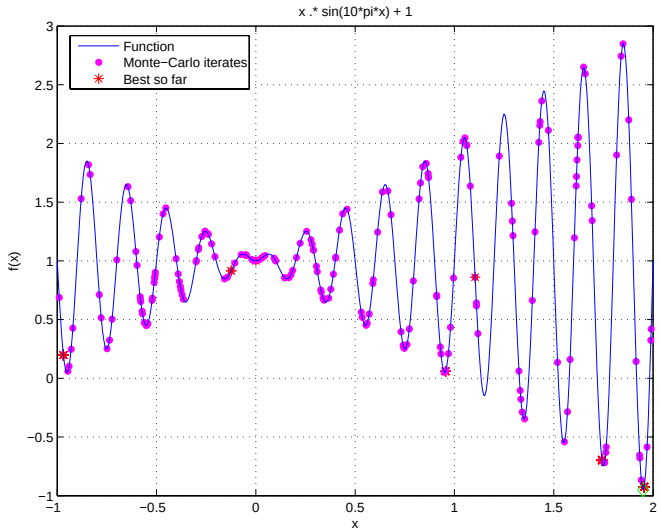
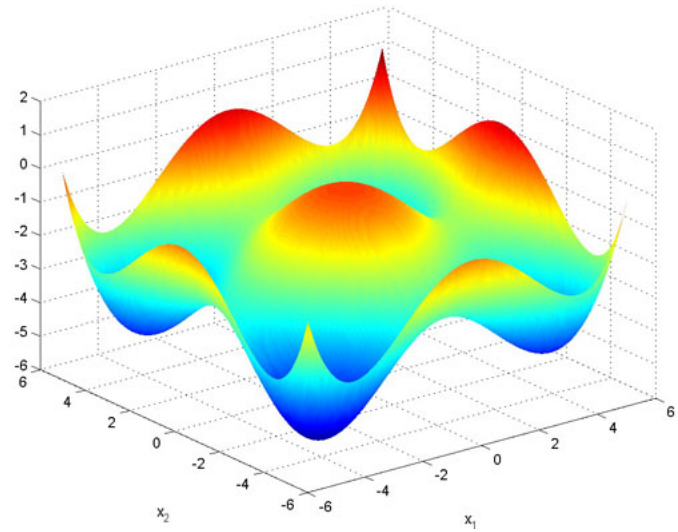
# Local and Global Optimization

## Formulation, Methods and Applications





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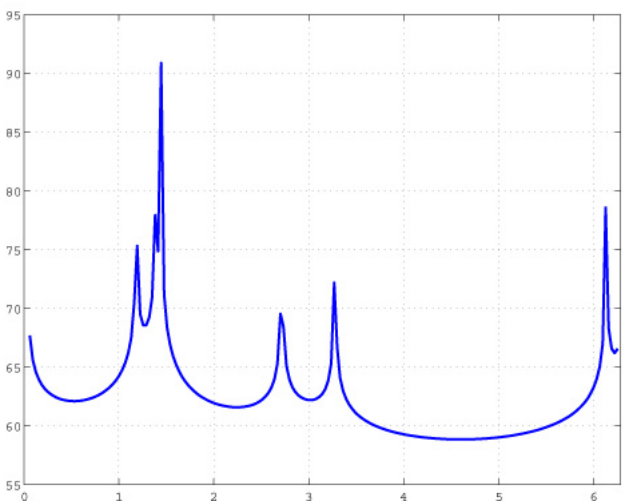
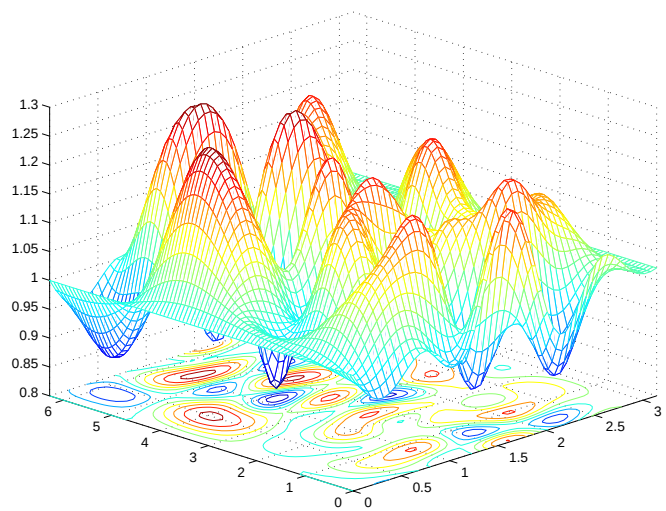
# Optimization

- Find values of the variable(s) $x$ to give the
  - ▷ best (minimum or maximum) of an
  - ▷ objective function $f(x)$
  - ▷ subject to any constraints (restrictions) $c(x) = 0$, $c(x) \leq 0$

  on what values the variables are allowed to take.
- Calculus, $x \in \mathbb{R} \Longrightarrow f'(x) = 0$ (stationary point)
  - ▷ $f''(x) > 0 \Longrightarrow$ min, $f''(x) < 0 \Longrightarrow$ max. Local vs Global



# Examples of optimization problems

- Choosing a course
  - ▷ Variables: which courses are available (continuous vs discrete)
  - ▷ Objective: compulsory, interesting (many, hard to quantify)
  - ▷ Constraints: one place at a time, pre-requisites
- How much should you invest in the bank, shares, property, ...
  - ▷ Variables: fraction of money in each asset (many variables)
  - ▷ Objective: maximize return, minimize risk (several competing objectives)
  - ▷ Constraints: money available, non-negative amounts, fractions in $[0, 1]$
- Optimality principles: Some form of optimality underlies many problems in
  - ▷ Science: physics, chemistry, biology, ...
  - ▷ Commerce, economics, management, ...
  - ▷ Engineering, Architecture, ...

# Finite dimensional optimization – variables

- Variables $x \in \mathbb{R}^n$: $x = (x_1, x_2, \ldots, x_n)^T, \quad x_i \in \mathbb{R}, i = 1, \ldots, n$
- $n$ = number of variables.
- $n = 1$, univariate; $\quad n \geq 2$, multivariate
- Ex 1 – What fraction of a portfolio should be invested in each asset class?
  - ▷ $n$ = number of assets;
  - ▷ $x_i$ = fraction invested in asset class $i$ for $i = 1, \ldots, n$.
- Ex 2 – In which order should a number of destinations be visited?
  - ▷ $n$ = number of destinations to be visited
  - ▷ $x$ = permutation of $\{1, \ldots, n\}$
  - ▷ $X_{ij} = 1$ if you go from destination $i$ to $j$; 0 otherwise
- Ex 3 – What are the positions of atoms/molecules in a stable compound?
  - ▷ $m$ = number of atoms; $n = 3m$ for positions $(x, y, z)$ in space
  - ▷ $x = [x_1, y_1, z_1, x_2, y_2, z_2, \ldots, x_m, y_m, z_m]$.

# Objective functions

- Objective function: Minimize $f(x)$
- Mathematical representation of "best"
- Maximize $\bar{f}(x) \iff$ Minimize $-\bar{f}(x)$
- Ex 1 – Maximize returns; minimize risk
  - ▷ Maximize return $r^T x = \sum_{i=1}^{n} r_i x_i$; $r_i$ = return on asset $i$
  - ▷ Minimize risk $x^T C x = \sum_{i=1}^{n} \sum_{j=1}^{n} x_i C_{ij} x_j$; Covariance matrix $C$
- Ex 2 – Minimize cost of visiting all destinations
  - ▷ Total cost $= \sum_{i=1}^{n} \sum_{j=1}^{m} X_{ij} C_{ij}$; $C_{ij}$ = cost of going from $i$ to $j$
- Ex 3 – Minimize the energy of the system
  - ▷ Distances between particles $\mathbf{x}_j = [x_j, y_j, z_j]$ for $j = 1, \ldots, m$
  - ▷ Energy $= \sum_{i=1}^{m} \sum_{j=1, j \neq i}^{m} \phi(|\mathbf{x}_i - \mathbf{x}_j|)$;
  - ▷ Potential $\phi(r)$, Coulomb $1/r$, Leonard-Jones,

# Constraints

- Constraints: $x \in \Omega \subseteq \mathbb{R}^n$, Feasible region $\Omega$
  - ▷ Simple bounds: $l \leq x \leq u \iff l_i \leq x_i \leq u_i, \quad i = 1, \ldots, n$
  - ▷ Linear constraints

$$\begin{array}{ll} Ax = b & \text{Equality constraints} \\ Ax \leq b & \text{Inequality constraints} \end{array}$$

$$Ax = b \iff \sum_{j=1}^{n} a_{ij} x_j = b_i, \quad i = 1, \ldots, m$$

  - ▷ Nonlinear constraints

$$\begin{array}{lll} c_i(x) = 0, & i = 1, \ldots, m_e & \text{Equality constraints} \\ c_i(x) \leq 0, & i = m_e + 1, \ldots, m & \text{Inequality constraints} \end{array}$$

