

# Current development work on ChemApp and SimuSage

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# Topics

- ChemApp
  - Semi-automatic charge balance correction
- SimuSage
  - Adding Nomad
  - Lazarus port



# Semi-automatic charge balance correction

- The situation:
  - In iterative calculations (input to an equilibrium calculation is based on the output of a previous equilibrium calculation) electroneutrality in phases with phase-internal electrons might not be given.
  - Typical reason: rounding errors
  - Primarily a problem when “streams” are used (as opposed to “global conditions”)
  - Solution: enable the user to specify that ChemApp should set the amount of phase-internal electrons to zero before an equilibrium calculation



# New subroutine: TQCONF

- `CALL TQCONF ('E', 0, 0, 0, NOERR)`
  - Sets amounts of all system components with names starting with 'e(', 'E(', or 'EA' to zero
- `CALL TQCONF ('E', I, 0, 0, NOERR)`
  - Sets amount of system component I (I begin an electron) to zero



# NOMAD in FactOptimal

Fact Optimal - [PROP #1: Temperature]

Recent... f Function Builder Help

Properties Variables Cost Constraints Parameters **Results**

Stop

Status: Done. Next Run >>

Number of FactSage calculations: 150

Best answer so far:

Temperature: **436.77 C**

Last solution:

Species	mol
Al	0.11539
Cu	0.02
Mg	0.75
Zn	0.11461

Open in Equilib

Save Pareto Points

Constraints:

Al+Cu=0.11539

Density=2.19982

Cost \$=2856.28076

0.115240478515625 0.020079101562500 0  
 0.115324707031250 0.020180175781250 0  
 0.115456542968750 0.020000000000000 0

**Results**

Temperature (C)

# of Calculations

# of Calculations	Temperature (C)
1	446
10	446
20	446
25	440
35	437.5
45	437.5
65	437
120	436.77

UNITS | Temperature : C , Mass : mol

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# NOMAD

- Nonlinear Optimization by Mesh Adaptive Direct Search
- C++ implementation of the Mesh Adaptive Direct Search (MADS) algorithm\*
- Designed for constrained optimization blackbox functions in the form:

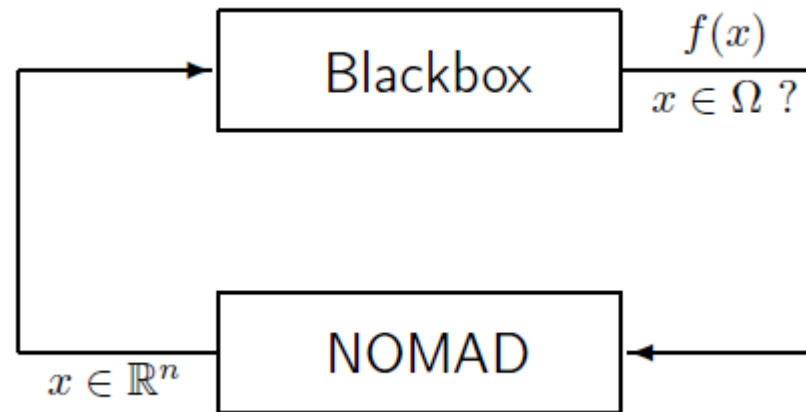
$$\min_{x \in \Omega} f(x)$$

\* Aued, C., and Dennis, J. (2006). Mesh Adaptive Direct Search Algorithm for Constrained Optimization. SIAM J. Opt. 17, 1, 188-217



