie de \mathbb{R}^N dans laquelle les critères admettent des gradients. Étant donné un point de conception $Y^0 \in \Omega$ qui n'est pas Pareto-stationnaire, on introduit les gradients $\{J'_i\}_{(i=1,\dots,n)}$ en $Y = Y^0$, et on les suppose linéairement indépendants. On considère également un ensemble de "facteurs d'échelles", $\{S_i\}_{(i=1,\dots,n)}$ ($S_i > 0, \forall i$), spécifiés par l'utilisateur, et considérés comme des constantes appropriées de normalisation des gradients. On montre alors que le processus d'orthogonalisation de Gram-Schmidt, lorsqu'on le conduit avec une calibration bien spécifique de la normalisation, produit un ensemble de vecteurs orthogonaux $\{u_i\}_{(i=1,\dots,n)}$ qui engendrent le même sous-espace que les gradients d'origine; de plus, l'élément de plus norme de l'enveloppe convexe de cette nouvelle famille, ω , se calcule explicitement, et les dérivées de Fréchet des critères dans la direction de ω sont égales et positives. Ce processus direct simplifie la mise en œuvre de l'*Algorithme de Descente à Gradients Multiples (MGDA)* défini précédemment.

Mots-clés : optimisation multiobjectif, direction de descente, enveloppe convexe, processus d'orthogonalisation de Gram-Schmidt

1 Introduction

We consider the context of the simultaneous minimization of n ($n \geq 2$) criteria, $\{J_i(Y)\}_{(i=1,\dots,n)}$, assumed to be smooth real-valued functions of the design vector $Y \in \Omega \subset \mathbb{R}^N$ ($n \leq N$) where Ω is the (open) admissible domain of \mathbb{R}^N over which these functions admit gradients. Let $Y^0 \in \Omega$, and let:

$$J'_i = \nabla J_i(Y^0) \quad (i = 1, \dots, n; J'_i \in \mathbb{R}^N) \quad (1)$$

be the gradients at the design-point Y^0 .

In [1] and [2], we have introduced the local notion of Pareto-stationarity, defined as the existence of a convex combination of the gradients that is equal to zero. We established there that Pareto-stationarity was a necessary condition to Pareto-optimality. If inversely, the Pareto-stationarity condition is not satisfied, vectors having positive scalar products with all the gradients $\{J'_i\}_{(i=1,\dots,n)}$ exist. We focus on the question of identifying such vectors.

Consider a family $\{u_i\}_{(i=1,\dots,n)}$ of n vectors of \mathbb{R}^N , and recall the definition of their convex hull:

$$\bar{U} = \left\{ u \in \mathbb{R}^N / u = \sum_{i=1}^n \alpha_i u_i; \alpha_i \geq 0 (\forall i); \sum_{i=1}^n \alpha_i = 1 \right\} \quad (2)$$

This set is closed and convex. Hence it admits a unique element ω of minimum norm. We established that:

$$\forall u \in \bar{U} : (u, \omega) \geq \|\omega\|^2 \quad (3)$$

By letting

$$u_i = J'_i \quad (i = 1, \dots, n) \quad (4)$$

and identifying the corresponding vector ω , we were able to conclude that either $\omega = 0$ and the design-point Y^0 is Pareto-stationary, or $-\omega$ is a descent direction common to all criteria.

This observation has led us to propose the *Multiple-Gradient Descent Algorithm (MGDA)* that is an iteration generalizing the classical steepest-descent method to the context of multiobjective optimization. At a given iteration, the design point Y^0 is updated by a step in the direction opposite to ω :

$$\delta Y^0 = -\rho \omega \quad (5)$$

Assuming the stepsize ρ is optimized, *MGDA* converges to a Pareto-stationary design point [1] [2].

Thus, *MGDA* provides a technique to identify Pareto sets when gradients are available, as demonstrated in [3].

We have also shown that the convex hull was isomorphic to the positive part of the sphere of \mathbb{R}^{n-1} (independently of N) and it can be parameterized by $n-1$ spherical coordinates. Hence, in the first version of our method, when $n > 2$, we proposed to identify the vector ω by actually finding numerically the minimum of $\|u\|^2$ in \bar{U} by optimizing the spherical coordinates, or more precisely, their cosines squared that are $n-1$ independent parameters varying in the interval $[0,1]$. This minimization can be conducted trivially when n is small, but can become difficult for large n .