  - ▷ Integrality constraints $x_i \in \mathbb{Z}$

$$\begin{array}{ll} x_i \in \{0, 1\} & \text{Zero-one variables} \\ x_i \in \{0, 1, 2, \ldots\} & \text{Nonnegative integer variables.} \end{array}$$

  - ▷ $\bar{c}_i(x) \geq 0 \iff -\bar{c}_i(x) \leq 0$

# Constraints – Examples

- Ex 1 – fraction of portfolio
  - ▷ fraction $0 \leq x_i \leq 1$ for $i = 1, \ldots, n$
  - ▷ fully invested $\sum_{i=1}^{n} x_i = 1$
  - ▷ investment guidelines $x_1 + x_2 + x_3 \leq 0.6$
  - ▷ minimum return $r^T x \geq 0.1$
  - ▷ maximum risk $x^T C x \leq 0.4$
- Ex 2 – visit all destinations exactly once
  - ▷ Go somewhere $\sum_{j=1}^{n} X_{ij} = 1$ for all $i$
  - ▷ Come from somewhere $\sum_{i=1}^{n} X_{ij} = 1$ for all $j$
  - ▷ $X_{ij} \in \{0, 1\}$
- Atoms/electrons/molecules
  - ▷ Particles on a surface $\mathcal{M}$: $x_j \in \mathcal{M}$
  - ▷ Bonds between particles
  - ▷ Geometry

# Dynamic constraints: Optimal Control

- Variables: a function $x(t)$
  - ▷ Time scales: $t \in [0, T]$
  - ▷ Space of functions (continuous, differentiable, ...)
- Objective is a function of $x$
  - ▷ Final state $x(T)$
  - ▷ $\int_0^T |x''(t)|\, dt$
- Constraints: Differential equations plus algebraic equations
  - ▷ Differential equations governing evolution of a system over time
  - ▷ Initial conditions $x(0)$ at $t = 0$, current state
  - ▷ Bounds: $a \leq x(t) \leq b$ for $t \in [0, T]$ – infinite number of constraints.

# Optimization problem classes (Terminology)

Optimization Technology Centre http://www.ece.northwestern.edu/OTC

- Combinatorial problems – finite but typically very large set of solutions
- Unconstrained problems – no constraints, any variables $x \in \mathbb{R}^n$ are allowed
- Linearly constrained problems – only linear constraints (simple bounds and/or general linear constraints)
- Nonlinearly constrained problems – at least one constraint is nonlinear
- Linear programming – objective and all constraints are linear, continuous variables
- Nonlinear programming – nonlinear objective or constraints, continuous variables
- Integer programming – variables are restricted to be integers
- Mixed integer programming – some variables are integers, some are continuous
- Stochastic optimization – some of the problem data is not deterministic

# Available information

- Objective function $f(x)$, $x \in \mathbb{R}^n$
- Objective gradient: $n$-vector,

$$\nabla f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix}$$

- Objective Hessian: $n$ by $n$ matrix

$$\nabla^2 f(x) = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_n x_1} & \cdots & \frac{\partial^2 f(x)}{\partial x_n^2} \end{bmatrix}$$

- Calculation: hand, symbolic (Maple, Mathematica), numerical (finite difference), automatic differentiation [6, 1]

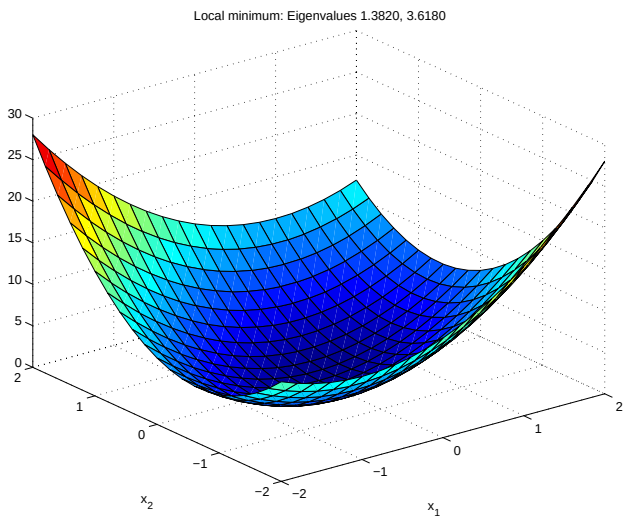
- Example:

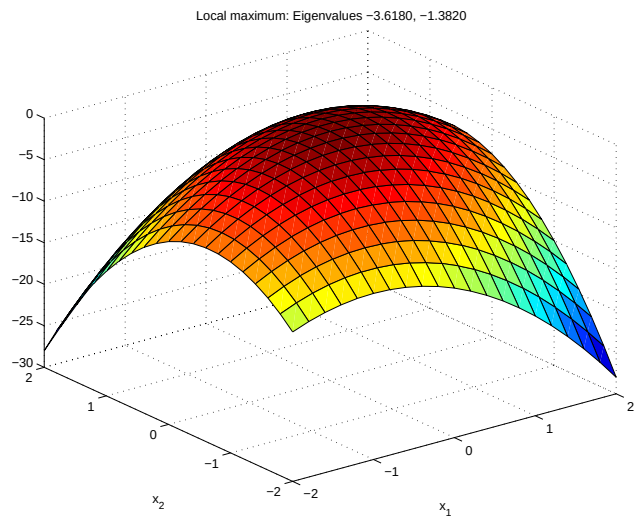
$$f(x) = 0.01 \sum_{i=1}^{3} \left( (x_i + 0.5)^4 - 30x_i^2 - 20x_i \right)$$

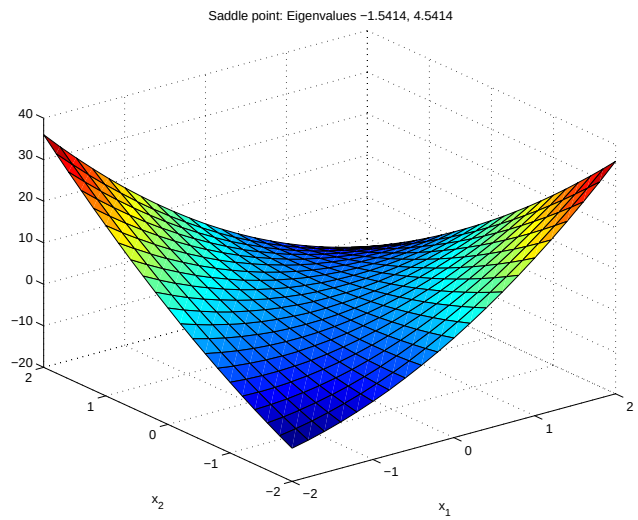
Find the gradient $\nabla f(x)$ and Hessian $\nabla^2 f(x)$ at $x = [0,\ 0,\ 0]^T$.

# Optimality – Unconstrained

- $x^*, f(x^*)$ local minimum $\Longrightarrow \nabla f(x^*) = 0$ (stationary point)
  - ▷ Can be minimum, maximum or saddle point
- Hessian information determines nature of stationary point:
  - ▷ Hessian positive definite (eigenvalues: all $> 0$) $\Longrightarrow$ local minimum
  - ▷ Hessian negative definite (eigenvalues: all $< 0$) $\Longrightarrow$ local maximum
  - ▷ Hessian indefinite (eigenvalues: some $> 0$, some $< 0$) $\Longrightarrow$ saddle point



# Problem Size

- Number of variables $n$, $x \in \mathbb{R}^n$
- Limitations
  - ▷ Compute time
  - ▷ Memory
- Example: If a method takes $n^3 + O(n^2)$ flops (floating point operations), what is the largest problem that can be solved in 24 hours on a 3 GHZ quad core workstation?

  **Ans:** $n \approx 10^5$
- Example: What is the largest Hessian ($n$ by $n$ symmetric matrix) that can be stored in IEEE double precision in 32 bit Windows (maximum 2 Gb addressable block)?