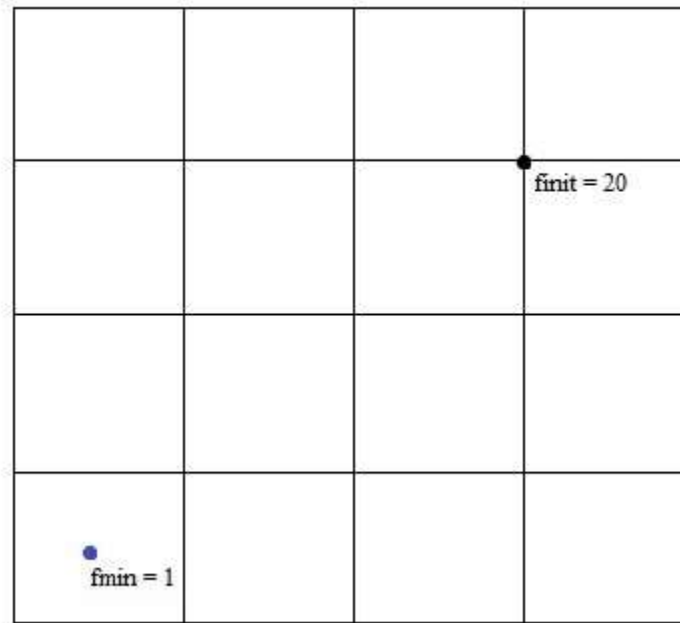
# Blackbox Problems

- Unknown internal structure of the target problem
- Function can have unreliable properties
- NOMAD is intended for time-consuming blackbox simulations with a small number of variables



