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A polynomial-time approximation scheme for monotonic optimization over the unit simplex

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Abstract

The problem of minimizing a function representable as the difference of two monotonic functions over the unit simplex has a potential for various practical applications. In this paper, we discretize the problem and develop a branch-and-bound algorithm for generating an approximate optimal solution within a polynomial number of function evaluations.

Key words: global optimization, increasing functions, difference of monotonic functions, branch-and-bound algorithm, polynomial-time approximation scheme.

1 Introduction

In this paper, we discuss optimization of a function representable as the *difference of monotonic (d.m.)* functions over the unit simplex. Monotonic optimization was first introduced by Rubinov et al. [10] in 2001 to solve optimization problems defined only with increasing functions. Since then, Tuy et al. extended it to handle d.m. functions and achieved remarkable results, including the polyblock algorithm for locating a globally optimal solution [11–14]. Monotonicity is commonly observed in real-world systems related to economics and engineering, and besides polynomials, often used in their mathematical modeling, are all d.m. functions. Therefore, monotonic optimization has a great potential for a broad range of real-world applications. In contrast to the objective function, the constraints of our problem are

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rather special and limit the feasible set of solutions to the unit simplex. However, our problem still includes various problems of practical and theoretical importance, e.g., the maximum clique problem [7], Lipschitz optimization [9], and so forth.

In [3], Bomze and de Klerk discretize the problem of minimizing a quadratic function over the unit simplex, and show that it admits a *polynomial-time approximation scheme* (*PTAS*). In [4,5], de-Klerk et al. extend this result and show that the problem of minimizing a polynomial of fixed degree also has a PTAS. Polynomials, including quadratic functions, are d.m., and their discretization technique is directly applicable to our problem. Although the number of feasible solutions to examine is a polynomial in the dimension, it is enormous when the tolerance for approximation is small enough to use in practical applications. To enumerate the feasible solutions of the discretized problem efficiently, we develop a branch-and-bound algorithm and show that it generates an approximate optimal solution within a polynomial number of function evaluations.

In Section 2, after describing the problem formulation, we present two major applications of the problem. In Section 3, we review some known results on discretization of the problem. In Sections 4 and 5, we devise a branching and a bounding procedures, respectively, which are the two main parts of the algorithm. In Section 6, we summarize the branch-and-bound algorithm.

2 Problem formulation and applications

Let us denote the unit n-cube and the unit $(n-1)$-simplex by $[0,1]^n$ and $\Delta_{n-1} = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{e}^\mathsf{T}\mathbf{x} = 1, \mathbf{x} \geq \mathbf{0}\}$, respectively, where $\mathbf{e}$ denote the all-ones n-vector. For $i = 1,2$, let $f_i : \mathbb{R}^n \to \mathbb{R}$ be a function increasing on $[0,1]^n$, i.e., for any $\mathbf{a},\mathbf{b} \in [0,1]^n$, we have $f_i(\mathbf{a}) \leq f_i(\mathbf{b})$ if $\mathbf{a} \leq \mathbf{b}$. Therefore, $[0,1]^n$ is assumed to be a subset of $\operatorname{dom} f_1 \cap \operatorname{dom} f_2$, where $\operatorname{dom} f_i$ denotes the effective domain of f_i. The difference of these increasing functions f_1 and f_2 is generally referred to as a *d.m.* (difference-of-monotonic) function [12], whose minimization on Δ_{n-1} is our problem considered in this paper:

$$\left|\begin{array}{ll} \text{minimize} & f_1(\mathbf{x}) - f_2(\mathbf{x}) \\ \text{subject to} & \mathbf{e}^\mathsf{T}\mathbf{x} = 1, \quad \mathbf{x} \geq \mathbf{0}. \end{array}\right. \tag{1}$$

Despite the simple appearance, (1) includes a wide variety of optimization problems, as will be seen below.

