Delaunay-based Derivative-free Optimization via Global Surrogate

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Outline

- Introduction
- Δ-Dogs for problems with a linear constraints.
- Δ-Dogs for problems with a general convex constraints.
- Minimizing the cost function that is derived by the infinite time-averaged.
- Conclusion.

Properties of the Derivative free Algorithms

Advantages

- Does not need any information about the derivative.
- Can handle problems with noisy or inaccurate cost function evaluations.
- Capability of the global Search

Disadvantages

- High computational cost with respect to the dimension of the problem.
- Slow speed of convergence.

General classification of the Derivative free methods

- Direct methods
- Nelder-Mead method
- Response surface methods
- Branch and bound algorithms
- Bayesian approaches
- Adaptive search algorithms
- Hybrid methods

General implementation of the response surface methods

- Design a model (interpolation) for the cost function based on the current data points.
- Find the most promising points for the global minimum based on the model.
- Calculate the cost function evaluation at the new data point.
- Add it to the data set, continue the algorithm until the global (local) minimum is found.

Optimization base on the kriging interpolations

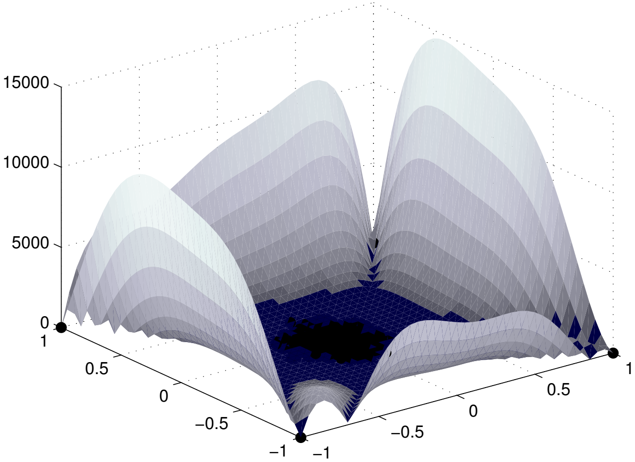
Advantages

- Have an estimation for both the cost function and its uncertainty at each feasible point.
- Can handle scattered data.
- Could be extended to high dimensional problems

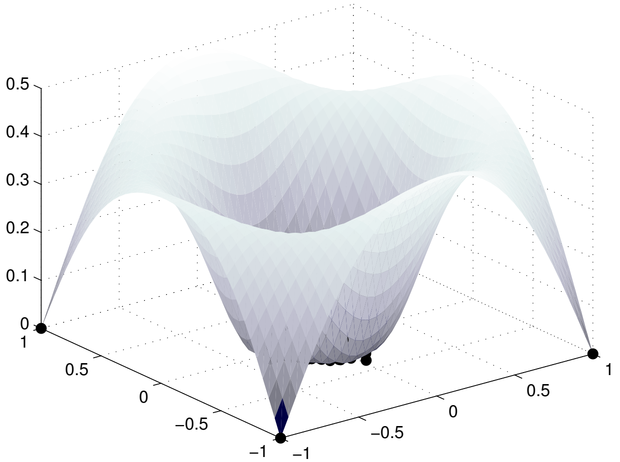
Disadvantages

- Has the numerical inaccuracy when the data points are clusttred in some region of the domain.
- Finding parameters of the Kriging interpolation is a hard non-convex subproblem.
- Minimizing the search function at each step is a non-smooth, non-convex optimization algorithm.

Performance of the Kriging for an illposed example



Performance of the polyharmonic spline for an illposed example



Initialization of the algorithm for problems with bounded Linear constraints

- In order to initialize the algorithm, a set of data points is needed that its convex hull is the feasible domain.
- The minimal subset of the feasible domain that its convex hull is our constraint is the set of vertices.
- There are some algorithms to find all vertices of a linear constrained problem.
- The box constraint is a special case which the corners are these vertices.

The Optimization Algorithm for the problems with linear constraints

- 1. Find all vertices of the feasible domain.

