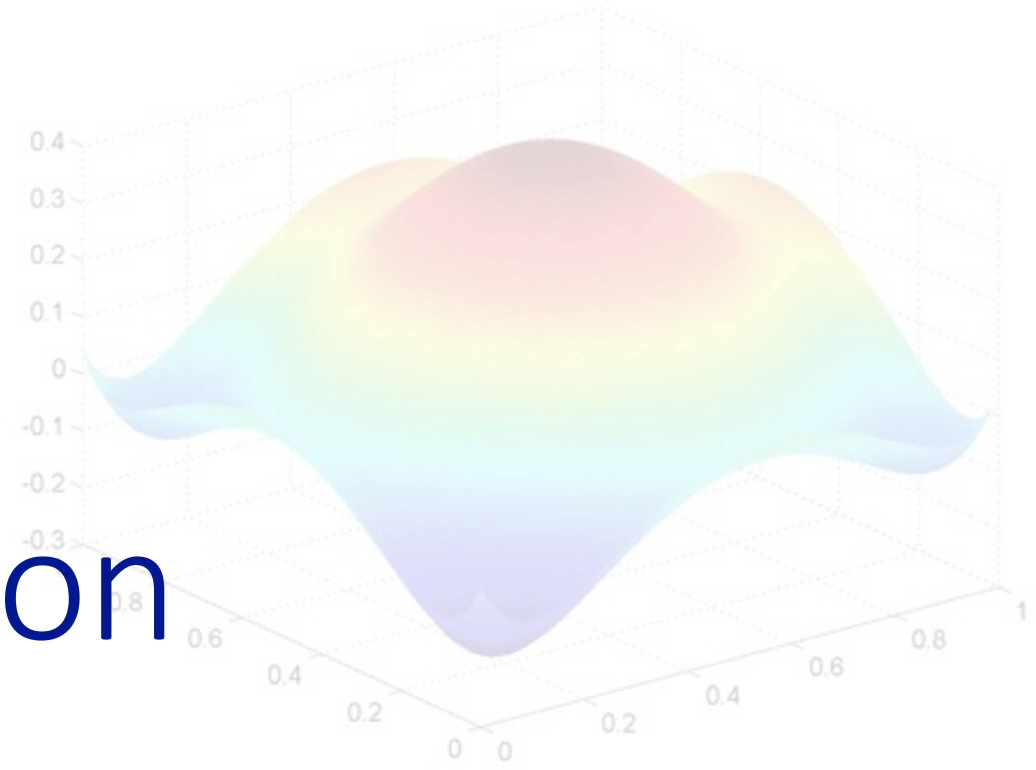


Parameter estimation

Lecture 6

Principles of Modeling for Cyber-Physical Systems

Instructor: Madhur Behl

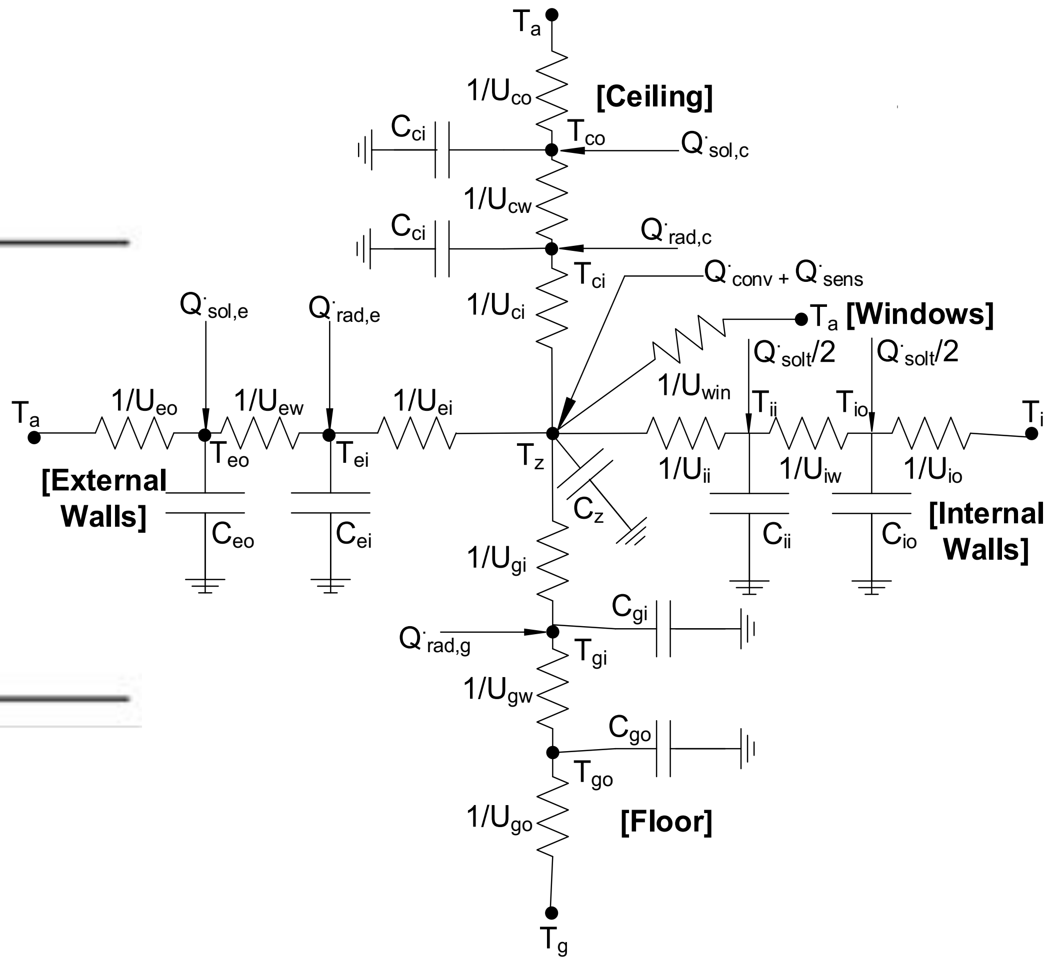
But first..

- **Worksheet 3 is out:**
  - Towards Matlab implementation of the model.
  - Nominal values of parameters from EnergyPlus IDF file.
  - Specify model structure in Matlab.
  - Collect training data.
  - Use the templates provided to save time.
  - Due in 1.5 week. Thursday, Oct 4, by 2:00pm

Previously..

