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Global Minimizer of Large Scale Stochastic Rosenbrock Function: Canonical Duality Approach

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Abstract. Canonical duality theory for solving the well-known benchmark test problem of stochastic Rosenbrock function is explored by two canonical transformations. Global optimality criterion is analytically obtained, which shows that the stochastic disturbance of these parameters could be eliminated by a proper canonical dual transformation. Numerical simulations illustrate the canonical duality theory is potentially powerful for solving this benchmark test problem and many other challenging problems in global optimization and complex network systems.

1 Preliminary

Almost all of benchmark test problems in previous literature are deterministic by parameters. However, it is usually more difficult for algorithms to deal with stochastic functions. In Yang's work [2], a stochastic parameter is introduced in Rosenbrock's function such that this well-known benchmark test problem can be proposed as

$$(\mathcal{P}): \min\left\{P(X) = \sum_{i=1}^{n-1} \left[(x_i - 1)^2 + 100\epsilon_i (x_{i+1} - x_i^2)^2 \right] \mid X \in \mathcal{X} \right\}, \quad (1)$$

where $X = \{x_i\} \in \mathcal{X} = \mathbb{R}^n$ is a real unknown vector, and the random parameters $\{\epsilon_i\}$ are drawn from a uniform distribution in [0, 1]. For stochastic functions, most deterministic algorithms such as hill climbing and Nelder-Mead downhill simplex method would simply fail.

2 Canonical dual approach

Following the standard procedures in the canonical dual transformation (see Gao, 2009), we first introduce the so-called geometrical operator $\xi = \Lambda(X)$: $\mathcal{X} \to \mathcal{E}_a \subset \mathbb{R}^{n-1}$

$$\xi = \{\xi_k\} = \epsilon_k^{\frac{1}{2}} (x_k^2 - x_{k+1}), \tag{2}$$

and a canonical function $V(\xi) = 100 \sum_{k=1}^{n-1} \xi_k^2$ such that the duality relation

$$\varsigma = \{\varsigma_k\} = \left\{\frac{\partial V(\xi_k)}{\partial \xi_k}\right\} = \{200\xi_k\}$$
(3)

is invertible. Thus, we have

$$\xi_k = \frac{1}{200} \varsigma_k \quad \forall k = 1, \dots, n-1, \tag{4}$$

and the conjugate function of $V(\xi_k)$ can be obtained uniquely by the Legendre transformation

$$V^{*}(\varsigma) = \sum_{k=1}^{n-1} \xi_{k}\varsigma_{k} - V(\xi)$$

=
$$\sum_{k=1}^{n-1} \{\xi_{k}\varsigma_{k} - 100\xi_{k}^{2}\} = \sum_{k=1}^{n-1} \frac{1}{400}\varsigma_{k}^{2}.$$
 (5)

Then, the total complementary function can be defined as

$$\Xi(X,\varsigma) = \sum_{k=1}^{n-1} (x_k - 1)^2 + \Lambda(X)^T \varsigma - V^*(\varsigma)$$

=
$$\sum_{k=1}^{n-1} \left[(x_k - 1)^2 + \epsilon_k^{\frac{1}{2}} (x_k^2 - x_{k+1}) \varsigma_k - \frac{1}{400} \varsigma_k^2 \right].$$
(6)

For a fixed ς in the canonical dual feasible space $S_a \subset \mathbb{R}^{n-1}$ defined by

$$\mathcal{S}_a = \left\{ \varsigma \in \mathcal{S} \mid \epsilon_k^{\frac{1}{2}} \varsigma_k + 1 \neq 0, \quad \forall k = 1, ..., n-2, \quad \varsigma_{n-1} = 0 \right\},\$$

the criticality condition $\nabla_X \Xi(X,\varsigma) = 0$ leads to the following analytical solution

$$X = \{x_k\} = \left\{\frac{\epsilon_{k-1}^{\frac{1}{2}}\varsigma_{k-1} + 2}{2(\epsilon_k^{\frac{1}{2}}\varsigma_k + 1)}\right\}.$$
(7)