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- 4. Perform a Delaunay triangulation among the points.

The Global Optimization Algorithm for the problems with linear constraints

- 5. For each simplex S_i
    - Calculate its circumcenter x_C and the circumradius R.

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  - Minimize the search function $c_i(x) = p(x) - K\, e_i(x)$ in this simplex.

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  - Minimize the search function $c_i(x) = p(x) - K\, e_i(x)$ in this simplex.
- 6. Take the minimum of the result of the minimization performed in each simplex and add it to the set of evaluation points.

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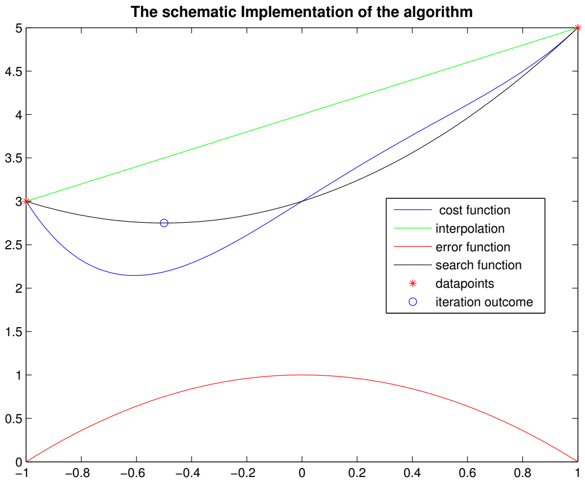
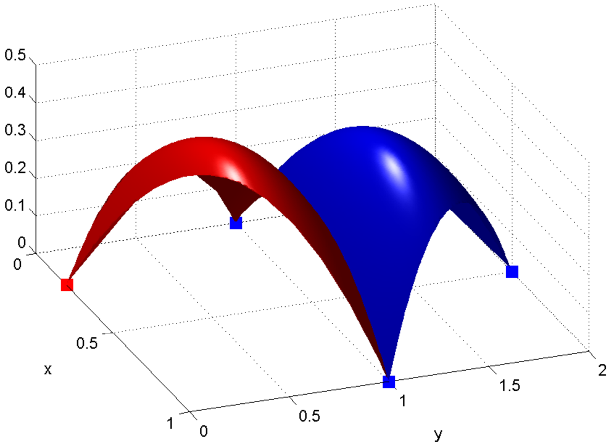
- 7. Repeat steps 3 to 6 until convergence.

Schematic implementation of the algorithm



Error function plots in 2 dimension



Minimizing the search function

- The search function $p(x) - Ke(x)$ has to be minimized in each simplex.
- A good initial estimate for the value of the minizer of this search function is derived by replacing $p(x)$ with the linear interpolation.
- For interpolation based on the radial basis functions, the gradient and Hessian of the search function is derived analytically; thus, the search function can be minimized by using the Newton method.
- If the linear constraints of the above optimization problems be relaxed with the whole feasible domian; the global minimizer of the search function is not changed.

Convergence Result

- The above algorithm will converge to the global minimum, if there is a K that for all steps of the algorithm, there is a point $\tilde{x}$ which

$$p_n(\tilde{x}) - K\ e_n(\tilde{x}) \leq f(x^*), \tag{1}$$

where $f(x^*)$, $p_n(x)$ and $e_n(x)$ are the global minimum, interpolating function and uncertainty functions at step n respectively.

- The above equation is true; if we have:

$$K \geq \lambda_{\max}(\nabla^2 f(x) - \nabla^2 p_n(x))/2, \tag{2}$$

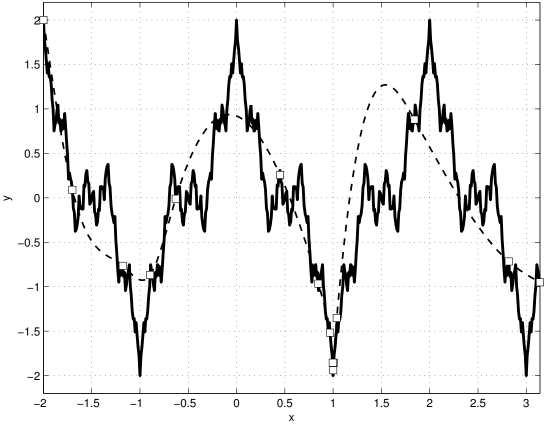
for all steps of the algorithm.