How to find the values of the parameters ?

$U_{\star o}$	convection coefficient between the wall and outside air
$U_{\star w}$	conduction coefficient of the wall
$U_{\star i}$	convection coefficient between the wall and zone air
U_{win}	conduction coefficient of the window
$C_{\star\star}$	thermal capacitance of the wall
C_z	thermal capacity of zone z_i
	g: floor; e: external wall; c: ceiling; i: internal wall

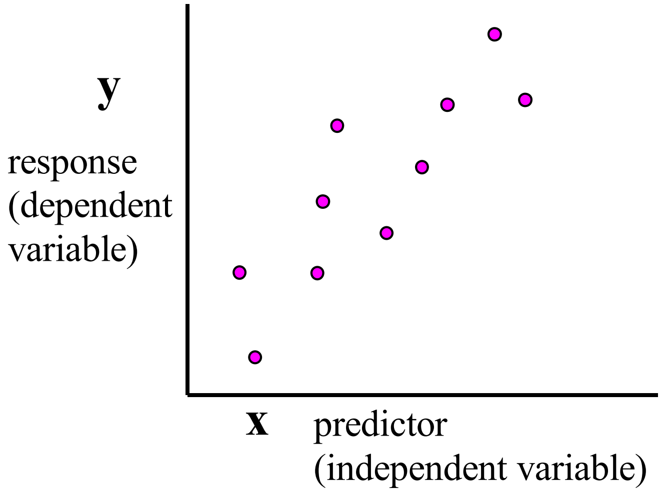


Parameter estimation overview

- Simple Linear Regression
- Least squares
- Non-linear least squares
- State-space sum of squared errors
- Non-linear optimization (estimation) methods
- Global and local search
- MATLAB implementations

Simple Linear Regression

Suppose we collect some data and want to determine the relation between the observed values, y, and the independent variable, x:



We can model the data using a **linear model**

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

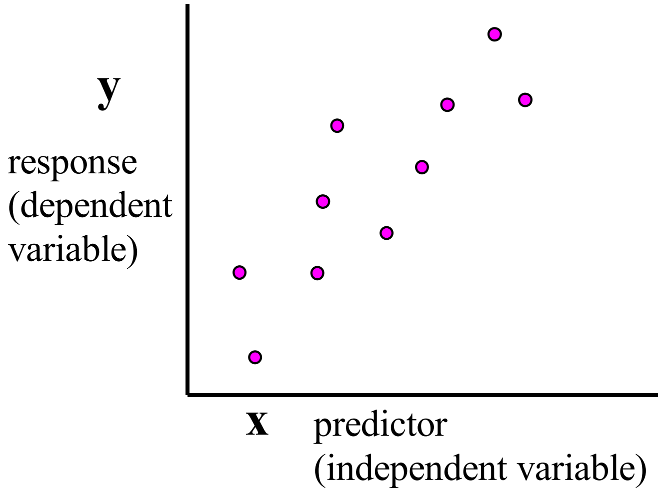
observed response — unknown intercept — unknown slope — unknown random error

Madhur Behl madhur.behl@virginia.edu

Simple Linear Regression

$$y_i = \beta_0 + \beta_1 x_i + \in_i$$

observed response	unknown intercept	unknown slope	unknown random error



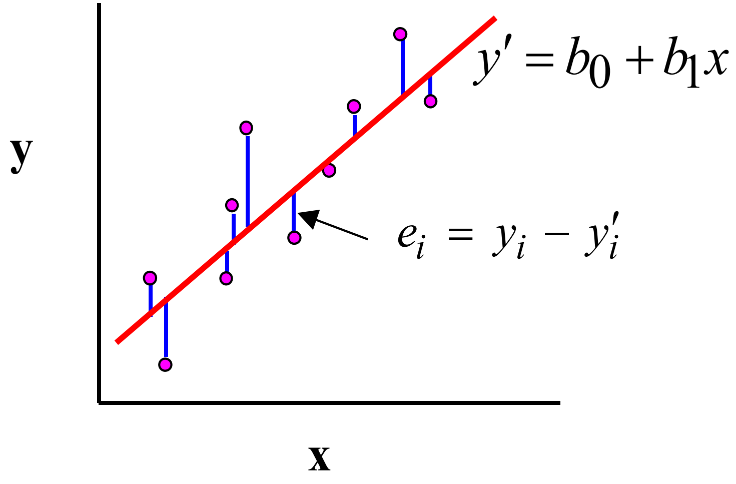
β_0 and β_1 are the **parameters** of this linear model.

- Don't know the true values of the parameters.
- Estimate them using the assumed model and the observations (data)

Simple Linear Regression

$$y_i = \overbrace{b_0 + b_1 x_i} + e_i$$

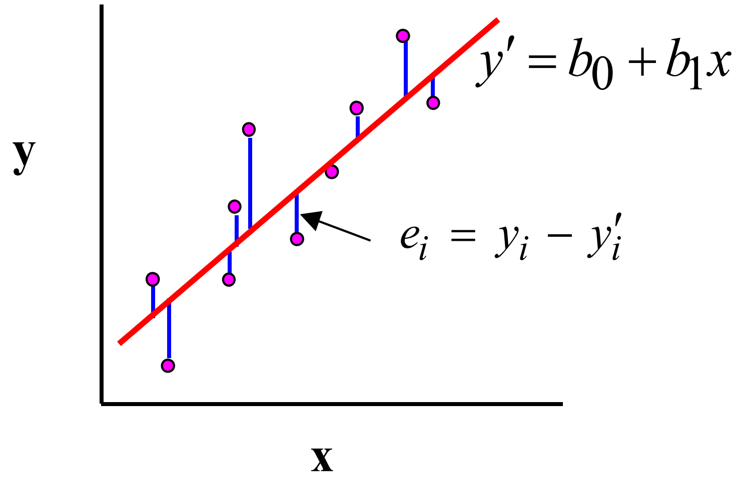
observed response — estimate of β_0 — estimate of β_1 — residual



- Estimate b_0 and b_1 to obtain the best fit of the simulated values to the observations.
- One method: **Minimize sum of squared errors, or residuals**.

