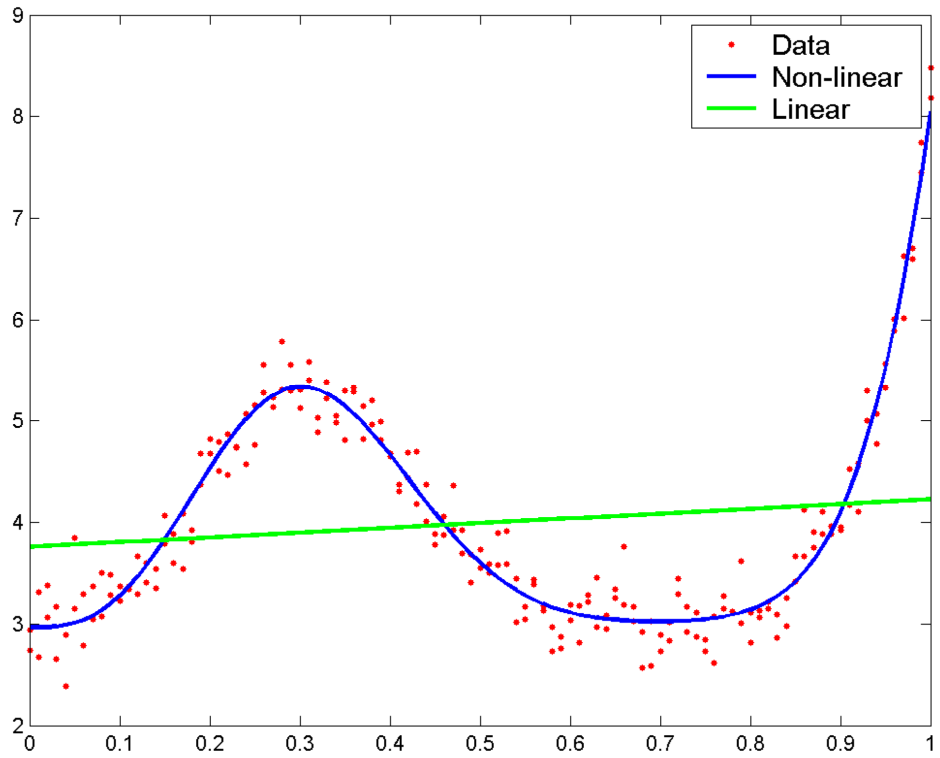
Introduction to Numerical Analysis for Engineers

- Minimization Problems
- Least Square Approximation
  - Normal Equation
  - Parameter Estimation
  - Curve fitting
- Optimization Methods
  - Simulated Annealing
    - Traveling salesman problem
  - Genetic Algorithms

