LOCAL PARETO ANALYSER FOR PRELIMINARY DESIGN

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Abstract

In the design process of complex systems, the designer has to solve an optimisation problem, which involves coupled disciplines and where all design criteria have to be optimised (traded-off) simultaneously. This problem is known as vector optimisation. Many numerical methods exist for obtaining solutions but in general, the solution is not unique. In such a case, the solution set is represented by a Pareto surface in the space of the objective functions. Regarding industrial applications, the multi-disciplinary optimisation problem is usually very time-consuming and the Pareto set rarely can be described analytically. The description of a Pareto surface is often reduced to a set of points lying onto the surface. Therefore, in the real design the set of Pareto solution is never exhaustively explored. Once a Pareto point is obtained, it may be very useful for the decision-maker to be able to perform a quick local approximation in order to obtain other approximate optimal solutions. In this paper, a local Pareto analyser is proposed. This concept is based on a local sensitivity analysis, which provides the relation between variations of the different objective functions under constraints. A method for obtaining a linear and quadratic local approximation of the Pareto surface is then derived. Application of the local Pareto analyser concept is demonstrated through the study of a few test cases.

1. Introduction

In the process of designing complex systems, contributions and interactions of multiple disciplines are taken into account to achieve a consistent design. The problem is made worse due to the fact that in a real industrial design setting, the decision maker (DM) has to take into account many different and often conflicting criteria. In fact, during the optimisation process, the DM often has to make compromises and look for trade-off solutions rather than a global optimum, which almost always does not exist.

Multi-disciplinary design has existed in the mind of designers for several decades but it is only with the emergence of new numerical methods and the development of computer power that this area has recently been recognised as a field of study: Multi-disciplinary Design Optimisation (MDO). MDO embodies a set of methodologies, which provide means of coordinating efforts and performing the optimisation of a complex system. Two fundamental issues associated with the MDO concept are the complexity of the problem (large number of variables, constraints and objectives) and the difficulty to explore the whole design space. Thus in practice the DM would benefit from obtaining information about the model without the need to run it extensively.

MDO analysis implies solving a non-linear vector optimisation problem. In general the solution of such a problem is not unique. In this respect a feasible solution, i.e. solutions satisfying all constraints, which cannot be optimised further with regard to any criteria without compromising at least one of the others leads to a Pareto optimal solution [1]. Every Pareto point is a solution of the multi-objective optimisation problem. Ultimately a designer has to select the final
design solution among the Pareto set; the decision can be based on additional requirements that were not taken into account in the mathematical formulation of the vector optimisation problem. In a real MDO problem, the Pareto front cannot often be described analytically and it is therefore desirable to have a sufficiently large number of Pareto points to obtain a good approximation for a quick local analysis. It is also important that the Pareto set be evenly distributed to ensure the representation of the Pareto surface is sufficient.

In spite of the existence of many numerical methods for non-linear vector optimisation, there are few methods suitable for real-design industrial applications, especially for preliminary design. In many applications, the design cycle includes time-consuming and expensive computations of each discipline. This is particularly true in the aerospace industry where many coupled disciplines such as aerodynamics and stress analysis are taken into account in the design process.

The objective of this work has been to develop a method for local Pareto analysis and approximation. The following section formally states the multi-objective optimisation problem. Section 3 describes the Pareto approximation concept for locally smooth Pareto surface while section 4 describes the analysis developed to identify non-differentiable Pareto points. The method is evaluated in section 5 with a few test cases. Finally conclusions are drawn and future work outlined in section 6.