# MADS Algorithm

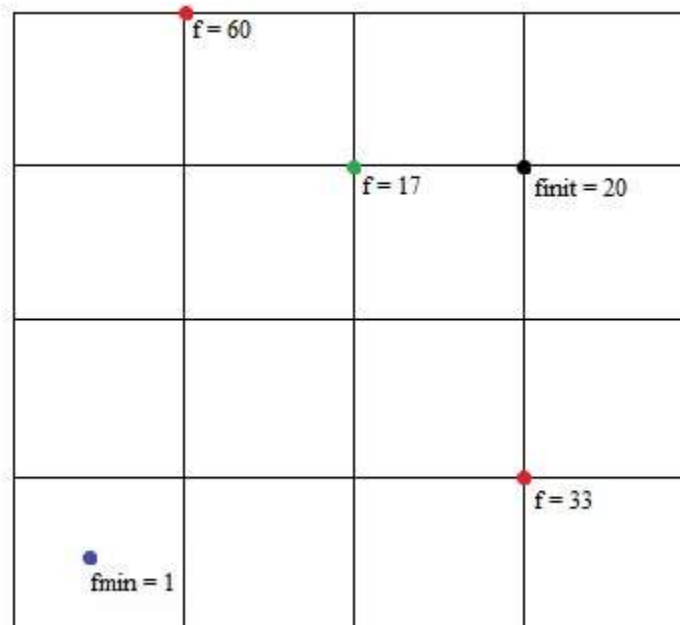
- Mesh Adaptive Direct Search





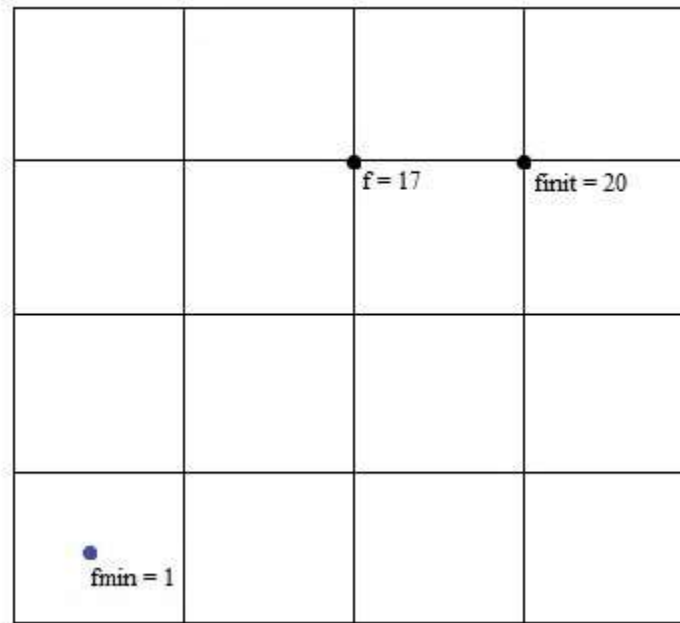
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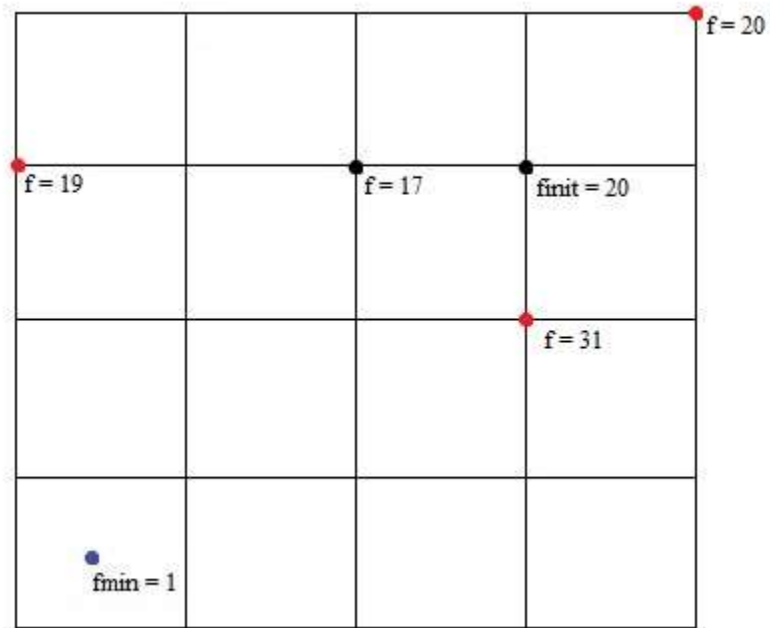
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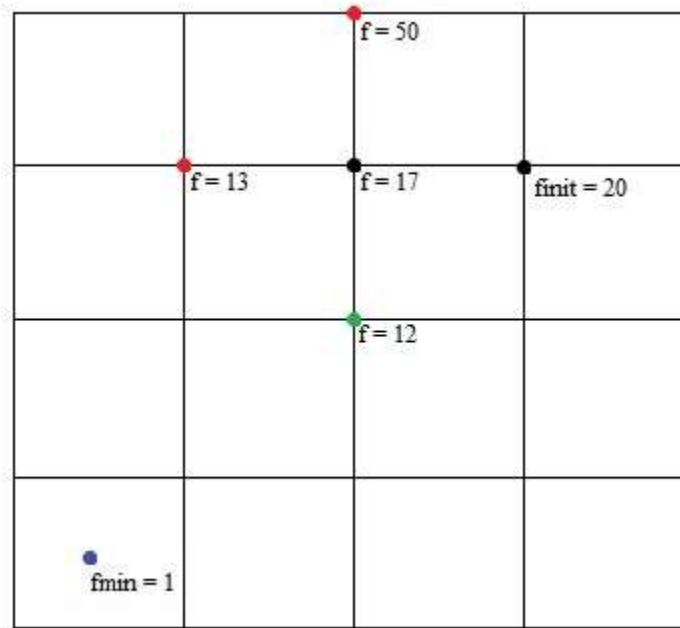
