An introduction to Numerical Optimization

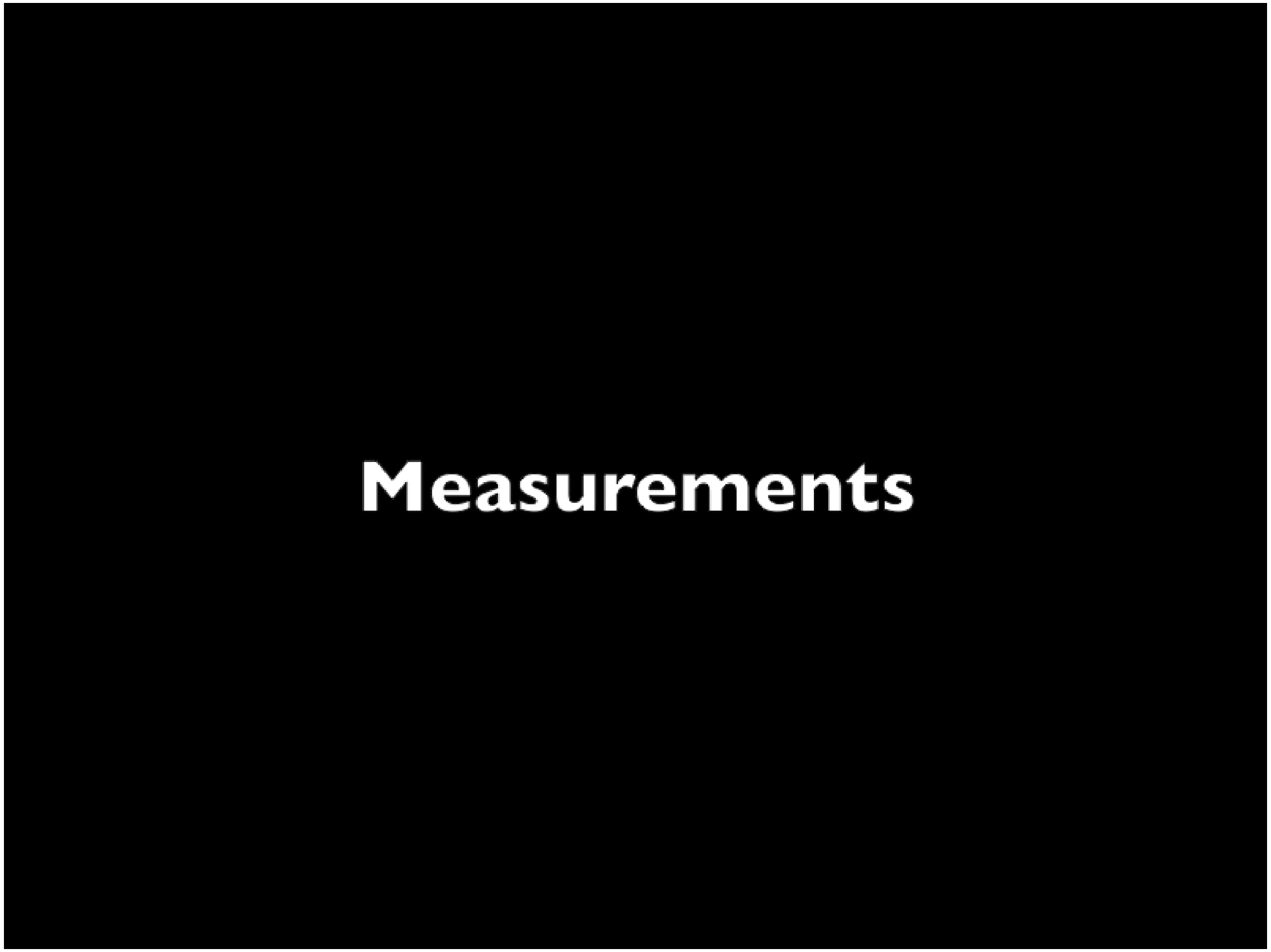
Stelian Coros

Plan for Today

- A fast and furious tour through numerical optimization
  - Unconstrained Optimization
    - Gradient Descent
    - Newton’s Method
  - Constrained Optimization
    - Newton’s Method
    - Quadratic Programming
  - Stochastic Optimization
  - Discrete Optimization

Optimization in Graphics

- Simulation and Material Parameter Estimation



Introduction to Optimization

- Optimization involves finding an "optimal value"

- i.e. Maximizing a profit, minimizing forces, etc…

$$\underbrace{\boxed{\min}}_{\text{minimize}}\ \overbrace{\boxed{f\left(x\right)}}^{\text{Cost Function}}$$

Introduction to Optimization

- Optimization involves finding an "optimal value"

- i.e. Maximizing a profit, minimizing an area etc…

$$\boxed{x^*} = \arg\min f(x)$$

Optimal Solution

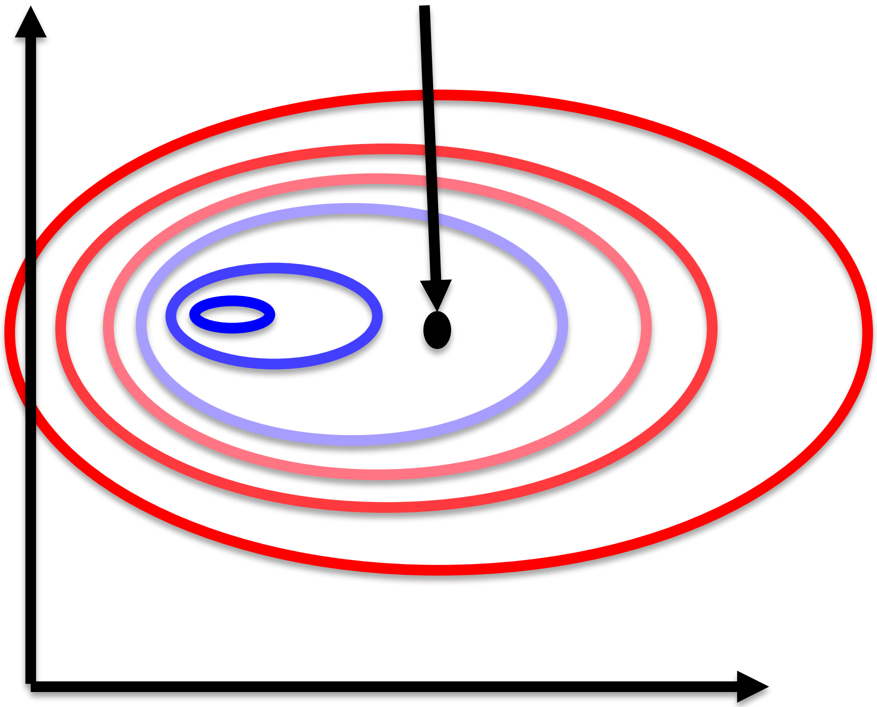
Types of Optimization

- Continuous vs. Discrete
- Constrained vs. Unconstrained

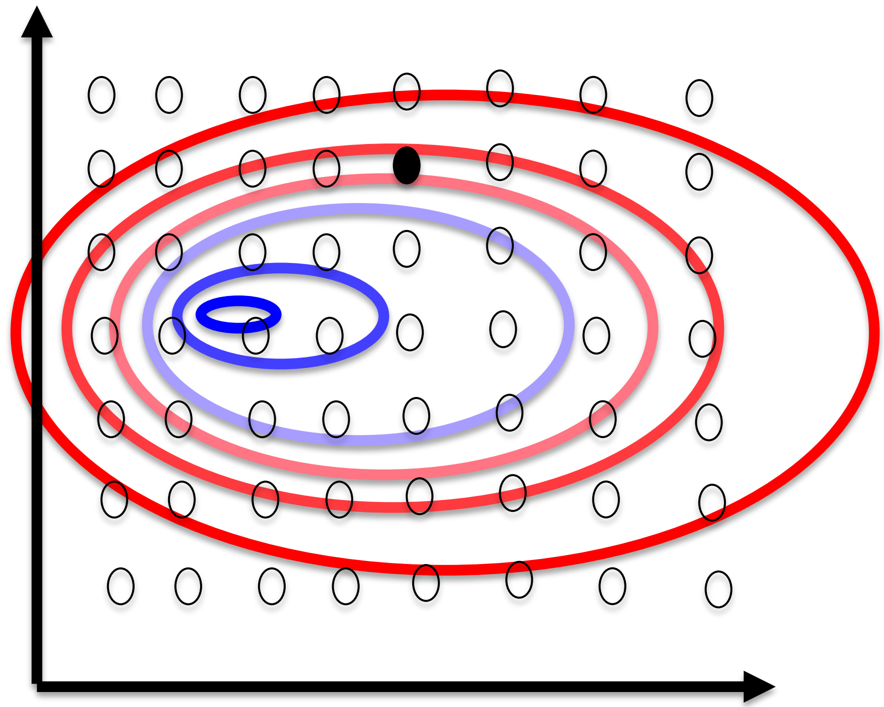
Continuous

Discrete

This point can move smoothly

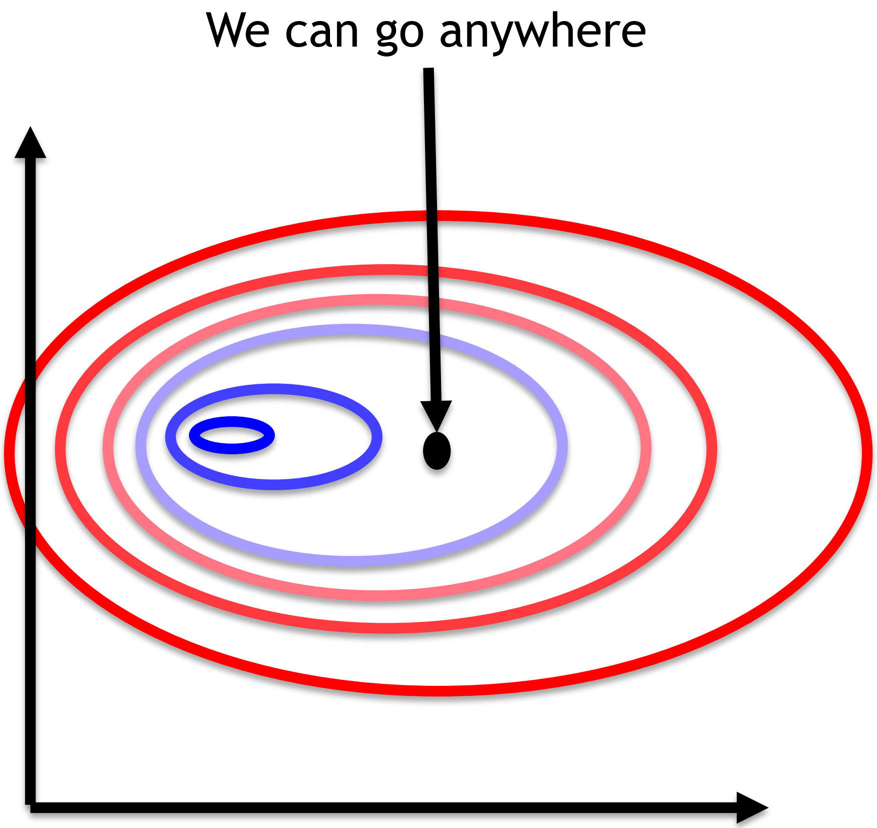


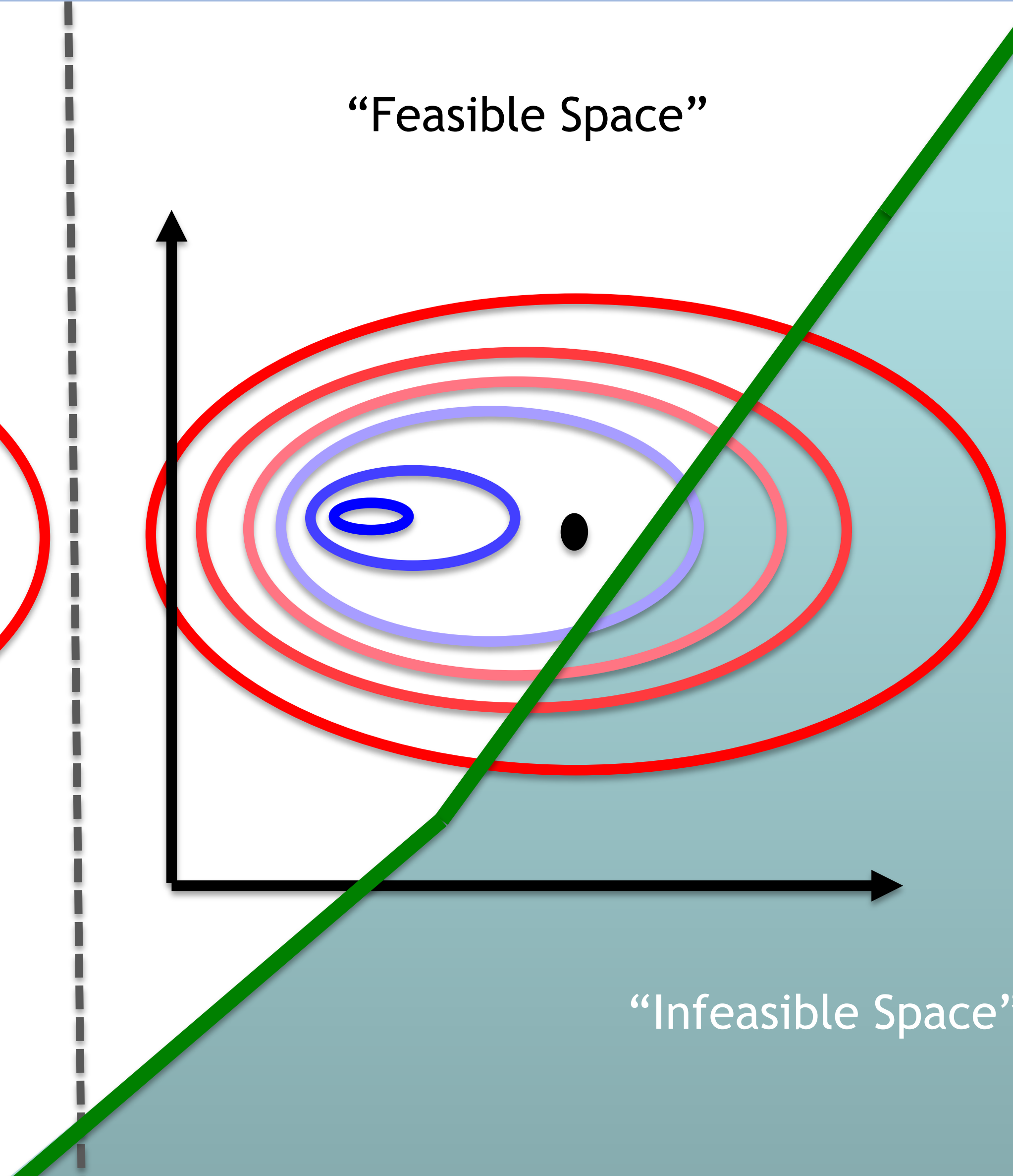
Choose from discrete points in parameter space



Unconstrained

Constrained





Types of Optimization

- $\boxed{\text{Continuous}}$ vs. Discrete
- Constrained vs. $\boxed{\text{Unconstrained}}$

Continuous Optimization

- We're solving

$$x^* = \arg\min f(x)$$

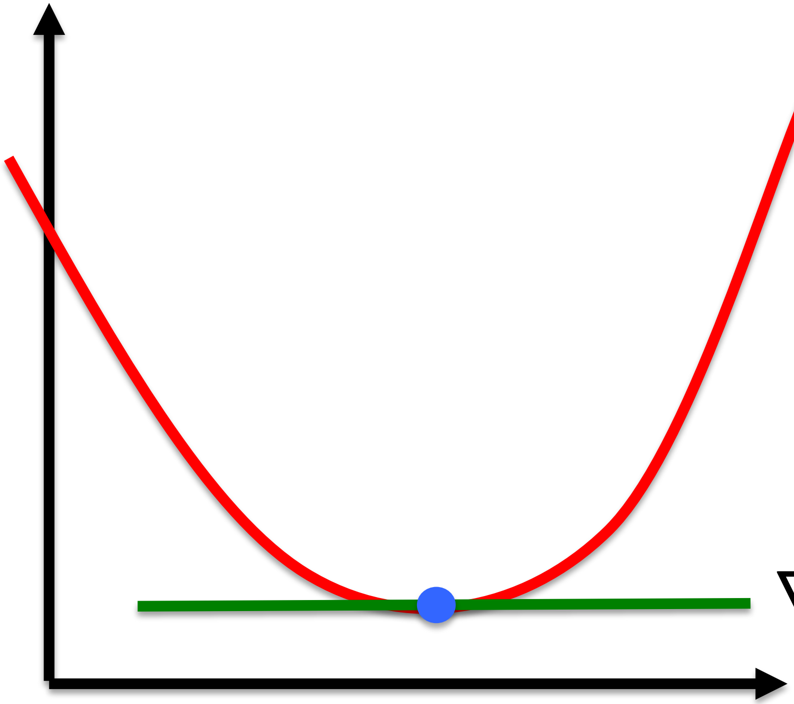
- How do we know we've found a potential solution?

IMPORTANT!!!!!

$$\nabla \mathbf{f}(\mathbf{x}^*) = \mathbf{0}$$

Potential Solutions

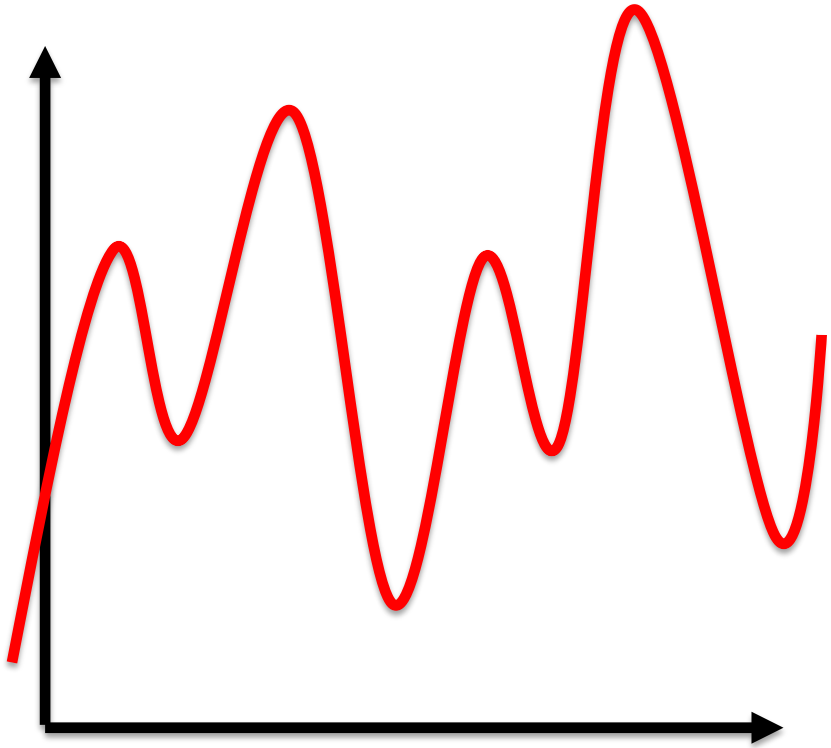
- Intuitively we look for a flat point on the cost function



$$\nabla \mathbf{f}\left(\mathbf{x}^*\right) = \mathbf{0}$$

Potential Solutions

- Sometimes that’s easier said than done



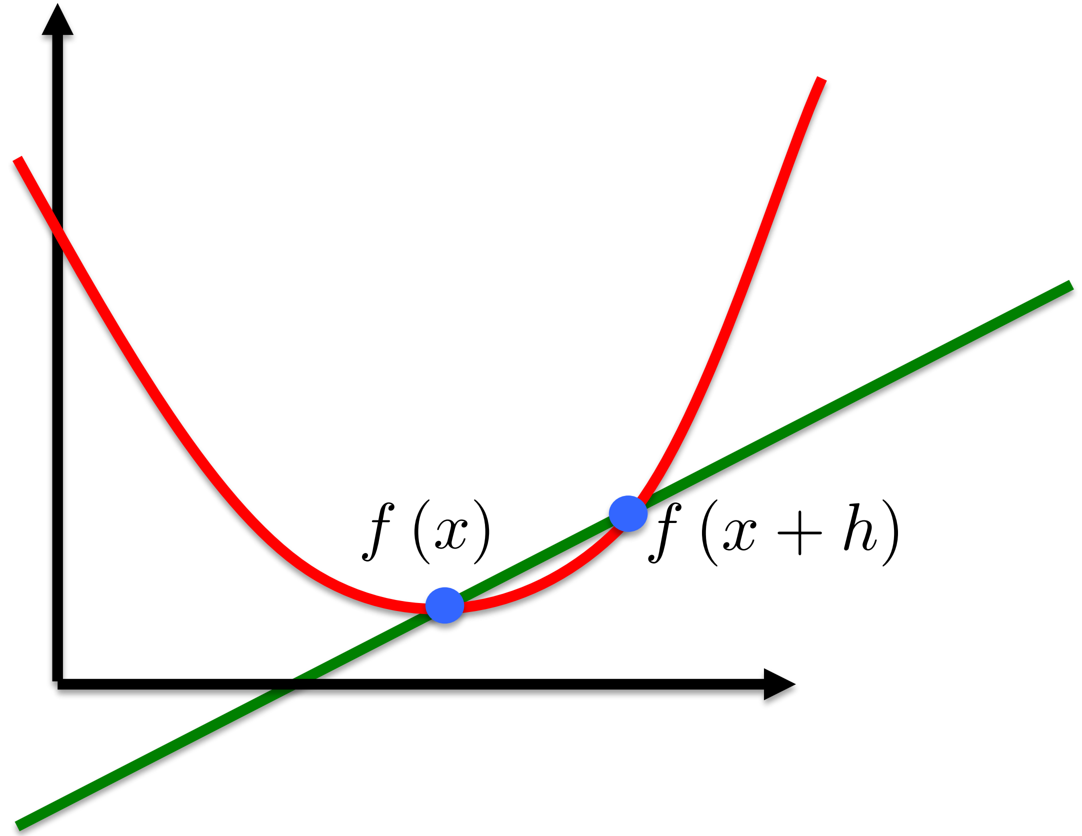
Computing Derivatives

- Analytically (pen and paper, mathematica)
- Finite Differences (via Taylor series)

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f^{(3)}(a)}{3!}(x-a)^3 + \ldots + \frac{f^{(n)}(a)}{n!}(x-a)^n + \ldots.$$

