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Numerical Analysis

Improving the identification of general Pareto fronts by global optimization

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Abstract

We present a controllability result for a second order dynamic system and its application to global optimization in the context of multi-criteria problems. In particular, we address the issue of reaching points on nonconvex regions of Pareto fronts. ***To cite this article: B. Mohammadi, P. Redont, C. R. Acad. Sci. Paris, Ser. I 347 (2009).***

Résumé

Optimisation globale et génération de fronts de Pareto. Nous présentons un résultat de controlabilité pour un système dynamique d'ordre deux et son utilisation en optimisation globale dans un context de minimisation multi-critère. En particulier, nous montrons comment atteindre les points sur des fronts de Pareto nonconvexes. ***Pour citer cet article : B. Mohammadi, P. Redont, C. R. Acad. Sci. Paris, Ser. I 347 (2009).***

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Les applications comportent souvent des problèmes d'optimisation multi-critère. Les fonctionnelles en jeu sont, en général, en conflit : on veut optimiser la performance d'un système dont on souhaite réduire le coût. Une première notion d'équilibre est celle de Pareto entre points non-dominés. En ces points de l'espace admissible il n'est pas possible d'obtenir une réduction pour toutes les fonctionnelles. La méthode la plus répandue est la minimisation de moyennes pondérées. En variant la pondération, on atteint différents points du front en utilisant une méthode de descente. Il est admis que cette approche ne peut atteindre les points situés sur les Pareto nonconvexes. Nous montrons que cet échec est lié à l'utilisation des méthodes de descente et non pas à la pondération. Les résultats de cette Note restent valablent avec un équilibre de Nash qui, si il existe, correspond à un point de l'espace admissible et la question d'atteignabilité reste posée.

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1. Introduction

Engineering design often deals with multiple and often conflicting objective functions $\vec{\mathbf{J}} = \{J_i(x),\ i = 1, \ldots, n\}$ [12,3,1,2,13]. For instance, one usually wants to maximize the performance of a system while minimizing its cost.

One optimality concept is known as Pareto equilibrium [12] defined by nondominated points: A point x is dominated by a point y if and only if $J_i(y) \leqslant J_i(x)$, with strict inequality for at least one of the objectives. Thus, a global Pareto equilibrium point is such that no improvement for all objectives can be achieved (i.e. by moving to any other feasible point). The results in this Note remain valid with a Nash definition of the equilibrium.

The classical method for multi-objective optimization is the weighted sum method [1,2,13]:

$$J(x) = \sum \alpha_i J_i(x), \quad \sum \alpha_i = 1,\ \alpha_i \in [0, 1].$$

A sampling in α_i enables to reach various points in the Pareto front using a descent method for $J(x)$. This method is extensively used because one knows that it has a solution for convex functionals.

It is admitted that the weighted sum approach does not find Pareto solutions in nonconvex regions of the Pareto front [7]. A geometric interpretation is that when the tangent to the Pareto front is parallel to one of the axes the corresponding functional has a plateau which cannot be crossed by a descent method.

In cases the front is nonconvex but the tangent never parallel to one of the axes one can still use a descent method for increasing power n in the functional [7]:

$$\tilde{J}(x) = \sum \alpha_i J_i^n(x), \quad \sum \alpha_i = 1,\ \alpha_i \in [0, 1].$$

One looks for the lowest n making the Pareto front convex because this approach has the disadvantage of degrading the conditioning of the optimization problem.

In this Note we would like to propose an alternative solution which is not submitted to the mentioned limitations. In particular, one aims at showing that the failure of the weighted sum approach is due to a lack in global minimization feature in descent methods and how controllability results for a second order dynamical system can be used to address this issue.

2. Controllability and global optimization

Consider the minimization of a functional $J(x) \in \mathbb{R}$, $x \in \mathcal{O}_{ad}$. We suppose the problem admissible (i.e. there exists at least one solution x_m to the problem: $J(x_m) = J_m$). Most minimization algorithms can be seen as discretizations of [11,6,5,4,9,10]:

$$\eta x_{tt} + M\big(x(t)\big)x_t = -d\big(x(t)\big), \quad x(t=0) = x_0, \quad x_t(t=0) = \dot{x}_0, \tag{1}$$

where M is positive definite and $M^{-1}d$ is built to be an admissible direction. Local minimization descent algorithms (steepest descent, Newton, ...) are recovered for $\eta = 0$.