2. Multi-objective optimisation problem

It is assumed that an optimisation problem is described in terms of a design variable vector \( \mathbf{x} = (x_1, x_2, \ldots, x_N)^T \) in the design space \( \mathbf{X} \subseteq \mathbb{R}^N \). A function \( \mathbf{f} \in \mathbb{R}^M \) evaluates the quality of a solution by assigning it to an objective vector

\[
\mathbf{y} = (y_1, y_2, \ldots, y_M)^T
\]

\( y_i = f_i(\mathbf{x}), \quad f_i : \mathbb{R}^N \rightarrow \mathbb{R}^i, i = 1, 2, \ldots, M \) in the objective space \( \mathbf{Y} \subset \mathbb{R}^M \). Thus, \( \mathbf{X} \) is mapped onto \( \mathbf{Y} \) by \( \mathbf{f} : \mathbf{X} \mapsto \mathbf{Y} \). A multi-objective optimisation problem may be formulated in the following form:

\[
\text{Minimize } |\mathbf{y}(\mathbf{x})| \quad (2.1)
\]

Subject to the \( K \) inequality constraints

\[
g_i(\mathbf{x}) \leq 0 \quad i = 1, \ldots, K \quad (2.2)
\]

which may also include equality constraints.

The feasible design space \( \mathbf{X}^* \) is defined as the set \( \{ \mathbf{x} | g_i(\mathbf{x}) \leq 0, i = 1, 2, \ldots, K \} \). A feasible design point is a point that does not violate any constraint. The feasible criterion (objective) space \( \mathbf{Y}^* \) is defined as the set \( \{ \mathbf{Y}(\mathbf{x}) | \mathbf{x} \in \mathbf{X}^* \} \).

A design vector \( \mathbf{a} (\mathbf{a} \in \mathbf{X}^*) \) is called a Pareto optimum iff it does not exist any \( \mathbf{b} \in \mathbf{X}^* \) such that \( y_i(\mathbf{b}) \leq y_i(\mathbf{a}) \), \( i = 1, \ldots, M \) and there exists at least one \( 1 \leq j \leq M \) such that: \( y_j(\mathbf{b}) < y_j(\mathbf{a}) \).

3. Pareto approximation

The local approximation is derived at a given Pareto point with account of active constraints. Constraints are active at some point of the design space \( \mathbf{X} \) if strict equality is valid at this point. It is assumed that constraints that are active at this particular point remain active in its vicinity. Thus, the sensitivity predicted at the given Pareto point is valid until the set of active constrains remains unchanged \([2, 7]\).

Let us note the set of active constraints as \( \mathbf{G} \). At a given point \( \mathbf{x}^* \) of the design feasible space \( \mathbf{X}^* \) that means:

\[
\mathbf{G}(\mathbf{x}^*) = \mathbf{0} \quad (3.1)
\]

Without violation of generality, we assume that the first \( P \) constraints are active and the
first $Q$ of those correspond to inequalities $(Q \leq P \leq K)$.

We assume that in the vicinity of $x^*$ the same set of constraints remains active. Locally the constraints can be written in a linear form:

$$J(x - x^*) = 0$$ (3.2)

where $J$ is the Jacobian of the active constraint set at $x^* : J = \nabla G$

If all gradients of the active constraints are linearly independent at a point, then this point is called a regular point [1]. We will say that a point $x^* \in X^*$ is regular if

$$\text{rank}(J) = n_f$$

The values of the gradient of any differentiable function $F$ at point $x^*$ under constraints are defined by the reduced gradient formula (see, e.g. [8]):

$$\nabla F_\beta = \nabla F$$ (3.3)

where $S$ is the surface defined by:

$$S = \{x | J(x - x^*) = 0\}$$ (3.4)

and $P$ is projection matrix onto this surface:

$$P = I - J^T(JJ^T)^{-1}J$$ (3.5)

Directional derivatives in the objective function space are given by:

$$\frac{dF}{df_i} = \frac{dF}{d\mathbf{x}} \frac{d\mathbf{x}}{df_i}$$ (3.6)

The last derivative can be represented via the gradients in the design space $X$ as follows.