STANDARD QUADRATIC OPTIMIZATION

Every polynomial such as a quadratic is d.m. on the nonnegative orthant $\mathbb{R}^n_+ = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{x} \geq \mathbf{0}\}$, because it can be divided into the sum of positive coefficient terms and the sum of negative coefficient terms. Therefore, (1) includes the standard quadratic optimization problem (standard QP) which minimizes $\mathbf{x}^\mathsf{T} Q\mathbf{x}$ on Δ_{n-1} for any $Q \in \mathbb{R}^{n\times n}$ [2,3]. An important example of this class is the maximum clique problem. Let $G = (V,E)$ be an undirected graph, where $V = \{1,\dots,n\}$ is the vertex set and $E \subset V \times V$ is the edge set, and let A denote the adjacency matrix of G, i.e., $a_{ij} = 1$ if $(i,j) \in E$, and $a_{ij} = 0$ otherwise. It is known [7] that finding a clique of maximum cardinality in G is equivalent to

$$\left|\begin{array}{ll} \text{minimize} & \mathbf{x}^\mathsf{T}(A+I)\mathbf{x} \\ \text{subject to} & \mathbf{x} \in \Delta_{n-1}, \end{array}\right. \tag{2}$$

where $I \in \mathbb{R}^{n\times n}$ is the identity matrix. Since all entries in $A+I$ are nonnegative, (2) is a special case of (1) where f_2 is absent. For other applications of the standard QP, the reader should refer to [2].

LIPSCHITZ OPTIMIZATION OVER A SIMPLEX

The problem (1) also includes Lipschitz optimization over the unit simplex:

$$\left|\begin{array}{ll} \text{minimize} & g(\mathbf{x}) \\ \text{subject to} & \mathbf{x} \in \Delta_{n-1}, \end{array}\right. \tag{3}$$

where g is Lipschitzian with Lipschitz constant $L > 0$, i.e., $|g(\mathbf{a}) - g(\mathbf{b})| \leq L\|\mathbf{a}-\mathbf{b}\|$ for any $\mathbf{a},\mathbf{b} \in \operatorname{dom} g$. In [9], it is shown that (3) can be reduced to minimization of an increasing positively homogeneous (IPH) function under the assumption where L is measured in the ℓ_1 norm. However, even if we do not impose such an assumption, (3) invariably belongs to the class (1). Let

$$h(\mathbf{x};\mathbf{y}) = g(\mathbf{y}) - L\|\mathbf{x}-\mathbf{y}\|.$$

Then we have $g(\mathbf{x}) \geq h(\mathbf{x};\mathbf{y})$ for any $\mathbf{x},\mathbf{y} \in \operatorname{dom} g$, where the equality holds if $\mathbf{x} = \mathbf{y}$. Assuming $[0,1]^n \subset \operatorname{dom} g$, let us define a function

$$f(\mathbf{x}) = \begin{cases} h\big(\mathbf{x};\mathbf{x}+(1-\mathbf{e}^\mathsf{T}\mathbf{x})\mathbf{e}\big) & \text{if } \mathbf{e}^\mathsf{T}\mathbf{x} \leq 1 \\ \mathbf{e}^\mathsf{T}\mathbf{x} + L\sqrt{n} + g(\mathbf{0}) & \text{otherwise.} \end{cases}$$

Obviously, we have $f(\mathbf{x}) = g(\mathbf{x})$ for any $\mathbf{x} \in \Delta_{n-1}$. Moreover, we can show that f is increasing on $[0,1]^n$.

Proposition 2.1 *Let* $\mathbf{a},\mathbf{b} \in [0,1]^n$*. If* $\mathbf{0} \le \mathbf{a} \le \mathbf{b}$*, then* $f(\mathbf{a}) \le f(\mathbf{b})$.

Thus, replacing the objective function g with f in (3), we have an equivalent d.m. optimization problem, which is again a special case of (1) where $f_2(\mathbf{x}) \equiv 0$. This class of (1) also includes minimization of ordinary IPH functions on the unit simplex, which is discussed in [1], because IPH functions are basically increasing on $\mathbb{R}^n_+$.