  **Ans:** $n \approx 16,000$

# Local search methods

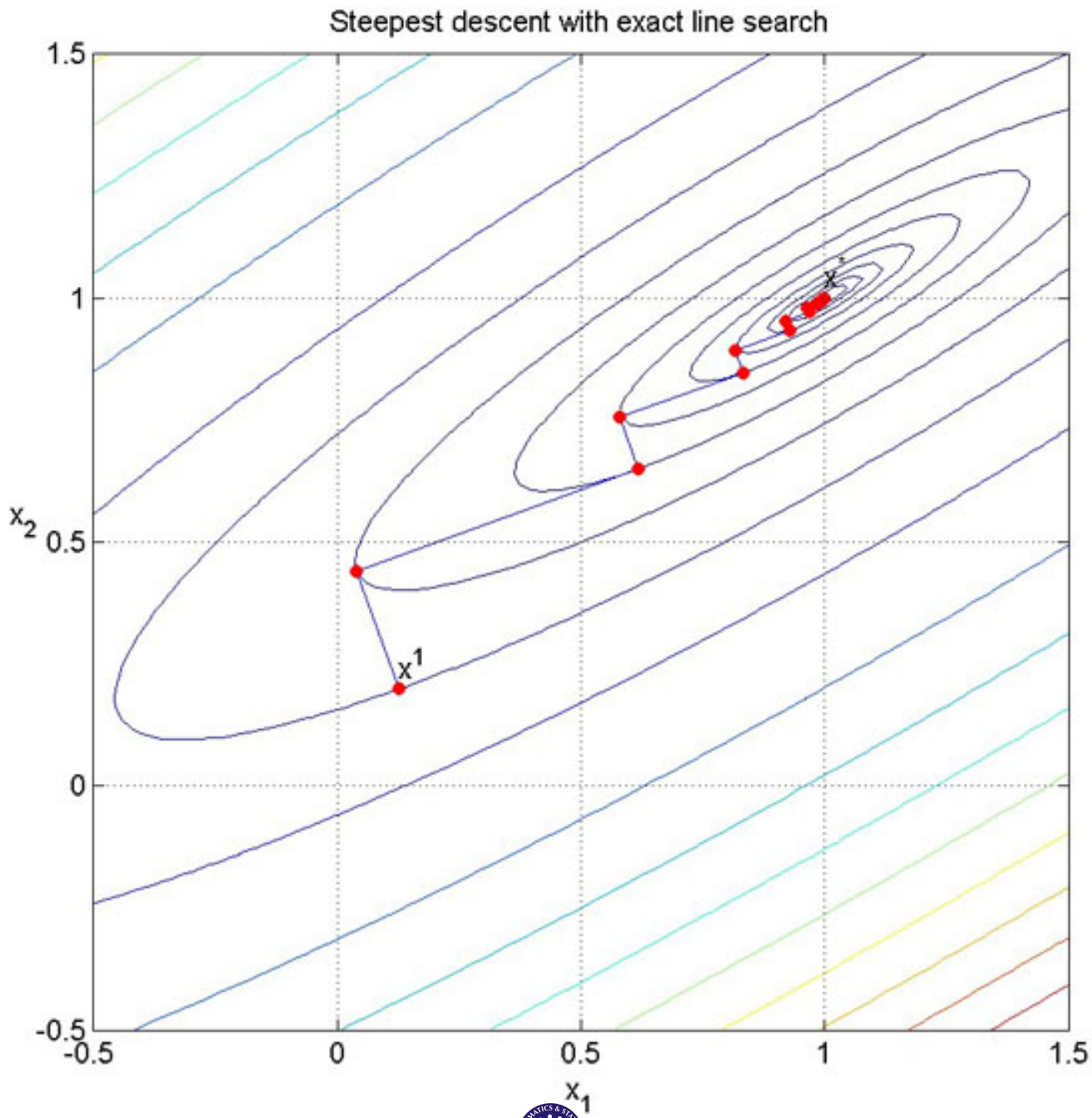
- Line search methods:
  - ▷ Given $x^{(1)}$ initial guess
  - ▷ At $x^{(k)}$ generate search direction $d^{(k)}$
  - ▷ Exact or approximate line search: $\alpha^{(k)} = \text{argmin}_{\alpha \geq 0} f\left(x^{(k)} + \alpha d^{(k)}\right)$
  - ▷ New points $x^{(k+1)} = x^{(k)} + \alpha d^{(k)}$
  - ▷ Descent method: $f\left(x^{(k+1)}\right) < f\left(x^{(k)}\right)$

- Steepest descent
  - ▷ $d^{(k)} = -\nabla f(x^{(k)})$
  - ▷ Global convergence: $x^{(k)} \to x^*$, $x^*$ stationary point ($\nabla f(x^*) = 0$) from **any** starting point
  - ▷ Arbitrarily slow linear rate of convergence $|x^{(k+1)} - x^*| \approx \beta |x^{(k)} - x^*|$, $0 < \beta < 1$.
  - ▷ Requires gradient $\nabla f(x)$, and $O(n)$ storage and work per iteration

- Newton's method
  - Solve linear system $\nabla^2 f(x^{(k)})d^{(k)} = -\nabla f(x^{(k)})$ for search direction $d^{(k)}$
  - Only locally convergent
  - Quadratic rate $|x^{(k+1)} - x^*| \approx |x^{(k)} - x^*|^2$ if $x^{(1)}$ sufficiently close to "nice" solution.
  - Requires $\nabla^2 f(x)$, $O(n^2)$ storage, $O(n^3)$ work per iteration

- Quasi-Newton methods
  - Solve $B^{(k)}d^{(k)} = -\nabla f(x^{(k)})$ for search direction $d^{(k)}$
  - Update $B^{(k+1)} \approx \nabla^2 f(x^{(k)})$
  - Superlinear rate $|x^{(k+1)} - x^*| \approx |x^{(k)} - x^*|^\tau$, $1 < \tau < 2$ under conditions
  - Requires $\nabla f(x)$, $O(n^2)$ storage, $O(n^2)$ work per iteration

- Conjugate Gradients methods
  - $d^{(k)} = -\nabla f(x^{(k)}) + \beta^{(k)} d^{(k-1)}$
  - Update $\beta^{(k)}$
  - Quadratic termination (conjugate directions)
  - Requires $\nabla f(x)$, $O(n)$ storage and work per iteration

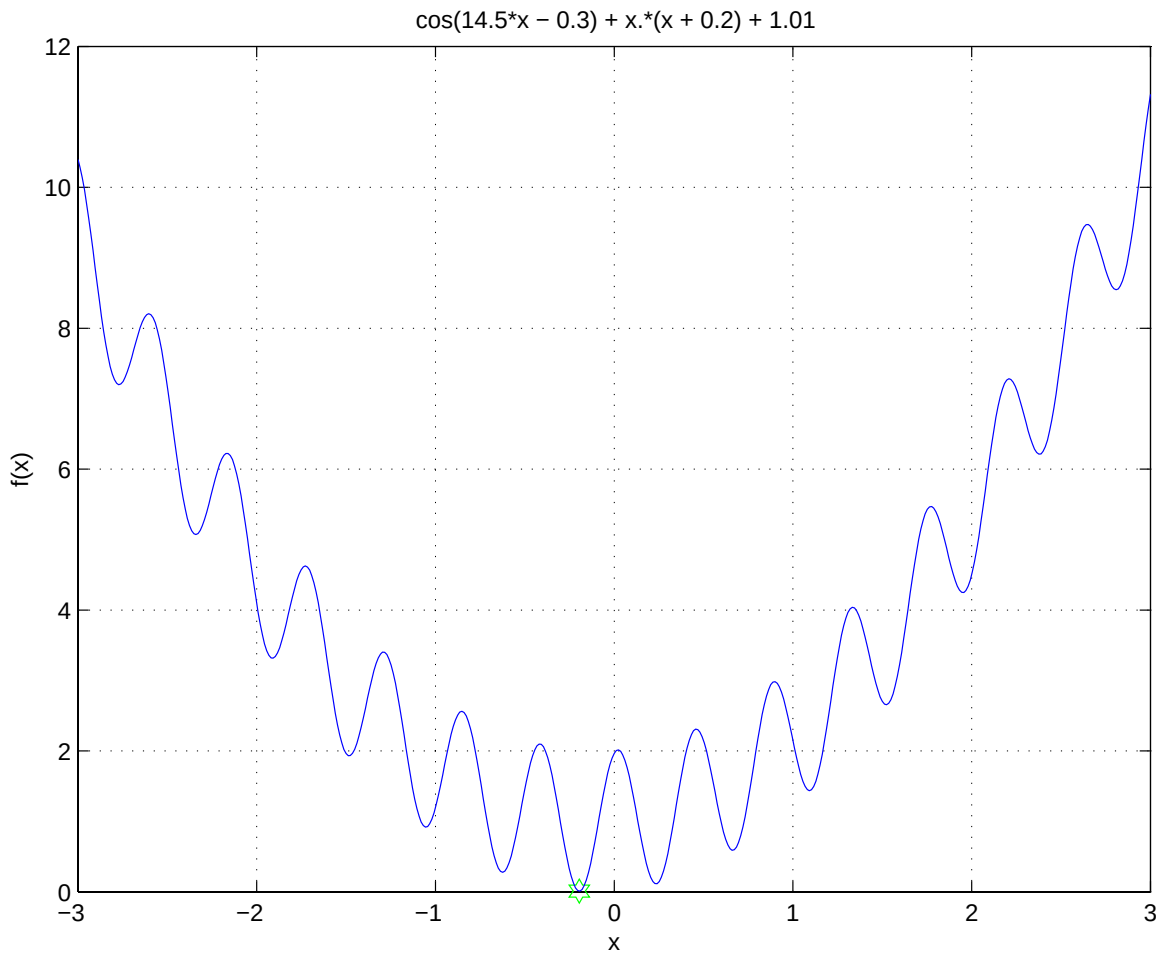

Steepest descent with exact line search
1.5
1
0.5
0
-0.5
-0.5
0
0.5
1
1.5
x2
x1
x1
x*

