Numerical Optimization

David Levin

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

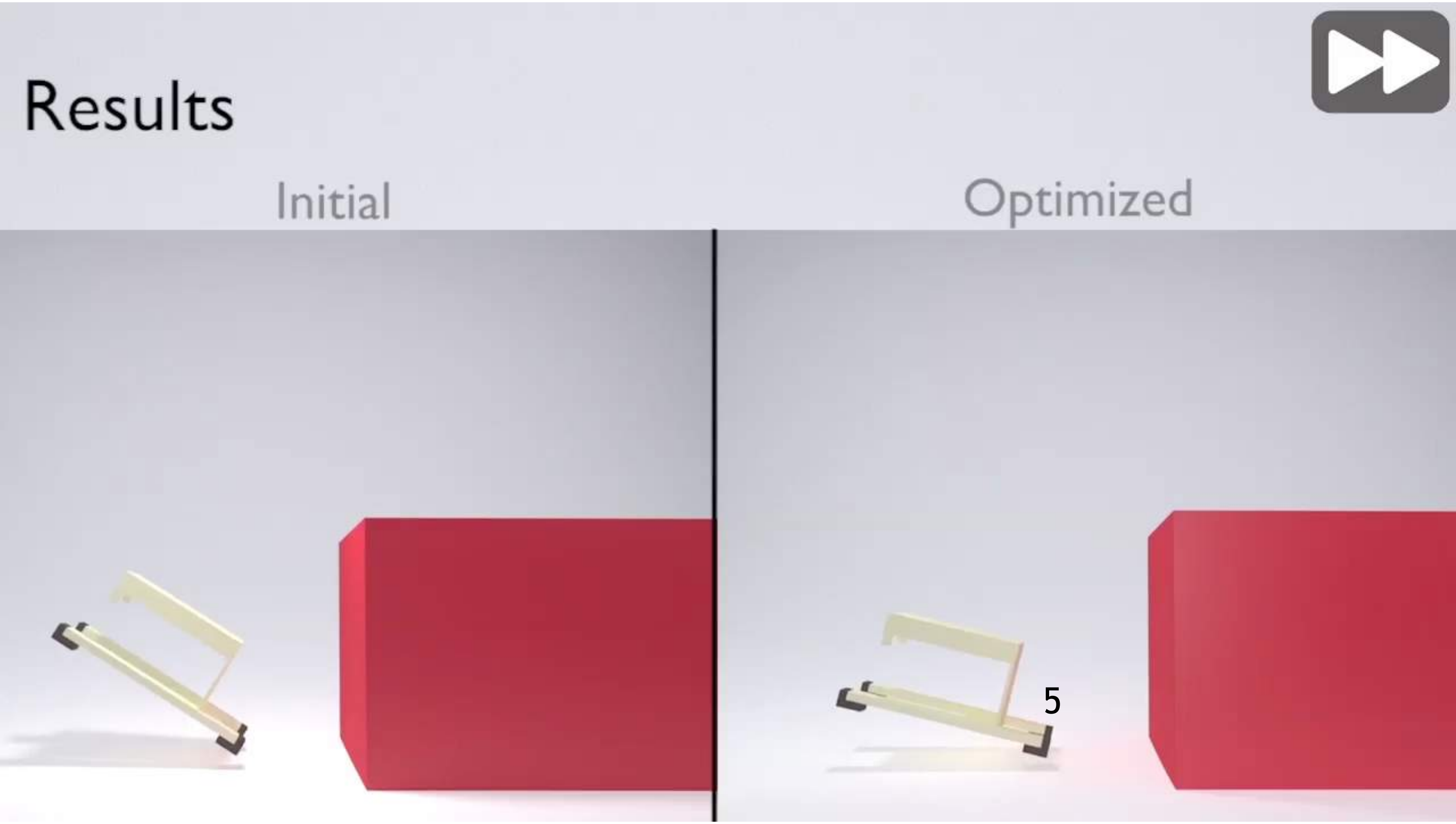
Plan for Today

- A fast and furious tour through numerical optimization
  - Discrete Optimization
    - Simulated Annealing
    - Branch and Bound

Warning

- Learning about optimization is a contact sport
- There will be math than (not too hard though!)

Example of a Design Optimization



Introduction to Optimization

- Optimization involves finding an “optimal value”
- i.e. Maximizing a profit, minimizing an area etc…

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

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

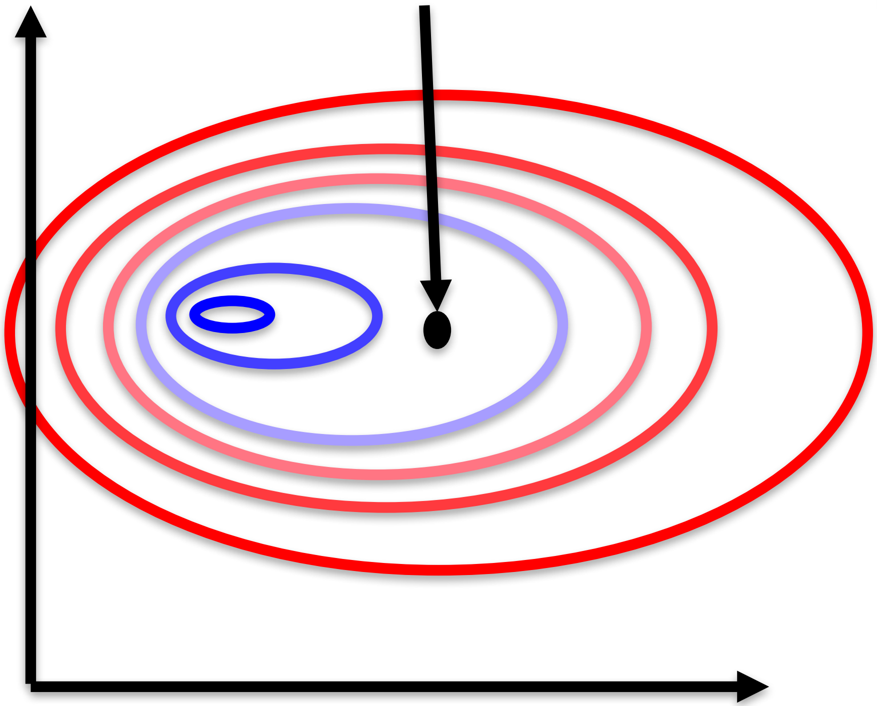
Types of Optimization

- Continuous vs. Discrete
- Constrained vs. Unconstrained

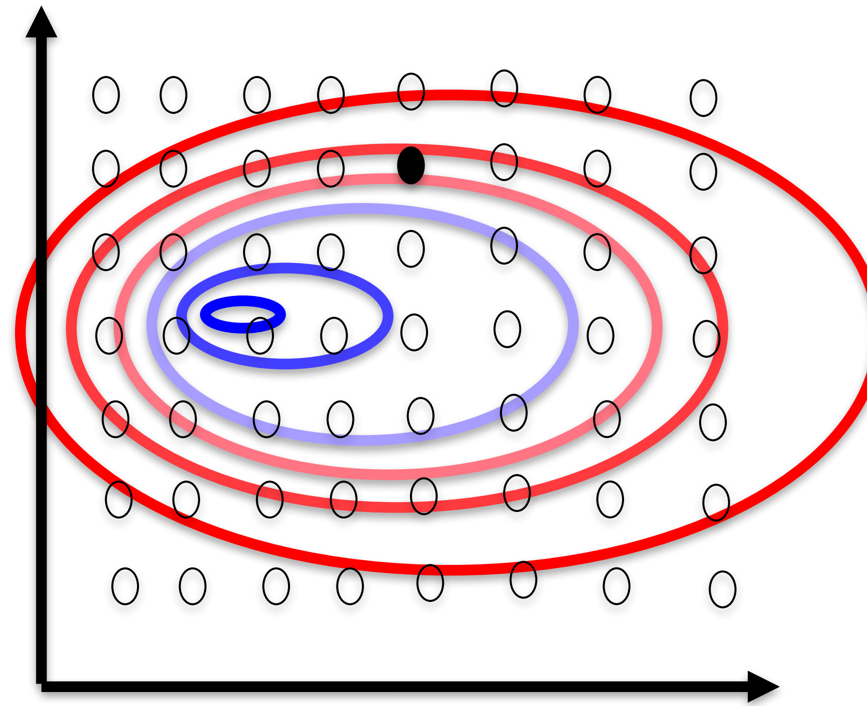
Continuous

Discrete

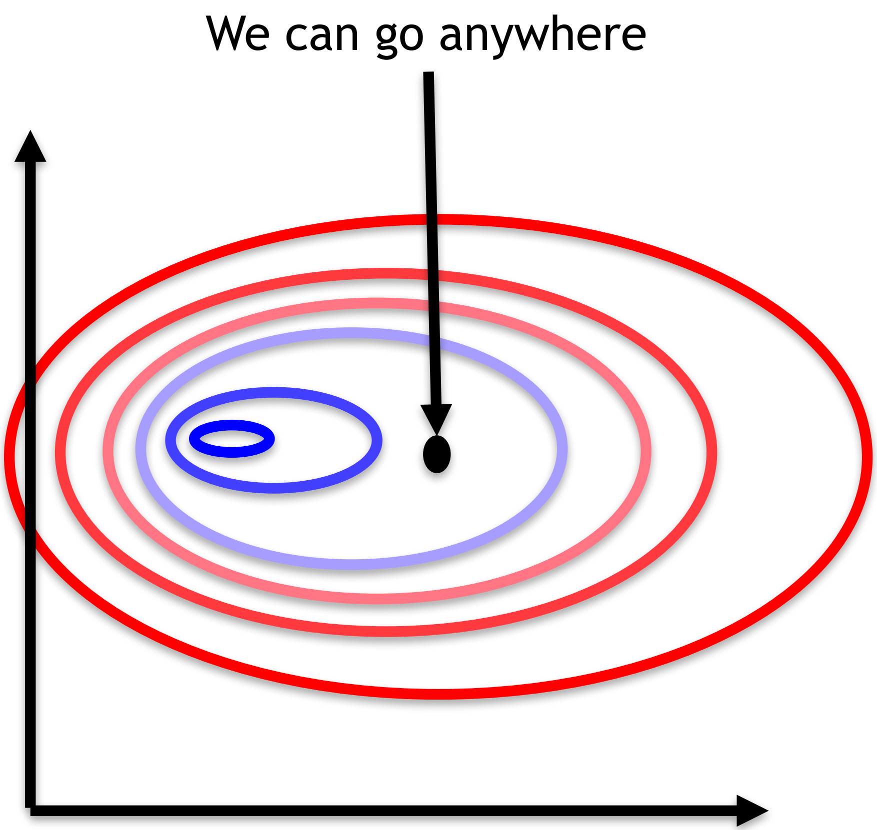
This point can move smoothly



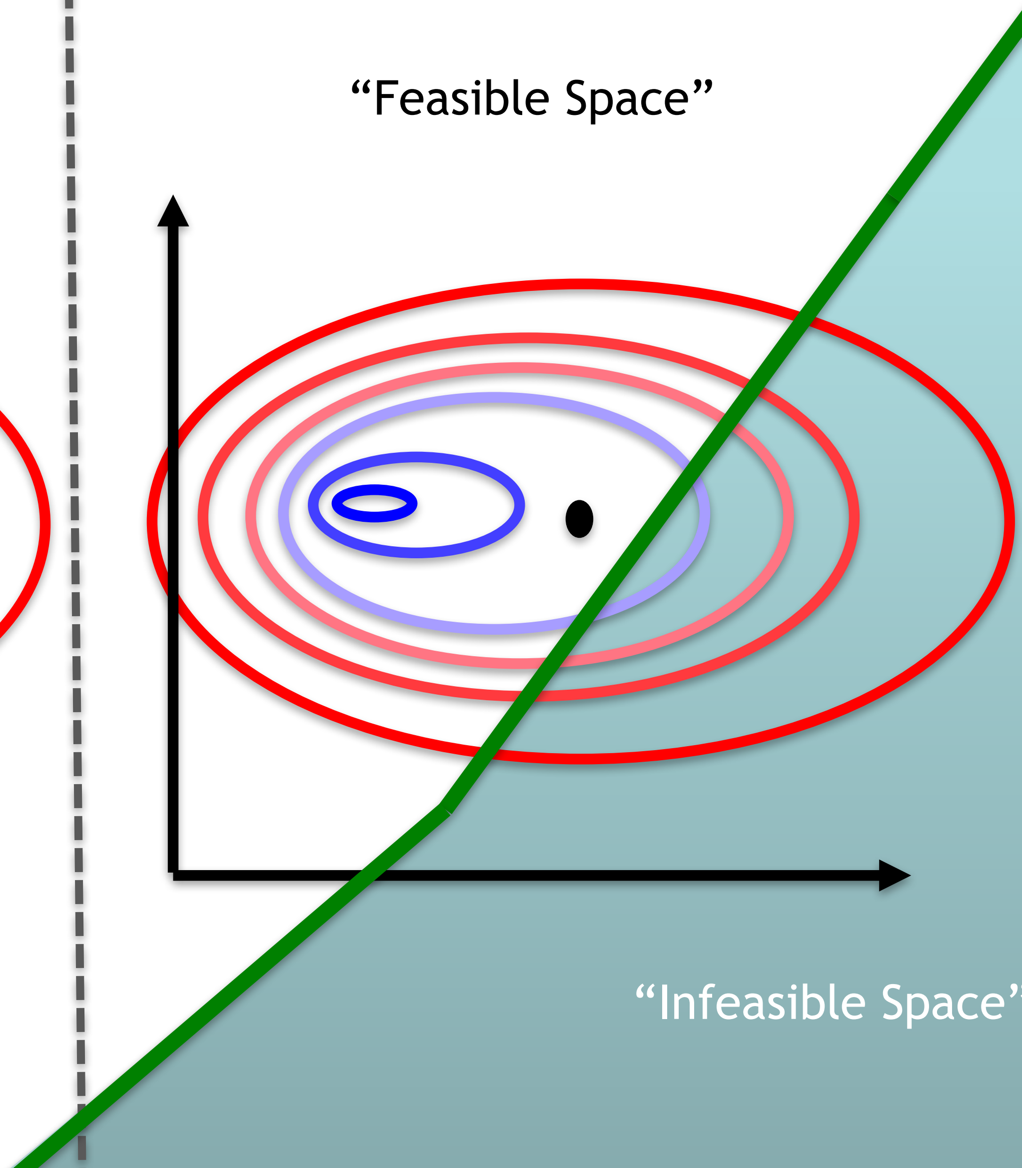
Choose from discrete points in parameter space



Unconstrained



Constrained



Types of Optimization

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

Continuous Optimization

- We're solving

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

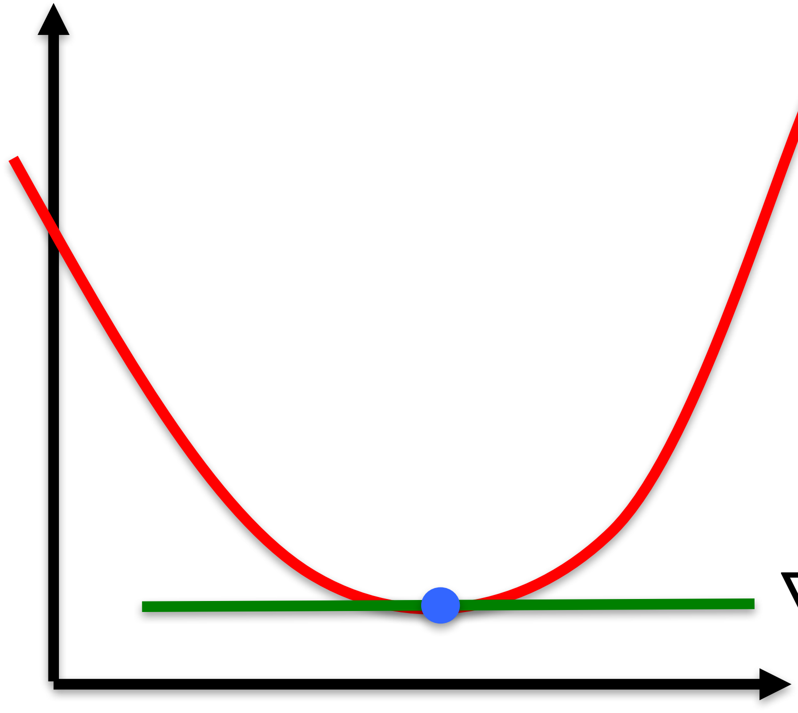
- How do we know we've found a potential solution?

IMPORTANT!!!!!

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

Potential Solutions

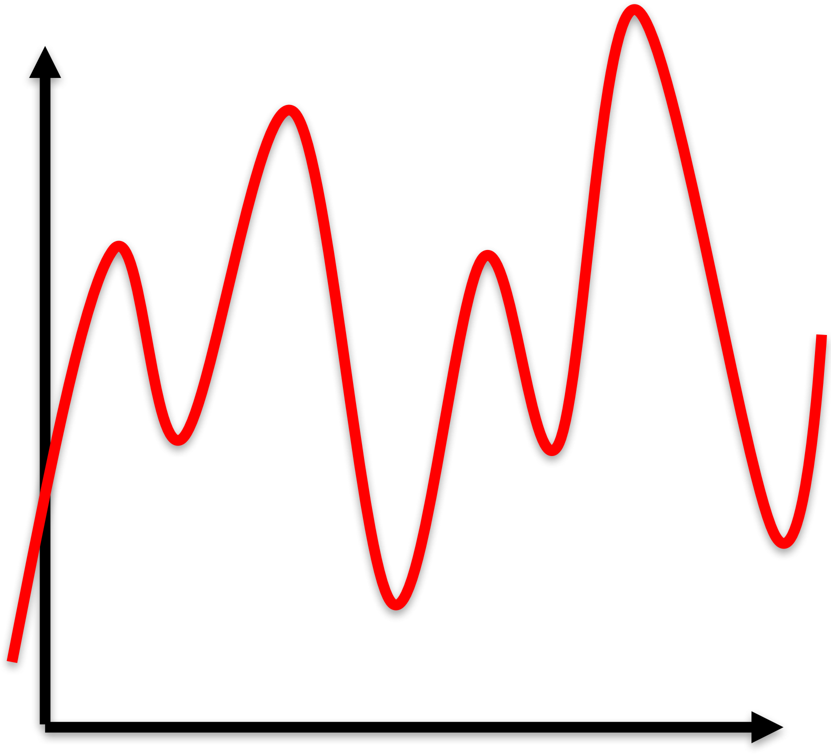
- Intuitively we look for a flat point on the cost function



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

Potential Solutions

- Sometimes that's easier said than done

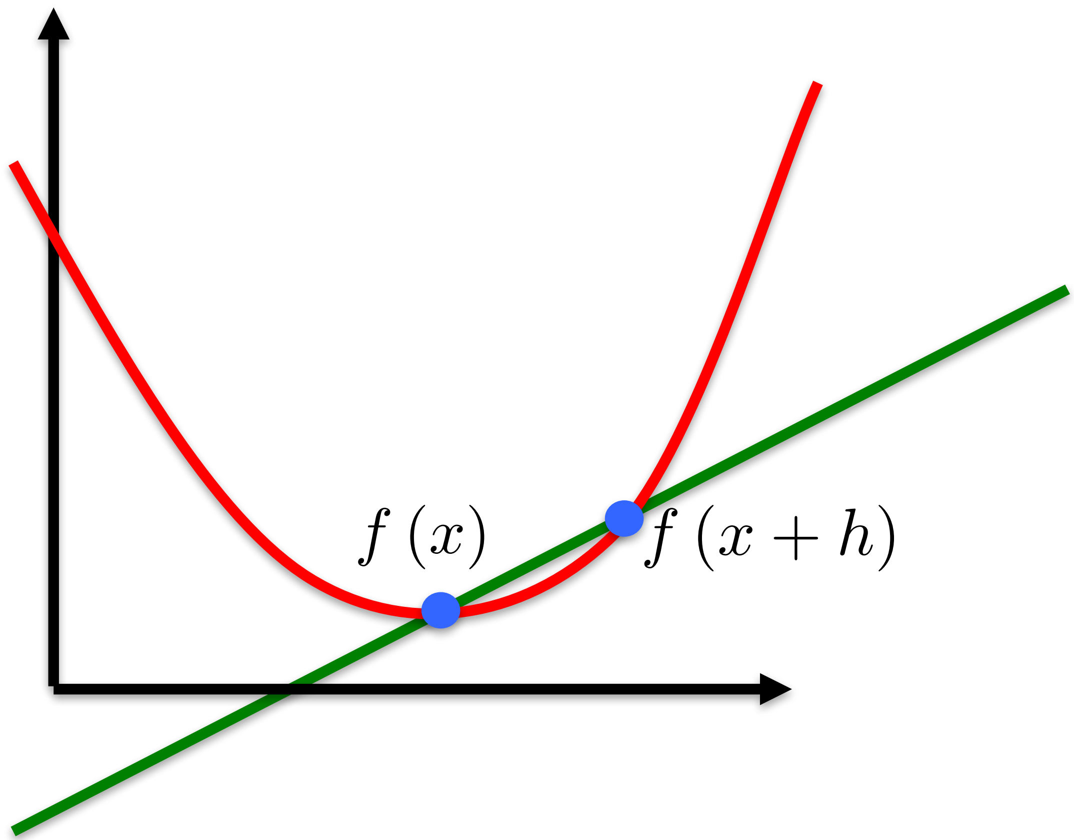


Computing the Gradient

- Analytically (pencil, paper, mathematica)
- Finite Differences

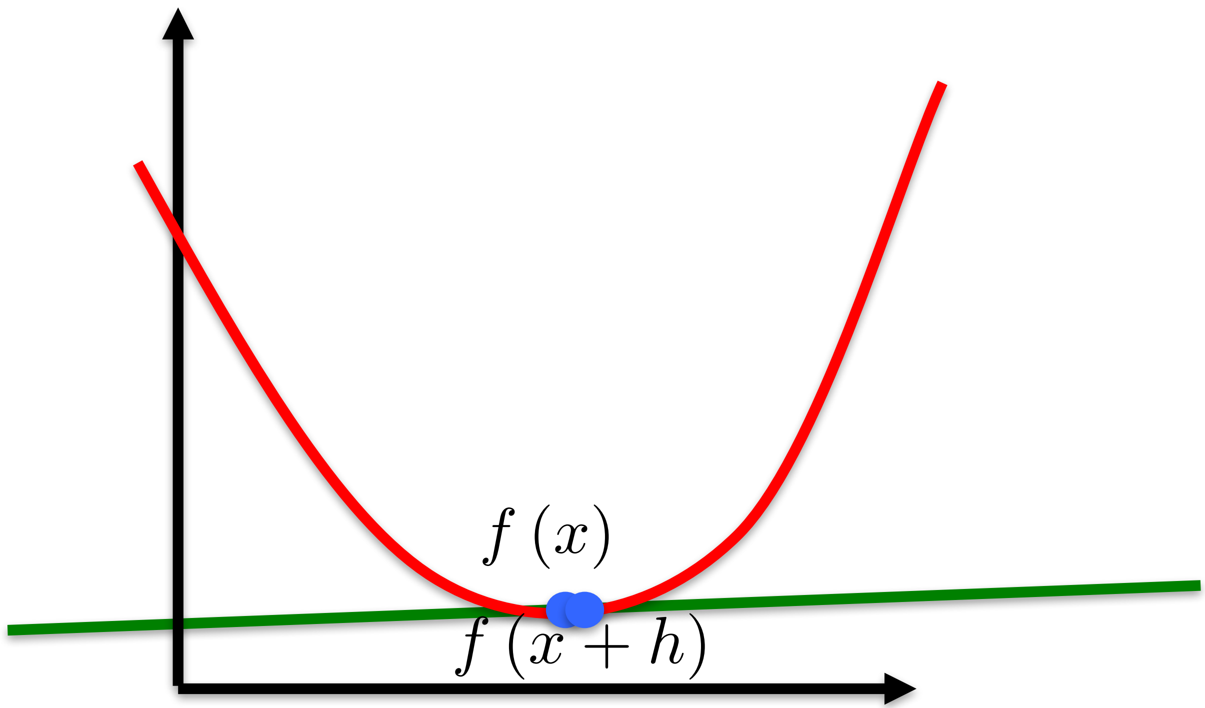
Potential Solutions

- Computing the gradient requires a limit



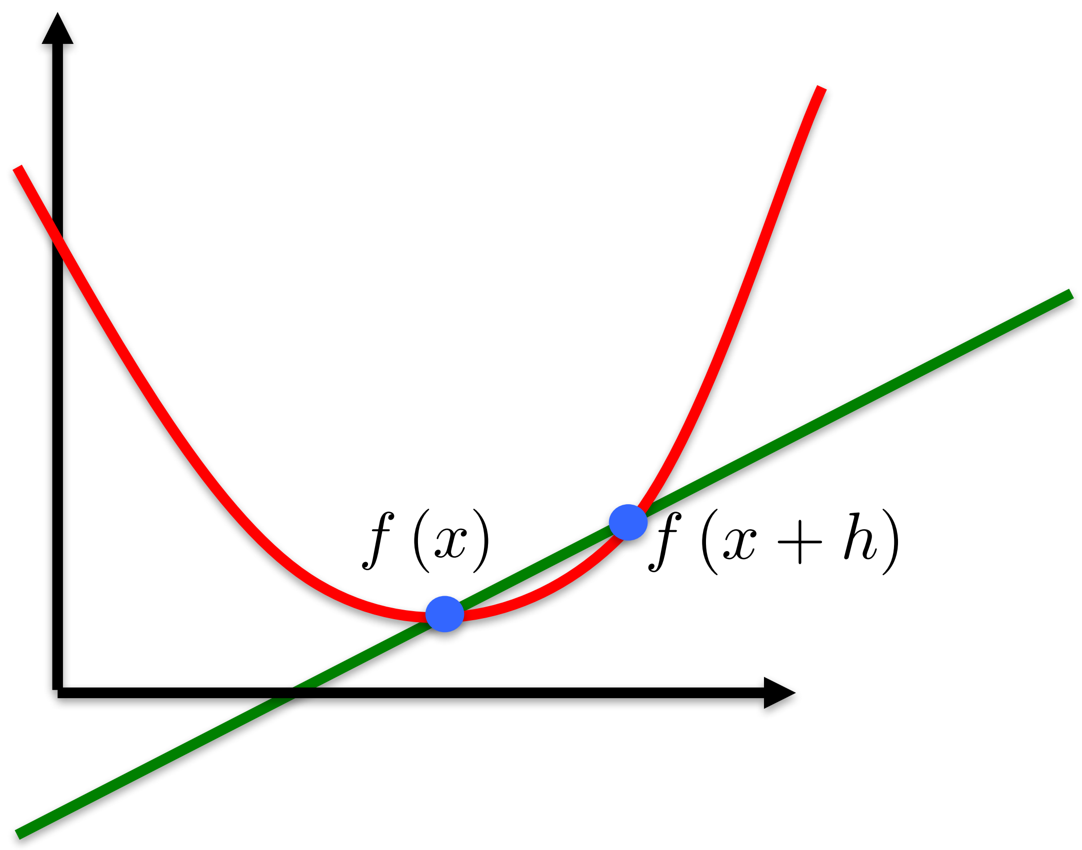
Potential Solutions

- Computing the gradient requires a limit



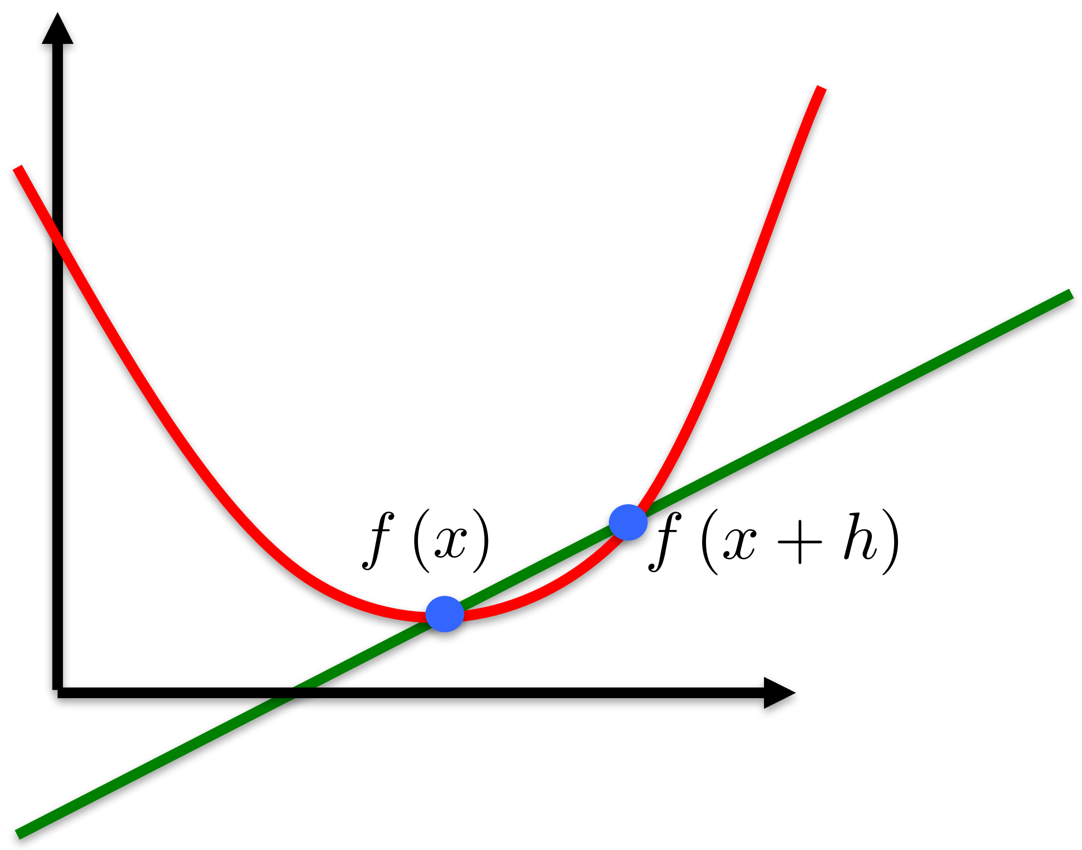
Potential Solutions

- In Finite Differencing we choose h and evaluate $\frac{1}{h} f(x+h) - f(x)$ numerically



Potential Solutions

- Matlab does this automatically which makes it easy to test out optimizations



Continuous Optimization

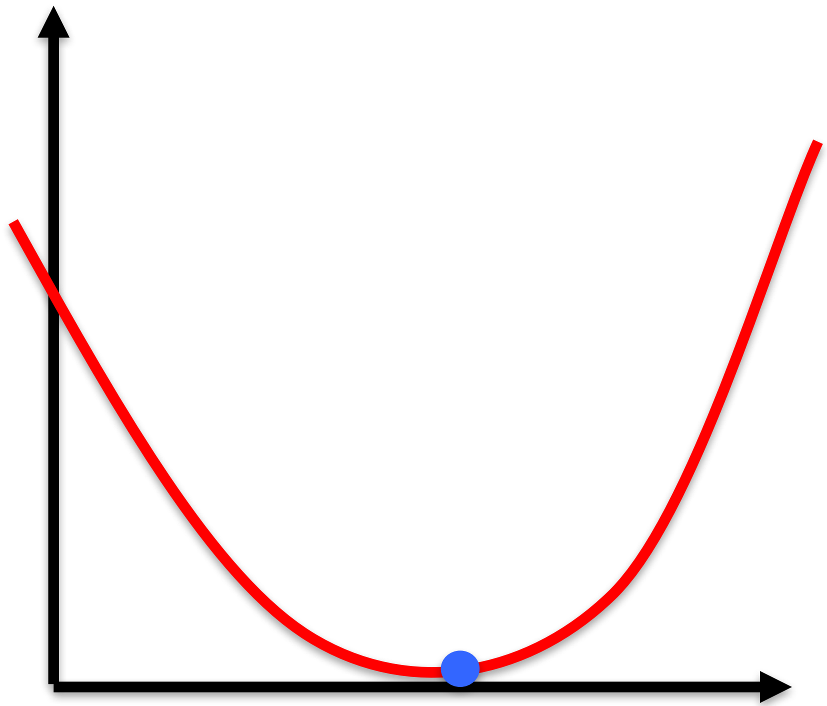
- General, continuous optimizations are difficult to solve
- We focus on certain classes of problems that are solvable

Convex Optimization

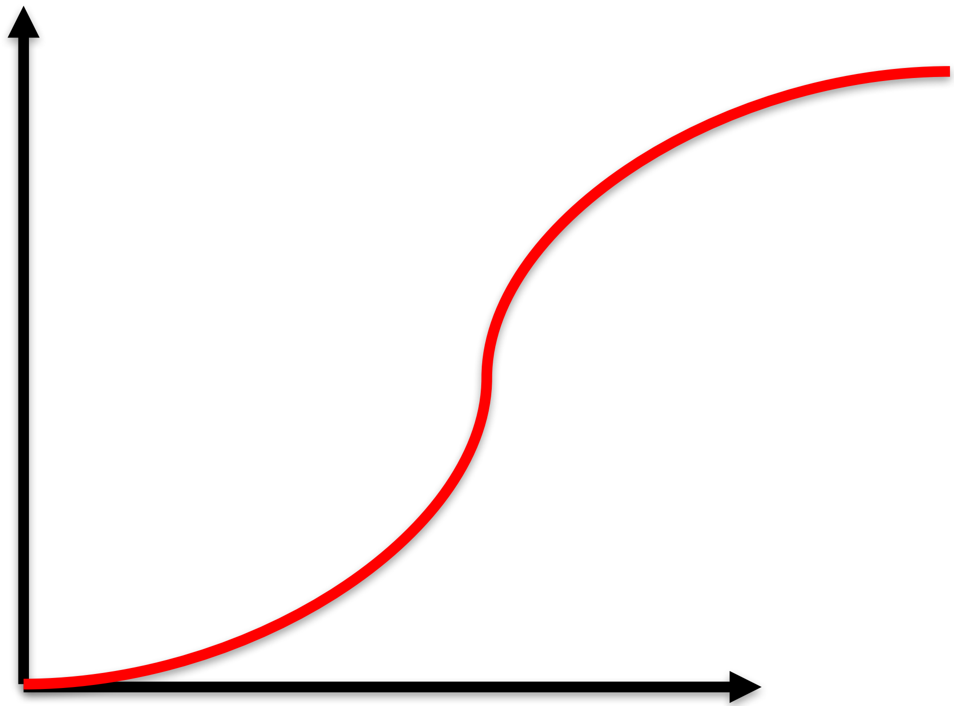
Convex Optimization

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

Convex Optimization



Is This Convex ?



