# Benchmarking the Hooke-Jeeves Method, MTS-LS1, and BSrr on the Large-scale BBOB Function Set

The BBOB-2022 workshop at Boston

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# Separability in black-box numerical optimization

## A $D$-dim. separable function $f$ can be $D$ 1-dim. functions

$$\arg\min_{\boldsymbol{x}} f(\boldsymbol{x}) = \left(\arg\min_{x_1} f(x_1, ..., ), ..., \arg\min_{x_D} f(\ldots, x_D)\right)$$

- Separable functions are easier to solve than nonseparable ones
  - If an optimizer can exploit the separability
  - E.g., Coordinate-wise optimizers

## IMHO, a separable real-world problem is very rare

- Some decision variables are likely to depend on each other
- The motivation to study optimizers for separable functions is weak
- Just in case, it is better for an algorithm portfolio to contain an optimizer that can exploit the separability
  - An efficient algorithm selection system is available [Tanabe 22] ☺

Ryoji Tanabe: Benchmarking Feature-based Algorithm Selection Systems for Black-box Numerical Optimization. IEEE Trans. Evol. Comput. in press (2022)

## Benchmarking three optimizers for separable functions on `bbob-largescale`

1. **The Hooke-Jeeves method (HJ) [Hooke 61]**
   - One of the most classical black-box optimizers
2. **Multiple trajectory search local search 1 (MTS-LS1) [Tseng 08]**
   - Designed for the CEC LSGO competition 2008
   - Some winners of the CEC (LSGO) competitions used MTS-LS1
   - Very similar to the Hooke-Jeeves method, but it has been overlooked
3. **Brent-STEP in a round-robin manner (BSrr) [Baudis 15]**
   - State-of-the-art for the five separable `bbob` functions $(f_1, \ldots, f_5)$
   - BSrr is a member of a portfolio in recent algorithm selection systems

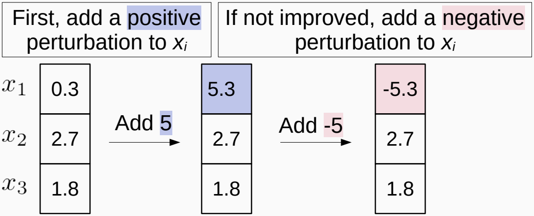
Robert Hooke, T. A. Jeeves: "Direct Search" Solution of Numerical and Statistical Problems. J. ACM 8(2): 212-229 (1961)

Lin-Yu Tseng, Chun Chen: Multiple trajectory search for Large Scale Global Optimization. IEEE Congress on Evolutionary Computation 2008: 3052-3059

Petr Baudis, Petr Posík: Global Line Search Algorithm Hybridized with Quadratic Interpolation and Its Extension to Separable Functions. GECCO 2015: 257-264

## The Hooke-Jeeves method: a pattern move (variable-wise operation)

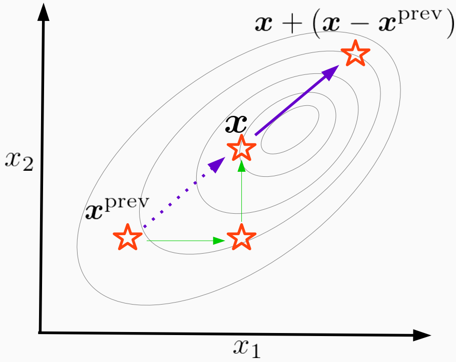
- HJ iteratively improves a search point $\boldsymbol{x} \in \mathbb{R}^D$ by two moves:
  1. a pattern move (variable-wise operation)
  2. an exploratory move (vector-wise operation)
- In the pattern move, HJ generates a new point $\boldsymbol{x}^{\mathrm{new}}$ by perturbing only one variable $x_i \in \boldsymbol{x}$ (from $i = 1$ to $D$)
  - $x_i^{\mathrm{new}} \leftarrow x_i + \sigma(x_i^{\mathrm{up}} - x_i^{\mathrm{low}})$ or $x_i^{\mathrm{new}} \leftarrow x_i - \sigma(x_i^{\mathrm{up}} - x_i^{\mathrm{low}})$
  - $\sigma$: step-size (the initial $\sigma^{\mathrm{init}} = 0.4$)
  - $x_i^{\mathrm{up}}$ and $x_i^{\mathrm{low}}$: the upper and lower bounds for the $i$-th variable




- When all trials for all variables were unsuccessful, $\sigma \leftarrow c \times \sigma$
  - $c$: learning rate (typically, $c = 0.5$?)