Potential Solutions

- Computing the gradient requires a limit



Potential Solutions

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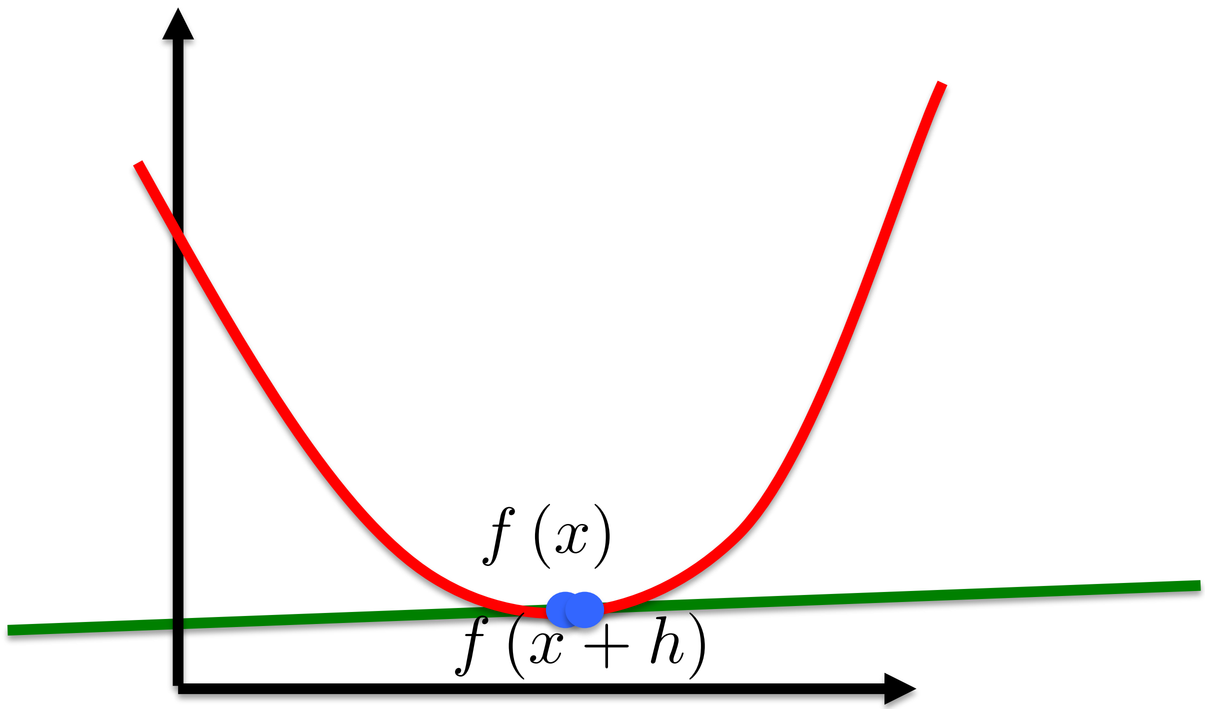
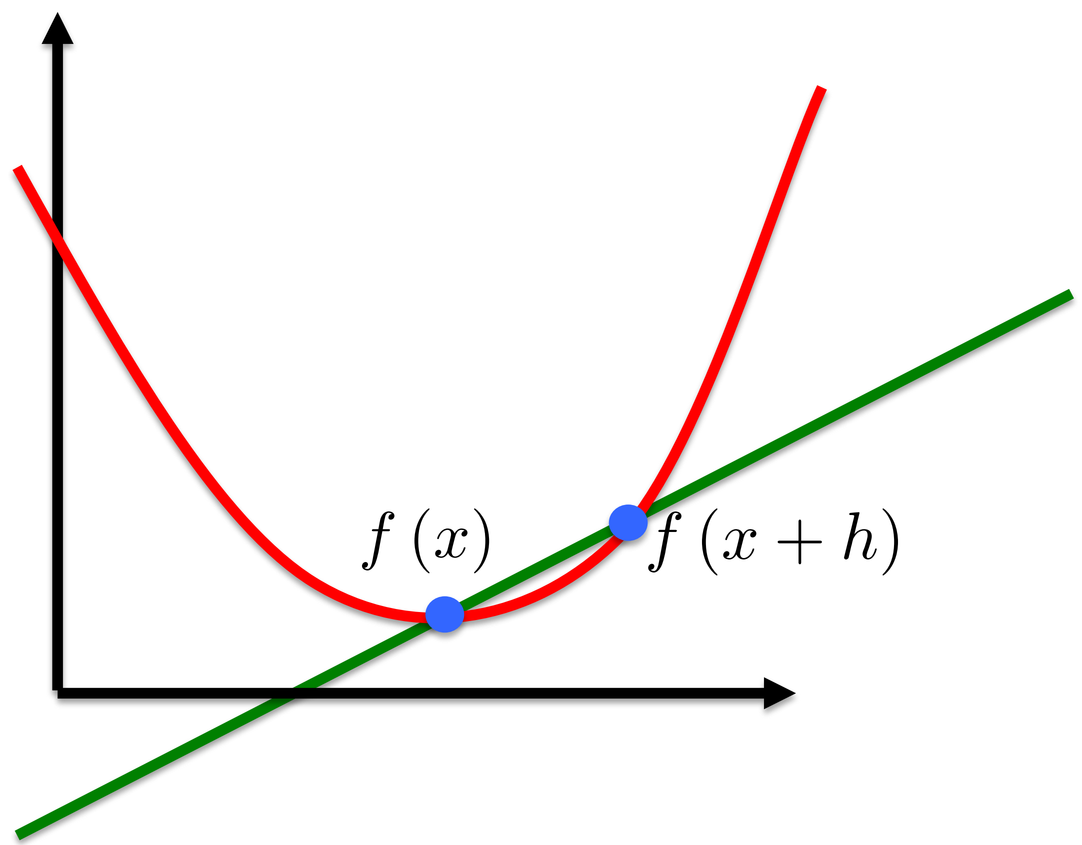


Potential Solutions

- In Finite Differencing we choose *h* and estimate the derivative numerically



Continuous Optimization

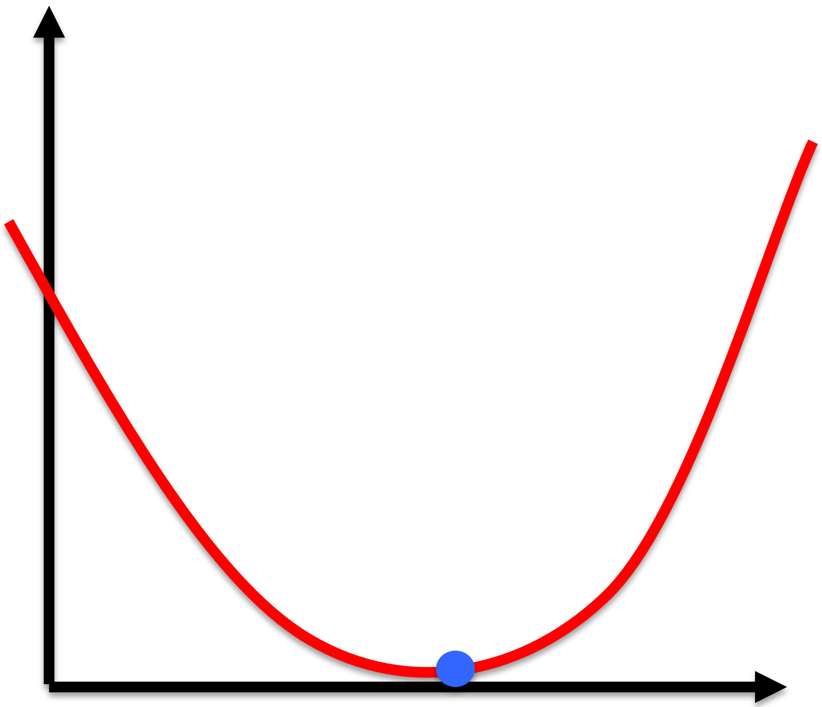
- General, continuous optimizations are difficult to solve – but we keep trying anyway
- We focus on certain classes of problems that are solvable

Convex Optimization

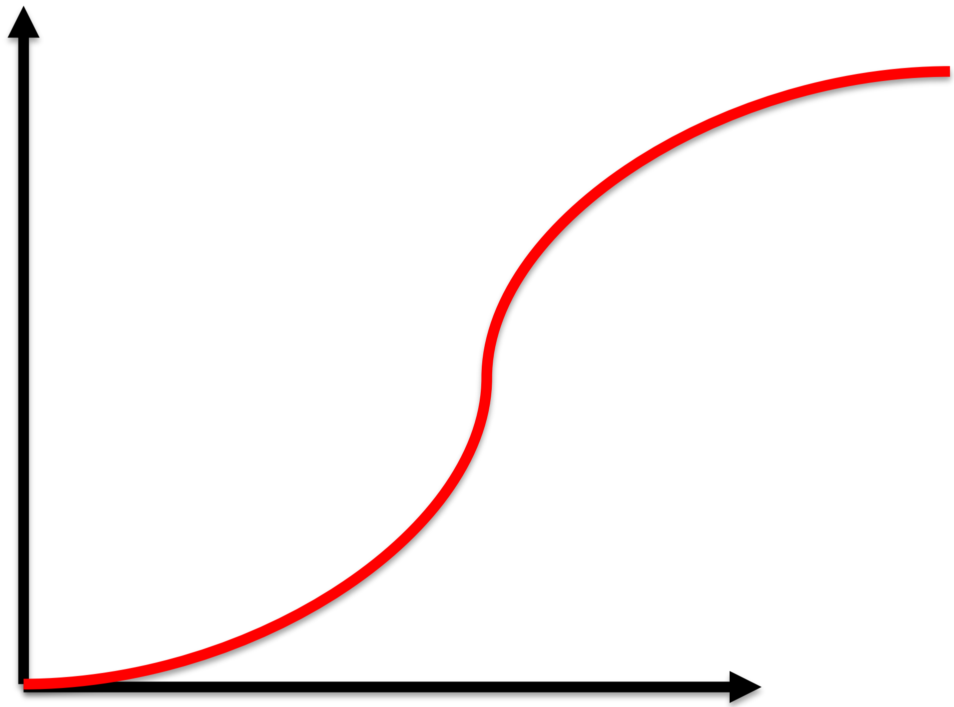
Convex Optimization

- Convex optimizations are ones that have a single minimum
- Let’s look at some examples of convex cost functions

Convex Optimization



Is This Convex ?



Descent Algorithms

- Idea: Follow search directions that reduce the cost!
- Two Types
  - Gradient Descent
  - Newton's Method

Gradient Descent

- Recall that the gradient of a function is given by

$$\nabla f\left(\mathbf{x}\right) = \begin{pmatrix} \frac{\partial f}{\partial \mathbf{x}_1} & \frac{\partial f}{\partial \mathbf{x}_2} & \cdots & \frac{\partial f}{\partial \mathbf{x}_n} \end{pmatrix}$$

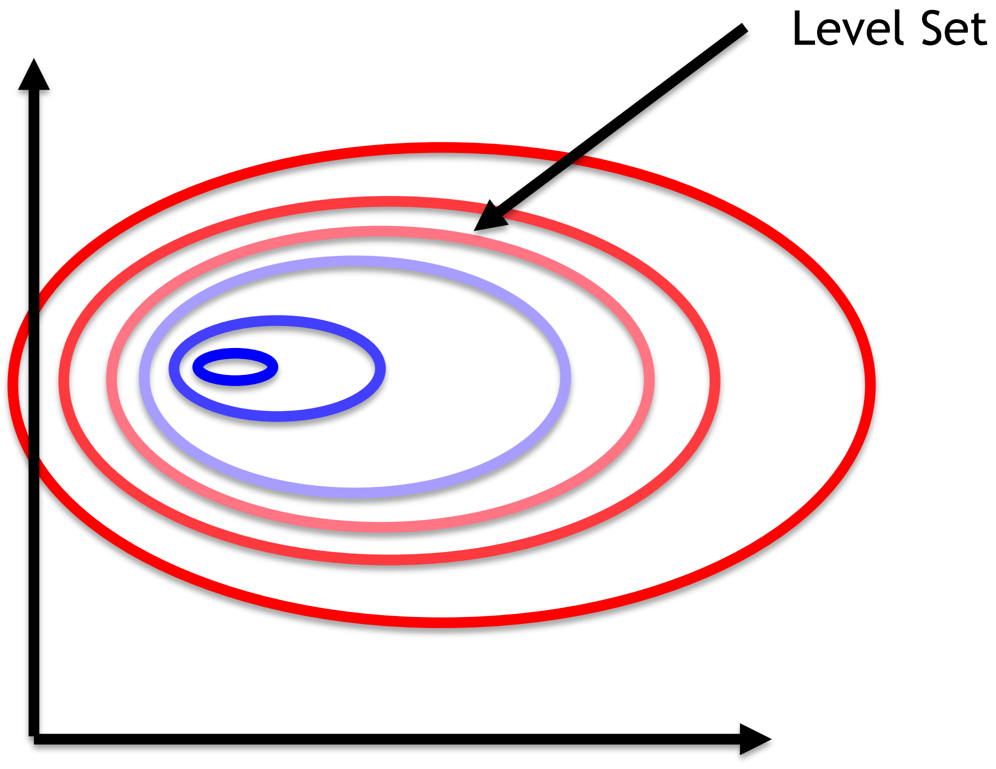
Gradient Descent

- Recall that the gradient of a function is given by

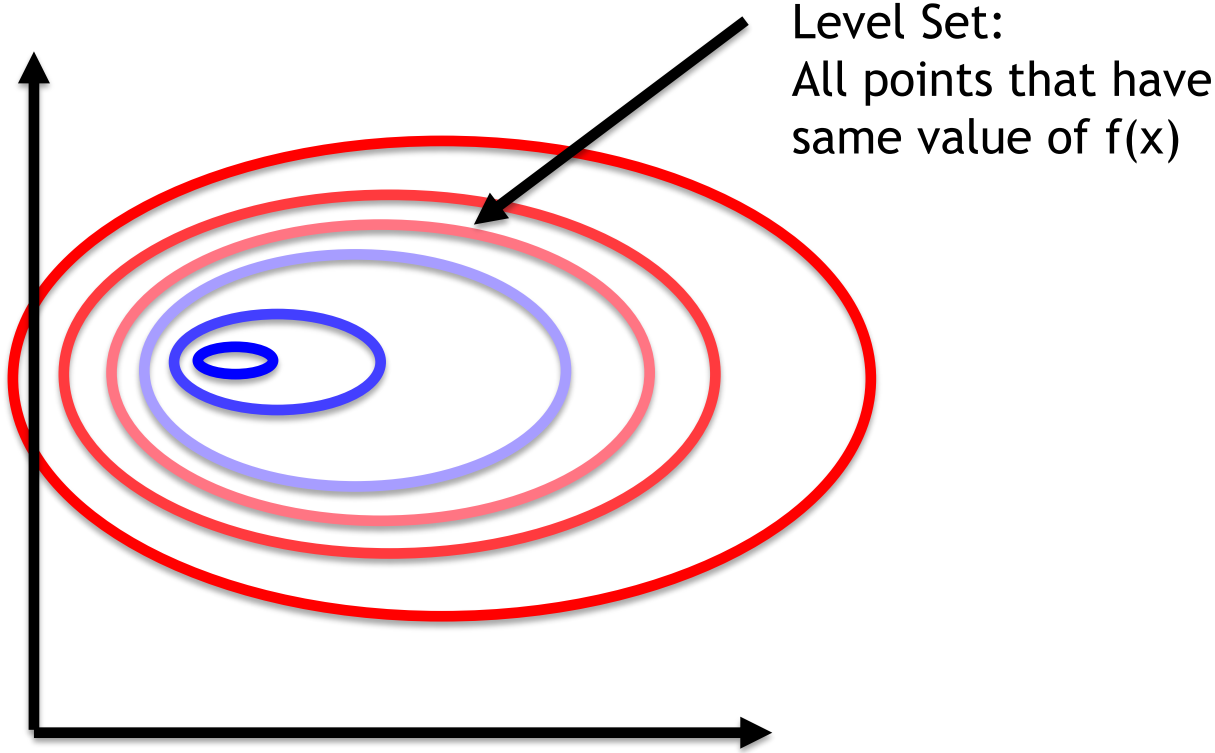
$$\nabla f(\mathbf{x}) = \begin{pmatrix} \frac{\partial f}{\partial \mathbf{x}_1} & \frac{\partial f}{\partial \mathbf{x}_2} & \cdots & \frac{\partial f}{\partial \mathbf{x}_n} \end{pmatrix}$$

- Points in direction of maximum ascent

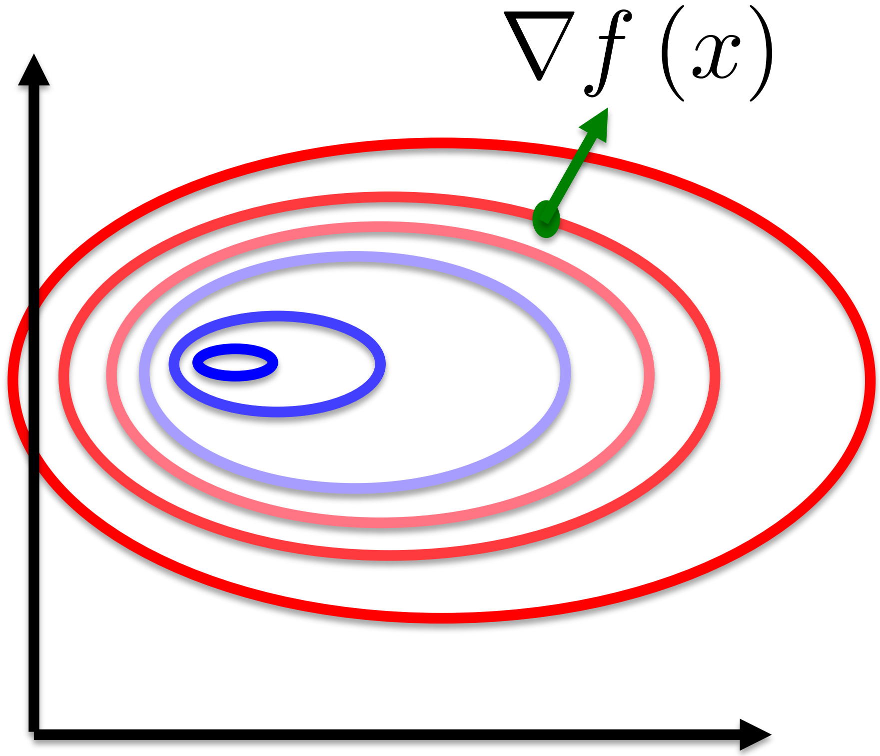
An Aside: Level Sets



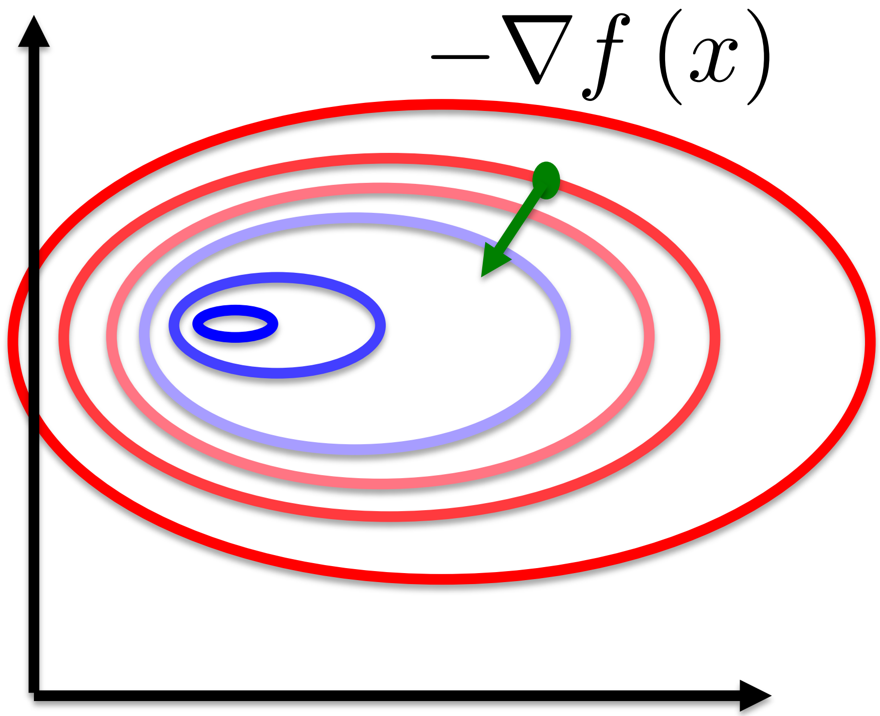
An Aside: Level Sets



Gradient Descent



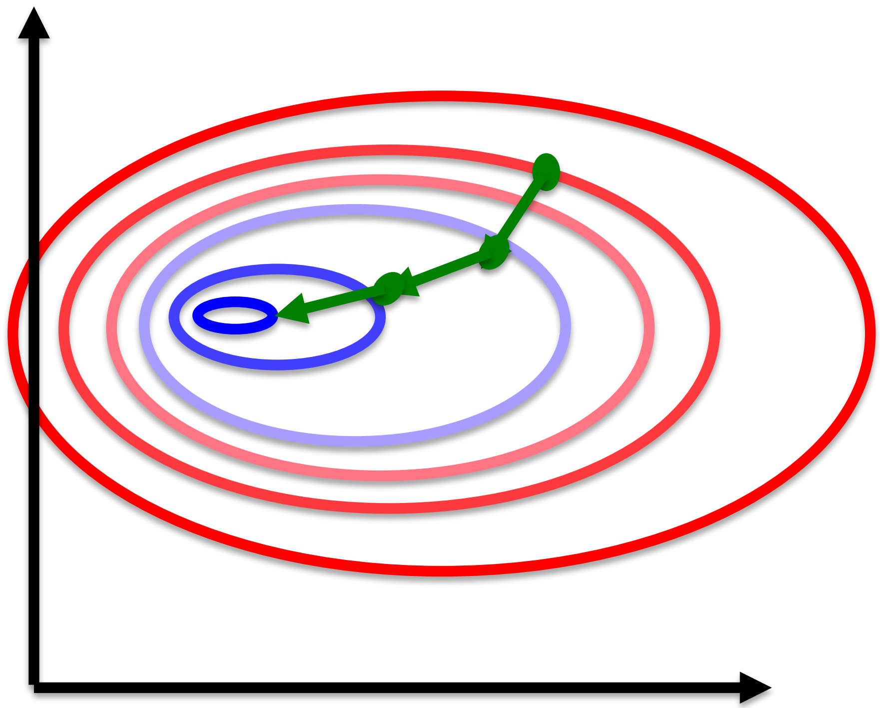
Gradient Descent



Simple Gradient Descent Algorithm

- While not at an optimal point
  - Compute the gradient at current point (x)
  - Move to new point $x = x - \boxed{h} \nabla f(x)$
  - Step size h: typically need line search

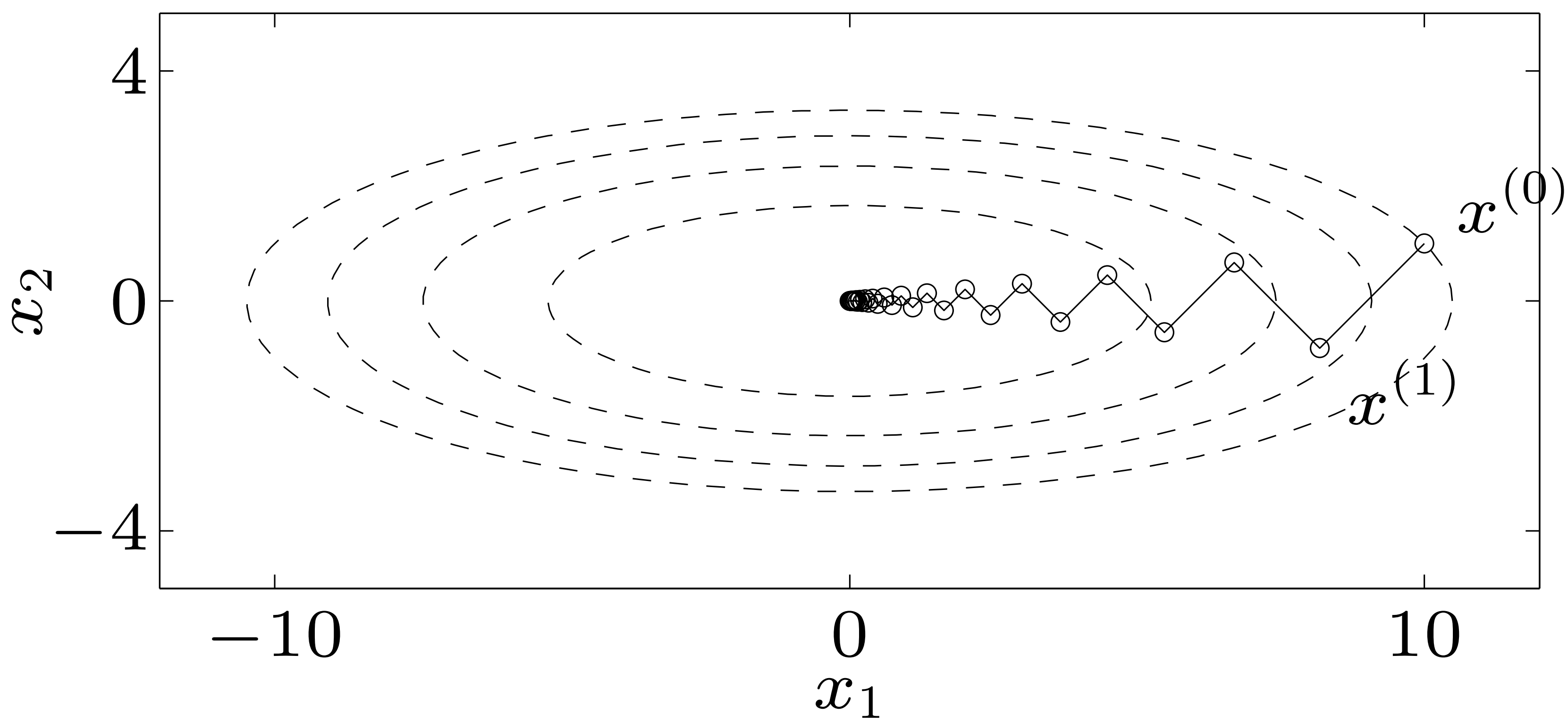
Gradient Descent



Gradient Descent

- Good:
  - Simple to implement
- Bad:
  - Sometimes converges badly

Gradient Descent

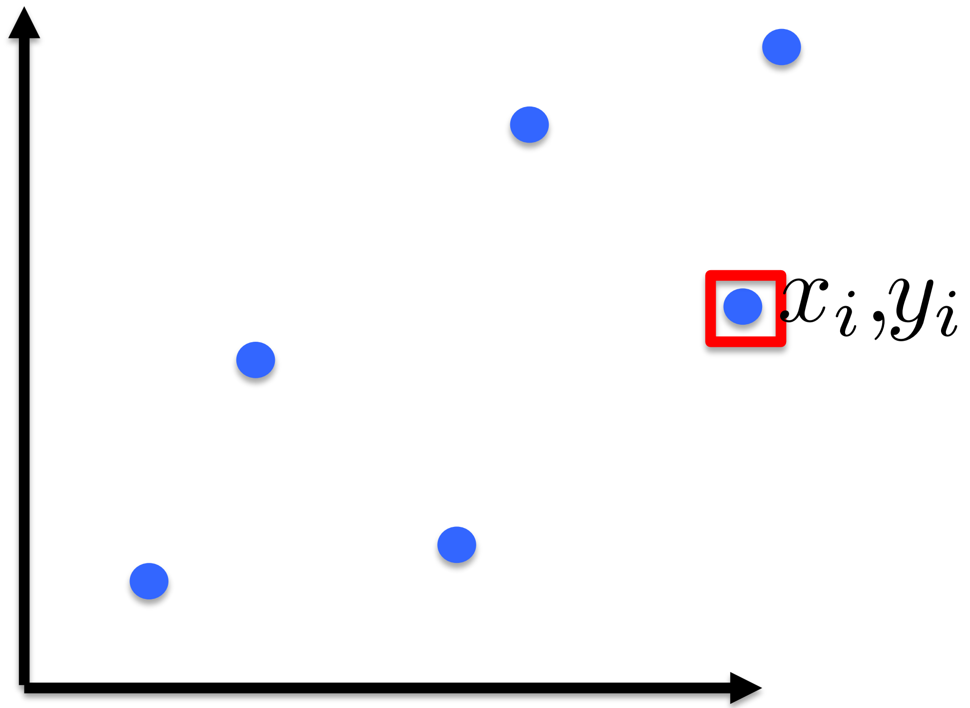


Newton’s Method

- Can we choose better search directions?
- Hint: quadratic functions are very nice!

