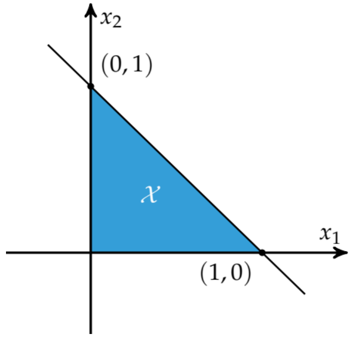
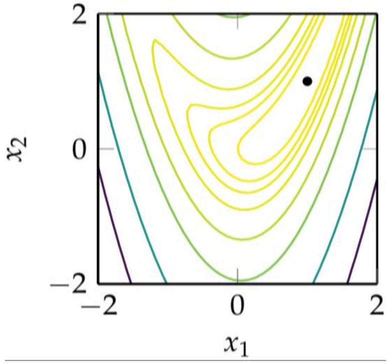
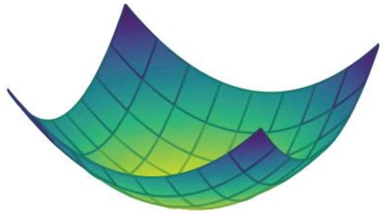
Tecnológico Nacional de México

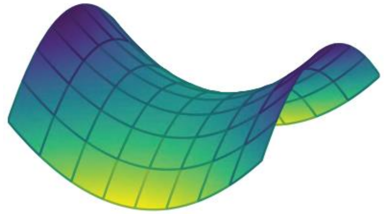
Instituto Tecnológico de Orizaba/Celaya

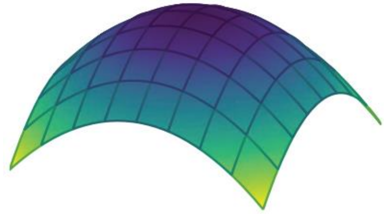
Modern Computing Algorithms for Process Optimization with Julia Programming











“7 – Direct Methods”

By:

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Postdoctoral Researcher/I.T. Celaya

Direct Methods

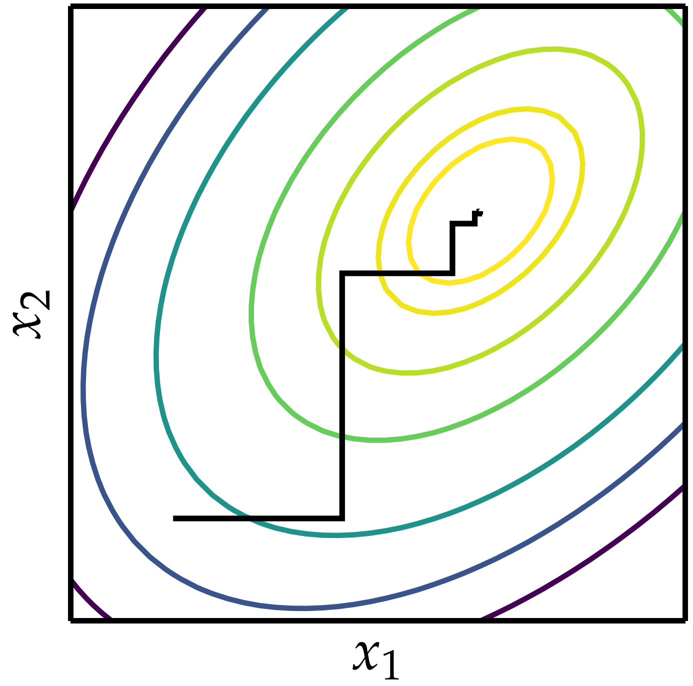
- Direct method search using function evaluations only
- Also called zero-order, black box, pattern search, or derivative-free methods

Cyclic Coordinate Search

- Also known as coordinate descent
- Performs line search in alternating coordinate directions

$$\mathbf{x}^{(2)} = \arg\min_{x_1} f(x_1, x_2^{(1)}, x_3^{(1)}, \ldots, x_n^{(1)})$$

$$\mathbf{x}^{(3)} = \arg\min_{x_2} f(x_1^{(2)}, x_2, x_3^{(2)}, \ldots, x_n^{(2)})$$



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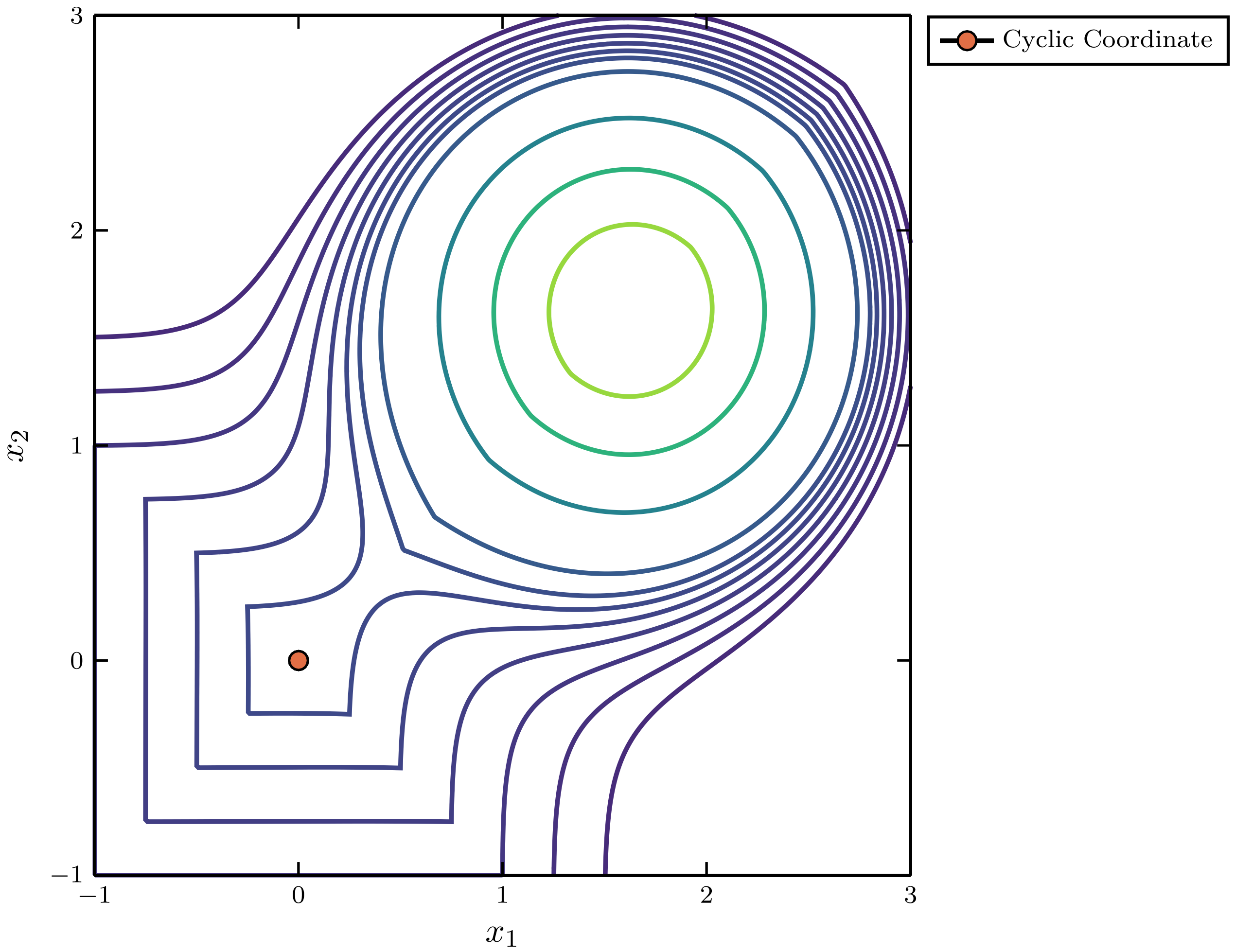
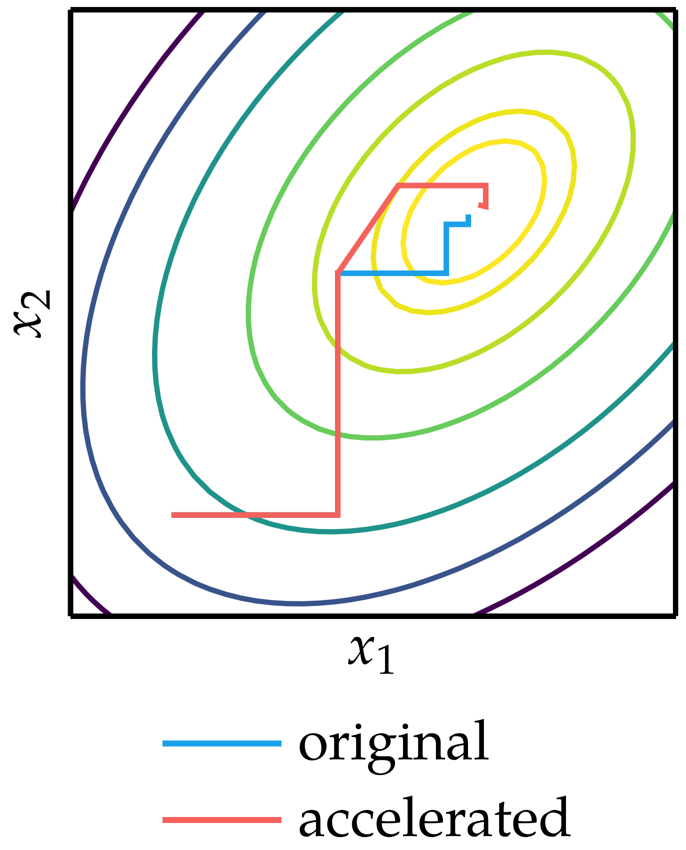
Cyclic Coordinate Search