Minimization Problems

Data Modeling – Curve Fitting



Linear Model

$$y = cx$$

Non-linear Model

$$y = c(x)$$

Minimimize Overall Error

$$(c) = \sum_i (y_i - c(x_i))^2$$

Objective: Find c that minimizes error

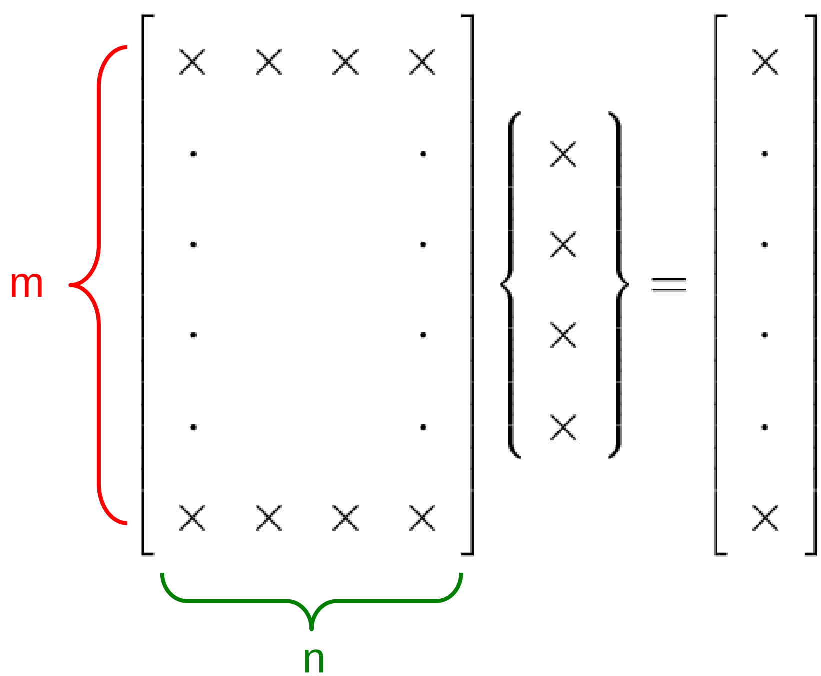
Least Square Approximation

Linear Measurement Model

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

n model parameters

m measurements



Overdetermined System

m measurements
n unknowns
m > n

Least Square Solution

Minimize Residual Norm

$$\overline{\mathbf{r}} = \overline{\mathbf{b}} - \overline{\overline{\mathbf{A}}}\,\overline{\mathbf{x}}$$

$$||r||_2 = (\overline{\mathbf{r}}^T \overline{\mathbf{r}})^{1/2}$$

Least Square Approximation

Theorem

$$\text{If } \overline{\overline{\mathbf{A}}}^T \left(\overline{\mathbf{b}} - \overline{\overline{\mathbf{A}}}\overline{\mathbf{x}}\right) = 0 \Rightarrow \forall\, y \left| \left\| \overline{\mathbf{b}} - \overline{\overline{\mathbf{A}}}\overline{\mathbf{x}} \right\|_2 \leq \left\| \overline{\mathbf{b}} - \overline{\overline{\mathbf{A}}}\overline{\mathbf{y}} \right\|_2 \right.$$

Proof

$$\left.\begin{aligned} \overline{\mathbf{r}}_x &= \overline{\mathbf{b}} - \overline{\overline{\mathbf{A}}}\overline{\mathbf{x}} \\ \overline{\mathbf{r}}_y &= \overline{\mathbf{b}} - \overline{\overline{\mathbf{A}}}\overline{\mathbf{y}} \end{aligned}\right\} \Rightarrow$$

$$\overline{\mathbf{r}}_y = (\overline{\mathbf{b}} - \overline{\overline{\mathbf{A}}}\overline{\mathbf{x}}) + (\overline{\overline{\mathbf{A}}}\overline{\mathbf{x}} - \overline{\overline{\mathbf{A}}}\overline{\mathbf{y}}) = \overline{\mathbf{r}}_x + \overline{\overline{\mathbf{A}}}(\overline{\mathbf{x}} - \overline{\mathbf{y}})$$

$$\overline{\mathbf{r}}_y^T\overline{\mathbf{r}}_y = \overline{\mathbf{r}}_x^T\overline{\mathbf{r}}_x + (\overline{\mathbf{x}} - \overline{\mathbf{y}})^T\overline{\overline{\mathbf{A}}}^T\overline{\overline{\mathbf{A}}}(\overline{\mathbf{x}} - \overline{\mathbf{y}}) + (\overline{\mathbf{x}} - \overline{\mathbf{y}})^T\overline{\overline{\mathbf{A}}}^T\overline{\mathbf{r}}_x + r_x^T\overline{\overline{\mathbf{A}}}(\overline{\mathbf{x}} - \overline{\mathbf{y}})$$

$$\begin{aligned} \overline{\overline{\mathbf{A}}}^T\overline{\mathbf{r}}_x &= \overline{\mathbf{0}} \\ \overline{\mathbf{r}}_x^T\overline{\overline{\mathbf{A}}} &= \left(\overline{\overline{\mathbf{A}}}^T\overline{\mathbf{r}}_x\right)^T = \overline{\mathbf{0}} \end{aligned}$$