Simple Linear Regression

$$\underbrace{y_i}_{\text{observed response}} = \overbrace{\underbrace{b_0}_{\text{estimate of } \beta_0} + \underbrace{b_1}_{\text{estimate of } \beta_1} x_i}^{\text{simulated values, } y_i'} + \underbrace{e_i}_{\text{residual}}$$



Sum of squared residuals: $$S(b_0, b_1) = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - y_i')^2 = \sum_{i=1}^{n} (y_i - b_0 - b_1 x)^2$$

To minimize: Set $$\frac{\partial S}{\partial b_0} = 0 \quad \text{and} \quad \frac{\partial S}{\partial b_1} = 0$$

Madhur Behl madhur.behl@virginia.edu

Simple Linear Regression

$$S(b_0,b_1) = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - y_i')^2 = \sum_{i=1}^{n} (y_i - b_0 - b_1 x)^2$$

Set $\dfrac{\partial S}{\partial b_0} = 0$ and $\dfrac{\partial S}{\partial b_1} = 0$

This results in the **normal equations**:

$$b_0 n + b_1 \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$$

$$b_0 \sum_{i=1}^{n} x_i + b_1 \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i$$

- Solve these equations to obtain expressions for b_0 and b_1, the parameter estimates that give the best fit of the simulated and observed values.

Linear Regression in Matrix Form

Linear regression model: $y_i = b_0 + b_1 x_i + e_i$, i=1.n ➔ $\underline{y} = \underline{X}\,\underline{b} + \underline{e}$

$$\underline{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \quad \underline{X} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \quad \underline{b} = \begin{bmatrix} b_0 \\ b_1 \end{bmatrix} \quad \underline{e} = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix}$$

vector of observed values

matrix of Predictors/ features

vector of parameters

vector of residuals

Linear Regression in Matrix Form

Linear regression model: $y_i = b_0 + b_1 x_i + e_i$, i=1.n ➔ $\underline{y} = \underline{X}\,\underline{b} + \underline{e}$

- The **normal equations** ($\underline{b}'$ is the vector of least-squares estimates of $\underline{b}$):

Using summations
And setting the derivative to 0

$$\boxed{\begin{aligned} b_0 n + b_1 \sum_{i=1}^{n} x_i &= \sum_{i=1}^{n} y_i \\ b_0 \sum_{i=1}^{n} x_i + b_1 \sum_{i=1}^{n} x_i^2 &= \sum_{i=1}^{n} x_i y_i \end{aligned}}$$

Using matrix notation:

$$\boxed{\underline{X}^T \underline{X}\,\underline{b}' = \underline{X}^T \underline{y} \quad ➔ \quad \underline{b}' = (\underline{X}^T \underline{X})^{-1} \underline{X}^T \underline{y}}$$

Ordinary least squares

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ \vdots \\ Y_n \end{bmatrix}_{n\times 1} = \begin{bmatrix} 1 & X_{11} & X_{21} & \dots & X_{k1} \\ 1 & X_{12} & X_{22} & \dots & X_{k2} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & X_{1n} & X_{2n} & \dots & X_{kn} \end{bmatrix}_{n\times k} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \vdots \\ \beta_n \end{bmatrix}_{k\times 1} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \vdots \\ \epsilon_n \end{bmatrix}_{n\times 1}$$

This can be rewritten more simply as:

$$y = X\beta + \epsilon$$

Ordinary least squares

$$e = y - X\hat{\beta}$$

The sum of squared residuals (RSS) is $e'e$.

$$\begin{bmatrix} e_1 & e_2 & \dots & \dots & e_n \end{bmatrix}_{1\times n} \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ \vdots \\ e_n \end{bmatrix}_{n\times 1} = \begin{bmatrix} e_1 \times e_1 + e_2 \times e_2 + \ldots + e_n \times e_n \end{bmatrix}_{1\times 1}$$

Ordinary least squares

The sum of squared residuals (RSS) is $e'e$.

$$\begin{aligned} e'e &= (y - X\hat{\beta})'(y - X\hat{\beta}) \\ &= y'y - \hat{\beta}'X'y - y'X\hat{\beta} + \hat{\beta}'X'X\hat{\beta} \\ &= y'y - 2\hat{\beta}'X'y + \hat{\beta}'X'X\hat{\beta} \end{aligned}$$

Ordinary least squares

$$e'e = y'y - 2\hat{\beta}'X'y + \hat{\beta}'X'X\hat{\beta}$$

$$\frac{\partial e'e}{\partial \hat{\beta}} = -2X'y + 2X'X\hat{\beta} = 0$$

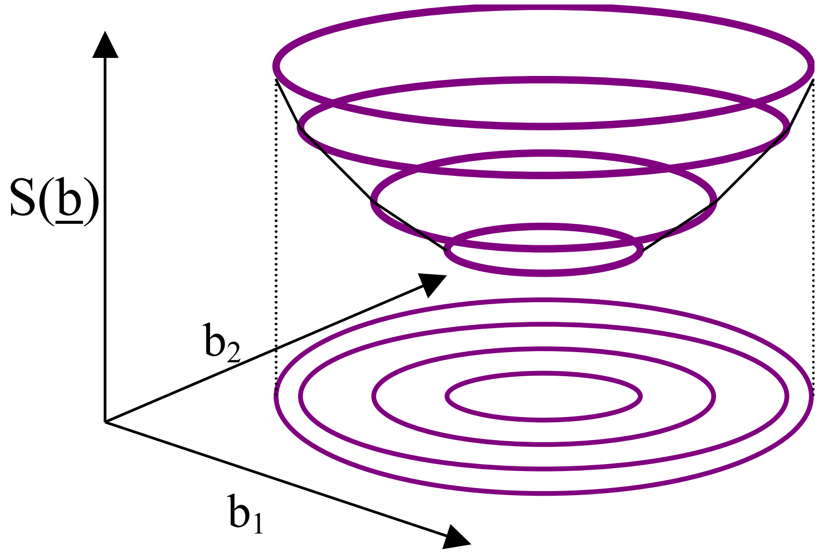
$$(X'X)\hat{\beta} = X'y \qquad \hat{\beta} = (X'X)^{-1}X'y$$