Cyclic Coordinate Search

- Can be augmented to accelerate convergence



Powell's Method

- Similar to Cyclic Coordinate Search, but can search in non-orthogonal directions

The algorithm maintains a list of search directions $\mathbf{u}^{(1)}, \ldots, \mathbf{u}^{(n)}$, which are initially the coordinate basis vectors, $\mathbf{u}^{(i)} = \mathbf{e}^{(i)}$ for all i. Starting at $\mathbf{x}^{(1)}$, Powell's method conducts a line search for each search direction in succession, updating the design point each time:

$$\mathbf{x}^{(i+1)} \leftarrow \texttt{line\_search}(f, \mathbf{x}^{(i)}, \mathbf{u}^{(i)}) \text{ for all } i \text{ in } \{1, \ldots, n\}$$

Powell's Method

Next, all search directions are shifted down by one index, dropping the oldest search direction, $\mathbf{u}^{(1)}$:

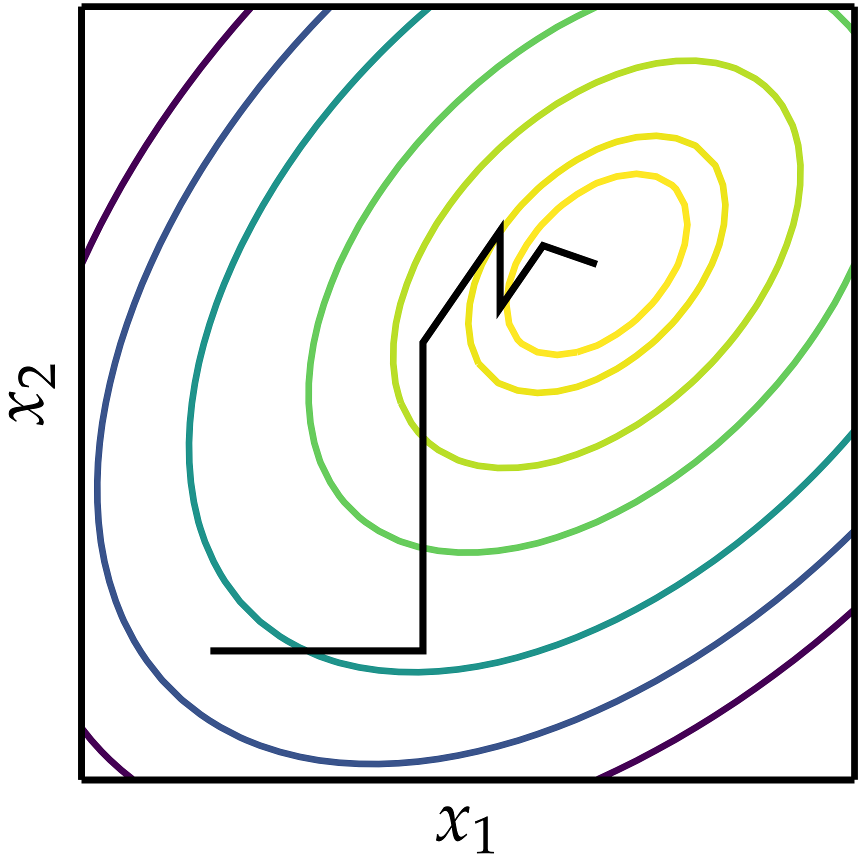
$$\mathbf{u}^{(i)} \leftarrow \mathbf{u}^{(i+1)} \text{ for all } i \text{ in } \{1, \ldots, n-1\}$$

The last search direction is replaced with the direction from $\mathbf{x}^{(1)}$ to $\mathbf{x}^{(n+1)}$, which is the overall direction of progress over the last cycle:

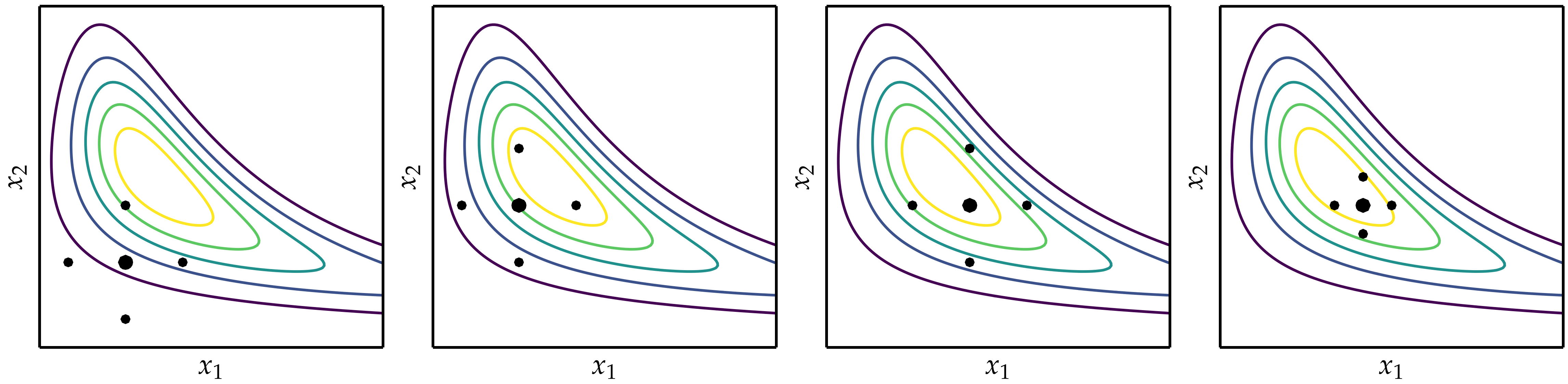
$$\mathbf{u}^{(n)} \leftarrow \mathbf{x}^{(n+1)} - \mathbf{x}^{(1)} \tag{7.6}$$

and another line search is conducted along the new direction to obtain a new $\mathbf{x}^{(1)}$.