Now, suppose J_m is known. Global optimization can be seen as finding $x(t)$ solution of:

$$\eta x_{tt} + M\big(x(t)\big)x_t = -d\big(x(t)\big), \quad x(t=0) = x_0, \quad J\big(x(T)\big) = J_m, \tag{2}$$

where the initial condition on x_t in (1) has been replaced by a final condition on $x(t)$ for some T, finite but a priori unknown.

In practice the final condition is not aimed at being exactly realized. Rather, one would like, for a given precision δ in the functional, to build at least one trajectory $(x(t), 0 \leqslant t \leqslant T_\delta)$ passing for finite T_δ in the ball $B_\delta(x_m)$. This can be summarized as:

$$\forall \delta > 0,\ \exists (v, T_\delta) \in \mathcal{O}_{ad} \times [0, +\infty[\quad \text{such that} \quad J\big(x_v(T_\delta)\big) - J_m \leqslant \delta. \tag{3}$$

T_δ also defines the maximum calculation complexity wanted. If J_m is unknown, setting $J_m = -\infty$, one retains the best solution obtained over $[0, T_\delta]$. In other words, one solves:

$$\forall (\delta, T_\delta) \in \mathbb{R}^+ \times [0, +\infty[,\ \exists (v, \tau) \in \mathcal{O}_{ad} \times [0, T_\delta] \quad \text{such that} \quad J\big(x_v(\tau)\big) - J_m \leqslant \delta. \tag{4}$$

The following theorem formalizes this controllability question with $M = Id$ and $d = \nabla J$:

Theorem. *Let $J : \mathbb{R}^n \to \mathbb{R}$ be a C^2-function such that $\min_{\mathbb{R}^n} J$ exists and is reached at $x_m \in \mathbb{R}^n$. Then for every $(x_0, \delta) \in \mathbb{R}^n \times \mathbb{R}^+$, there exists $(\sigma, t') \in \mathbb{R}^n \times \mathbb{R}^+$ such that the solution of the following system:*

$$\eta x_{tt}(t) + x_t(t) = -\nabla J\big(x(t)\big), \quad t \geqslant 0, \qquad x(0) = x_0, \qquad x_t(0) = \sigma, \tag{5}$$

with $\eta \in \mathbb{R}$, passes at time $t' = t$ into the ball $B_\delta(x_m)$.

Proof. We assume $x_0 \neq x_m$ ($x_0 = x_m$ is a trivial case). Let $\varepsilon > 0$, we consider first the initial value problem:

$$\eta y_{tt}(t) + \varepsilon y_t(t) = -\varepsilon^2 \nabla J\big(y(t)\big), \quad t \geqslant 0, \qquad y(0) = x_0, \qquad y_t(0) = \varrho(x_m - x_0), \tag{6}$$

with $\varrho \in \mathbb{R}^+ \backslash \{0\}$.

Let us show that $y(\cdot)$ passes at some time into the ball $B_\delta(x_m)$:

– If $\varepsilon = 0$, we obtain the following system:

$$\eta y_{tt,0}(t) = 0, \quad t \geqslant 0, \qquad y_0(0) = x_0, \qquad y_{t,0}(0) = \varrho(x_m - x_0). \tag{7}$$

System (7) describes a straight line of origin x_0 and passing at some time $\theta_\varrho = \frac{1}{\varrho}$ by the point x_m, i.e. $y_0(\theta_\varrho) = x_m$.

– If $\varepsilon \neq 0$, system (6) can be rewritten as $(w_2)_t = f(\eta, w, \varepsilon)$, with $w = (w_1, w_2)^T = (y(t), \eta y_t(t))^T$ and $f = -\varepsilon w_2/\eta - \varepsilon^2 \nabla J(w_1(t))$ satisfying the Cauchy–Lipschitz conditions (J is a C^2 function). Then $\lim_{\varepsilon \to 0} |y_\varepsilon(\theta_\varrho) - y_0(\theta_\varrho)| = 0$. Thus, for every $\delta \in \mathbb{R}^+ \backslash \{0\}$, there exists ε_δ such that for every $\varepsilon < \varepsilon_\delta$:

$$\big| y_\varepsilon(\theta_\varrho) - x_m \big| < \delta. \tag{8}$$

Finally, let us consider the change of variables $t' = \varepsilon_\delta t$ and $x(t') = y_{\varepsilon_\delta}(\frac{t'}{\varepsilon_\delta})$. Then system (6) becomes:

$$\eta x_{t't'}(t') + x_{t'}(t') = -\nabla J\big(x(t')\big), \quad t' \geqslant 0, \qquad x(0) = x_0, \qquad \dot{x}(0) = \frac{\varrho}{\varepsilon_\delta}(x_m - x_0). \tag{9}$$