## The Hooke-Jeeves method: an exploratory move (vector-wise operation)

- If the pattern move was successful for at least one variable, HJ performs a bonus operation
- HJ generates a new point $\boldsymbol{x}^{\text{new}}$ by taking the difference from the previous one $\boldsymbol{x}^{\text{prev}}$ to the current one $\boldsymbol{x}$
  - $\boldsymbol{x}^{\text{new}} \leftarrow \boldsymbol{x} + (\boldsymbol{x} - \boldsymbol{x}^{\text{prev}})$



## The overall procedure of the Hooke-Jeeves method

Initialize $\boldsymbol{x}$, $\sigma \leftarrow \sigma^{\mathrm{init}}$;
**while** *not happy* **do**
  $\boldsymbol{x}^{\mathrm{prev}} \leftarrow \boldsymbol{x}$;
  `/* The pattern move (variable-wise operation) */`
  **for** $i \in \{1, \ldots, D\}$ **do**
    $\boldsymbol{x}^{\mathrm{new}} \leftarrow \boldsymbol{x}$;
    $x_i^{\mathrm{new}} \leftarrow x_i + \sigma(x_i^{\mathrm{up}} - x_i^{\mathrm{low}})$;
    **if** $f(\boldsymbol{x}^{\mathrm{new}}) < f(\boldsymbol{x})$ **then** $\boldsymbol{x} \leftarrow \boldsymbol{x}^{\mathrm{new}}$ ;
    **else**
      $\boldsymbol{x}^{\mathrm{new}} \leftarrow \boldsymbol{x}$;
      $x_i^{\mathrm{new}} \leftarrow x_i - \sigma(x_i^{\mathrm{up}} - x_i^{\mathrm{low}})$;
      **if** $f(\boldsymbol{x}^{\mathrm{new}}) < f(\boldsymbol{x})$ **then** $\boldsymbol{x} \leftarrow \boldsymbol{x}^{\mathrm{new}}$ ;
  `/* The exploratory move (vector-wise operation) */`
  **if** $f(\boldsymbol{x}) < f(\boldsymbol{x}^{\mathrm{prev}})$ **then**
    $\boldsymbol{x}^{\mathrm{new}} \leftarrow \boldsymbol{x} + (\boldsymbol{x} - \boldsymbol{x}^{\mathrm{prev}})$;
    **if** $f(\boldsymbol{x}^{\mathrm{new}}) < f(\boldsymbol{x})$ **then** $\boldsymbol{x} \leftarrow \boldsymbol{x}^{\mathrm{new}}$ ;
  **else** $\sigma \leftarrow c \times \sigma$ ;

## Two main differences between MTS-LS1 and the Hooke-Jeeves method

1. MTS-LS1 does not adopt the exploratory move (vector-wise operat.)
2. MTS-LS1 reinitializes the step-size $\sigma$ when $\sigma$ is too small

# The Hooke-Jeeves method vs. MTS-LS1

## The Hooke-Jeeves method

Initialize $\boldsymbol{x}$, $\sigma \leftarrow \sigma^{\text{init}}$;
**while** *not happy* **do**
    $\boldsymbol{x}^{\text{prev}} \leftarrow \boldsymbol{x}$;
    **for** $i \in \{1, \ldots, D\}$ **do**
        $\boldsymbol{x}^{\text{new}} \leftarrow \boldsymbol{x}$;
        $x_i^{\text{new}} \leftarrow x_i + \sigma(x_i^{\text{up}} - x_i^{\text{low}})$;
        **if** $f(\boldsymbol{x}^{\text{new}}) < f(\boldsymbol{x})$ **then**
          $\boldsymbol{x} \leftarrow \boldsymbol{x}^{\text{new}}$ ;
        **else**
            $\boldsymbol{x}^{\text{new}} \leftarrow \boldsymbol{x}$;
            $x_i^{\text{new}} \leftarrow x_i$
            $- \sigma(x_i^{\text{up}} - x_i^{\text{low}})$;
            **if** $f(\boldsymbol{x}^{\text{new}}) < f(\boldsymbol{x})$ **then**
                $\boldsymbol{x} \leftarrow \boldsymbol{x}^{\text{new}}$
    **if** $f(\boldsymbol{x}) < f(\boldsymbol{x}^{\text{prev}})$ **then**
        $\boldsymbol{x}^{\text{new}} \leftarrow \boldsymbol{x} + (\boldsymbol{x} - \boldsymbol{x}^{\text{prev}})$;
        **if** $f(\boldsymbol{x}^{\text{new}}) < f(\boldsymbol{x})$ **then**
          $\boldsymbol{x} \leftarrow \boldsymbol{x}^{\text{new}}$ ;
    **else** $\sigma \leftarrow c \times \sigma$ ;