Powell's Method

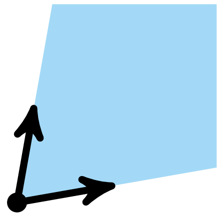


Hooke-Jeeves

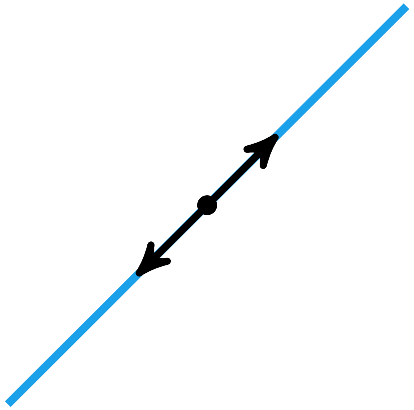


Generalized Pattern Search

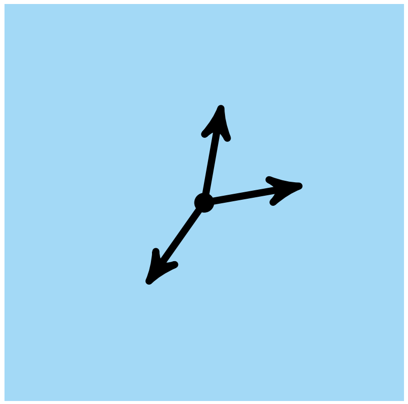
- Generalization of Hooke-Jeeves method
- Searches in set of directions that positively spans search space



only positively spans the cone



only positively spans 1d space



positively spans $\mathbb{R}^2$

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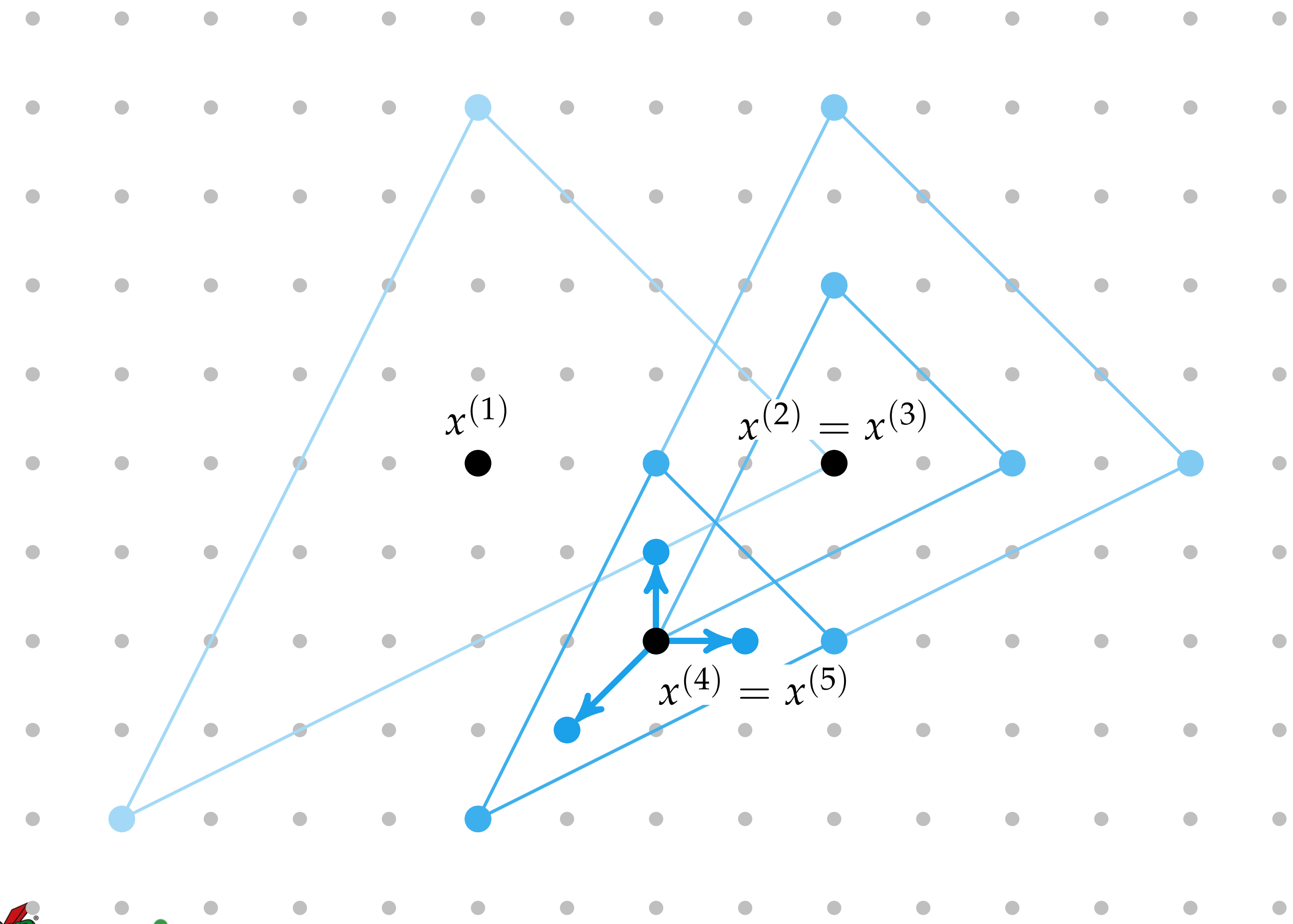
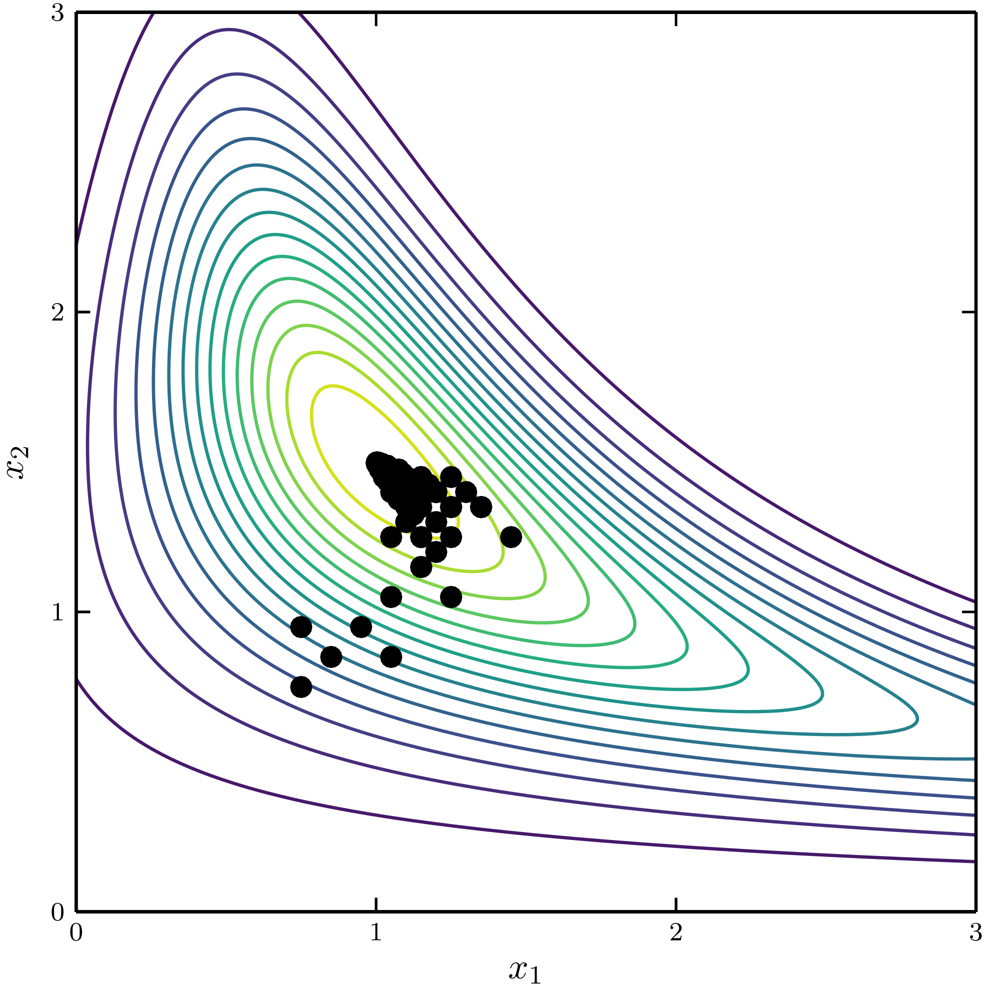
Generalized Pattern Search