A Simple Example: Least Squares

- Least Squares Fitting of a Curve



- Want to find a line, mx + c, that is a “best fit”

A Simple Example: Least Squares

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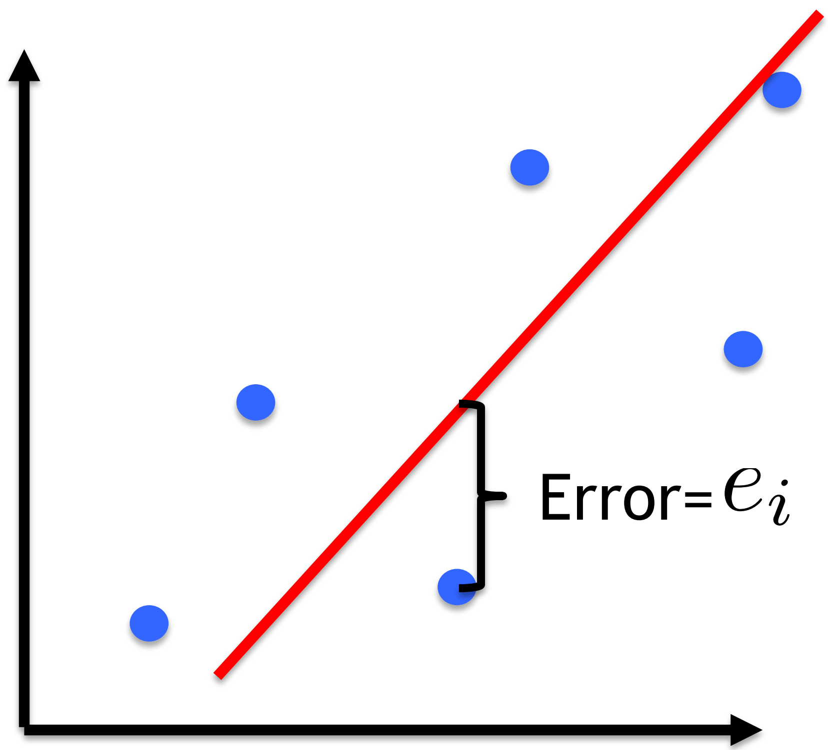

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A Simple Example: Least Squares

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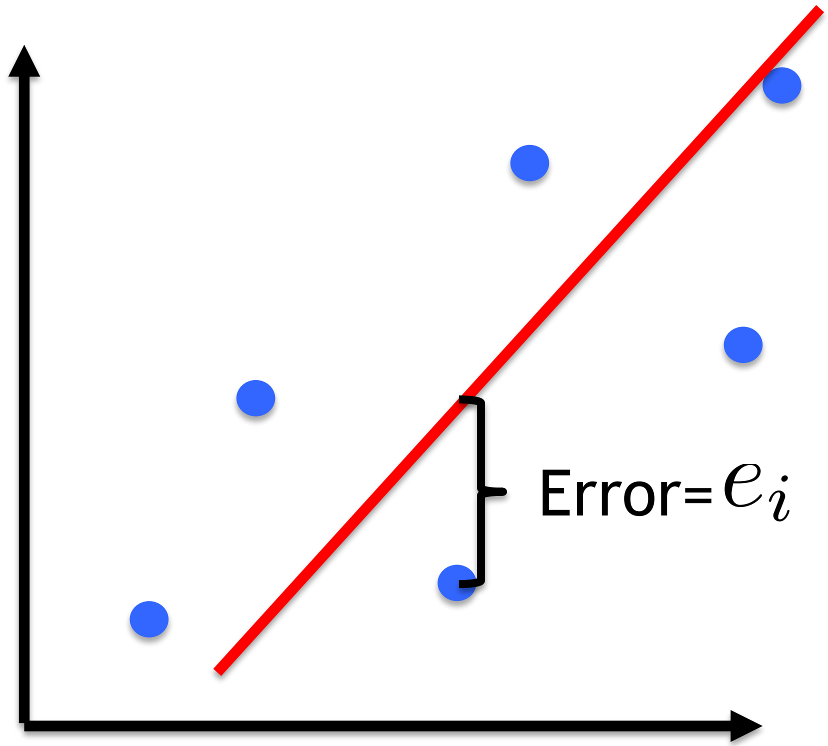
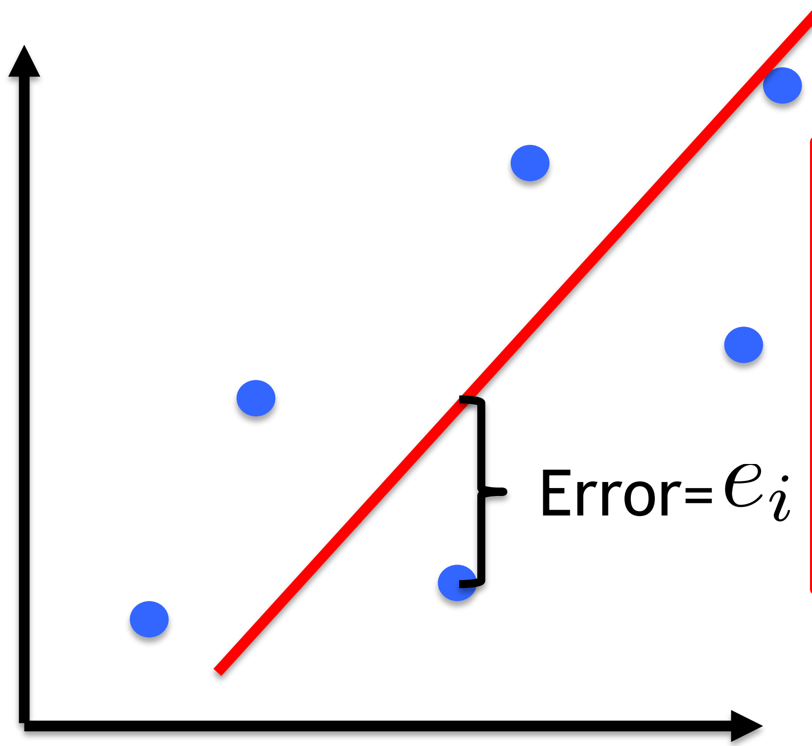


$$e_i = y_i - mx_i - c$$

A Simple Example: Least Squares

- Minimize sum of squared errors



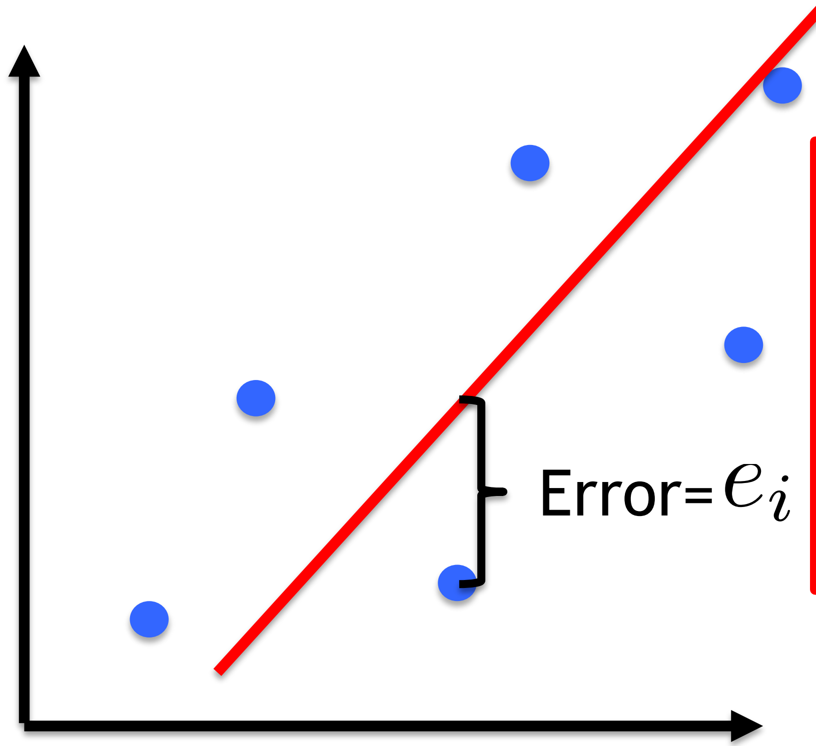
$$\mathbf{A} = \begin{pmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \\ x_n & 1 \end{pmatrix}$$

Total Error = $\|\mathbf{A}\theta - \mathbf{y}\|^2$

A Simple Example: Least Squares

- Minimize sum of squared errors

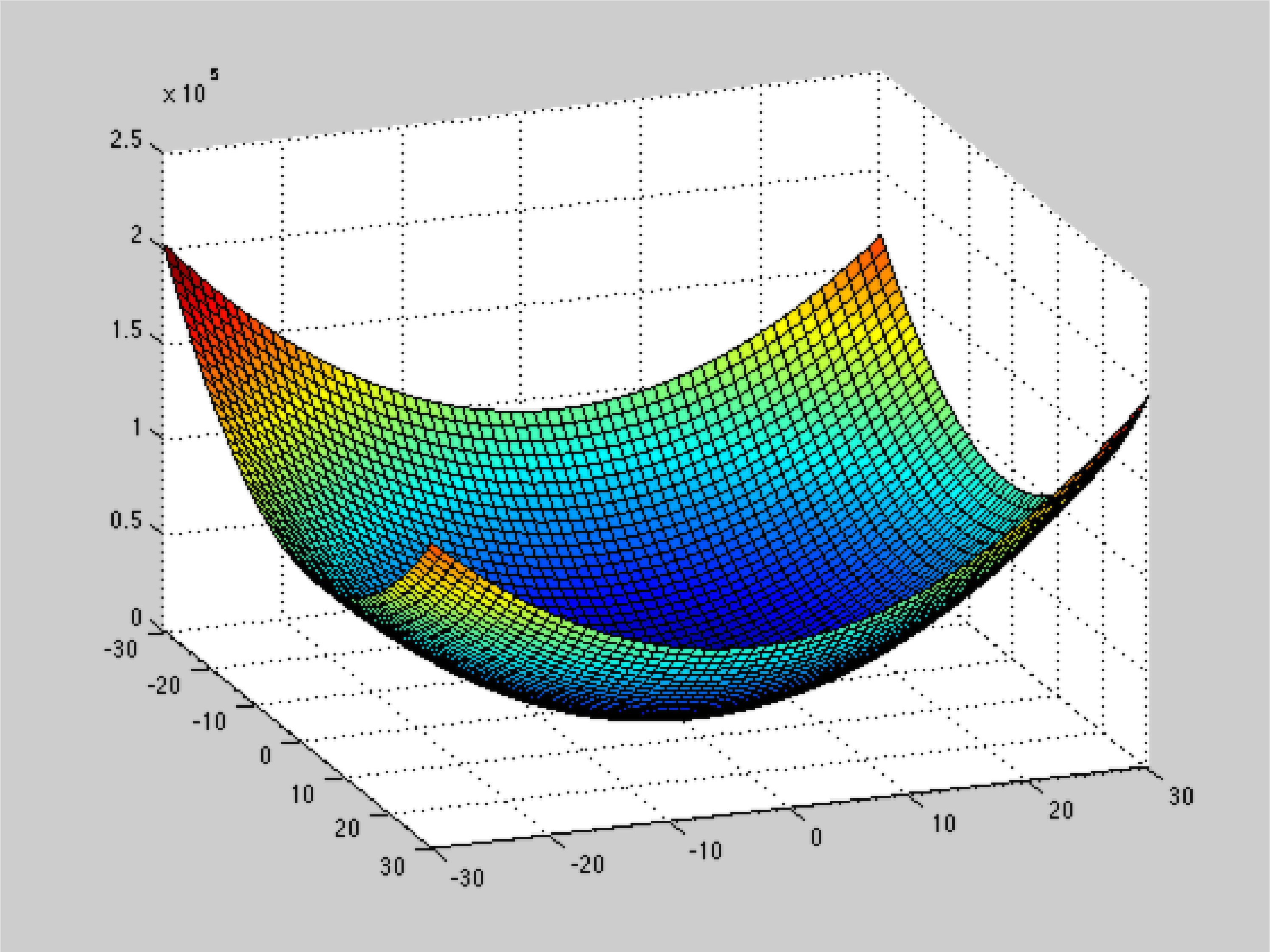
$$\boxed{\theta = \begin{pmatrix} m \\ c \end{pmatrix}}$$



$$\boxed{\mathbf{A} = \begin{pmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \\ x_n & 1 \end{pmatrix}}$$

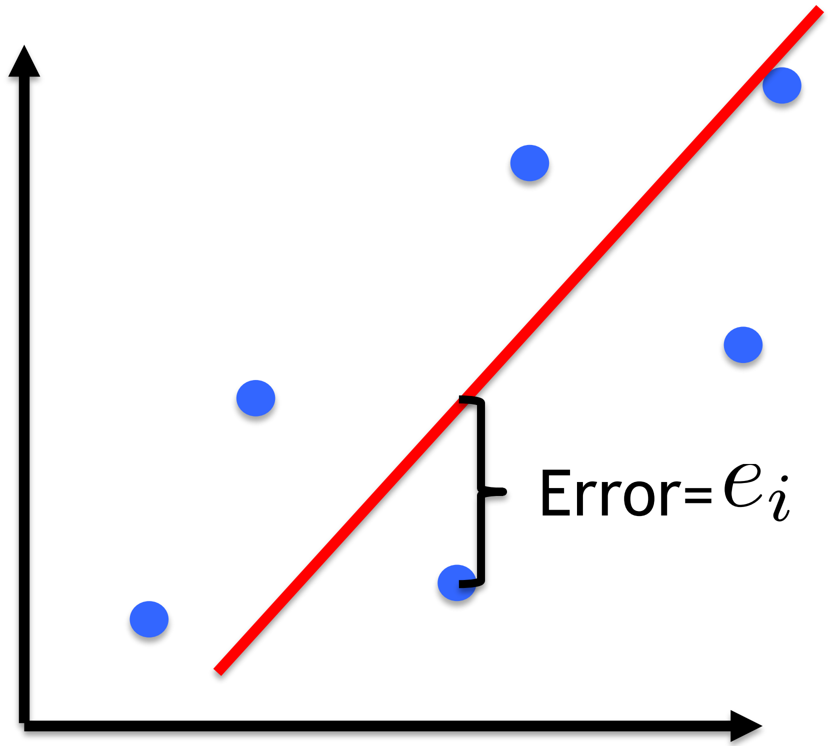
Sum of Squared Error = f(x) = $||\mathbf{A}\theta - \mathbf{y}||^2$

Simple Example: Least Squares



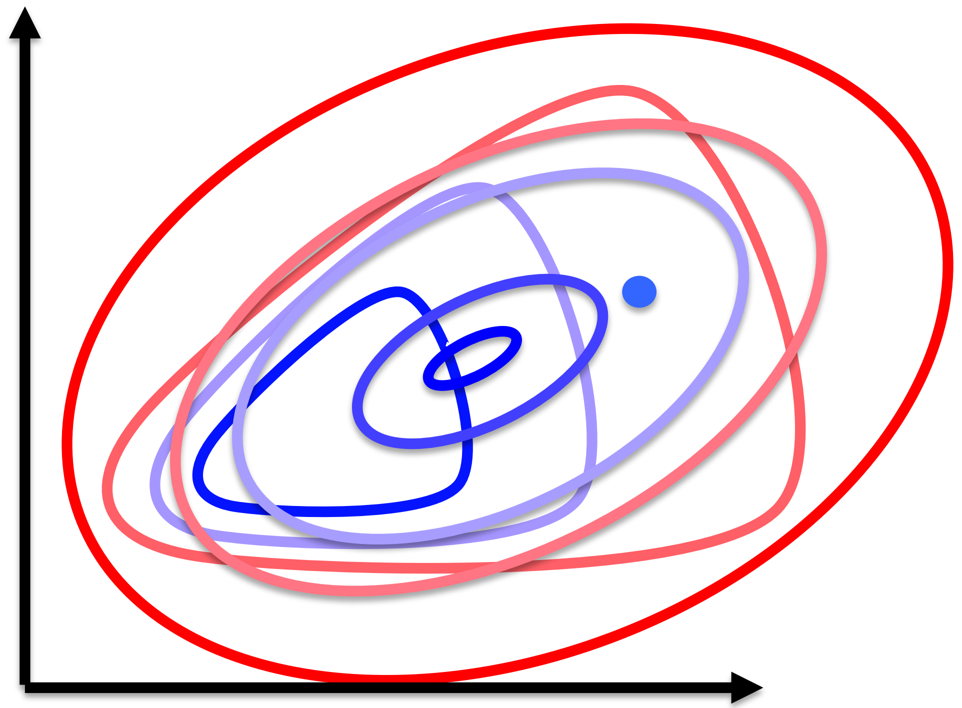
A Simple Example: Least Squares

- Solution given by the normal equations



Solution = $\boxed{\left(\mathbf{A}^T\mathbf{A}\right)^{-1}\mathbf{A}^T\mathbf{y}}$ $\nabla \mathbf{f}\left(\mathbf{x}^*\right) = \mathbf{0}$

Newton's Method



Choose best descent direction according to quadratic approximation

Newton's Method

- How do we get an approximation ?
- Taylor Series!

$$f\left(\mathbf{x}^c + \Delta\mathbf{x}\right) \approx f\left(\mathbf{x}^c\right) + \Delta\mathbf{x}^T\mathbf{g} + \frac{1}{2}\Delta\mathbf{x}^T\mathbf{H}\Delta\mathbf{x}$$

$$\boxed{\nabla f\big|_{\mathbf{x}^c}}$$

$$\boxed{H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1\,\partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1\,\partial x_n} \\ \frac{\partial^2 f}{\partial x_2\,\partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2\,\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n\,\partial x_1} & \frac{\partial^2 f}{\partial x_n\,\partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}}$$

Newton's Method

- We minimize the model problem
- Find where the gradient is zero

$$f\left(\mathbf{x}^c\right) + \Delta\mathbf{x}^T\mathbf{g} + \frac{1}{2}\Delta\mathbf{x}^T\mathbf{H}\Delta\mathbf{x}$$

Newton's Method

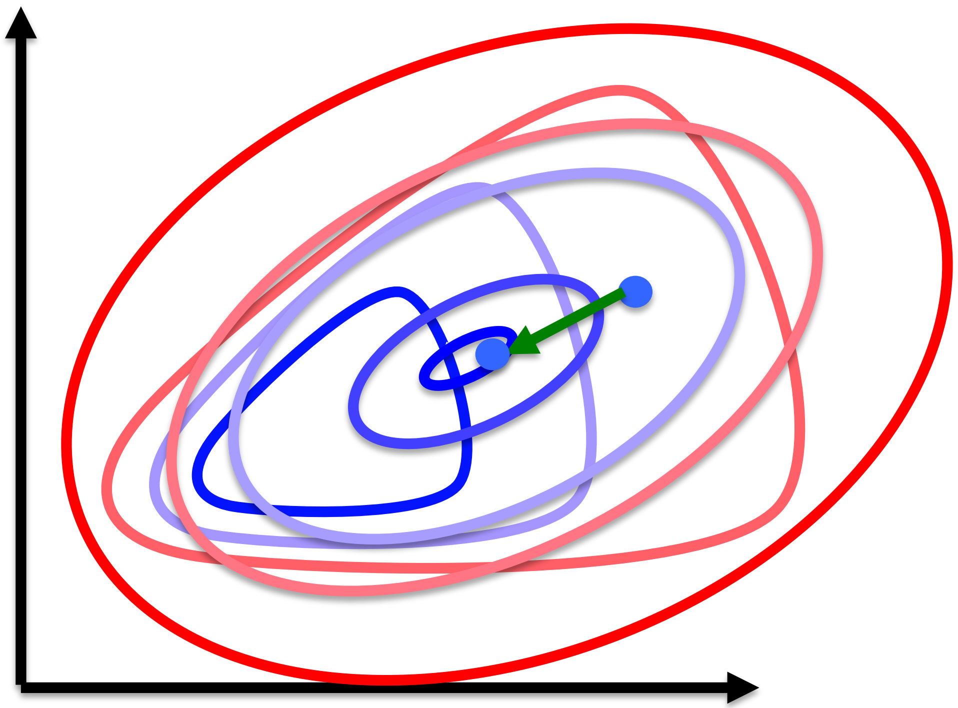
- We minimize the model problem
- Find where the gradient is zero

Model: $f\left(\mathbf{x}^c\right) + \Delta\mathbf{x}^T\mathbf{g} + \frac{1}{2}\Delta\mathbf{x}^T\mathbf{H}\Delta\mathbf{x}$