# Local vs global optimization

- Local minimum $f^* = f(x^*)$, local minimizer $x^*$
  - ▷ smallest function value in some feasible neighbourhood
  - ▷ $x^* \in \Omega$
  - ▷ there exists a $\delta > 0$ such that $f^* \leq f(x)$ for all $x$ in $\{ x \in \Omega : |x - x^*| \leq \delta \}$
- Global minimum $f^* = f(x^*)$, global minimizer $x^*$
  - ▷ smallest function value over **all** feasible points
  - ▷ $f^* \leq f(x)$ for all $x$ in $\Omega$
- There can be many local minima which are not global minima
- In the context combinatorial problems, global optimization is NP-hard
- Special properties (eg. convexity) of feasible region $\Omega$ and objective function $f$ imply that any local solution is a global solution.
- References: Pinter [20]

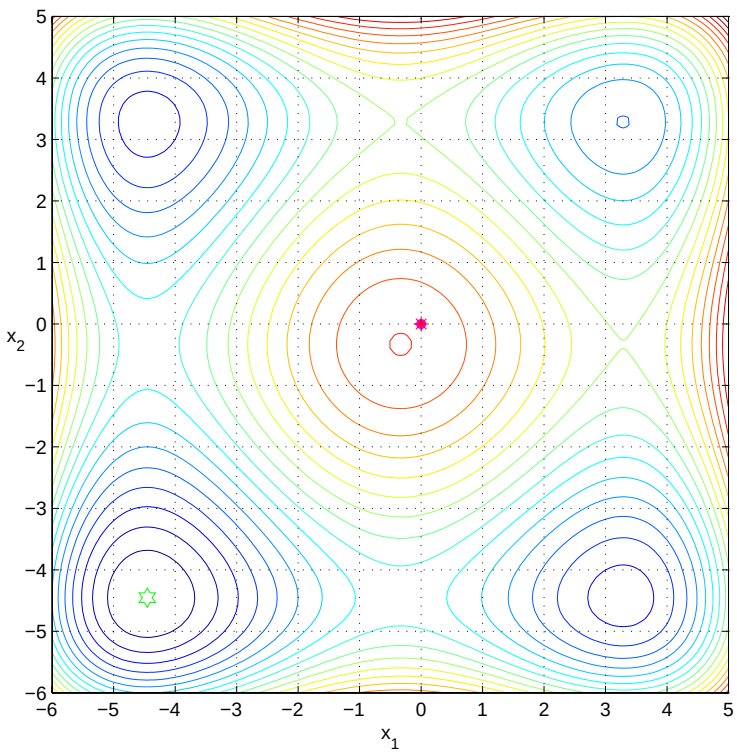
# One-dimensional example

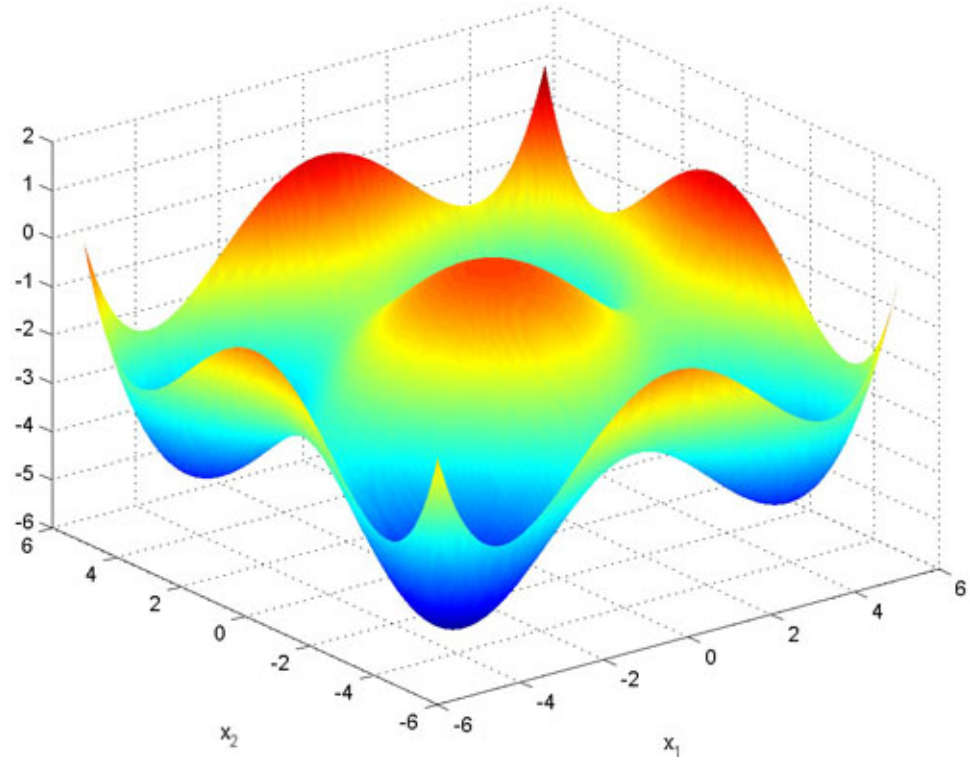
- $f(x) = \cos(14.5x - 0.3) + x(x + 0.2) + 1.01$
- $\Omega = [-3, 3]$



# Two-dimensional example

- $f(x) = \left( \sum_{i=1}^{2} (x_i + 0.5)^4 - 30x_i^2 - 20x_i \right) / 100$
- $\Omega = \{ x \in \mathbb{R}^2 : -6 \leq x_i \leq 5, \quad i = 1, 2 \}$