Choose the optimal value for K

- If we have a lower bound for the global minimum (y_0), we could minimize $\frac{p(x)-y_0}{e(x)}$ instead of the above search function.
- If y_0 is the global minimum; the second method is equivalent to the optimal choice for the tuning parameter K.
- This new approach will converge to the global minimum even if the search function is not globally minimized at each step.

Results

$$f(x) = \sum_{i=0}^{N} \frac{1}{2^i} \cos(3^i \pi x), \;\; N = 300;$$



Results

$$f(x,\ y) = x^2 + y^2$$

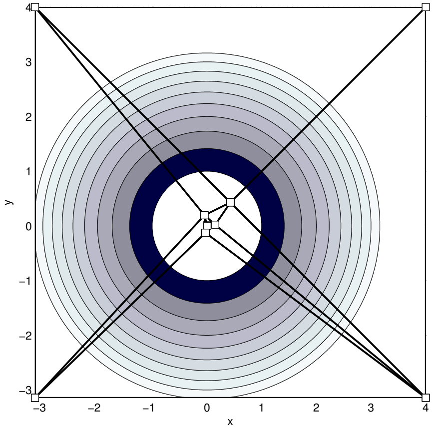


Figure : parabola function

Results

$$f(x,y) = -x sin(\sqrt{|x|}) - y sin(\sqrt{|y|})$$

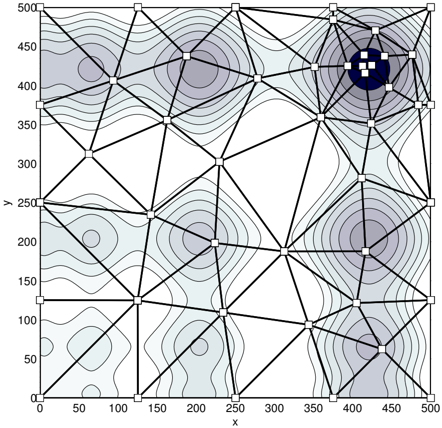


Figure : Schwefel function

Results

$$f(x) = (1 - x_1)^2 + 100(x_2 - x_1^2)^2$$

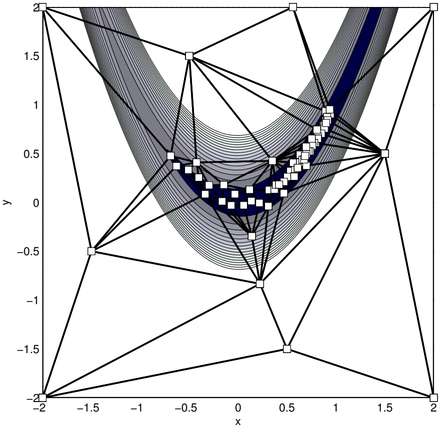


Figure : Rosenbrock function

Perturbed Rosenbrock function

$$f_P(x) = f(x) + \frac{10}{\pi N} sin(N\pi x_1)^2 sin(N\pi x_2)^2 \quad N \to \infty$$