Let $\vartheta = \varepsilon_\delta \theta_\varrho$. Under this assumption, $x(\vartheta) = y_{\varepsilon_\delta}(\theta_\varrho)$. Thus, due to (8): $|x(\vartheta) - x_m| < \delta$. We have found $\sigma = \frac{\varrho}{\varepsilon_\delta}(x_m - x_0) \in \mathbb{R}^n$ and $t_b = \vartheta \in \mathbb{R}^+$ such that the solution of system (5) passes at time t_b into the ball $B_\delta(x_m)$. □

2.1. Algorithmic considerations

The previous proof is instructive and permits to derive an efficient global minimization algorithm which requires $\delta > 0$, the infimum J_m and $0 \leqslant T < \infty$ [11,6,5,9,4]. We then minimize the functional $h_{\delta,T,J_m} : \mathcal{O}_{ad} \to \mathbb{R}^+$:

$$h_{\delta,T,J_m}(v) = \min_{\mathcal{A}} \big(J\big(x_v(\tau)\big) - J_m \big), \tag{10}$$

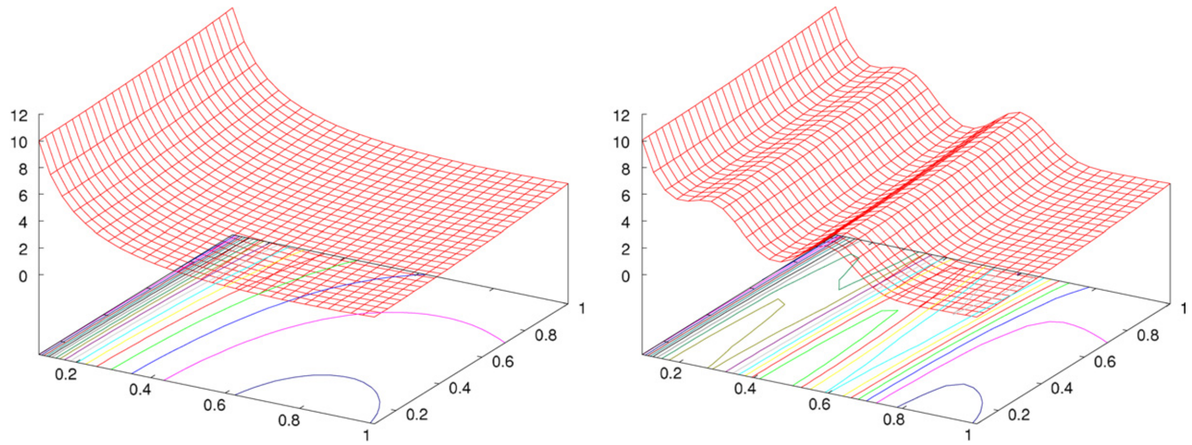

Fig. 1. $J_2(x)$ for $\beta = 0$ and $\beta = 3$. The Pareto front generation will require a global minimization algorithm when the functional has local minima.

Fig. 1. $J_2(x)$ avec $\beta = 0$ et $\beta = 3$. La génération du front de Pareto requiert l'utilisation d'un algorithme de minimization globale si une des fonctionnelles admet des minimas locaux.

where $\mathcal{A} = \{x_v(\tau) \in \mathcal{O}_{ad},\ \tau \in [0, T]\}$. Hence, global minimization becomes a nested minimization problem where one looks to improve the initial impulse v for an internal minimization sub-problem to generate the trajectory $(x_v(\tau), 0 \leqslant \tau \leqslant T)$ by:

$$\eta x_{tt} + M\big(x(t)\big)x_t = -d\big(x(t)\big), \quad x(t=0) = x_0, \quad x_t(t=0) = v, \quad t \in [0, T]. \tag{11}$$