# Travelling Salesman Problem (TSP)

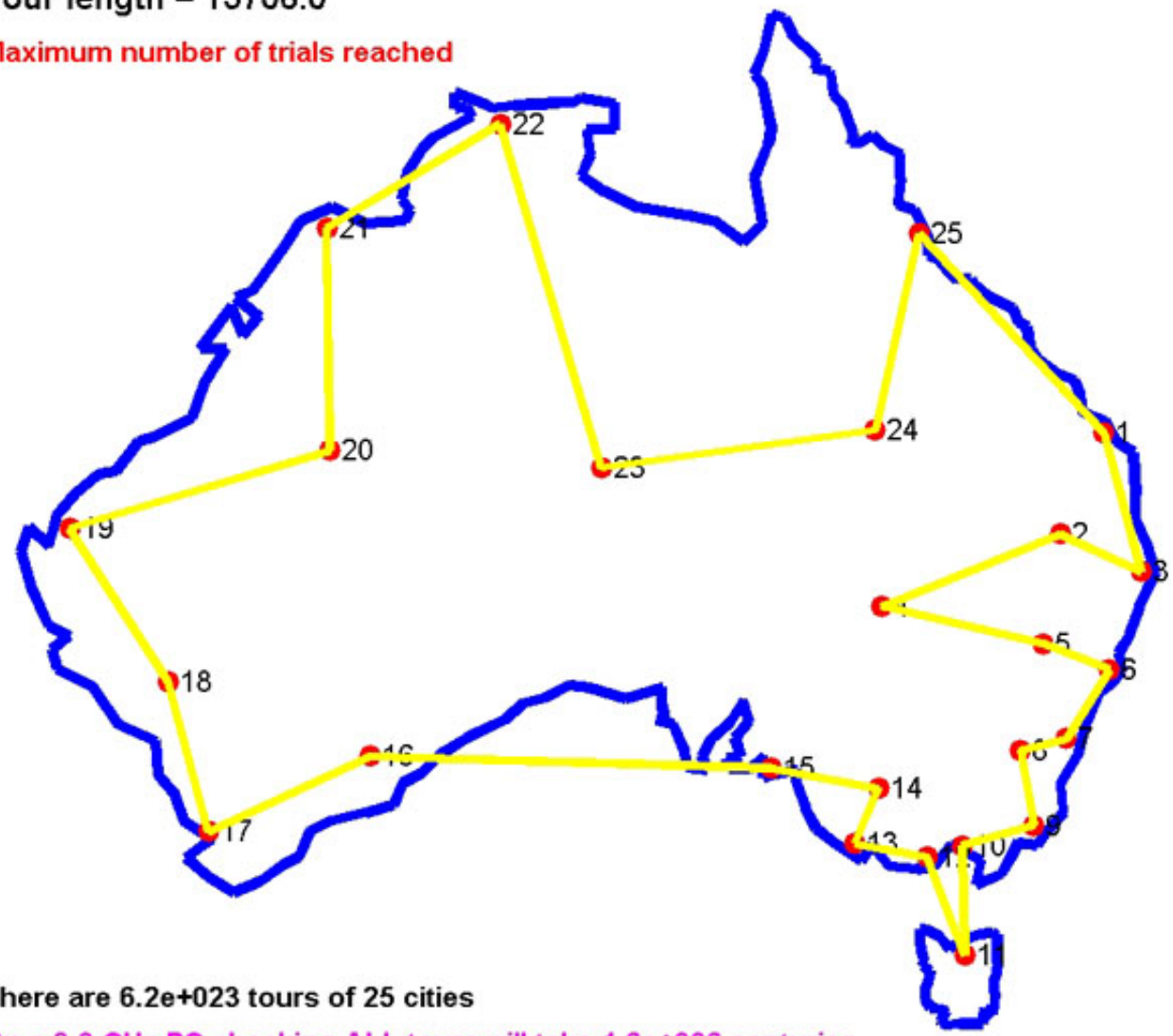
A salesman must visit every one of $n$ cities exactly once and return to their starting city. If the cost of going from city $i$ to city $j$ is $C_{ij}$, find the route that minimizes the total cost.

- Variables
  - ▷ $X_{ij} = 1$ if go from city $i$ to city $j$; 0 otherwise
  - ▷ $x_i = i$th city visited; Permutation of $\{1, 2, \ldots, n\}$
- Objective
  - ▷ $f(X) = \sum_{i=1}^{n} \sum_{j=1}^{n} C_{ij} X_{ij}$
  - ▷ $f(x) = \sum_{i=1}^{n} C_{i,x_i}$
- Combinatorial optimization problem
  - ▷ $(n-1)!$ possible tours
  - ▷ Enumerating all tours, comparing costs $\Longrightarrow n!$ operations
  - ▷ Impossible except for small numbers of cities
  - ▷ NP-hard
  - ▷ References [14]

Initial tour length = 15751.0

Tour length = 15706.0

Maximum number of trials reached




There are 6.2e+023 tours of 25 cities

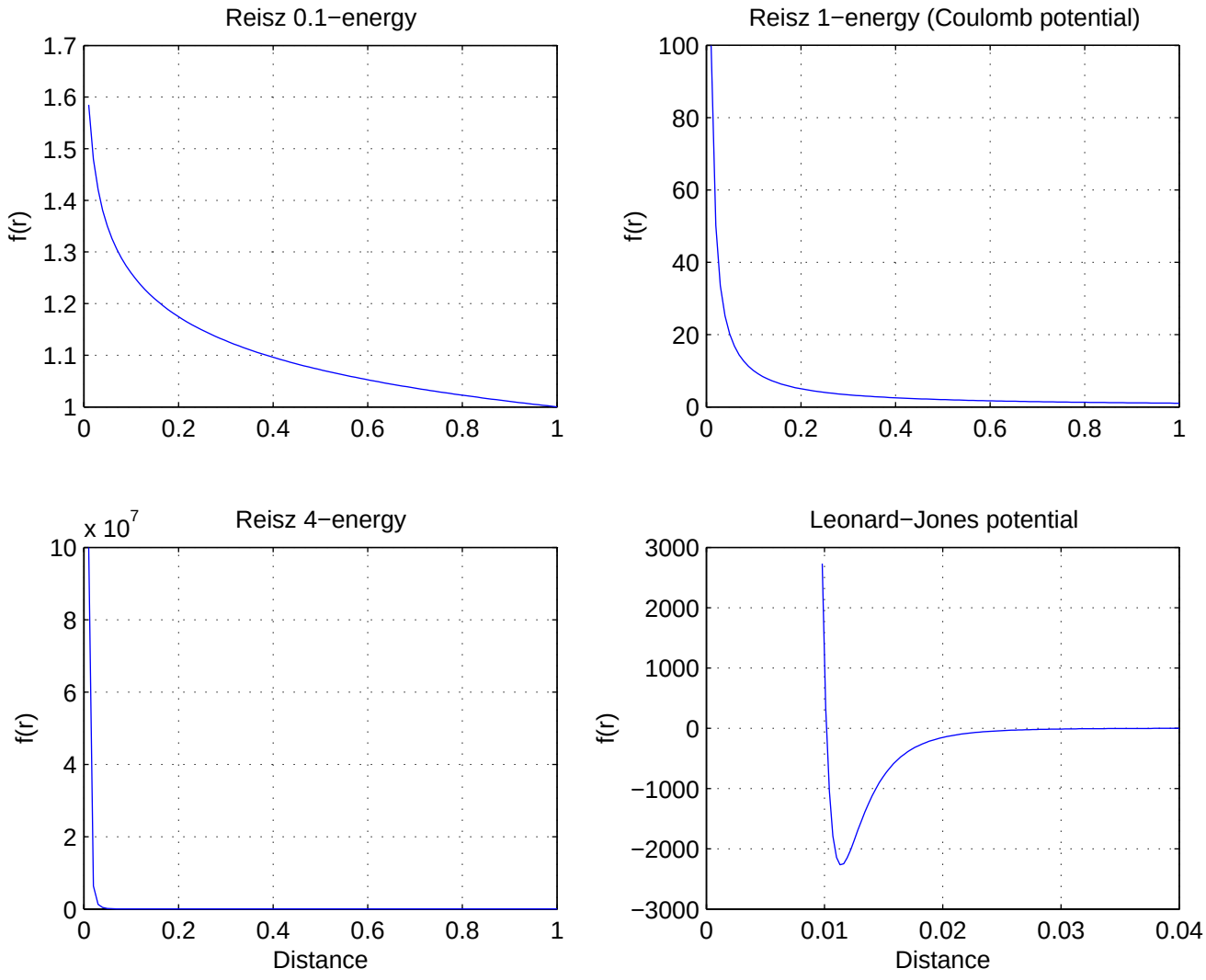
On a 3.0 GHz PC checking ALL tours will take 1.6e+006 centuries

# Minimum Energy Problems

The optimal geometry is one which minimizes the total energy of the system.

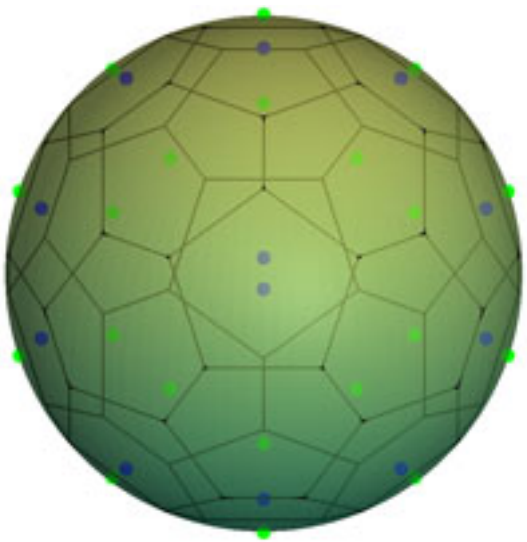
- Protein folding: find the 3-dimensional protein structure given the sequence of amino acids of the protein
  - ▷ Variables: Positions of each amino acid, or relative positions (distances, angles)
  - ▷ Objective: Stretching, bending, torsion, electrostatic energy
  - ▷ Constraints: given order of amino acids,
- Example potentials
  - ▷ Reisz $s$-energy: $V(r) = 1/r^s$ ($s = 1$ Coulomb potential)
  - ▷ Leonard-Jones $V(r) = c_{12}/r^{12} - c_6/r^6$
- Characteristic: Many local minima
  - ▷ Number of local minima grows exponentially with problem size
  - ▷ Many local minima close to global minima
- General mathematical survey by Neumaier [17], others [19]