Gradient: $\mathbf{H}\Delta\mathbf{x} + \mathbf{g} = \mathbf{0}$

Increment: $\Delta\mathbf{x} = -\mathbf{H}^{-1}\mathbf{g}$

Newton’s Method



Newton's Method

- Initialize $\mathbf{x}^c$
- While not at optimal point
  - Compute gradient (**g**) and Hessian (**H**)
  - Compute $\Delta\mathbf{x} = -\mathbf{H}^{-1}\mathbf{g}$
  - Update $\mathbf{x}^c = \mathbf{x}^c + \Delta\mathbf{x}$

Gradient Descent vs. Newton's Method

- Gradient Descent is very simple
- Newton's Method converges faster (near solution, quadratic vs linear)
- Available Newton's Method Implementations:
  - MATLAB: fminunc
- Quasi-Newton Methods
  - LBFGS: http://www.chokkan.org/software/liblbfgs/

Examples of Optimization in Engineering

- Static Equilibrium: Find the minimum energy state of a deformable object
- Typically done using a Newton's method

Examples from Engineering

ENGINEERPEDIA

Types of Optimization

- Continuous vs. Discrete
- Constrained vs. Unconstrained

Constrained Optimization

- Optimization involves finding an “optimal value”

- i.e. Maximizing a profit, minimizing an area etc…

$$\min f\left(x\right)$$
$$s.t\ \boxed{\mathbf{c}_i\left(\mathbf{x}\right)} = 0$$

Equality Constraints

Constrained Optimization

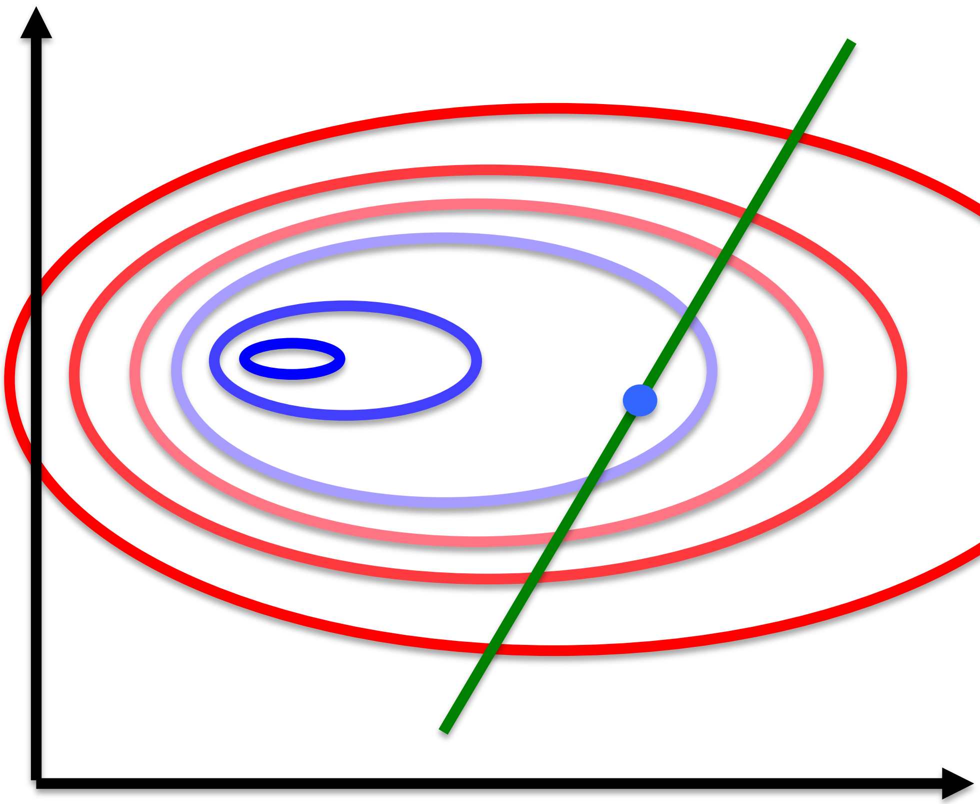
- Optimization involves finding an “optimal value”

- i.e. Maximizing a profit, minimizing an area etc…

$$\min f\left(x\right)$$
$$s.t\ \boxed{Ax} = \mathbf{b}$$

Equality Constraints

Constrained Optimization



Constrained Optimization: method of Lagrange multipliers

- Solve a different, *unconstrained* optimization problem instead

- Compute stationary (critical) points of the Lagrangian:

$$f + \boxed{\lambda} c$$

Lagrange Multipliers!

At Optimal Solution, we have:

$$\mathbf{c}_i(\mathbf{x}) = 0$$

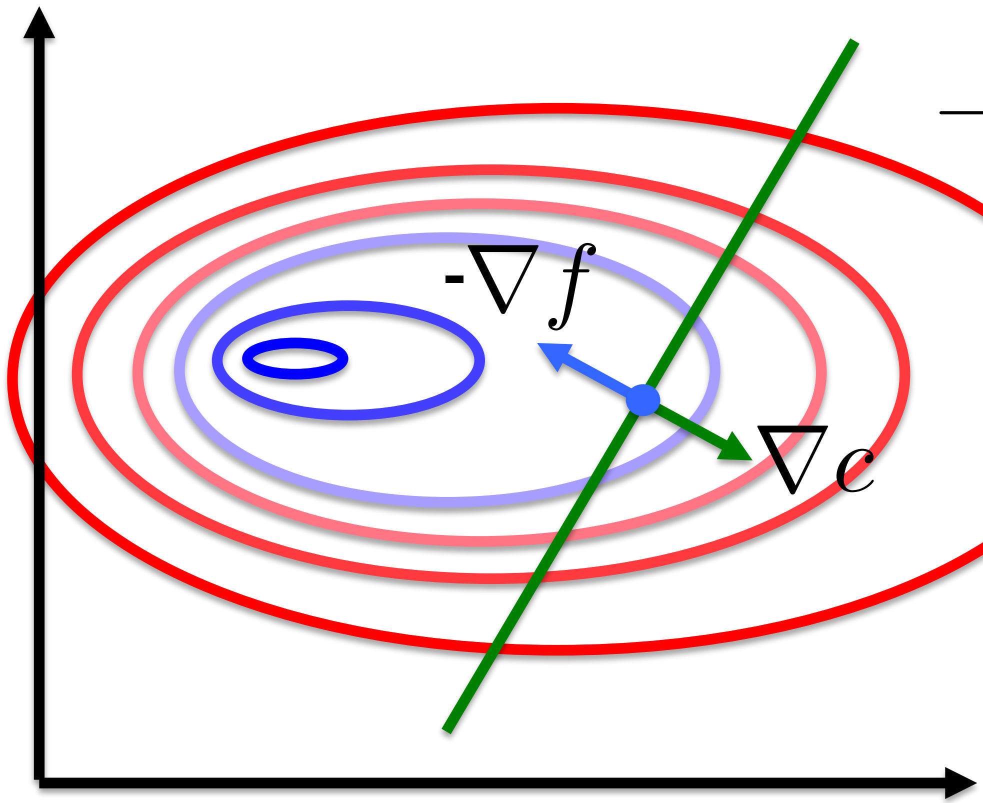
$$-\nabla f = \lambda \nabla c$$

Constrained Optimization

At Optimal Point

$$\mathbf{c}_i\left(\mathbf{x}\right) = 0$$

$$-\nabla f = \lambda \nabla c$$



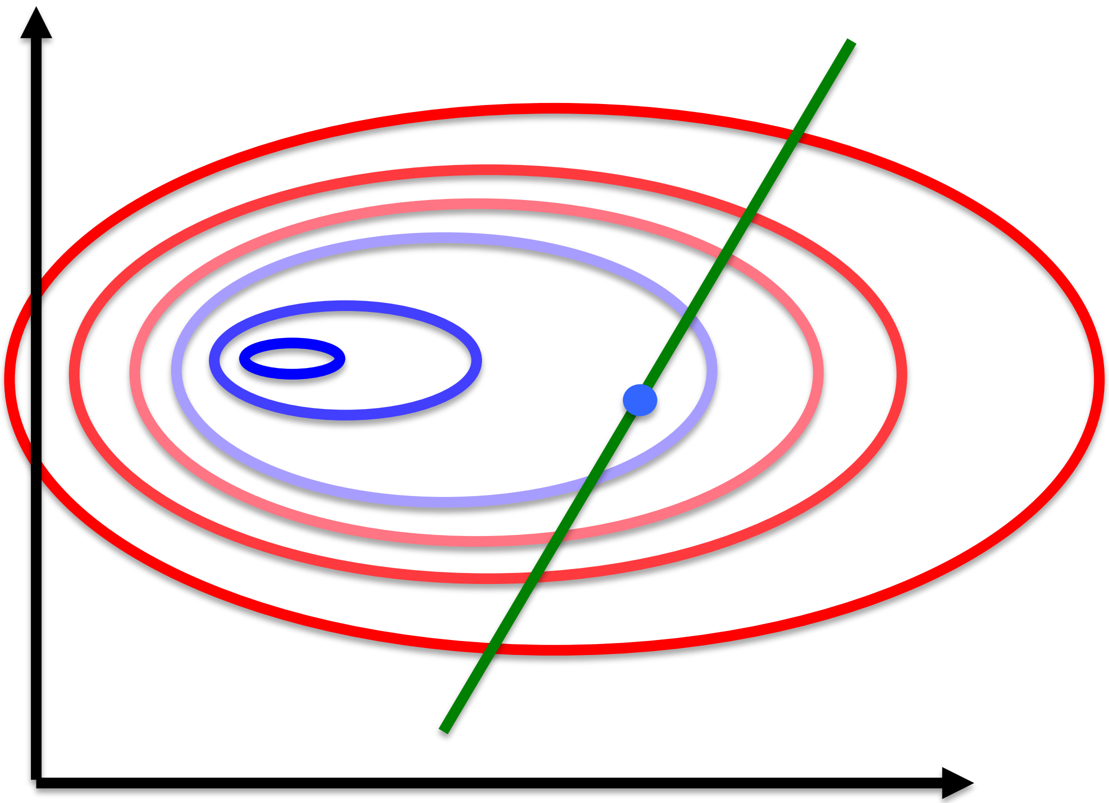
Constrained Optimization

- Very useful for general equality constrained problems
- Available in MATLAB as fmincon
- Easy to modify unconstrained Newton Code

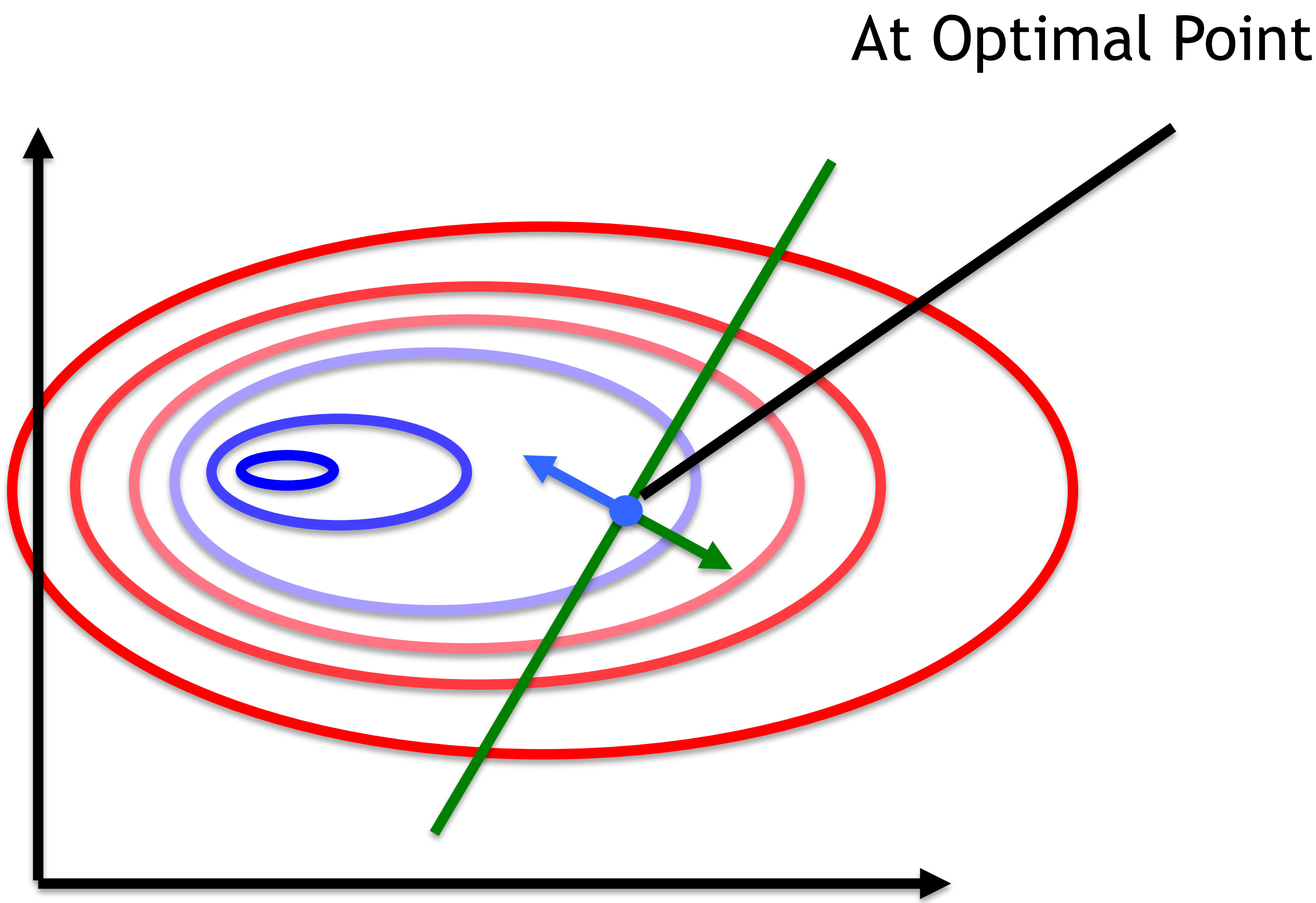
Next: Inequality Constrained Optimization

- Specifically we will work up to a particular type of problem called a Quadratic Program