## MTS-LS1

Initialize $\boldsymbol{x}$, $\sigma \leftarrow \sigma^{\text{init}}$;
**while** *not happy* **do**
    $\boldsymbol{x}^{\text{prev}} \leftarrow \boldsymbol{x}$;
    **for** $i \in \{1, \ldots, D\}$ **do**
        $\boldsymbol{x}^{\text{new}} \leftarrow \boldsymbol{x}$;
        $x_i^{\text{new}} \leftarrow x_i - \sigma(x_i^{\text{up}} - x_i^{\text{low}})$;
        **if** $f(\boldsymbol{x}^{\text{new}}) < f(\boldsymbol{x})$ **then**
          $\boldsymbol{x} \leftarrow \boldsymbol{x}^{\text{new}}$ ;
        **else**
            $\boldsymbol{x}^{\text{new}} \leftarrow \boldsymbol{x}$;
            $x_i^{\text{new}} \leftarrow x_i$
            $+0.5\sigma \, (x_i^{\text{up}} - x_i^{\text{low}})$;
            **if** $f(\boldsymbol{x}^{\text{new}}) < f(\boldsymbol{x})$ **then**
                $\boldsymbol{x} \leftarrow \boldsymbol{x}^{\text{new}}$
    **if** $f(\boldsymbol{x}) = f(\boldsymbol{x}^{\text{prev}})$ **then**
        $\sigma \leftarrow c \times \sigma$;
        **if** $\sigma(x_1^{\text{up}} - x_1^{\text{low}}) < 10^{-15}$ **then**
            $\sigma \leftarrow \sigma^{\text{init}}$

## The Brent-STEP method for $1$-dimensional optimization

**The Brent method (e.g., `fminbnd` in Matlab)**

- It simultaneously performs the bisection and the secant methods
- Pros : It performs very well on unimodal functions
- Cons : It performs poorly on multimodal functions

**Select The Easiest Point (STEP) [Langerman 94]**

- It sequentially selects an interval with the smallest `difficulty`
- Pros : It performs well on multimodal functions
- Cons : It generally converges slow

**The Brent-STEP method aims to take their pros**

- First, it runs the Brent method
- If the search fails (i.e., on multimodal functions), it then runs STEP

Richard Peirce Brent. Algorithms for Minimization without Derivatives. Englewood Cliffs, 1973

Stefan Langerman, Gregory Seront, Hugues Bersini: S.T.E.P.: The Easiest Way to Optimize a Function. International Conference on Evolutionary Computation 1994: 519-524

## BSrr: An extension of the Brent-STEP method to $D$-dimensional opt.

- BSrr applies Brent-STEP to each variable in a round-robin manner
  - It is competitive with more sophisticated ones [Posík 15]

Initialize $\boldsymbol{x}$;
**while** *not happy* **do**
    **for** $i \in \{1, \ldots, D\}$ **do**
        $\boldsymbol{x}^{\mathrm{new}} \leftarrow \boldsymbol{x}$;
        $x_i^{\mathrm{new}} \leftarrow$ Apply a single iteration of `brent_step` to $x_i$;
        **if** $f(\boldsymbol{x}^{\mathrm{new}}) < f(\boldsymbol{x})$ **then**
            $\boldsymbol{x} \leftarrow \boldsymbol{x}^{\mathrm{new}}$;
            Update internal parameters of $D$ `brent_step`;

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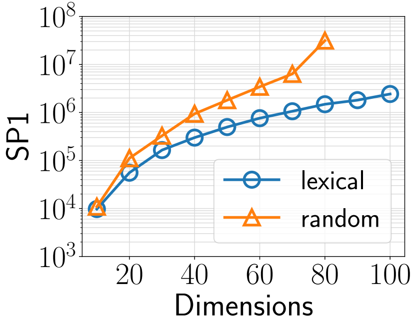
Petr Posík, Petr Baudis: Dimension Selection in Axis-Parallel Brent-STEP Method for Black-Box Optimization of Separable Continuous Functions. GECCO (Companion) 2015: 1151-1158

# The three optimizers are sensitive to the order of variables

**Results of MTS-LS1 on Schwefel 1.2**




- $f(\boldsymbol{x}) = \sum_{i=1}^{D}(\sum_{j=1}^{i} x_j)^2$
- Similar to LeadingOnes, the first $i$ variables are dependent
- lexical: $x_1, x_2, x_3, x_4, \ldots$
- random: $x_9, x_1, x_8, x_3, \ldots$
- Max. fevals = $10^5 \times D$
- N. runs = 31