Substituting this result into the total complementary function $\Xi(X,\varsigma)$, the canonical dual problem can be finally formulated as

$$(\mathcal{P}^d): P^d(\varsigma) = \max\left\{ n - 1 - \sum_{k=1}^{n-1} \left[\frac{(\epsilon_{k-1}^{\frac{1}{2}}\varsigma_{k-1} + 2)^2}{4(\epsilon_k^{\frac{1}{2}}\varsigma_k + 1)} + \frac{1}{400}\varsigma_k^2 \right] \mid \varsigma \in \mathcal{S}_a^+ \right\},$$
(8)

where

$$\mathcal{S}_a^+ = \{\varsigma \in \mathcal{S}_a \mid \epsilon_k^{\frac{1}{2}}\varsigma_k + 1 > 0, \quad \forall k = 1, ..., n-2\}.$$
(9)

By introducing $G(\varsigma), F(\varsigma)$ and \mathcal{S}_a^+ such that

$$G(\varsigma) = \begin{bmatrix} \epsilon_1^{\frac{1}{2}}\varsigma_1 + 1 & & \\ & 2(\epsilon_2^{\frac{1}{2}}\varsigma_2 + 1) & & \\ & & \dots & \\ & & & 2(\epsilon_{n-2}^{\frac{1}{2}}\varsigma_{n-2} + 1) \\ & & & & 2 \end{bmatrix}$$
(10)

$$F(\varsigma) = \begin{bmatrix} 1\\ \epsilon_1^{\frac{1}{2}}\varsigma_1 + 2\\ \cdots\\ \epsilon_{n-3}^{\frac{1}{2}}\varsigma_{n-3} + 2\\ \epsilon_{n-2}^{\frac{1}{2}}\varsigma_{n-2} + 2 \end{bmatrix}.$$
 (11)

We have the following theorem (see Gao, 2009)

Theorem 1. If $\bar{\varsigma}$ is a critical point of (\mathcal{P}^d) , then the vector

$$\bar{X} = G^{-1}(\bar{\varsigma})F(\bar{\varsigma}) \tag{12}$$

is a critical point of (\mathcal{P}) and

$$P(\bar{X}) = P^d(\bar{\varsigma}). \tag{13}$$

If $\bar{\varsigma} \in S_a^+$, then $\bar{\varsigma}$ is the global maximizer of the canonical dual problem (\mathcal{P}^d) on S_{a^+} . The vector \bar{X} is a global minimal to the primal problem, and

$$P(\bar{X}) = \min_{X \in \mathcal{X}} P(X) = \max_{\varsigma \in \mathcal{S}_a^+} P^d(\varsigma) = P^d(\bar{\varsigma}).$$
(14)

The proof of this Theorem can be intuitively derived from the paper by Gao (2003).

3 An Alternative Transformation

In this section, we choose an alternative canonical dual transformation for stochastic function, which shows analytically that the stochastic perturbation of this problem would never change the global minimal elements.

Let $\xi = \{\xi_k\} = \{x_k^2 - x_{k+1}\} \in \mathbf{R}^{n-1}$. The canonical function $V(\xi)$ has the form of

$$V(\xi) = 100 \sum_{k=1}^{n-1} \epsilon_k \xi_k^2.$$
 (15)

Thus, the associated canonical dual variable $\varsigma = \{\varsigma_k\} = \nabla V(\xi) = \{200\epsilon_k\xi_k\}$ and

$$V^*(\varsigma) = \sum_{k=1}^{n-1} \frac{1}{400\epsilon_k} \varsigma_k^2.$$
 (16)

Correspondingly, the total complementary function can be written as

$$\Xi(X,\varsigma) = \sum_{k=1}^{n-1} \left[(x_k - 1)^2 + (x_k^2 - x_{k+1})\varsigma_k - \frac{1}{400\epsilon_k}\varsigma_k^2 \right].$$
 (17)