Linear versus Nonlinear Models

Linear models: Sensitivities of the output are **not** a function of the model parameters:

$$y_i' = b_0 + b_1 x_i$$

$$\frac{\partial y_i'}{\partial b_0} = 1 \text{ and } \frac{\partial y_i'}{\partial b_1} = x_i \text{ ; recall } \underline{X} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$$

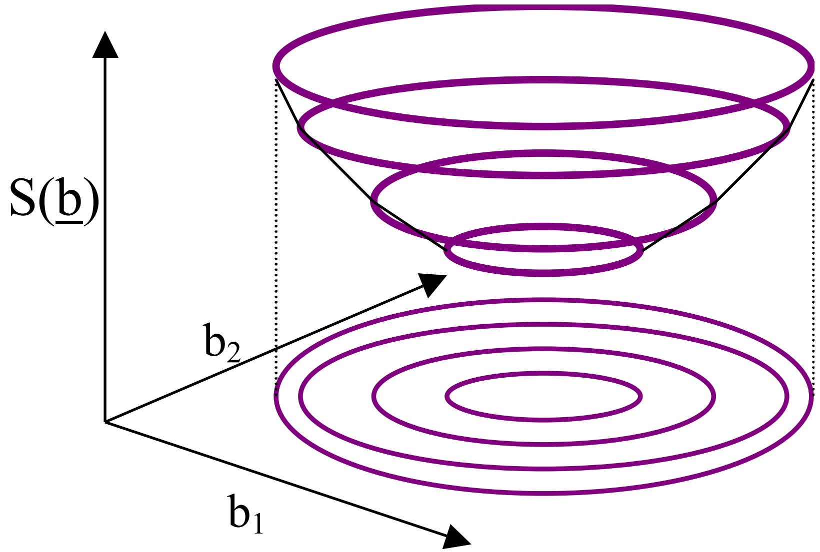


Linear versus Nonlinear parameters

- Linear models have elliptical objective function surfaces.
- i.e. the level sets of the objective function (sum of errors squared) are ellipsis.

One step to get to the minimum.

Nonlinear parametric models: Sensitivities **are** a function of the model parameters.



With two parameter

Nonlinearity is in parameter space.

$$x(k+1) = A_\theta(k)x(k) + B_\theta(k)u(k)$$

$$y(k) = C_\theta(k)x(k) + D_\theta(k)u(k)$$

Elements of A, B, C, and D could be non-linear in the parameter θ

Nonlinear Estimation

Suppose that we have collected data on the output/response Y (n samples),

- $(y_1, y_2, \ldots y_n)$

corresponding to n sets of values of the independent variables/predictors/features $X_1, X_2, \ldots$ and X_p

- $(x_{11}, x_{21}, \ldots, x_{p1})$,
- $(x_{12}, x_{22}, \ldots, x_{p2})$,
- … and
- $(x_{1n}, x_{2n}, \ldots, x_{pn})$.

Nonlinear Estimation

For possible values $\theta_1, \theta_2, \ldots, \theta_q$ of the parameters, the residual sum of squares function

$$S(\theta_1, \theta_2, \ldots, \theta_q) = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} \left[y_i - f(x_{1i}, x_{2i}, \ldots, x_{pi} | \theta_1, \theta_2, \ldots, \theta_q) \right]^2$$

$$\hat{y}_i = f(x_{1i}, x_{2i}, \ldots, x_{pi} | \theta_1, \theta_2, \ldots, \theta_q)$$

Nonlinear Estimation

$$S(\theta_1, \theta_2, \ \ldots, \theta_q) = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} \left[y_i - f(x_{1i}, x_{2i}, \ \ldots, x_{pi} | \theta_1, \theta_2, \ \ldots, \theta_q) \right]^2$$

The least squares estimates of θ_1, θ_2, ... , θ_q, are values which minimize S(θ_1, θ_2, ... , θ_q).

Nonlinear Estimation

$$S(\theta_1, \theta_2, \ \ldots, \theta_q) = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} \left[y_i - f\left(x_{1i}, x_{2i}, \ \ldots, x_{pi} \middle| \theta_1, \theta_2, \ \ldots, \theta_q \right) \right]^2$$

To find the least squares estimate we need to determine when all the derivatives S(θ_1, θ_2, ... , θ_q) with respect to each parameter θ_1, θ_2, ... and θ_q are equal to zero.

This will involve, terms with partial derivatives of the non-linear function f.

$$\frac{\delta f(\ldots)}{\delta \theta_1}, \frac{\delta f(\ldots)}{\delta \theta_2}, \ldots, \frac{\delta f(\ldots)}{\delta \theta_q}$$

Nonlinear Estimation

$$\frac{\delta f(\dots)}{\delta \theta_1}, \frac{\delta f(\dots)}{\delta \theta_2}, \dots, \frac{\delta f(\dots)}{\delta \theta_q}$$

Closed form analytical solutions are not possible.

It is usually necessary to develop an iterative technique for solving them

Recall..

$$x(k+1) = A_\theta(k)x(k) + B_\theta(k)u(k)$$

$$y(k) = C_\theta(k)x(k) + D_\theta(k)u(k)$$

$$\Downarrow$$

$$\hat{y}(k) = f(\hat{x}(k), u(k), \hat{\theta}_1, \dots, \hat{\theta}_q)$$

Madhur Behl madhur.behl@virginia.edu

How can we compute the sum of squared error for state-space models ?

$$x(k+1) = A_\theta x(k) + B_\theta u(k)$$

$$y(k) = C_\theta\ (k) + D_\theta u(k)$$

Consider the LTI model

sum of squared error for state-space models

Given $x(0) = x_0, and\ u(k), k = 1, \ldots N$

$$y(0) = C_\theta x(0) + D_\theta u(0)$$

$$x(1) = A_\theta x(0) + B_\theta u(1)$$

$$y(1) = C_\theta x(1) + +D_\theta u(1)$$

$$y(1) = C_\theta A_\theta x(0) + C_\theta B_\theta u(1) + D_\theta u(1)$$

$$x(2) = A_\theta x(1) + B_\theta u(2)$$

$$x(2) = A_\theta A_\theta x(0) + A_\theta B_\theta u(1) + B_\theta u(2)$$

$$y(2) = C_\theta x(2) + D_\theta u(2)$$

$$y(2) = C_\theta A_\theta A_\theta x(0) + C_\theta A_\theta B_\theta u(1) + C_\theta B_\theta u(2) + D_\theta u(2)$$

sum of squared error for state-space models

$$\begin{pmatrix} y(0) \\ y(1) \\ \vdots \\ y(N-1) \end{pmatrix} = \boldsymbol{\mathcal{O}}\, x(0) + \boldsymbol{\mathcal{T}} \begin{pmatrix} u(0) \\ u(1) \\ \vdots \\ u(N-1) \end{pmatrix}$$