- MTS-LS1 perturbs variables in a lexical order (from $x_1$ to $x_D$)
  - It can unintentionally exploit the order of variables
- Their operators are not permutation-invariant [Lehre 12]
- This issue can be very very easily addressed
  - by randomly shuffling the order of perturbations

Per Kristian Lehre, Carsten Witt: Black-Box Search by Unbiased Variation. Algorithmica 64(4): 623-642 (2012)

# Experimental setup

- The 24 `bbob-largescale` functions [Varelas 20]
  - Dimension $D \in \{20, 40, 80, 160, 320, 640\}$
  - The results of L-BFGS were taken from [Varelas 19] as a base line
- The Hooke-Jeeves method and MTS-LS1
  - We implemented them in C (`https://github.com/ryojitanabe/largebbob2022`)
  - The maximum number of function evaluations: $10^4 \times D$
  - The initial step size $\sigma^{\text{init}} = 0.4$ (is this best for HJ?)
  - The learning rate $c = 0.5$ and $0.9$
    - "HJ-5" and "MTS-LS1-5" are HJ and MTS-LS1 with $c = 0.5$
    - "HJ-9" and "MTS-LS1-9" are HJ and MTS-LS1 with $c = 0.9$
- BSrr
  - We used the Python implementation of BSrr (`https://github.com/pasky/step`)
    - Default setting
  - The maximum number of function evaluations: $10^3 \times D$

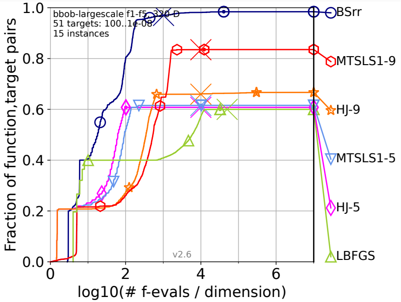
Konstantinos Varelas, Ouassim Ait ElHara, Dimo Brockhoff, Nikolaus Hansen, Duc Manh Nguyen, Tea Tušar, Anne Auger: Benchmarking large-scale continuous optimizers: The bbob-largescale testbed, a COCO software guide and beyond. Appl. Soft Comput. 97: 106737 (2020)

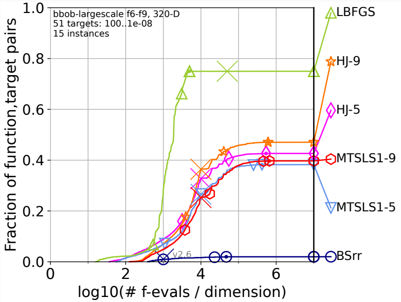
Konstantinos Varelas: Benchmarking large scale variants of CMA-ES and L-BFGS-B on the bbob-largescale testbed. GECCO (Companion) 2019: 1937-1945

## Aggregated results on the separable function group ($f_1, \ldots, f_5$) and the moderate conditioning function group ($f_6, \ldots, f_9$) for $D = 320$

**BSrr, HJ-9, and MTSLS1-9 outperform L-BFGS on $f_1, \ldots, f_5$**

- BSrr performs the best on $f_1, \ldots, f_5$ for all $D$
- HJ-5 and MTSLS1-5 (with the learning rate $c = 0.5$) do not work
  - $c = 0.5$ is recommended for CEC functions, but unsuitable for BBOB?
- They are outperformed by L-BFGS on $f_6, \ldots, f_9$

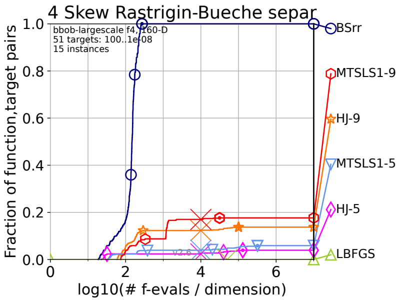


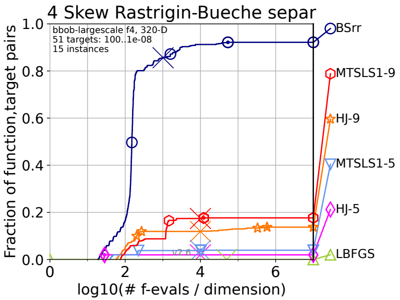



# Performance deterioration of BSrr on $f_2$ and $f_4$ for $D \geq 320$

**BSrr could not reach $x^*$ on $f_2$ and $f_4$ for $D \geq 320$**

- But, BSrr still performs better than the other optimizers
- The small max. fevals $(10^3 \times D)$ may be the reason