Assume that matrix $\nabla F\mathbf{f}$ has $n_f < M$ linearly independent columns. Without violation of generality, we can suppose that the first $n_f$ objective functions originate the linear independent columns of $\nabla F\mathbf{f}$. Then, let us introduce vector $\tilde{f} \equiv (f_1, \ldots, f_{n_f})^T$. It is possible to show that

$$\frac{dx}{df} = A \equiv \nabla \tilde{f}[(\nabla \tilde{f})^T P \nabla \tilde{f}]^{-1}$$ (3.7)

Then, for any $i \leq n_f$, from (3.3), (3.6) and (3.7) we obtain

$$\frac{dF}{df_i} = A_i^T P \nabla F$$ (3.8)

where

$$A = (A_1, A_2, \ldots, A_{n_f})$$

Hence

$$\frac{df_j}{df_i} = A_i^T P \nabla f_j$$ (3.9)

In this case $f_j$ is considered as a dependable variable and not included in $P \nabla \tilde{f}$.

It is important to note that only if all vectors in $P \nabla \tilde{f}$ are orthogonal, (3.9) coincides with the appropriate formula obtained in [3]:

$$\frac{df_j}{df_i} = \frac{\langle P \nabla f_j, P \nabla f_i \rangle}{\langle P \nabla f_i, P \nabla f_i \rangle}$$ (3.10)

In the general case formula (3.10) only gives some approximation of the derivative.

Similarly, it is possible to obtain the reduced Hessian as follows:

$$\frac{d^2F}{df_i df_j} = A_i^T P \nabla \left(A_j^T P \nabla F \right)$$ (3.11)

If $F = f_j$, then we obtain the sensitivity of an objective $f_j$ along the feasible descent direction of an objective $f_i$.

Assuming that in the objective space $Y$ the Pareto surface is given by:

$$S(y) = 0$$ (3.12)

and at point $y^* = f(x^*)$ function $S \subset C^2$. Then, the Pareto surface can be locally represented as either a linear hyperplane:

$$\sum_{i=1}^{n_f} \frac{dS}{df_i} \Delta f_i = 0$$ (3.13)

or a quadratic surface:
\[
\sum_{i=1}^{n_f} \frac{dS}{df_i} \Delta f_i + \frac{1}{2} \sum_{j,k=1}^{n_f} \frac{d^2 S}{df_j df_k} \Delta f_j \Delta f_k = 0 \quad (3.14)
\]

where \( \Delta f = f - \hat{f}^{*} \).

Approximations (3.13) and (3.14) can be rewritten with respect to the trade-off relation between the objective functions as follows:

\[
f_p = f_p^{*} + \sum_{i=1}^{n_p} \frac{df_p}{df_i} \Delta f_i \quad (3.15)
\]

and

\[
f_p = f_p^{*} + \sum_{i=1}^{n_p} \frac{df_p}{df_i} \Delta f_i + \frac{1}{2} \sum_{j,k=1}^{n_p} H^{(p)}_{jk} \Delta f_j \Delta f_k \quad (3.16)
\]

for \((p = n_f + 1, \ldots, M)\)

where \(H^{(p)}_{jk} = \frac{d^2 f_p}{df_j df_k}\).

4. Pareto front analysis

In the SA, due to a perturbation \( \delta f \) and the appropriate displacement \( \delta x \) some constraints which are inactive at point \( \mathbf{x}^{*} \) can become either violated or active. The exact verification of the constraints validation may be time consuming. In [6], it was suggested to perform local linear analysis of the degree of the inactive constraint violation.

In order to fulfill the SA let us consider small perturbations of the objective functions in some direction tangential to the Pareto surface. At this direction we choose the descent direction \( \mathbf{S}_\Psi \) of some test function \( \Psi \):

\[
\{ \Psi = \Psi(f), \frac{\partial \Psi}{\partial f_i}(\mathbf{x}_p) \geq 0, \quad i = 1, 2, \ldots, P \} \quad \text{which is determined by:}
\]

\[
\mathbf{S}_\Psi = -\nabla \Psi - \mathbf{J}^T \mathbf{\mu} = \mathbf{P}(-\nabla \Psi) \quad (4.1)
\]

where

\[
\mathbf{\mu} = (\mathbf{J} \mathbf{J}^T)^{-1} \mathbf{J} \nabla \Psi \quad (4.2)
\]

Assume that the gradient \( \nabla \Psi \) is directed from the point \( P \) into the feasible direction \( \mathbf{e} \) [9]. Further, we will consider only normal (hence regular) Pareto points [9].