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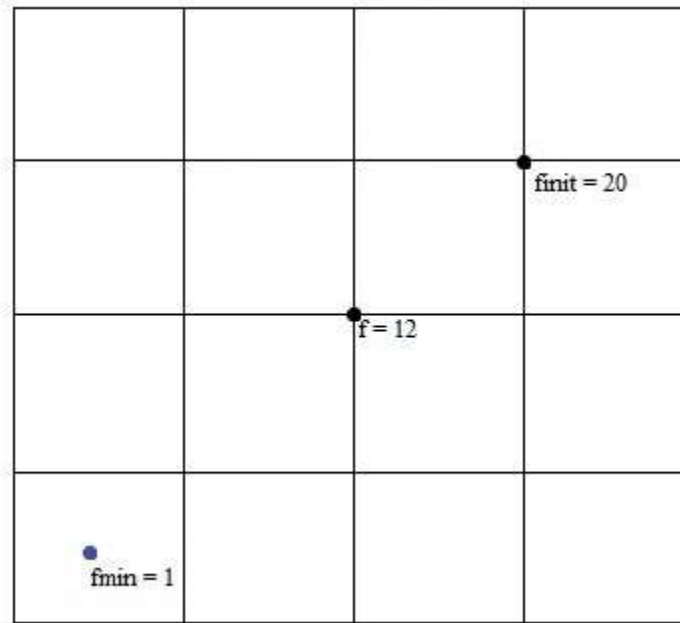
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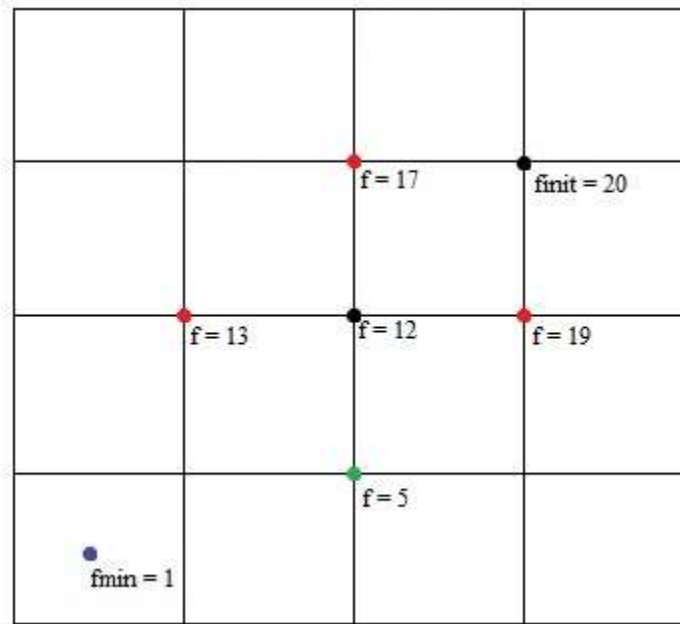
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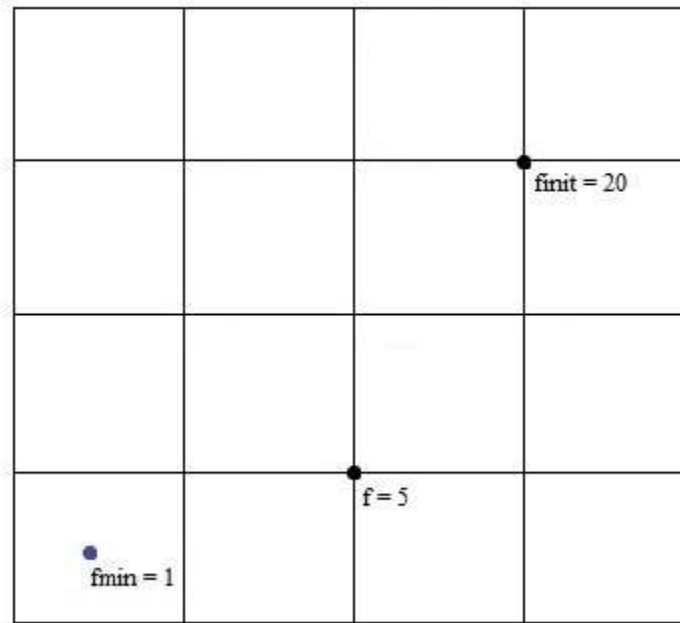
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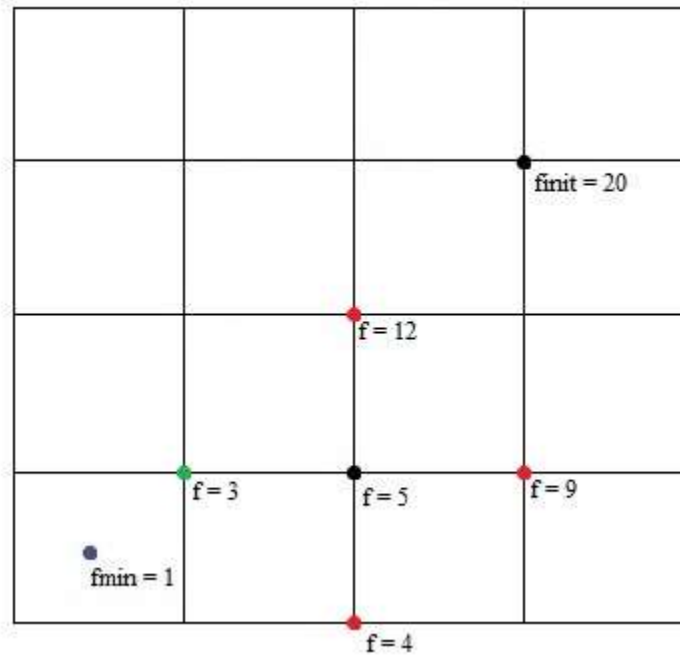
