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On regular simplex subdivision in Branch-and-Bound algorithms for blending problems *

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Abstract One of the aspects of Branch-and-Bound (B&B) algorithms is the use of an effective rejection (also called pruning) tests. Blending problems have the unit simplex as search space. The aim of this article is to study division schemes that generate new B&B sub-problems. The division scheme aims to increase the success of rejection tests and to decrease the number of vertex and simplex evaluations. In this way a division scheme improves the performance of the algorithm. [3] show that a simplex can be rejected if it is covered by infeasibility spheres centered at its vertices. In general, a regular simplex has more chance to be covered than an irregular one due to the equal distance between its vertices. Unfortunately, regular division without overlapping is not known for d-simplices, with $d > 2$. This work shows empirically the advantages of a regular partition in blending problems. Therefore, it is important to solve issues associated to overlap in regular division. Some strategies are described.

Keywords: Branch-and-Bound, blending, simplex partition, covering.

1. Introduction

Consider the following formulation of a mixture design problem which actually consists of identifying mixture products, each represented by a vector $x \in \mathbb{R}^n$, which meet certain requirements [3, 8]. The set of possible mixtures is mathematically defined by the unit simplex

$$S = \left\{ x \in \mathbb{R}^n \mid \sum_{j=1}^{n} x_j = 1.0;\ 0 \le x_j \le 1 \right\}, \tag{1}$$

where the variables x_j represent the fraction of the components in a product x. In mixture design (blending) problems, the objective is to minimize the cost of the material,

$$f(x) = e^T x, \tag{2}$$

where vector e gives the costs of the raw materials. In the model under study, linear inequality constraints and bounds define the design space $X \subset S$. The requirements are defined as

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quadratic inequalities.

$$g_i(x) = x^T A_i x + b_i^T x + c_i \leq 0; \;\; i = 1, \ldots, m, \tag{3}$$

in which A_i is a symmetric n by n matrix, b_i is an n-vector and c_i is a scalar. In this way we formulate the problem to be solved as finding elements of the set of "satisfactory" (feasible) products

$$D = \{x \in S \mid g_i(x) \leq 0; \;\; i = 1, \ldots, m\}. \tag{4}$$

Finding a point $x \in X \cap D$ defines the quadratic mixture design problem (QMDP), as studied in [7]. From practical considerations, this problem was extended towards robust solutions. One can define robustness $R(x)$ of a design $x \in D$ with respect to D as

$$R(x) = \max\{R \in \mathbb{R}^+ \mid (x+h) \in D, \; \forall h \in \mathbb{R}^n, \; \|h\| \leq R\} \tag{5}$$

Notice that for mixture problems $x + h$ is projected on the unit simplex. Additionally, variables has semi-continuity property related to a minimum acceptable dose md that the practical problems reveal. Therefore, we are merely interested in methods for finding an ϵ-robust solution with minimum cost, i.e.

$$\begin{array}{lll} \min & f(x) & \text{(Cost} \quad (2)) \\ \text{s.t.} & x \in X \cap D & \text{(Feasibility} \quad (4)) \\ & R(x) \geq \epsilon & \text{(Robustness} \quad (5)) \\ & x_j = 0 \text{ or } x_j \geq md & \text{(Minimal dose)} \end{array} \tag{6}$$

Independently of the application, we are dealing with a B&B algorithm where the search region defined as a simplex is decomposed iteratively [8]. The left hand side graph of Figure 1 shows the initial search space for $n = 2$, which is composed of two 0-simplices (one raw material) and one 1-simplex (two raw materials). The right hand side graph of Figure 1 shows the initial search space for $n = 3$, which consists of three 0-simplices, three 1-simplices and one 2-simplex.