Constrained Optimization



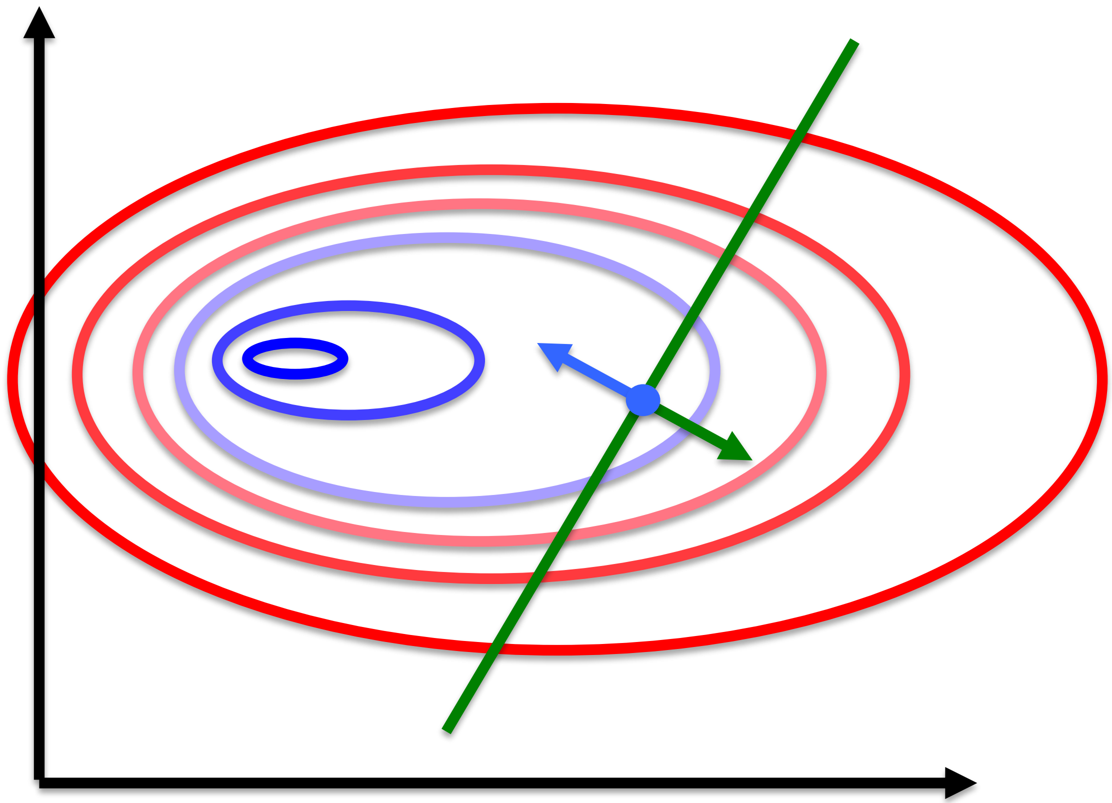
Constrained Optimization



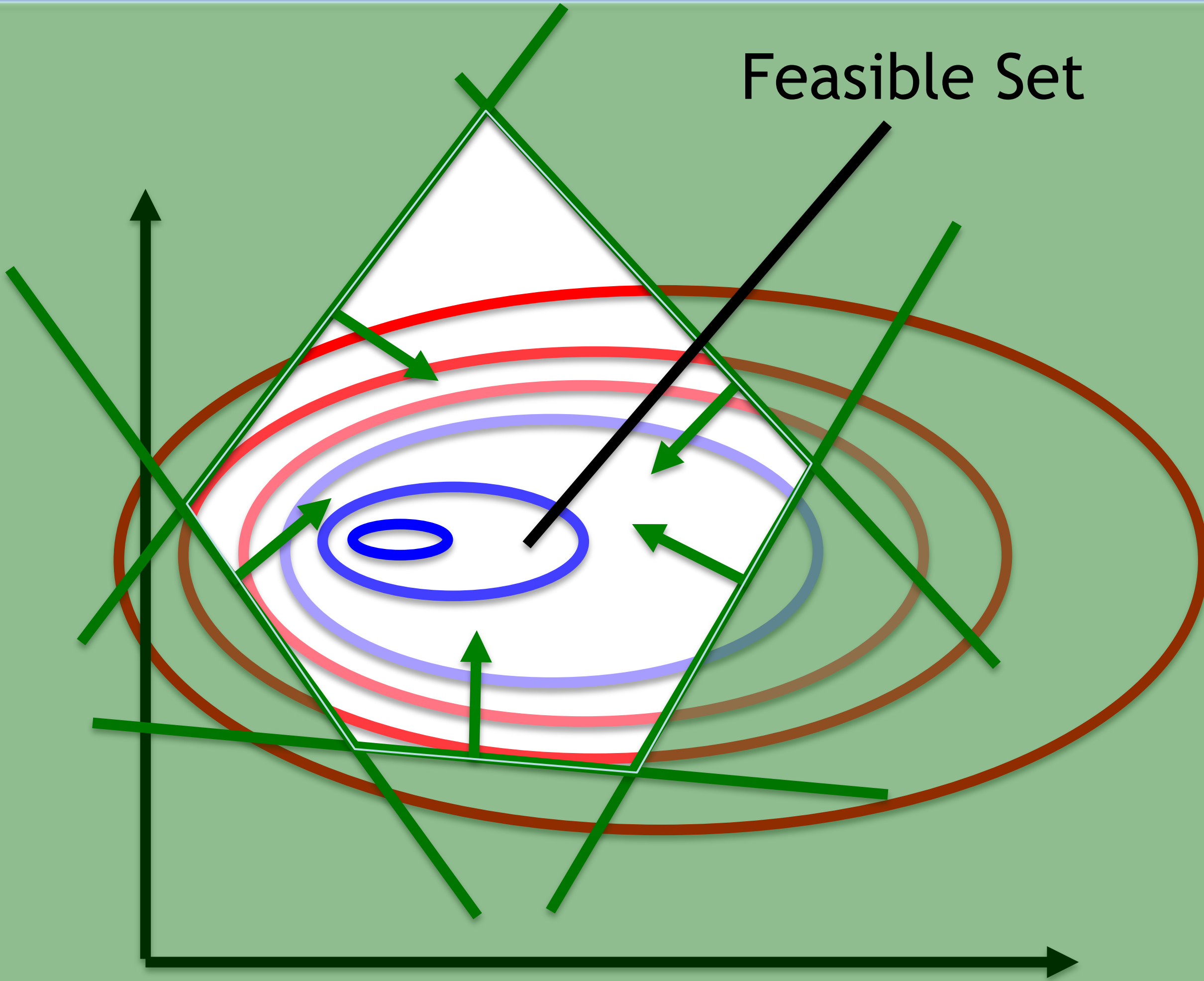
Inequality Constrained Optimization

$$\min f(x)$$
$$s.t\ c_i(\mathbf{x}) \boxed{\leq} 0$$

Equality Constrained Optimization



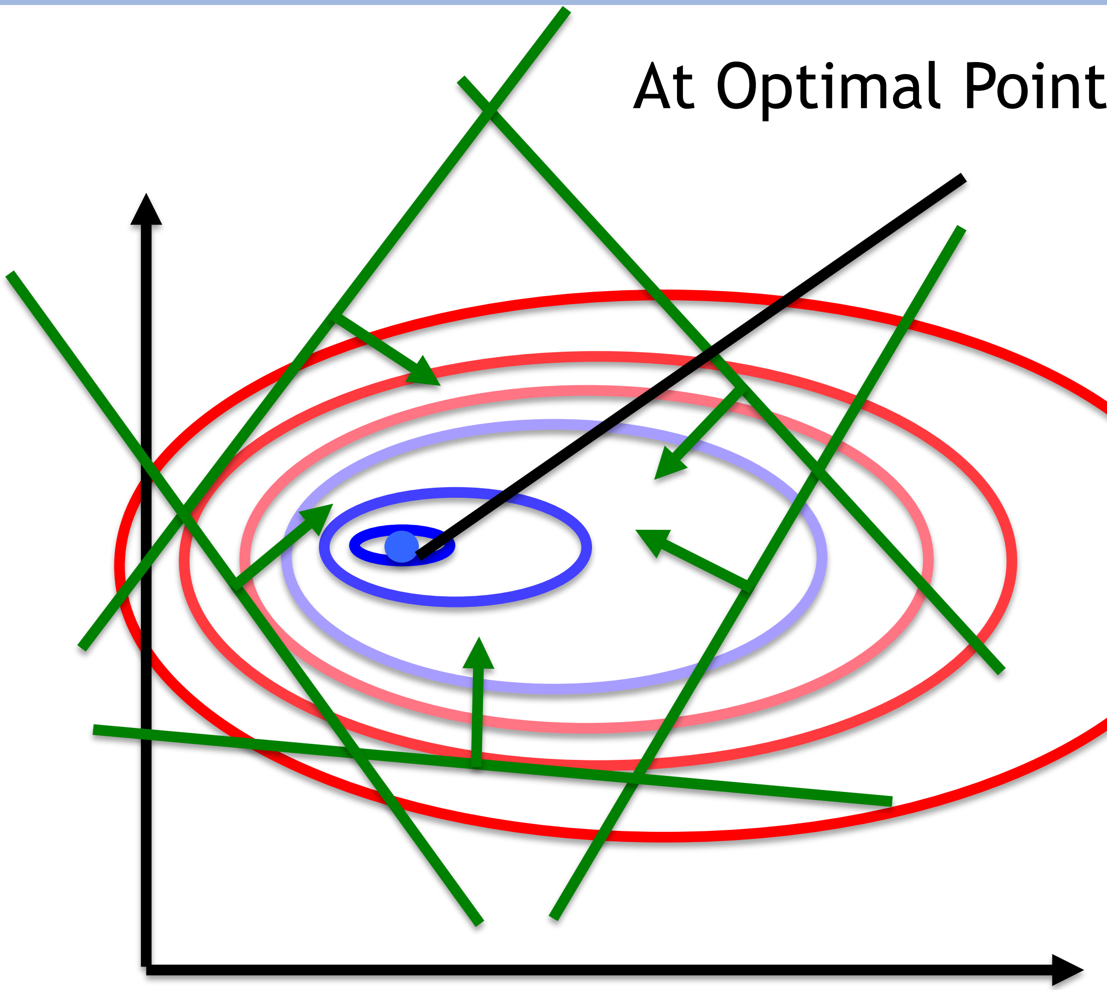
Inequality Constrained Optimization



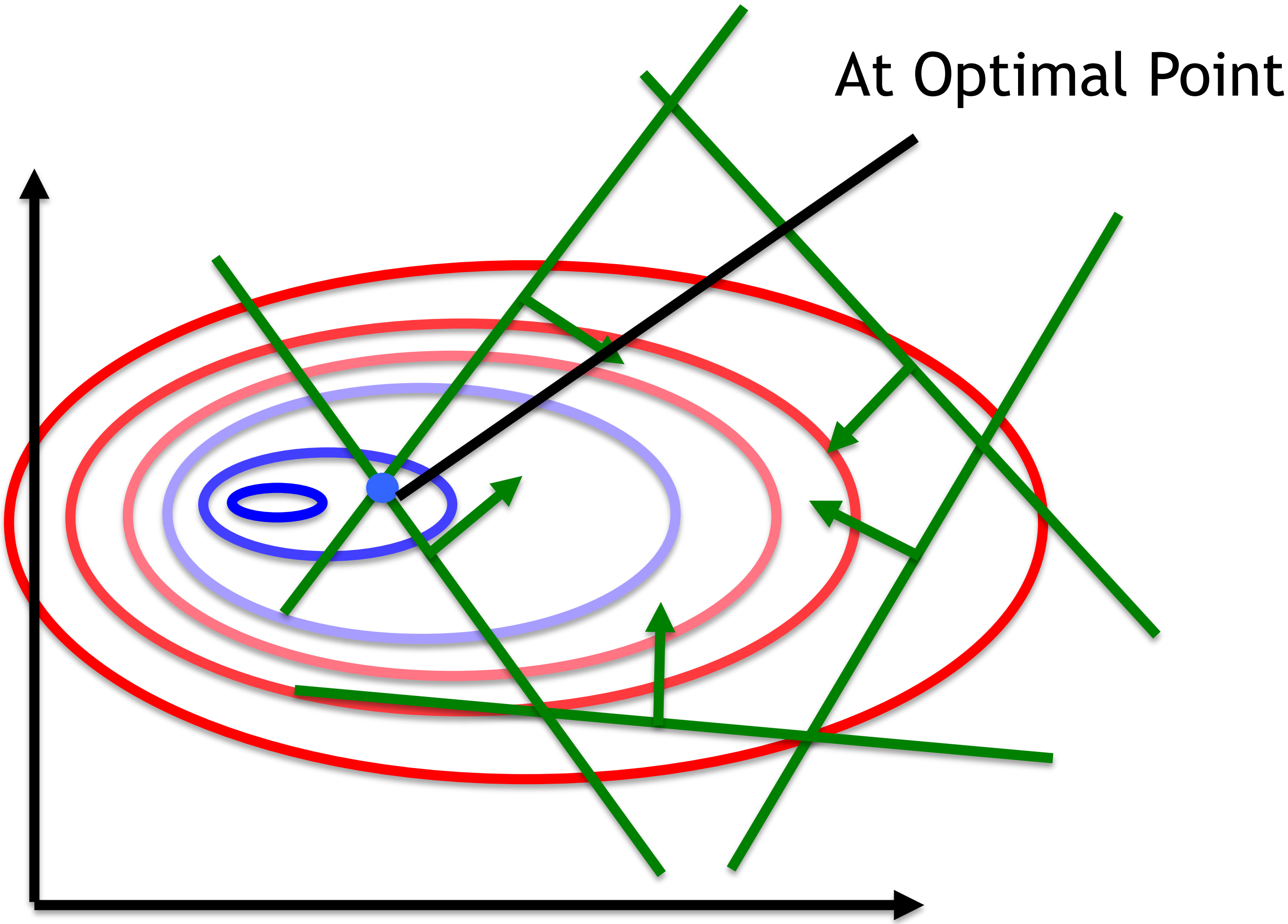
The Active Set

- Hidden inside of each inequality constrained optimization is an equality constrained optimization
- There are two cases for our optimal point…

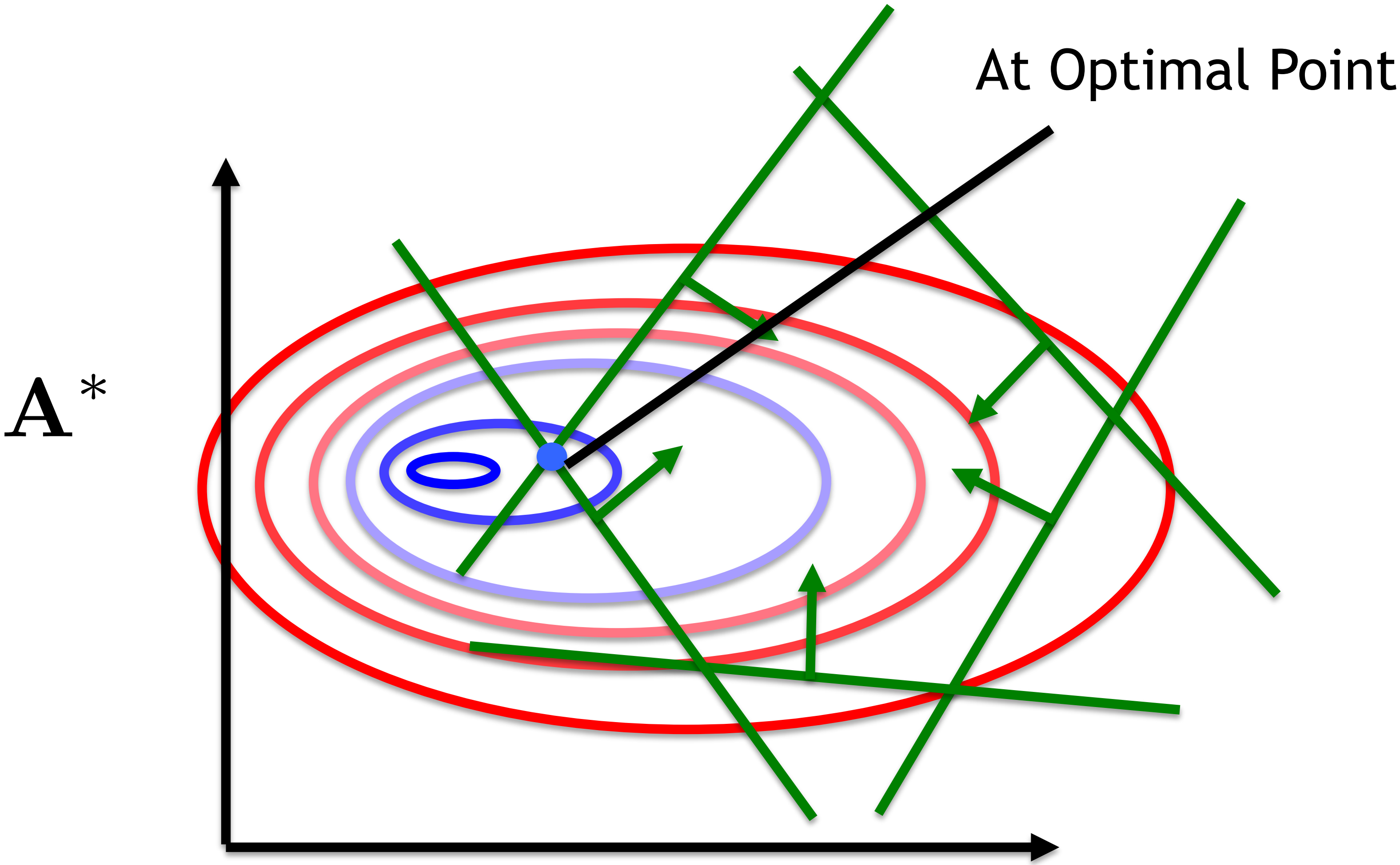
Case 1: Optimal Value Inside Feasible Set



Case 2: Optimal Value On Boundary



Case 2: Optimal Value On Boundary



The Active Set

- On the boundary we satisfy

$$\min f(x)$$

$$s.t\ \boxed{\mathbf{A}}^{*}\mathbf{x} = \mathbf{b}$$

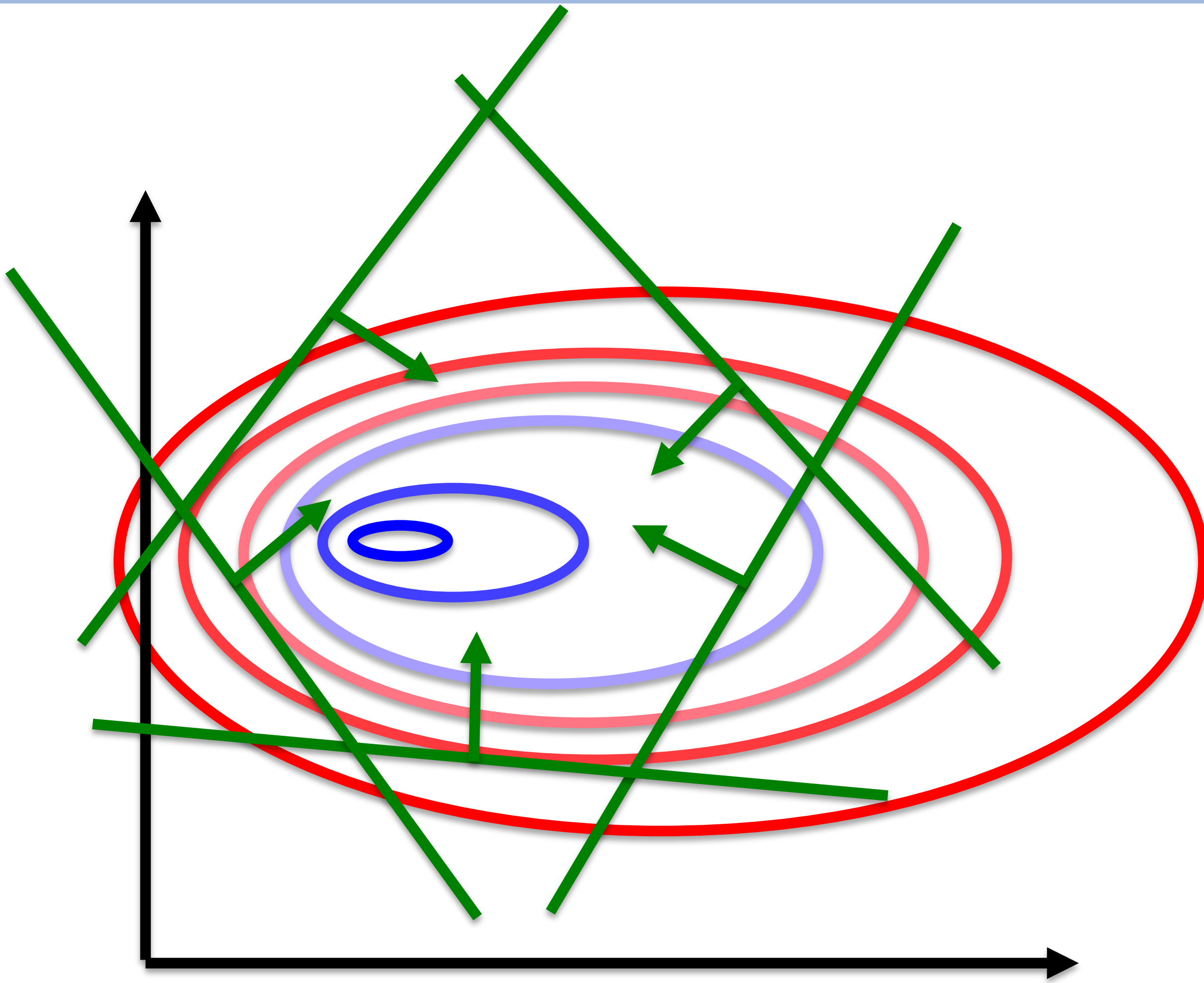
Active Set

Quadratic Programs

- Quadratic objective, linear constraints

$$\min \mathbf{x}^T \mathbf{H} \mathbf{x} + \mathbf{x}^T \mathbf{d}$$
$$s.t.\ \mathbf{A}\mathbf{x} = \mathbf{b}$$
$$s.t.\ \mathbf{L}\mathbf{x} \leq \mathbf{m}$$

Quadratic Programs



Quadratic Program

- How do we solve this ?
- Active Set: Try different combinations of constraints until the minimum is found
- Interior Point: …

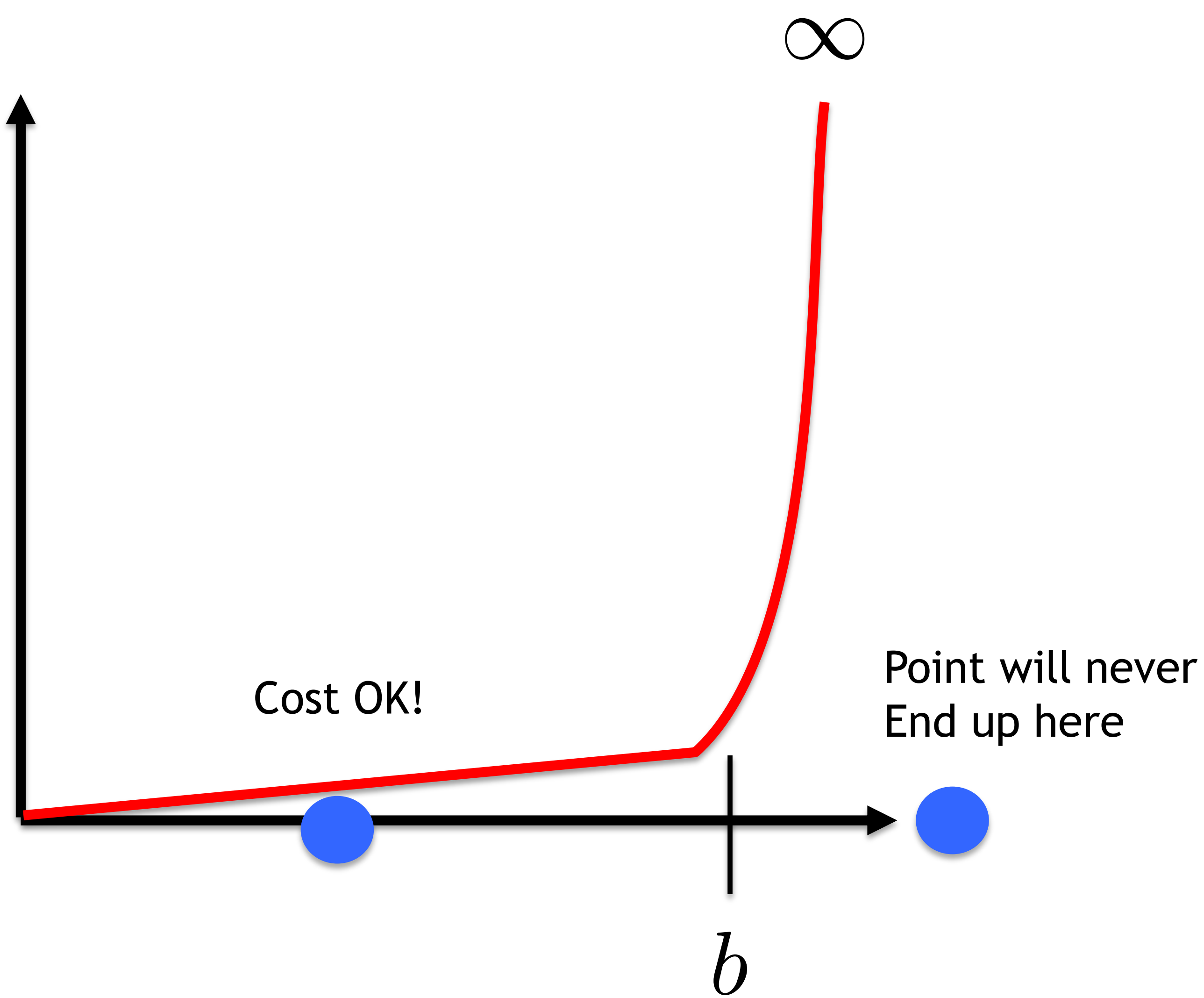
Interior Point Methods

- Replace inequality constraints with special barrier functions

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) + (\mathbf{A}\mathbf{x} - \mathbf{b})^T \lambda + \sum_i \boxed{c_i}(\mathbf{x})$$

Special "Constraint" Function

Interior Point: barrier functions



Interior Point Methods

- Replace inequality constraints with special barrier functions

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) + (\mathbf{A}\mathbf{x} - \mathbf{b})^T \lambda + \sum_i \boxed{c_i}(\mathbf{x})$$

Special "Constraint" Function

- Now use Newton's method

Quadratic Programs and Interior Point

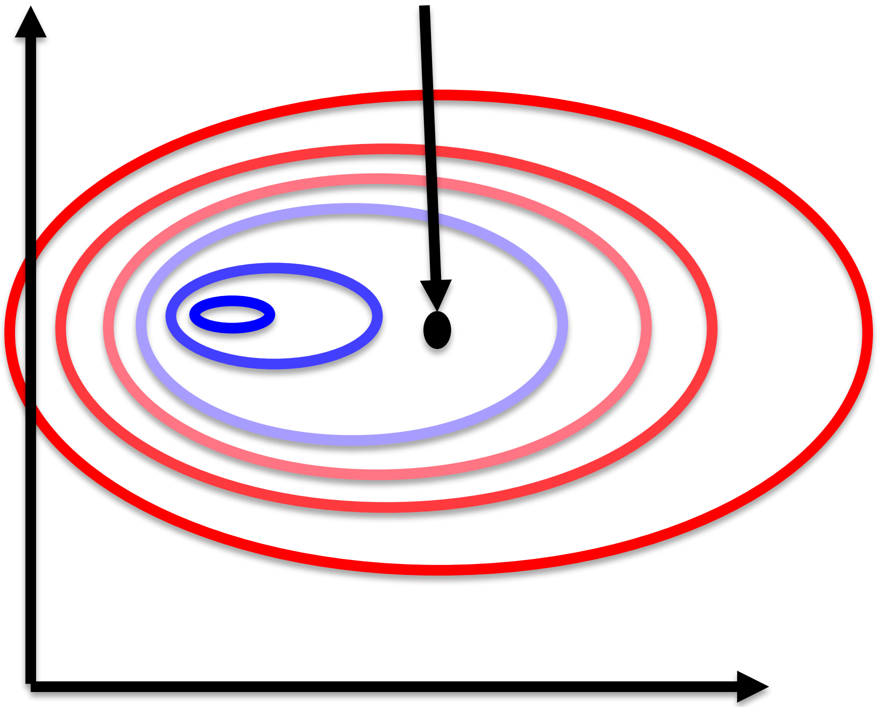
- Quadratic Programs (Active Set)
  - Quadprog++ (http://quadprog.sourceforge.net)
  - MATLAB: quadprog
- Interior Point
  - Ipopt (https://projects.coin-or.org/Ipopt)

Types of Optimization

- Continuous vs. Discrete
- Constrained vs. Unconstrained

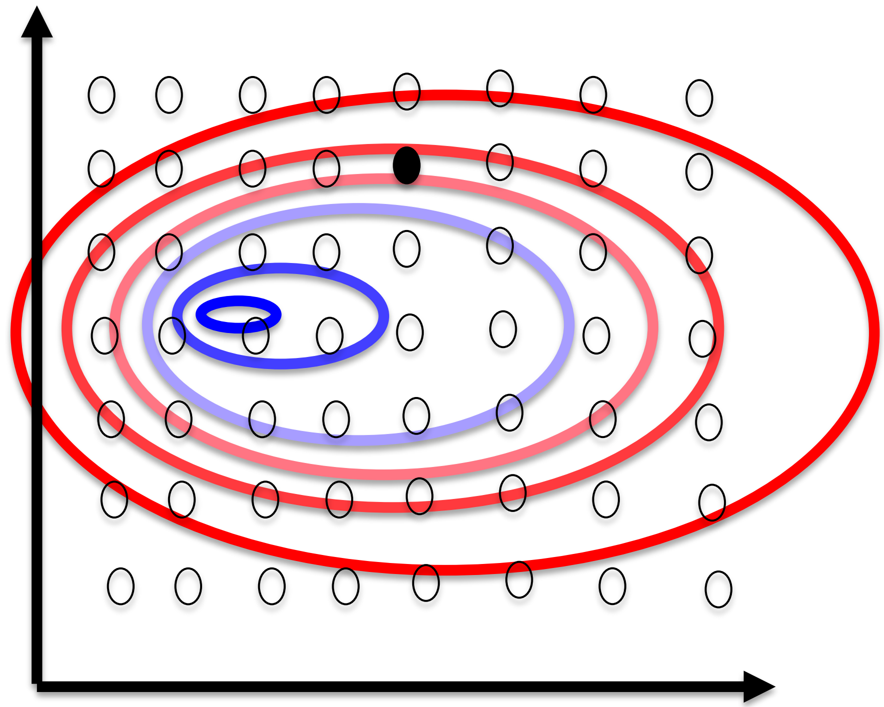
Continuous

This point can move smoothly



Discrete

Choose from discrete points in parameter space



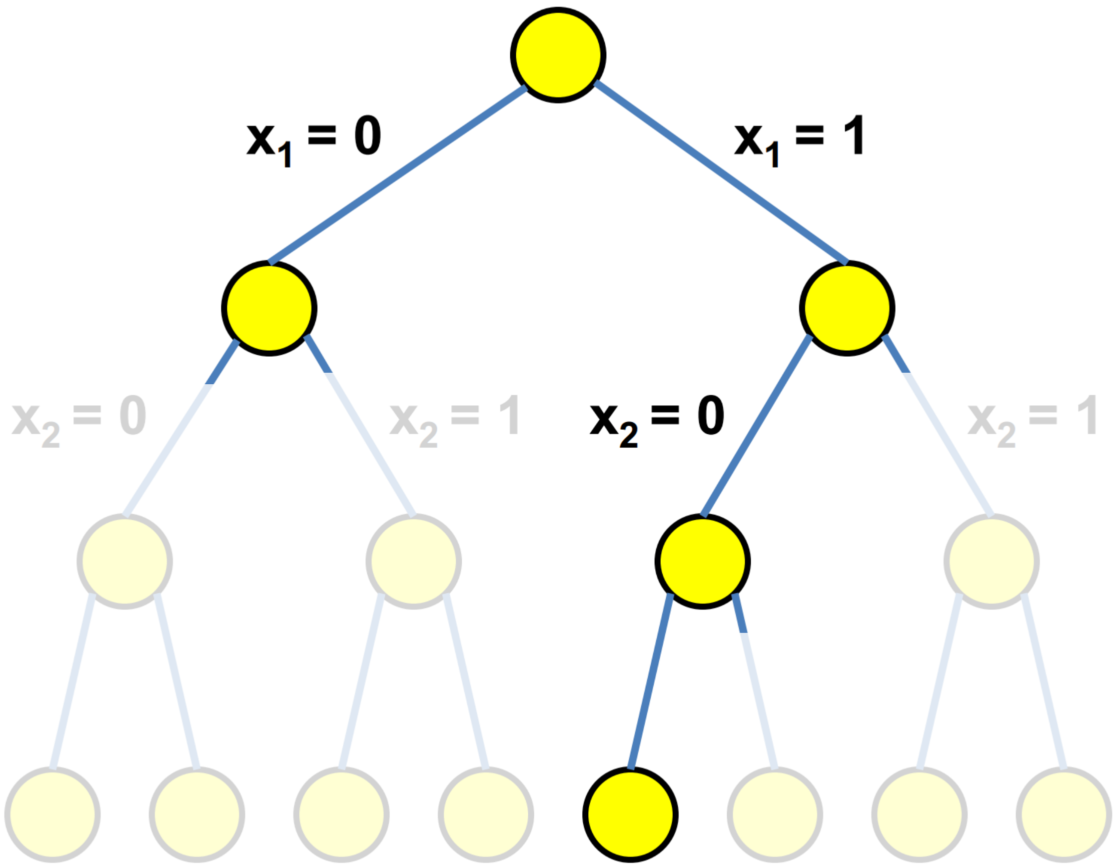
Branch and Bound Optimizations

- most commonly used tool for solving NP-hard optimization problems
- An optimization technique with 3 phases
  - Branch (divide the solution space into a number of subspaces)
  - Bound (compute some upper and lower bound for the cost of each subspace – worst case, conservative but feasible solution, best case, optimistic, usually through relaxation)
  - Prune (remove subspaces with upper bounds worse than the lower bounds of other subspaces)