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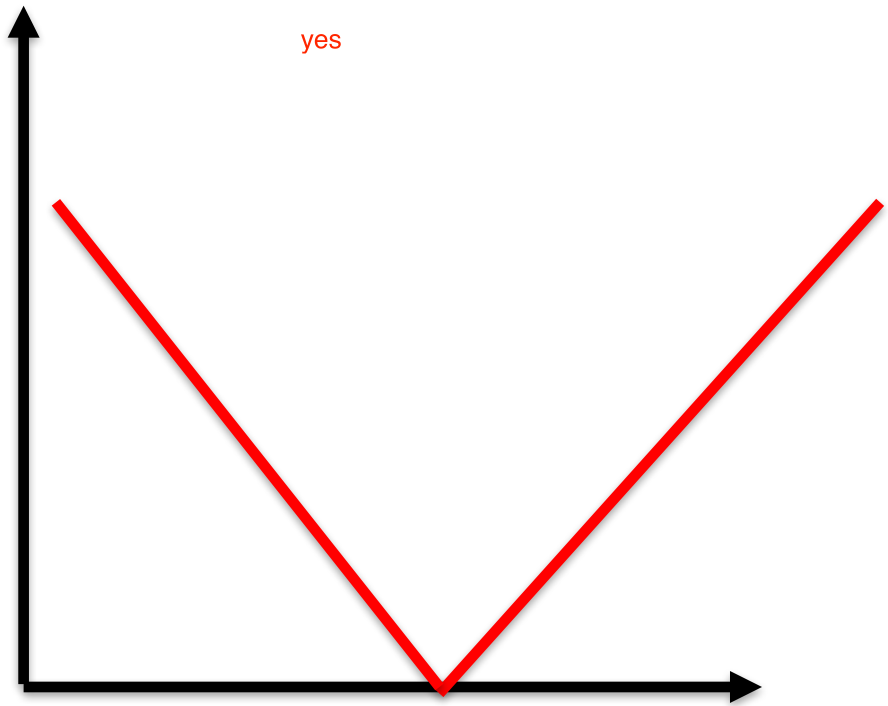
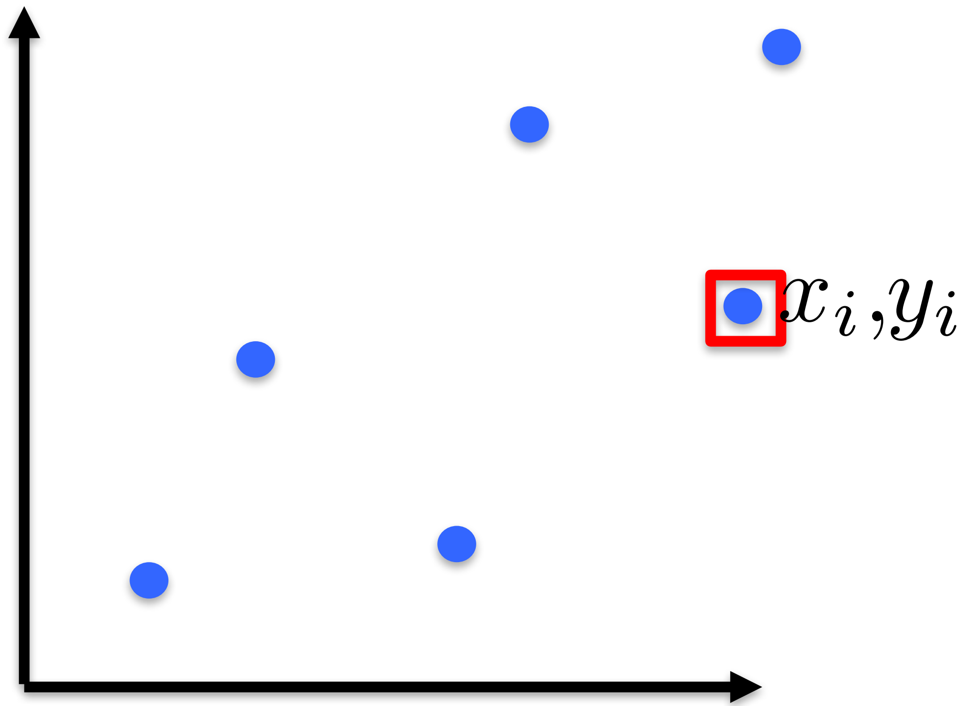


A Simple Example: Least Squares

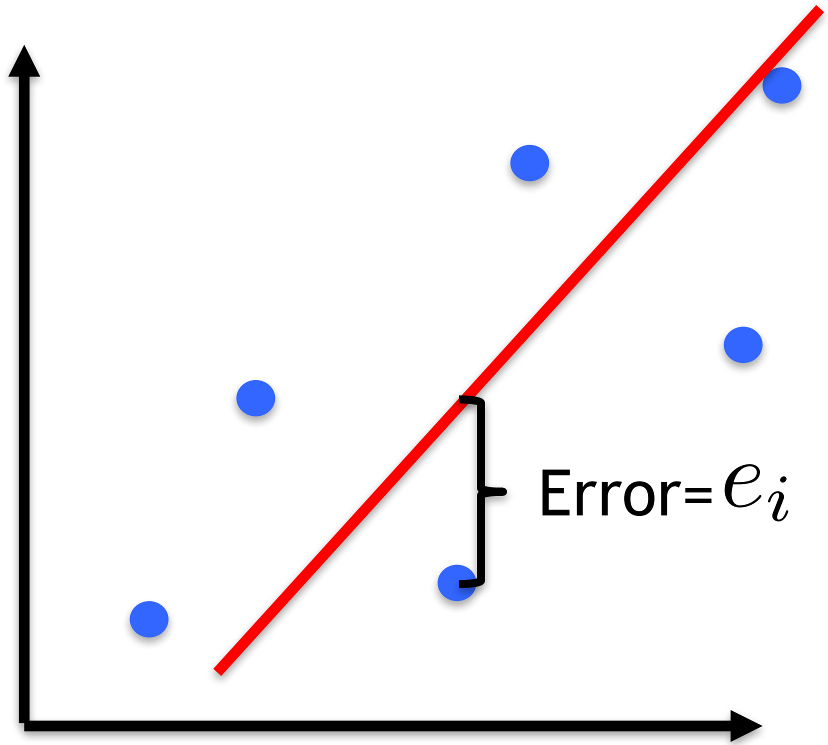
- Least Squares Fitting of a Curve



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

A Simple Example: Least Squares

- 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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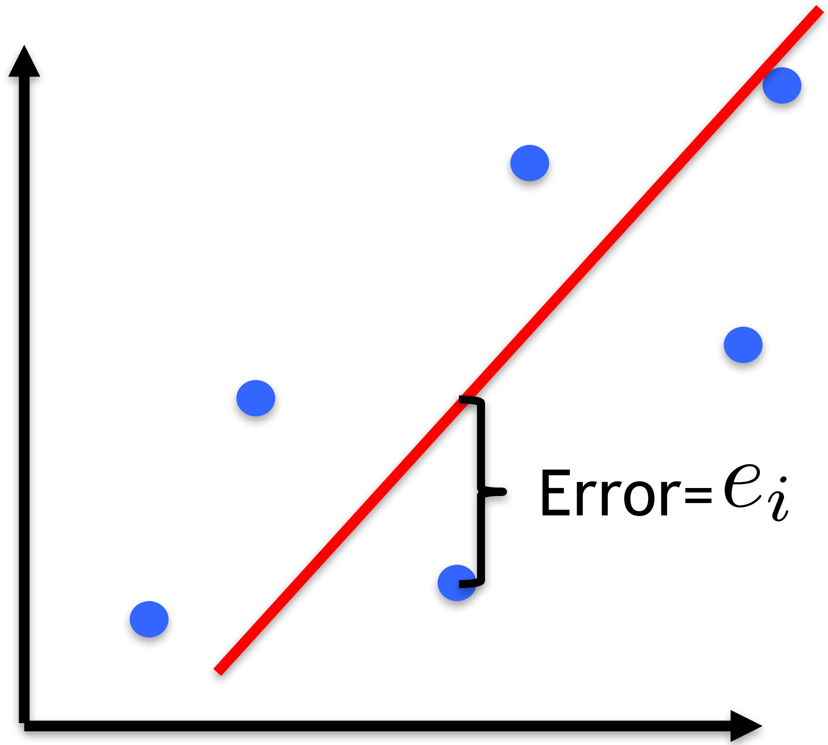
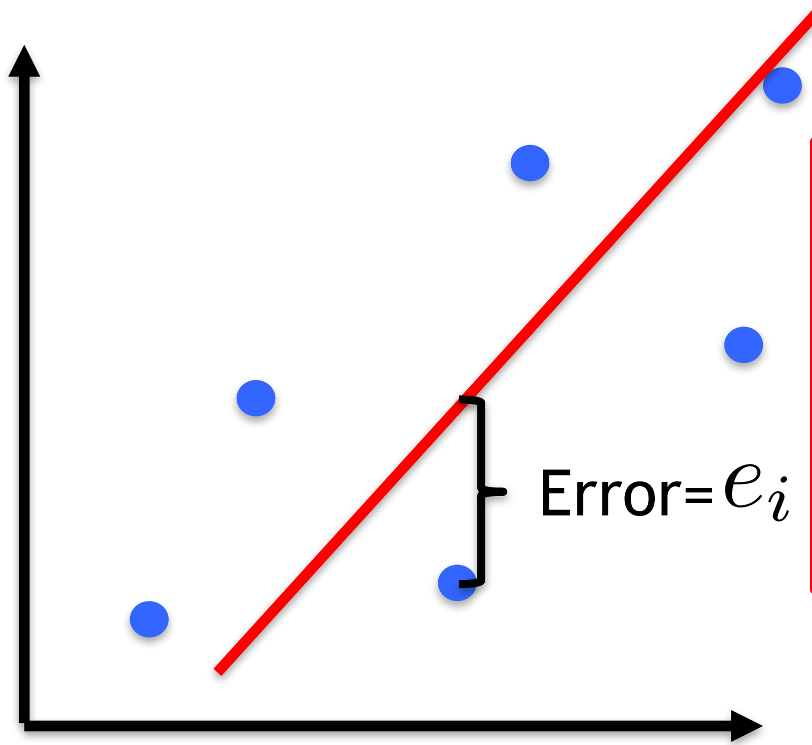


$$e_i = y_i - mx_i - c$$

A Simple Example: Least Squares

- Minimize sum of squared errors



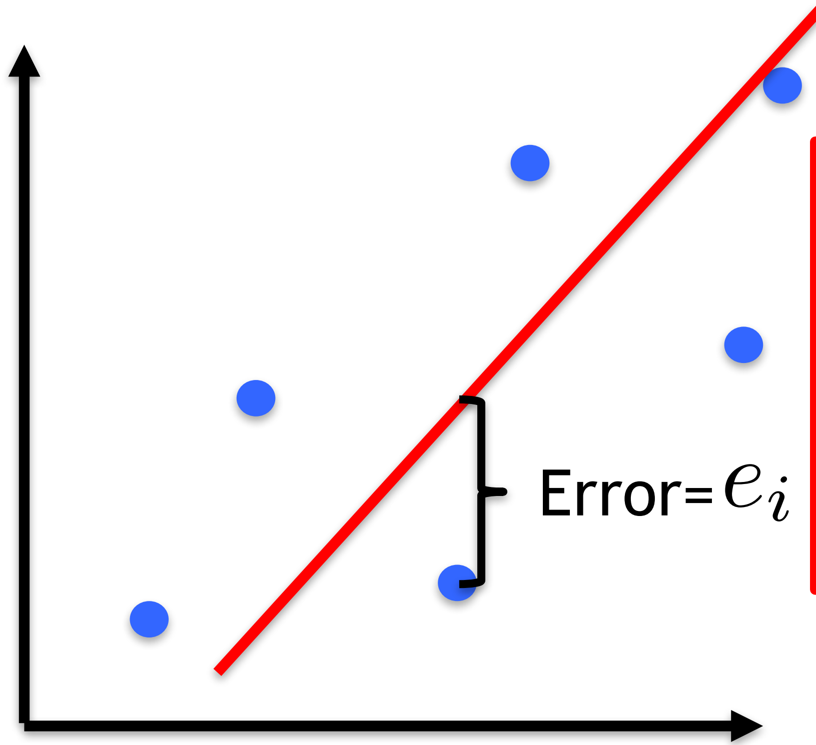
$$\boxed{\mathbf{A} = \begin{pmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \\ x_n & 1 \end{pmatrix}}$$

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

A Simple Example: Least Squares

- Minimize sum of squared errors

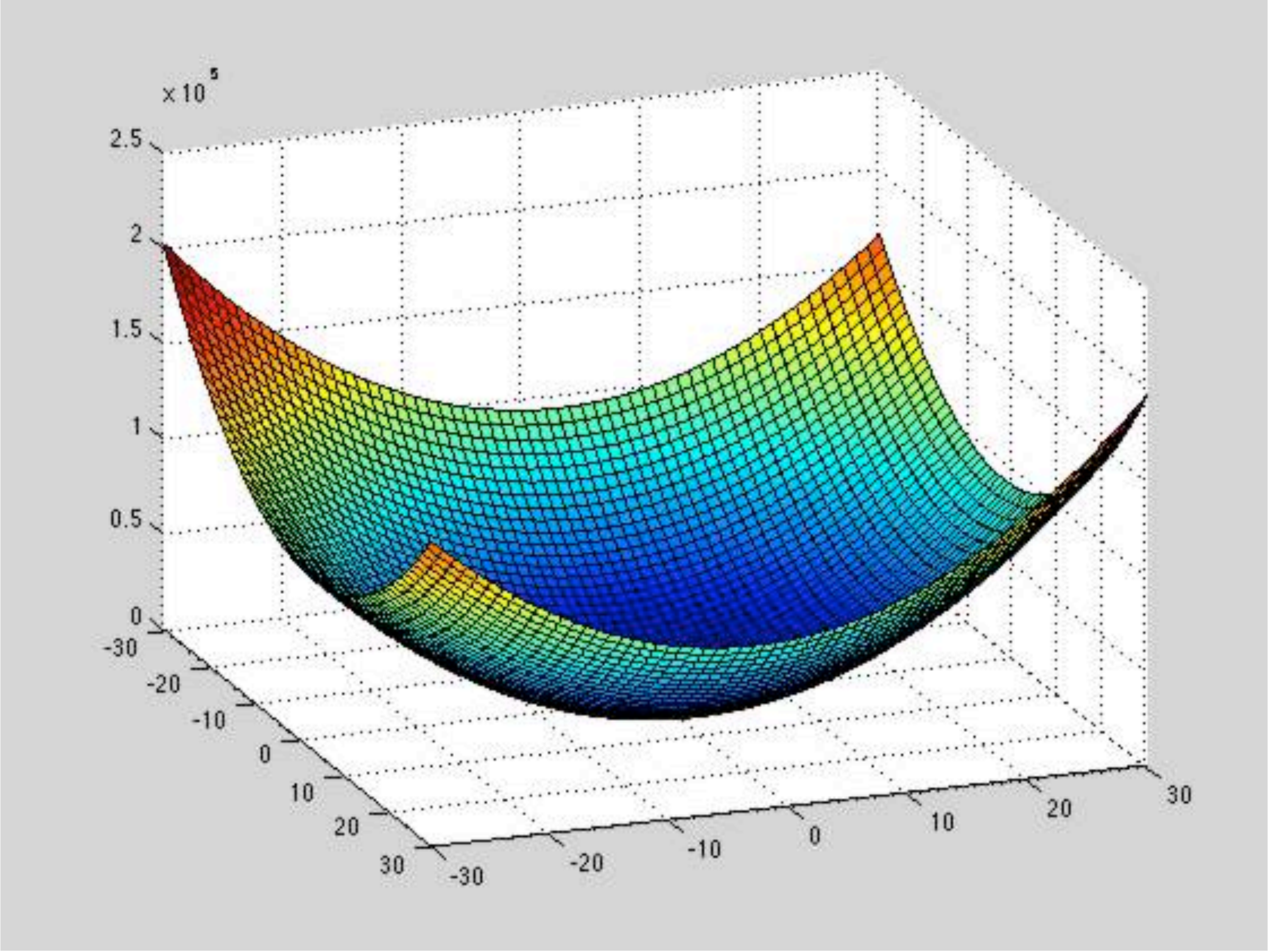
$$\boxed{\theta = \begin{pmatrix} m \\ c \end{pmatrix}}$$



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

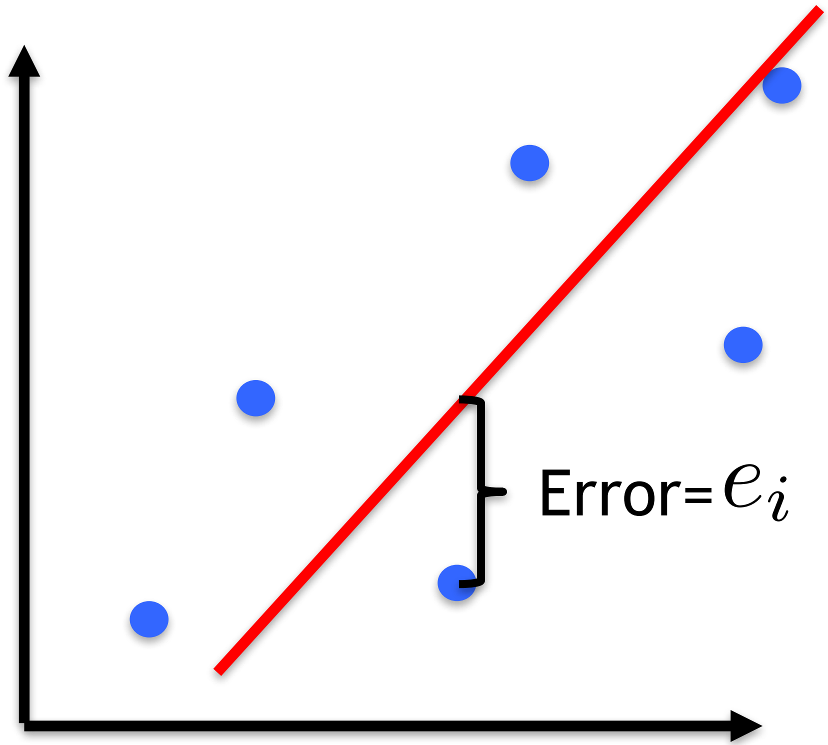
Sum of Squared Error = f(x) = $||\mathbf{A}\theta - \mathbf{y}||^2$

Simple Example: Least Squares



A Simple Example: Least Squares

- Solution is the normal equations



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

Descent Algorithms

- Used when cost function is more complicated
- 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

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

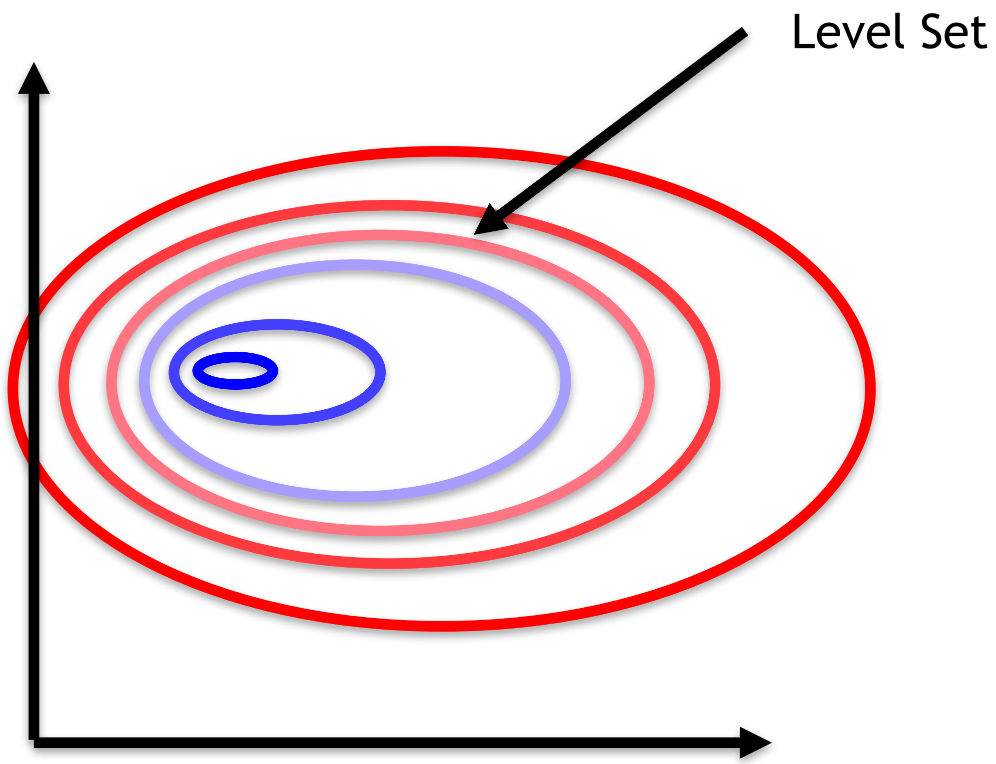
Gradient Descent

- Recall that the gradient of a function is given by

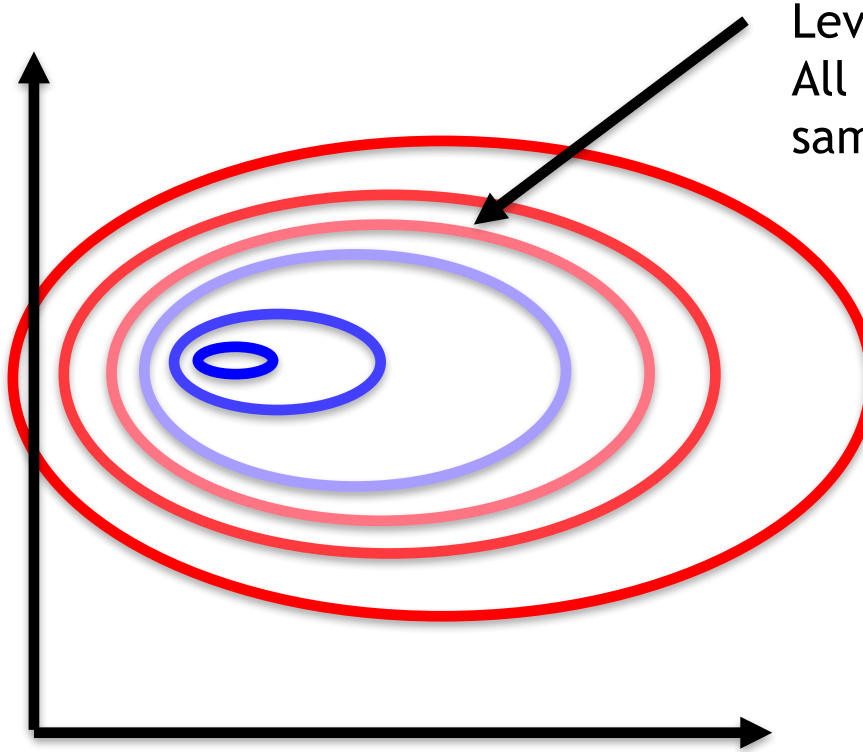
$$\nabla f\left(\mathbf{x}\right) = \begin{pmatrix} \frac{\partial f}{\partial \mathbf{x}_1} & \frac{\partial f}{\partial \mathbf{x}_2} & \cdots & \frac{\partial f}{\partial \mathbf{x}_n} \end{pmatrix}$$

- Points in direction of maximum ascent

An Aside: Level Sets

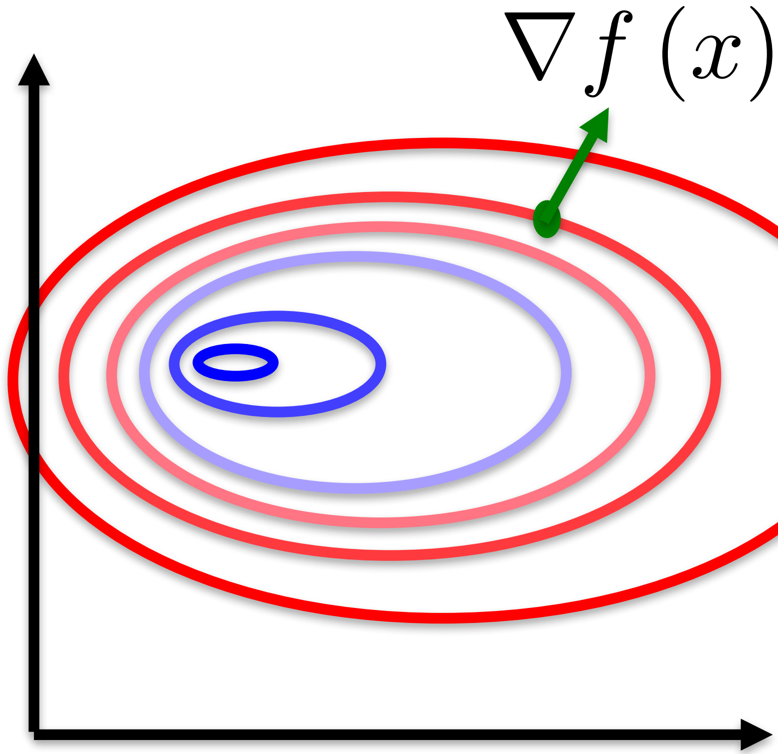


An Aside: Level Sets

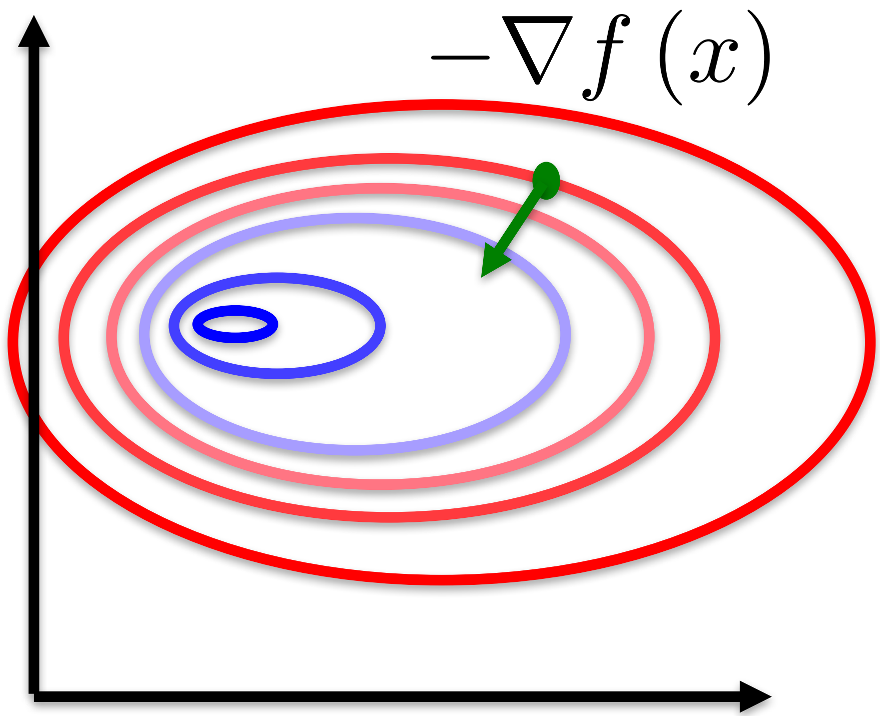


Level Set:
All points that have same value of f(x)