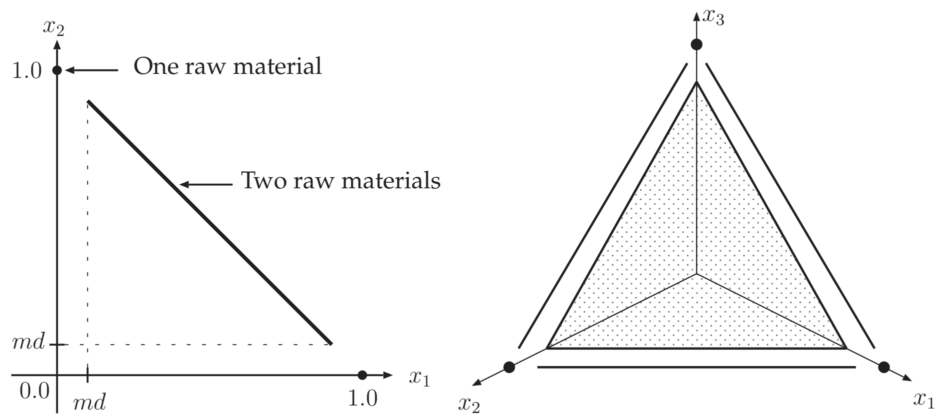

Figure 1. n=2 and n=3 initial simplices by removing the minimum dose region

B&B methods can be characterized by four rules: *Branching*, *Selection*, *Bounding*, and *Elimination* [10, 11]. For continuous problems, like the mixture design problem, a termination criterion has to be incorporated; i.e, one has to establish a minimum sampling precision α. A detailed description of these rules can be found in [8]. Here we focus on *Division rule* because it affects the effectiveness of the elimination tests. The use of simplicial sets in B&B and several ways of splitting them has been studied extensively in [4–6, 9]. Bisection of the longest edge (BLE), as shown in Figure 2a, is most used because it is simple and for all the generated simplices the length of the longest edge is at most twice the size of the shortest edge.

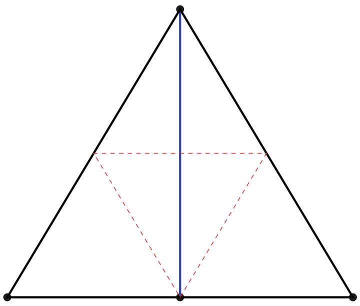

Figure 2a. BLE.
Bisect the Longest Edge.

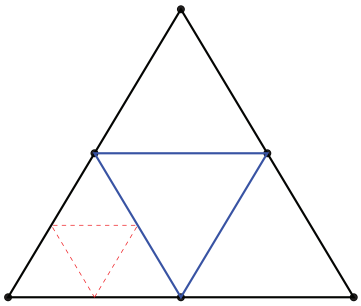

Figure 3b. BAE.
Bisect All Edges.

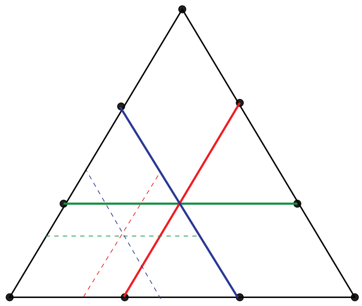

Figure 4c. ROD.
Regular Overlapping Division.

In general, regular shaped simplices give better bounding results than nonregular ones as can be found among others in [2]. A regular partition of a simplex similar to bisecting all edges (BAE), as in Figure 3b, has not been found for dimension higher than 3. Therefore we develop and investigate the potential of a simplicial subdivision which is regular, but is not a partition. Figure 4c shows an example of a regular overlapping division (ROD) for $n = 3$. The number of simplices generated is n and the length of its edges is $(n - 1)/n$, as shown by [4]. Dashed lines in Figures 2a to 4c are possible future divisions.

2. Experimental results for blending problems

Results for B&B algorithm using bisection of the largest edge are shown in [8]. Among several rejection tests, we want to highlight here those based on covering the simplex by infeasibility spheres centered at its vertices. A summary of them is:

- SCTest (Single Cover Test): One sphere covers all the simplex.
- MCTest (Multiple Cover Test): A simplex S can be rejected if a point $p \in S$ is covered by all spheres. The correctness of the test was proved in [3]. The proposed p in [8] is heuristic and can be calculated at low computational cost.
- θ-Test: The point θ to be covered is determined by a system of equations in [2]. If one sphere covers θ all spheres cover it, even if $\theta \notin S$. Even if θ is not covered, there exist cases where the covering of S can be determined from θ with additional computational cost, but we will not consider them in this experimentation.

Table 1 shows the efficiency of different division schema for problems defined in [8]. The efficiency is measured in terms of number of simplex (NSimplex) and vertex evaluations (NVertex). The rejection tests: SCTest, MCTest and θ-test, with others shown in [8], are checked in order.

