A Randomized Algorithm to Approximate the Star Discrepancy Based on Threshold Accepting

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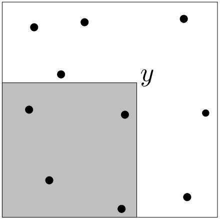
Star Discrepancy: Definition

$X \subset [0,1]^d$ n-point set, $[0,y) := [0,y_1) \times \cdots \times [0,y_d)$ "test box".

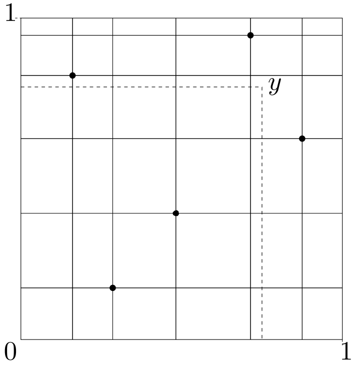


Local discrepancy: $$\delta(y) = \delta(y,X) = \mathrm{vol}([0,y)) - \frac{1}{n}|X \cap [0,y)|$$

Star discrepancy: $$\mathrm{disc}^*(X) = \sup_{y \in [0,1]^d} |\delta(y,X)|$$

Known Methods for Calculation

Elementary Method for Exact Calculation



Simple Observation: It suffices to consider $2(n+1)^d$ test boxes to calculate the discrepancy.

Known Methods for Calculation

Elementary Method for Exact Calculation

For $X = \{x^1, \dots, x^n\} \subset [0,1]^d$ put

$$\Gamma_j(X) := \{x_j^i \,|\, i = 1, \dots, n\} \cup \{1\}, \; j = 1, \dots, d,$$
$$\Gamma(X) := \Gamma_1(X) \times \cdots \times \Gamma_d(X)$$

Then $\mathrm{disc}^*(X) =$

$$\max_{y \in \Gamma(X)} \max \left\{ \mathrm{vol}([0,y)) - \frac{1}{n} \big| [0,y) \cap X \big| , \; \frac{1}{n} \big| [0,y] \cap X \big| - \mathrm{vol}([0,y)) \right\}$$

Thus $\mathrm{disc}^*(X)$ can be calculated by considering at most $2(n+1)^d$ test boxes.

Further Methods for Calculation

Improvements of the Elementary Method:

Exact formula for the star discrepancy in dimension $d = 1$ by Niederreiter '72 ($d = 1$).

Faster methods than the elementary one by De Clerck '86 ($d = 2$) and Bundschuh and Zhu '93 ($d \geq 3$). Time to calculate the star discrepancy still $O(n^d)$.

Fastest algorithm to calculate the star discrepancy needs time $O(n^{1+d/2})$ [Dobkin, Eppstein, Mitchell '96].

Known Methods for Calculation

Observation: Exact calculation of star discrepancy is discrete optimization problem.

Bad news from Discrete Complexity Theory:

Theorem [G., Srivastav, Winzen '09].
The calculation of the star discrepancy is NP-hard.

Theorem [Giannopoulos, Knauer, Wahlström, Werner '11].
Calculation of star discrepancy is $W[1]$-hard with respect to parameter d.

Methods for Approximation

Algorithms with error guarantee

- Algorithms from [Thiémard '00, '01a] to approximate the star discrepancy up to some user-specified error δ.
  Cost of the algorithms is $\geq \Omega(d\delta^{-d})$ [G.'08].

Algorithms based on optimization heuristics

- Algorithm from [Thiémard'01b] formulates problem as integer linear program (ILP) and relies on cutting plane and branch-and-bound techniques.
- Algorithm of Winker & Fang '97 is a local search algorithm relying on the meta heuristic "Threshold Accepting".
- Genetic algorithm of Shah '10.

Randomized Approach

Idea: Calculate lower bound for star discrepancy by choosing test boxes randomly within a (refined) local search algorithm

Algorithm of Winker & Fang ("Threshold Accepting")

Threshold values $T_1 > T_2 > \cdots > T_I \geq 0$

Local neighborhood structure for $y \in \Gamma(X)$

$N_k(y) \simeq$ subgrid of $\Gamma(X)$ of cardinality $(2k+1)^d$ with center y,

with Laplace measure as probability measure.

Algorithm of Winker & Fang

For $y \in [0,1]^d$ put

$$\delta(y) := \mathrm{vol}([0,y)) - \frac{1}{n}\big|[0,y) \cap X\big|, \quad \overline{\delta}(y) := \frac{1}{n}\big|[0,y] \cap X\big| - \mathrm{vol}([0,y)),$$

and $\delta^*(y) := \max\{\delta(y), \overline{\delta}(y)\}$.

Concrete Algorithm

Choose x randomly from $\Gamma(X)$ and put $x^* := x$.