Gradient Descent



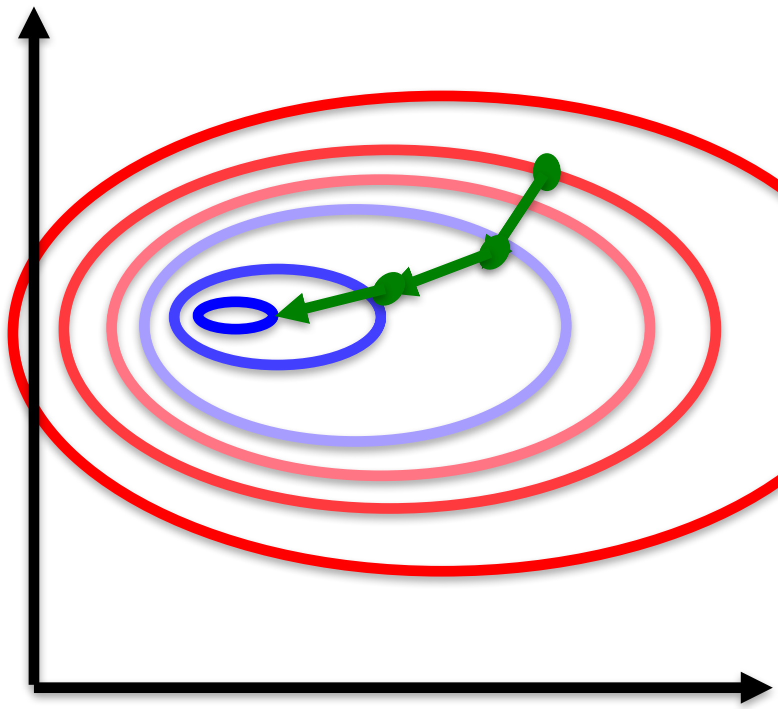
Gradient Descent



Simple Gradient Descent Algorithm

- While not at an optimal point
  - Compute the gradient at current point (x)
  - Move to new point $x = x - \boxed{h} \nabla f(x)$

Gradient Descent



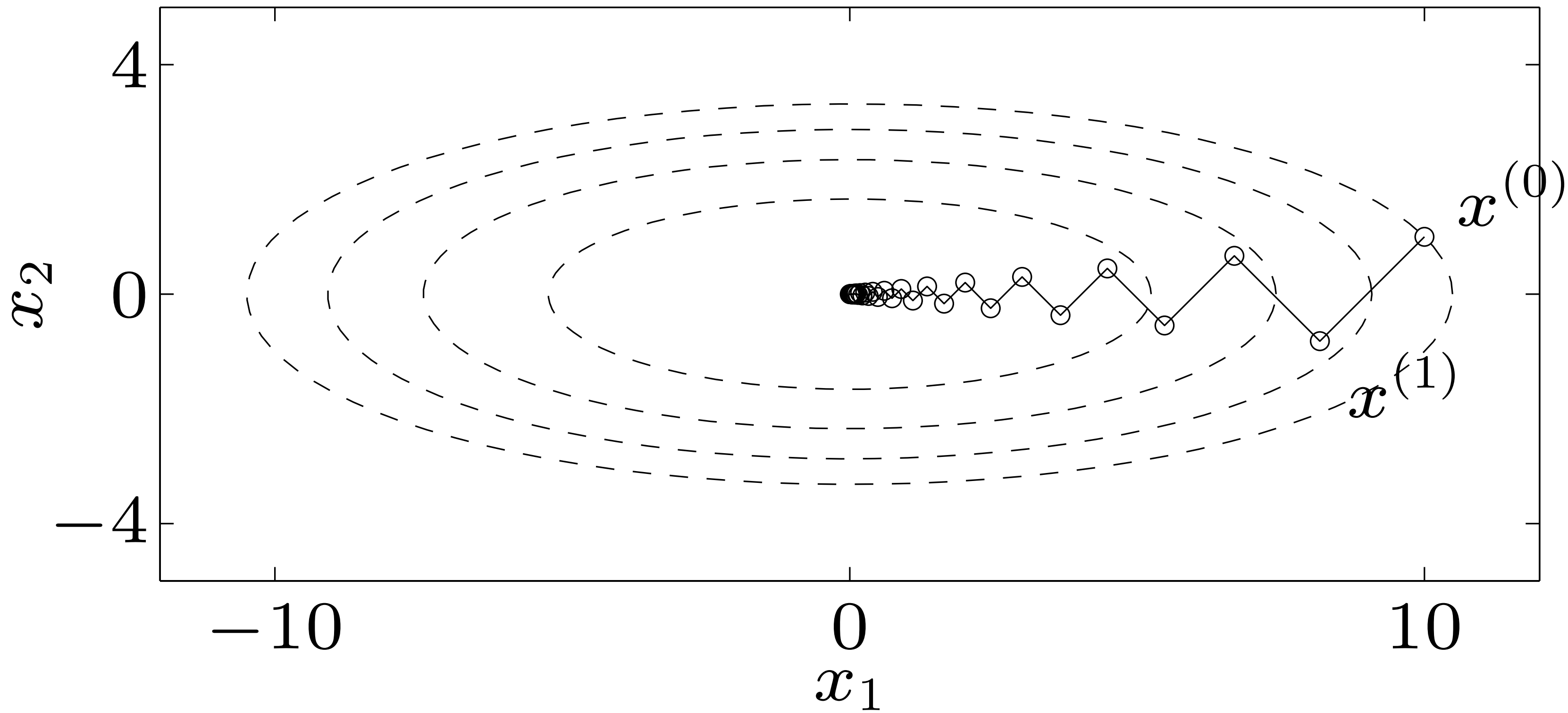
Simple Gradient Descent Algorithm

- While not at an optimal point
  - Compute the gradient at current point (x)
  - Move to new point $x = x - \boxed{h} \nabla f(x)$

Gradient Descent

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

Gradient Descent



Newton’s Method

- Can we choose better search directions ?
- This is the goal of Newton’s Method
- Newton’s Method needs access to the “Hessian” of a function

An Aside: The Hessian

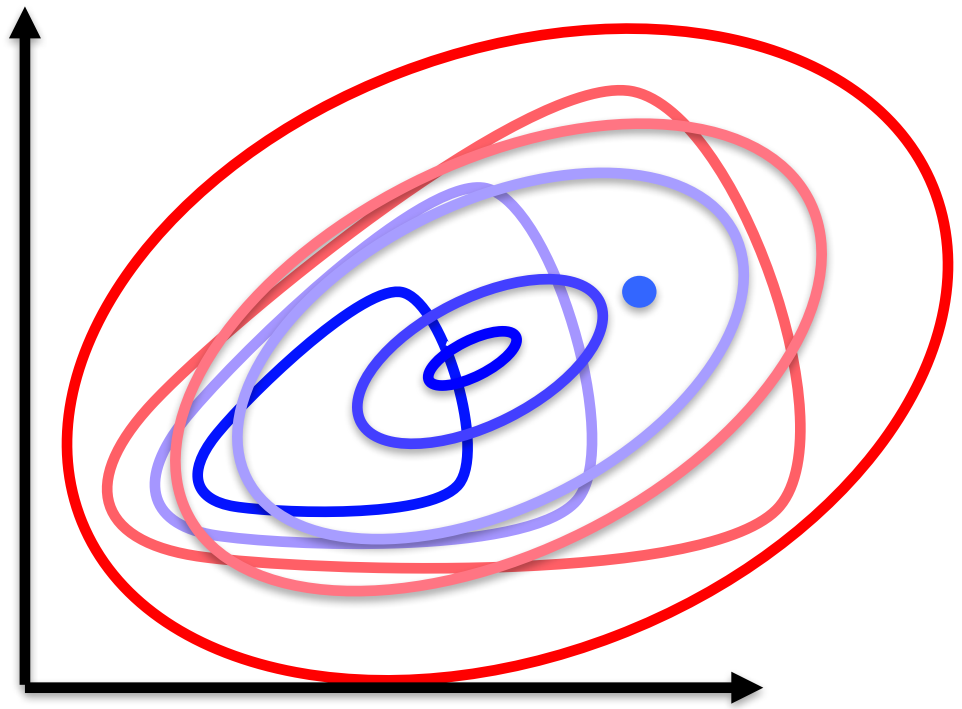
- The Hessian of a function $f(\mathbf{x})$

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

Newton's Method

- In Newton's Method we approximate our function using a quadratic model
- Use that model to compute the best step length

Newton’s Method



Choose best descent direction according to approximation

Newton's Method

- How do we get our approximation ?
- Taylor Expansion (we saw this in lecture 1)

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

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

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

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

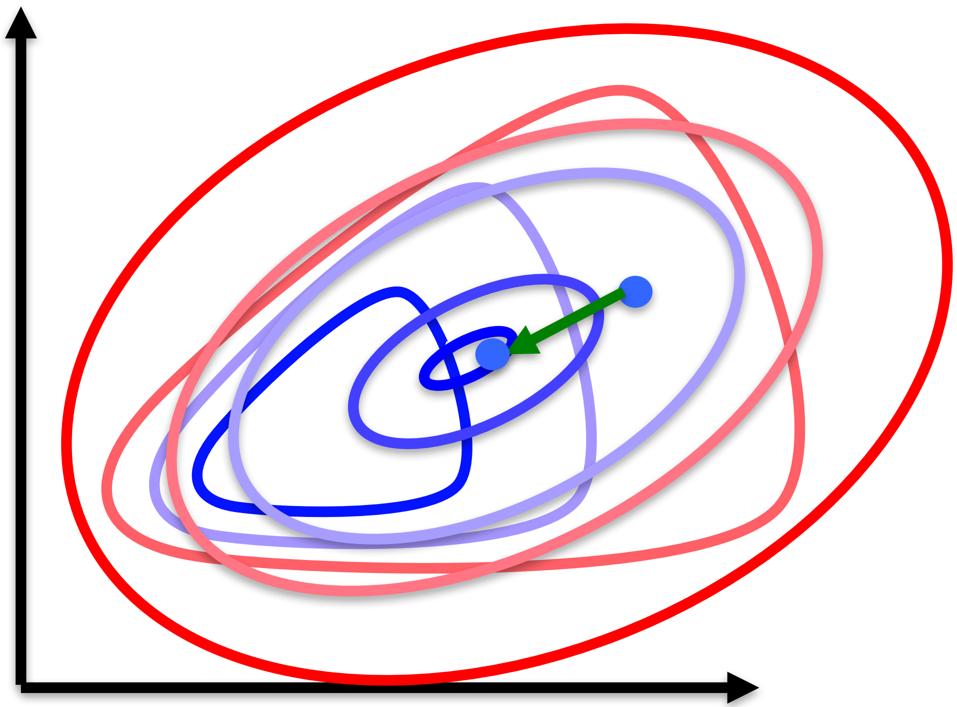
- We minimize the model problem
- Find where the gradient is zero

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 $\mathbf{x}^c = \mathbf{x}^c + h\Delta\mathbf{x}$
  - Update $\Delta\mathbf{x} = -\mathbf{H}^{-1}\mathbf{g}$

Aside: Hessian for Black Box Functions

- Centered Finite Differences:

$$\frac{\partial f}{\partial \mathbf{x}_i}\left(\mathbf{x}\right) \approx \frac{f\left(\mathbf{x} + \epsilon \mathbf{e}_i\right) - f\left(\mathbf{x} - \epsilon \mathbf{e}_i\right)}{2\epsilon}$$

- Second order accurate

The Hessian via Finite Differences

- Each entry of the Hessian: $\dfrac{\partial f^2}{\partial^2 \mathbf{x}}$

- Can apply finite differences twice to get a formula for each entry.

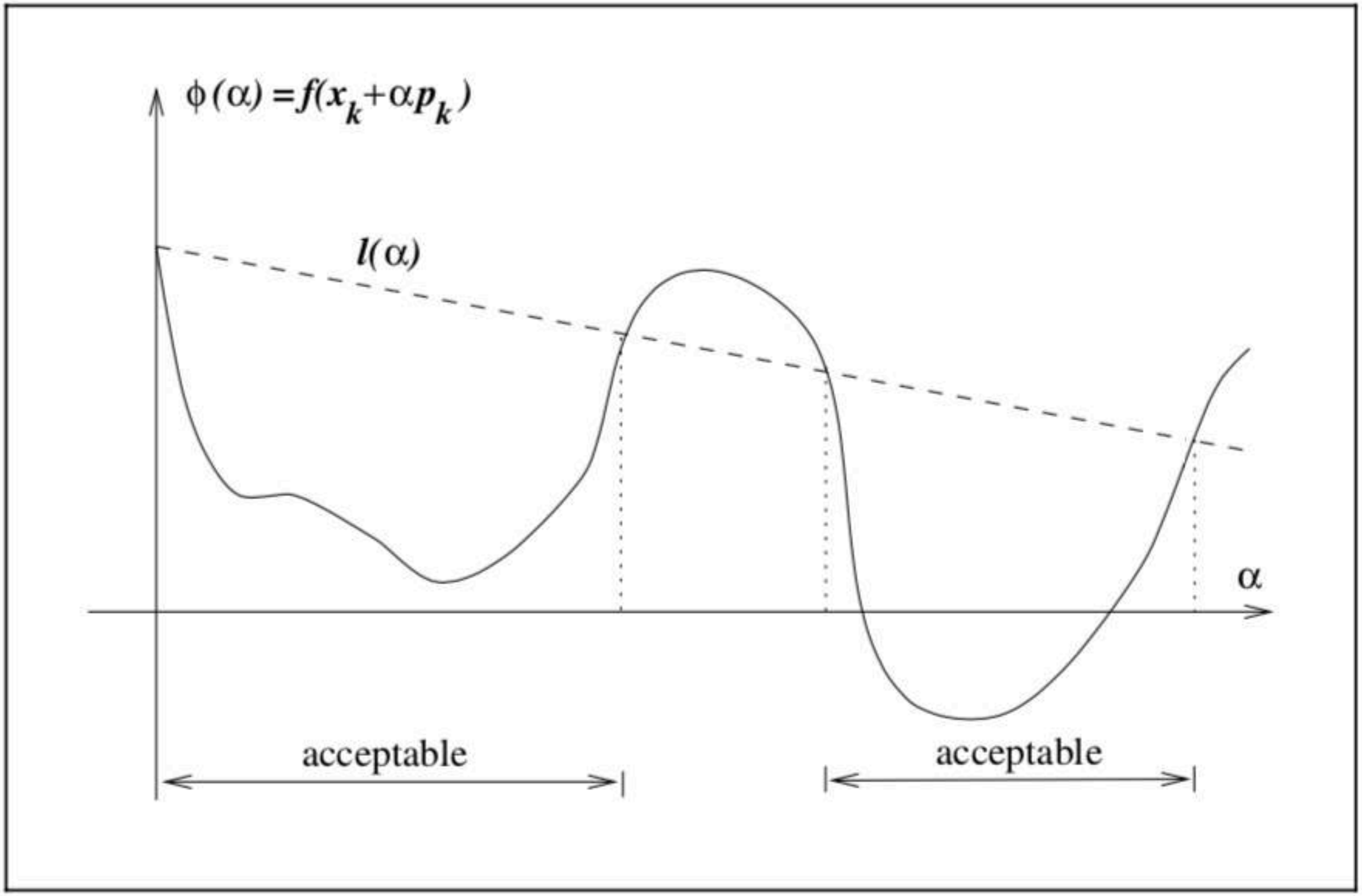
Gradient Descent vs. Newton's Method

- Gradient Descent is simpler
- Newton's Method converges faster, esp. near the solution
- Available Newton's Method Implementations:
  - MATLAB: fminunc
  - LBFGS: http://www.chokkan.org/software/liblbfgs/

Search Direction vs. Step Length

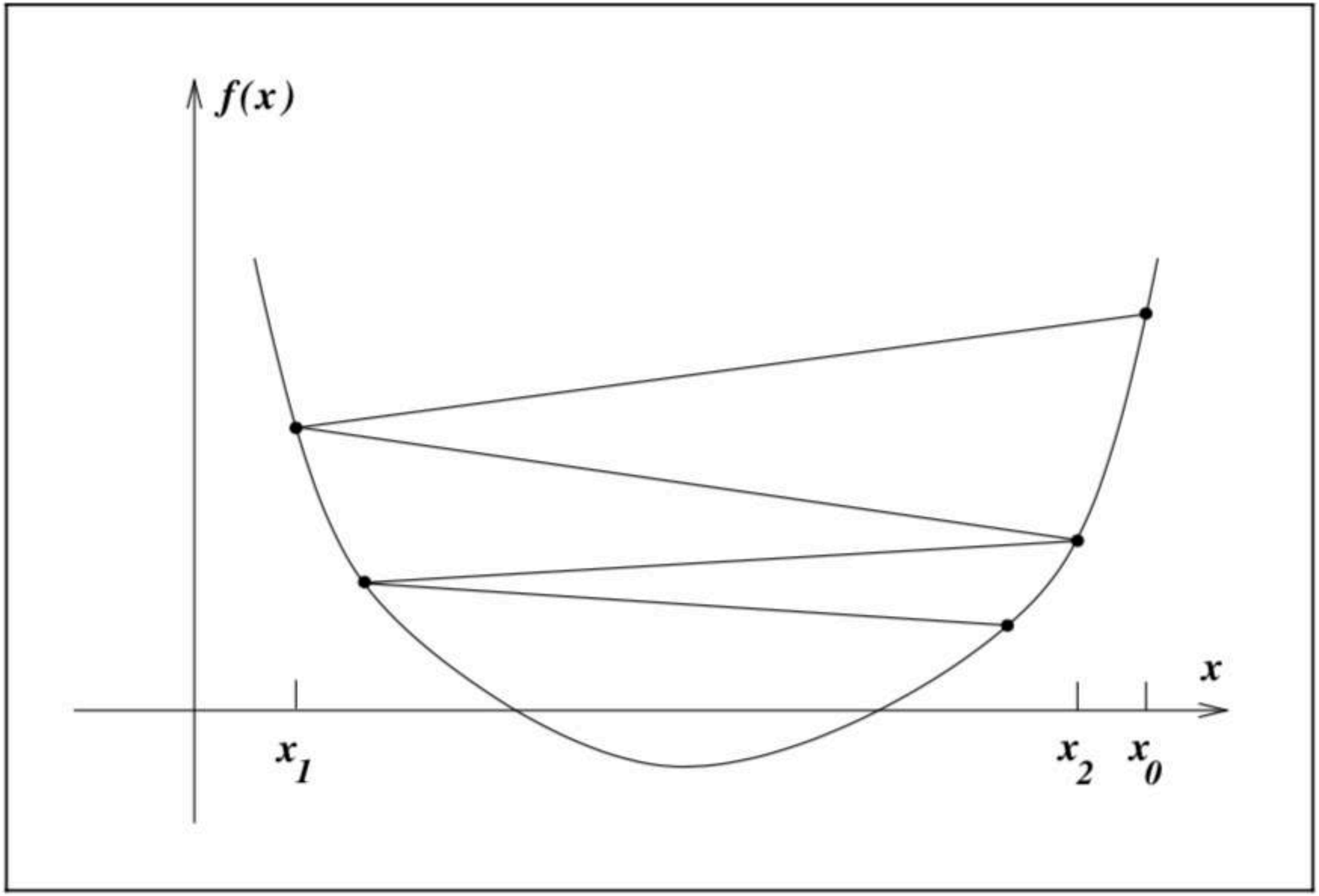
- While not at optimal point
  - Compute gradient (**g**) and Hessian (**H**)
  - Compute $\Delta\mathbf{x} =$ **?**
  - Update $\mathbf{x}^c = \mathbf{x}^c + h\Delta\mathbf{x}$

When Good Optimizations Go Bad



Numerical Optimization – Nocedal and Wright, pg. 33

When Good Optimizations Go Bad



Numerical Optimization – Nocedal and Wright, pg. 32

Choosing step length automatically

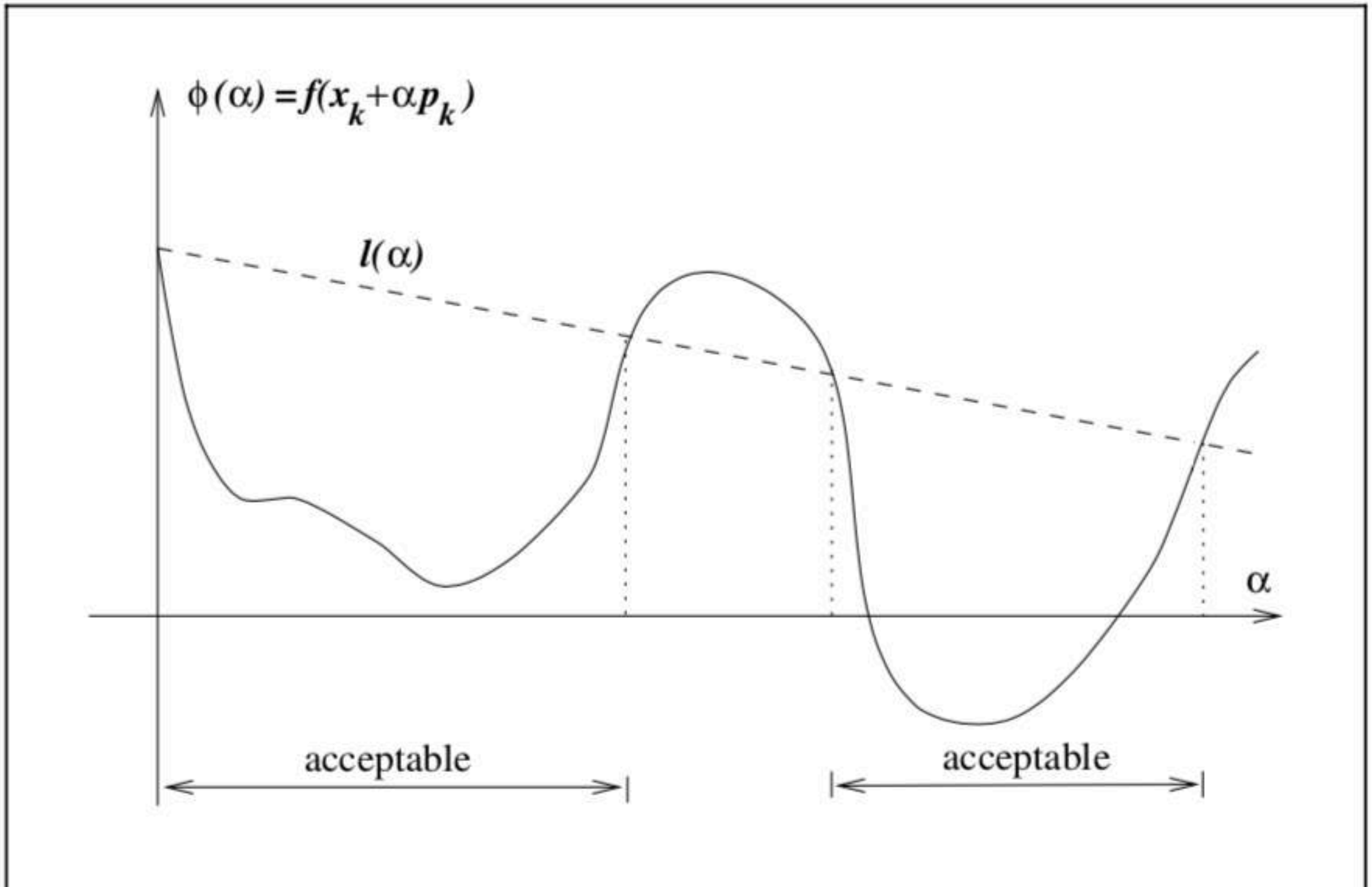
- While not at optimal point
  - Compute gradient (**g**) and Hessian (**H**)
  - Compute $\Delta\mathbf{x} = $ **?**
  - Update $\mathbf{x}^c = \mathbf{x}^c + h\Delta\mathbf{x}$

Characteristics of a Good Optimization Step

- We've seen that just guaranteeing a decreasing cost function is not enough
- We need sufficient decrease in the cost function
- How do we define sufficient decrease ?

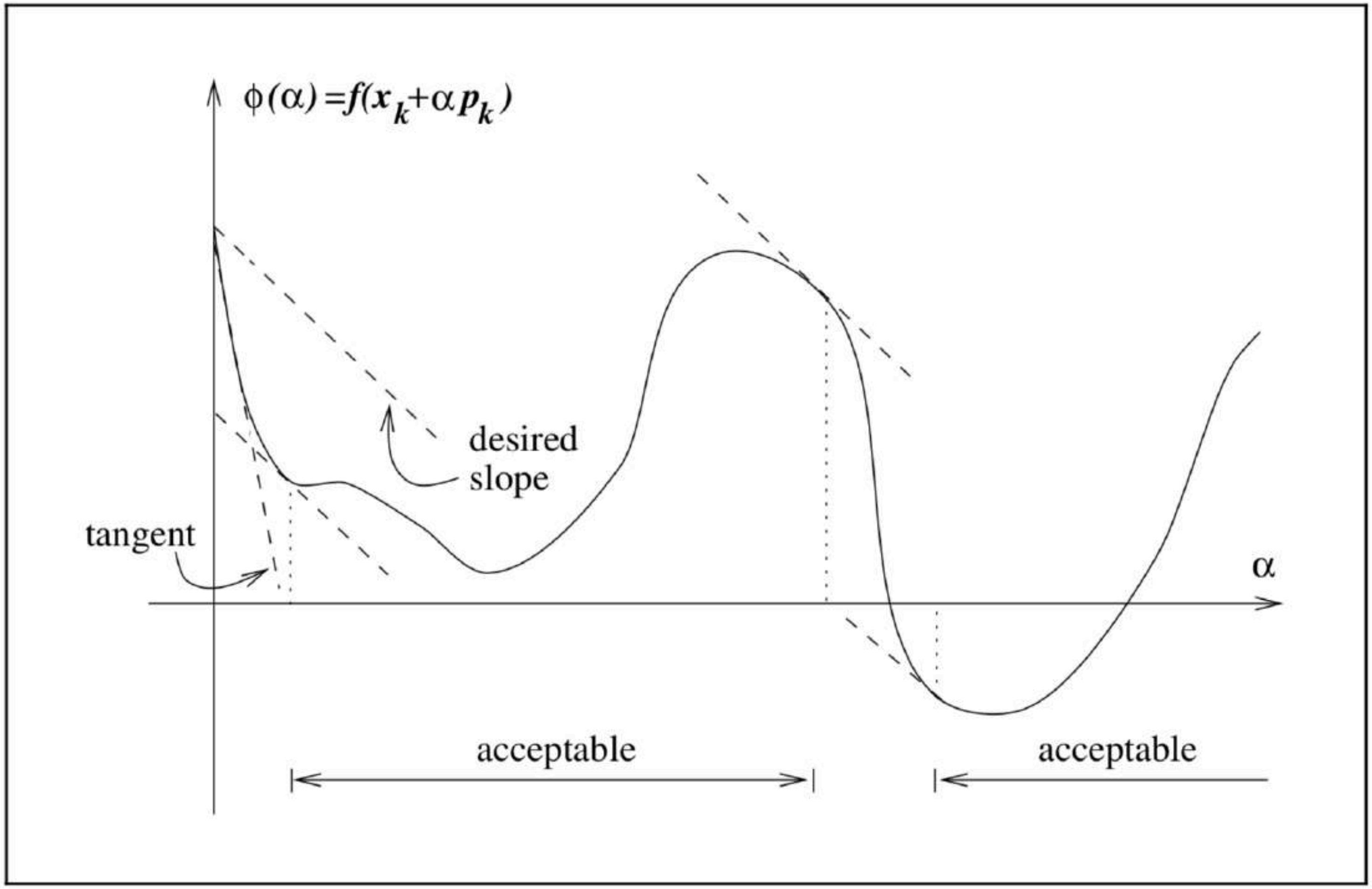
Sufficient Decrease

$$f(x_k + \alpha p_k) \leq f(x_k) + c_1 \alpha \nabla f_k^T p_k,$$



Curvature Condition

$$\nabla f(x_k + \alpha_k p_k)^T p_k \geq c_2 \nabla f_k^T p_k.$$



Wolfe Conditions

$$f(x_k + \alpha p_k) \le f(x_k) + c_1 \alpha \nabla f_k^T p_k,$$

$$\nabla f(x_k + \alpha_k p_k)^T p_k \ge c_2 \nabla f_k^T p_k,$$

- Typical values
  - C1=1e-8 to 1e-4
  - C2 = 0.1 to 0.9

Backtracking Line Search

Algorithm 3.1 (Backtracking Line Search).

Choose $\bar{\alpha} > 0$, $\rho \in (0, 1)$, $c \in (0, 1)$; Set $\alpha \leftarrow \bar{\alpha}$;

repeat until $f(x_k + \alpha p_k) \le f(x_k) + c\alpha \nabla f_k^T p_k$

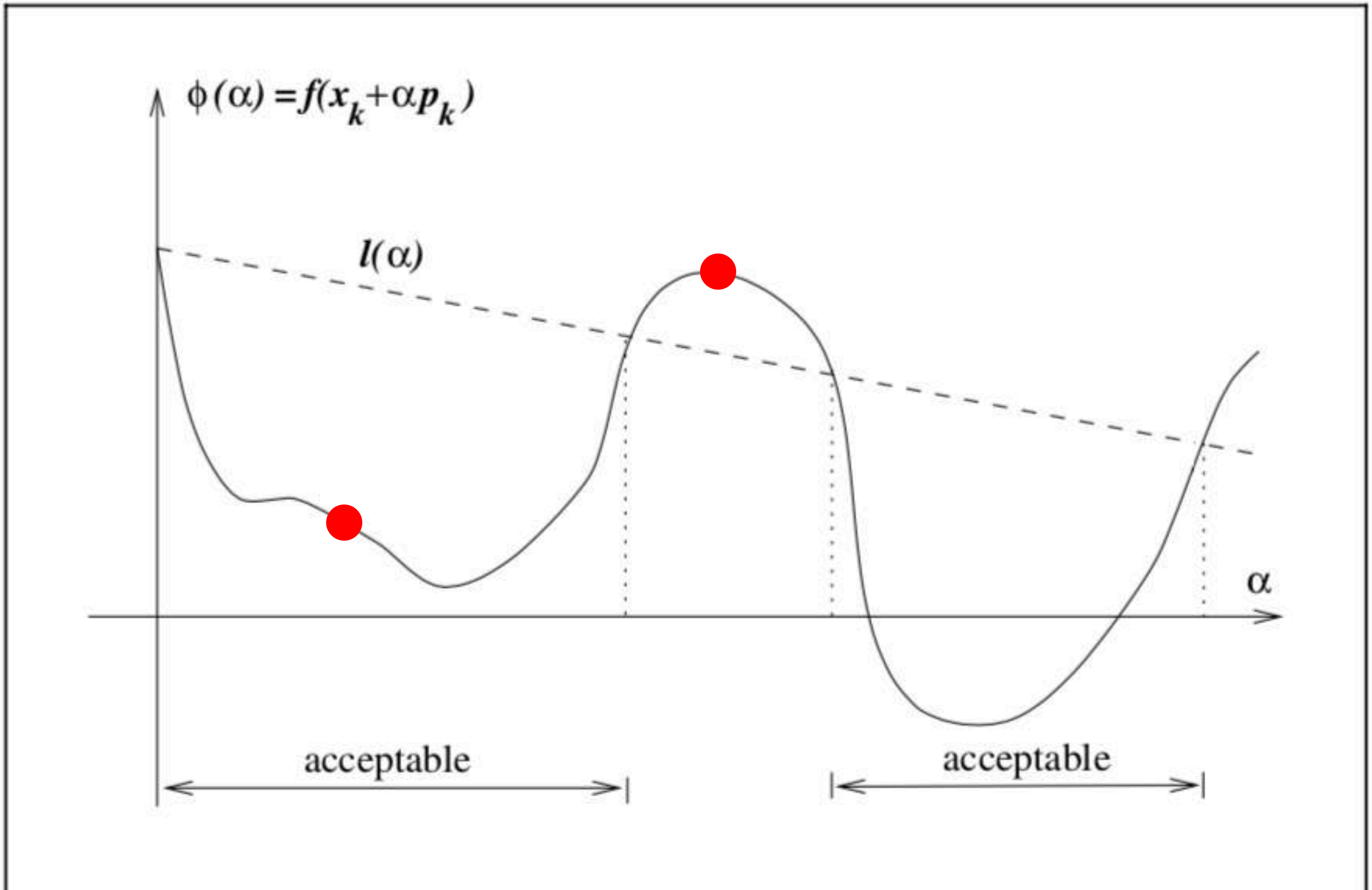
$\alpha \leftarrow \rho\alpha$;

end (repeat)

Terminate with $\alpha_k = \alpha$.