Suppose that the \( \mathbf{S}_\Psi \) is a null-vector. If the first \( Q \) Lagrange multipliers \( \mathbf{\mu} \) are non-negative \( (\mathbf{\mu} \in \Omega_{P,Q}) \), then no descent direction exists and the test function \( \Psi \) reaches the minimum at the Pareto point as well as the AOF. This follows immediately from the KKT theorem (see, e.g., [8]), at least under some additional general assumptions such as the convexity of the Pareto frontier.

If some of the first \( Q \) multipliers are negative \( (\mathbf{\mu} \notin \Omega_{P,Q}) \), then the appropriate inequality constraints become inactive in the direction \( \mathbf{S}_\Psi \) which is treated as the direction of a perturbation. In other words, these constraints become inactive in the case of further reduction of \( \Psi \). The Pareto solution can correspond to a non-differentiable point of the Pareto frontier. In [5, 6], where only inequality constraints are considered, it is suggested to remove the constraints corresponding to negative components of \( \mathbf{\lambda} \) and repeat the analysis reconsidering active constraints. The analysis is performed with respect to the weighted-sum representation of \( \Psi \). A similar analysis can be done in application to the AOF. Let us consider now the requirements for the test function \( \Psi \). This question was not addressed in [5, 6].

The vector \( \mathbf{S}_\Psi \) is represented by a linear combination of the vectors normal to the hyperplanes of the active constraints:

\[
\nabla \Psi = -\sum_{i=1}^{P} \mu_i \nabla \mathbf{g}_i \quad (4.3)
\]

Then, the gradient \( \nabla \Psi \) belongs to the constraint cone \( K \), [9]:

\[
K = \{ \mathbf{y} \in \mathbb{R}^M \ | \ \mathbf{y} = -\sum_{i=1}^{P} \mu_i \nabla \mathbf{g}_i, \ \mathbf{\mu} \in \Omega_{P,Q} \} \quad (4.4)
\]
Meanwhile, for any normal point the tangent cone \( T \) coincides with the cone \( K^* \) polar to \( K \): 
\[
K^* = \{ z \in R^M \mid z^T y \geq 0 \ \forall y \in K \} (4.5)
\]

On the other hand, if the function \( \Psi \) reaches a minimum then for any vector \( e \in T \) the following condition must be valid:
\[
e^T \nabla \Psi \geq 0 \quad (4.6)
\]

This fact means the gradient \( \nabla \Psi \) belongs to the convex cone \( T^* \) which is the positive polar cone to the cone \( T \).

Let us analyse now mutual location of the cones \( K \) and \( K^* = T \). Assume that \( K \subset K^* = T \). If \( \nabla \Psi \in T \setminus K \), \( \mu \notin \Omega_{P,E} \) and there is a direction along which the function \( \Psi \) can be further diminished. Let us assume that \( \mu_q < 0 \) (\( q \leq Q \)). By removing the \( q \)-th active constraint we obtain the reduced matrix \( J_r \). Then, the descent vector \( \tilde{S}_q \) is defined by the rest active constraints as follows:
\[
\tilde{S}_q = - \nabla \Psi - J_r^T \mu_r \quad (4.7)
\]

Vector \( \tilde{S}_q \) defines a feasible direction along which the \( q \)-th constraint becomes inactive. Along this direction in the vicinity of the point \( P \) we have:

\[
\nabla (\Psi + \sum_{q=Q} \mu_q g_q) = - \sum_{i=1}^P \mu_i \nabla g_i \quad (4.8)
\]

All coefficients \( \mu_i \) at the right-hand side are positive. Thus, the necessary condition for the minimum of the function \( \Psi^* = \Psi + \mu_q g_q \) is valid. In the objective space, the normal direction to the Pareto surface coincides with the gradient \( \nabla_j \Psi^* \).