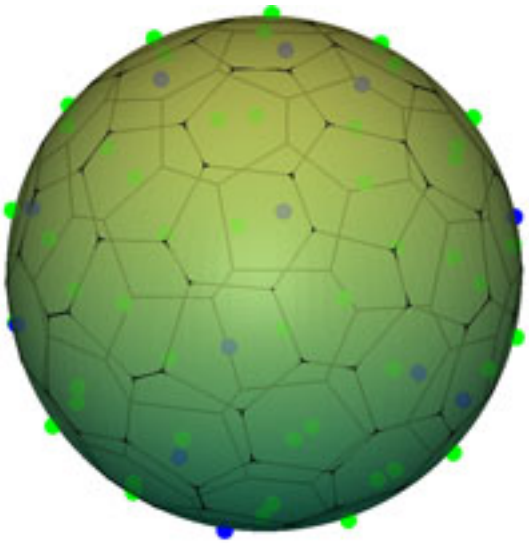
# Potential between two particles



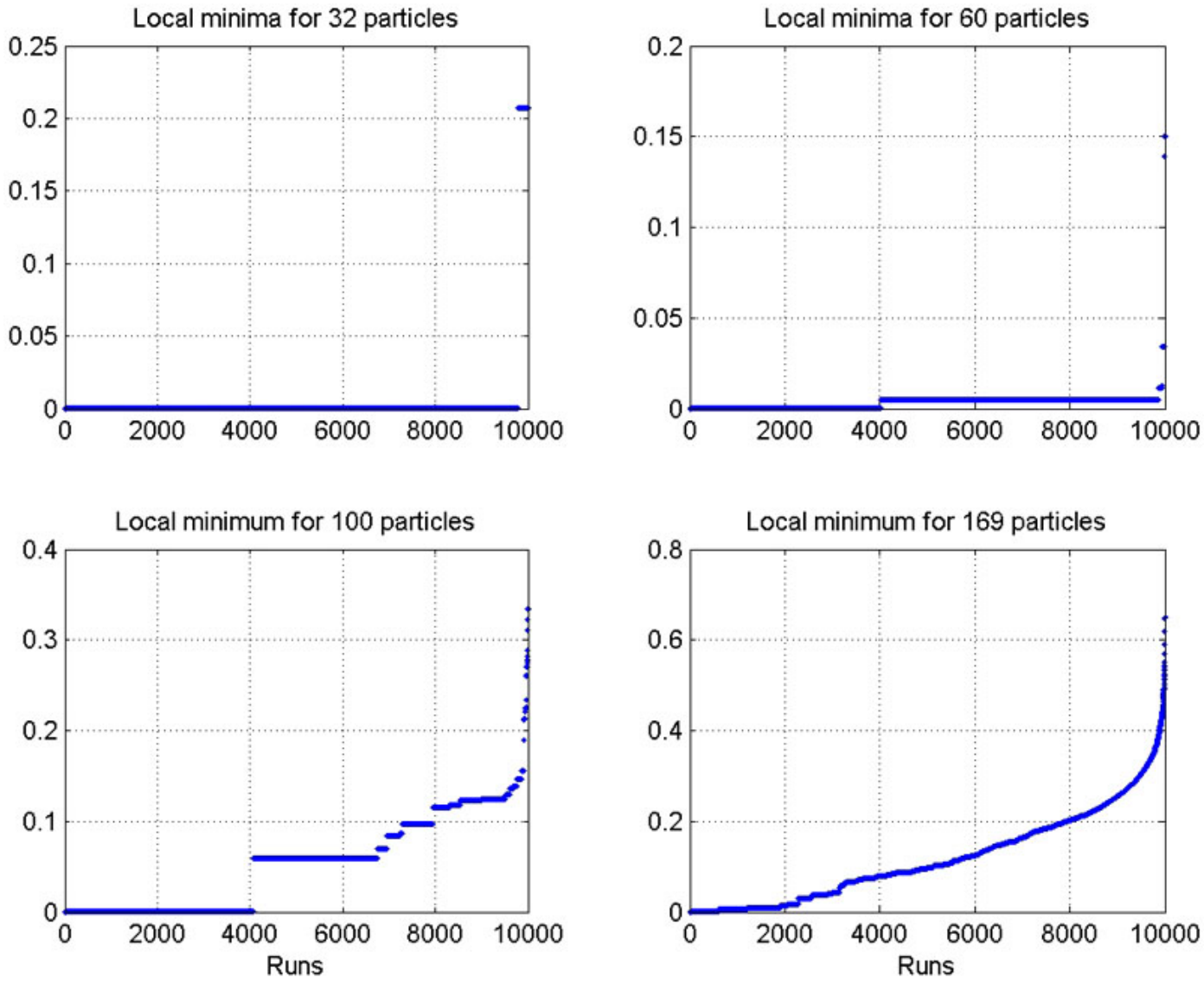
# Minimum Energy on the Sphere

- Particles (electrons) on the surface of the unit sphere
- Using Coulomb potential
- Voronoi cells around each particle gives positions of atoms
- 32 electrons gives $C_{60}$, other Carbon fullerenes
- Stable configurations have few local minima, unstable configurations many





# Minimum energy – Local minima

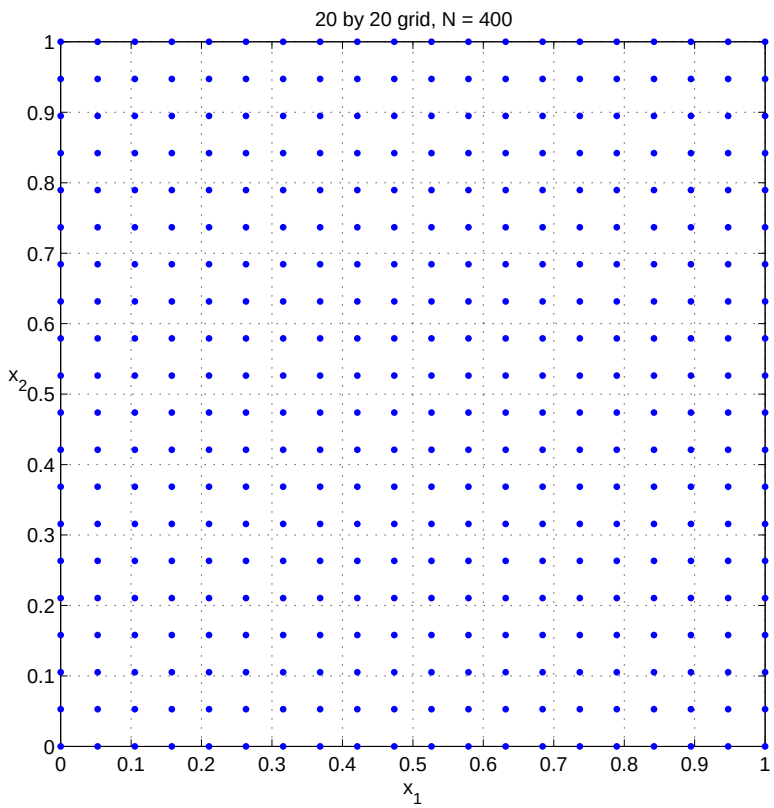


# Exact methods

- Enumeration
  - ▷ Only possible for combinatorial problems
  - ▷ Exponential explosion makes only very small problems possible
- Branch and Bound
  - ▷ Bound: Relax some constraints $\Longrightarrow$ bound on objective value
  - ▷ Branch: Add constraints to remove infeasible points
- Interval methods
- References
  - ▷ Hansen [7], [9, 10]