In this new report, we propose a variant of *MGDA* in which the direction ω is found by a direct process, assuming the family of gradients $\{J'_i\}_{(i=1,\dots,n)}$ is linearly independent.

2 Direct calculation of the minimum-norm element

In [2], the following remark was made:

Remark 1

If the gradients are not normalized, the direction of the minimum-norm element ω is expected to be mostly influenced by the gradients of small norms in the family, as the case $n = 2$ illustrated in Figure 1 suggests. In the course of the iterative optimization, these vectors are often associated with the criteria that have already achieved a fair degree of convergence. If this direction may yield a very direct path to the Pareto front, one may question whether it is adequate for a well-balanced multiobjective iteration. Some on-going research is focused on analyzing various normalization procedures to circumvent this undesirable trend. In these alternatives, the gradient J'_i is replaced by one of the following formulas:

$$\frac{J'_i}{\|J'_i\|}, \frac{J'_i}{J_i(Y^0)}, \frac{J_i(Y^0)}{\|J'_i\|^2} J'_i, \text{ or } \frac{\max(J_i^{(k-1)}(Y^0) - J_i^{(k)}(Y^0), \delta)}{\|J'_i\|^2} J'_i \quad (6)$$

(k : iteration number; $\delta > 0$, small). The first formula is a standard normalization: it has the merit of providing a stable definition; the second realizes equal logarithmic first variations of the criteria whenever ω belongs to the interior \mathbf{U} of the convex hull since then, the Fréchet derivatives (u_i, ω) are equal; the last two are inspired from Newton's method (assuming $\lim J_i = 0$ for the first). This question is still open.

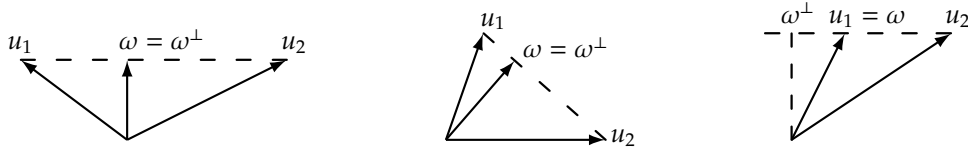


Figure 1: Case $n = 2$: possible positions of vector ω with respect to the two gradients u_1 and u_2

Thus, accounting for the above remark, we consider a given set of strictly-positive “scaling factors” $\{S_i\}_{(i=1,\dots,n)}$, intended to normalize the gradients appropriately. We apply the Gram-Schmidt orthogonalization process to the gradients with the following special calibration of the normalization:

$$u_1 = \frac{J'_1}{A_1} \quad (7)$$

where $A_1 = S_1$, and, for $i = 2, 3, \dots, n$:

$$u_i = \frac{J'_i - \sum_{k<i} c_{i,k} u_k}{A_i} \quad (8)$$

where:

$$\forall k < i : c_{i,k} = \frac{(J'_i, u_k)}{(u_k, u_k)} \quad (9)$$

and

$$A_i = \begin{cases} S_i - \sum_{k<i} c_{i,k} & \text{if nonzero} \\ \varepsilon_i S_i & \text{otherwise} \end{cases} \quad (10)$$

for some arbitrary, but small ε_i ($0 < |\varepsilon_i| \ll 1$).

Then :

In general, the vectors $\{u_i\}_{(i=1,\dots,n)}$ are not of norm unity. But they are orthogonal, and this property

makes the calculation of the minimum-norm element of the convex hull, ω , direct. For this, note that:

$$\omega = \sum_{i=1}^n \alpha_i u_i \quad (11)$$

and

$$\|\omega\|^2 = \sum_{i=1}^n \alpha_i^2 \|u_i\|^2. \quad (12)$$

To determine the coefficients $\{\alpha_i\}_{(i=1,\dots,n)}$, anticipating that ω belongs to the interior of the convex hull, the inequality constraints are ignored, and the following Lagrangian is made stationary:

$$\mathcal{L}(\alpha, \lambda) = \|\omega\|^2 - \lambda \left(\sum_{i=1}^n \alpha_i - 1 \right) = \sum_{i=1}^n \alpha_i^2 \|u_i\|^2 - \lambda \left(\sum_{i=1}^n \alpha_i - 1 \right) \quad (13)$$