3. Recovering Pareto fronts

We saw how to link any couple of points in the admissible space in finite time with some given accuracy by a trajectory solution of a second order dynamical system. If the problem is admissible, a point in a Pareto front

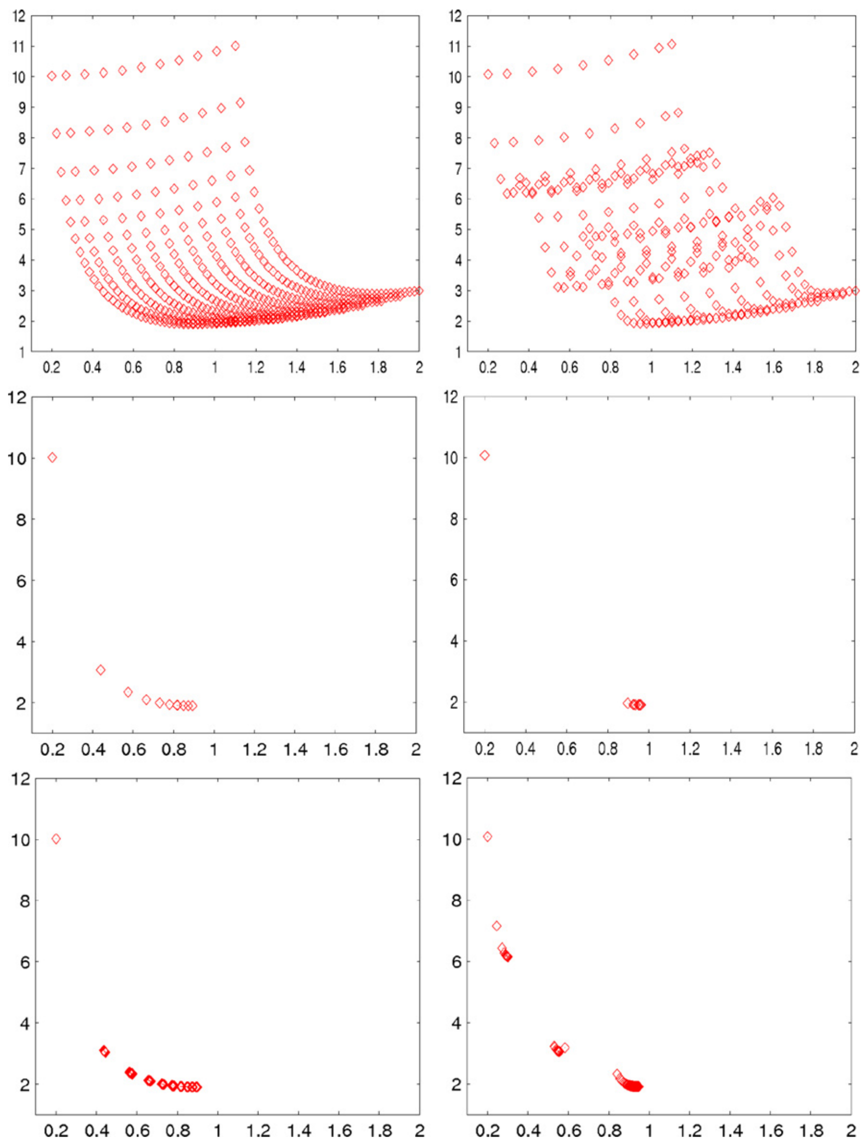

Fig. 2. Pareto fronts generation. (J_1, J_2) generated after sampling of the control space for $\beta = 0$ and 3 (upper line). Solutions of minimization by first (middle line) and second order (lower line) dynamical systems for an uniform 10 points sampling of $\alpha \in [0, 1]$. On the right, the front is not connected.

Fig. 2. Générations de fronts de Pareto. (J_1, J_2) généré avec un échantillonnage de l'espace de contrôle et $\beta = 0$ et 3 (ligne du haut). Solutions de minimisation avec un système d'ordre un (milieu) et deux (bas) pour des problèmes d'optimisation correspondant à un échantillonnage uniforme en 10 points de $\alpha \in [0, 1]$. A droite, le front n'est pas connexe.

corresponds to a point in the admissible control space. It shall be reached in finite time from any initial condition in the admissible space by a trajectory solution of our second order system. The algorithm above can therefore be used to recover any point in a Pareto front with:

$$h_{\delta,T,\vec{\mathbf{J}}_m}(v) = \min_{\mathcal{A}} \big\| \vec{\mathbf{J}}\big(x_v(\tau)\big) - \vec{\mathbf{J}}_m \big\|. \tag{12}$$

Obviously, $\vec{\mathbf{J}}_m$ is unknown in general. Still, this means that one shall use a minimization method which has global search features to cross escape local minima in the case of nonconvex Pareto fronts.