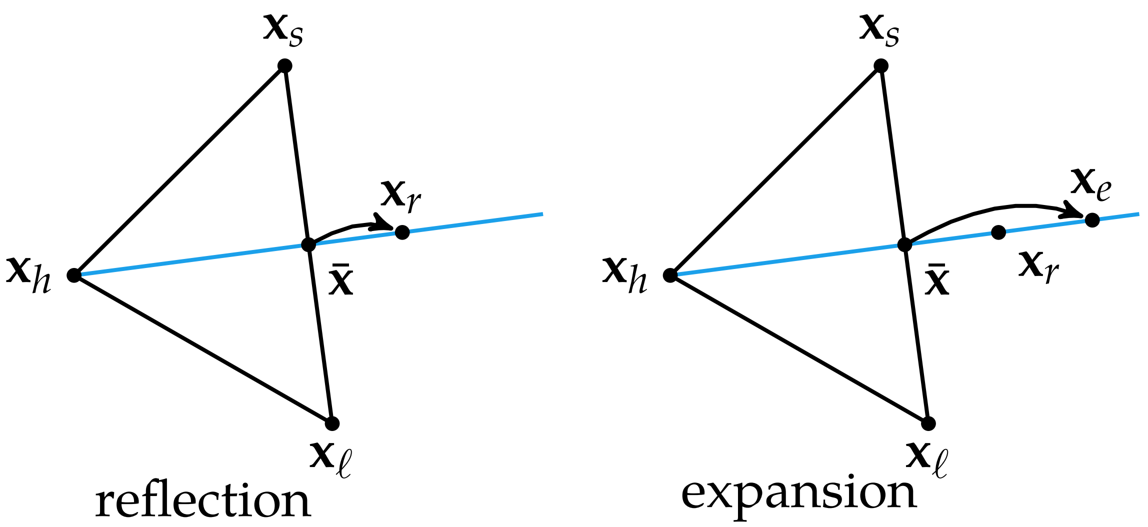


Generalized Pattern Search

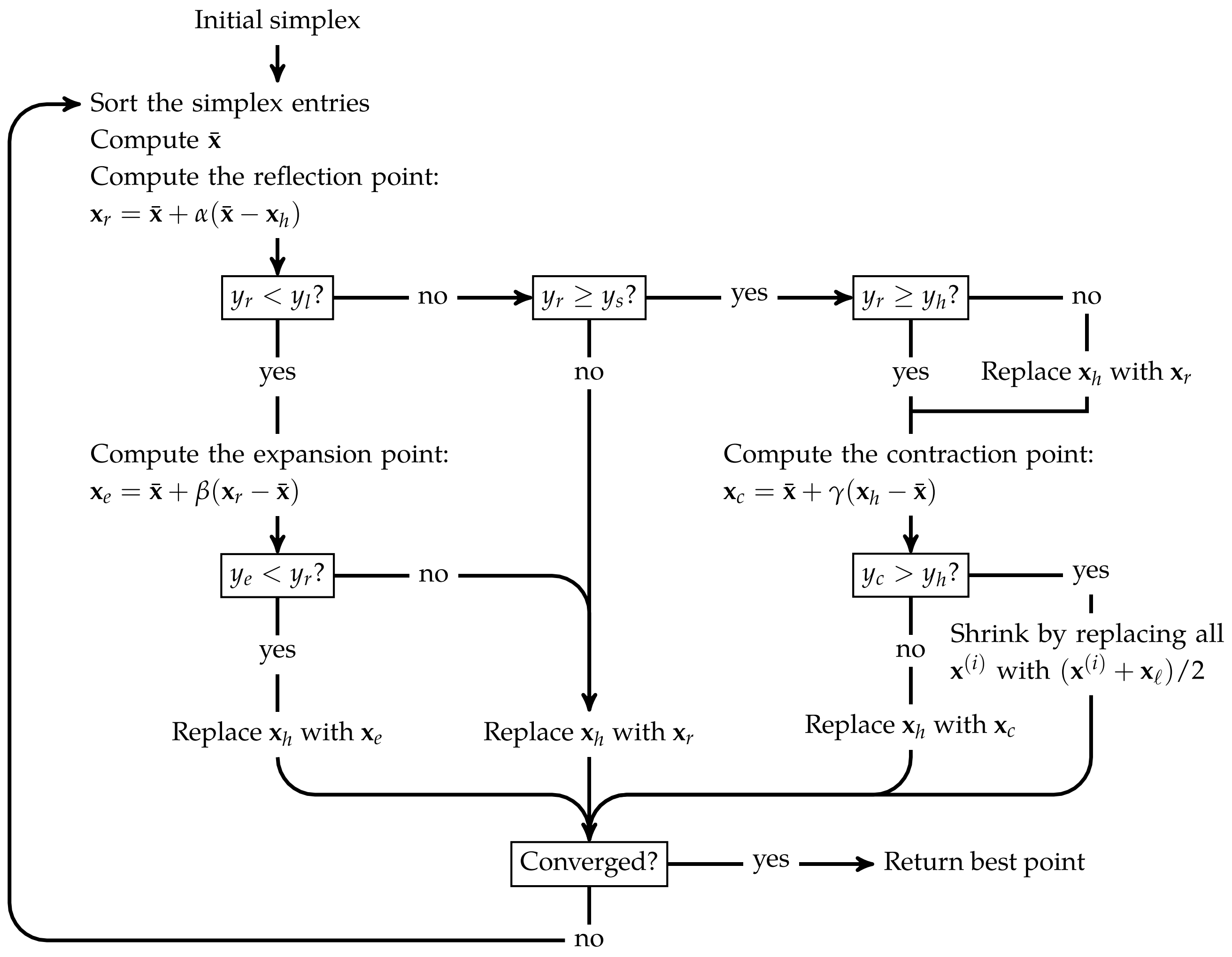


Nelder-Mead Simplex Method

- Uses simple algorithm to traverse search space using set of points defining a simplex