Numerical Optimization – Nocedal and Wright, pg. 37

Backtracking Line Search



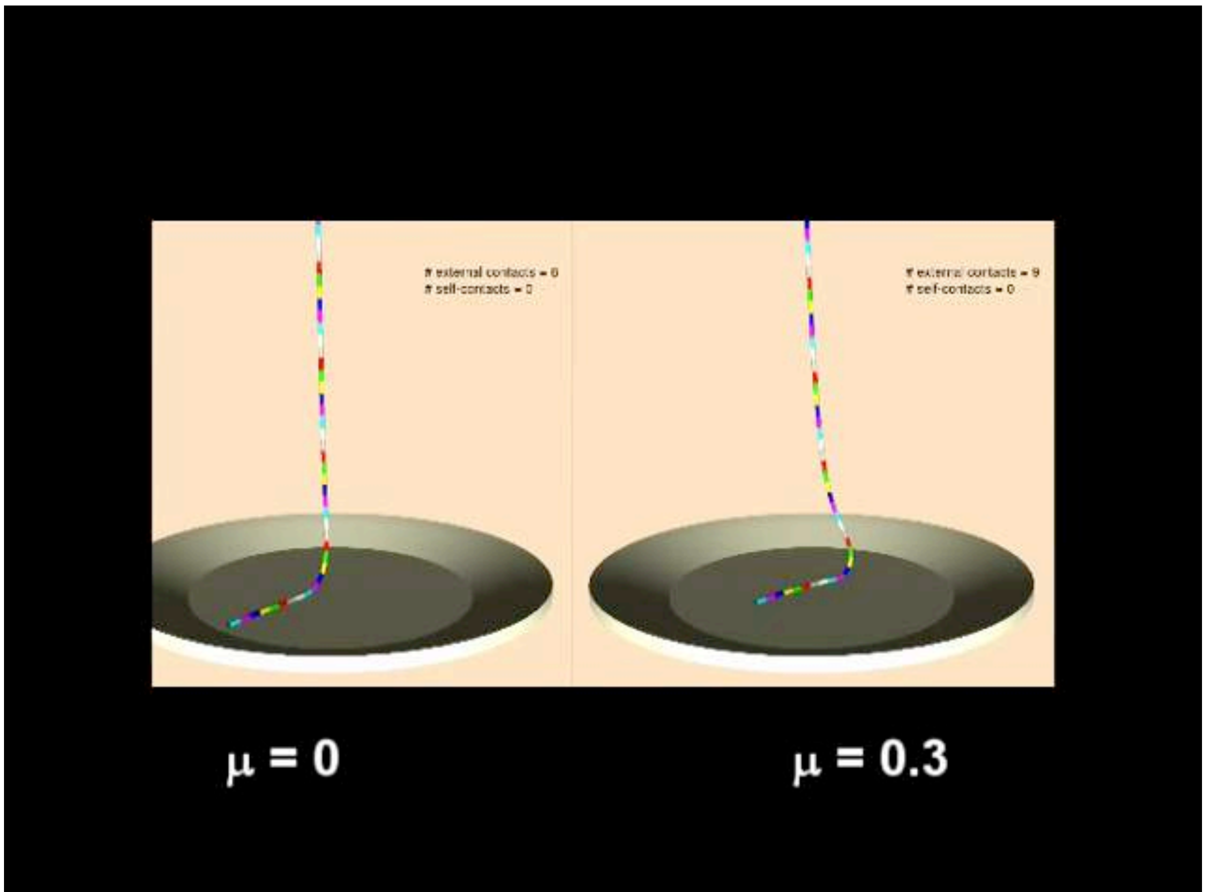
Examples of Optimization in Engineering

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

Examples from Engineering

Examples in Graphics

- Newton's method is used to compute frictional force between hairs



Types of Optimization

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

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

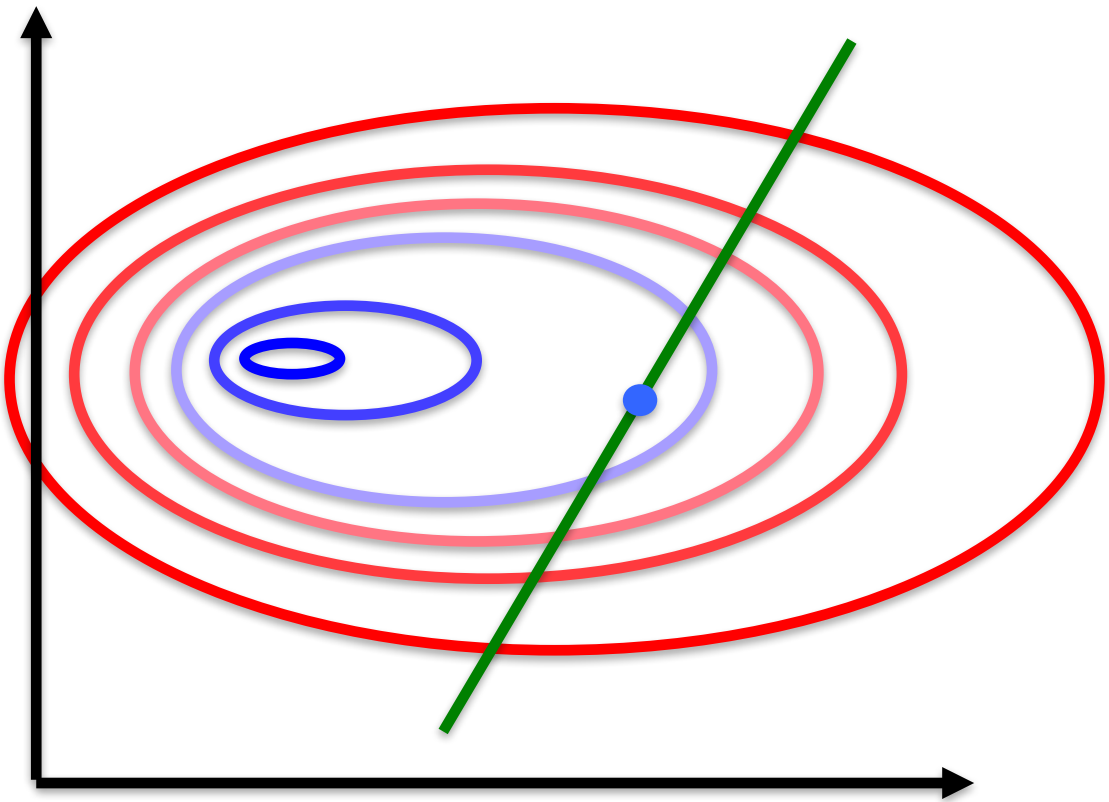
- Optimization involves finding an "optimal value"

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

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

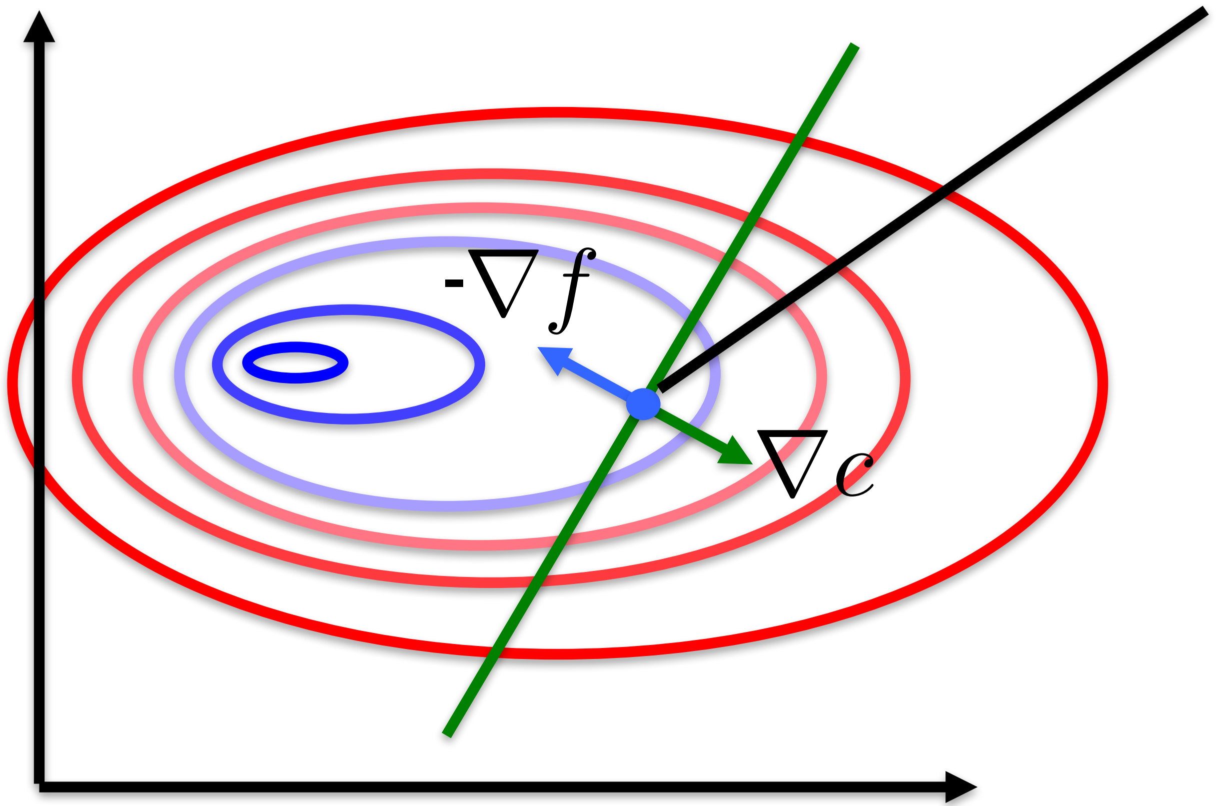
Equality Constraints

Constrained Optimization



Constrained Optimization

At Optimal Point



Constrained Optimization

- Equation from Geometry

$$-\nabla f = \boxed{\lambda}\nabla c$$

Lagrange Multipliers!

Constrained Optimization

- Equation from Geometry

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

$$\nabla f + \lambda \nabla c = 0$$

$$\nabla \left(f + \lambda c \right) = 0$$

$$\boxed{\min \left(f + \lambda c \right)}$$

Minimize old cost function + constraints · Lagrange Multipliers

Constrained Optimization

- Find Optimal Point!

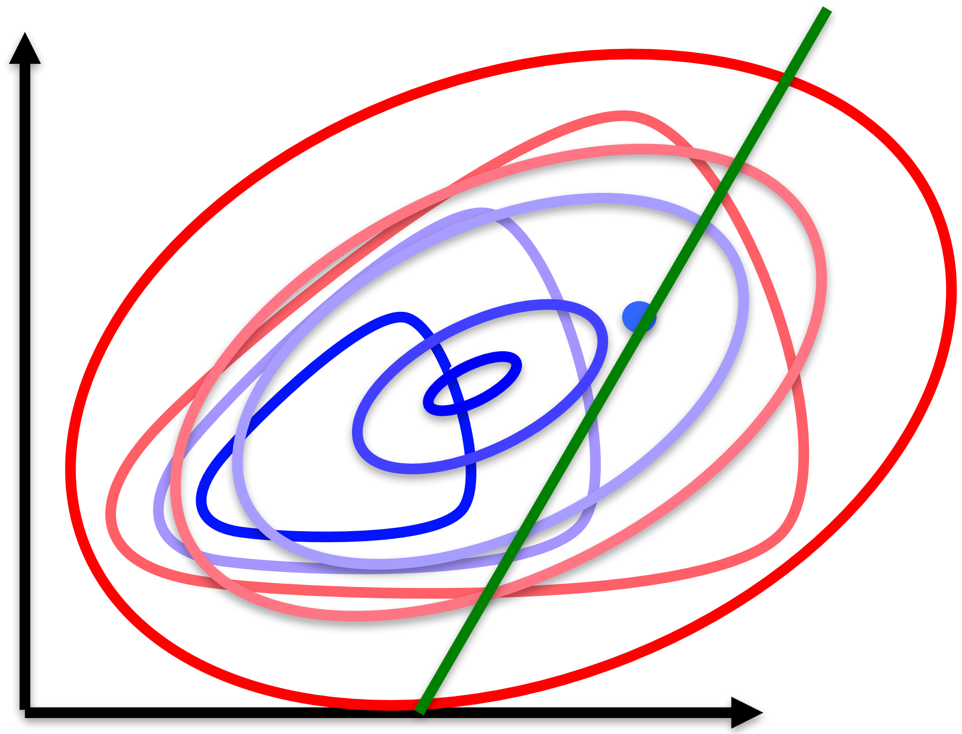
$$\nabla_{\mathbf{x}} f\left(\mathbf{x}\right) + \mathbf{A}^T \lambda = 0$$

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

Constrained Optimization

- This simple tool is incredibly powerful
- Let’s use it to build an equality constrained Newton’s Method

Equality Constrained Newton's Method



Newton's Method

- How do we get our approximation ?
- Taylor Expansion!!!!

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

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

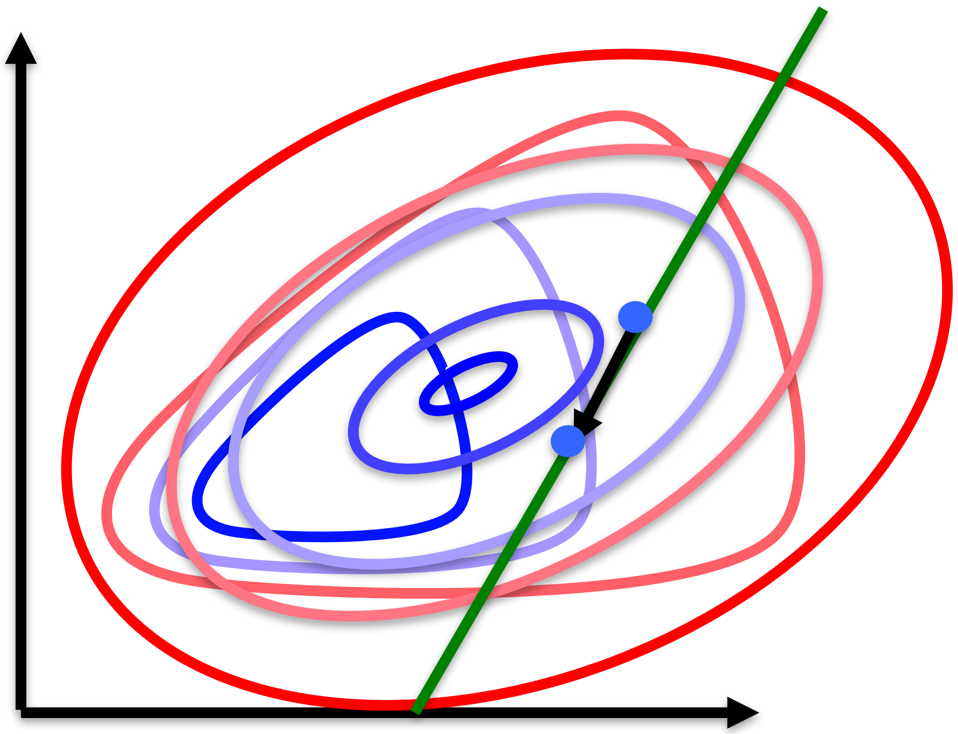
$$\boxed{H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1\,\partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1\,\partial x_n} \\ \frac{\partial^2 f}{\partial x_2\,\partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial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

Equality Constrained Newton

- Add constraints to model problem

$$\Delta x = \arg\min f\left(\mathbf{x}^c\right) + \Delta\mathbf{x}^T\mathbf{g} + \frac{1}{2}\Delta\mathbf{x}^T\mathbf{H}\Delta\mathbf{x}$$
$$s.t.\ \mathbf{A}\mathbf{x} = \mathbf{b}$$

Equality Constrained Newton's Method



Equality Constrained Newton

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

So Far !

- Gradient Descent

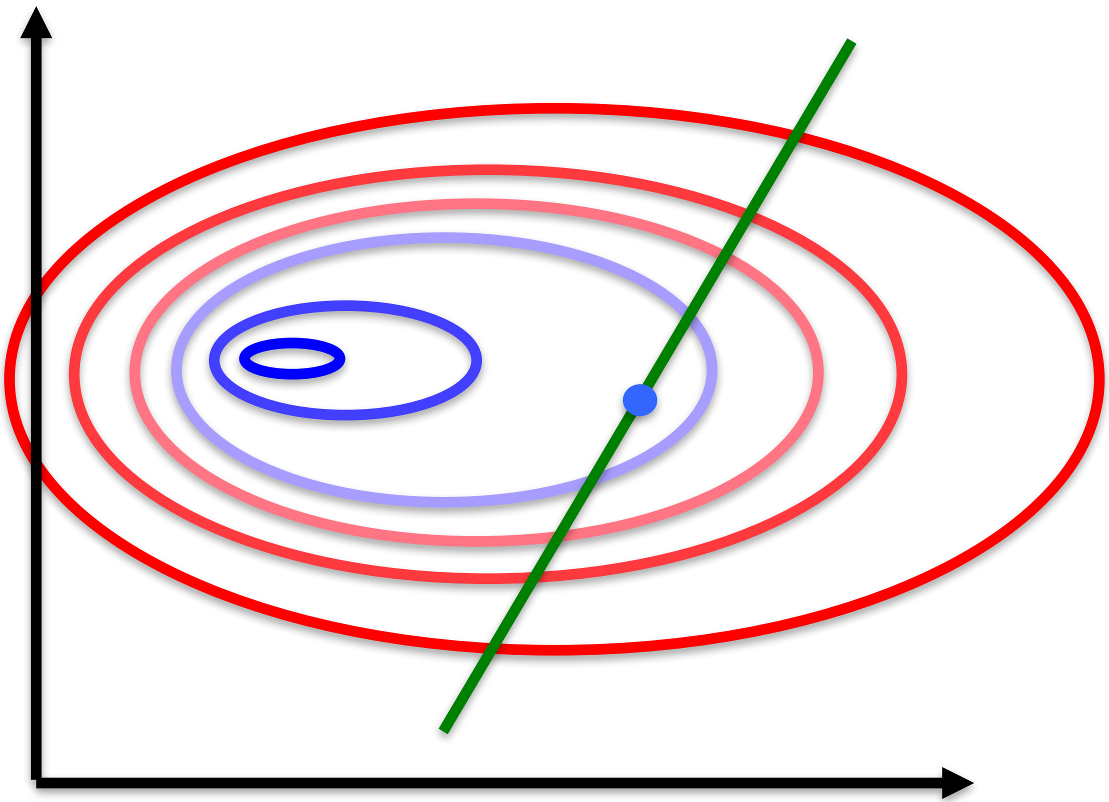
- Newton’s Method

- Equality Constrained Newton’s Method

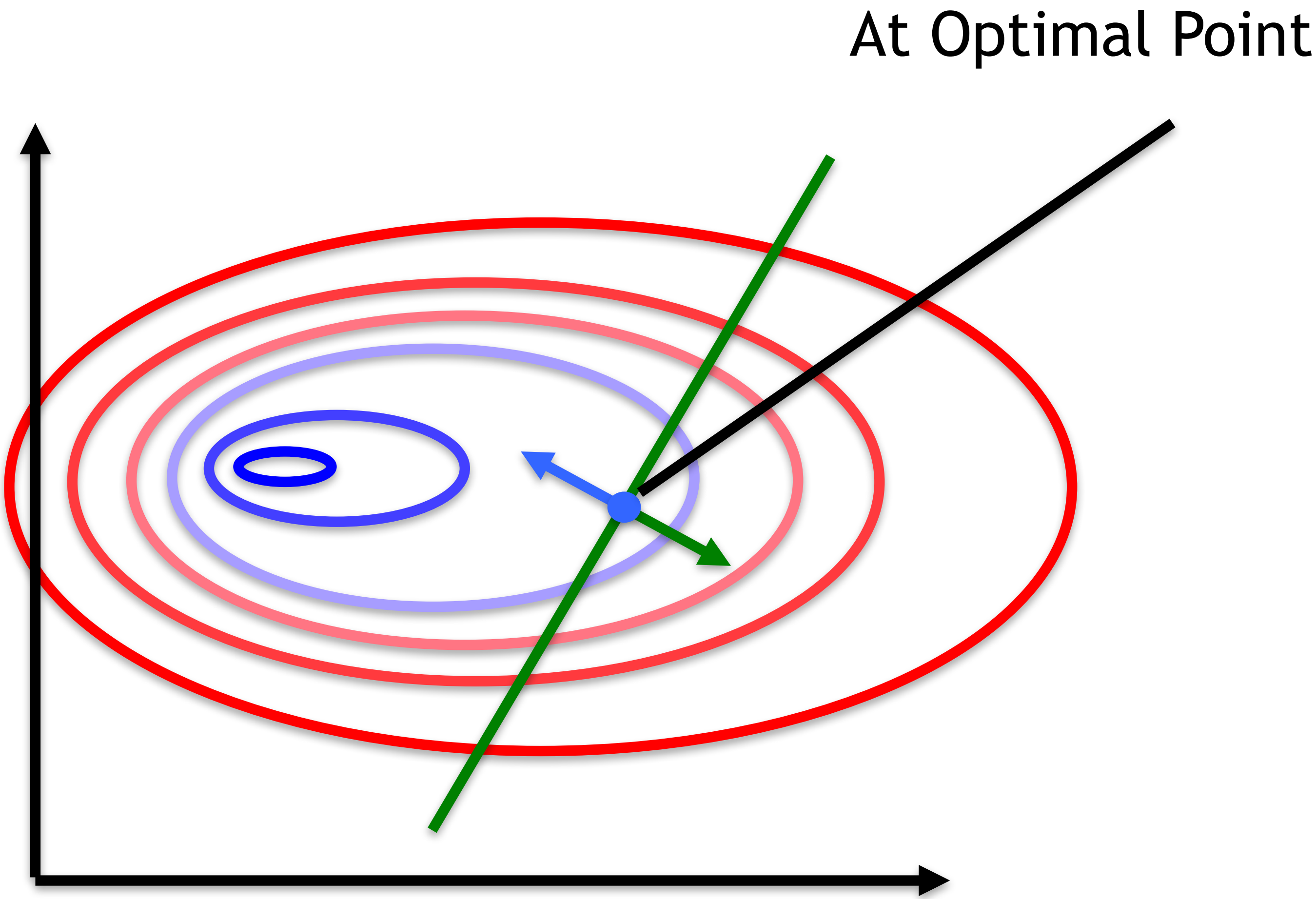
Next: Inequality Constrained Optimization

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

Constrained Optimization



Constrained Optimization



Inequality Constrained Optimization

- Optimization involves finding an "optimal value"

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

$$\min f(x)$$

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

Inequality Constraints

Inequality Constrained Optimization

- Optimization involves finding an "optimal value"

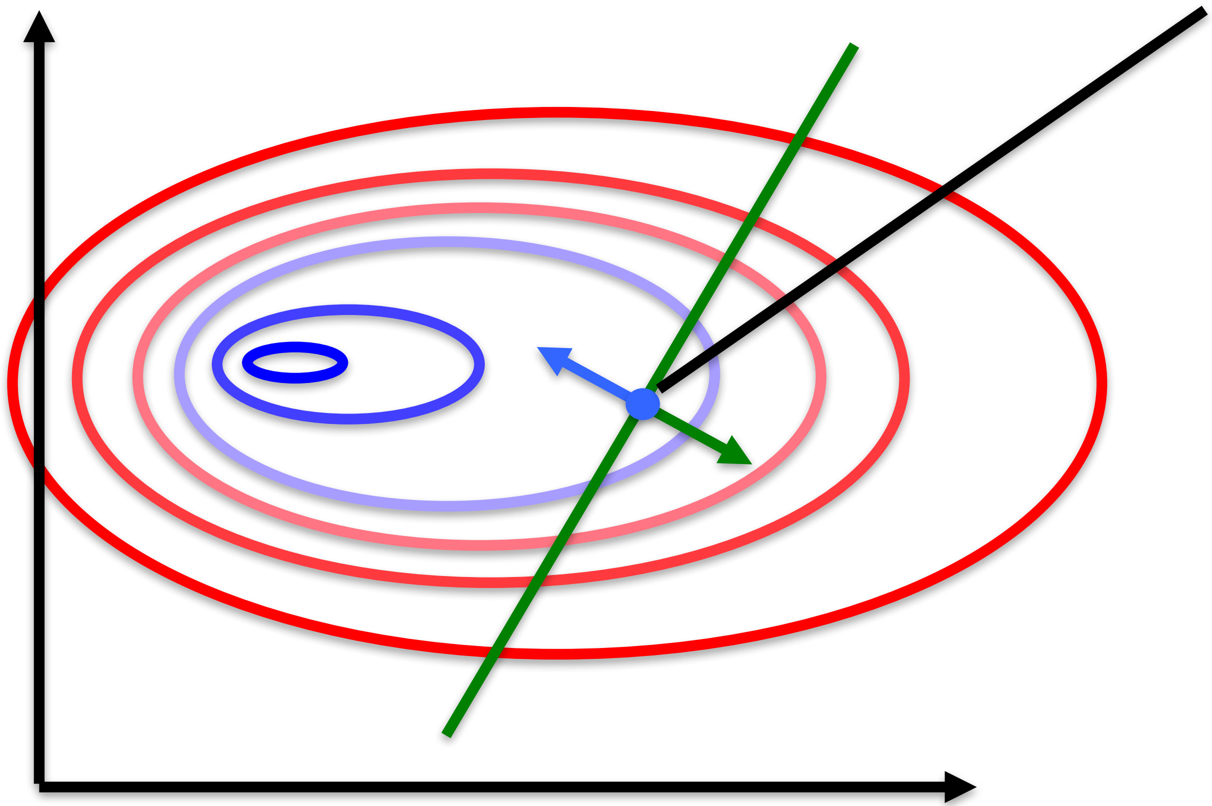
- i.e. Maximizing a profit, minimizing an area etc…