Branch and Bound Example

$$\begin{array}{ll} \text{maximize} & 15x_1 + 12x_2 + 4x_3 + 2x_4 \\ \text{subject to} & 8x_1 + 5x_2 + 3x_3 + 2x_4 \leq 10 \\ & x_k \text{ binary for } k = 1 \text{ to } 4 \end{array}$$

Branch and Bound Example



Enumerating all solutions is not feasible – exponential explosion

Simulated Annealing

- Has four ingredients
  - Cost function
  - Configuration (made of discrete or continuous elements)
  - Neighbor Generator
  - Annealing Schedule

Simulated Annealing

- Basic Idea taken from cooling of materials in metallurgy
- At high “heat” atoms undergo rigorous motion
- As they are cooled they move less
- Explore trade-off between exploration and exploitation

Simulated Annealing

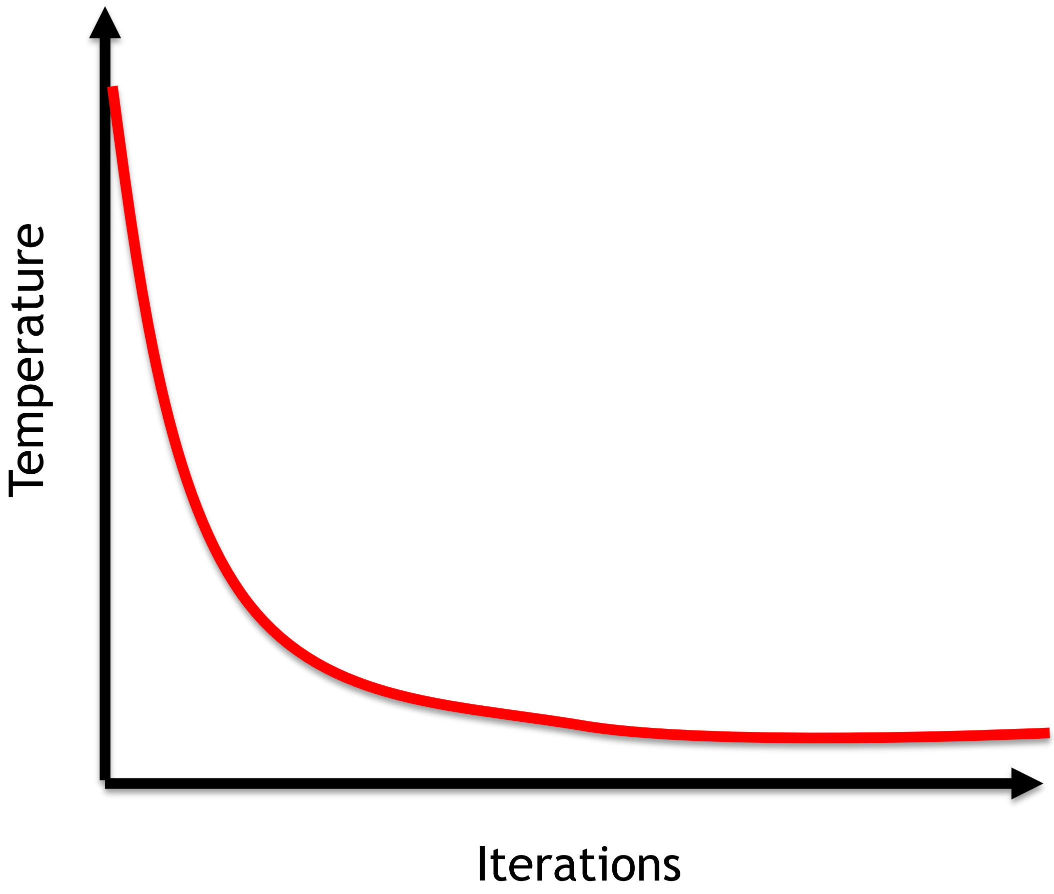
- Cost function: $f(\mathbf{q})$

Simulated Annealing

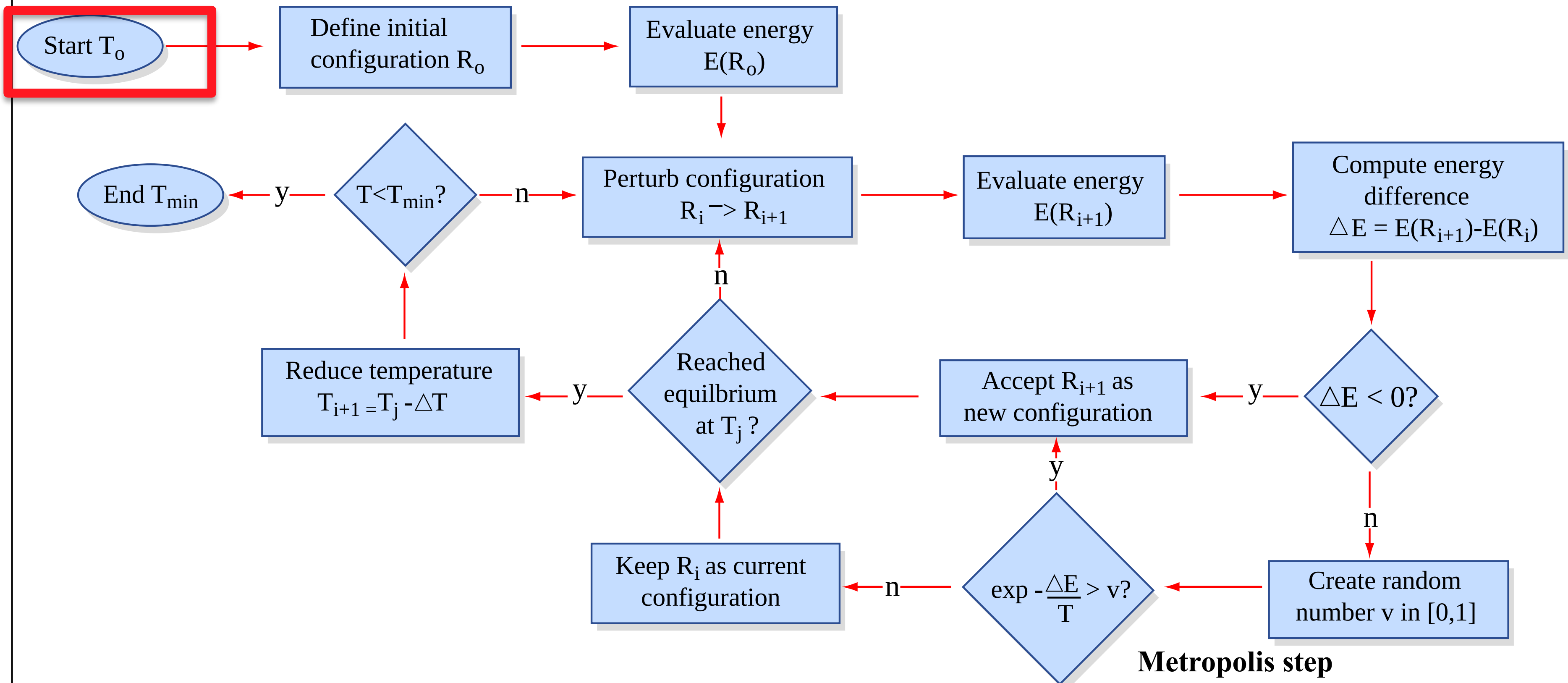
- Cost function: $f(\mathbf{q})$
- Neighbor Generator: Rearrange Configuration
  - Change **q** to something nearby
- Annealing Schedule

Simulated Annealing

- Annealing Schedule



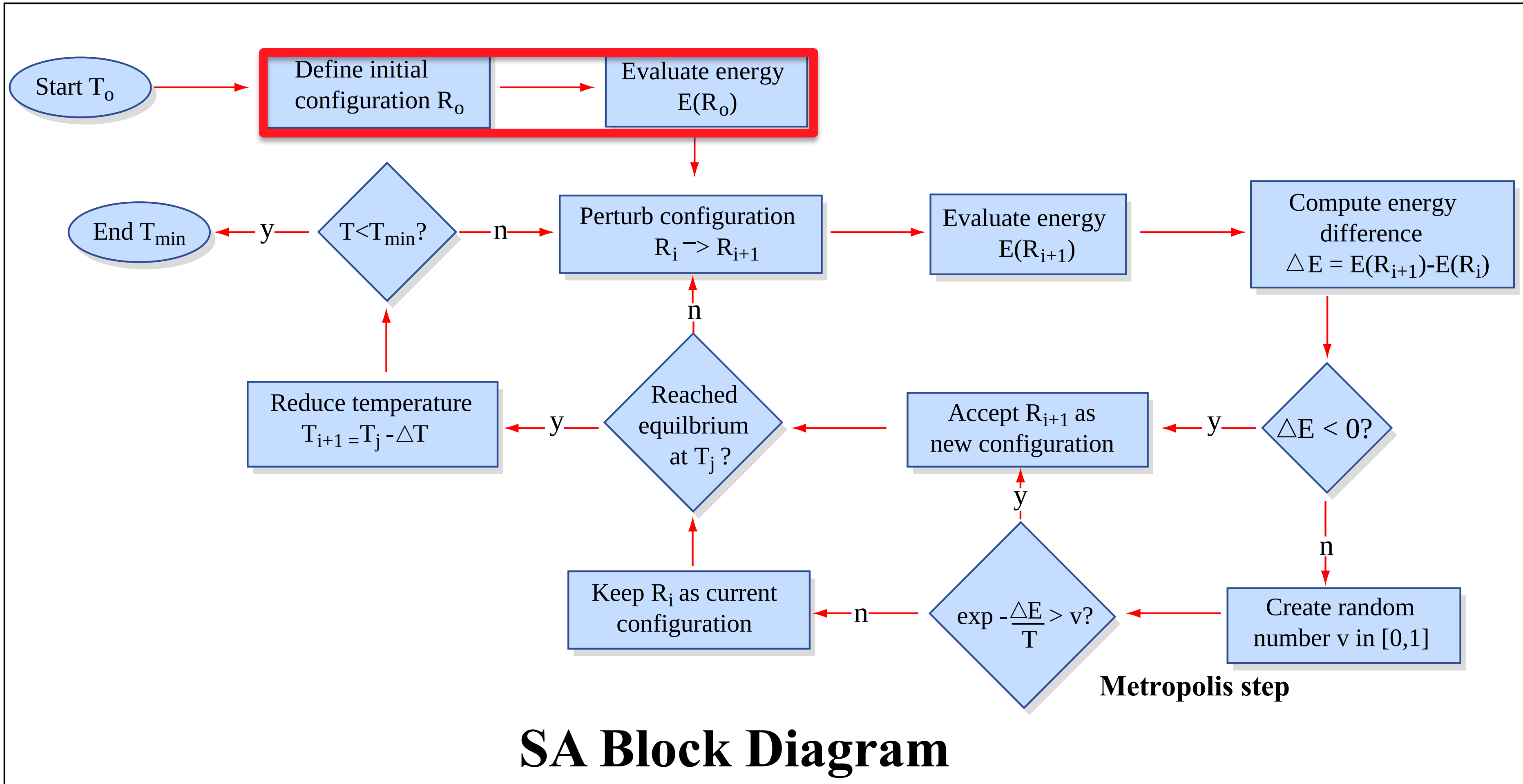
Simulated Annealing



SA Block Diagram

Image by MIT OpenCourseWare.

Simulated Annealing



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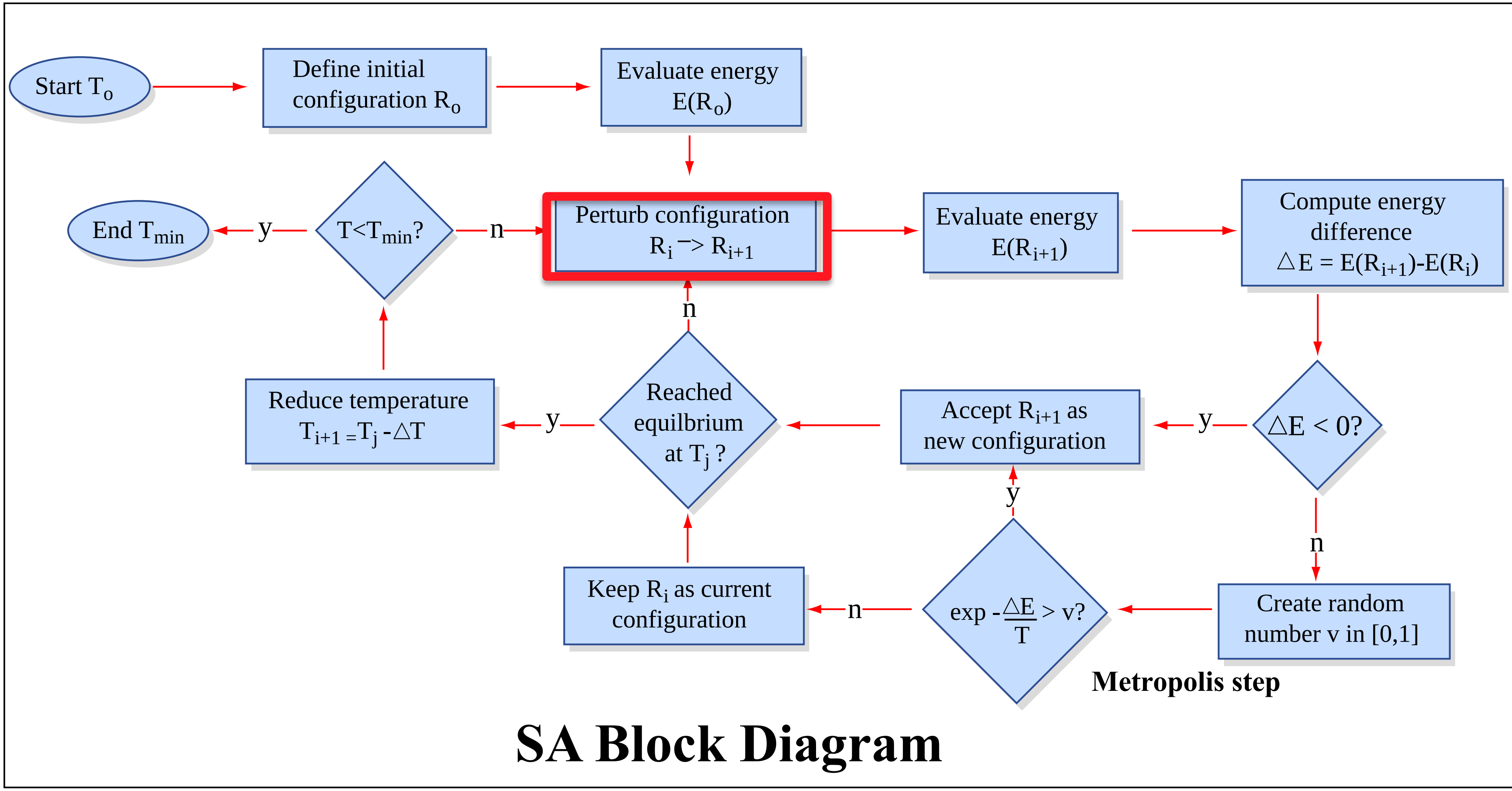
Simulated Annealing



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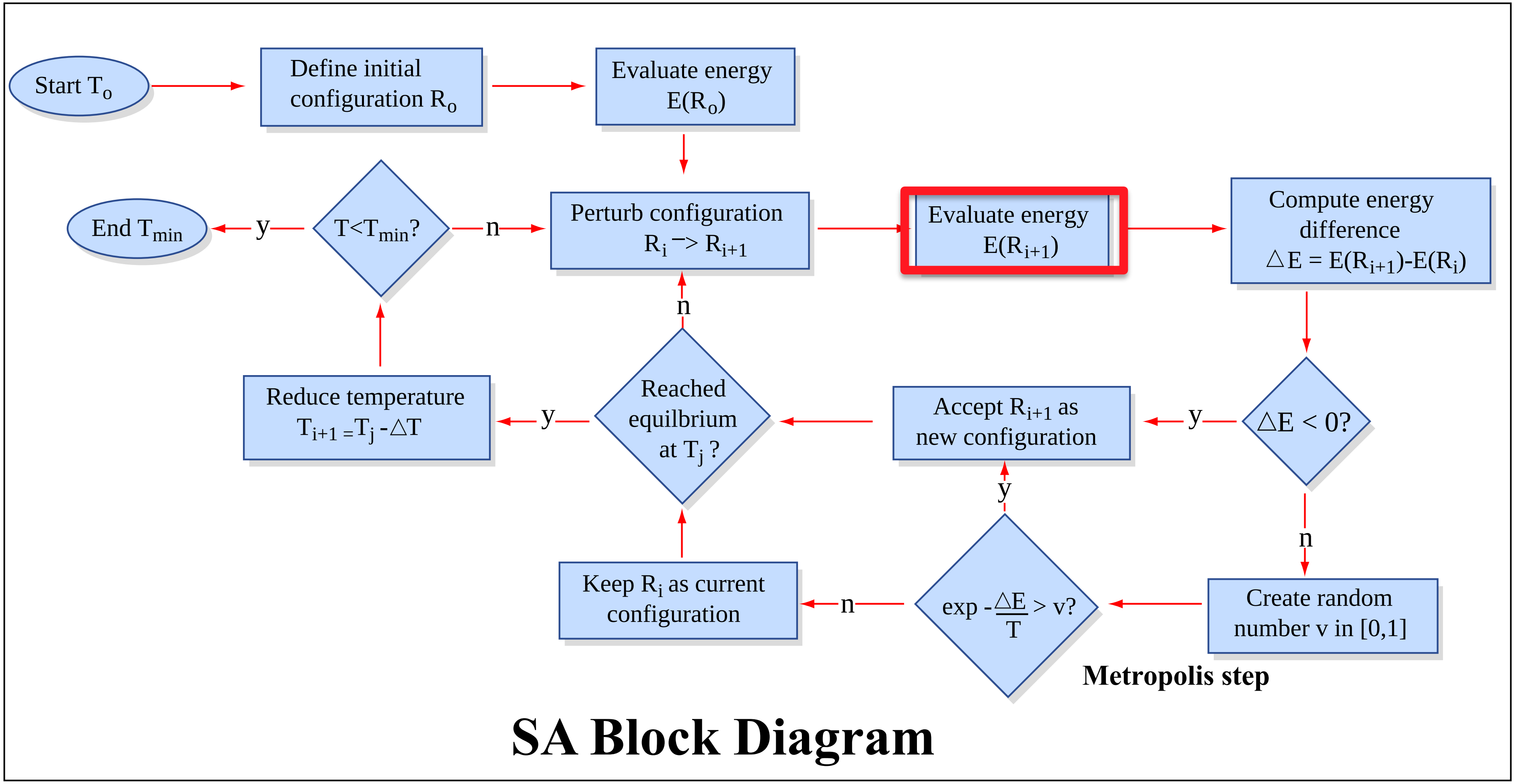
Simulated Annealing



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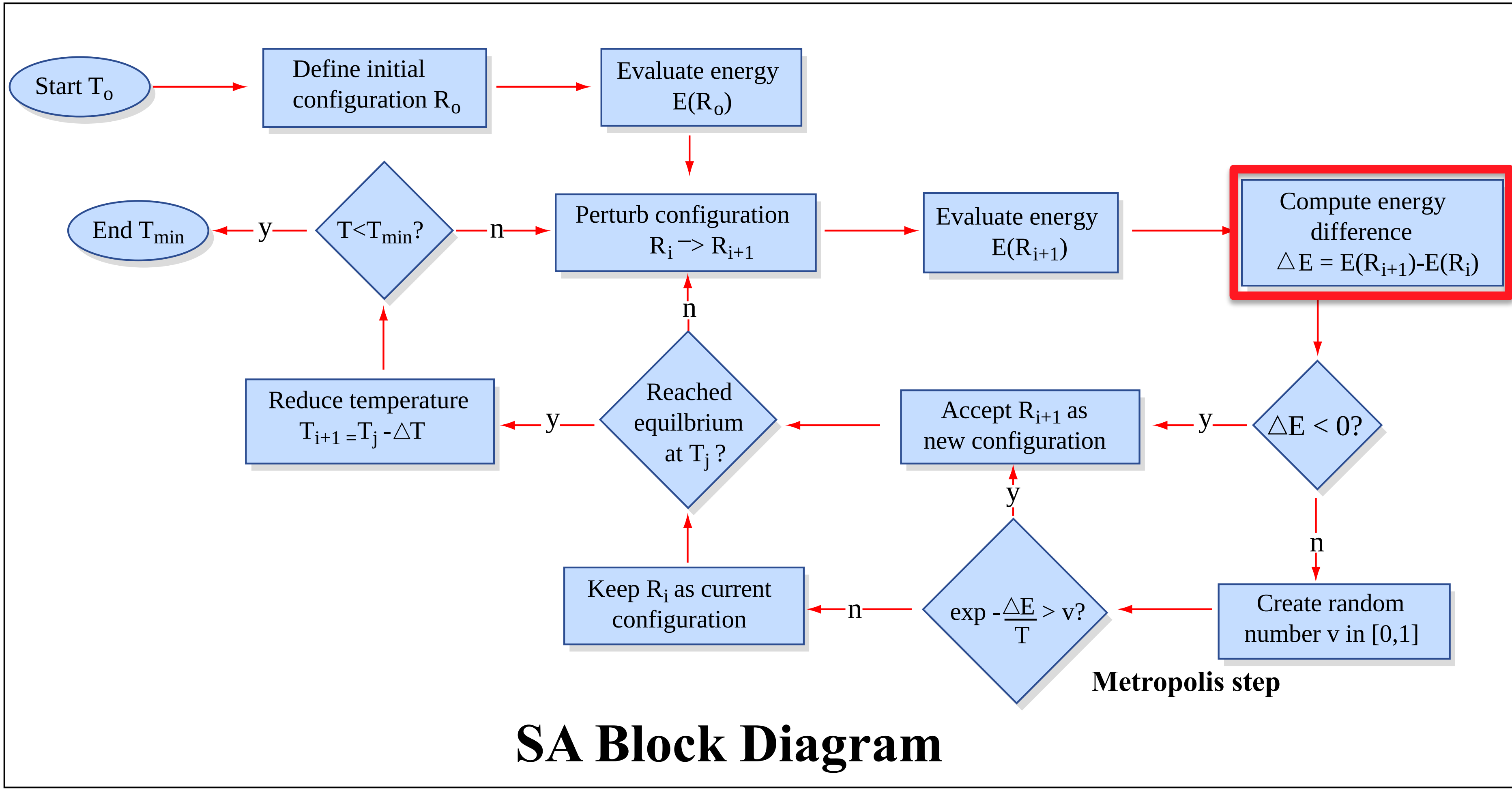
Simulated Annealing



