Proceedings of TOGO 2010, pp. 1 – ??.

The averaged problem*

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Abstract We consider a particular global optimization problem whose special structure permits the use of a decomposition algorithm optimizing globally only in search spaces of lower dimension. Roughly speaking, this problem involves the optimization of a weighted average of objective function values, subject to the same weighted average of constraints, where the weights are to be determined. We present theoretical results and an algorithmic approach to solve problems of this class.

Keywords: Gibbs free energy, decomposition, convexity, phase equilibrium

1. Definition of the problem

We consider in this talk a particular global optimization problem which, first, has various applications (for instance, in chemical engineering and in resource allocation), and, secondly, whose special structure permits the use of a decomposition algorithm optimizing globally only in search spaces of lower dimension. We call this problem the averaged problem. It has the following form:

$$\begin{aligned} \min_{K,x,y} F(K,x,y) &:= \sum_{k=1}^{K} y_k f(x_k) \\ \text{subject to} \quad \sum_{k=1}^{K} y_k g(x_k) &= b, \\ y &\in S_K, \\ x &\in X^K, \\ K &\in \mathbb{N}^+, \end{aligned} \tag{P}$$

where

$$S_K := \{y : \sum_{k=1}^{K} y_k = 1, y_k \geq 0, \quad k = 1, 2, \ldots, K\};$$

$X \subseteq \mathbb{R}^n$; f and g are given functions $f : X \to \mathbb{R}$, $g : X \to \mathbb{R}^m$; m is a given positive integer; and b is a given vector of $\mathbb{R}^m$. The optimization variables are: K, a positive integer, $y \in \mathbb{R}^K$, where y_k denotes the kth component of vector y, and $x_k \in X$, x being the vector $(x_1, x_2, \ldots, x_K) \in X^K := X \times \cdots \times X$. We note that the dimension, K, of the optimization variables is itself an optimization variable.

*ACKNOWLEDGEMENT: This work has been supported by French National Research Agency (ANR) through COSINUS program (project ID4CS no. ANR-09-COSI-005)

Roughly speaking, this problem involves the optimization of a weighted average of objective function values, subject to the same weighted average of constraints, where the weights, y_k's, are to be determined. By analogy with the specific chemical engineering instances of the averaged problem, we shall say that K is the number of phases and we shall call y_k, and x_k respectively the weight, and the composition of the kth phase.

2. Motivation

This problem was introduced by Whittle [5] four decades ago in order to take into account Lagrangian duality when convexity is lacking. To our knowledge, no one worked on the practical resolution of the averaged problem.

Various applications motivate our study. Special instances of the averaged problem are:

PEP The phase equilibrium problem.

Case where $f(x) := \min\{f_{\text{Liquid}}(x), f_{\text{Vapour}}(x)\}$, X is an open simplex, $g(x) := x$, and f_{Liquid} (respectively f_{Vapour}) is some given coercive smooth function whose specific form depends on the thermodynamic model chosen to describe a liquid phase (respectively a vapour phase). One must determine the number, types, proportions and compositions of each phase. See for instance [4] and references therein;

CEP The chemical equilibrium problem.

The same case except for the fact that g has rather the form $g(x) := Ax$, where A is an $m \times n$ real matrix of rank m related to the amount of each chemical element per unit amount of each substance involved in the chemical reaction (see again for instance [4] and references therein);

RA Resource allocation.

A very simple example involves choosing among many processes for producing a material. Given the production costs, $f_i(x)$ of producing at a rate x per hour with process i, $i \in \tau$ (where τ is some finite index set), find the least-cost way of producing at a given rate b, assuming that only one process can operate at the time, assuming that adequate storage is available, and that the costs of storage, changing production process or production rate are negligible. In such a case, we consider $f(x) := \min_{i \in \tau}\{f_i(x)\}$.