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

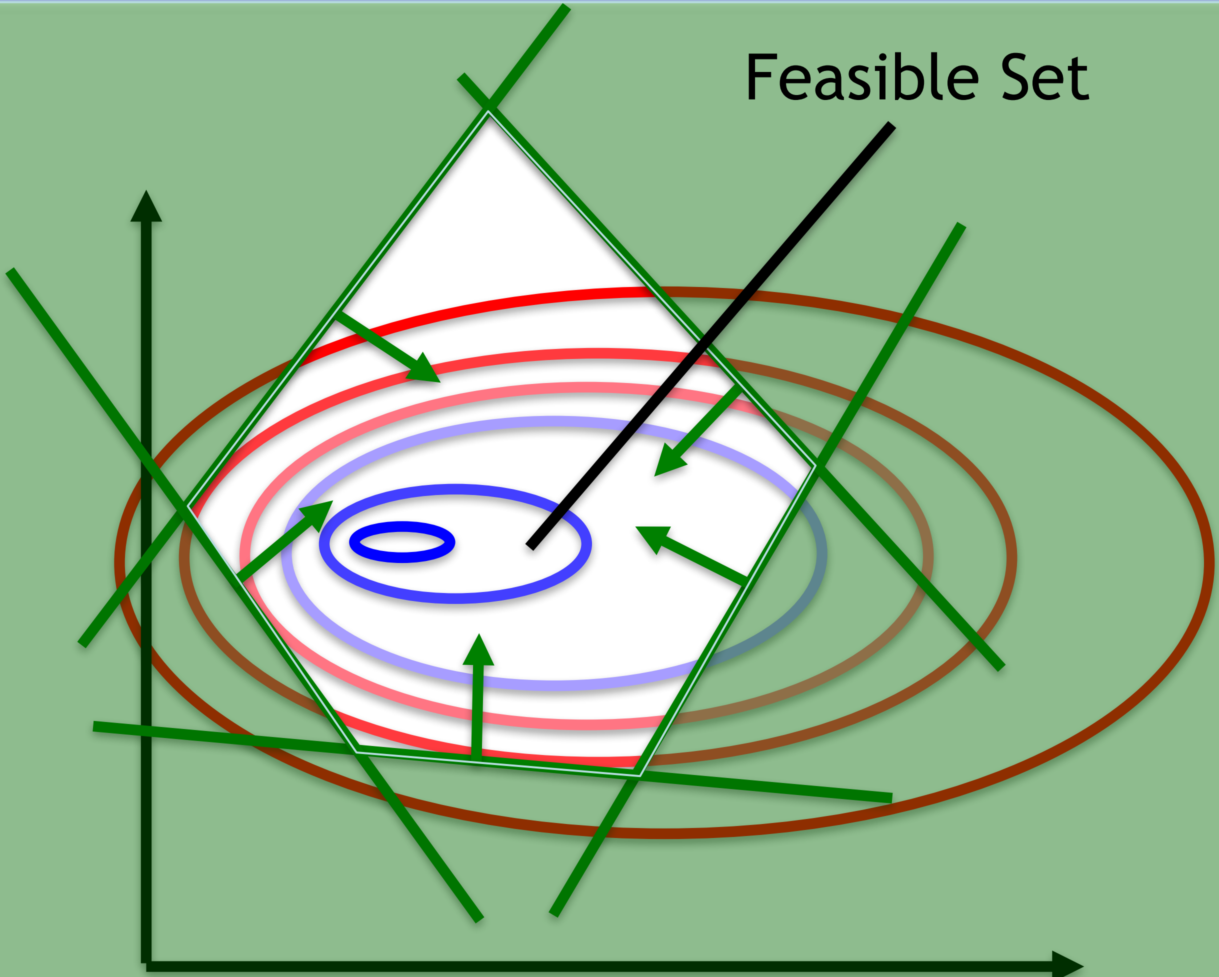
Inequality Constraints

Equality Constrained Optimization

At Optimal Point



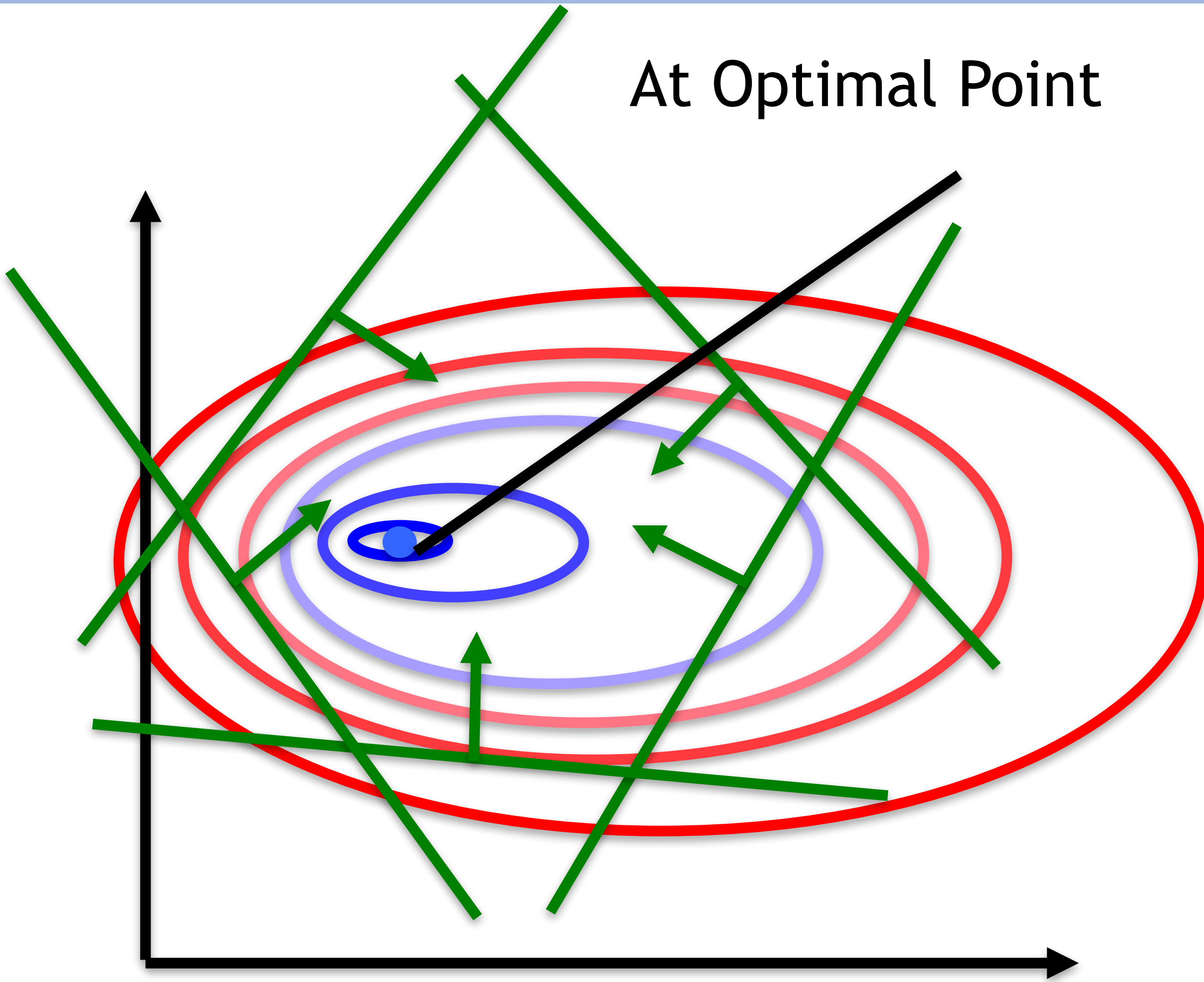
Inequality Constrained Optimization



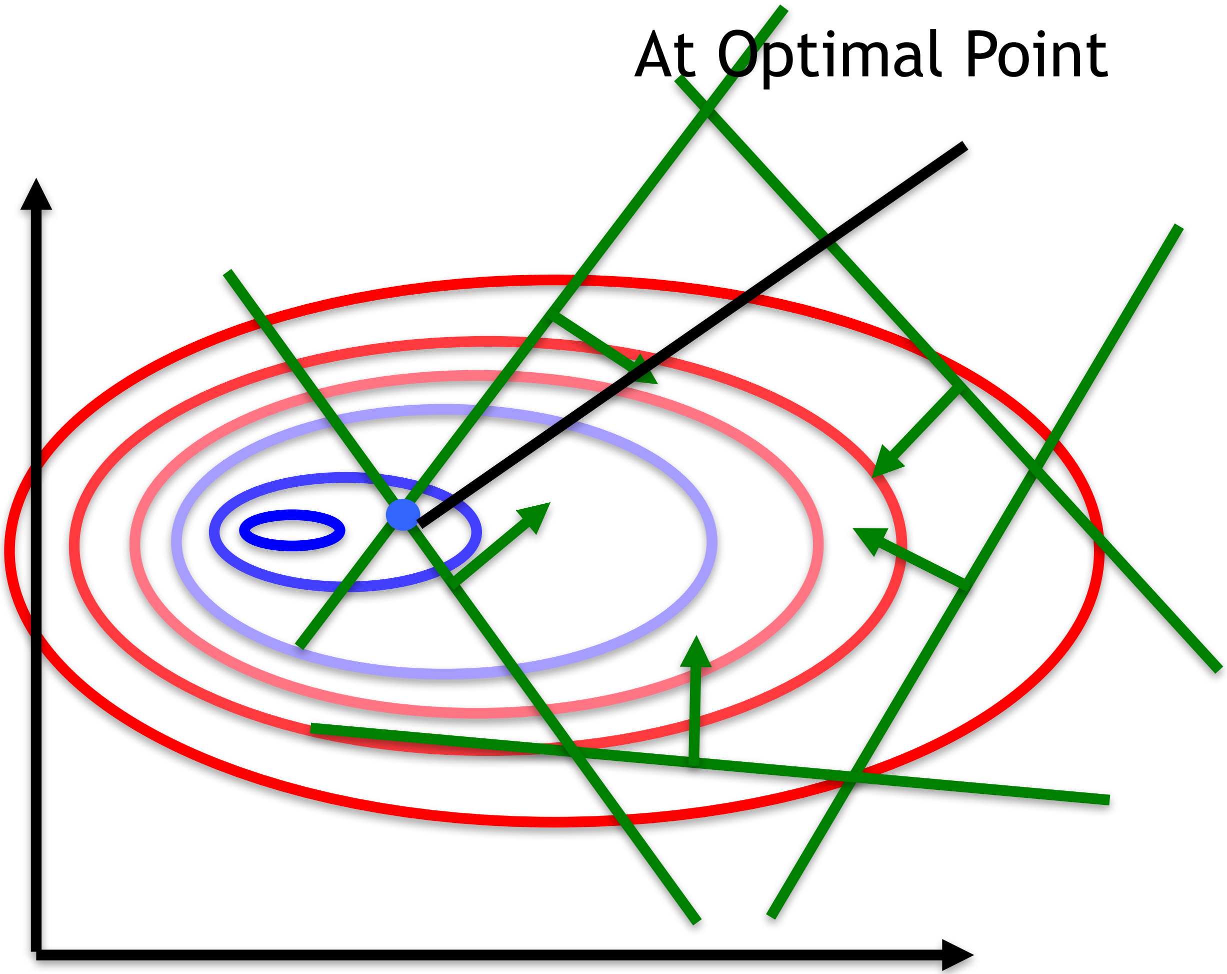
The Active Set

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

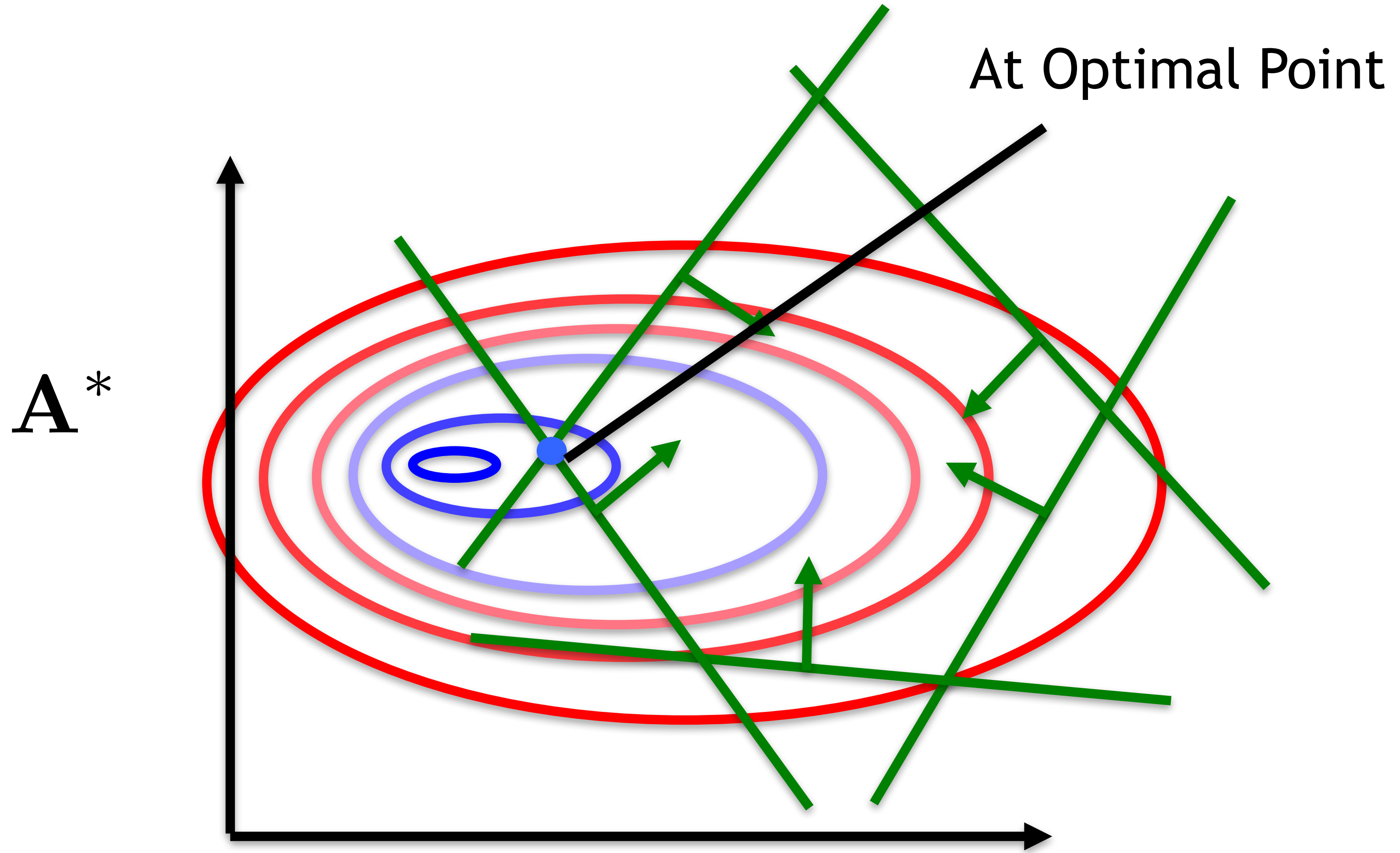
Case 1: Optimal Value Inside Feasible Set



Case 2: Optimal Value On Boundary



Case 2: Optimal Value On Boundary



The Active Set

- On the boundary we satisfy

$$\min f(x)$$

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

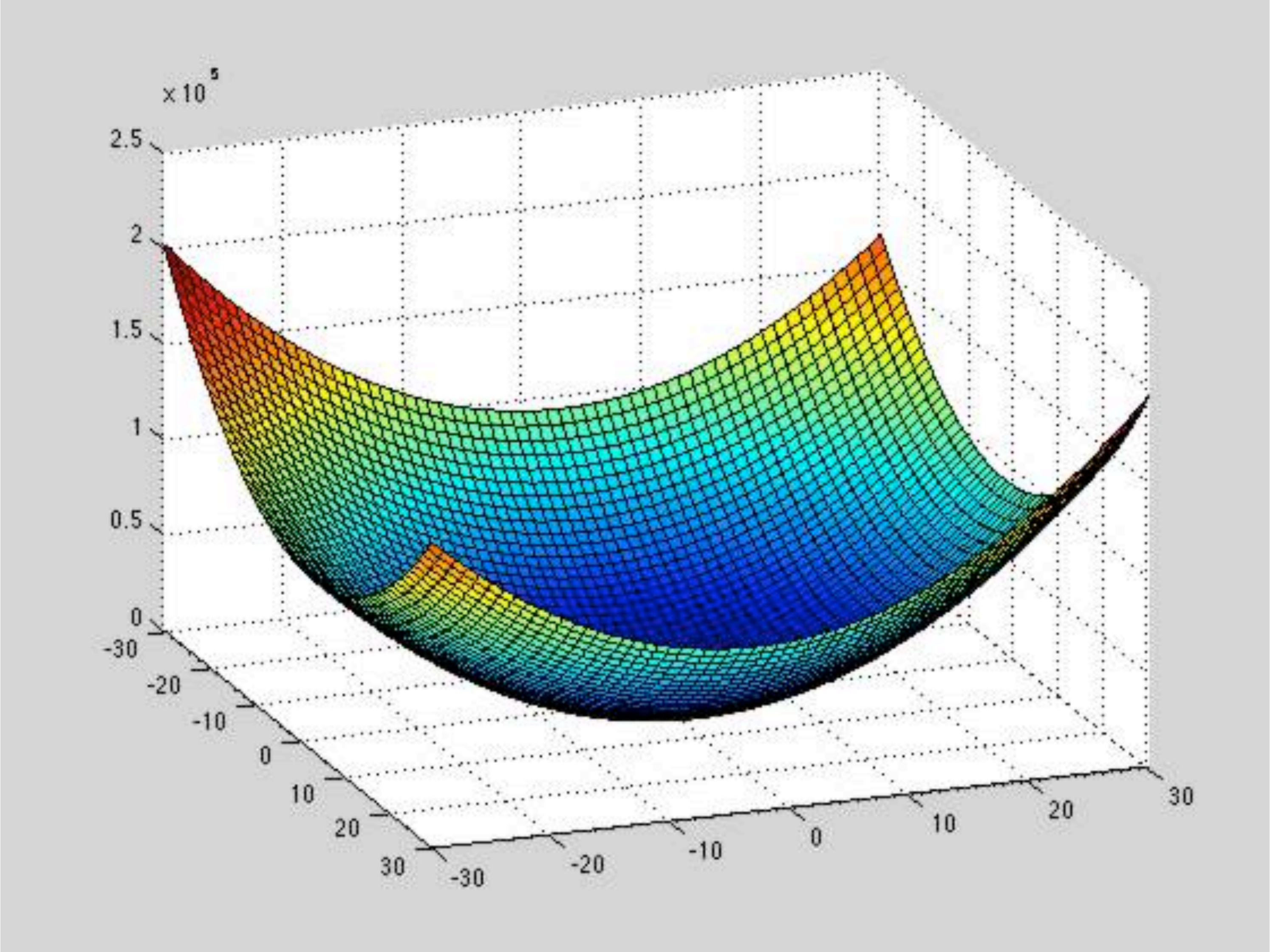
Active Set

Quadratic Programs

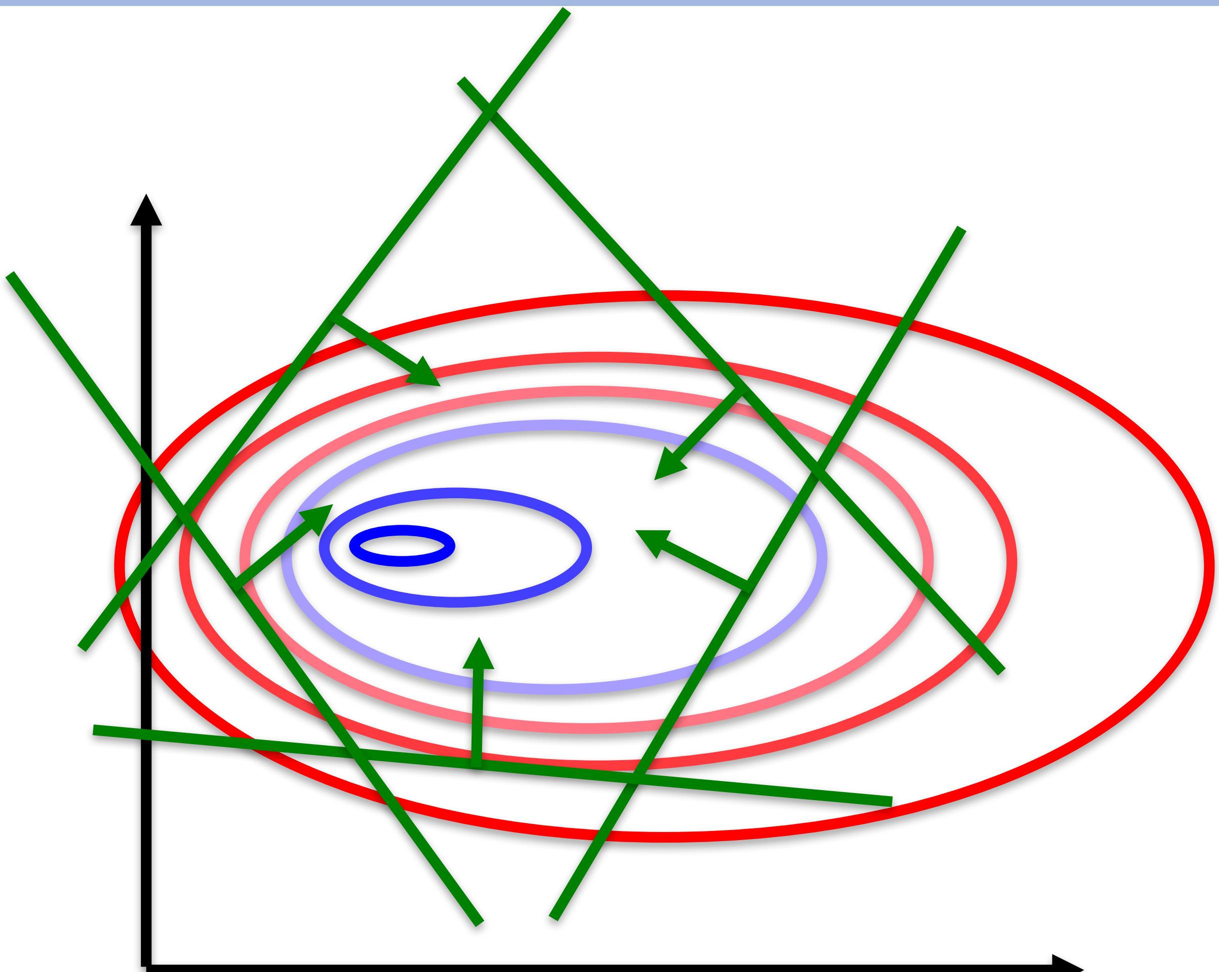
- It's got a quadratic cost function!

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

Quadratic Program



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

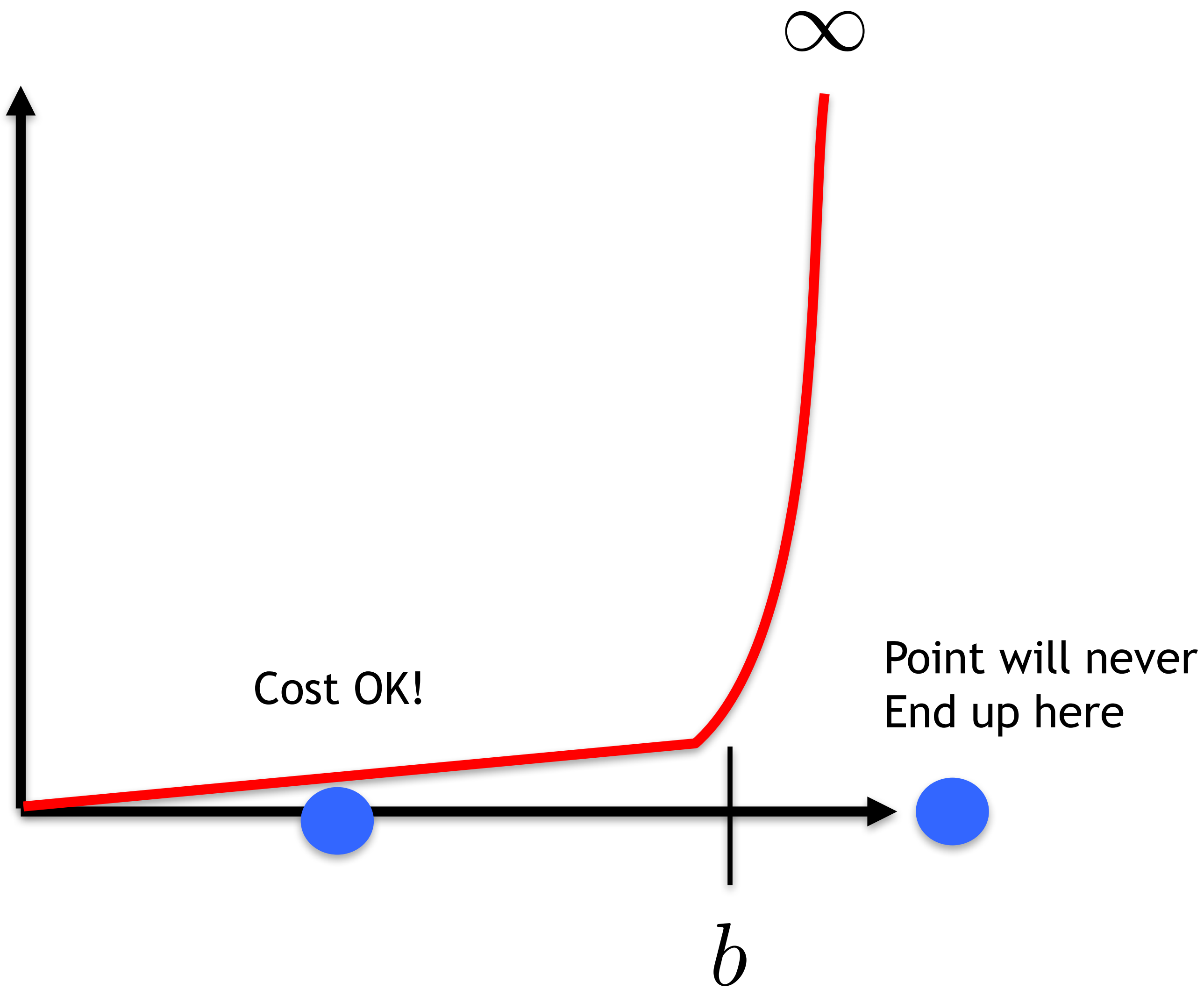
- Replace inequality constraints with functions

$$L\left(\mathbf{x},\lambda\right)=f\left(\mathbf{x}\right)+\left(\mathbf{A}\mathbf{x}-\mathbf{b}\right)^T\lambda$$

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

Special "Constraint" Function

Interior Point



Interior Point Methods

- Replace inequality constraints with functions

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

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

Special "Constraint" Function

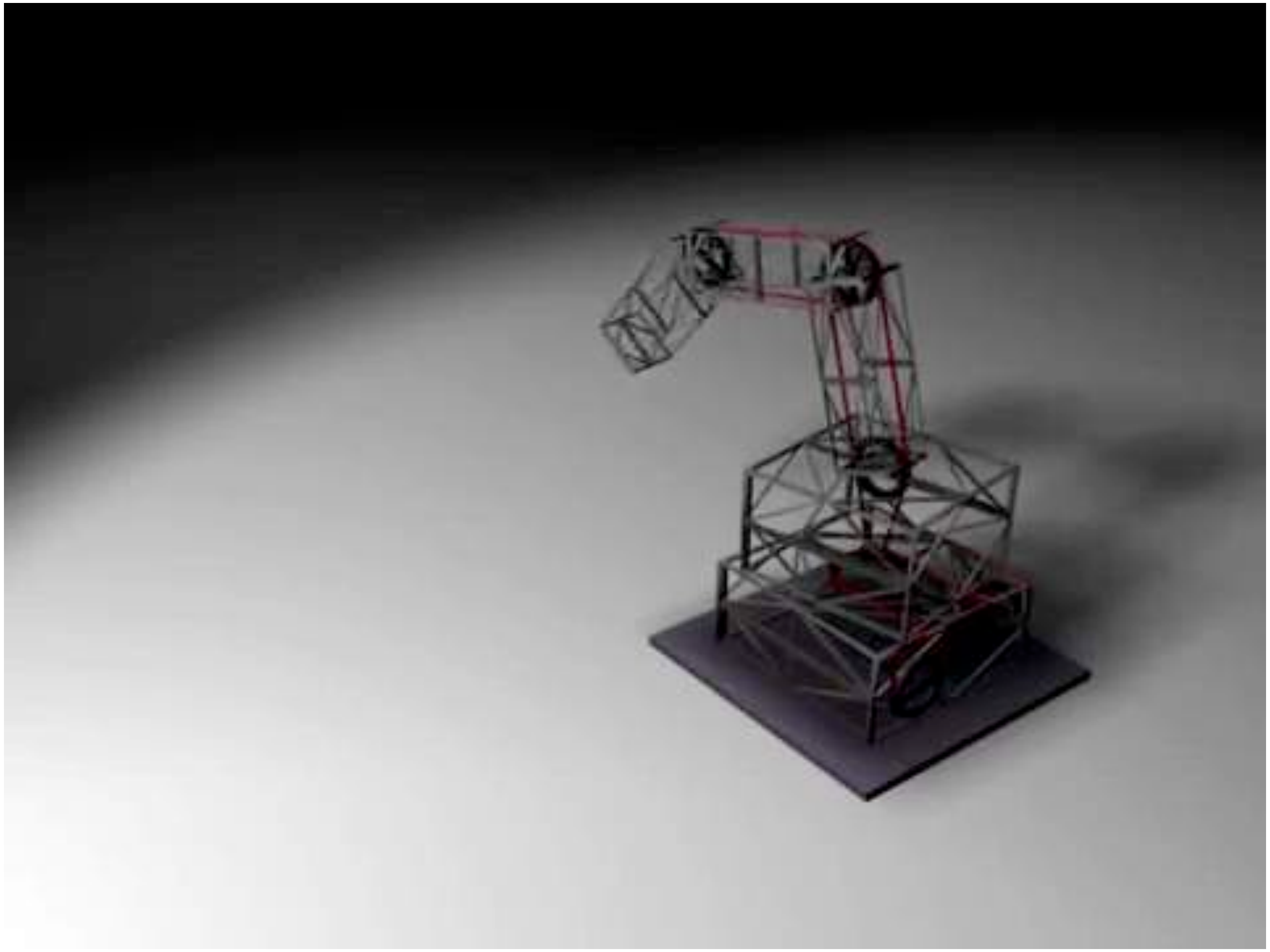
- Now use Equality Constrained Newton!!!

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)

Examples of Quadratic Programming

Examples of Quadratic Programming

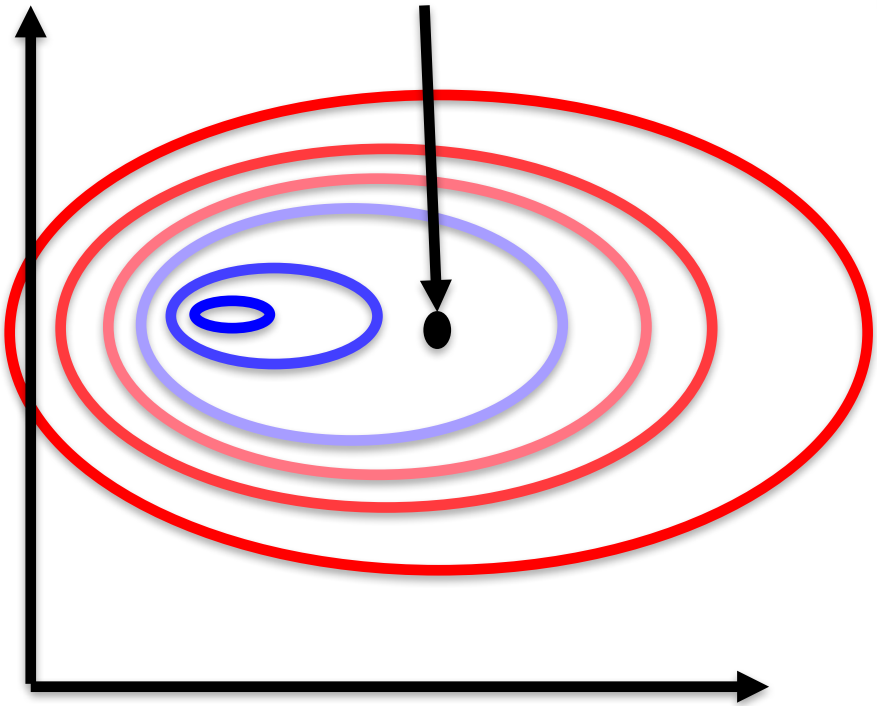


Types of Optimization

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

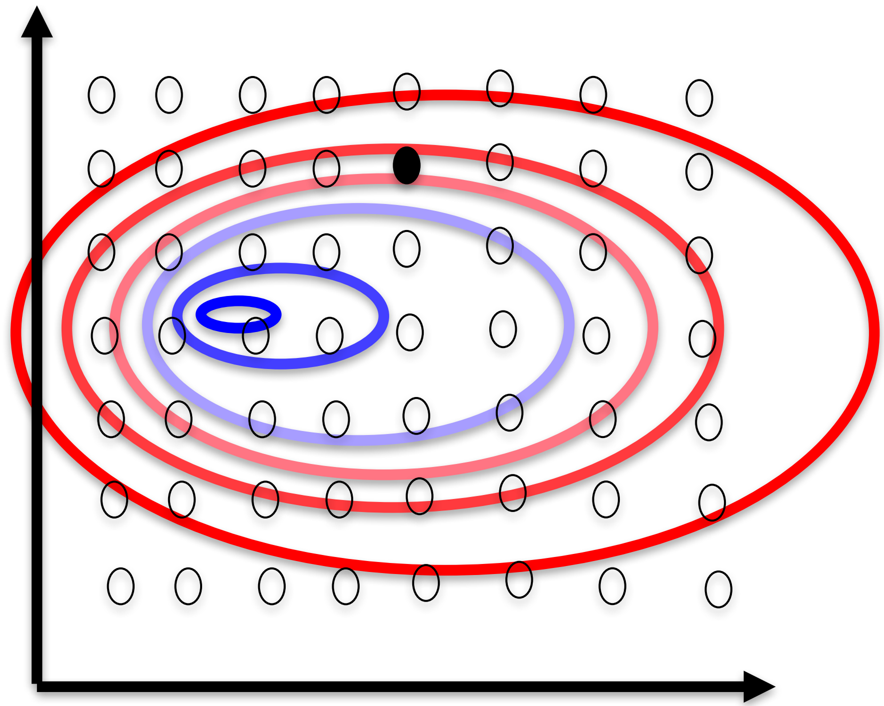
Continuous

This point can move smoothly



Discrete

Choose from discrete points in parameter space



Branch and Bound Optimizations

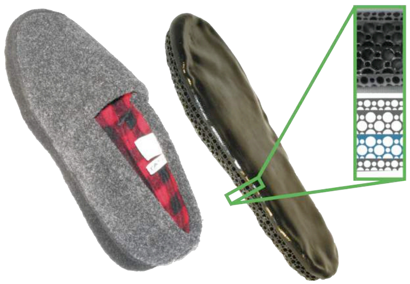
- An optimization technique with 3 phases
  - Branch (divide the solution space into a number of subspaces)
  - Bound (compute some upper and lower bound for the cost of each subspace)
  - Prune (remove subspaces with upper bounds higher than the lower bounds of the least costly subspaces)