Nelder-Mead Simplex Method



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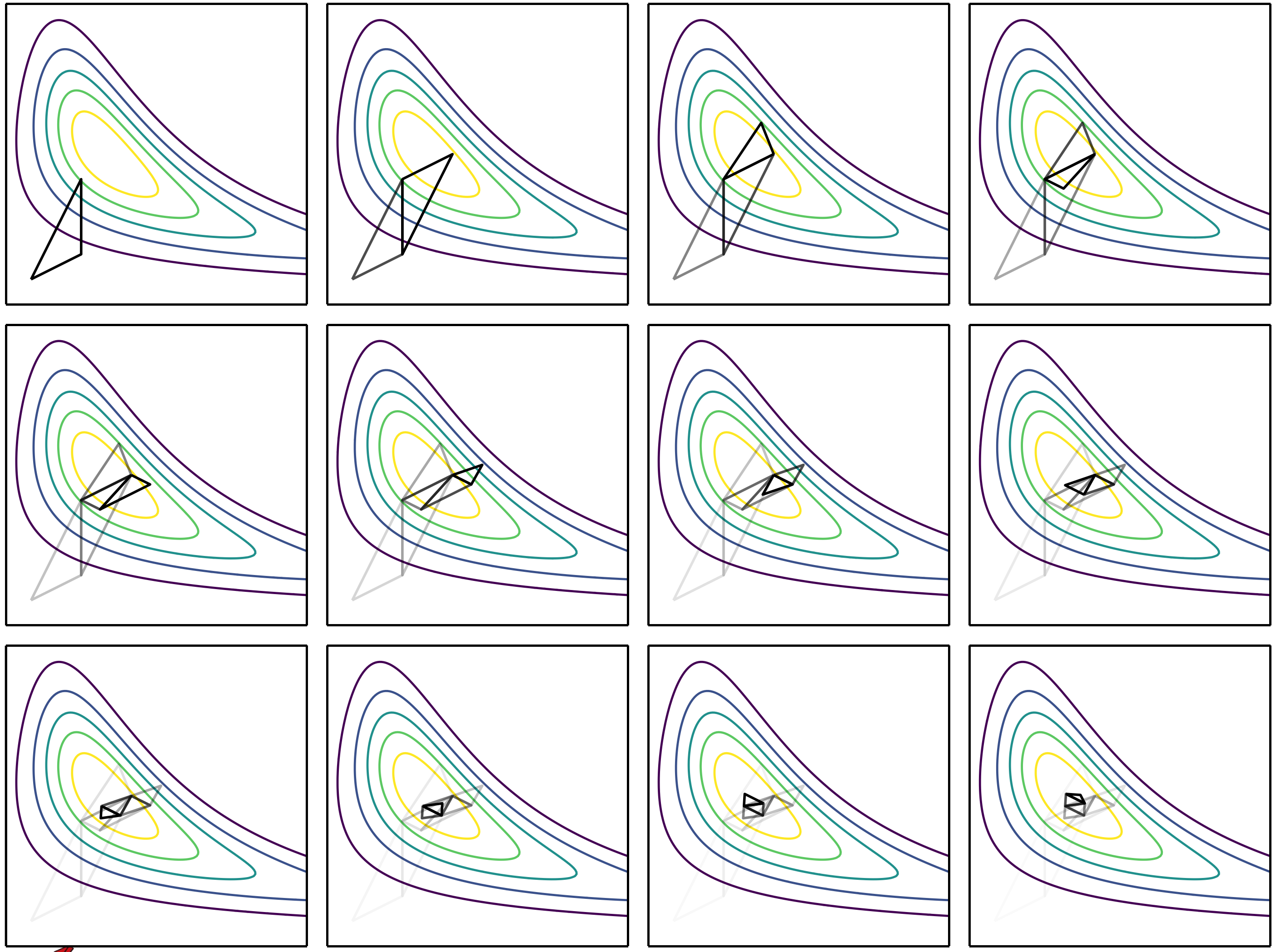
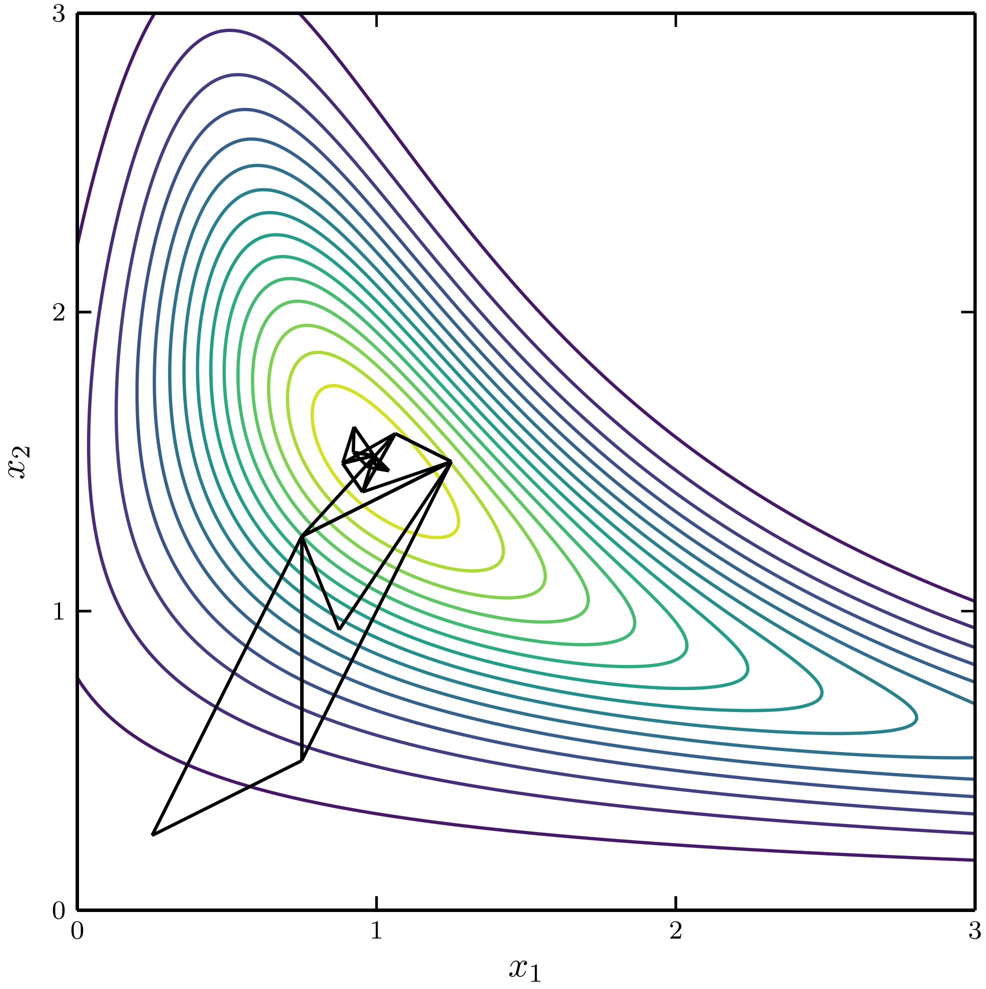
Nelder-Mead Simplex Method



Nelder-Mead Simplex Method

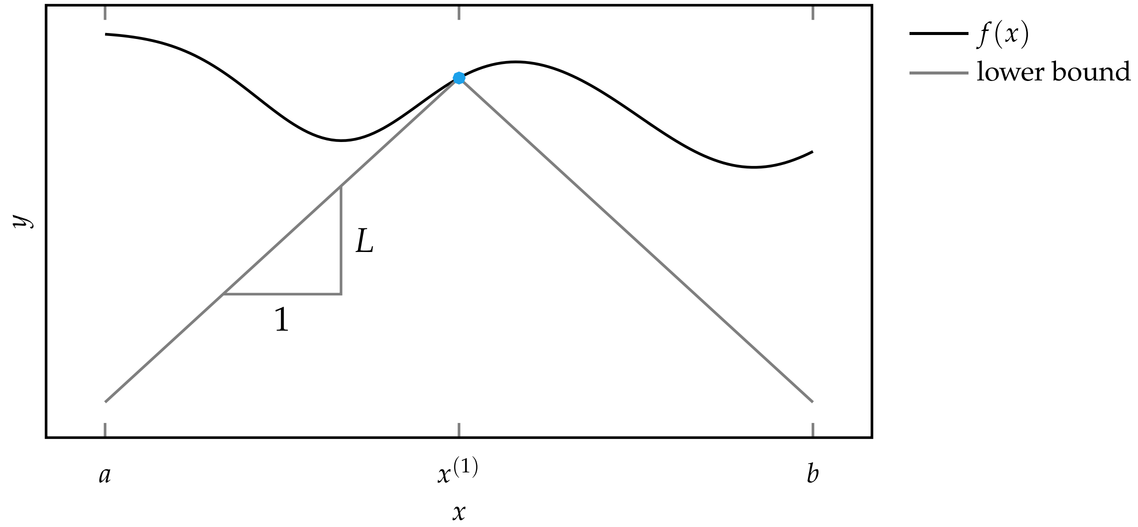


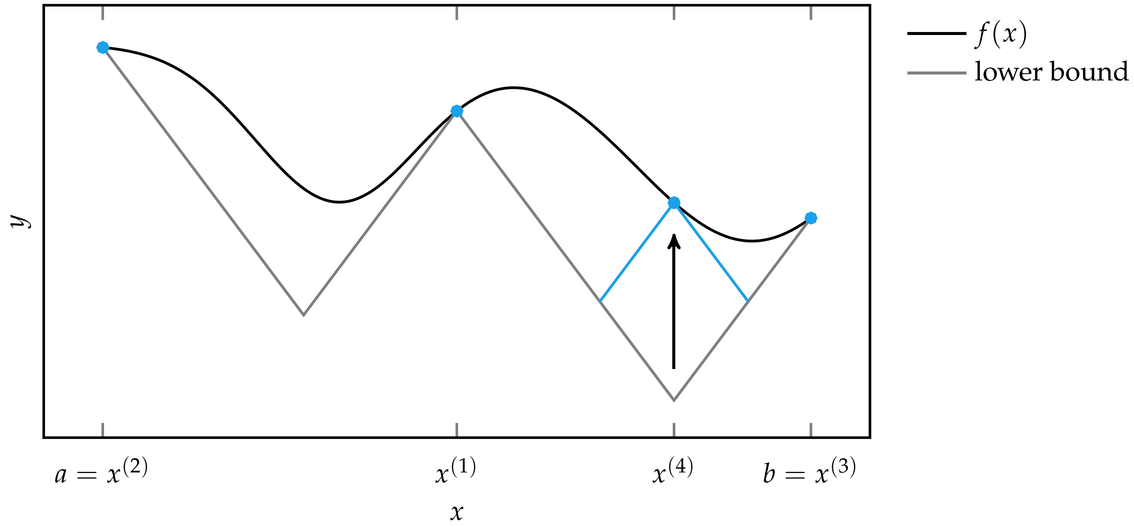
Divided Rectangles

- Also called DIRECT for Divided RECTangles
- Same approach as Shubert-Piyavskii method, but does not need to specify Lipschitz constant and is more efficiently expanded to multiple dimensions