For a given estimate of θ , this is the $\hat{y}$ vector

$$S(\theta_1, \theta_2, \ldots, \theta_q) = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

sum of squared error for state-space models

$$\mathcal{O} = \begin{pmatrix} C_\theta \\ C_\theta A_\theta \\ \vdots \\ C_\theta A_\theta^{N-1} \end{pmatrix} \qquad \mathcal{T} = \begin{pmatrix} D_\theta & 0 & \dots & \\ C_\theta B_\theta & D_\theta & 0 & \dots \\ \vdots & \vdots & \vdots & \\ C_\theta A_\theta^{N-2} B_\theta & C_\theta A_\theta^{N-3} B_\theta & \dots C_\theta B_\theta & D_\theta \end{pmatrix}$$

Nonlinear Estimation

Let $\mathcal{Z}^N$ be the given data-set $\{\boldsymbol{u}_k, \boldsymbol{x}_{\mathbf{0}}, k = 1, \dots, N\}$

$$\widehat{\boldsymbol{\theta}}_N = \widehat{\boldsymbol{\theta}}_N(\mathcal{Z}^N) = \arg\min_{\boldsymbol{\theta} \in \Theta} S_N(\boldsymbol{\theta}, \mathcal{Z}^N)$$

$S_N(\boldsymbol{\theta}, \mathcal{Z}^N)$ is the squared error i.e. $S_N(\boldsymbol{\theta}, \mathcal{Z}^N) = \sum_{k=1}^{N} \boldsymbol{e}_k(\boldsymbol{\theta})\, \boldsymbol{e}_k^T(\boldsymbol{\theta})$

$$\boldsymbol{e}_k(\boldsymbol{\theta}) = \underbrace{\boldsymbol{y}_k}_{\text{Measured}} - \underbrace{\widehat{\boldsymbol{y}}_k(\boldsymbol{\theta})}_{\text{Predicted (for a particular value of } \boldsymbol{\theta}\text{)}}$$

Non-linear least squares

We will cover the following methods:

1) Steepest descent (or Gradient descent) and Newton's method,
2) Gauss Newton and Linearization, and
3) Levenberg-Marquardt's procedure.

1. In each case a iterative procedure is used to find the least squares estimators : $\hat{\theta}_1, \hat{\theta}_2, \ldots, \hat{\theta}_q$
2. That is an initial estimates, $\theta_1^0, \theta_2^0, \ldots, \theta_q^0$,for these values are determined.
3. Iteratively find better estimates, $\theta_1^i, \theta_2^i, \ldots, \theta_q^i$ that hopefully converge to the least squares estimates,

Steepest Descent

- The steepest descent method focuses on determining the values of $\theta_1, \theta_2, \ldots, \theta_q$ that minimize the sum of squares function, $S(\theta_1, \theta_2, \ldots, \theta_q)$.
- The basic idea is to determine from an initial point, $\theta_1^0, \theta_2^0, \ldots, \theta_q^0$

and the tangent plane to $S(\theta_1, \theta_2, \ldots, \theta_q)$ at this point, the vector along which the function $S(\theta_1, \theta_2, \ldots, \theta_q)$ will be decreasing at the fastest rate.

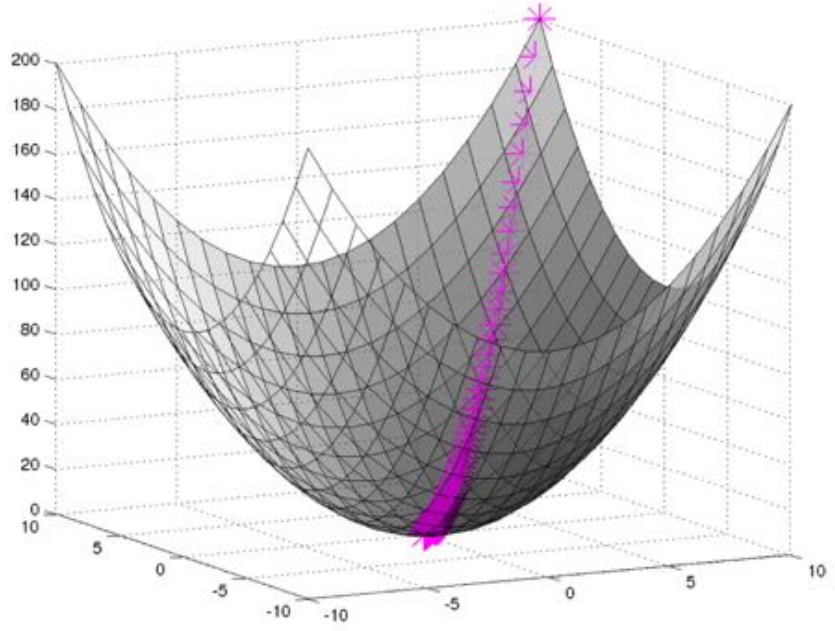
- The method of steepest descent than moves from this initial point along the direction of steepest descent until the value of $S(\theta_1, \theta_2, \ldots, \theta_q)$ stops decreasing.