# Grids – Curse of Dimensionality

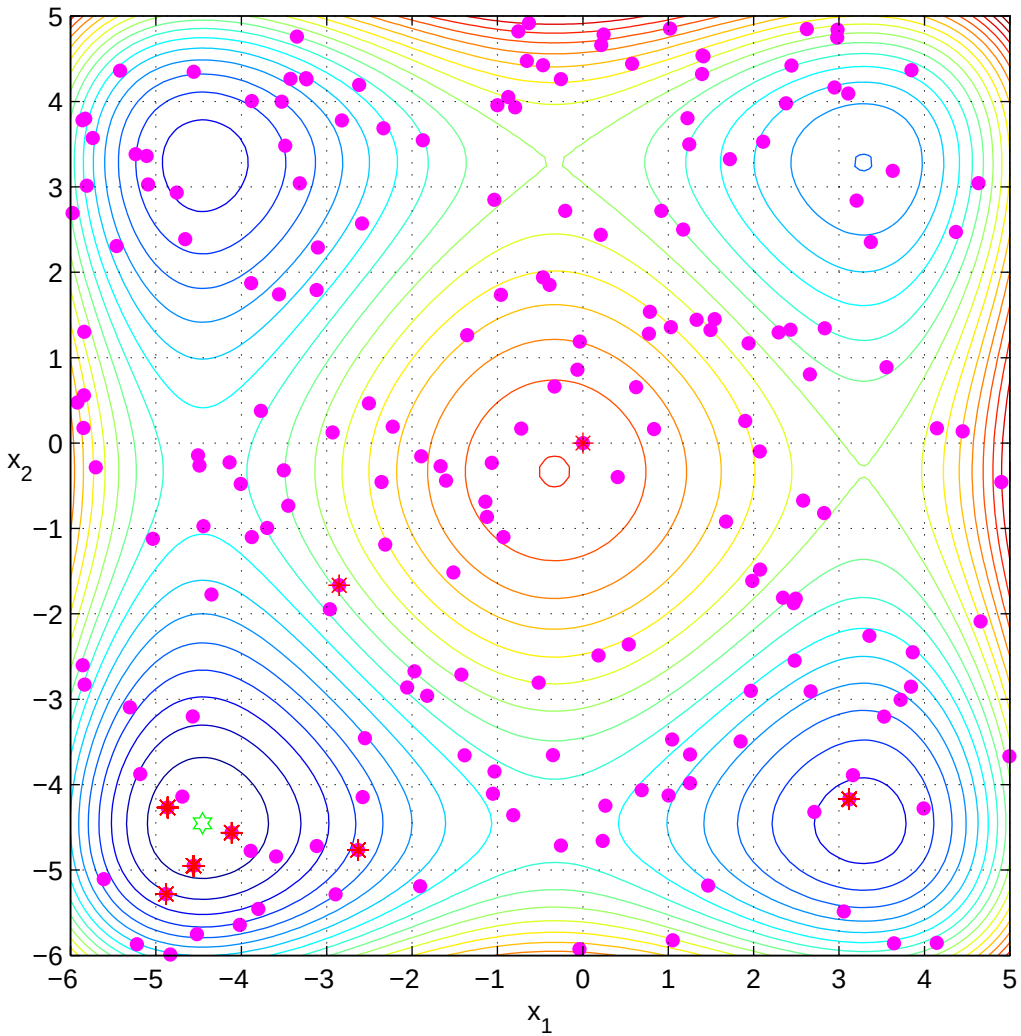
- $k$ points in each variable; $n$ variables
- Tensor product grid has $N = k^n$ points (**Curse of Dimensionality**)
- Example: $\Omega = [0,1]^n$, $n = 1000$, $k = 2 \Longrightarrow N = 2^{1000} \approx 10^{300}$

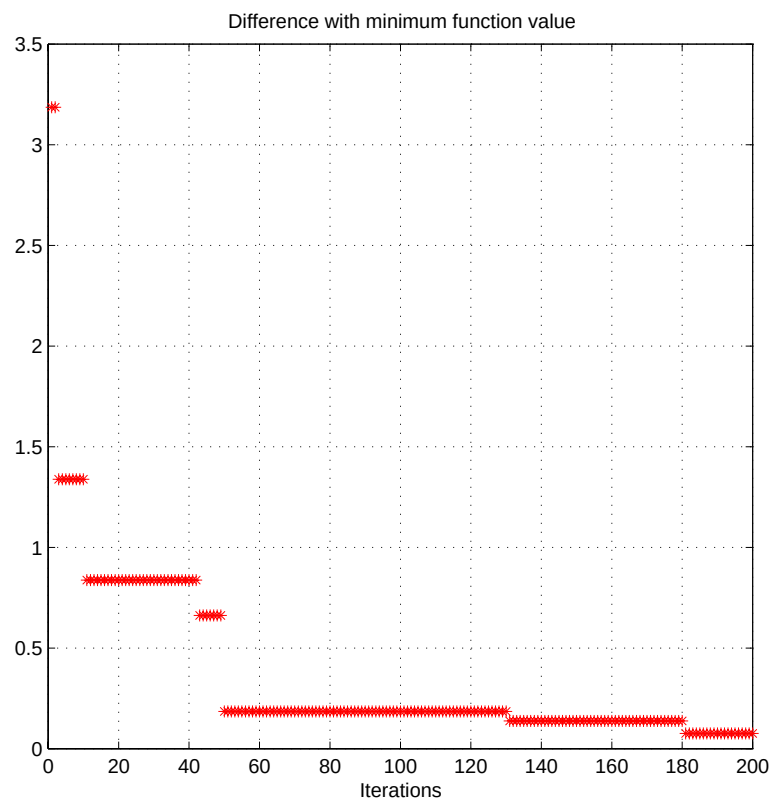


# Monte-Carlo Methods

- Minimize $f(x)$ over $x \in \Omega$
  - ▷ $f_{\min} = \infty$
  - ▷ For $k = 1, \ldots, N$
  - ▷ Generate $x^{(k)} \in \Omega$ uniformly distributed in $\Omega$
  - ▷ Evaluate $f^{(k)} = f(x^{(k)})$
  - ▷ If $f^{(k)} < f_{\min}$ then $f_{\min} = f^{(k)}; \quad x_{\min} = x^{(k)}$
- Generate $x^{(k)}$ by making random changes to $x^{(k-1)}$
- Rate of convergence: Probabilistic
  - ▷ Expected value of error $O\left(N^{-1/2}\right)$ (slow)
  - ▷ Independent of dimension $n$ (very nice)
- Issues
  - ▷ Convergence/number of iterations