$$\overline{\mathbf{r}}_y^T\overline{\mathbf{r}}_y = \overline{\mathbf{r}}_x^T\overline{\mathbf{r}}_x + (\overline{\mathbf{x}} - \overline{\mathbf{y}})^T\overline{\overline{\mathbf{A}}}^T\overline{\overline{\mathbf{A}}}(\overline{\mathbf{x}} - \overline{\mathbf{y}})$$

$$\Rightarrow$$

$$||\overline{\mathbf{r}}_y||_2^2 = ||\overline{\mathbf{r}}_x||_2^2 + \left\|\overline{\overline{\mathbf{A}}}(\overline{\mathbf{x}} - \overline{\mathbf{y}})\right\|_2^2 \geq ||\overline{\mathbf{r}}_x||_2^2$$

q.e.d

Normal Equation

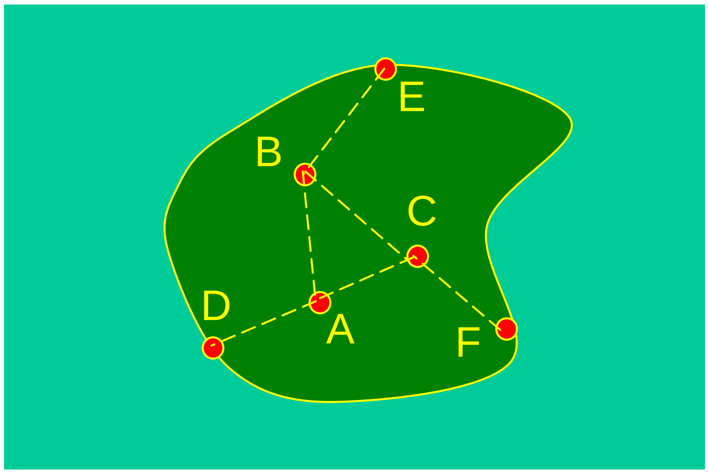
$$\left(\overline{\overline{\mathbf{A}}}^T\overline{\overline{\mathbf{A}}}\right)\overline{\mathbf{x}} = \overline{\overline{\mathbf{A}}}^T\overline{\mathbf{b}}$$

$$\overline{\overline{\mathbf{C}}} = \overline{\overline{\mathbf{A}}}^T\overline{\overline{\mathbf{A}}}$$

Symmetric n x n matrix. Non-singular if columns of A are linearly independent

Least Square Approximation
Parameter estimation

Example
Island Survey



Points D, E, and F at sea level. Find altitude of inland points A, B, and C.

```
A=[ [1 0 0 -1 0 -1]' [0 1 0 1 -1 0]' [0 0 1 0
b=[1 2 3 1 2 1]';
C=A'*A
c=A'*b
% Least square solution
z=inv(C)*c
% Residual
r=b-A*z
rn=sqrt(r'*r)
```

lstsq.m

Measured Altitude Differences

$$h_{DA} = 1\ ,\ h_{EB} = 2\ ,\ h_{FC} = 3\ ,\ h_{AB} = 1\ ,\ h_{BC} = 2\ ,\ h_{AC} = 1$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \\ -1 & 0 & 1 \end{bmatrix} \begin{Bmatrix} z_A \\ z_B \\ z_C \end{Bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 1 \\ 2 \\ 1 \end{bmatrix}$$