Another example is the allocation of discharge of water among generating units of a hydro-electric generating station so as to maximize power output within operating constraints. To each type of unit corresponds a particular power-output function of the discharge. Here b is the average discharge through the station in m^3/s.

LP Classical linear programming is itself a special case of the averaged problem. Indeed, in the case where a positive integer K, some scalars c_k, and some vectors a_k are given, and where $X := \{1, 2, \ldots, K\}$ (discrete index set), $f(x) = c_k$ if $x = k$ and $g(x) = a_k$ if $x = k$ $(k = 1, 2, \ldots, K)$, then the averaged problem (P) simply reduces to the linear programming problem.

Incidentally, we shall see in this talk that the chemical and phase equilibrium global optimization algorithm GILO, introduced in [4] and described in the next section, can be viewed as an extension of the simplex method for linear programming. This is obvious when substituting

here y for x in order to respect the notational conventions of linear programming:

$$\begin{array}{rcl} \min\limits_{x} \sum\limits_{k=1}^{K} x_k c_k & := & z, \\ \text{subject to} \quad Ax & = & b, \\ \sum\limits_{k=1}^{K} x_k & = & 1, \\ x & \geq & 0, \end{array} \tag{LP}$$

where A is an $m \times n$ matrix having a_k as kth column. From Dantzig's fundamental book [1], when evoking the simplex interpretation of the simplex method:

> It was in this geometry that the simplex method was first seriously proposed after it had been earlier set aside as unpromising. The variables x_k were interpreted as non-negative weights to be assigned to a system of points $A_k = (a_k, c_k)$ in the space (u, v), $u \in I\!R^m$ and $v \in I\!R$, so that their weighted average (center of gravity) is a point $(b, \text{Min } z)$. That is to say the $x_k \geq 0$ are chosen so that the center of gravity lies on the "requirement line" $u = b$ (constant), and such that the v-coordinate is minimum.

3. Algorithm GILO and its extension to the averaged problem

The algorithm GILO (Global Improvement Local Optimization) was introduced as an alternative to solving the phase or chemical equilibrium problem as a single optimization problem. GILO rather iterates between a local minimization problem and a global search in a lower dimensional space, taking advantage of the special structure of the problem. Under mild assumptions, the GILO algorithm is guaranteed to find a global minimizer [3, 4]. The proofs of convergence are based on results in [2] which derives the global optimality conditions for the problem.

The global optimization algorithm we shall present is a further generalization. The proofs behind GILO relied on the fact that X be an open set, and that f tend towards infinity as its argument approaches the frontier of X. It is hence not readily extendable to the more general case of the averaged problem, where no such assumptions are made.

4. Summary

The phase and chemical equilibrium problem involving multiple phase classes is a difficult global optimization problem. Necessary and sufficient conditions for global optimality based on the tangent-plane criterion has been derived as well as an algorithmic approach, called GILO, that reduces this global optimization problem to a finite sequence of local optimization (LO) steps and global optimization (GI) steps in a smaller search space. This algorithmic approach can be extended to the more general averaged problem which has further applications such as resource allocation.

References

[1] George B. Dantzig. Linear Programming and Extensions. Princeton University Press, 1963.

[2] Y. Jiang, W. R. Smith, and G. R. Chapman. Global optimality conditions and their geometric interpretation for the chemical and phase equilibrium problem. SIAM Journal on Optimization, 5(4):813–834, 1995.

[3] K. I. M. McKinnon, C. G. Millar, and M. Mongeau. Global optimization for the chemical and phase equilibrium problem using interval analysis. In C. Floudas and P.M. Pardalos, editors, State of the Art in Global Optimization, pages 365–382. Kluwer, 1996.

[4] K. I. M. McKinnon and M. Mongeau. A generic global optimization algorithm for the chemical and phase equilibrium problem. Journal of Global Optimization, 12(4):325–351, 1998.

[5] P. Whittle. Optimization Under Constraints. Wiley-Interscience, 1971.