Divided Rectangles

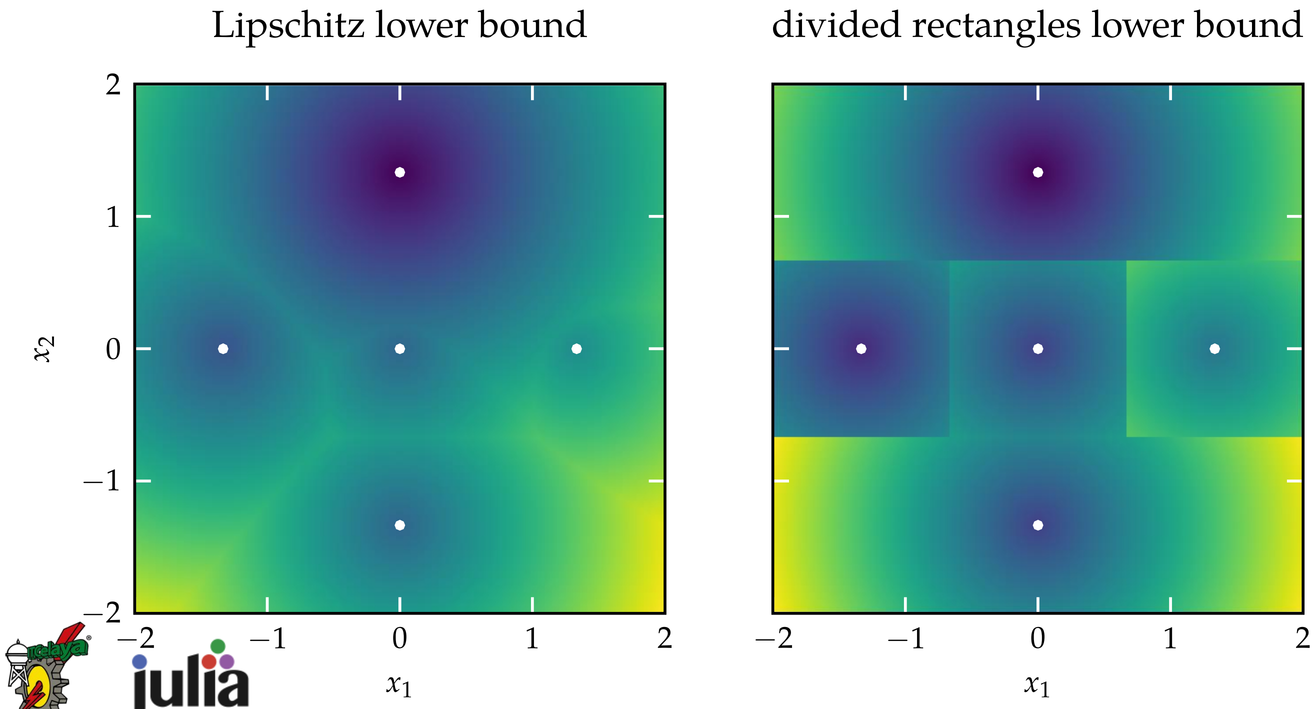
- Recall from Shubert-Piyavskii, a Lipshitz constant is used to provide a lower bound on the function, and a function evaluation is made where this bound is lowest





Divided Rectangles

- In multiple dimensions, the geometry of these cone intersections can become very complicated
- DIRECT simplifies geometry using subdivided rectangles



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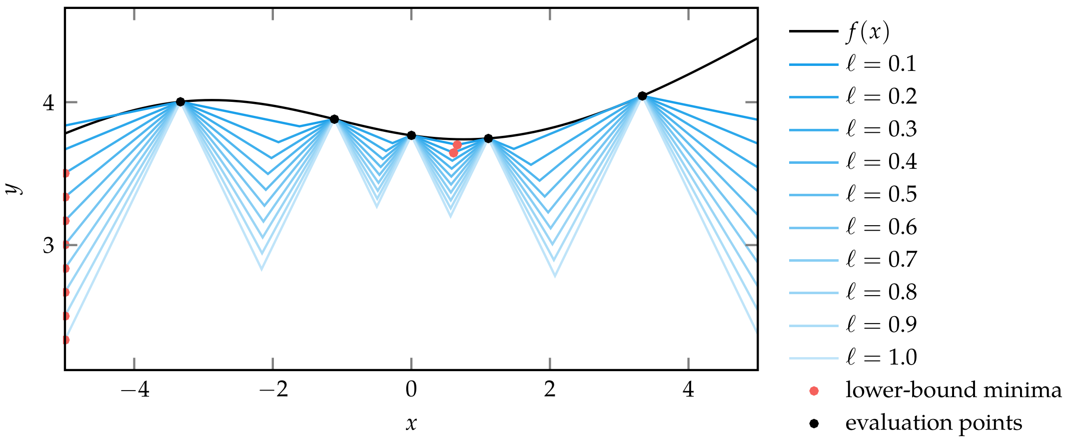
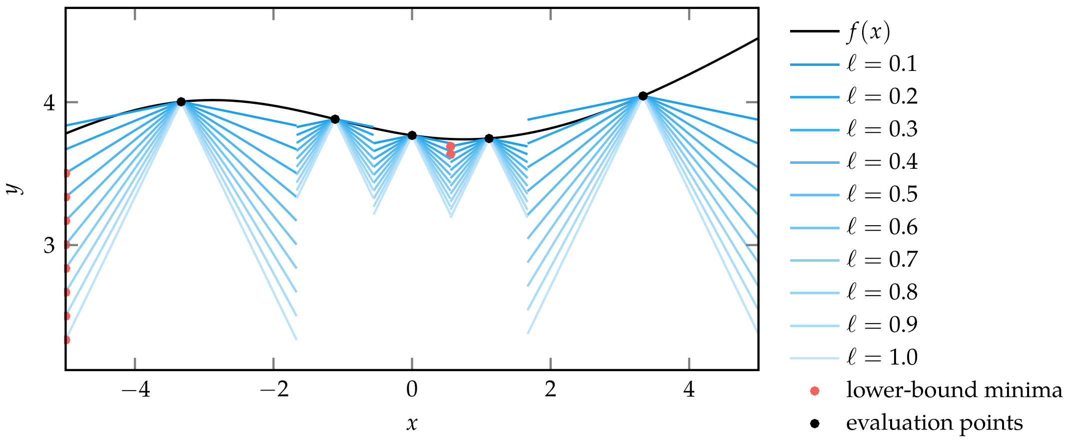
Divided Rectangles

