Energy Minimisation Cheat Sheet

by Nimisha (lemonbuzz) via cheatography.com/132716/cs/41241/

Definitions

Minimisation algorithm	Identifies geometries corresponding to minimum points on the energy surface
Saddle point	Highest points on the path between two minima/maxima i.e. a transition structure
At a minimum point, first derivatives are zero, and second derivatives are positive	
Parameter coordinates	Molecular mechanics – Cartesian (3N) Quantum mechanics – Internal (3N-6)
Categories of min algo	1. Derivative 2. Non-derivative
Derivative methods	- Obtained analytically or numerically - Analytical preferred - If only numerical, non-derivative may be more effective
Numerical derivative	Change in energy divided by change in coordinates

Non-derivative methods

Simplex method	- Non derivative (zeroth order) - Locates minimum on energy surface by moving around like an amoeba
Simplex	M cartesian coord => M+1 vertices M internal coord => M-5 vertices
- Direction of first derivative => Minima location - Magnitude of deriv. => Steepness of local slope	
Movements	Reflection - Reflection and Expansion - Contraction -

Derivative methods

- Direction of first derivative => Minima location
- Magnitude of deriv. => Steepness of local slope
- Second derivative => curvature of function

Force = -dV(r)/dr

First order algos	- steepest descent - conjugate gradient

STEEPEST DESCENT

- moves in dir. || net force (walking straight downhill
- both gradient and direction orthogonal

1) line search (2) arbitrary step (3) lanrange multipliers

- robust when starting point is far from minimum
- relieves higest energy features

1D Line search	- bracket search - computationally expensive
Arbitrary step	- random step size - if lower energy, step size increased by multiplication factor - higher energy, step size reduced - more steps but less function evaluations
Cons	- forced to make right angles - path oscillates, overcorrects, and reintroduces errors

CONJUGATE GRADIENT

- no oscillation
- gradient orthogonal but direction **conjugate**
- for quadratic function of M variables, min reached in M steps
- can be used from 2nd step (1st step SD)

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