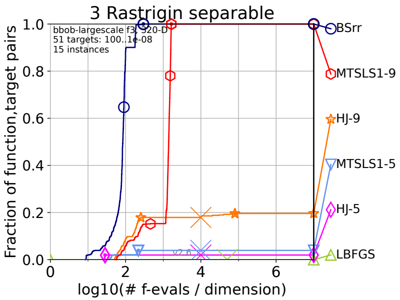


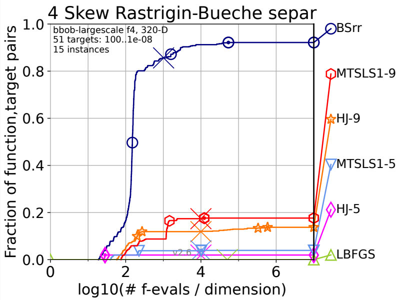



## Poor performance of MTS-LS1 on $f_4$

**MTS-LS1 works well for $f_3$, but does not work for $f_4$**

- MTS-LS1 uses (almost) the symmetric operation
- MTS- LS1 can perform poorly on a function with a asymmetric landscape structure, e.g., $f_4$



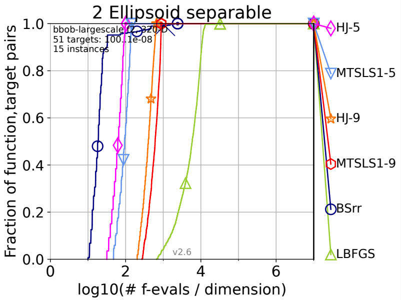
## Comparison of HJ and MTS-LS1 on $f_2$ and $f_3$ for $D = 320$

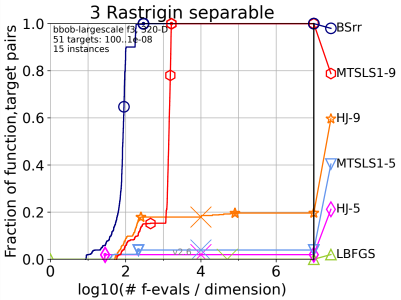
**HJ can outperform MTS-LS1 on unimodal functions, e.g., $f_2$**

- HJ adopts the the exploratory move (vector-wise operat.)

**MTS-LS1 can outperform HJ on multimodal functions, e.g., $f_3$**

- MTS-LS1 adopts the reinitialization strategy for the step-size $\sigma$
- HJ can be improved by a restart strategy or the reinitialization for $\sigma$



## Conclusion

**Benchmarking HJ, MTS-LS1, and BSrr on** `bbob-largescale`

- BSrr generally performs the best on $f_1, ..., f_5$
  - BSrr can complement L-BFGS and CMA-ES variants ☺
  - Its performance deterioration was observed on $f_2$ and $f_4$
- MTS-LS1 cannot handle the asymmetricity in $f_4$
  - Due to the symmetric operation
  - The same is true for HJ
- HJ performs better than MTS-LS1 on unimodal functions
  - But, HJ is outperformed by MTS-LS1 on multimodal functions
  - A restart strategy or the reinitialization for $\sigma$ is needed

**Future work**

- Benchmarking the winners of the CEC LSGO competitions
  - E.g., MOS, SHADE-ILS, and CC-RDG3
  - Especially, variable-decomposition-based approaches

## Computation time of the three optimizers ($10^{-5}$ seconds)

The C code is much faster than the Python code

| Optimizers | Languages | 20-D | 40-D | 80-D | 160-D | 320-D | 640-D |
|---|---|---|---|---|---|---|---|
| HJ | C | Na | 4.2 | 5.9 | 11 | 21 | 41 |
| MTS-LS1 | C | 4.1 | 2.0 | 5.8 | 11 | 21 | 42 |
| BSrr | Python | 13 | 20 | 33 | 62 | 120 | 270 |

- CPU time to run the three optimizers on the 24 `bbob-largescale` functions for $2D$ function evaluations
- Computation environment
  - Ubuntu 18.04
  - Intel(R) 52-Core Xeon Platinum 8270 (26-Core$\times 2$) 2.7GHz
  - Compile options `-O2`
- $f_{21}$ for $D = 640$ may be particularly time-consuming
  - $f_{21}$: the Gallagher's Gaussian 101-me Peaks function

## Unexpected results on $f_{19}$ for any $D$ pointed out by a reviewer (Thanks!)

**The initialization method significantly influences the results**

- The initial point in HJ-5, HJ-9, MTSLS1-5, and MTSLS1-9
  - The center of the search space $(0, ..., 0)$
- The initial point in L-BFGS and BSrr
  - randomly generated in the search space
- The solution at $(0, ..., 0)$ may have a good objective value
  - Known issue? (`https://github.com/numbbo/coco/issues/1851`)