BLE, BAE and ROD has been evaluated for 3-dimensional problems Case2 and RumCoke. BAE outperform BLE in efficiency. If the rejection test is not very successful it is better to do multisection, as it is shown for boxes in [1]. Additionally, the SCTest rejects more simplices at earlier stages of the algorithm because they are regular. BAE reduces the need of MCTest and only one expensive θ-Test is needed for Case2 and none for RumCoke. On the other hand, ROD is the worst of all divisions due to the fact that one simplex is overlapped by several simplices. So, unnecessary redundant computation is done. Additionally, it lacks vertex reusability.

Table 1 shows the necessary development of a regular division for larger dimensional problems. The number of congruent classes of simplices generated by BLE is $n!/2$ [6]. This hinders the success of SCTest. We research how to avoid redundant computation in ROD division, increasing the vertex reusability at the same time. Some strategies are designed but they deserve a complete article.

Table 1. Experimental results for different division schema. $\alpha = \epsilon = \sqrt{(}2)/100$, $md = 0.03$.

Problem	n	Division	NSimplex	NVertex	SCTest	NCTest	θ-Test
Case2	3	BLE	393	136	58	18	3
		BAE	291	153	66	6	1
		ROD	5,946	11,878	745	37	16
RumCoke	3	BLE	569	179	70	31	6
		BAE	341	172	86	13	0
		ROD	9,038	18,059	1,141	100	23
UniSpec1	7	BLE	72,419	7,561	11,146	5,442	780
UniSpec5b	7	BLE	94,422,861	1,962,173	15,135,582	9,546,656	1,108,185

3. Conclusions

Regular partition seems to outperform bisection and increases the performance of simple rejection tests. Unfortunately, regular division for dimension greater than 3 is only known with overlapping divisions. New methods to avoid redundant computation and to increase the vertex reusability in regular division are investigated. They will be shown in the final paper.

References

[1] L. G. Casado, I. García, and T. Csendes. A New Multisection Technique in Interval Methods for Global Optimization. *Computing*, 65(3):263–269, 2000. doi:10.1007/s006070070010.

[2] L. G. Casado, I. García, B. G.-Tóth, and E.M.T. Hendrix. On determining the cover of a simplex by spheres centered at its vertices. *Journal of Global Optimization*, 2010. doi:10.1007/s10898-010-9524-x.

[3] L. G. Casado, E.M.T. Hendrix, and I. García. Infeasibility spheres for finding robust solutions of blending problems with quadratic constraints. *Journal of Global Optimization*, 39(2):215–236, 2007. doi:/10.1007/s10898-006-9072-6.

[4] J. Claussen and A. Zilinskas. Subdivision, sampling and initialization strategies for simplical branch and bound in global optimization. *Computers and Mathematics with Applications*, 44:943–955, 2002.

[5] Herbert Edelsbrunner and Daniel R. Grayson. Edgewise subdivision of a simplex. In *SCG '99: Proceedings of the fifteenth annual symposium on Computational geometry*, pages 24–30, New York, NY, USA, 1999. ACM.

[6] Eduardo N. Gonçalves, Reinaldo M. Palhares, Ricardo H. C. Takahashi, and Renato C. Mesquita. Algorithm 860: Simples—an extension of freudenthal's simplex subdivision. *ACM Trans. Math. Softw.*, 32(4):609–621, 2006.

[7] E. M. T. Hendrix and J. D. Pintér. An application of Lipschitzian global optimization to product design. *Journal of Global Optimization*, 1:389–401, 1991.

[8] E.M.T. Hendrix, L. G. Casado, and I. García. The semi-continuous quadratic mixture design problem: Description and branch-and-bound approach. *European Journal of Operational Research*, 191(3):803–815, 2008. doi:10.1016/j.ejor.2007.01.056.

[9] R. Horst. On generalized bisection of n-simplices. *Mathematics of Computation*, 66(218):691–698, 1997.

[10] T. Ibaraki. Theoretical comparisons of search strategies in branch and bound algorithms. *Int. J. Comput. Inform. Sci.*, 5:315–344, 1976.

[11] L. G. Mitten. Branch and bound methods: general formulation and properties. *Operations Research*, 18:24–34, 1970.