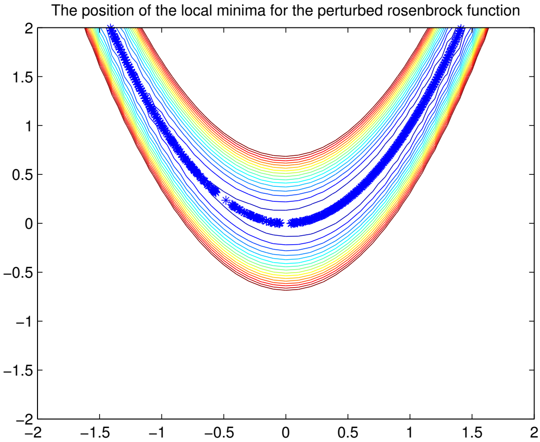


Figure : Rosenbrock function

Generalization of the algorithm for problems with convex constraints

- Above algorithm in restricted to convex hull of the available evaluation points.
- The modification that solves above problems is to project the a search point at each step to the feasible boundary if the search point is out (or on the boundary) of the this convex hull from an interior points.
- We proved the convergence of the above algorithm if the feasible boundary is smooth or the global minizer is an interior point.
- This algorithm is efficient if the feasibility check is a cheap process.
- The new modified algorithms needs $d+1$ initial points instead of 2^d points.

Results

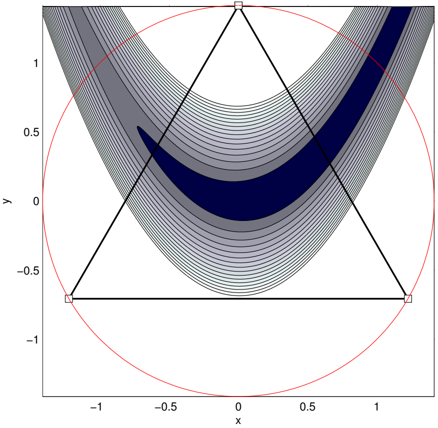


Figure : Rosenbrock function in a circle

Results

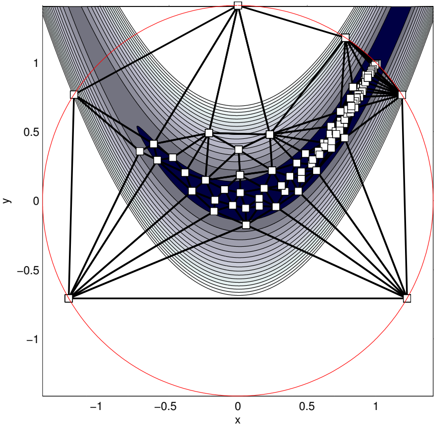


Figure : Rosenbrock function in a circle

Minimizing the long time averaged statistics

The objective function that has been considered is as follow:

$$\min_{x} \lim_{T \to \infty} \frac{1}{T} \int_0^T F(x,t)dt \tag{3}$$

Assumptions

- F(x,t) is the only accessible value that is derived with a simulation or an experiment.
- F(x,t) is a stationary process.
- Above function is a non-convex function.
- The dimension of the design parameters is small.

Construct the model for the problem

The mathematical model that is designed for the above problem is

$$F(x,t) = f(x) + v(x,t) \tag{4}$$

$$v(x,t) = \mathcal{N}(0,\sigma^2) \tag{5}$$

$$g(x,N) = \frac{1}{N}\sum_{i=1}^{N} F(x, i\Delta t) \tag{6}$$

- The computational cost of calculating $g(x,N)$ is proportional to N.
- $g(x,N)$ is an approximate for $f(x)$ that is more accurate as N increased.
- An estimation for the error of $g(x,N)$ has been derived based on the long-memory process theory.

The process of the algorithm for Weierstrass test function

The outcome of the algorithm for Weierstrass test function

Conclusions

- A new optimization algorithm has been developed that found the global minimum with a minimum number of function evaluations.
- Any smooth interpolating function can be used in this algorithm.
- This algorithm is not sensitive to the noisy or inaccurate cost function evaluations.
- The global minimum can be approximate pretty fast, yet the speed of the convergence for the algorithm is slow.
- This method can be combined a local method to develop a fast converging algorithm.
- This algorithm can deal with problems with general convex constraints.
- A new method that uses Δ-Dogs has been developed which minimized the simulated based optimization problems in which the cost function evaluations are derived from infinite-time-average statistics.