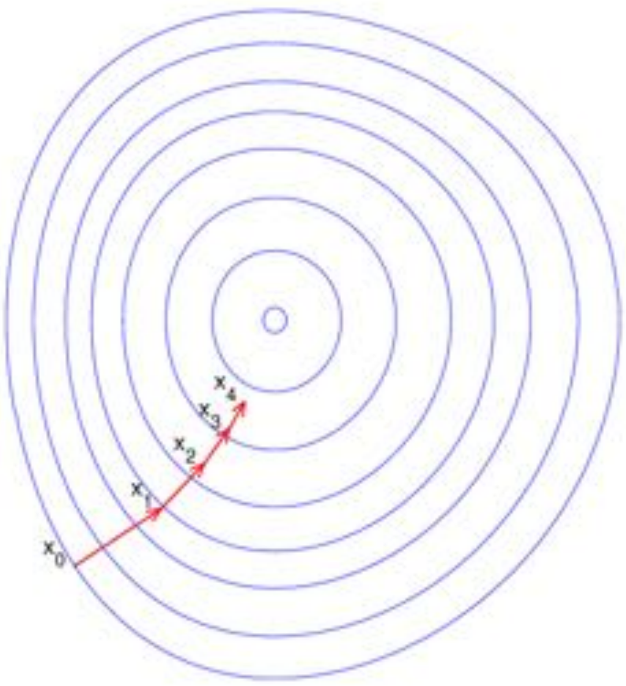
Steepest Descent

- It uses this point, $\theta_1^1, \theta_2^1, \ldots, \theta_q^1$ as the next approximation to the value that minimizes S(θ_1, θ_2, ... , θ_q).
- The procedure than continues until the successive approximation arrive at a point where the sum of squares function, S(θ_1, θ_2, ... , θ_q) is minimized.
- At that point, the tangent plane to S(θ_1, θ_2, ... , θ_q) will be horizontal and there will be no direction of steepest descent.

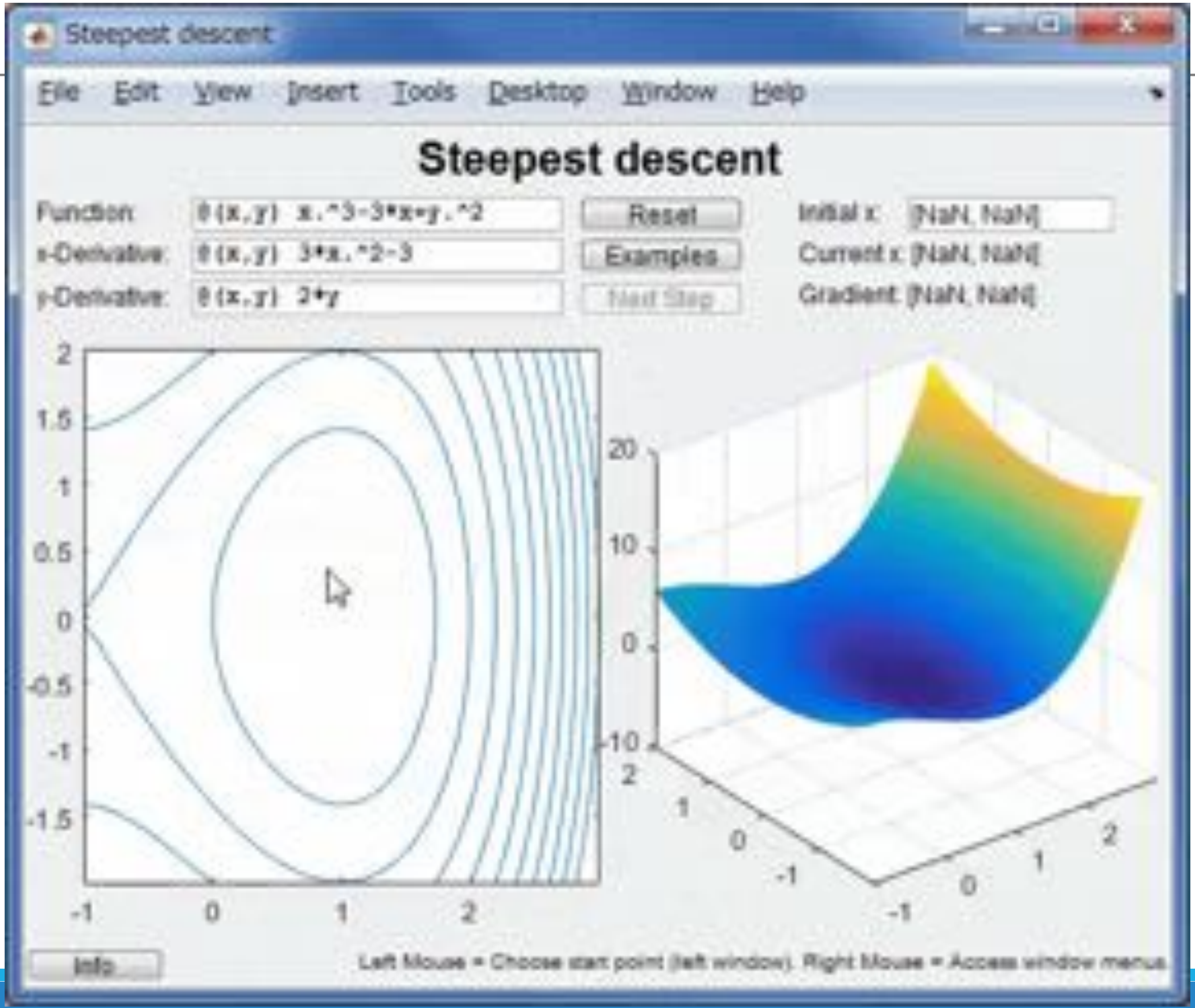
Steepest Descent

To find a local minimum of a function using steepest descent, one takes steps proportional to the *negative* of the gradient of the function at the current point.