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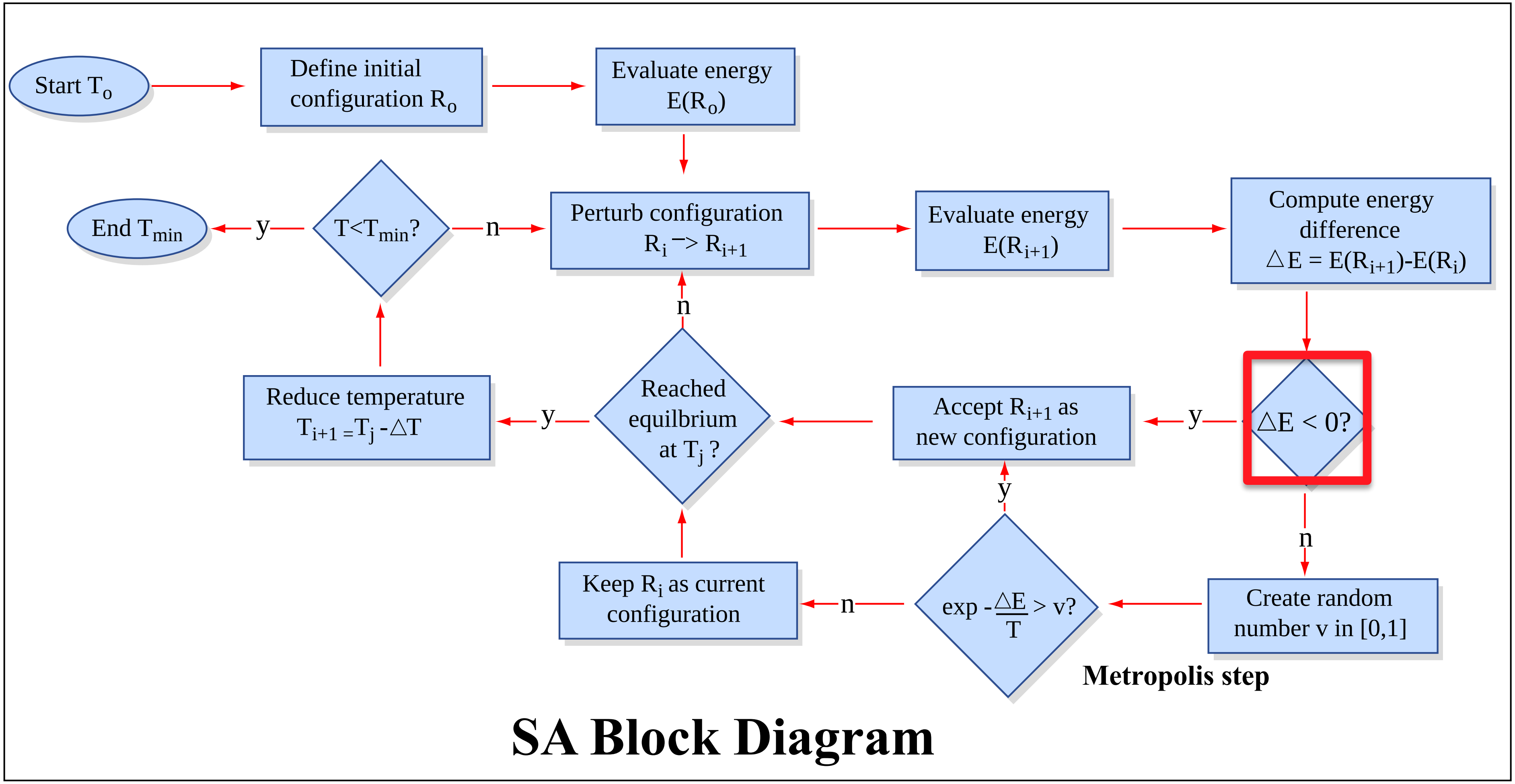

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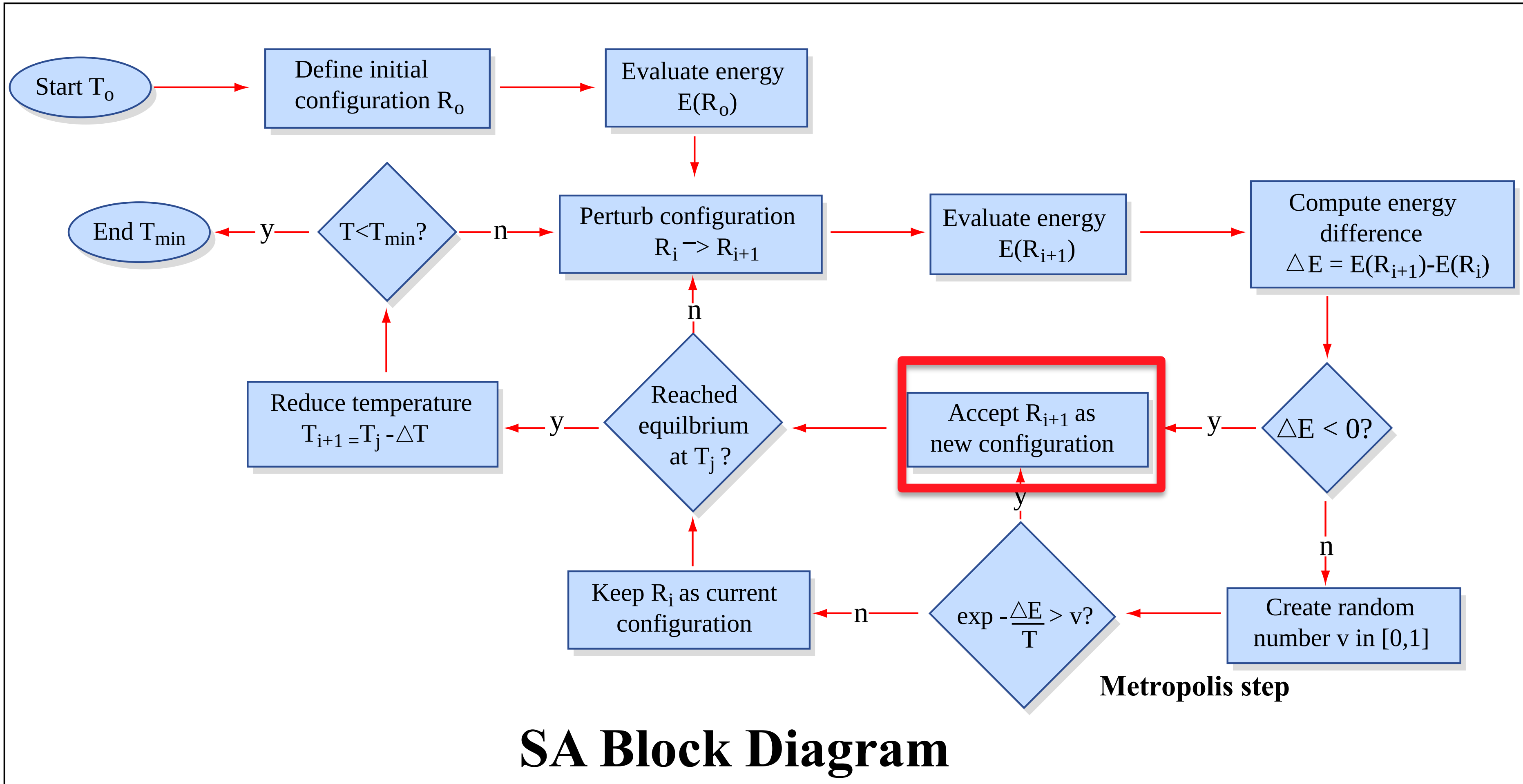

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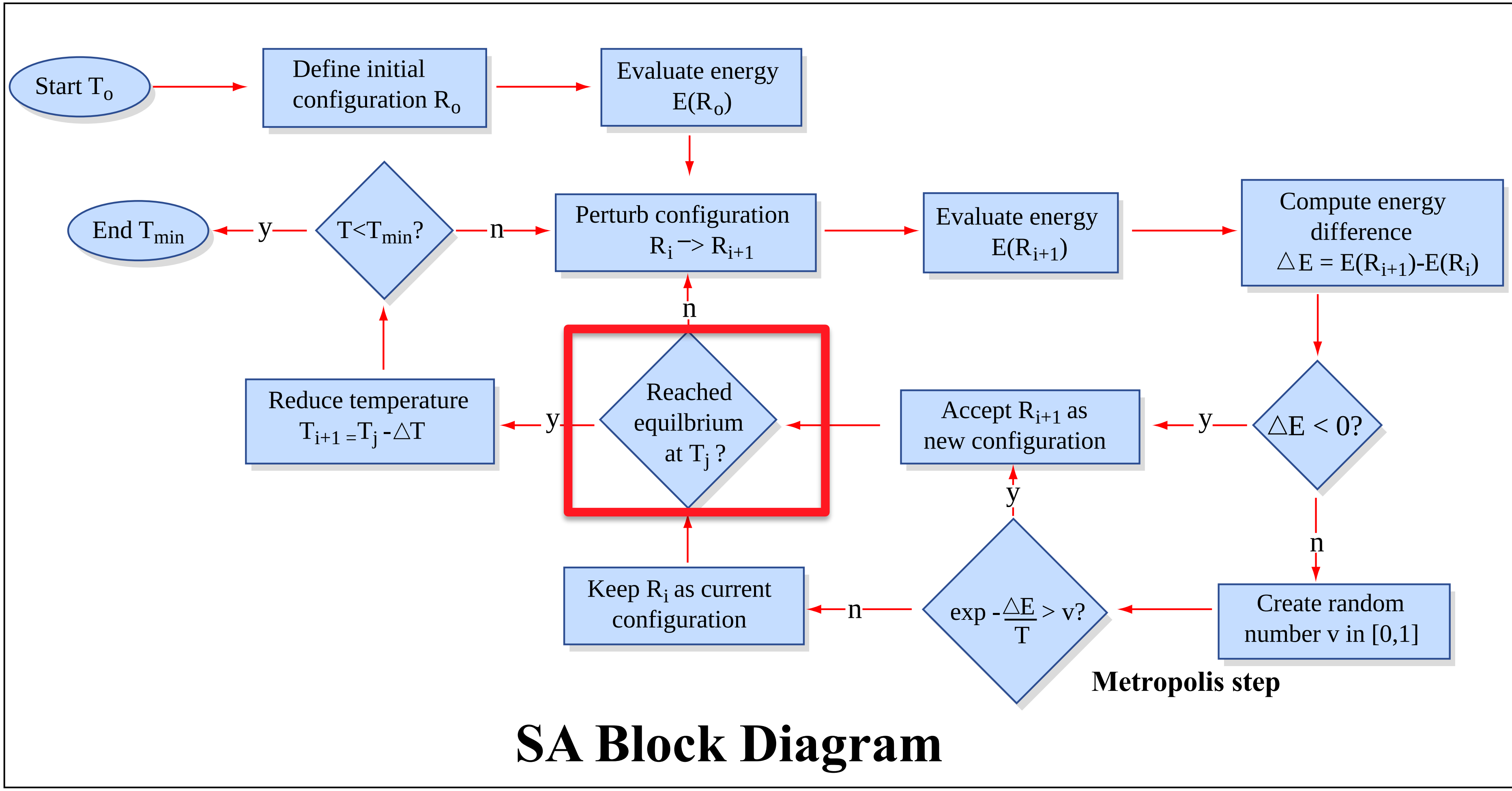

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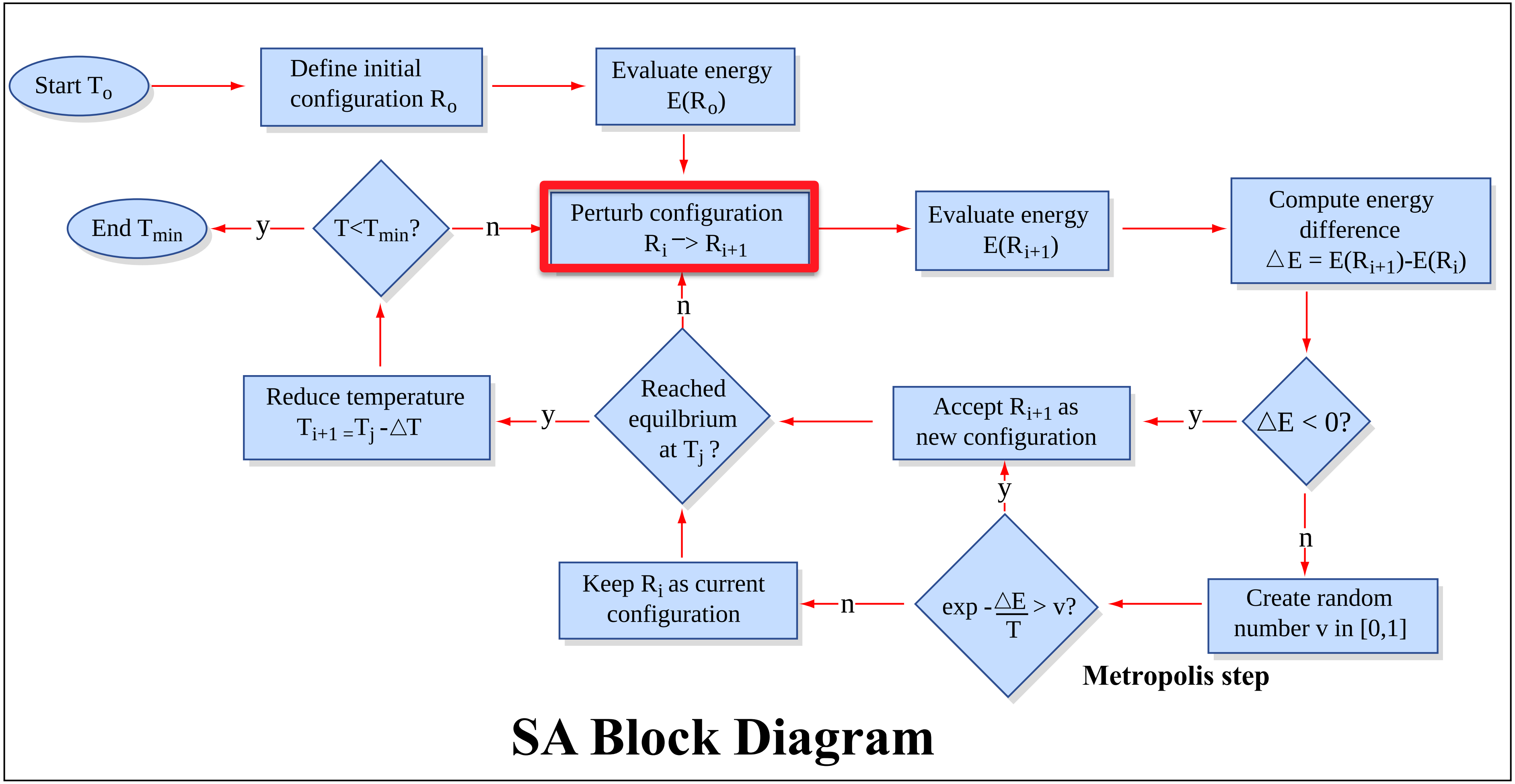

Image by MIT OpenCourseWare.

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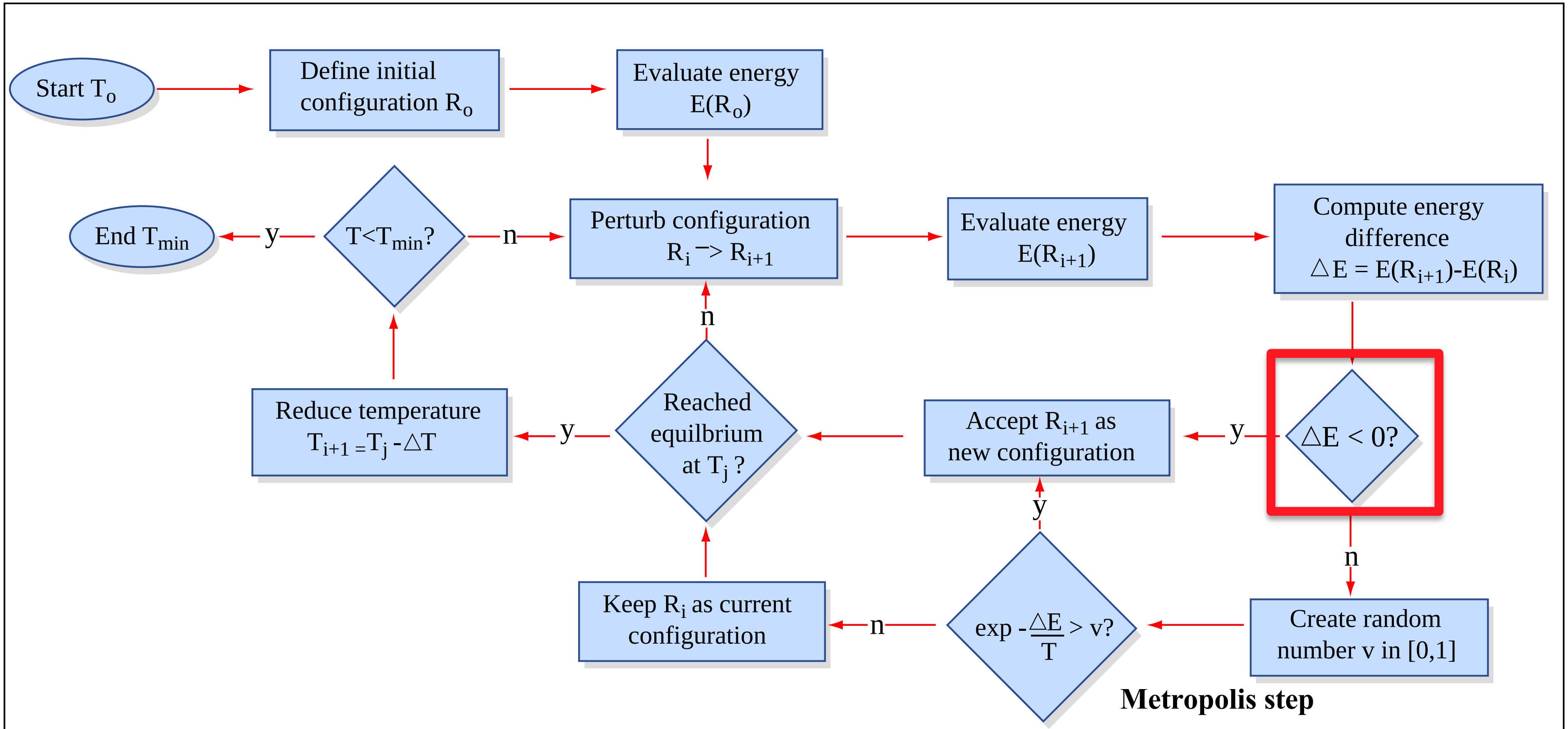
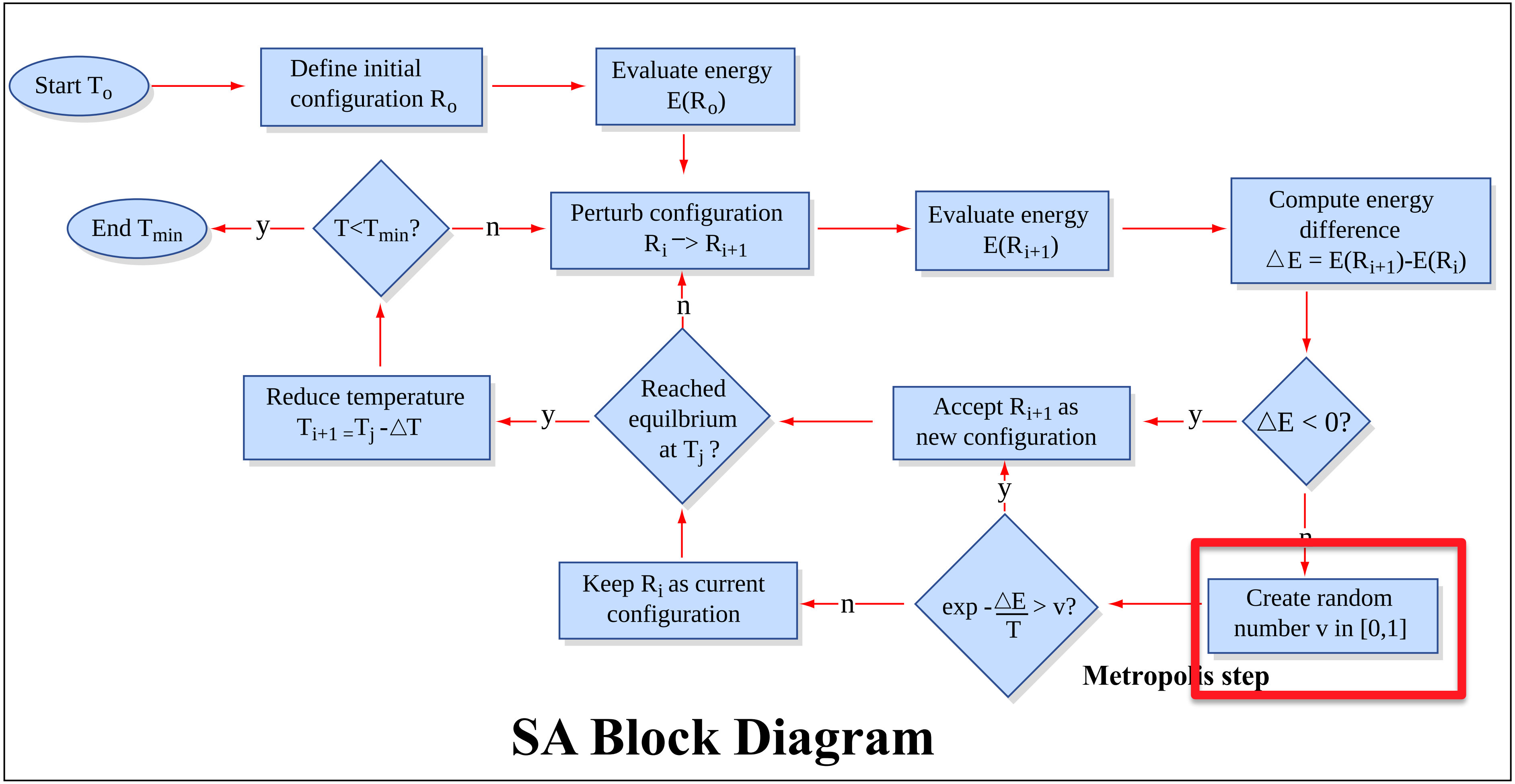


SA Block Diagram

Image by MIT OpenCourseWare.