By which, the second type of the canonical dual problem can be formulated as

$$(\mathcal{P}^d): P^d(\varsigma) = \max\left\{ \{n - 1 - \frac{1}{2}F(\varsigma)^T G^{-1}(\varsigma)F(\varsigma) - \frac{1}{400\epsilon}\varsigma^T\varsigma \mid \varsigma \in \mathcal{S}_a^+ \right\}$$
(18)

where

$$G(\varsigma) = \begin{bmatrix} \varsigma_1 + 1 & & \\ & 2(\varsigma_2 + 1) & & \\ & & \ddots & \\ & & & 2(\varsigma_{n-2} + 1) \\ & & & & 2 \end{bmatrix}$$
(19)

$$F(\varsigma) = \begin{bmatrix} \varsigma_1 + 2 \\ ... \\ \varsigma_{n-3} + 2 \\ \varsigma_{n-2} + 2 \end{bmatrix}$$
(20)

$$\mathcal{S}_{a}^{+} = \{ \varsigma \in \mathbb{R}^{n-1} \mid \varsigma_{k} > -1, \quad \forall k = 1, ..., n-2, \ \varsigma_{n-1} = 0 \}.$$
(21)

Theorem 1 still holds for this second canonical dual problem. However, by numerical experiments we can see that the stochastic perturbation does not have any impact on the global optimal solution.

4 Illustration

In this section we list some numerical examples with different dimensions, which are more general than normal Rosenbrock function. **Example 1.** Consider

$$(\mathcal{P}): \quad \min \quad \left\{ P(X) = \sum_{i=1}^{3} \left[(x_i - 1)^2 + 100\epsilon_i (x_{i+1} - x_i^2)^2 \right] \mid X \in \mathcal{X} \right\}. \quad (22)$$

This problem has the global minimum of all ones and a local minimum near $(x_1, x_2, x_3, x_4) = (-1, 1, 1, 1)$. Correspondingly, the canonical dual problem is

$$\max\left\{ P^{d}(\varsigma) = 3 - \sum_{k=1}^{3} \left[\frac{(\epsilon_{k-1}^{\frac{1}{2}}\varsigma_{k-1} + 2)^{2}}{4(\epsilon_{k}^{\frac{1}{2}}\varsigma_{k} + 1)} + \frac{1}{400}\varsigma_{k}^{2} \right] \mid \varsigma \in \mathcal{S}_{a}^{+} \right\}$$
(23)

where S_a^+ is defined by (9). And an alternative canonical dual problem is

$$\max\left\{ P^{d}(\varsigma) = 3 - \sum_{k=1}^{3} \left[\frac{(\varsigma_{k-1}+2)^{2}}{4(\varsigma_{k}+1)} + \frac{1}{400\epsilon_{k}}\varsigma_{k}^{2} \right] \mid \varsigma \in \mathcal{S}_{a}^{+} \right\}$$
(24)

where S_a^+ is defined by (21). Obviously, it is easy to find results by Matlab optimization tools FMINCON. Note that $\varsigma_3 = 0$, the contour of dual problem can be obtained directly(see Fig. 1). Thus, the global maximum of dual problem is $(\varsigma_1,\varsigma_2,\varsigma_3)=(0, 0, 0)$ and the global minimum of primal problem is $(x_1,x_2,x_3,x_4)=(1, 1, 1, 1)$.



Fig. 1. (a) Dual problem n=3 determined by (24); (b) Dual problem n=3 determined by (25)

Example 2. Consider N= 1000, 3000, 5000, 10000, 20000. The global minimum is inside a long, narrow, banana shaped flat valley. In this case, it is difficult to solve exactly the primal problem (\mathcal{P}) by gradient methods. Fortunately, the canonical dual problem is concave maximization over a cone, which can be solved easily, fast and exactly by gradient method.

For (22) and (23), the initial points are chosen randomly from -5 to 5 with the constraints (9) and (21), respectively. With these numerical computation settings, L-BFGS method can quickly solve all these test problems and accurately converge to the global maximizer $\varsigma = (0, 0, ..., 0)$ with the optimal value $P^d(\varsigma) = 0(10^{-8})$.

All of numerical experiments have been carried out in Intel(R)Core i5-2430M @2.40GHz Windows 7 Home Basic personal notebook computer.

5 Conclusion

This paper illustrates that the well-known benchmark test problem of Rosenbrock function with stochastic parameters can be easily solved by the canonical duality theory. Numerical examples show that even though the nonconvex primal problem has been disturbed by stochastic parameters, the canonical duality theory can avoid defective influence to achieve global optimal solution stably. The canonical duality theory can be used for solving some more challenging problems in global optimization and complex network systems.

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