Continuum Mechanics and Fabrication

- Example: Cloning Object Behavior

We want to control the printed shoes response to applied force

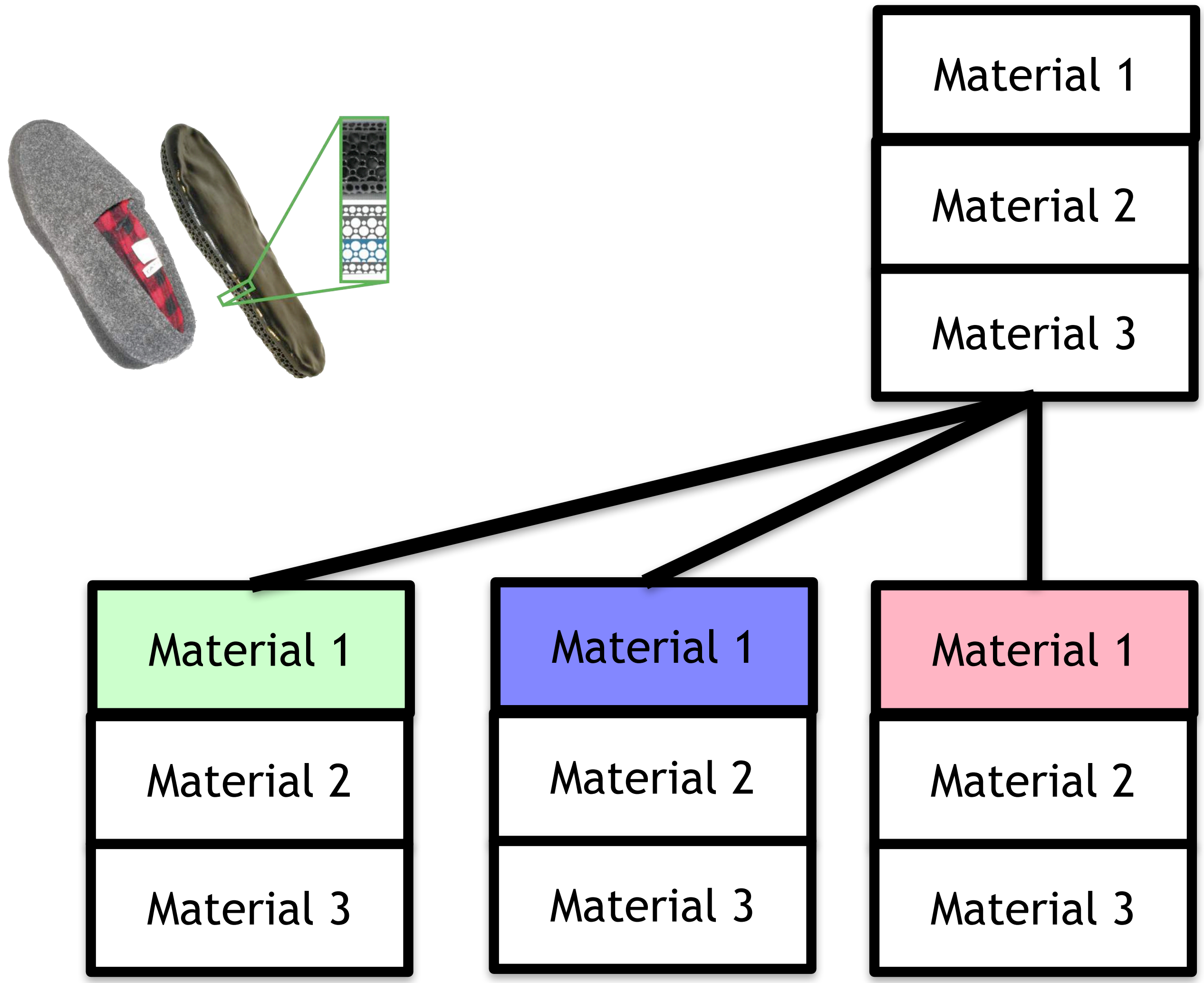
Material Assignment



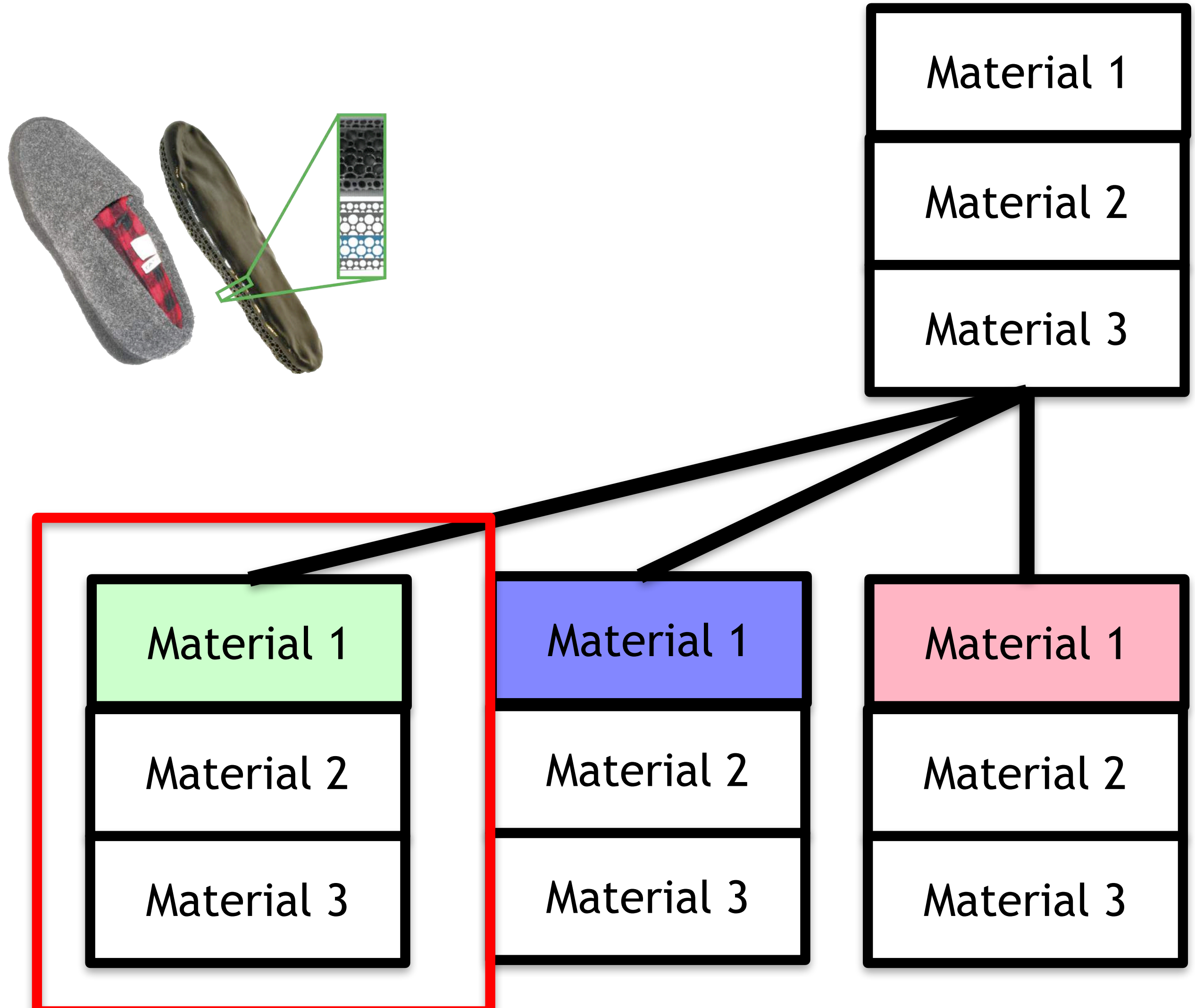
Match Goal Displacement G

Material 1	Material 1	Material 1	Material 1
Material 2	Material 2	Material 2	Material 2
Material 3	Material 3	Material 3	Material 3

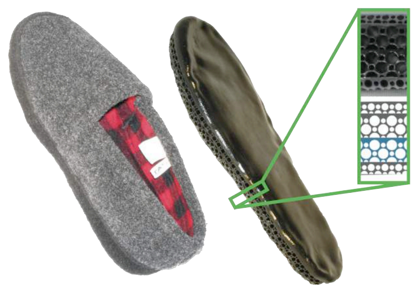
Material Assignment



Bounding Material Assignment



Bounding Material Assignment



Material 1
Material 2
Material 3

Material 1
Material 2
Material 3

Material 1
Material 2
Material 3

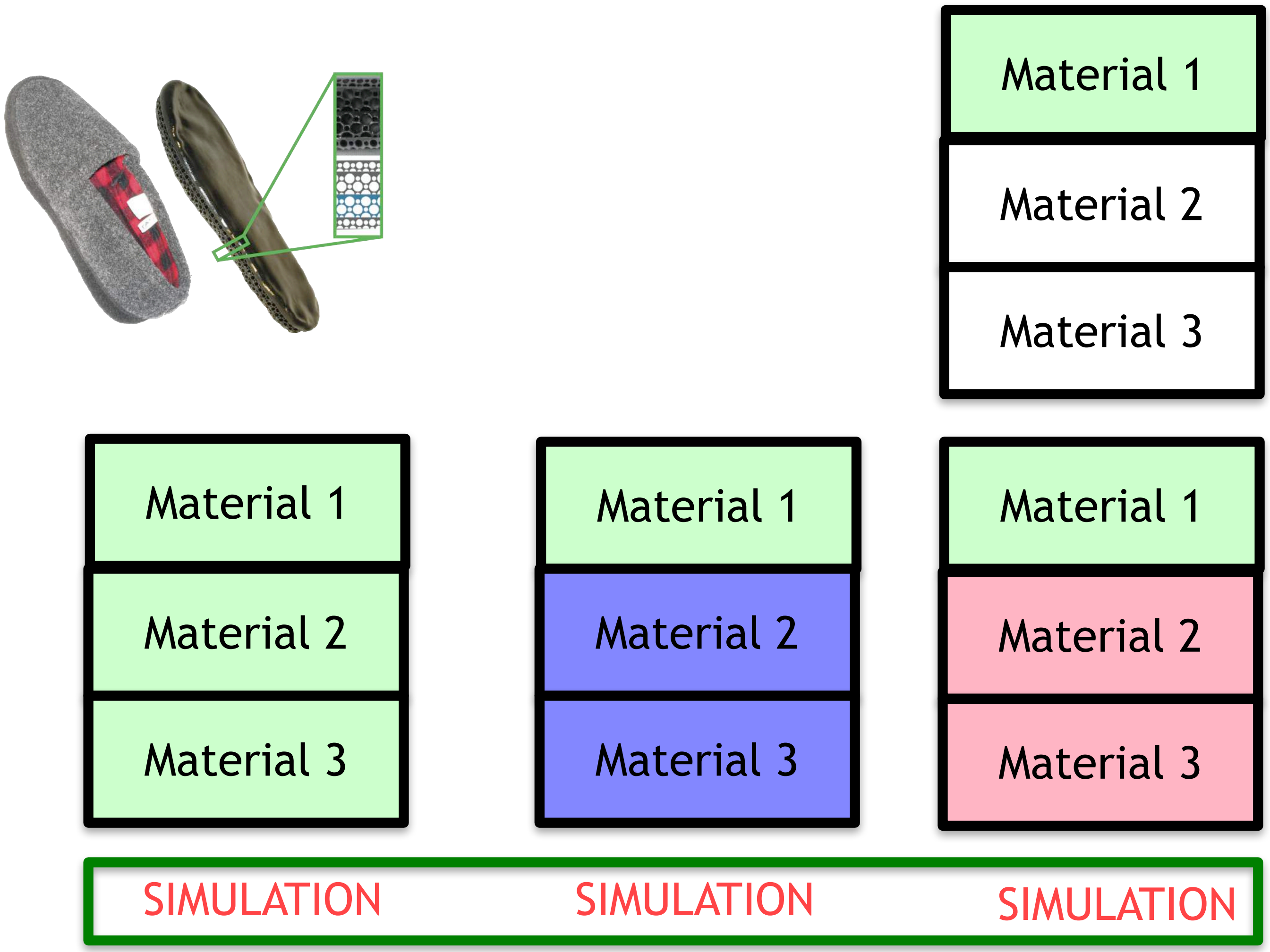
Material 1
Material 2
Material 3

SIMULATION

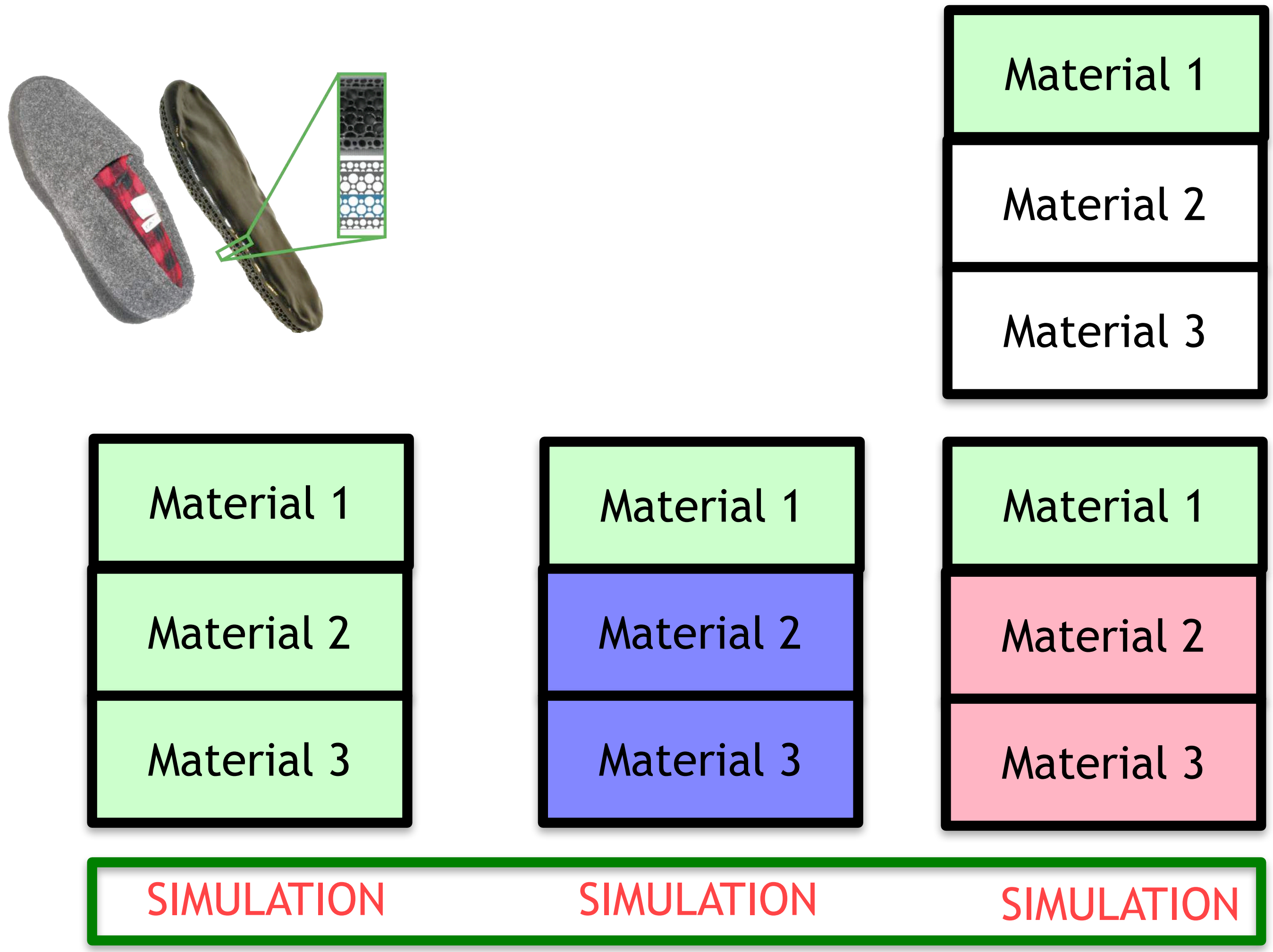
SIMULATION

SIMULATION

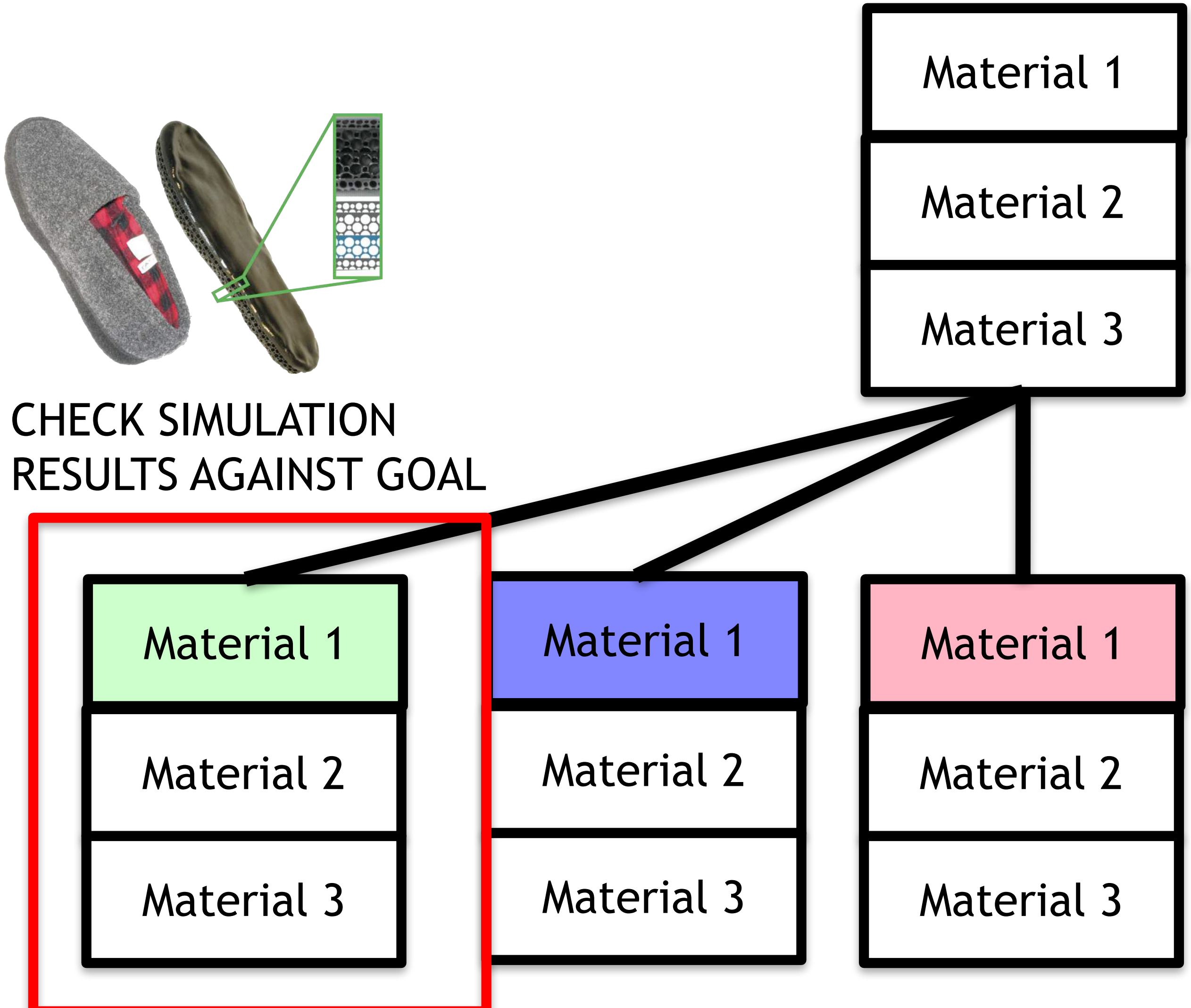
Bounding Material Assignment



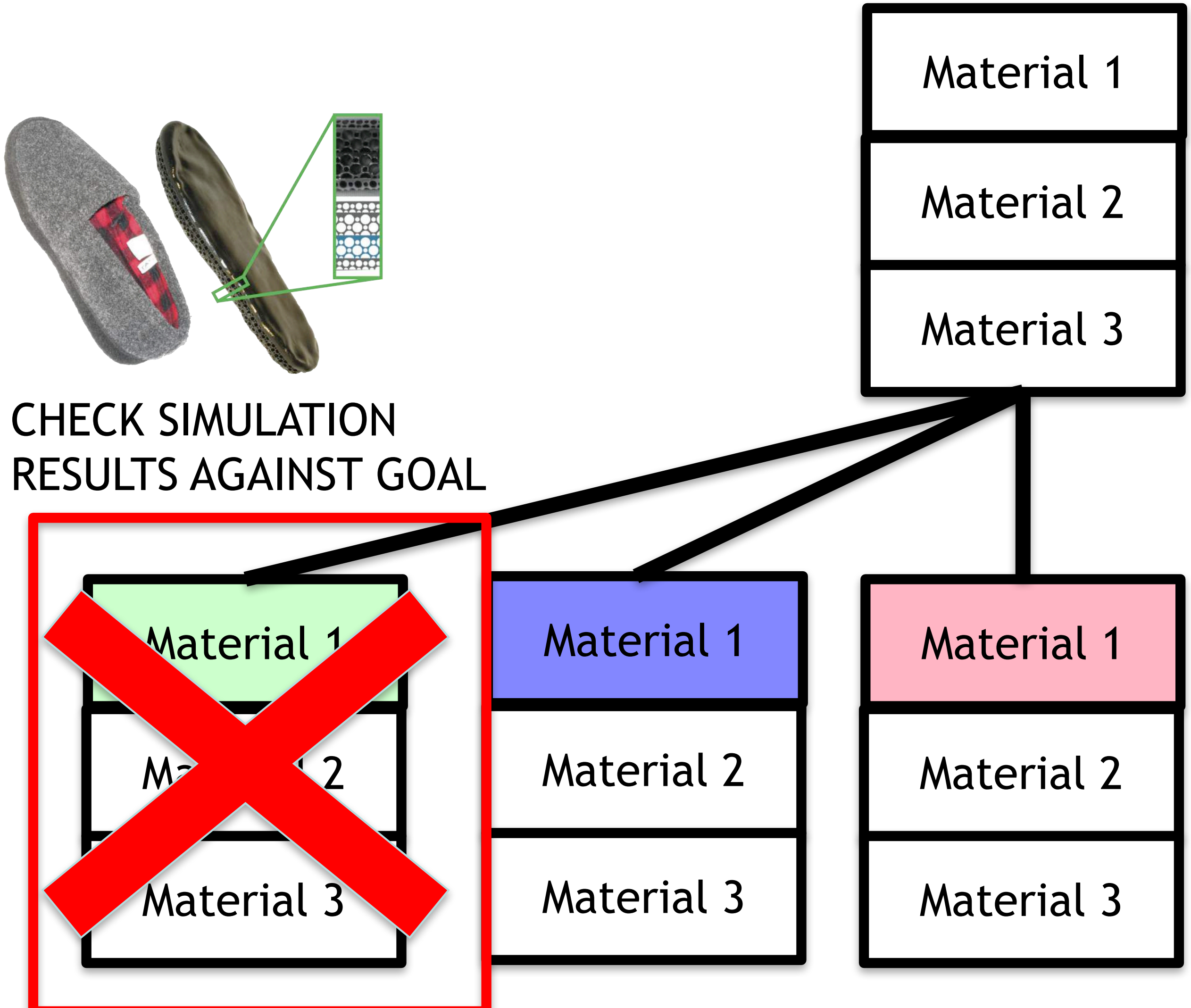
Bounding Material Assignment



Bounding Material Assignment



Bounding Material Assignment



Simulated Annealing

- Has four ingredients
  - Cost function
  - Configuration (made of discrete 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

Simulated Annealing

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

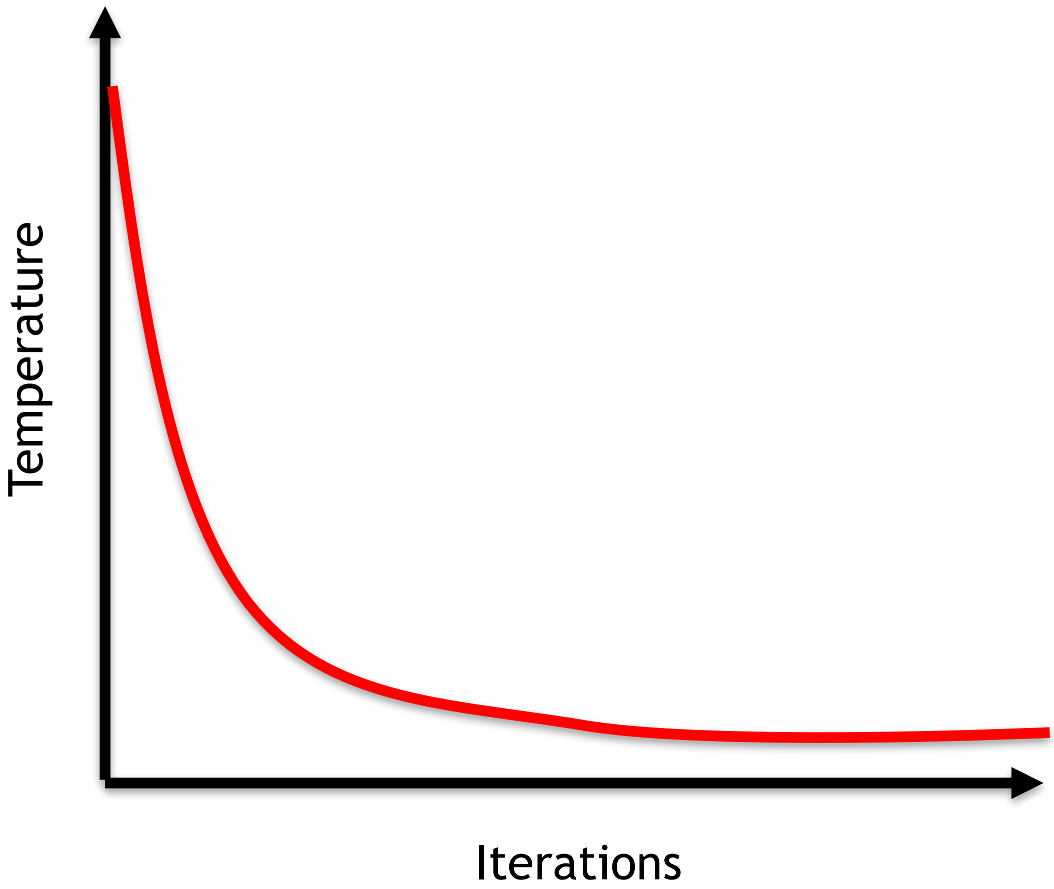
Configuration

Simulated Annealing

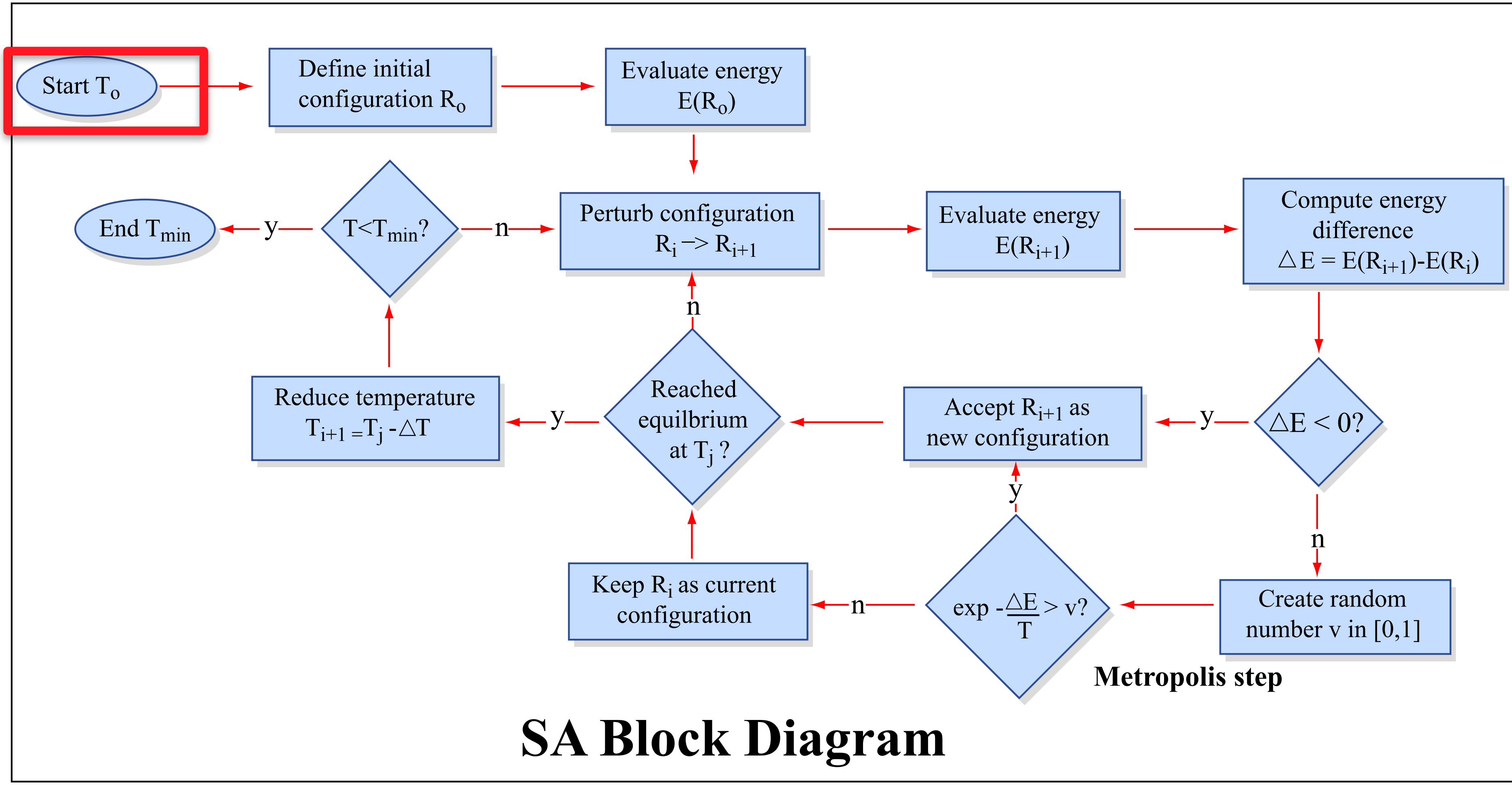
- Cost function: $f\left(\mathbf{q}\right)$
- Configuration: $\mathbf{q}$ e.g. Material Assignments
- Neighbor Generator: Rearrange Configuration
  - e.g. Change some materials to ones with nearby stiffness
- Annealing Schedule