Steepest Descent



Steepest Descent

Initialize k=0, choose θ_0

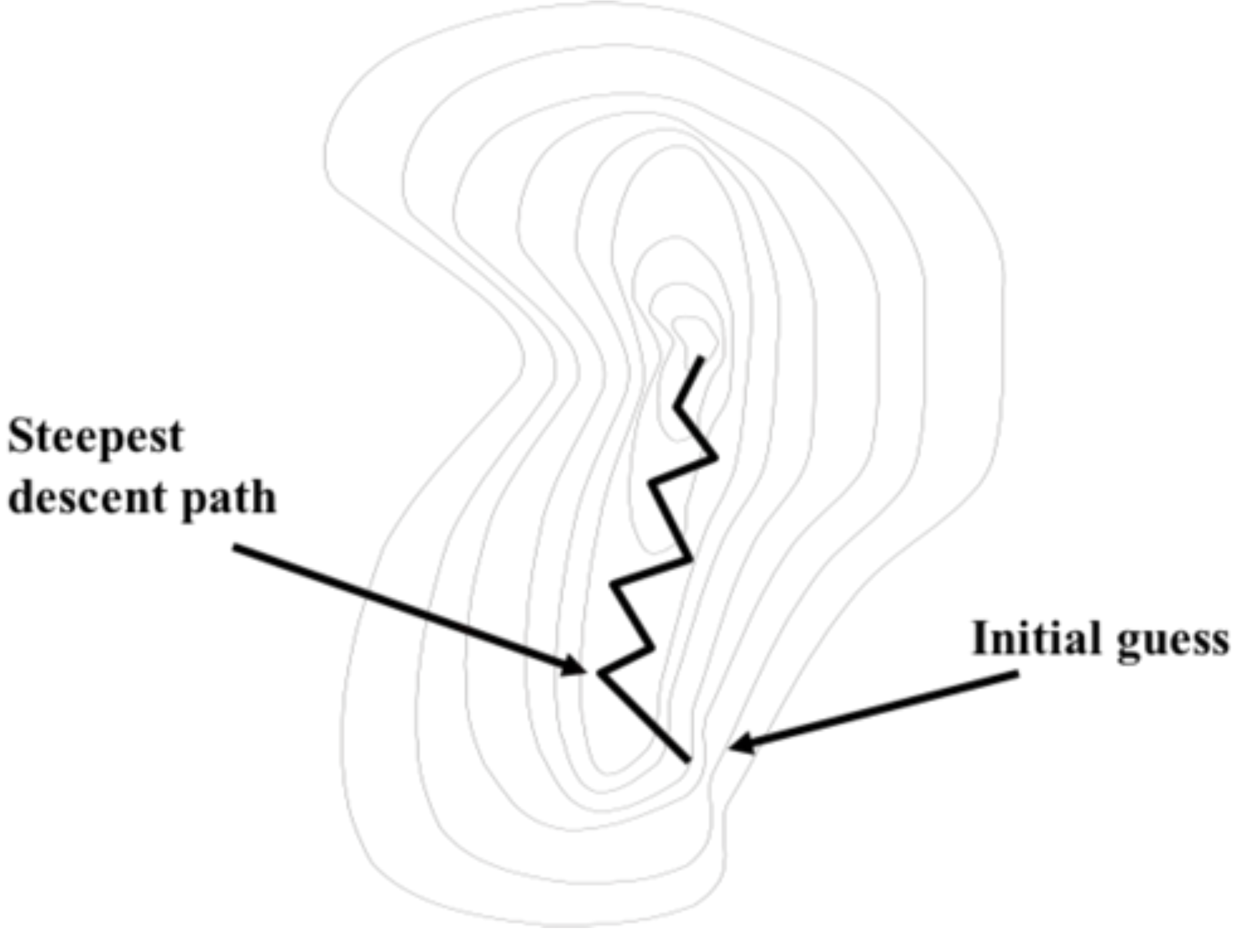
While $k<k_{max}$

$$\theta_k = \theta_{k-1} - \underbrace{\nabla F(\theta_{k-1})}_{\text{Gradient}}$$