This gives:

$$\frac{\partial \mathcal{L}}{\partial \alpha_i} = 2 \|u_i\|^2 \alpha_i - \lambda \implies \alpha_i = \frac{\lambda}{2 \|u_i\|^2} \quad (14)$$

The equality constraint, $\sum_{i=1}^n \alpha_i = 1$, then gives:

$$\frac{\lambda}{2} = \frac{1}{\sum_{i=1}^n \frac{1}{\|u_i\|^2}} \quad (15)$$

and finally:

$$\alpha_i = \frac{1}{\|u_i\|^2 \sum_{j=1}^n \frac{1}{\|u_j\|^2}} = \frac{1}{1 + \sum_{j \neq i} \frac{\|u_i\|^2}{\|u_j\|^2}} < 1 \quad (16)$$

which confirms that ω does belong to the interior of the convex hull, so that:

$$\forall i : \alpha_i \|u_i\|^2 = \frac{\lambda}{2} \quad (\text{a constant}), \quad (17)$$

and:

$$\forall k : (u_k, \omega) = \alpha_k \|u_k\|^2 = \frac{\lambda}{2}. \quad (18)$$

Now:

$$(J'_i, \omega) = (A_i u_i + \sum_{k < i} c_{i,k} u_k, \omega) = \left(A_i + \sum_{k < i} c_{i,k} \right) \frac{\lambda}{2} = S_i \frac{\lambda}{2}, \quad \text{or } S_i (1 + \varepsilon_i) \frac{\lambda}{2} \quad (\forall i). \quad (19)$$

Lastly, convening that $\varepsilon_i = 0$ in the regular case ($S_i \neq \sum_{k < i} c_{i,k}$), and otherwise by modifying slightly the definition of the scaling factor according to

$$S'_i = (1 + \varepsilon_i) S_i, \quad (20)$$

the following holds:

$$\boxed{(S_i^{-1} J'_i, \omega) = \frac{\lambda}{2} \quad (\forall i)} \quad (21)$$

that is, the same positive constant.

3 Conclusion

We have considered the multiobjective optimization problem of the simultaneous minimization of n ($n \geq 2$) criteria, $\{J_i(Y)\}_{(i=1,\dots,n)}$, assumed to be smooth real-valued functions of the design vector $Y \in \Omega \subset \mathbb{R}^N$ ($n \leq N$) where Ω is the (open) admissible domain of \mathbb{R}^N over which these functions admit gradients. Given a design point $Y^0 \in \Omega$ that is not Pareto-stationary, we have introduced the gradients $\{J'_i\}_{(i=1,\dots,n)}$ at $Y = Y^0$, and assumed them to be linearly independent. We have also considered the possible “scaling factors”, $\{S_i\}_{(i=1,\dots,n)}$ ($S_i > 0, \forall i$), as specified appropriate normalization constants for the gradients. Then we have shown that the Gram-Schmidt orthogonalization process, if conducted with a particular calibration of the normalization yields a new set of orthogonal vectors $\{u_i\}_{(i=1,\dots,n)}$ spanning the same subspace as the original gradients; additionally, the minimum-norm element of the convex hull corresponding to this new family, ω , is calculated explicitly, and the Fréchet derivatives of the criteria in the direction of ω are all equal and positive.

This new result has led us to reformulate the definition of the *MGDA*, in which the descent direction common to all criteria is now calculated by a direct process.

Finally, we make the following two remarks:

Remark 2

In the exception case where $\sum_{k < i} c_{i,k} = S_i$, for some i , the corresponding vector u_i has a large norm. Consequently, this vector has a weak influence on the definition of ω .

Remark 3

As the Pareto set is approached, the family of gradients becomes closer to linear dependence, as the Pareto-stationarity condition requires. At this stage, this variant may experience numerical difficulties, making the more robust former approach preferable.

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