4. Numerical examples

We consider the functionals $J_1 = x_1 + x_2$ and $J_2 = (1/x_1 + \|x\|^2) + \beta(\exp(-100(x_1 - 0.3)^2) + \exp(-100(x_1 - 0.6)^2))$ for $x \in [0.1, 1]^2$. Fig. 1 shows J_2 for $\beta = 0$ and 3. Fig. 2 shows examples of convex and nonconvex Pareto fronts generation with two functionals and in a two dimensional search space. The pictures are for $\beta = 0$ and 3. The first situation can be solved using a steepest descent method with optimal step size. Here, the points could have been eventually better distributed with a more clever choice of the weights [7]. The second case requires a global optimization method to reach regions where the front is either not connected or nonconvex. We have solved 10 minimization problems based on uniform sampling of $\alpha \in [0, 1]$ in the weighted sum. We have then solved the minimization problems starting from the same point ($x(t = 0) = (1, 1)^T$) in the admissible space using an algorithm based on discrete forms of second order (11) dynamical systems with $M = Id, d = \alpha\nabla J_1 + (1 - \alpha)\nabla J_2$ and with $\eta = 0$ and $\eta = 1$. For the second order system the initial impulse is variable as mentioned in (5). On sees that second order dynamics is necessary to recover general Pareto fronts. Similar problems have been considered in [8] and the recovered Pareto fronts feature also the fact that global optimization is necessary.

References

[1] I. Das, J.E. Dennis, A closer look at drawbacks of minimizing weighted sums of objectives for Pareto set generation in multicriteria optimization problems, Struct. Optim. 14 (1997) 63–69.

[2] I. Das, J.E. Dennis, Normal-boundary intersection: A new method for generating Pareto optimal points in multicriteria optimization problems, SIAM J. Optim. 8 (1998) 631–657.

[3] K. Deb, Multi-objective genetic algorithms: Problem difficulties and construction of test problems, IEEE J. Evolutionary Comp. 7 (1999) 205–230.

[4] L. Dumas, B. Ivorra, P. Redont, B. Mohammadi, Semi-deterministic vs. genetic algorithms for global optimization of multichannel optical filters, Int. J. Comput. Sci. Eng. 2 (3-4) (2006) 170–188.

[5] B. Ivorra, D. Hertzog, B. Mohammadi, J.F. Santiago, Global optimization for the design of fast microfluidic protein folding devices, Int. J. Numer. Meth. Eng. 26 (6) (2006) 319–333.

[6] B. Ivorra, B. Mohammadi, A. Ramos, Semi-deterministic global optimization method and application to the control of Burgers equation, JOTA 135 (1) (2007) 549–561.

[7] A. Messac, G.J. Sundararaj, R. Tappeta, J.E. Renaud, Ability of objective functions to generate points on non-convex Pareto frontiers, AIAA J. 38 (6) (2000) 155–163.

[8] E. Miglierina, E. Molhob, M.C. Recchionici, Box-constrained multi-objective optimization: A gradient-like method without a priori scalarization, Eur. J. Oper. Res. 188 (2008) 662–682.

[9] B. Mohammadi, Optimal transport, shape optimization and global minimization, C. R. Acad. Sci. Paris, Ser. I. 344 (2007) 591–596.

[10] B. Mohammadi, O. Pironneau, Applied Shape Optimization for Fluids, second ed, Oxford Univ. Press, 2009.

[11] B. Mohammadi, J.H. Saiac, Pratique de la simulation numérique, Dunod, Paris, 2003.

[12] V. Pareto, Manuale di Economia Politica, Societa Editrice Libraria, Milano, Italy, 1906. Translated into English by Schwier, A.S, Manual of Political Economy, Macmillan, New York, 1971.

[13] W. Stadler, A survey of multicriteria optimization, or the vector maximum problem, JOTA 29 (1979).