If several Lagrange multipliers are negative in (3.3), the approach is similar. In this case, we have:

\[
\nabla (\Psi + \sum_{q=Q} \mu_q g_q) = - \sum_{i=Q}^* \mu_i \nabla g_i, \quad (4.9)
\]

\[
\Psi^* = \Psi + \sum_{q=Q} \mu_q g_q, \quad (4.9)
\]

\[
\mu_i > 0 \quad \text{if} \quad i \in Q^*, \mu_q < 0 \quad \text{if} \quad q \in Q^-
\]

where \( \sum^+ \) corresponds to the sum of all positive Lagrange multipliers while negative multipliers are included in the sum \( \sum^- \).

The descent direction is determined by
\[
\tilde{S}_q = - \nabla \Psi - J_r^T \mu_r = \sum_q^- \mu_q \nabla g_q \quad (4.10)
\]

Here, the reduced matrix \( J_r \) and the vector \( \mu_r \) are obtained by removing all rows corresponding to the negative Lagrange multipliers. The direction \( \tilde{S}_q \) is feasible if the following inequalities are valid:

\[
\nabla g_j^T \tilde{S}_q = \sum_{q=Q}^- \mu_q \nabla g_q \nabla g_j < 0 \quad (4.11)
\]

\[
j, q \in Q^-
\]

In order to prove inequality (4.11), let us consider the convex cone generated by the vectors \( \nabla g_j \) (\( j \in Q^- \)):
\[
C = \{ y \in E^M \mid y = \sum_{q=Q}^- \alpha_q \nabla g_q, \ \alpha_q \geq 0 \} \quad (4.12)
\]

Inequality (4.11) is equivalent to the requirement that \( \nabla g_j \) (\( j \in Q^- \)) belongs to the positive polar cone \( C^* \). This follows immediately from our assumption that the tangent cone \( K \) includes the polar cone \( K^* \) and the Polar theorem: \( (K^*)^* = K \).

Thus, to verify the differentiability of a Pareto point it is necessary to choose a function \( \Psi \) such that:

\[
\{ \nabla \Psi \in R^P, \nabla \Psi \in T \setminus K, \frac{\partial \Psi}{\partial f_i}(x_p) \geq 0, \ i = 1, ..., P \} \quad (4.13)
\]
It is to be noted that such a vector does not always exist. It is worth noting that the equality constraints effect on the matrix $J$ but do not effect on the SA related with the recognition of non-differentiable points. This follows from the fact that for the equality constraints the signs of the Lagrange multipliers are determined and the feasible direction is limited by equalities. On the other hand, if the polar cone $K$ includes the tangent cone $K^*$ ($T \subset K$), then a Pareto point can be non-differentiable while the appropriate vector $\mu \in \Omega_{P,Q}$. This means that although all first Lagrange multipliers are positive for any differentiable function $\Psi$: $\{S_\Psi = 0\}$ the Pareto point is non-differentiable. With regard to the described analysis, it is important to be able to determine the polar cone $K^*$. It can be obtained using Tamura method [10].

5. Test cases

The approach described above is illustrated using a few test cases related to vector optimisation.

The first example is related to a smooth local approximation of the Pareto surface.