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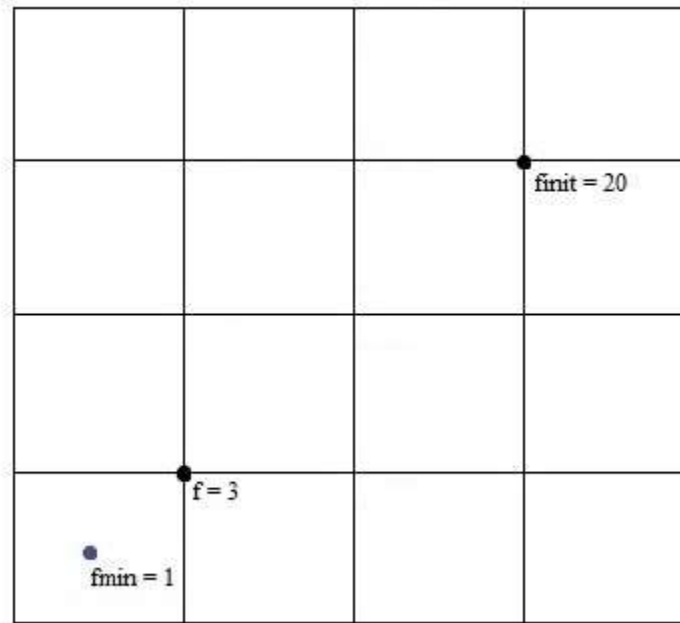
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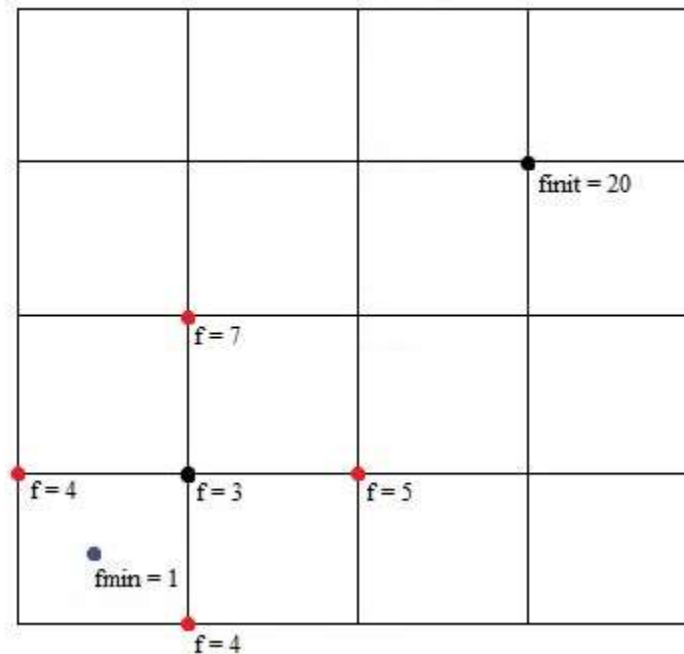
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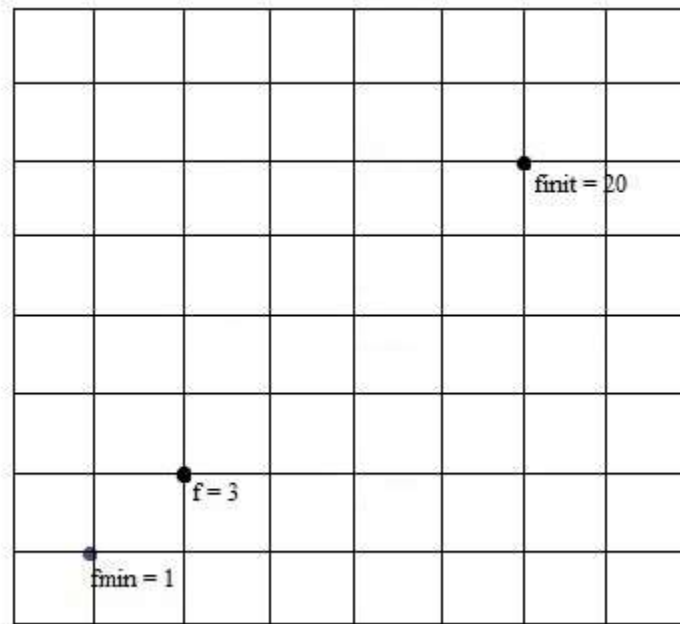
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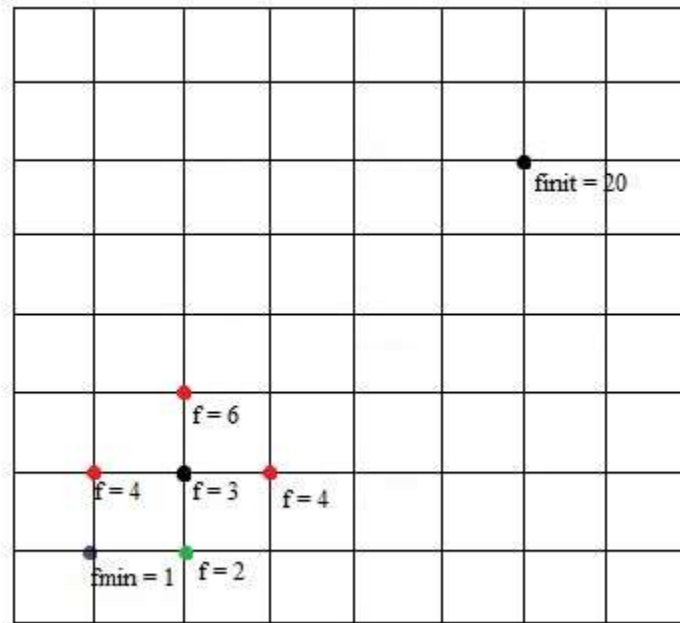