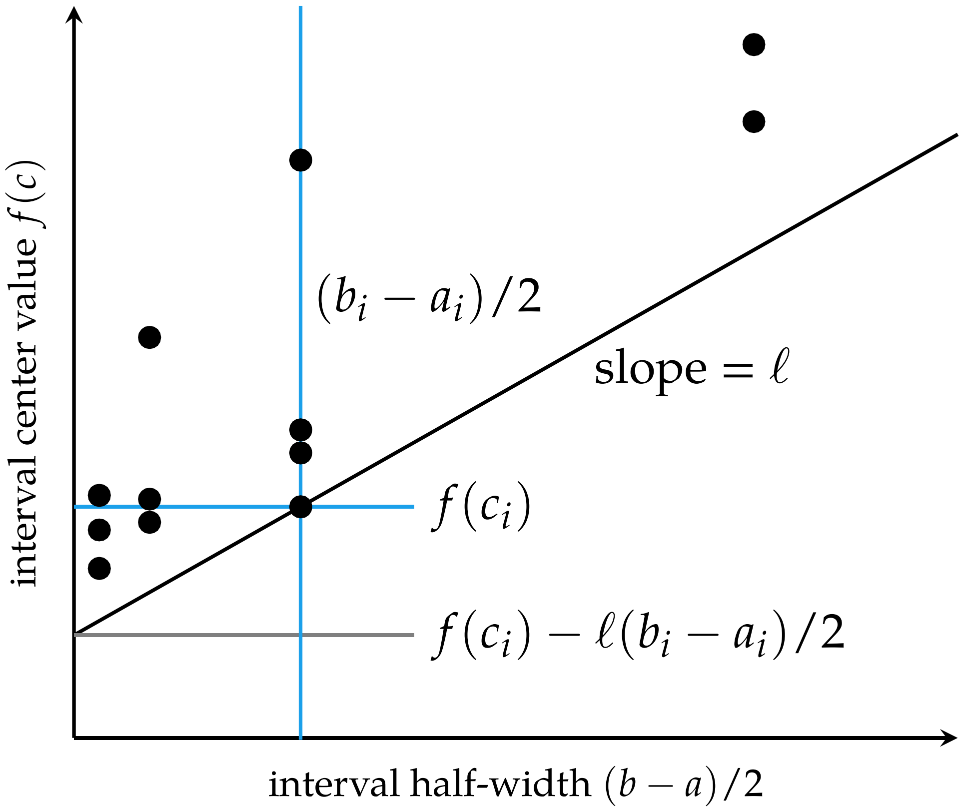
- DIRECT does not assume a Lipschitz constant is known

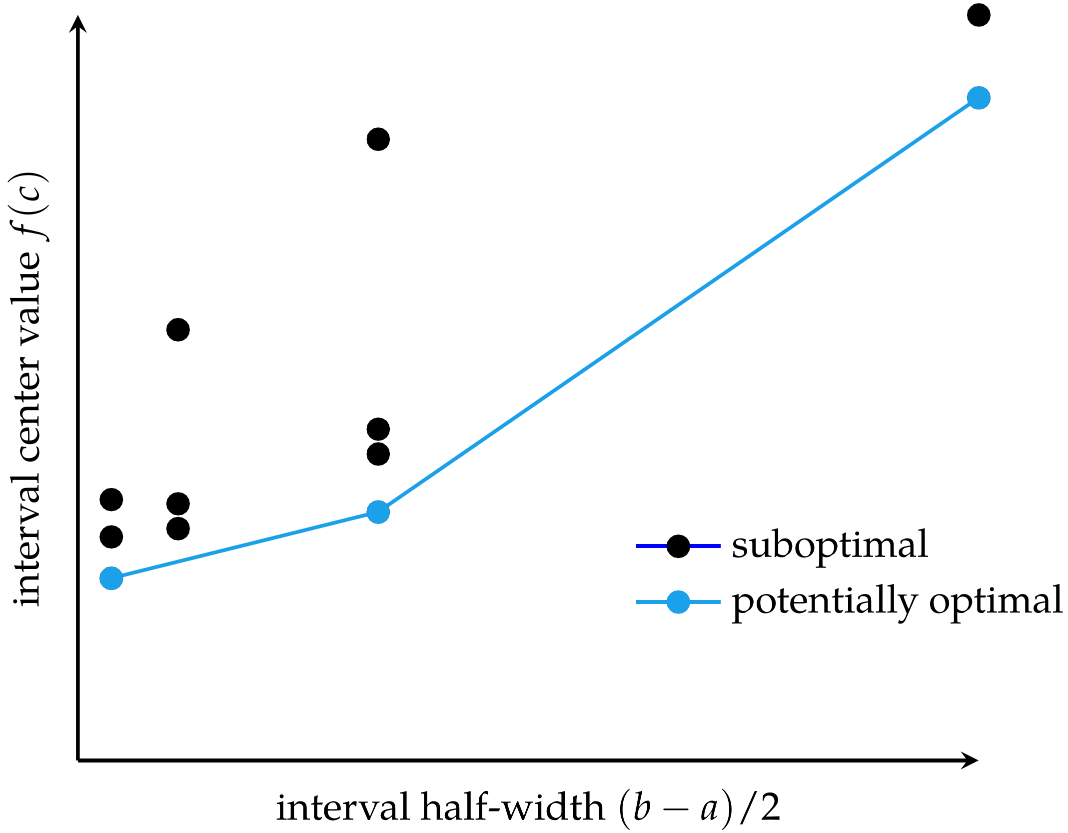




Divided Rectangles

- Univariate DIRECT





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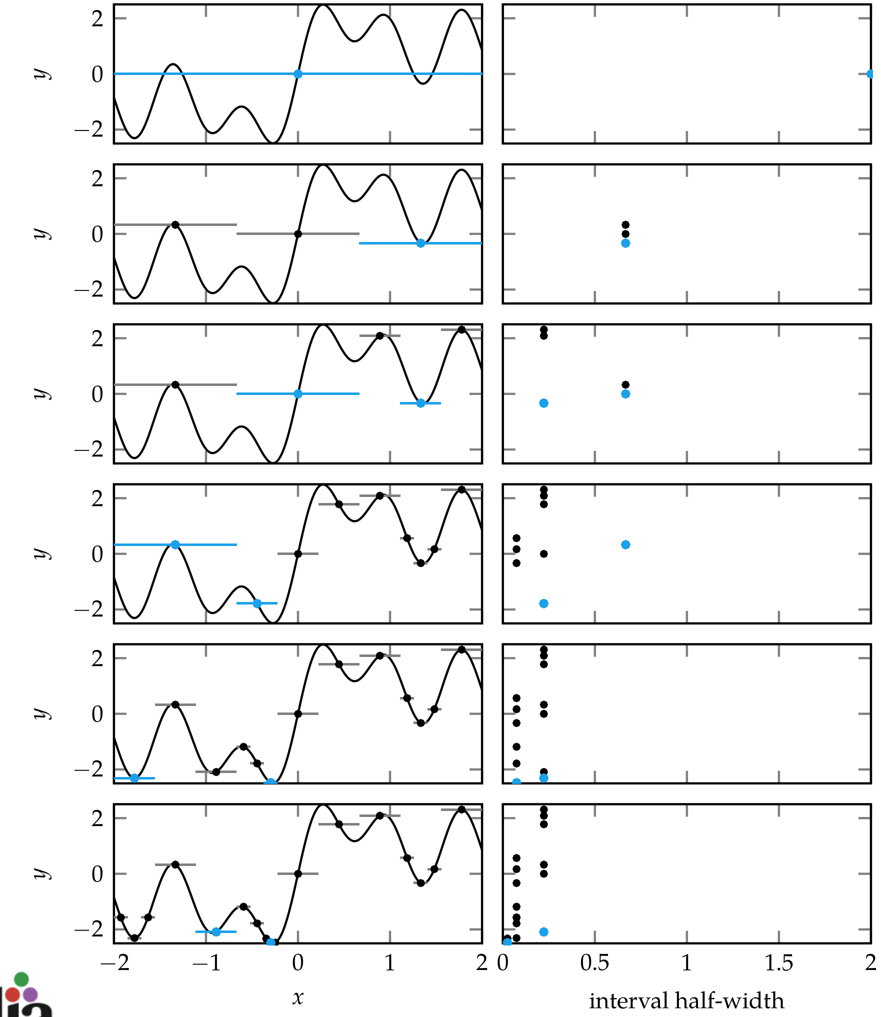
Divided Rectangles