Example 1:

Minimise: $F(x) = \{f_1(x), f_2(x), f_3(x)\}$
Subject to: $g(x) = 12 - x_1^2 - x_2^2 - x_3^2 \geq 0$

and the objective functions are given by:

$$
\begin{align*}
&f_1 = 25 - (x_1^2 + x_1^2(1 + x_2 + x_3) + x_2^2 + x_3^2)/10 \\
&f_2 = 35 - (x_1^3 + 2x_2^2 + x_3^3(1 + x_1 + x_3) + x_3^2)/10 \\
&f_3 = 50 - (x_1^3 + x_2^2 + 3x_3^3 + x_3^2(1 + x_1 + x_2))/10
\end{align*}
$$

In this 3D test case, the Pareto frontier is concave. The linear and quadratic approximations obtained by the analysis derived in section 3 are given in Figure 1 and Figure 2 respectively.

As expected, Figure 3 shows that a much better estimate of the Pareto surface in the vicinity of the Pareto point under investigation is obtained with the quadratic approximation.
In the next examples only non-differentiable Pareto surfaces are considered. The Pareto analysis is used to detect non-differentiable Pareto points and its limits are discussed.

**Example 2:**

The linear bi-criteria test case taken from [6] is considered.

\[
\begin{align*}
\min(x, y) \\
g_1(X) &= -\frac{x}{4} - \frac{y}{4} + 1 \leq 0, \\
g_2(X) &= -\frac{x}{3} - \frac{y}{6} + 1 \leq 0, \\
g_3(X) &= -x \leq 0, \\
g_4(X) &= -y \leq 0
\end{align*}
\]

A particularity of this example is that the variables are minimised, therefore the design space coincide with the objective space. For this test case, each point of the Pareto set is a point of the design space for which at least a constraint is active.

As illustrated in Figure 5, it is obvious that a function \( \Psi \) that satisfies (4.13) can be obtained. Therefore, according to the analysis given in the previous section, the Pareto point under study is non-differentiable.

**Example 3:**

In this example, the quadratic bi-criteria test case under linear constraints described as follows is considered:

\[
\begin{align*}
\min(f_1, f_2) \\
g_1(X) &= y - 2x + 1 \leq 0, \\
g_2(X) &= -y + \frac{x}{2} + \frac{1}{2} \leq 0
\end{align*}
\]

with

\[
\begin{align*}
f_1(X) &= \left(y - \frac{3}{2}x - \frac{1}{2}\right)^2 \\
f_2(X) &= \left(y - \frac{2}{3}x + \frac{1}{2}\right)^2
\end{align*}
\]

A representation of the feasible space of the optimisation problem is given in Figure 6.
Only the two contour lines corresponding to the minimum value of the objectives are represented in the design space. For each objective, isovalue contour lines are parallel to the minimum value contour line. The consequence of the difference between the slope of the minimum value contour lines and the slope of the borders of the feasible space is that under constraints, both objectives cannot be minimised together. It results that the solution set of the optimisation problem is a Pareto set as given in Figure 7.

The Pareto point obtained when both constraints \( g_1 \) and \( g_2 \) are active (i.e. \( g_1 = 0 \) and \( g_2 = 0 \)) is clearly a non-differentiable point in the objective space. Moving away from this point along the Pareto surface, the set of active constraints is changed.

The tangent cone \( T = K' \) and its polar cone \( K \) are built in the design space as shown in Figure 8.

In this test case, \( K' \subset K \). It is therefore impossible to find a function \( \Psi \) that satisfies (4.13). From the analysis described previously, it results that no conclusion on the differentiability of the Pareto point can be drawn.

6. Conclusion

A method for local approximation of the Pareto frontier is presented. The formulas for the first and the second order approximations have been derived. Both the linear and quadratic approximations are based on the Taylor approximation analysis. An approach is suggested to evaluate the vicinity of the Pareto solution where the local analysis is valid. The cases of non-differentiable Pareto points are also considered. The technique based on the gradient-projection method is applied and analysed in detail. The limits of this technique are also discussed. The developed concept of the Local Pareto Analyser allows the decision maker to
perform a local analysis of the Pareto solutions and trade-off between different objectives. Future work will concentrate on testing and application of the method to complex MDO industrial test cases.

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7. Literature