3 Discretization of the problem

Instead of dealing with (1) directly, we propose to discretize it, using a prescribed integer $m > 0$, into an approximation problem:

$$\left| \begin{array}{ll} \text{minimize} & f_1(\mathbf{x}) - f_2(\mathbf{x}) \\ \text{subject to} & \mathbf{e}^\top\mathbf{x} = 1, \quad \mathbf{x} \ge \mathbf{0}, \quad m\mathbf{x} \in \mathbb{Z}^n. \end{array} \right. \tag{4}$$

For any $c \ge 0$, let

$$M(c,n,m) = c\Delta_{n-1} \cap \frac{1}{m}\mathbb{Z}^n,$$

where $c\Delta_{n-1} = \{c\mathbf{x} \in \mathbb{R}^n \mid \mathbf{x} \in \Delta_{n-1}\}$. Then $M(1,n,m)$ represents the feasible set of (4), which is the set of grid points generated by subdividing each edge of Δ_{n-1} into m segments of length $\sqrt{2}/m$. Since the number of gird points is identical to the $(m+1)$th $(n-1)$-simplex number, the figurate number for an $(n-1)$-simplex [6], the total number of feasible solutions to this approximation problem (4) is bounded from above by

$$|M(1,n,m)| = \binom{n+m-1}{m},$$

which is a polynomial in n. Therefore, as discussed in [3–5], the problem (4) is polynomial-time solvable if f_1 and f_2 can be evaluated in time polynomial in n. A typical such case is when both f_1 and f_2 are polynomials of fixed degree. In that case, we can also estimate the approximation quality of (4) beforehand.

Let us denote the optimal values of (1) and (4) by $\underline{z}$ and z^*, respectively. Also let $\overline{z}$ denote the optimal value of

$$\left| \begin{array}{ll} \text{maximize} & f_1(\mathbf{x}) - f_2(\mathbf{x}) \\ \text{subject to} & \mathbf{e}^\top\mathbf{x} = 1, \quad \mathbf{x} \ge \mathbf{0}. \end{array} \right. \tag{5}$$

In [3, 4], the following result is proven:

Proposition 3.1 *If both* f_1 *and* f_2 *are polynomials of degree* d *and* $m \ge d$*, then*

$$z^* - \underline{z} \le \left(1 - \frac{m!}{m^d(m-d)!}\right)\binom{2d-1}{d} d^d(\overline{z} - \underline{z}).$$

Especially if $d = 2, 3$, this bound can be tightened, respectively, into

$$z^* - \underline{z} \le \frac{1}{m}(\bar{z} - \underline{z}), \quad z^* - \underline{z} \le \frac{4}{m}(\bar{z} - \underline{z}).$$

For any given tolerance $\varepsilon > 0$ and any polynomials f_1 and f_2 of fixed degree d, we can choose an integer $m \ge d$ to satisfy

$$\varepsilon \le \left(1 - \frac{m!}{m^d(m-d)!}\right)\binom{2d-1}{d} d^d(\bar{z} - \underline{z}).$$

The number of feasible solutions to (4) derived from this integer m is $|M(1,n,m)|$, which is polynomial in n as seen above. These two facts imply that our target problem (1) allows a *polynomial-time approximation scheme (PTAS)* (see e.g., [8]) when both f_1 and f_2 are polynomials of fixed degree. Even though it is polynomial, $|M(1,n,m)|$ is an enormous number when the tolerance ε is reasonably small. In the rest of this section, we develop a branch-and-bound algorithm for implicitly enumerating all points in the feasible set $M(1,n,m)$ of (4).

4 Branching procedure

Let $\mathbf{a} \in \mathbb{R}^n$ be a nonnegative vector satisfying $\mathbf{e}^\mathsf{T}\mathbf{a} < 1$, $\mathbf{0} \le m\mathbf{a} \in \mathbb{Z}^n$, and let $c = 1 - \mathbf{e}^\mathsf{T}\mathbf{a}$. Obviously, mc is a positive integer. For $K = \{j_1, \ldots, j_k\} \subset N = \{1, \ldots, n\}$, consider a subproblem of the approximation problem (4):

$$\mathrm{P}(\mathbf{a},K)\left|\begin{array}{ll} \text{minimize} & f_1(\mathbf{x}) - f_2(\mathbf{x}) \\ \text{subject to} & \mathbf{e}^\mathsf{T}\mathbf{x} = 1, \quad \mathbf{x} \ge \mathbf{0}, \quad m\mathbf{x} \in \mathbb{Z}^n \\ & x_j \ge a_j, \quad j \in K \\ & x_j = a_j, \quad j \notin K, \end{array}\right.$$

which is equivalent to

$$\left|\begin{array}{ll} \text{minimize} & f_1(\mathbf{x}) - f_2(\mathbf{x}) \\ \text{subject to} & \mathbf{y} \in M(c,k,m) \\ & y_i = x_{j_i} - a_{j_i}, \quad i = 1, \ldots, k \\ & x_j = a_j, \qquad j \notin K. \end{array}\right. \tag{6}$$