For $i = 1$ to I
    For $j = 1$ to J
        Choose $x \in N_k(x^*)$ randomly
        If $\delta^*(x^*) - \delta^*(x) \leq T_i$ then $x^* := x$
Return $\delta^*(x^*)$

Improving on the W&F-Algorithm

Modified Neighborhoods:

$C_k(x) := \mathrm{conv}(N_k(x))$, endowed with probability measure

$$\mu_d := \bigotimes_{j=1}^{d} dy_j^{d-1}\,\lambda(\mathrm{d}y_j)\,,$$

λ the Lebesgue measure on $\mathbb{R}$.

After choosing $y \in C_k(x)$, round each y_j up (down) to the next number in $\Gamma_j(X)$ to get $y^+ \in \Gamma(X)$ ($y^- \in \Gamma(X)$).

We want to maximize

$$\hat{\delta}(y) := \max\{\delta(y^+), \overline{\delta}(y^-)\}$$

Modified Measure is Superior in High Dimension

GLP-sets: $0 < h_1 < h_2 < \cdots < h_d < n, \quad \exists j : \gcd(h_j, n) = 1$

$$T := \{t^1, \ldots, t^n\}, \; t^i_j := \left\{\frac{2ih_j - 1}{2n}\right\}, \; i = 1, \ldots, n, \; j = 1, \ldots, d$$

Mean values of coordinates of optimal test boxes for randomly chosen GLP-sets:

$$d = 4 : \quad 0.799743$$
$$d = 5 : \quad 0.840825$$
$$d = 6 : \quad 0.873523$$

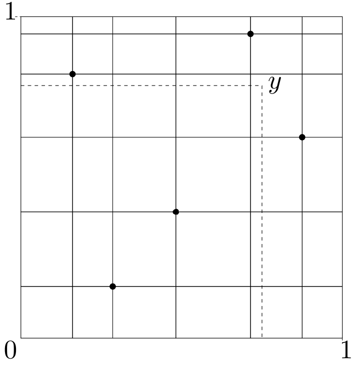
Expectation of coordinates of randomly chosen y with respect to μ_d is $d/(d+1)$:

$$d = 4 : \quad 0.8$$
$$d = 5 : \quad 0.8\overline{3}$$
$$d = 6 : \quad 0.857143$$

Further Improvement on the W&F-Algorithm

Procedures "snapping up" and "snapping down":

Rounding y^+ and y^- up and down to critical test boxes $y^{+,\mathrm{sn}}$ and $y^{-,\mathrm{sn}}$.



Some Numerical Results

			$\mathrm{disc}^*(\cdot)$	TA improved		Winker & Fang	
Name	d	n	found	Hits	Best-of-10	Hits	Best-of-10
Faure	7	343	0.1298	100	0.1298	0	0.1143
Faure	8	121	0.1702	100	0.1702	0	0.1573
Faure	9	121	0.2121	100	0.2121	0	0.1959
Faure	10	121	0.2574	100	0.2574	0	0.2356
Faure	11	121	0.3010	100	0.3010	0	0.2632
Faure	12	169	0.2718	100	0.2718	0	0.1708
Sobol'	50	2000	0.1030^*	0	0.1024	0	0.0005
Sobol'	50	4000	0.0677^*	0	0.0665	0	0.00025
Faure	50	2000	0.3112^*	100	0.3112	0	0.0123
Faure	50	4000	0.1979^*	0	0.1978	0	0.0059
GLP	50	2000	0.1465^*	0	0.1450	0	0.0005
GLP	50	4000	0.1205^*	0	0.1201	0	0.0003

Table: New instance comparisons. Discrepancy values marked with a star are lower bounds only (i.e., largest discrepancy found over all executions of algorithm variants). All data is computed using 100 trials of $100,000$ iterations; reported is the average value of best-of-10 calls, and number of times (out of 100) that the optimum (or a value matching the largest known value) was found.

Further Numerical Results

				TA improved		Shah	
Class	d	n	$\mathrm{disc}^*(\cdot)$	Hits	Best-of-10	Hits	Best Found
Halton	5	50	0.1886	100	0.1886	81	0.1886
Halton	7	50	0.2678	100	0.2678	22	0.2678
Halton	7	100	0.1714	100	0.1714	13	0.1714
Halton	7	1000	0.0430	81	0.0430	$8^{(1)}$	$0.0430^{(1)}$
Faure	10	50	0.4680	100	0.4680	97	0.4680
Faure	10	100	0.2483	100	0.2483	28	0.2483
Faure	10	500	0.0717*	100	0.0717	$0^{(1)}$	$0.0689^{(1)}$

Table: Comparison against point sets used by Shah. Reporting average value of best-of-10 calls, and number of times (out of 100) that the optimum was found; for Shah, reporting highest value found, and number of times (out of 100) this value was produced. The discrepancy value marked with a star is lower bound only (i.e., largest value found by any algorithm). Values marked (1) are recomputed using the same settings as in [Sha'10].