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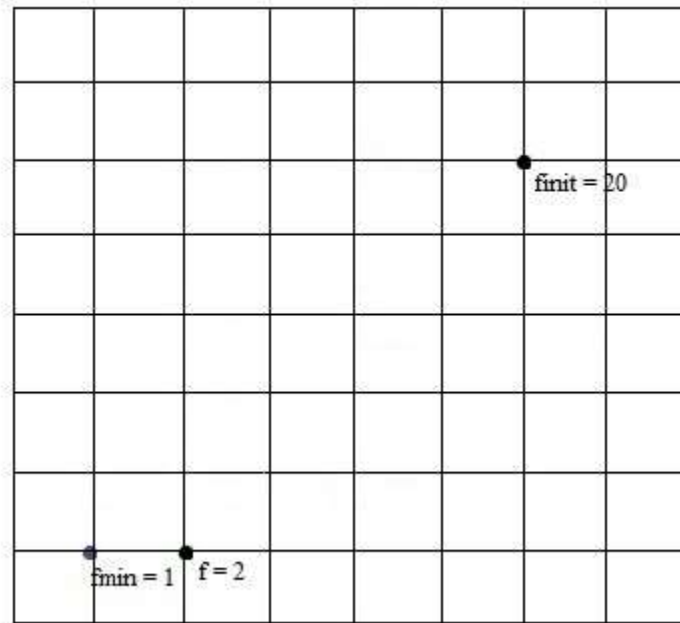
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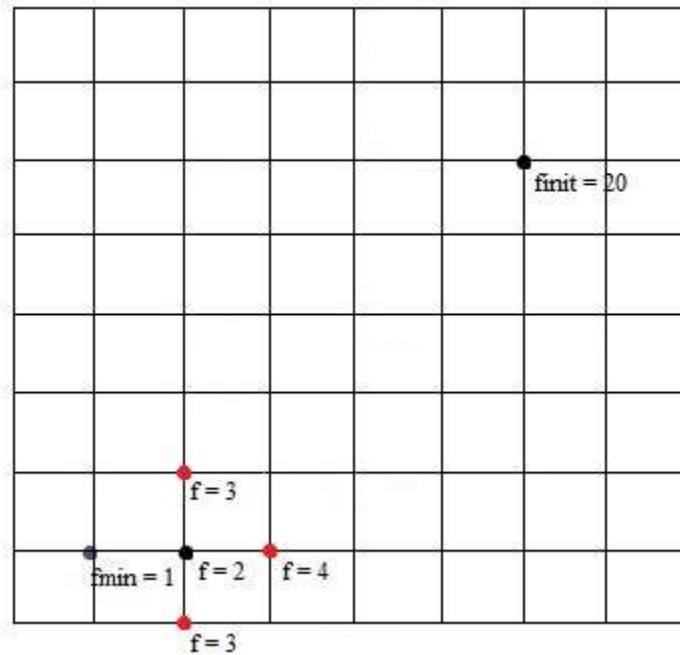
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# MADS Algorithm

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**Some examples...**



***Thank you for your  
attention!***