By definition, $M(c,k,m)$ is the set of grid points generated by subdividing each edge of the $(k-1)$-simplex $c\Delta_{k-1}$ into mc segments of length $\sqrt{2}/m$. The number of grid points is given by

$$|M(c,k,m)| = \binom{k+mc-1}{mc}, \tag{7}$$

which is the number of evaluations of f_1 and f_2 required to solve $\mathrm{P}(\mathbf{a},K)$. To perform this recursively, we first select an index, say r, from K. Then we divide $\mathrm{P}(\mathbf{a},K)$ into two problems:

$$\mathrm{P}(\mathbf{a}+\mathbf{e}_r/m,K)\left|\begin{array}{ll}\text{minimize} & f_1(\mathbf{x})-f_2(\mathbf{x})\\ \text{subject to} & \mathbf{e}^{\mathrm{T}}\mathbf{x}=1,\quad \mathbf{x}\geq\mathbf{0},\quad m\mathbf{x}\in\mathbb{Z}^n\\ & x_j\geq a_j,\quad j\in K\setminus\{r\}\\ & x_r\geq a_r+1/m\\ & x_j=a_j,\quad j\notin K,\end{array}\right.$$

and

$$\mathrm{P}(\mathbf{a},K\setminus\{r\})\left|\begin{array}{ll}\text{minimize} & f_1(\mathbf{x})-f_2(\mathbf{x})\\ \text{subject to} & \mathbf{e}^{\mathrm{T}}\mathbf{x}=1,\quad \mathbf{x}\geq\mathbf{0},\quad m\mathbf{x}\in\mathbb{Z}^n\\ & x_j\geq a_j,\quad j\in K\setminus\{r\}\\ & x_r=a_r\\ & x_j=a_j,\quad j\notin K,\end{array}\right.$$

where $\mathbf{e}_r$ is the rth standard basis n-vector. These are rewritten, respectively, as follows:

$$\left|\begin{array}{lll}\text{minimize} & f_1(\mathbf{x})-f_2(\mathbf{x}) & \\ \text{subject to} & \mathbf{y}\in M(c-1/m,k,m) & \\ & y_i=x_{j_i}-a_{j_i}, & i=1,\ldots,k-1\\ & y_k=x_r-a_r-1/m & \\ & x_j=a_j, & j\notin K,\end{array}\right. \tag{8}$$

and

$$\left|\begin{array}{lll}\text{minimize} & f_1(\mathbf{x})-f_2(\mathbf{x}) & \\ \text{subject to} & \mathbf{y}\in M(c,k-1,m) & \\ & y_i=x_{j_i}-a_{j_i}, & i=1,\ldots,k-1\\ & x_r=a_r & \\ & x_j=a_j, & j\notin K.\end{array}\right. \tag{9}$$

Note that

$$|M(c-1/m,k,m)|=\binom{k+mc-2}{mc-1},\quad |M(c,k-1,m)|=\binom{k+mc-2}{mc}.$$

Since the following relation is well-known:

$$\binom{k+mc-1}{mc}=\binom{k+mc-2}{mc-1}+\binom{k+mc-2}{mc},$$

we have

$$|M(c,k,m)| = |M(c-1/m,k,m)| + |M(c,k-1,m)|.$$

If the same procedure is applied to both $\mathrm{P}(\mathbf{a}+\mathbf{e}_r/m,K)$ and $\mathrm{P}(\mathbf{a},K\setminus\{r\})$ recursively, we eventually have $\binom{k+mc-1}{mc}$ subproblems, each of which is a trivial problem with a single feasible solution corresponding to some grid point in the feasible set $M(c,k,m)$ of (4).

If we start this branching procedure from $\mathrm{P}(\mathbf{0},N)$, the original discretized problem (4), then $\binom{n+m-1}{m}$ trivial subproblems are generated. Simultaneously, we have a branching binary tree T rooted at $\mathrm{P}(\mathbf{0},N)$ with $\binom{n+m-1}{m}$ leaves.