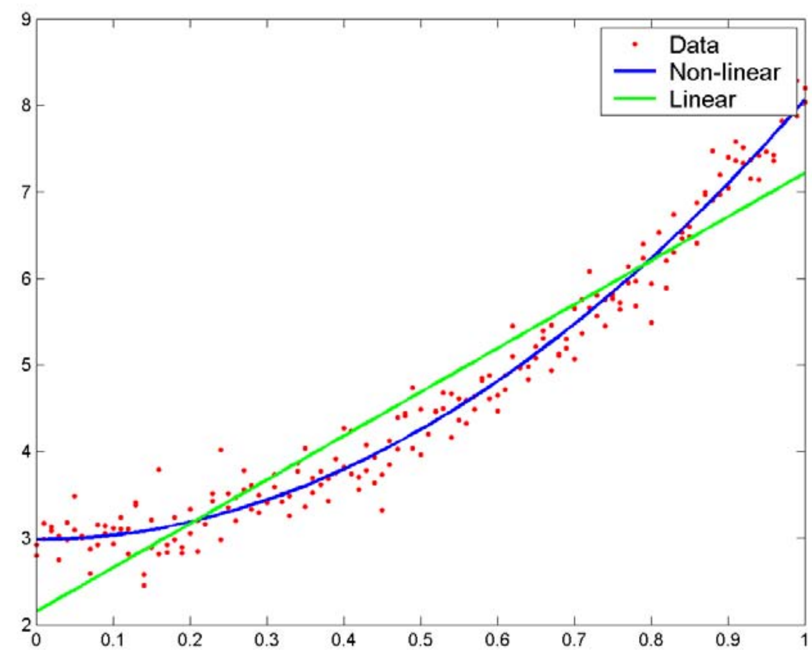
$$\begin{bmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{bmatrix} \begin{Bmatrix} z_A \\ z_B \\ z_C \end{Bmatrix} = \begin{bmatrix} -1 \\ 1 \\ 6 \end{bmatrix} \Rightarrow \begin{cases} z_A = \frac{5}{4} \\ z_B = \frac{7}{4} \\ z_C = 3 \end{cases}$$

$$\bar{\mathbf{r}} = \frac{1}{4}[-1, 1, 0, 2, 3, -3]^T$$

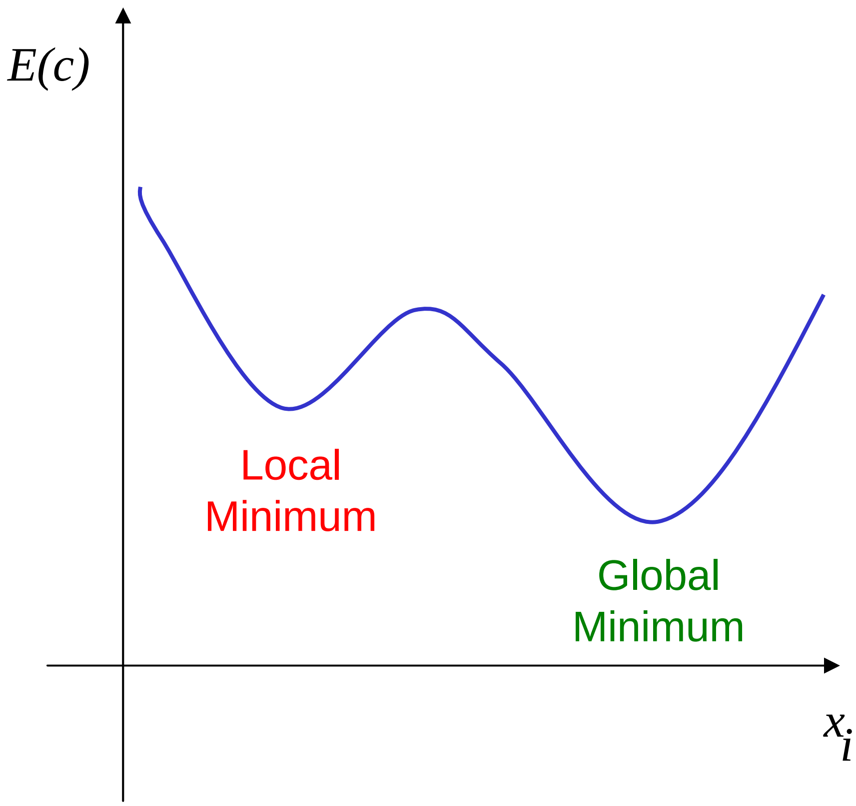
Least Square Approximation
Curve Fitting