Simulated Annealing

- Annealing Schedule



Simulated Annealing



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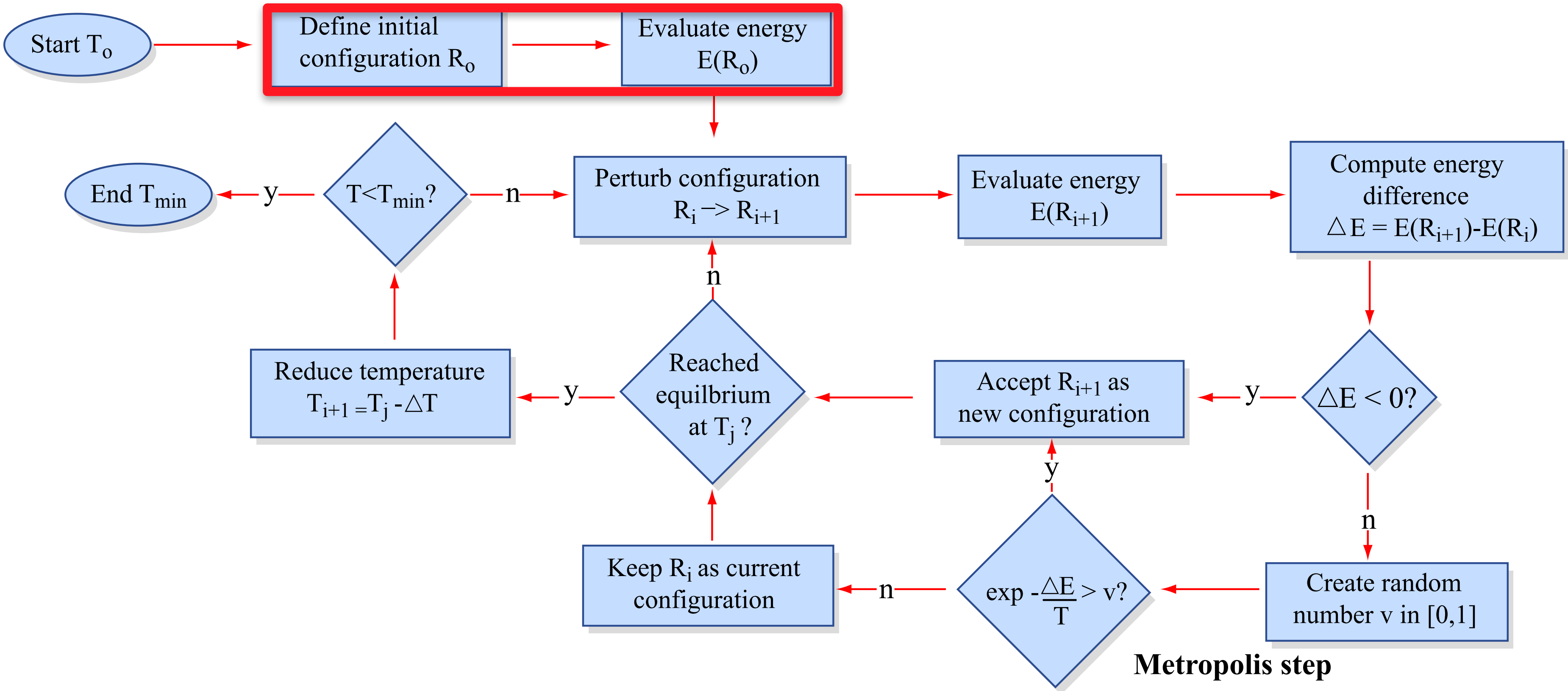
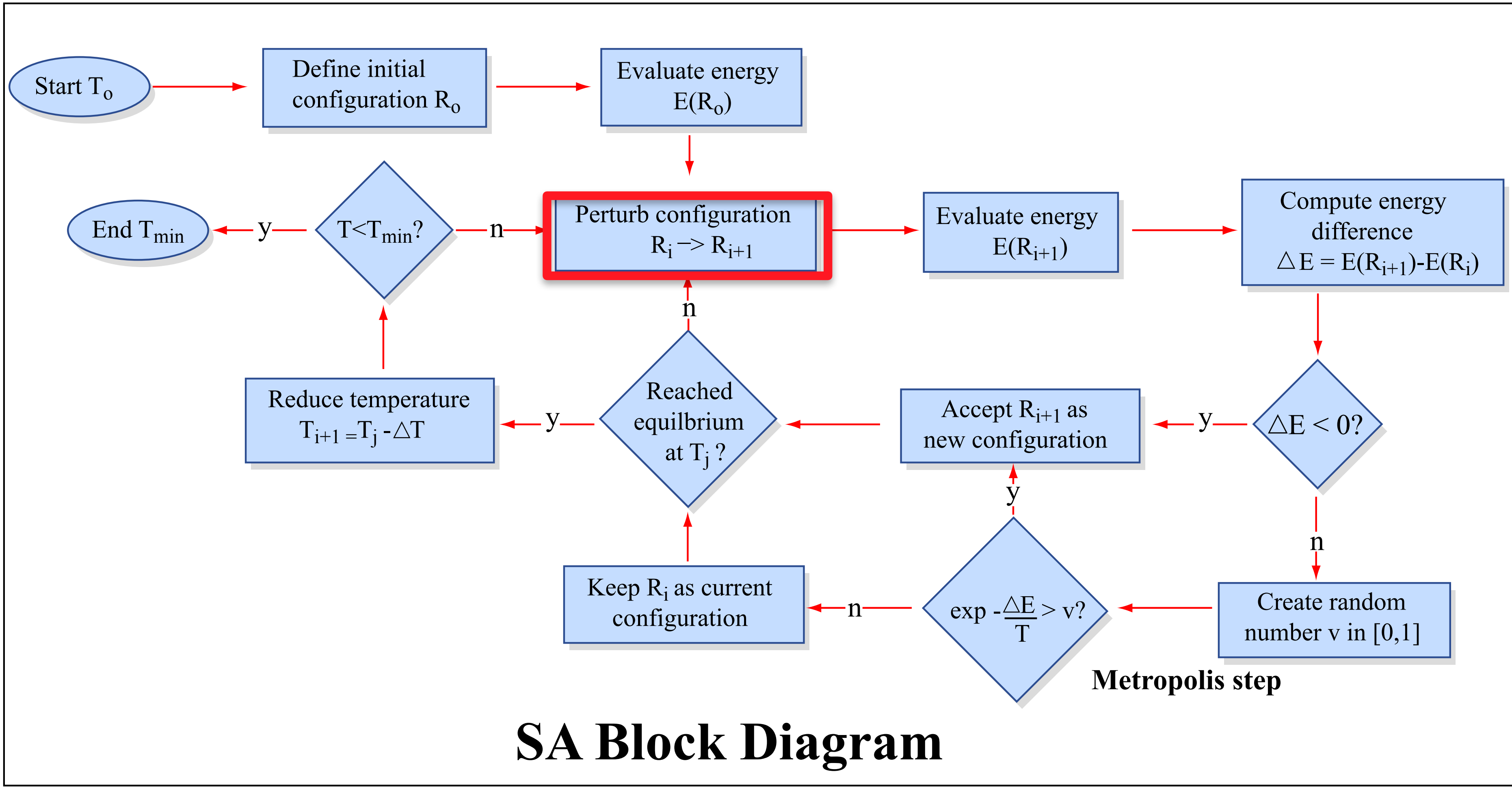
Simulated Annealing



SA Block Diagram

Image by MIT OpenCourseWare.

Simulated Annealing



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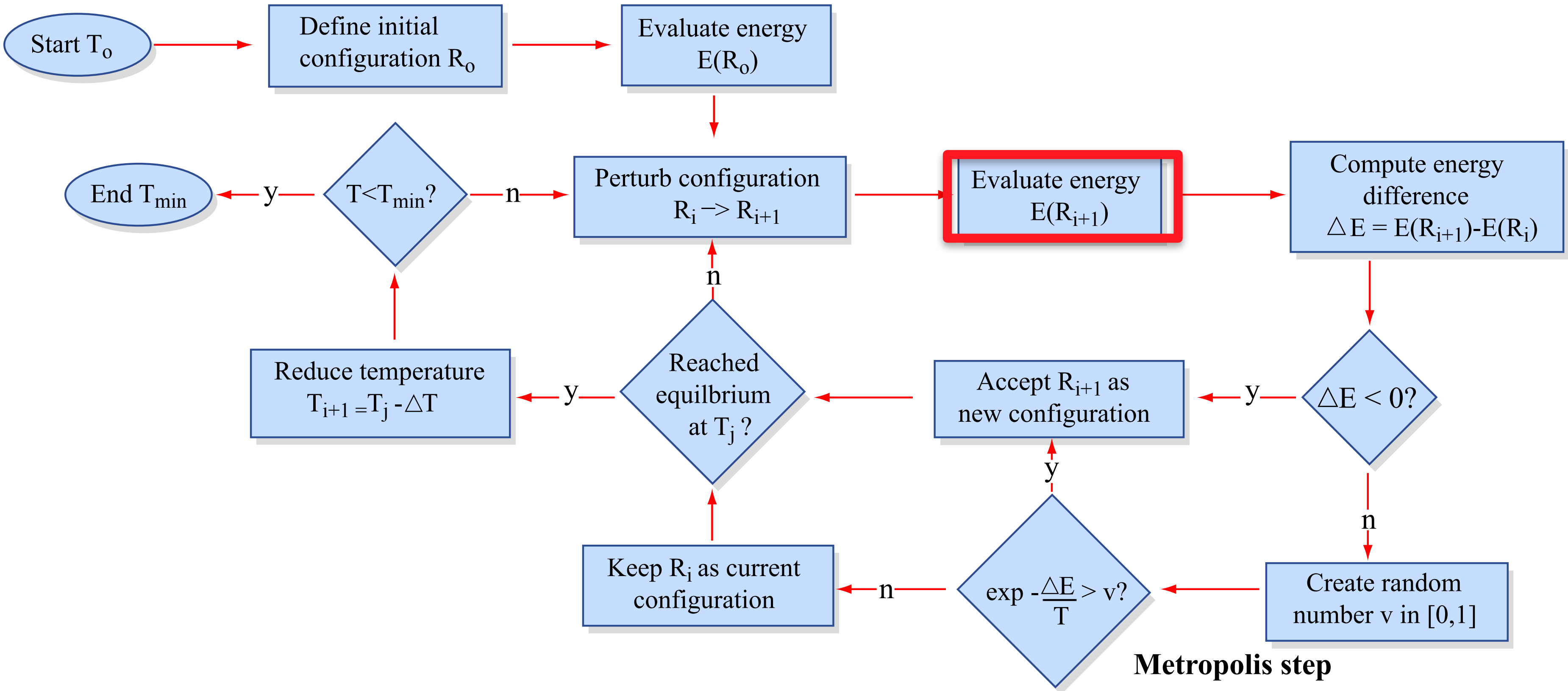
Simulated Annealing



SA Block Diagram

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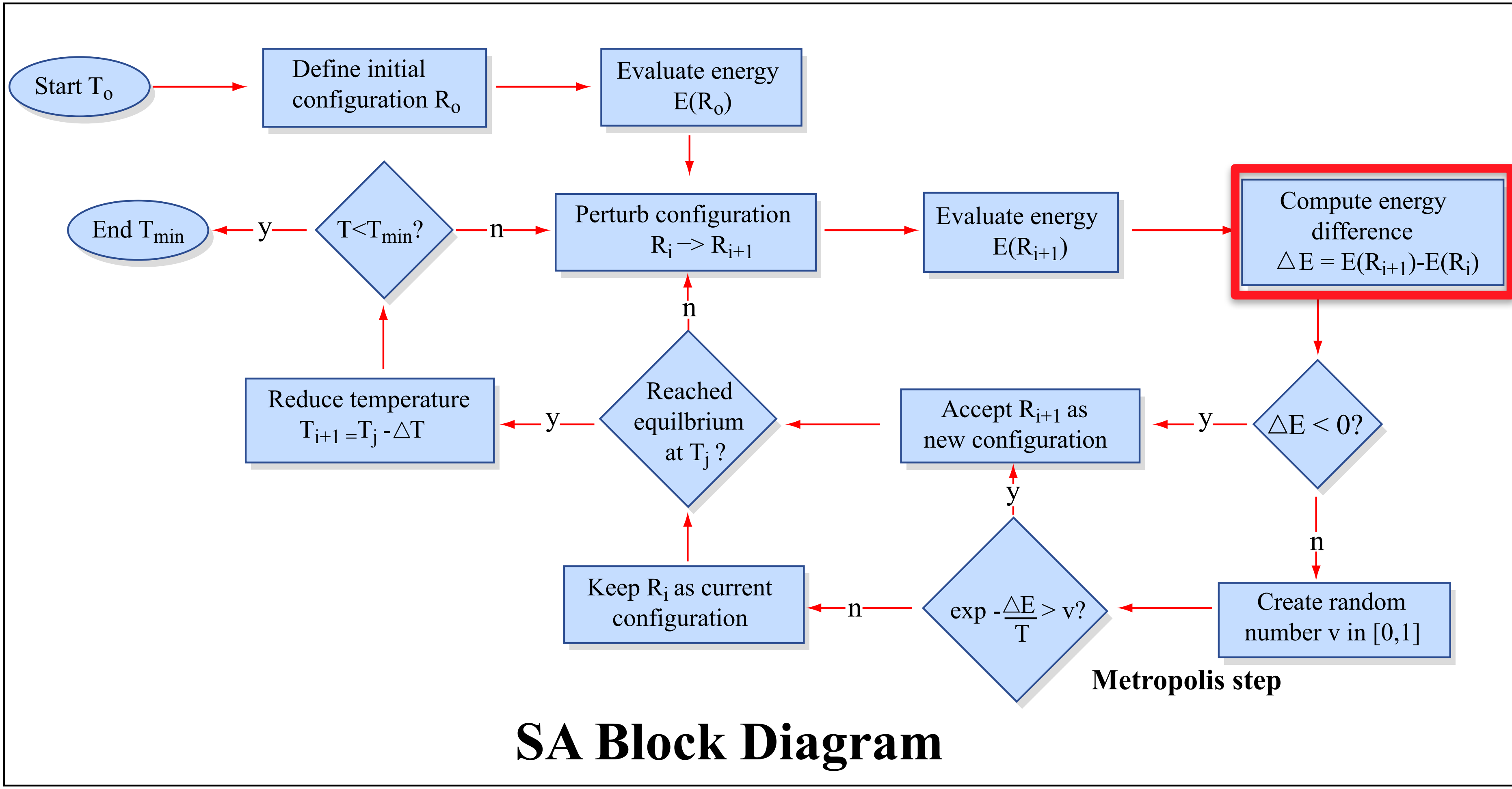
Simulated Annealing



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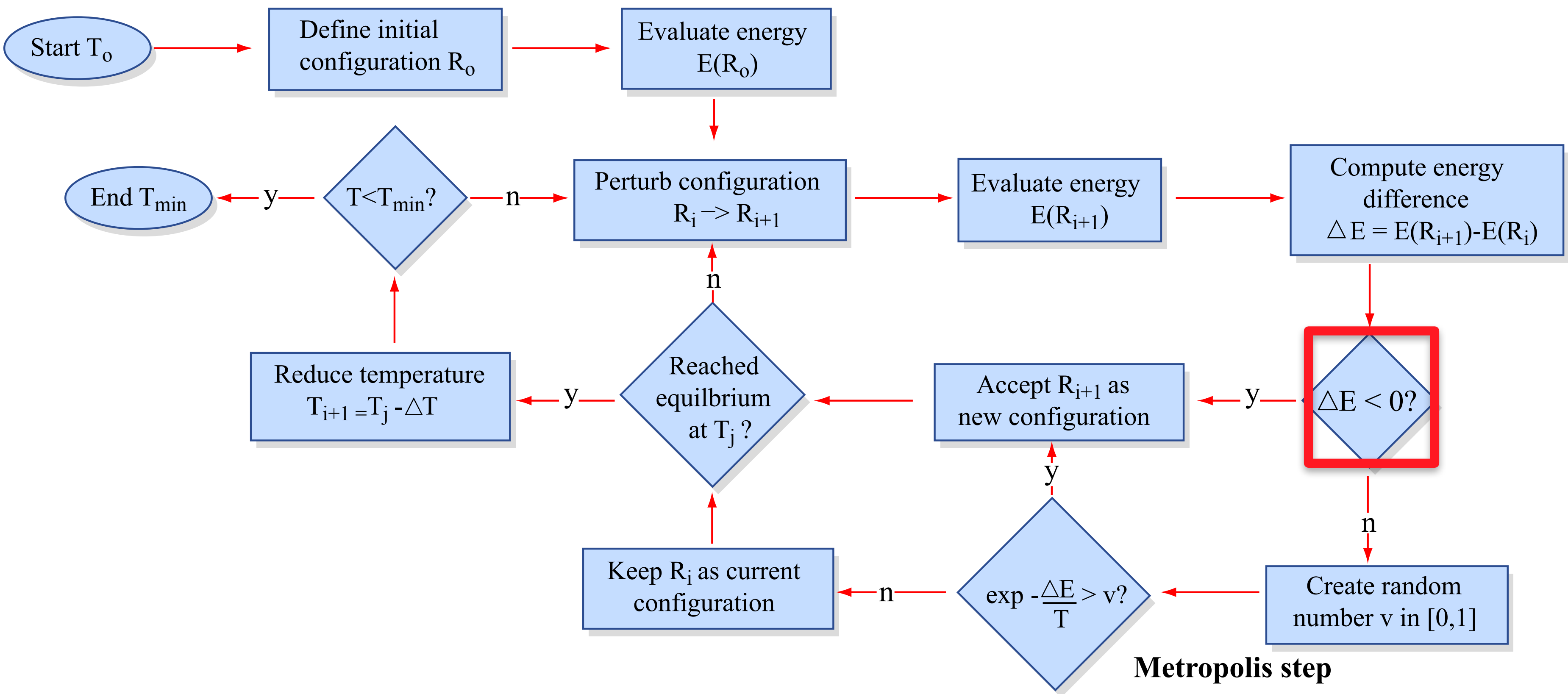
Simulated Annealing



SA Block Diagram

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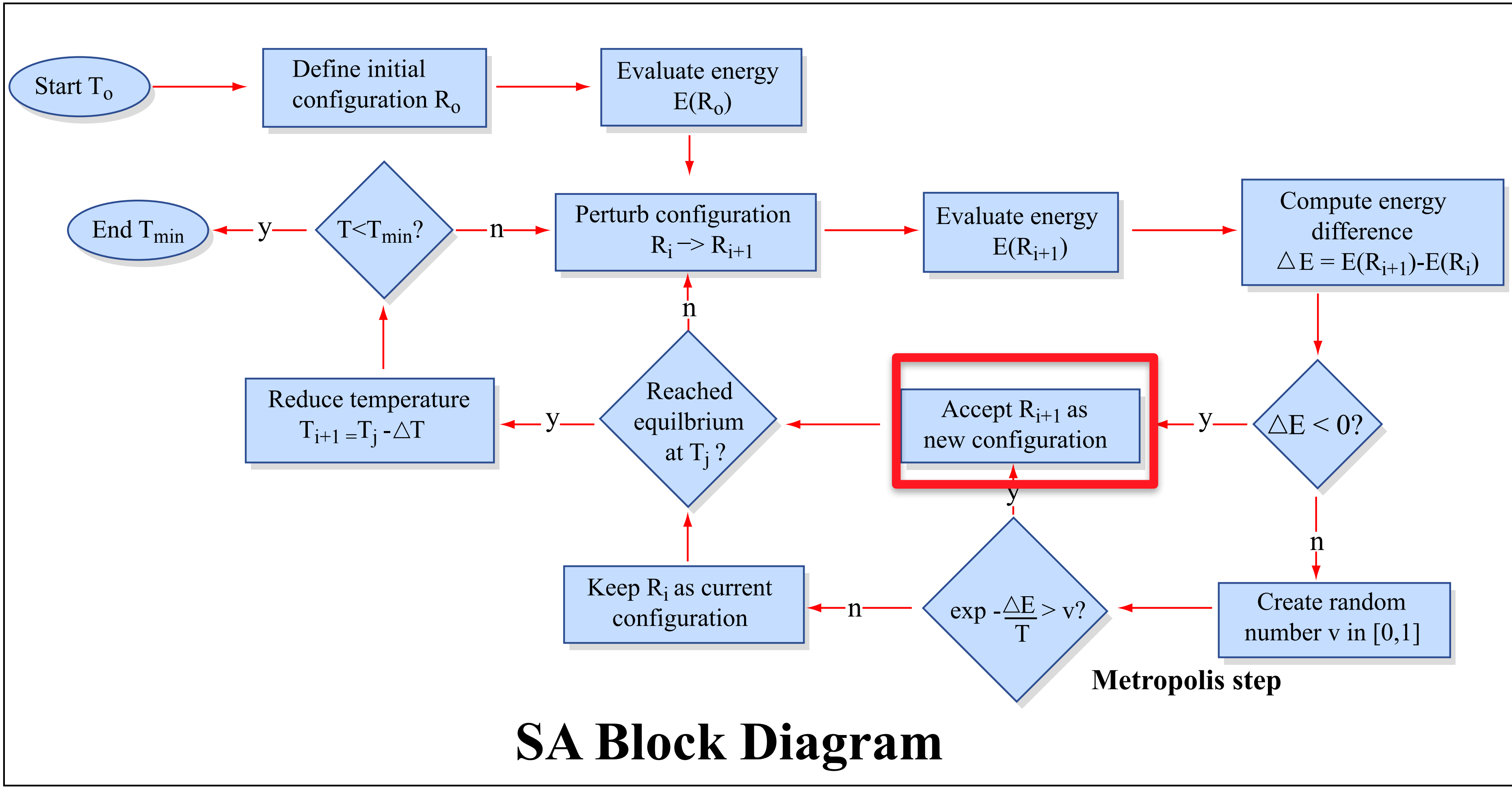
Simulated Annealing



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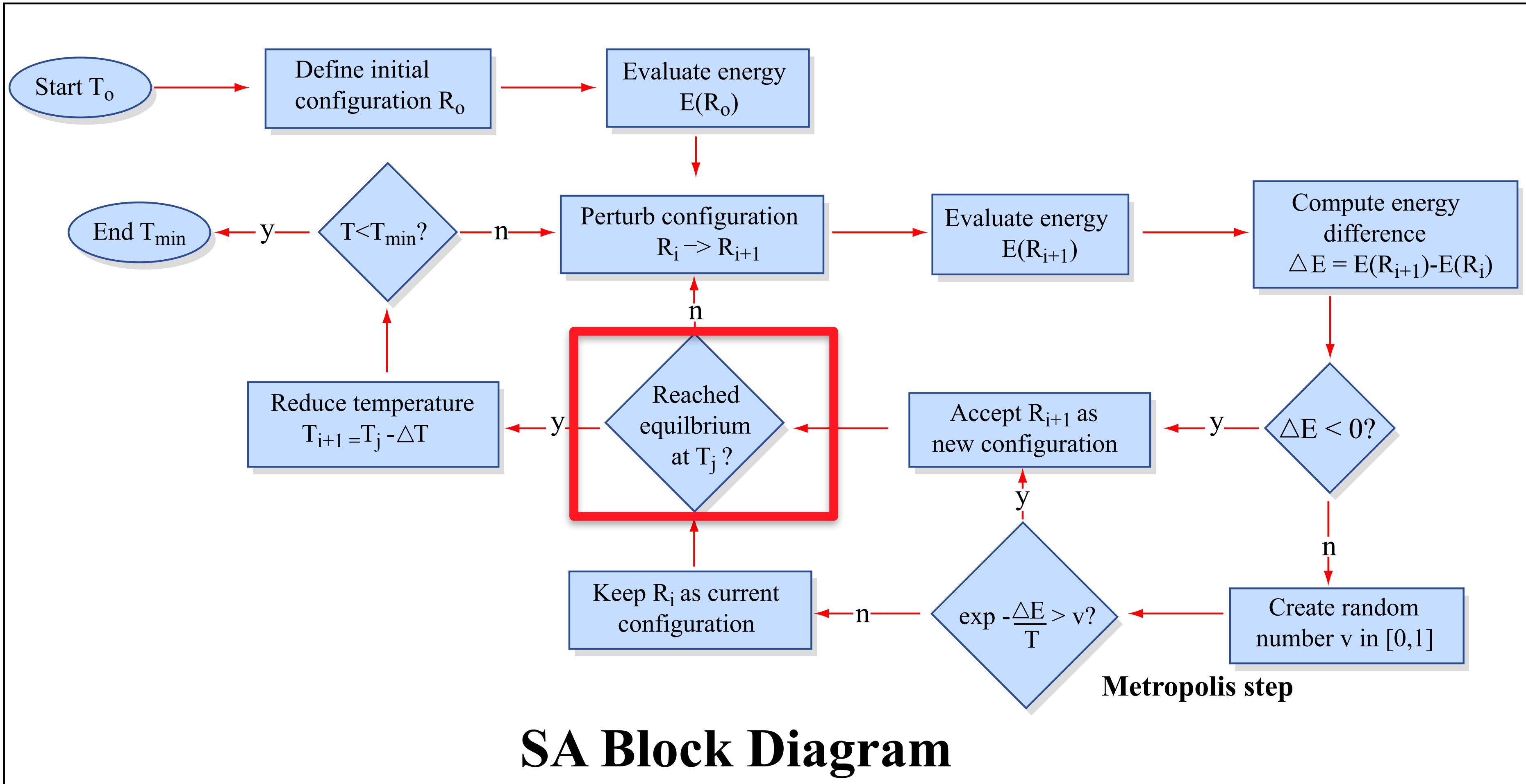
Simulated Annealing



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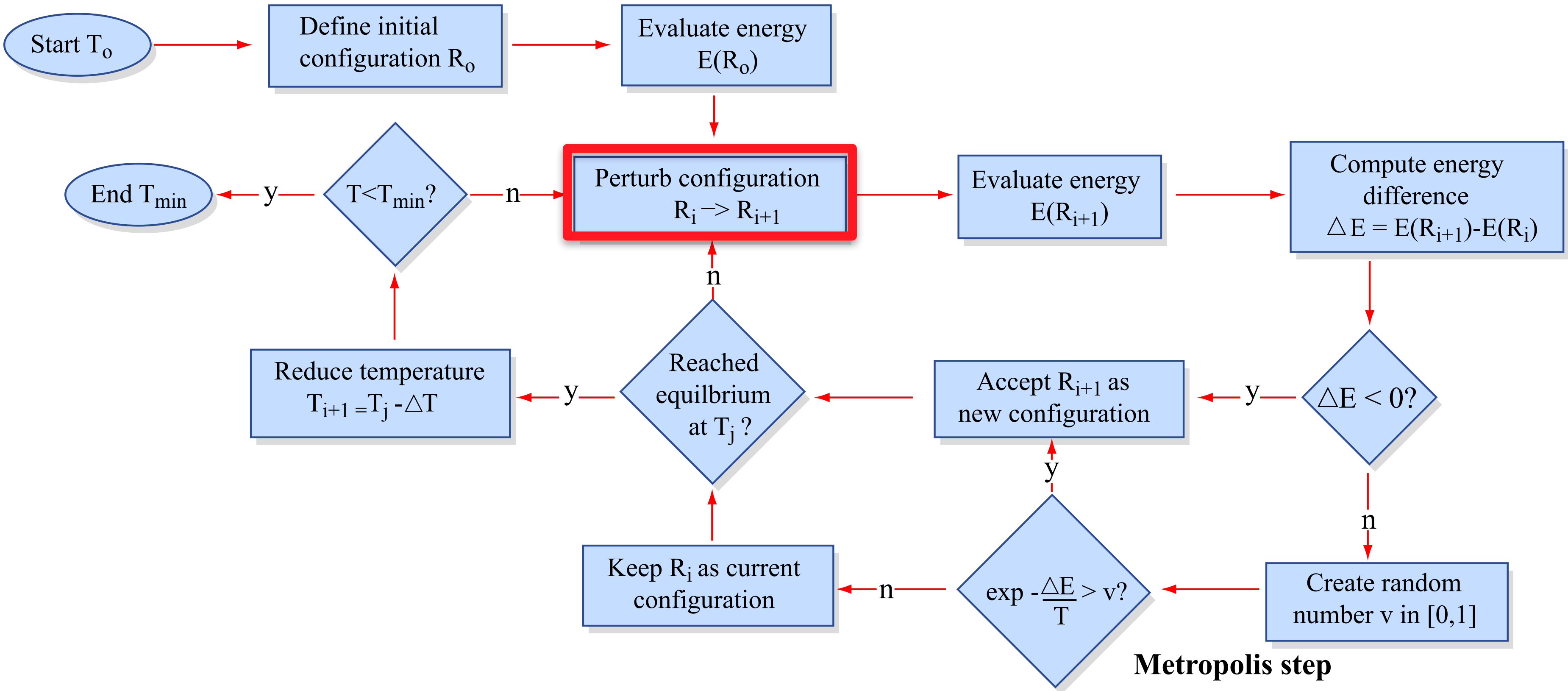
Simulated Annealing



SA Block Diagram

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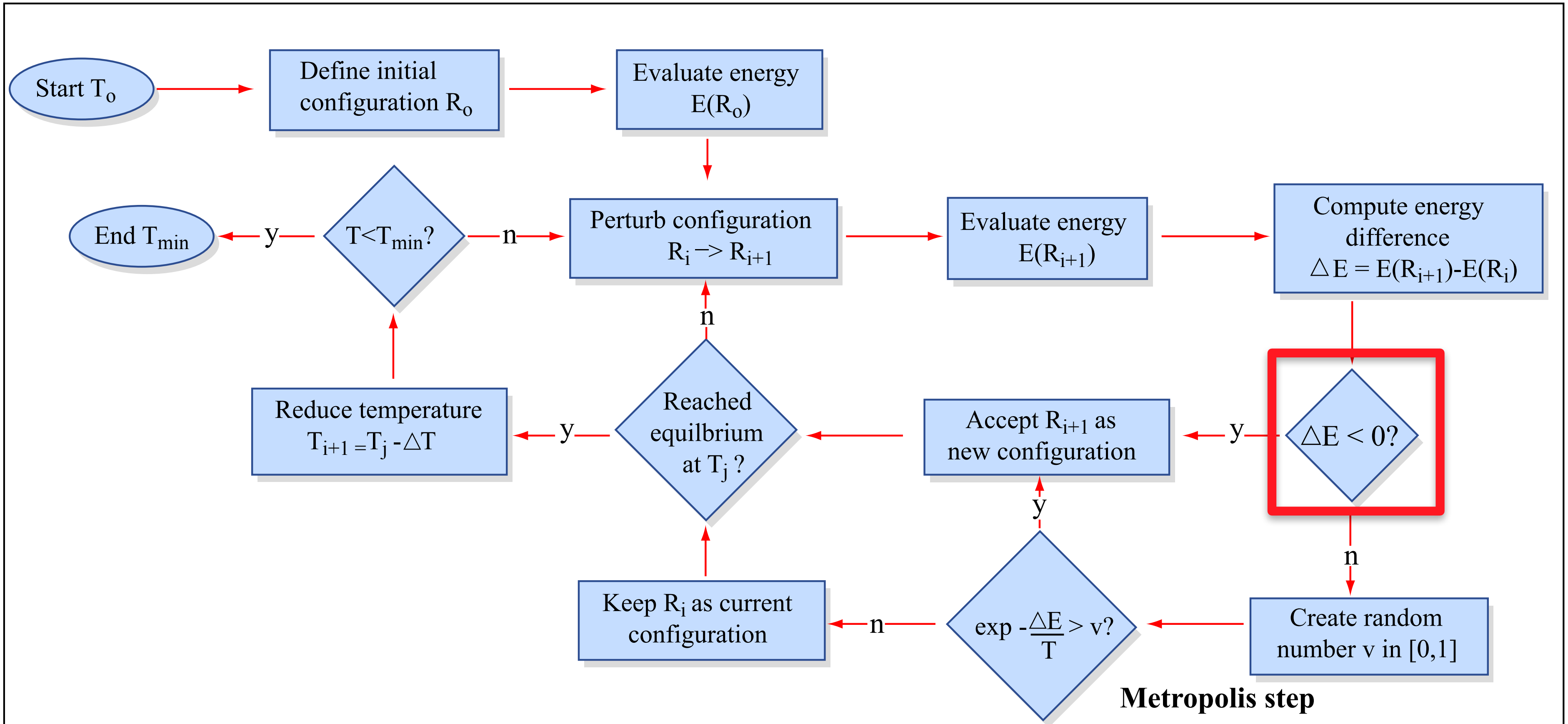
Simulated Annealing