Lemma 4.1 *The total number of nodes in T is* $2\binom{n+m-1}{m}-1$.

5 Bounding procedure

Again, consider the subproblem $\mathrm{P}(\mathbf{a},K)$, or equivalently (6), of the approximation problem (4). To simplify the illustration, let $K=\{1,\ldots,k\}$ and $N\setminus K=\{k+1,\ldots,n\}$. Also let $\mathbf{a}_K=(a_1,\ldots,a_k)^\mathsf{T}$ and $\mathbf{a}_{N\setminus K}=(a_{k+1},\ldots,a_n)^\mathsf{T}$. Introducing the following functions defined on $\mathbb{R}^k$:

$$f_{i,K}(\mathbf{y}) = f_i(\mathbf{y}+\mathbf{a}_K,\mathbf{a}_{N\setminus K}), \quad i=1,2,$$

we can rewrite $\mathrm{P}(\mathbf{a},K)$ and (6) in a more tidy form:

$$\left|\begin{array}{ll} \text{minimize} & f_{1,K}(\mathbf{y}) - f_{2,K}(\mathbf{y}) \\ \text{subject to} & \mathbf{y}\in M(c,k,m). \end{array}\right. \tag{10}$$

We also see that $\mathrm{P}(\mathbf{a},K)$ is an approximation problem of

$$\left|\begin{array}{ll} \text{minimize} & f_{1,K}(\mathbf{y}) - f_{2,K}(\mathbf{y}) \\ \text{subject to} & \mathbf{y}\in c\Delta_k. \end{array}\right. \tag{11}$$

Let $z^*(\mathbf{a},K)$ and $\underline{z}(\mathbf{a},K)$ denote the optimal values of (10) and (11), respectively. Needless to say, $z^*(\mathbf{a},K)$ is the optimal value of $\mathrm{P}(\mathbf{a},K)$, and greater than or equal to $\underline{z}(\mathbf{a},K)$. It should also be noted that $z^*(\mathbf{0},N)=z^*$ and $\underline{z}(\mathbf{0},N)=\underline{z}$.

Note that $M(c,k,m)\subset c\Delta_k\subset c[0,1]^k=\{\mathbf{x}\in\mathbb{R}^k \mid \mathbf{0}\le\mathbf{x}\le c\mathbf{e}\}$. Since $f_{i,K}$ is still increasing on $c[0,1]^k$ for each i, we have a lower bound on $z^*(\mathbf{a},K)$ immediately as follows:

$$u_1(\mathbf{a},K) = f_{1,K}(\mathbf{0}) - f_{2,K}(c\mathbf{e}) = f_1(\mathbf{a}) - f_2(\mathbf{a}_K+c\mathbf{e},\mathbf{a}_{N\setminus K}). \tag{12}$$

If $u_1(\mathbf{a},K)\ge f_1(\mathbf{x}^*)-f_2(\mathbf{x}^*)$ for some $\mathbf{x}^*\in M(1,n,m)$ obtained in the course of the algorithm, we can prune $\mathrm{P}(\mathbf{a},K)$ from the branching tree. This lower bound $u_1(\mathbf{a},K)$ is handy to obtain, but unfortunately it is not strong enough.

To strengthen the lower bound for $\mathrm{P}(\mathbf{a},K)$, let us consider k cubes, each of which is a proper subset of $[0,1]^k$:

$$B_j = \frac{1}{n}\left((n-1)[0,1]^k + \mathbf{e}_j\right) = \left\{ \mathbf{x} \in \mathbb{R}^k \;\middle|\; \begin{array}{l} 0 \le x_i \le 1-1/n, \quad i \neq j \\ 1/n \le x_j \le 1 \end{array} \right\}, \quad j \in K,$$

where $\mathbf{e}_j$ is the jth standard basis k-vector. Since $cB_j \subset c[0,1]^k$ for each $j \in K$, the minimum and the maximum of $f_{i,K}$ on cB_j are achieved at the vertices $(c/n)\mathbf{e}_j$ and $(c/n)\left((n-1)\mathbf{e}+\mathbf{e}_j\right)$, respectively. Let