curve.m

```
% Quadratic data model
fxy='a*x.^2+b'
f=inline(fxy,'x','a','b');
x=[0:0.01:1]; x=reshape([x' x']',1,2*length(x));
n=length(x); y=zeros(n,1);
a=5;  b=3;
% Generate noisy data
amp=0.05*(max(f(x,a,b))-min(f(x,a,b)));
for i=1:n
    y(i) =f(x(i),a,b)+random('norm',0,amp);
end
figure(1); clf; hold off; p=plot(x,y,'.r');
set(p,'MarkerSize',10)
% Non-linear, quadrati model
A=ones(n,2); A(:,1)=f(x,1,0)'; bb=y;
%Normal matrix
C=A'*A; c=A'*bb;
z=inv(C)*c
% Residuals
r=bb-A*z; rn=sqrt(r'*r)/n
hold on; p=plot(x,f(x,z(1),z(2)),'b'); set(p,'LineWidth',2)
% Linear model
A(:,1)=x';
C=A'*A; c=A'*bb;
z=inv(C)*c
% Residuals
r=bb-A*z; rn=sqrt(r'*r)/n
hold on; p=plot(x,z(1)*x+z(2),'g'); set(p,'LineWidth',2)
p=legend('Data','Non-linear','Linear'); set(p,'FontSize',14);
```



Optimization Problems
Non-linear Models



Non-linear models

$$y = c(x)$$

Minimimize Overall Error

$$E(c) = \sum_i (y_i - c(x_i))^2$$

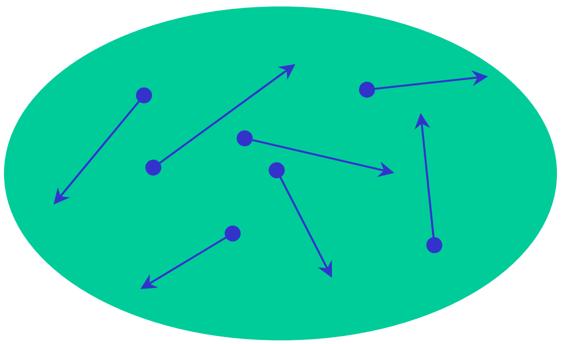
Measured values (y_i) — Model Parameters (c)

Non-linear models often have multiple, local minima. A locally linear, least square approximation may therefore find a local minimum instead of the global minimum.

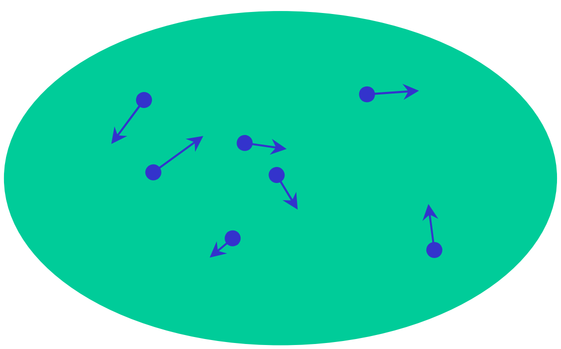
Optimization Algorithms
Simulated Annealing

Analogy: Freezing of a Liquid

High temperature T



Low temperature T



Crystal: Minimum energy of system.
Slow cooling -> crystal..
Fast cooling -> glass.

