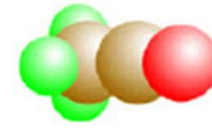


Optimization Techniques

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강정원

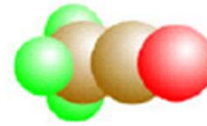
Introduction



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- Optimization
 - Finding stationary point of a function
- Methods
 - Steepest Descent
 - Conjugate Gradient Method
 - Newton-Raphson Method
 - Locating the Global Minimum and Conformal Sampling
 - Stochastic and Monte Carlo Method
 - Molecular Dynamics
 - Simulated Annealing
 - Genetic Algorithm
 - Diffusion Method
 - Distance Geometry Method

Local Minimum vs. Global Minimum

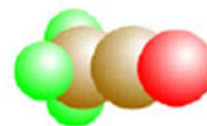


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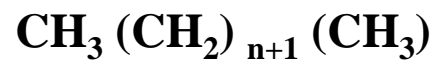
- Steepest Descent
- Conjugate Gradient Method
- Newton' Method
 - Local Minimum Methods (“Nearest minimum”)

- A global optimization is an extremely difficult task for a multidimensional problem
 - Multiple minima
 - Combinatorial explosion

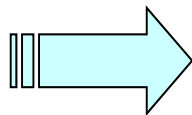
Possible conformation for linear alkanes



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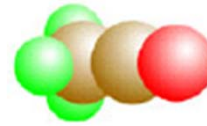
N	No. of possible conformation 3^n	Time 1 conformation = 1 s
1	3	3s
5	243	4 min
10	59049	16 h
15	14348907	166 d



Combinatorial explosion !

The systematic (or grid) search is only possible for small molecules

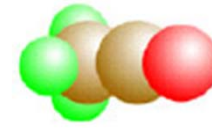
Stochastic and Monte Carlo Method



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- Similar to MC simulation of properties
- Procedure
 - Random “kick” is generated to one or more atoms
 - New geometry is accepted if the lower energy
 - Otherwise Boltzmann factor is calculated and compared with random number between (0,1)

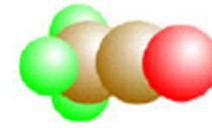
Molecular Dynamics



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- Solves Newton's second law of motion for atoms on an energy surface
- Available energy = (kinetic) + (potential)
 - Molecules are able to overcome barriers separating minima if sufficient kinetic energy is given
 - Closely related to the temperature of the system
 - Require long simulation time

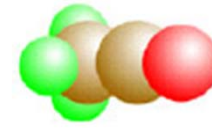
Simulated Annealing



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- MC and MD employ a temperature as guiding parameter
- At sufficiently high T and long time, conformation space is sampled
- Simulated Annealing (SA)
 - Initial T is chosen to be high (2000-3000K)
 - MC and MD run
 - T is slowly reduced (Trapped in minimum)

Genetic Algorithm



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- Concept and terminology from biology
- Children = mixture of parent genes
 - Allowing mutation of parent genes
 - Best population are selected based on Darwin's principle