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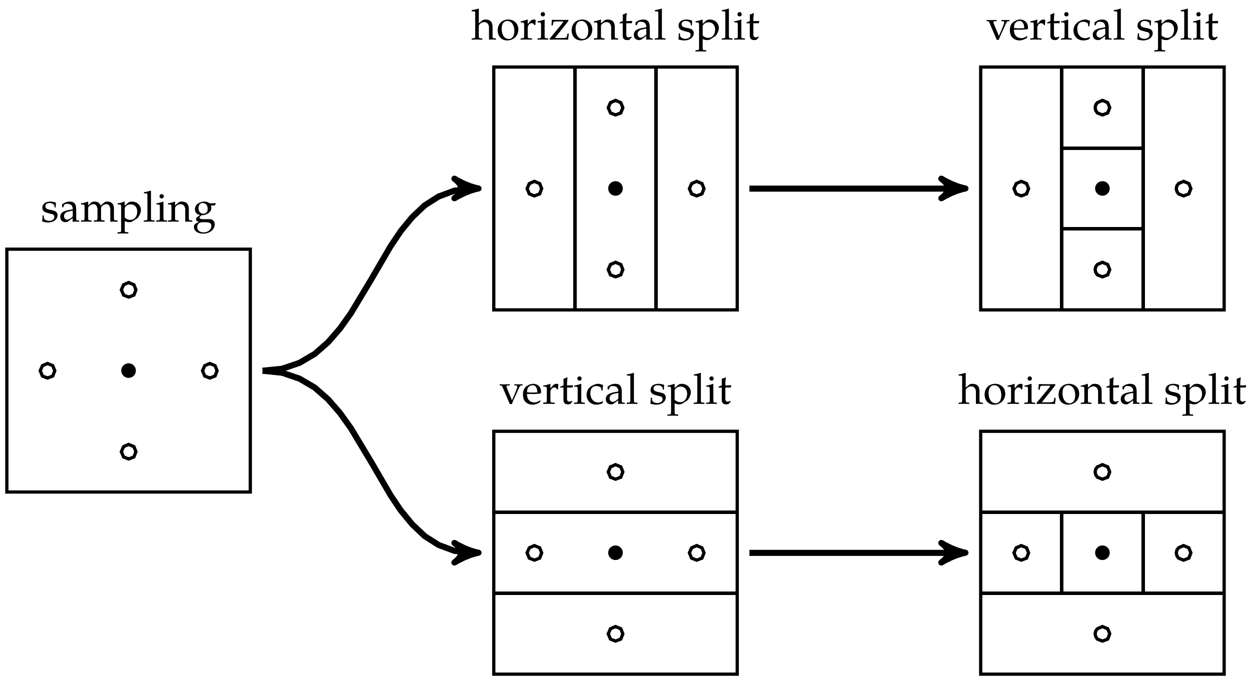
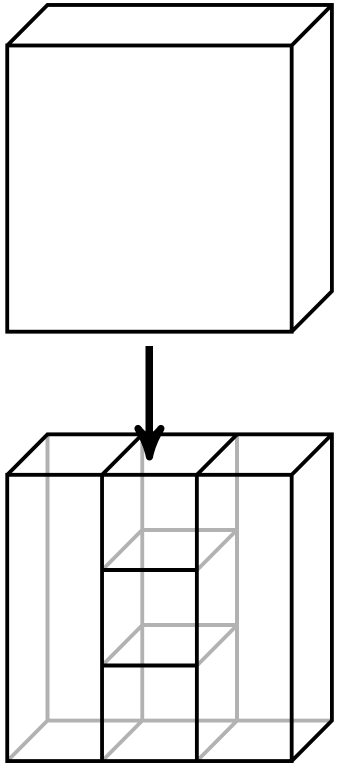
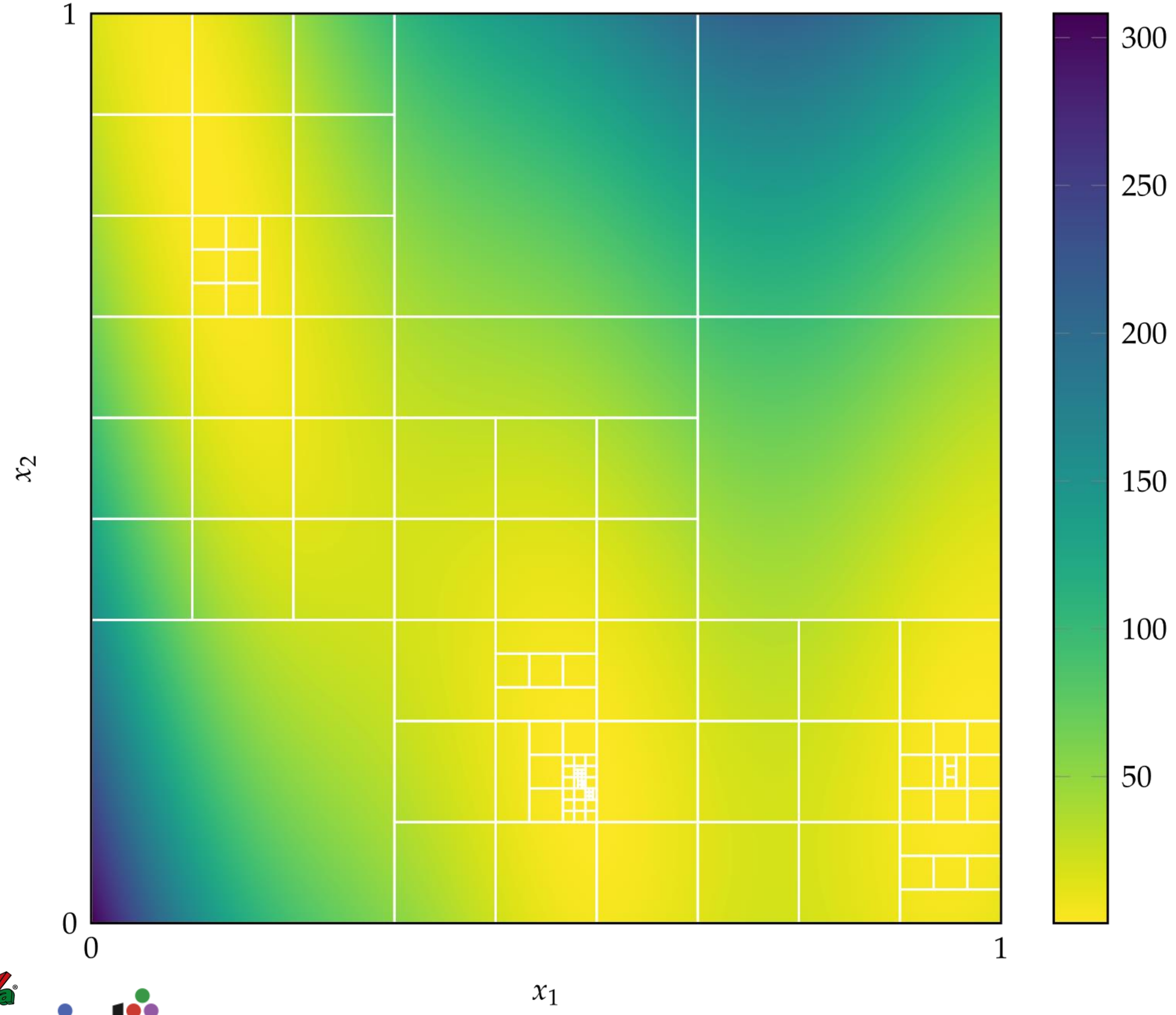
Divided Rectangles

- Multivariate DIRECT





Divided Rectangles



Summary

- Direct methods rely solely on the objective function and do not use derivative information.
- Cyclic coordinate search optimizes one coordinate direction at a time.
- Powell’s method adapts the set of search directions based on the direction of progress.
- Hooke-Jeeves searches in each coordinate direction from the current point using a step size that is adapted over time.

Summary

- Generalized pattern search is similar to Hooke-Jeeves, but it uses fewer search directions that positively span the design space.
- The Nelder-Mead simplex method uses a simplex to search the design space, adaptively expanding and contracting the size of the simplex in response to evaluations of the objective function.
- The divided rectangles algorithm extends the Shubert-Piyavskii approach to multiple dimensions and does not require specifying a valid Lipschitz constant.