$$v_j = f_{1,K}\left(\frac{c}{n}\mathbf{e}_j\right), \quad w_j = f_{2,K}\left(\frac{c}{n}\left((n-1)\mathbf{e}+\mathbf{e}_j\right)\right), \quad j \in K,$$

and let

$$u_2(\mathbf{a},K) = \min\{v_j \mid j \in K\} - \max\{w_j \mid j \in K\}.$$

Proposition 5.1 *The following inequalities hold:*

$$u_1(\mathbf{a},K) \le u_2(\mathbf{a},K) \le z^*(\mathbf{a},K).$$

For each $j \in K$, if we further replace B_j with the union of k cubes

$$B_{j\ell} = \frac{1}{n}\left((n-1)B_j + \mathbf{e}_\ell\right), \quad \ell \in K,$$

and define

$$v'_j = \min\{f_{1,K}(\mathbf{y}) \mid \mathbf{y} \in \bigcup_{\ell \in K} cB_{j\ell}\}, \quad w'_j = \max\{f_{2,K}(\mathbf{y}) \mid \mathbf{y} \in \bigcup_{\ell \in K} cB_{j\ell}\}, \quad j \in K.$$

Then we obtain another lower bound on $z^*(\mathbf{a},K)$:

$$u_3(\mathbf{a},K) = \min\{v'_j \mid j \in K\} - \max\{w'_j \mid j \in K\},$$

which is expected to be tighter than $u_2(\mathbf{a},K)$. In principle, by applying this procedure recursively to $B_{j\ell}$'s, we can strengthen the lower bound for $\mathrm{P}(\mathbf{a},K)$ endlessly. The polyblock algorithm for solving more general class of monotonic optimization problems is essentially based on the same idea [11–14]. However, while u_1 requires a single function evaluation for each of f_1 and f_2, the strengthened bounds u_2 and u_3 need $O(n)$ and $O(n^2)$ function evaluations, respectively. As a tool for bounding, this kind of lower bound would be too expensive to use if we expected it to be tighter than u_3.

6 Algorithm description and performance

Let us summarize the discussion so far into a branch-and-bound algorithm. For prescribed integers $m > 0$ and $s \in \{1,2,3\}$, it can be described as follows:

```
algorithm dm_branch_bound(f_1, f_2, m, s)
  𝒫 ← {P(0, {1,...,n})}; x* ← null; z* ← +∞; a ← 0;
  while 𝒫 ≠ ∅ do
    select a subproblem P(a, {j_1,...,j_k}) from 𝒫;
    K ← {j_1,...,j_k}; c ← 1 − e^T a; x° ← a;
    select a point y° ∈ cS^k;                          # extraction of a solution
    for i = 1,...,k do
      x°_{j_i} ← x°_{j_i} + y°_i
    end for;
    if f_1(x°) − f_2(x°) < z* then                     # update of the incumbent
      x* ← x°; z* ← f_1(x°) − f_2(x°);
    end if;
    compute a lower bound u_s(a, K) for P(a, K);       # bounding process
    if u_s(a, K) < z* then
      select an index r from K;                        # branching process
      𝒫 ← (𝒫 \ {P(a, K)}) ∪ {P(a + e_r/m, K), P(a, K \ {r})}
    end if
  end while;
  return x*
end.
```

It should be remarked in this description that $\mathbf{y}^\circ$ is chosen from the simplex $c\Delta_k$, not from the set of grid points $M(c,k,m)$. As a result, the output $\mathbf{x}^*$ of the algorithm might not a feasible solution to the approximation problem (4). However, $\mathbf{x}^*$ is still feasible for the original problem (1), and besides never inferior to any feasible solution of (4).

Theorem 6.1 *The algorithm* dm_branch_bound *terminates after* $2\binom{n+m-1}{m} - 1$ *iterations at most, and generates a feasible solution* $\mathbf{x}^*$ *of (1) satisfying*

$$f_1(\mathbf{x}^*) - f_2(\mathbf{x}^*) \leq f_1(\mathbf{x}) - f_2(\mathbf{x}), \quad \forall \mathbf{x} \in \Delta_m \cap \frac{1}{m}\mathbb{Z}^n.$$

Numerical results of the algorithm dm_branch_bound will be reported in details elsewhere.

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