SA Block Diagram

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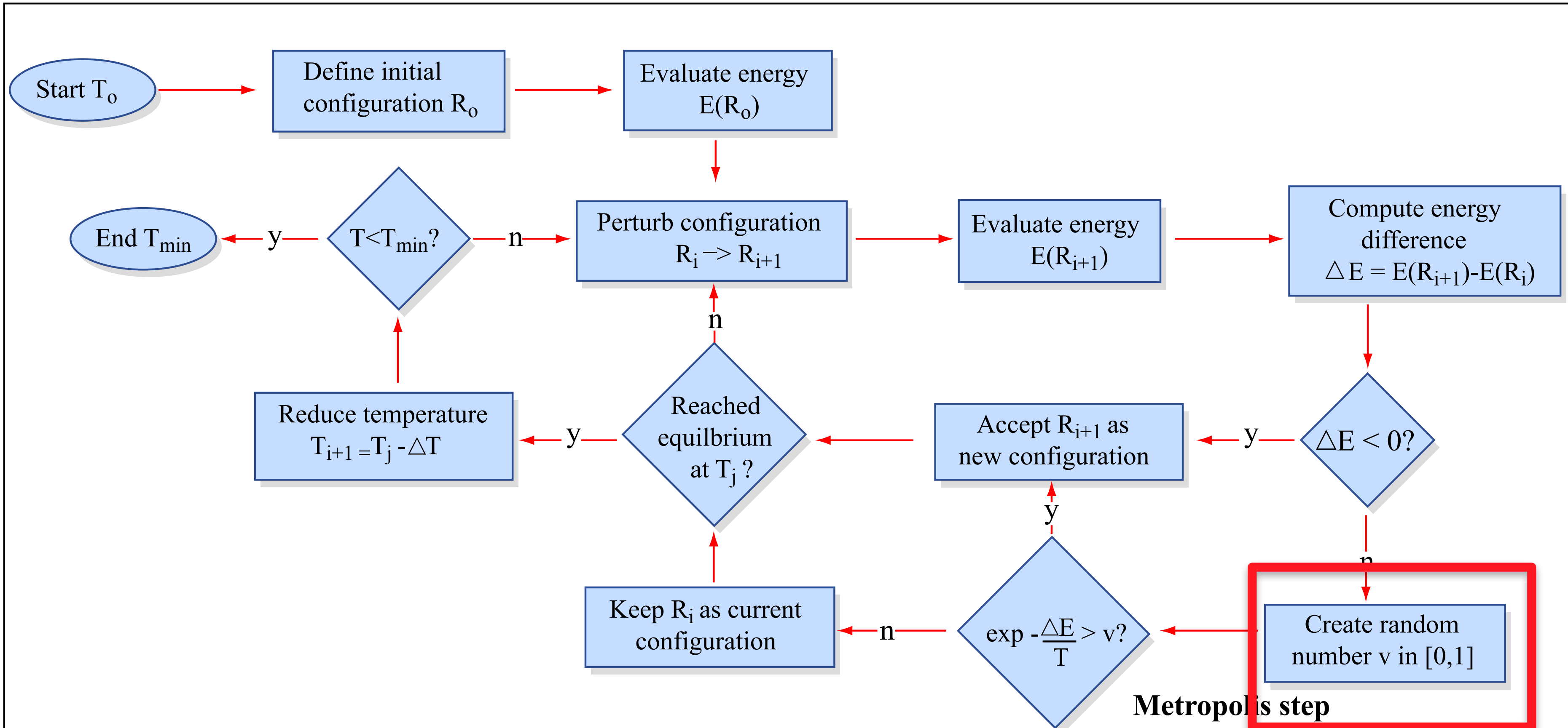
Simulated Annealing



SA Block Diagram

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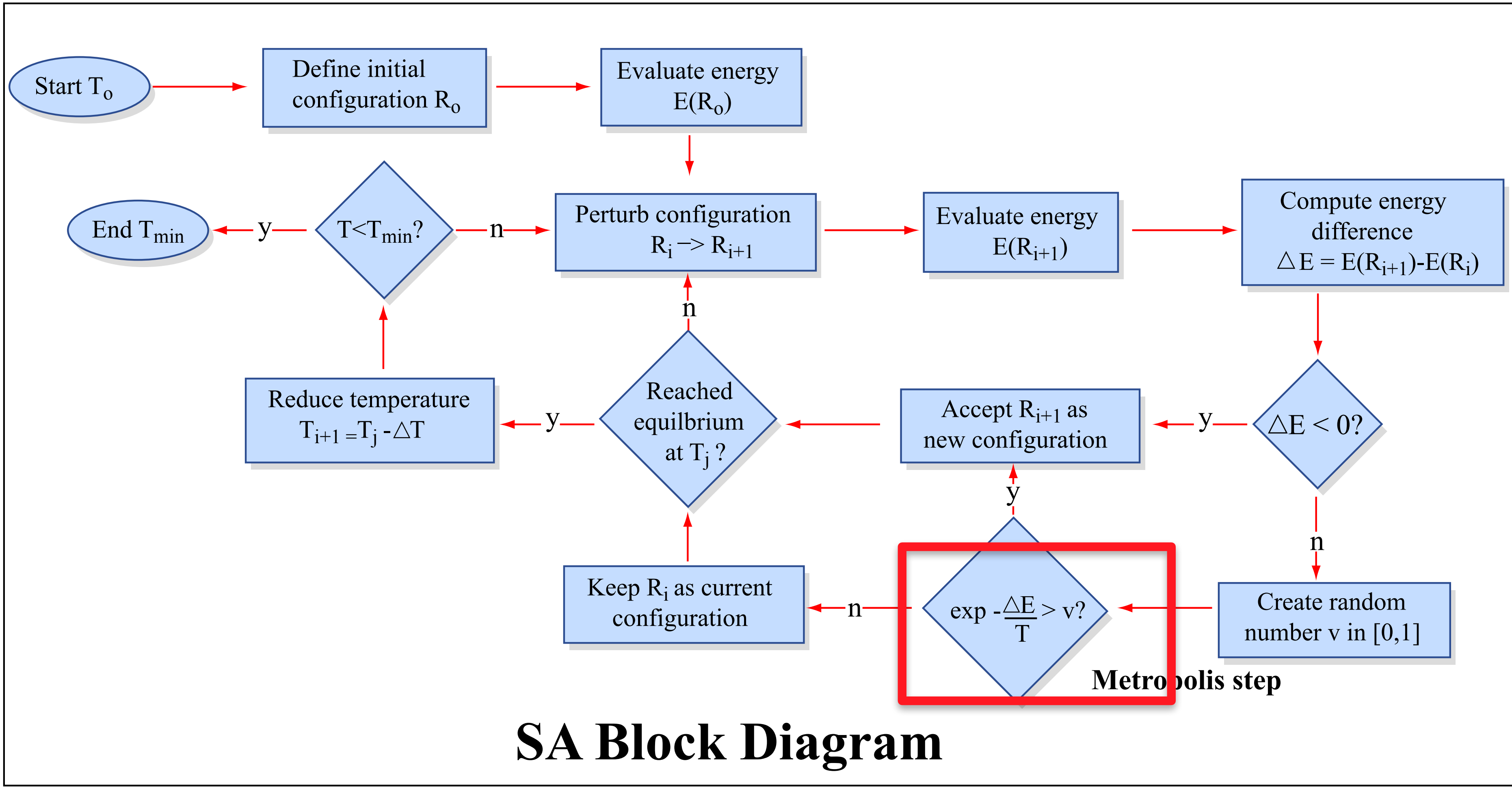
Simulated Annealing



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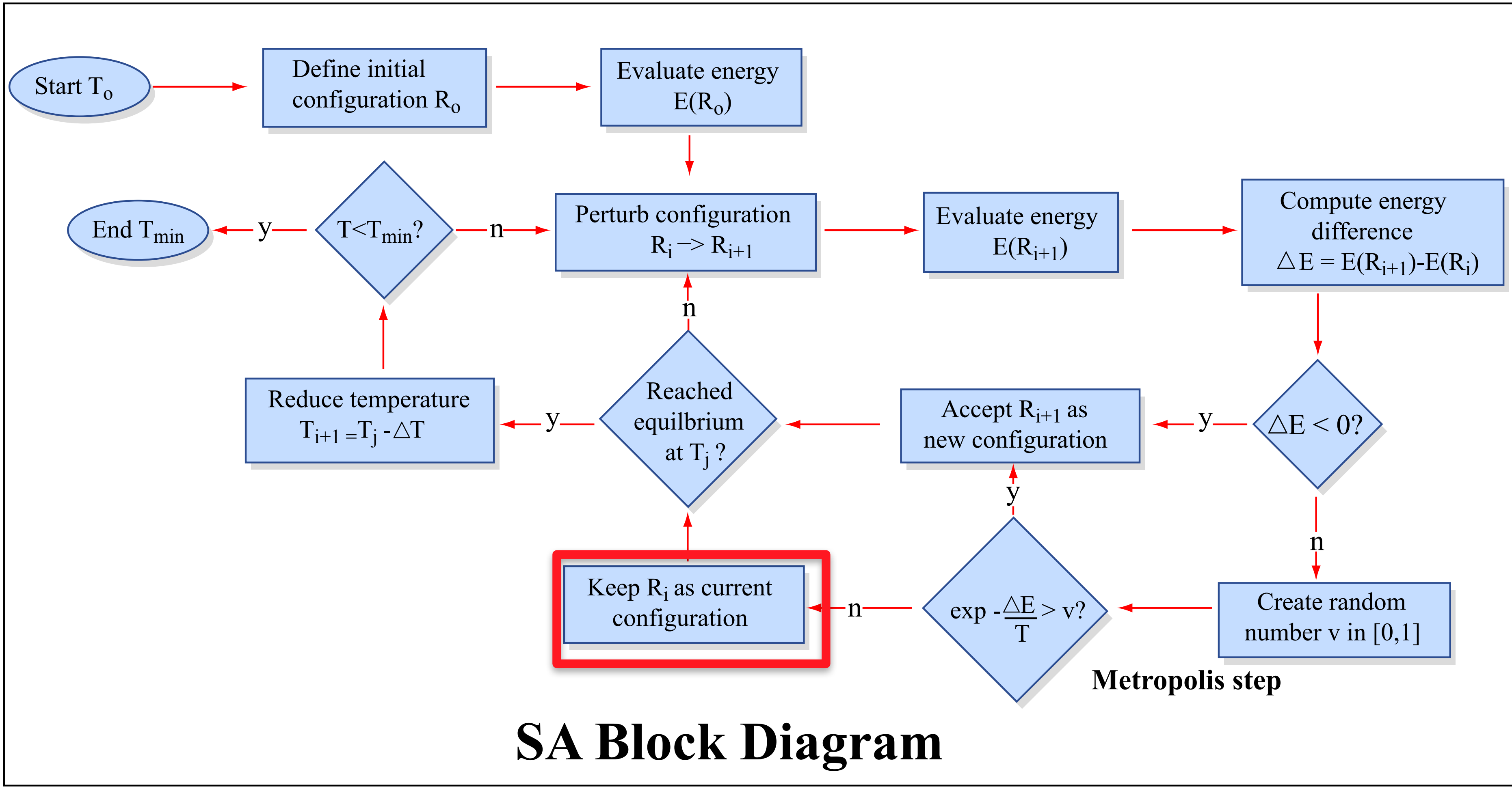
Simulated Annealing



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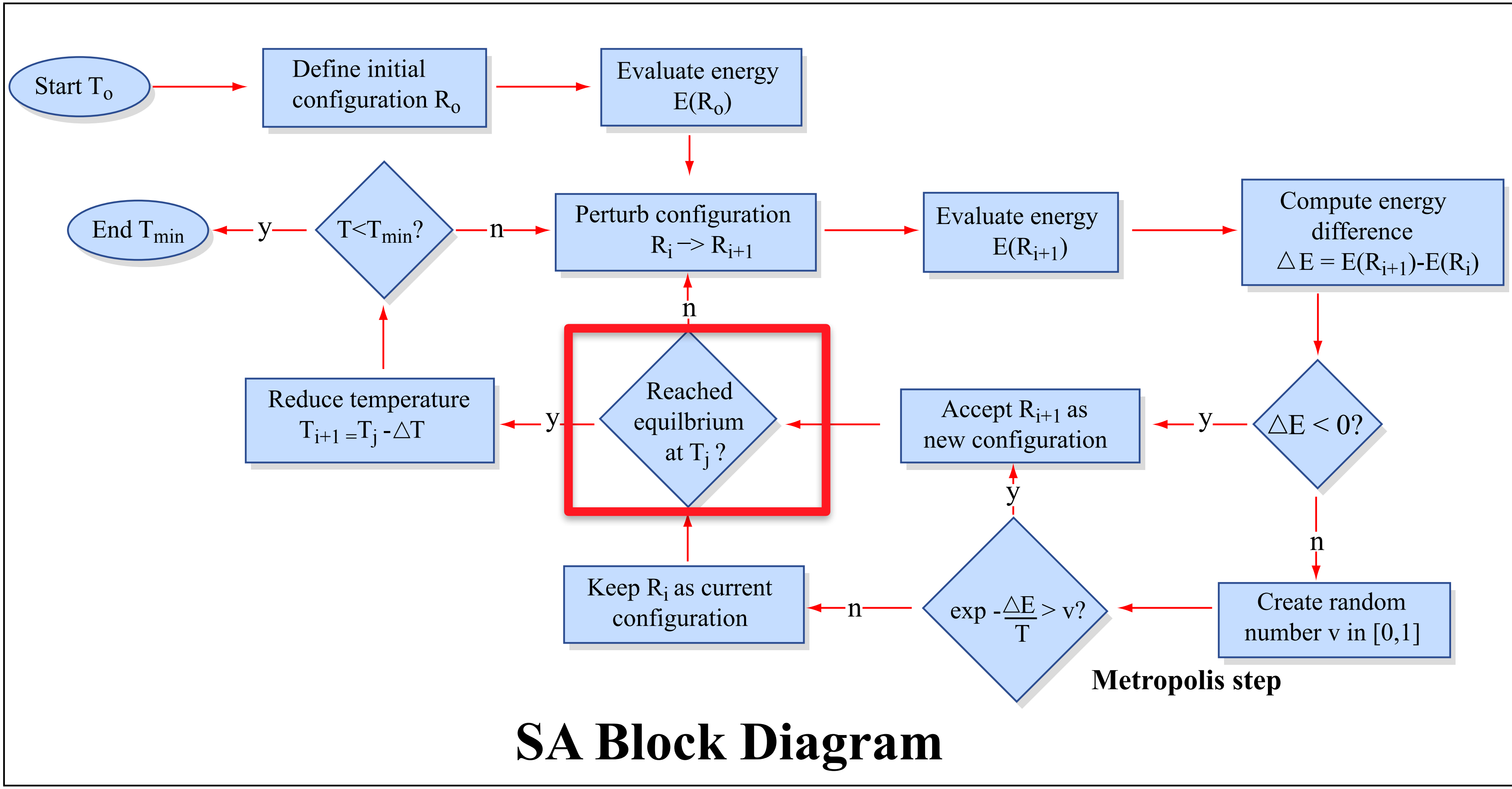
Simulated Annealing



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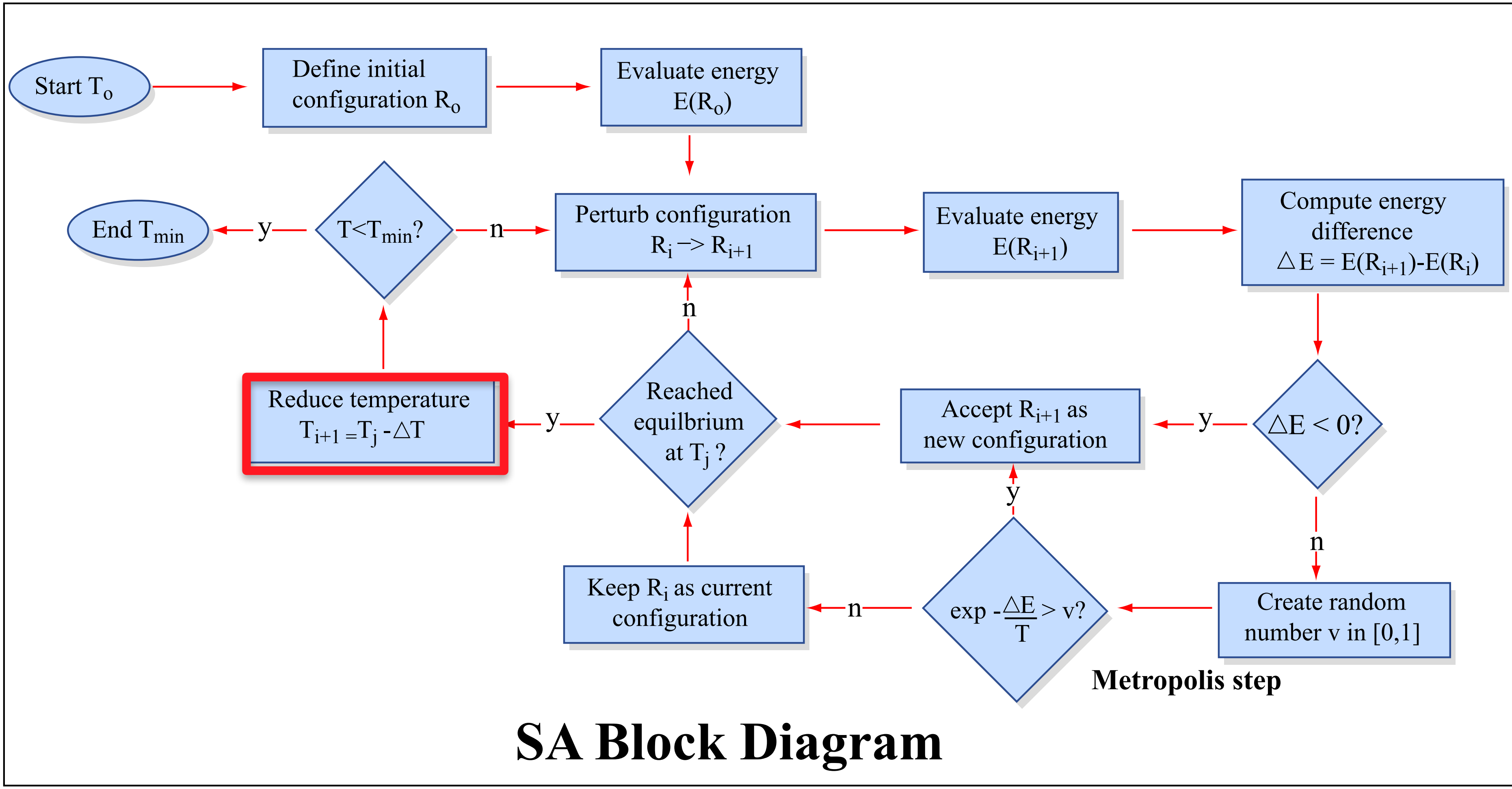
Simulated Annealing



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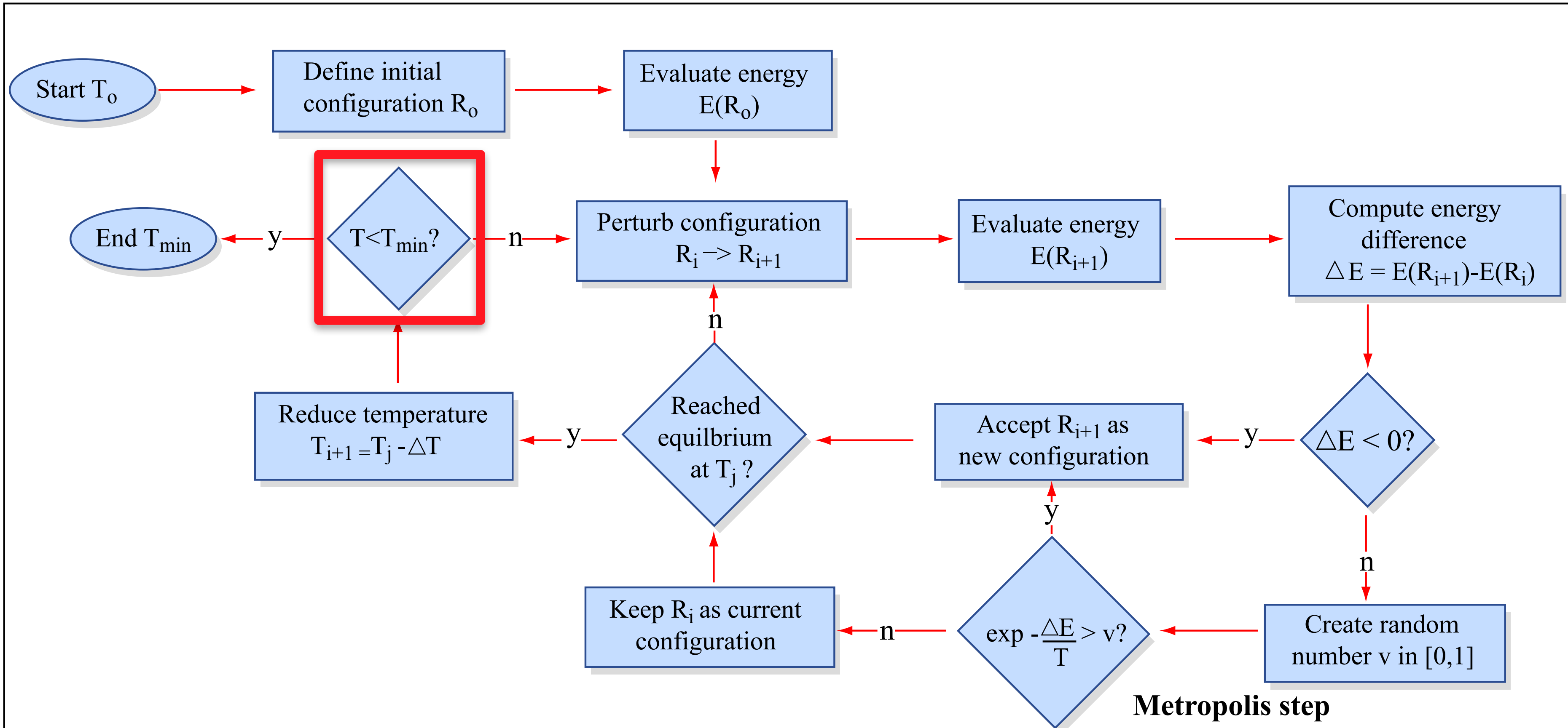
Simulated Annealing



SA Block Diagram

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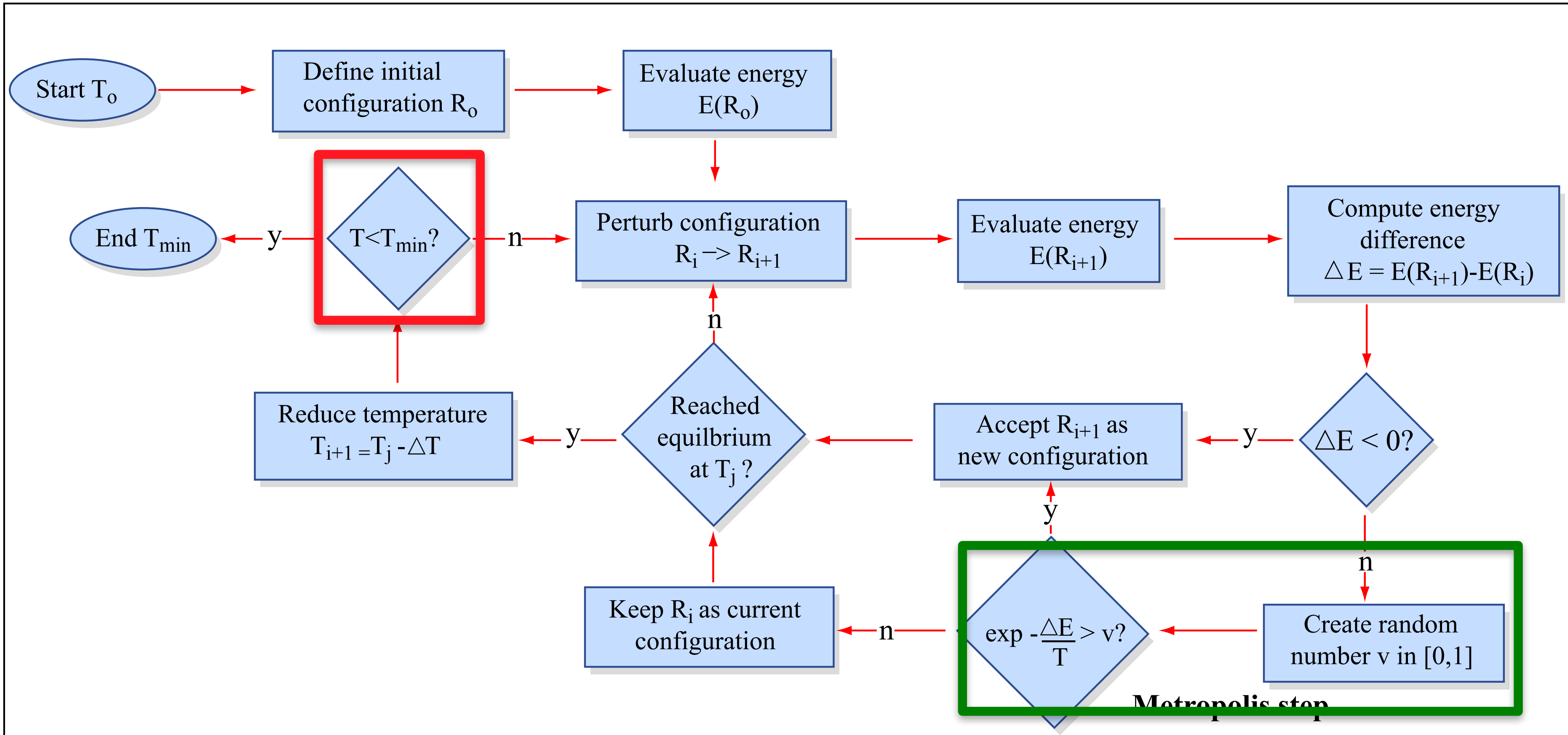
Simulated Annealing



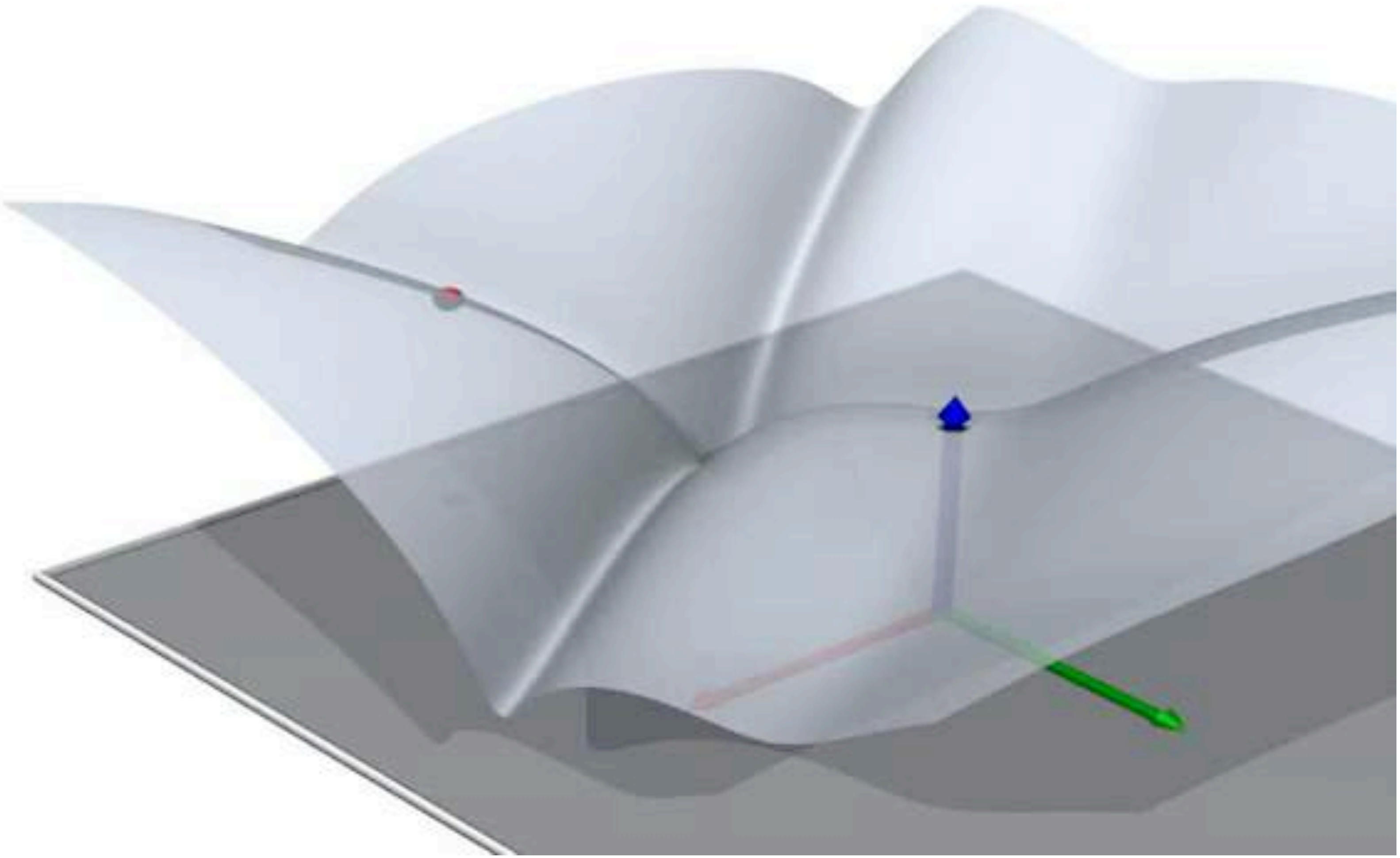
SA Block Diagram

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

The End

- This is the last topic lecture for the course
- The remainder of the lectures will be on current research in computational fabrication