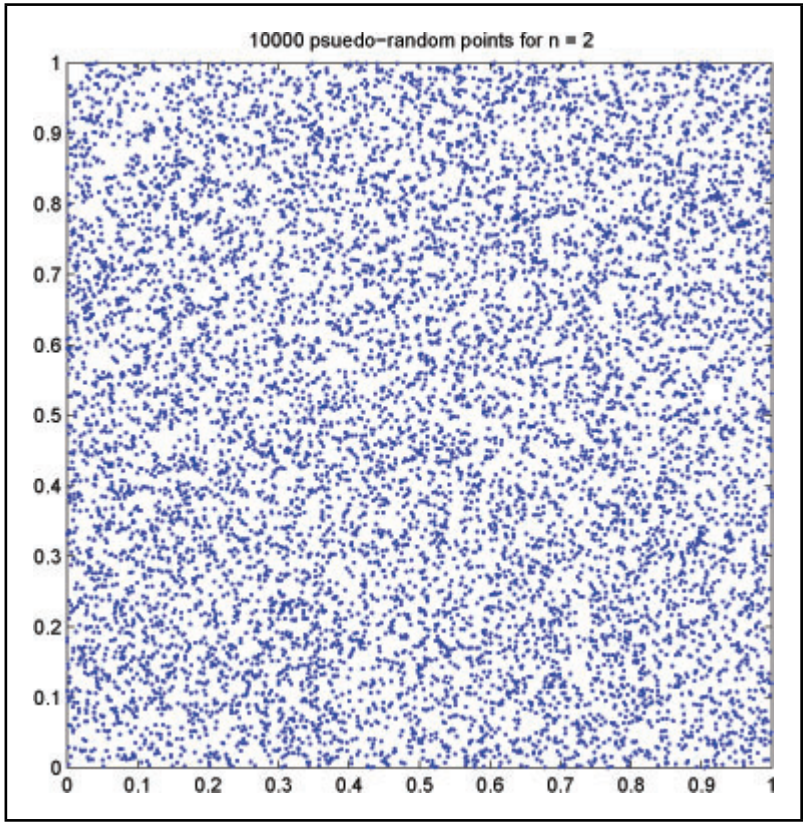
# Two dimensional example

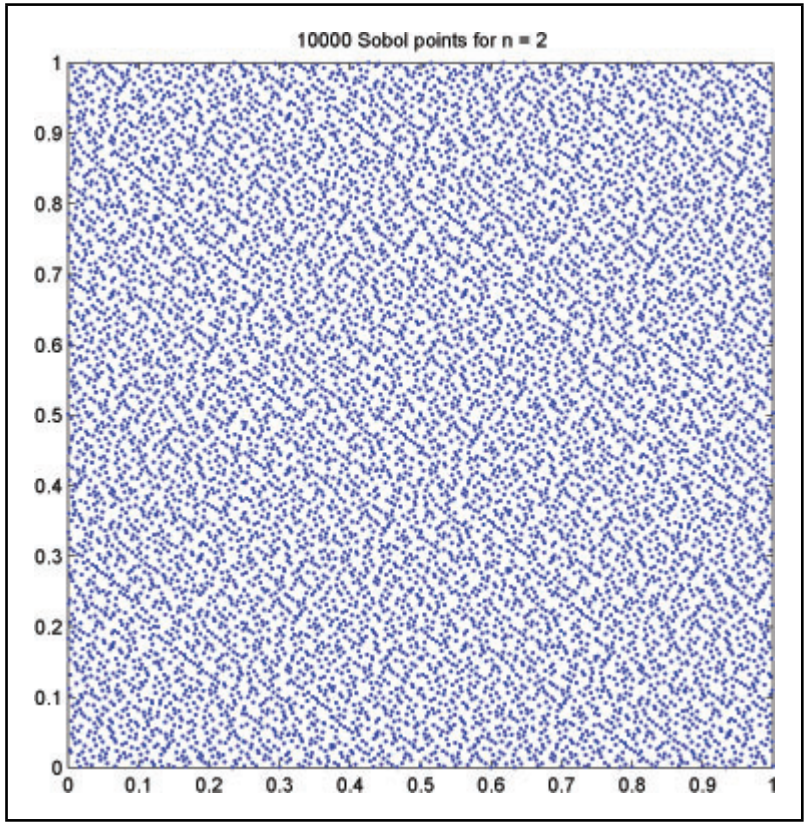


# Quasi Monte-Carlo (QMC) Methods

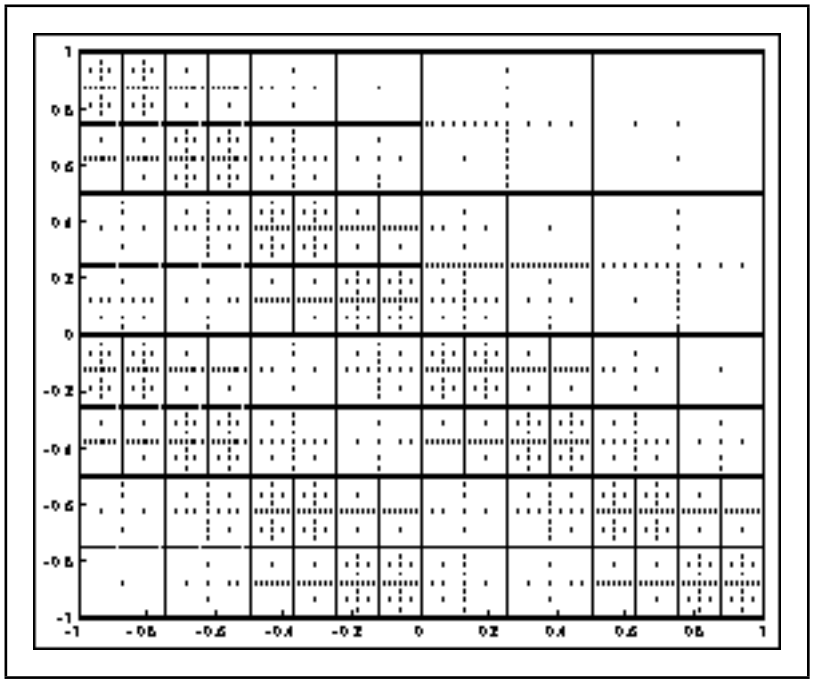
- QMC points are chosen deterministically to be "well distributed" in $[0,1]^n$.
- Examples: Sobol, Halton ,Faure, Niedereitter [18] $(s,t)$-nets, Lattices
- Pseudo-random vs Sobol points



# Sparse Grids

- Selective points are chosen to explore very high dimensional space
- Jochen Garcke, Sparse Grid Tutorial [4].
- Michael Griebel `http://wissrech.ins.uni-bonn.de/main/`



From: `http://wissrech.iam.uni-bonn.de/research/projects/zumbusch/fd.html`

# Simulated Annealing

- Annealing: a molten substance, initially at a high temperature and disordered, is slowly cooled so the the system is approximately in equilibrium. The frozen (minimum energy) ground state at $T = 0$ is ordered
- Generate new state $x^{(k+1)}$ of system:
  - ▷ If energy $f(x^{(k+1)}) < f(x^{(k)})$, accept new state $x^{(k+1)}$;
  - ▷ If the change in energy $\Delta f^{(k)} = f(x^{(k+1)}) - f(x^{(k)}) > 0$, accept $x^{(k+1)}$ with probability $\sim e^{-K\Delta f^{(k)}/T}$
- Issues:
  - ▷ Generating new state;
  - ▷ Initial temperature $T_0$; Cooling schedule
- References
  - ▷ Metropolis (1953) [15]; Kirkpatrick (1983) [13], Cermy (1985) [2]
  - ▷ Numerical Recipes [21] - Second edition.
  - ▷ Ingber Adaptive Simulated Annealing code (ASA) [11, 12]

# Evolutionary Algorithms

- Inspired by Genetic Algorithms: natural selection and survival of fittest
- Algorithm outline
  - ▷ Population: many individuals $x^{(k)}$, with fitness $-f(x^{k)})$
  - ▷ New population using genetic operators: recombination (crossover), mutation, ...
  - ▷ Use fitness of individuals to select those who survive
- GA usually applied to combinatorial optimization problems, with binary representation of population.
- Convergence to global optimum in weak probabilistic sense
- Continuous variables versions (Michalewicz)
- Nonlinear constraints difficult: many individuals not feasible
- References
  - ▷ Holland (1975) [8], Goldberg (1989) [5], Michalewicz [16] and [3]

## References

[1] AD, *Automatic differentiation*, tech. report, Univeristy of Aachen and Argonne National Laboratory, 2005. http://www.autodiff.org/.

[2] V. Cerny, *Thermodynamical approach to the travelling salesman problem: An efficient simulation algorithm*, Journal of Optimization Theory and Applications, 45 (1985), pp. 51–51.

[3] L. Davis, ed., *Handbook of Genetic Algorithms*, Van Nostrand Reinhold, New York, 1991.

[4] J. Garcke, *Sparse grid tutorial*, tech. report, Technical University of Berlin, 2007. http://www.math.tu-berlin.de/~garcke/paper/sparseGridTutorial.pdf.

[5] D. E. Goldberg, *Genetic Algorithms in Search, Optimization and Machine Learning*, Addison-Wesley, Reading, 1989.

[6] A. Griewank, *Evaluating derivatives: principles and techniques of algorithmic differentiation*, SIAM, Philadelphia, 2000.

[7] E. R. Hansen, *Global Optimization using Interval Analysis*, Marcel Dekker, New York, 1992.

[8] J. H. Holland, *Adaption in Natural and Artificial Systems*, University of Michigan Press, 1975. Reprinted by MIT Press, Cambridge MA, 1992.

[9] R. Horst and P. M. Pardalos, eds., *Handbook of Global Optimization*, Kluwer Academic, 1995.

[10] R. Horst, P. M. Pardalos, and N. V. Thoai, eds., *Introduction to Global Optimization*, Kluwer Academic, 2nd ed., 2000.

[11] L. Ingber, *Very fast simulated re-annealing*, Mathematical and Computer Modelling, 12 (1989), pp. 967–973.

[12] L. Ingber and B. Rosen, *Genetic algorithms and very fast simulated reannealing: A comparison*, Mathematical and Computer Modelling, 16 (1992), pp. 87–100.

[13] S. Kirkpatrick, C. D. Gelatt Jr., and M. P. Vecchi, *Optimization by simulated annealing*, Science, 220 (1983), pp. 671–680.

[14] E. L. Lawler, J. K. Lenstra, A. H. G. R. Kan, and D. B. Shmoys, *The Traveling Salesman Problem : A Guided Tour of Combinatorial Optimization*, John Wiley, 1985.

[15] N. Metropolis, A. Rosenbluth, A. Teller, and E. Teller, *Equation of state calculations by fast computing machines*, Journal of Chemical Physics, 21 (1953), pp. 1–87–1092.

[16] Z. Michalewicz, *Genetic Algorithms + Data Structures = Evolution Programs*, Springer-Verlag, Berlin, second ed., 1994.

[17] A. Neumaier, *Molecular modelling of proteins and mathematical prediction of protein structure*, SIAM Review, 39 (1997), pp. 407–460.

[18] H. Niederreiter, *Random Number Generation and Quasi-Monte Carlo Methods*, SIAM, Philadelphia, 1992.

[19] P. M. Pardalos, D. Shalloway, and G. Xue, *Optimization methods for computing global minima of nonconvex potentail energy functions*, Journal of Global Optimization, 4 (1994), pp. 117–133.

[20] J. D. Pinter, *Global Optimization in Action*, Kluwer, Dordrecht, 1995.

[21] W. M. Press, B. Flannery, S. Teuklosky, and W. Vettering, *Numerical Recipes in C: The Art of Scientific Computing*, Cambridge University Press, New York, 2nd ed., 1992. http://www.nr.com//.