Boltzman Probability Distribution

Energy probabilistically distributed among all states.
Higher energy states possible even at low temperature!

$$p(E) \sim exp(-E/kT)$$

Optimization Problem: Minimize residual 'energy'

$$E(x) = \bar{\mathbf{r}}^T(x)\bar{\mathbf{r}}(x) = ||\bar{\mathbf{r}}(x)||_2$$

Simulated thermodynamic system changes its energy from E_1 to E_2 with probability

$$p = exp(-(E_2 - E_1)/kT)$$

Lower energy always accepted

$$E_2 < E_1 : \qquad p > 1 \Rightarrow p = 1$$

Higher energy accepted with probability p

$$E_2 > E_1 : \qquad p = exp(-(E_2 - E_1)/kT)$$

Elements of Metropolis algorithm

1. Description of possible system configurations
2. Random number generator for changing parameters
3. Cost function – 'energy' E
4. Control parameter – 'temperature' T.

Simulated Annealing
Example: Traveling Salesman Problem

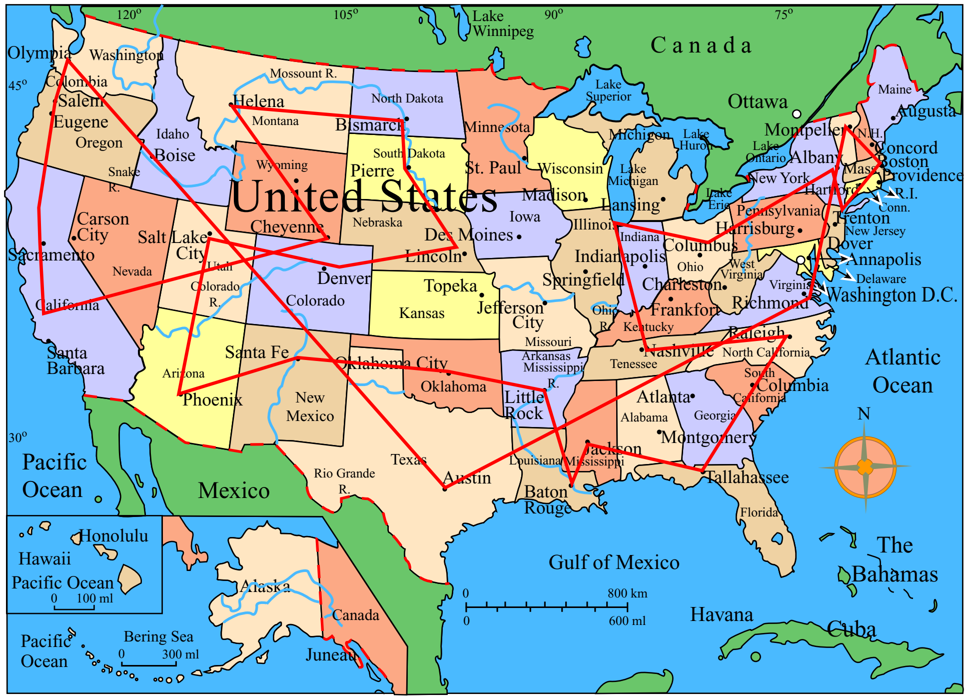


Figure by MIT OCW.

Objective:
Visit N cities across the US in arbitrary order, in the shortest time possible.

Metropolis Algorithm

1. Configuration: Cities I = 1,2, …N. Order can vary
2. Rearrangements: Change the order of any two cities.
3. Cost function: Distance traveled, number of Mississippi crossings.
4. Annealing schedule. Experimentation with ‘cooling’ schedule. T held constant for e.g. 100 reorderings (heat-bath method).

Cost function: Distance Traveled

$$E = \sum_{i=1}^{N} \sqrt{(x_i - x_{i+1})^2 + (y_i - y_{i+1})^2}$$

Penalty for crossing Mississippi

$$E = \sum_{i=1}^{N} \sqrt{(x_i - x_{i+1})^2 + (y_i - y_{i+1})^2 + \lambda(\mu_i - \mu_{i+1})^2}$$

East: μ_i = 1

West: μ_i = -1