Simulated Annealing



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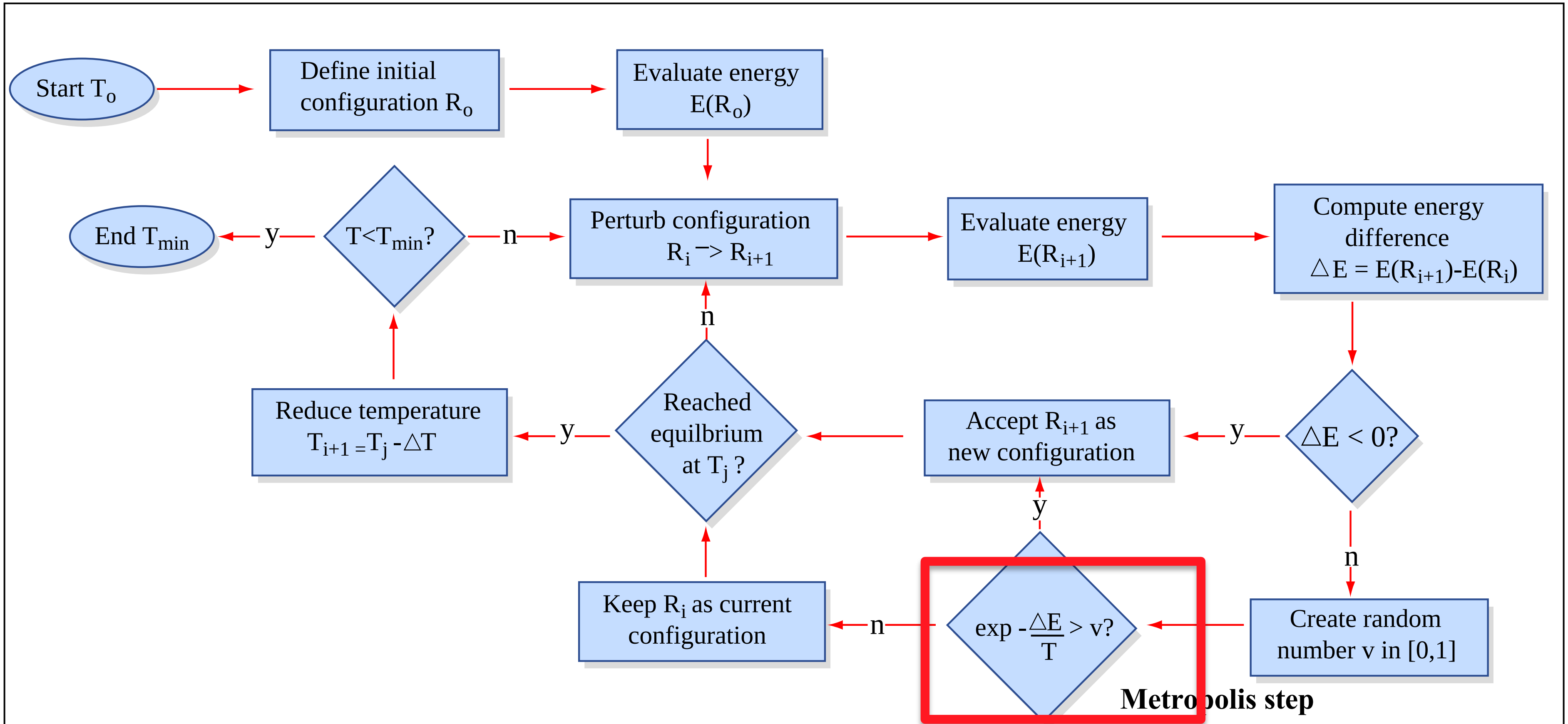
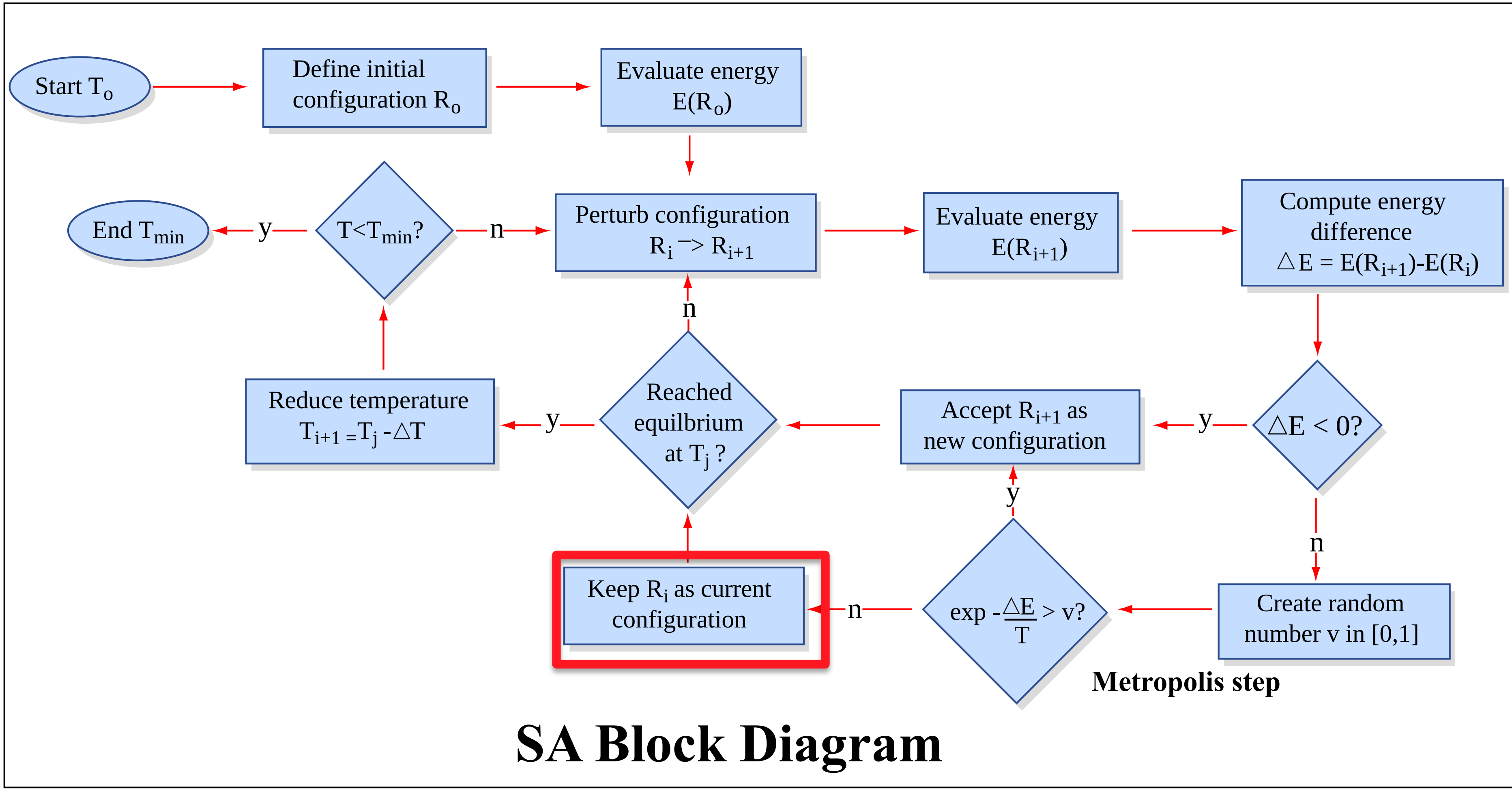
Simulated Annealing



SA Block Diagram

Image by MIT OpenCourseWare.

Simulated Annealing



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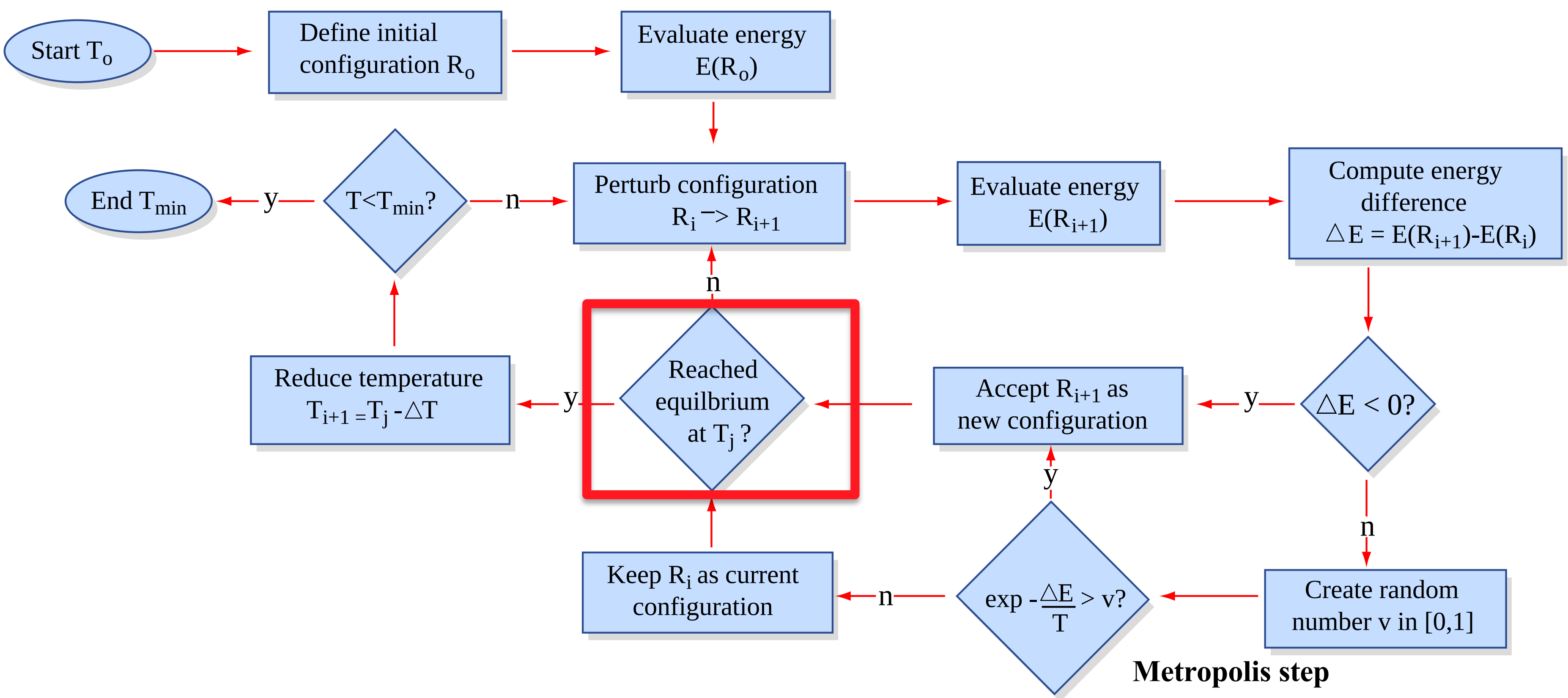
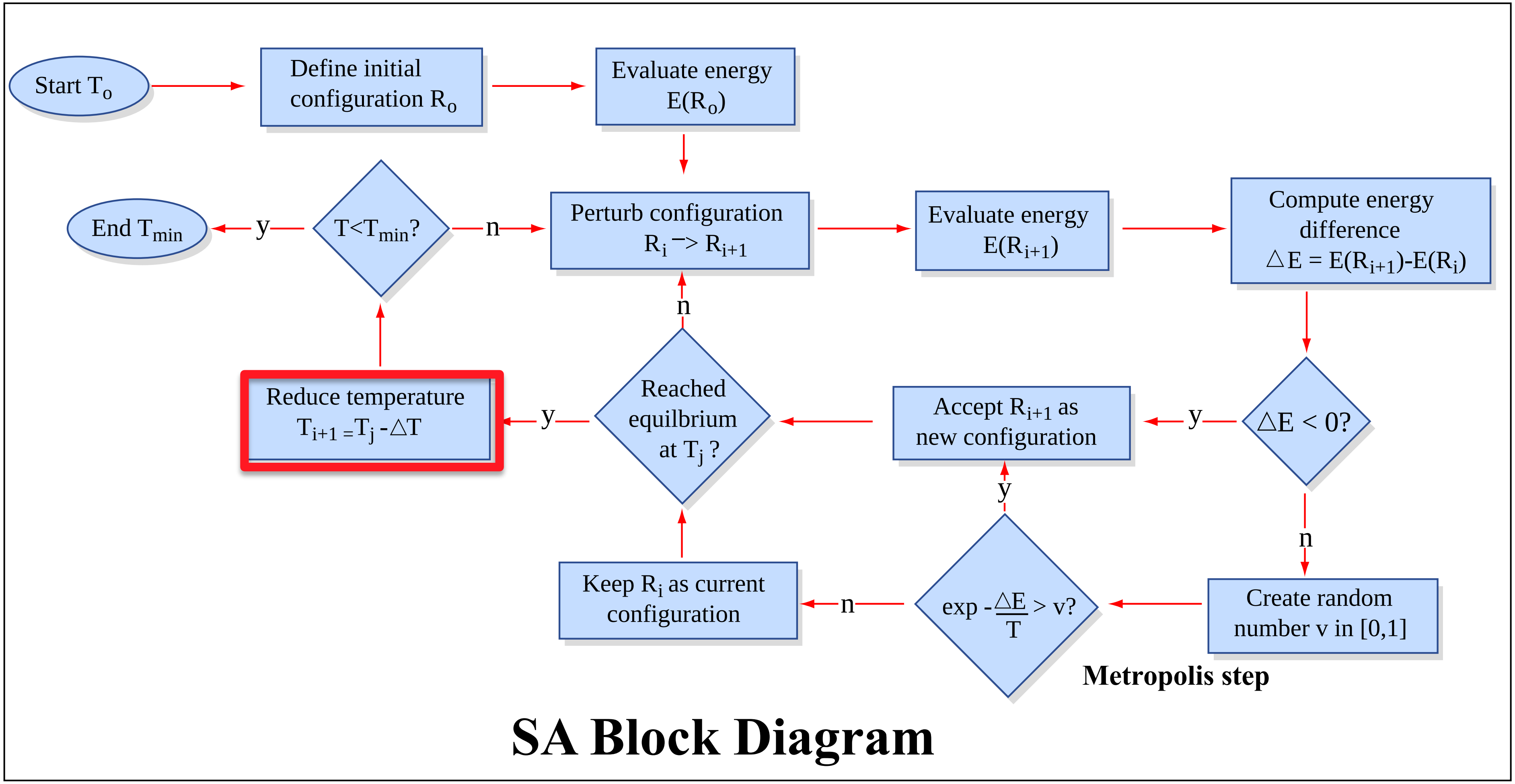
Simulated Annealing



SA Block Diagram

Image by MIT OpenCourseWare.

Simulated Annealing



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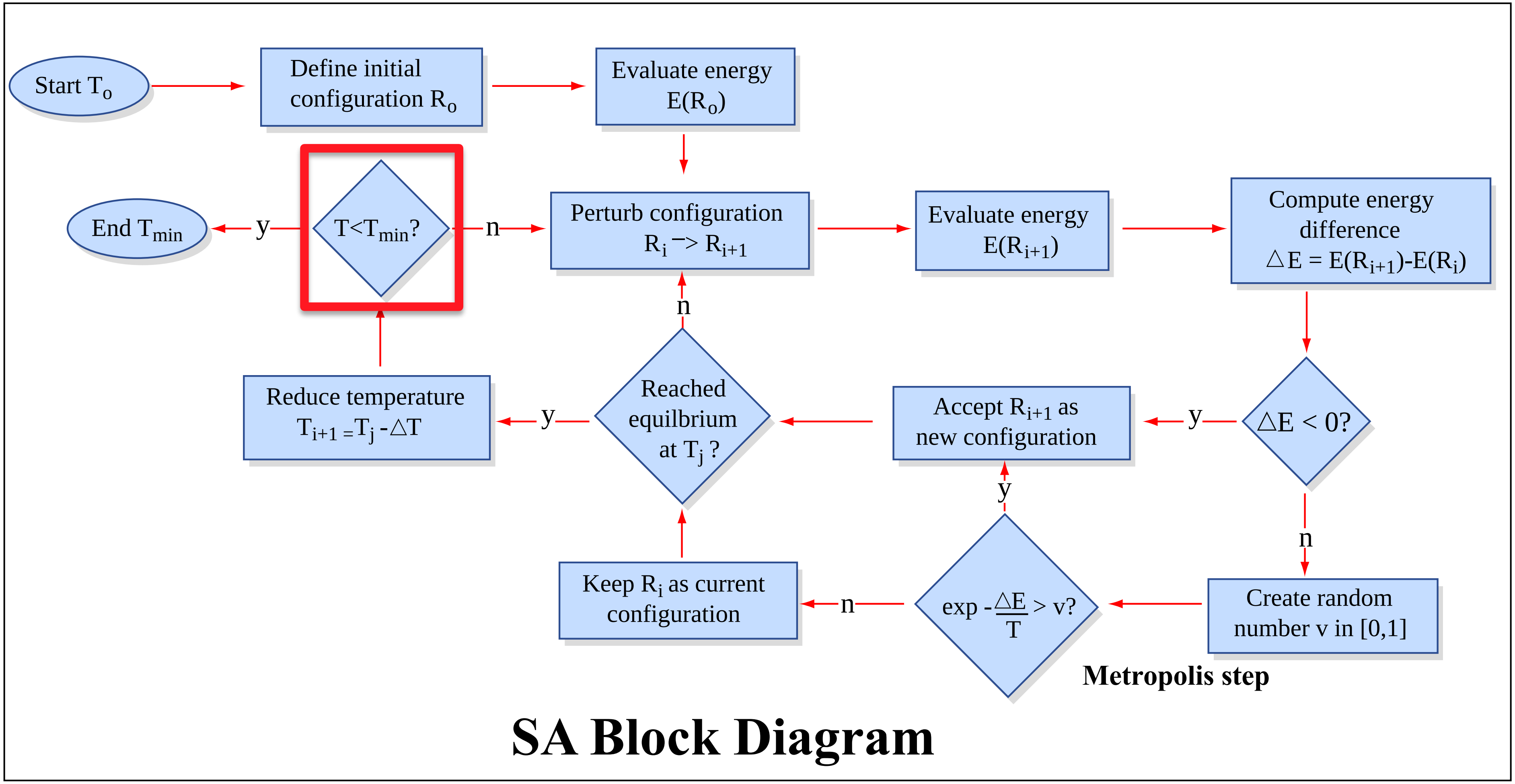
Simulated Annealing



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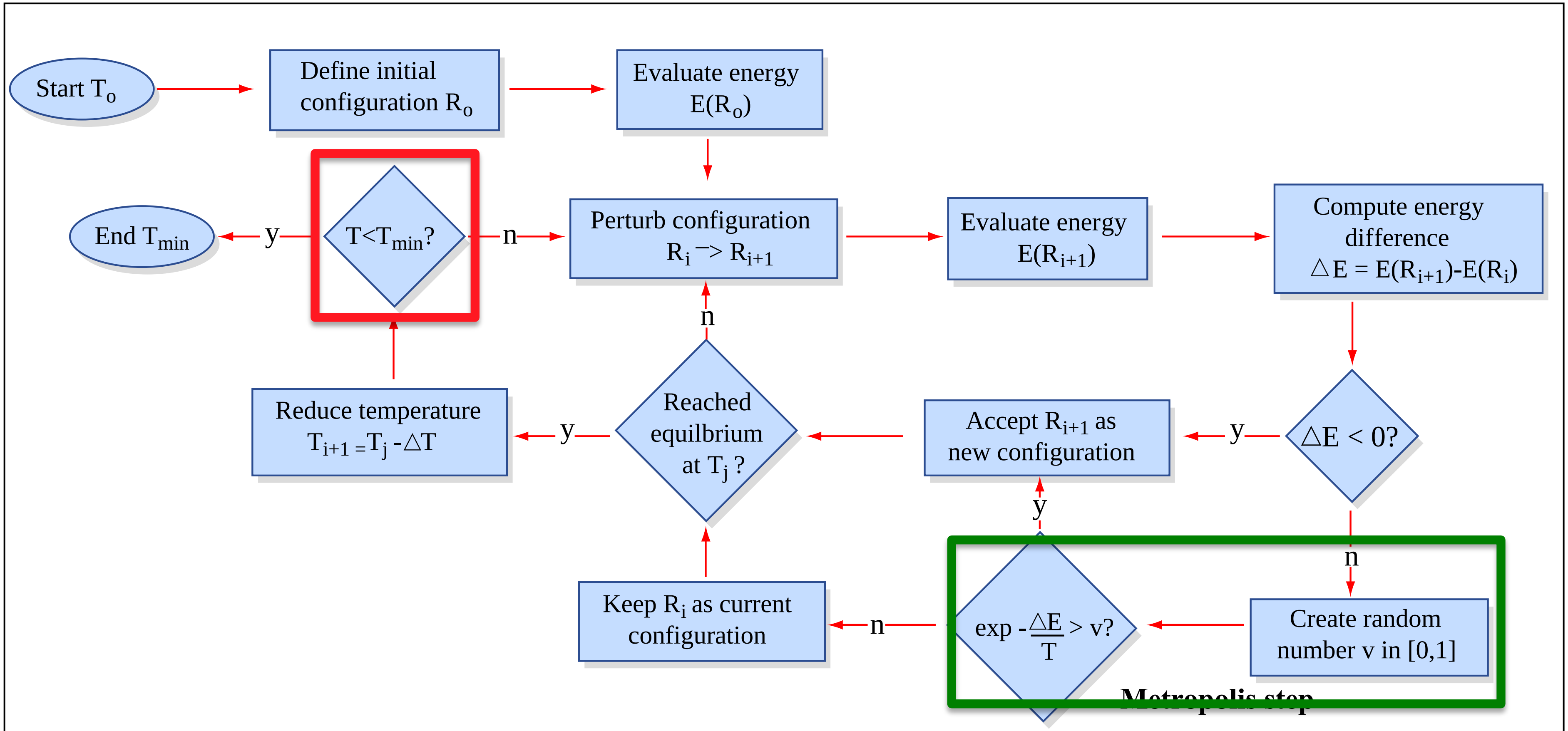
Simulated Annealing



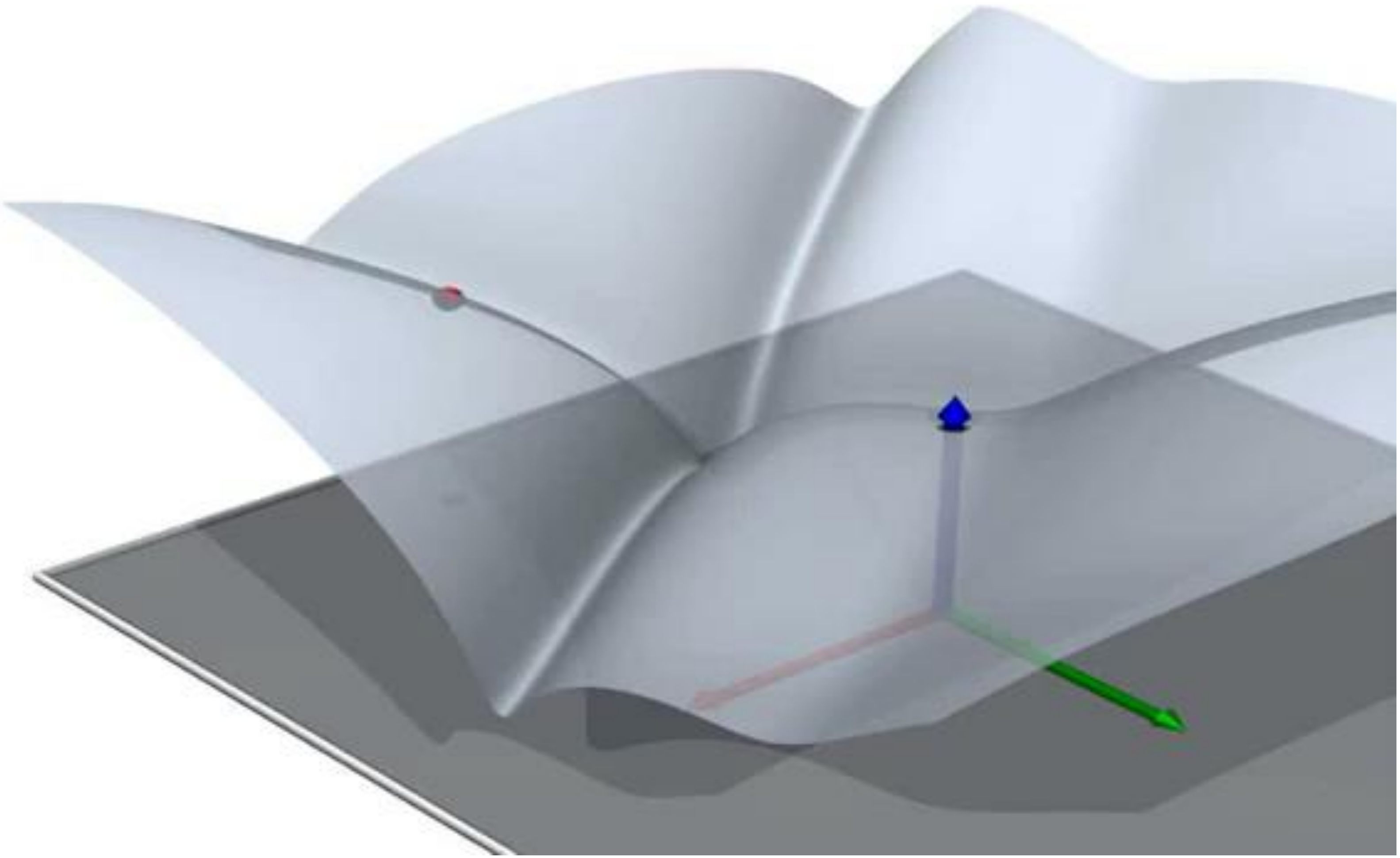
SA Block Diagram

Image by MIT OpenCourseWare.

Simulated Annealing

- Global optimization
- Combinatorial optimization
- Difficult to define good annealing schedule and neighbor generation scheme

Simulated Annealing



Examples from Graphics