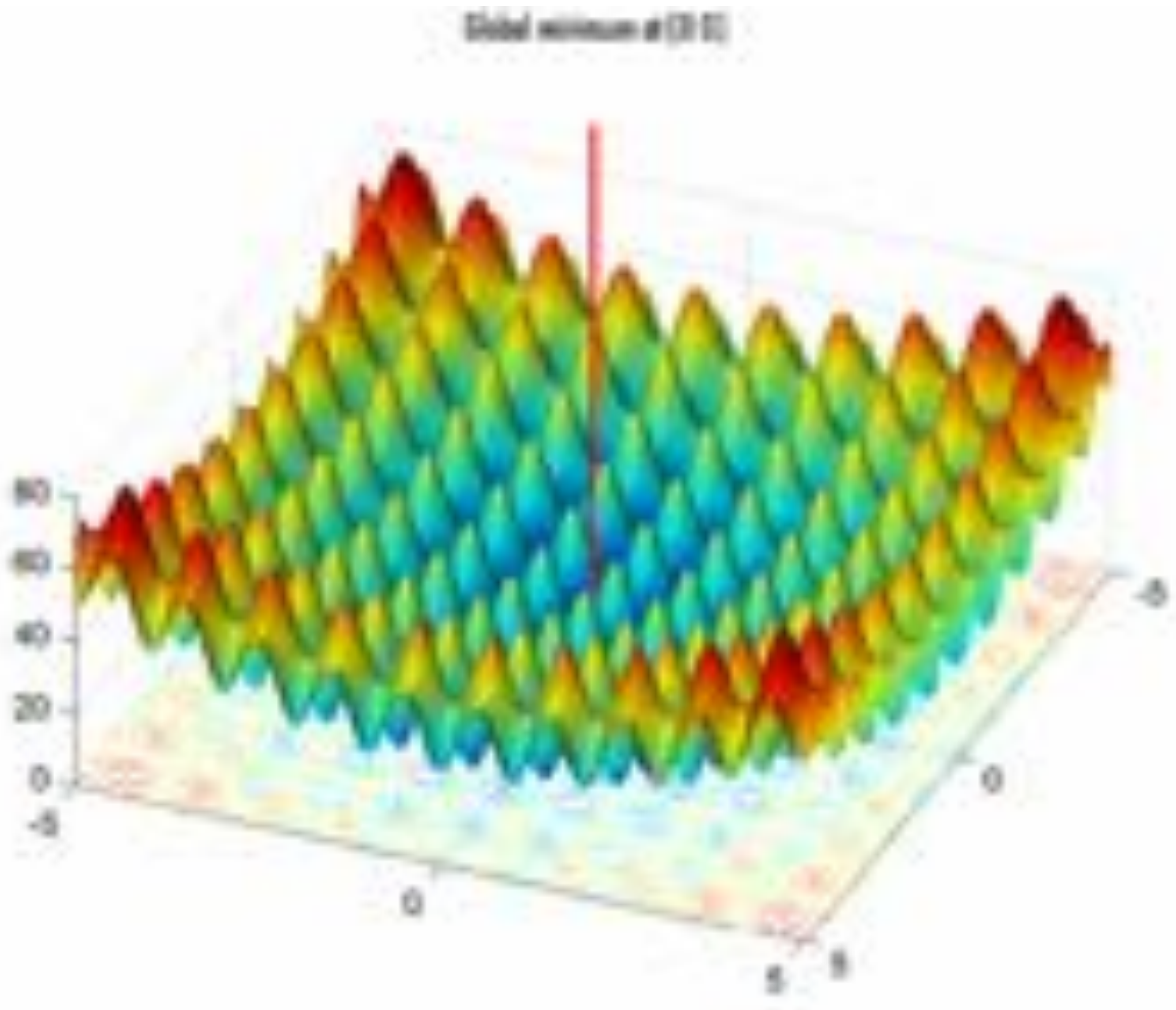
Steepest Descent

- While, theoretically, the steepest descent method will converge, it may do so in practice with agonizing slowness after some rapid initial progress.
- Slow convergence is particularly likely when the $S(\theta_1, \theta_2, \ldots, \theta_q)$ contours highly curved and it happens when the path of steepest descent zigzags slowly up a narrow ridge, each iteration bringing only a slight reduction in $S(\theta_1, \theta_2, \ldots, \theta_q)$.
- A further disadvantage of the steepest descent method is that it is not scale invariant.
- The steepest descent method is, on the whole, slightly less favored than the linearization method (described later) but will work satisfactorily for many nonlinear problems

Steepest Descent



Steepest Descent



Gradient descent is a *local* optimization method

Least squares in general

Most optimization problem can be formulated as a nonlinear least squares problem

$$x^* = \arg\min_x \frac{1}{2} \sum_{i=1}^{m} (f_i(x))^2$$

$$x^* = \arg\min_x \frac{1}{2} f(x)^T f(x)$$

Where $f_i : \; R^n \mapsto R$, i=1,…,m are given functions, and m>=n

Newton's Method

Quadratic approximation

$$f(x+\Delta x) \approx f(x) + f'(x)\Delta x + \frac{1}{2} f''(x)\Delta x^2$$

What's the minimum solution of the quadratic approximation

$$\Delta x = -\frac{f'(x)}{f''(x)}$$

Newton's Method

High dimensional case:

$$F(x+\Delta x) \approx F(x) + \nabla F(x)\Delta x + \frac{1}{2}\Delta x^T H(x)\Delta x$$

What's the optimal direction?

$$\Delta x \approx -H(x)^{-1}\nabla F(x)$$

Newton's Method

Initialize k=0, choose x_0

While $k<k_{max}$

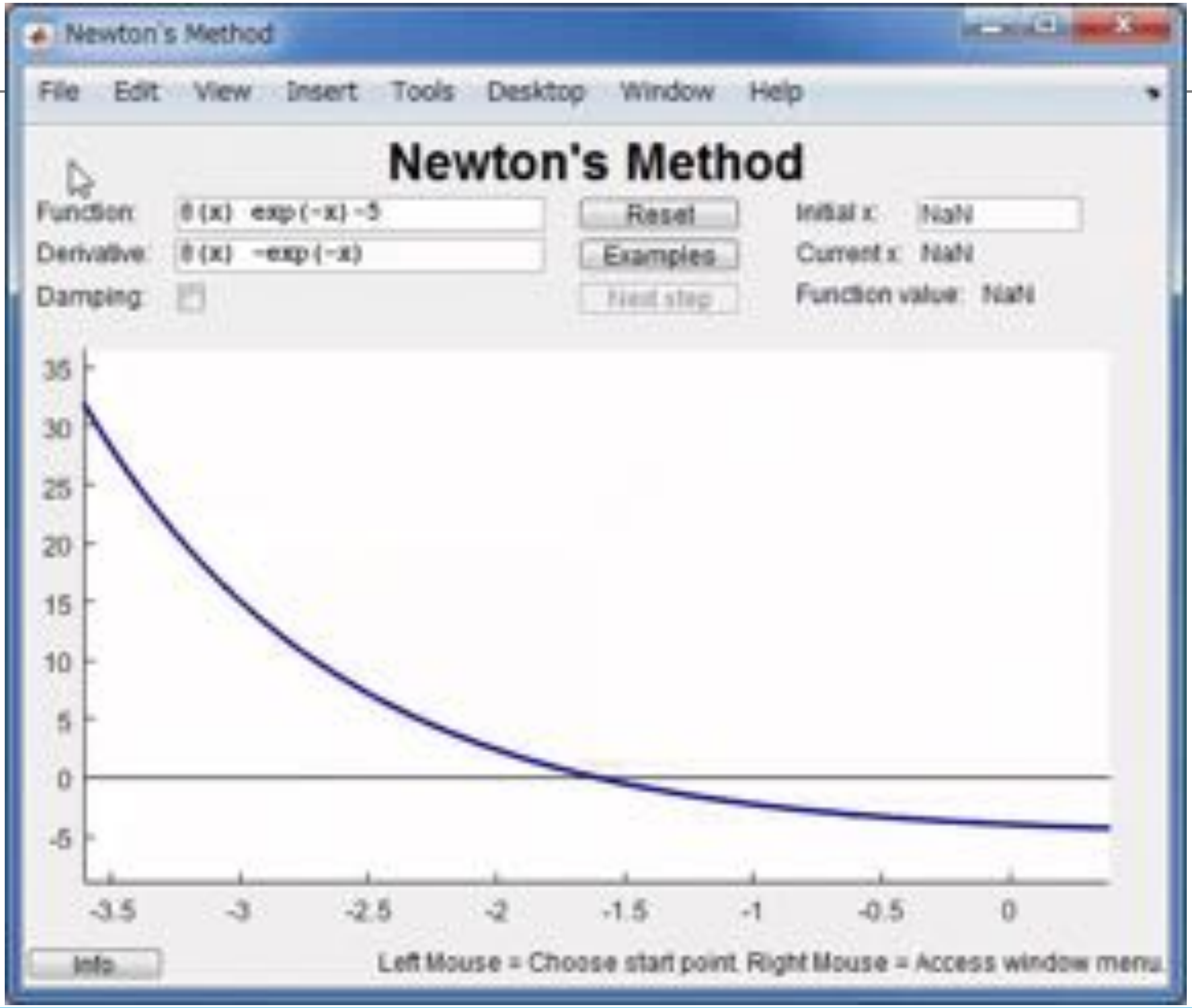
$$x_k = x_{k-1} - \lambda H(x)^{-1} \nabla F(x_{k-1})$$

Newton's Method

- Finding the inverse of the Hessian matrix is often expensive

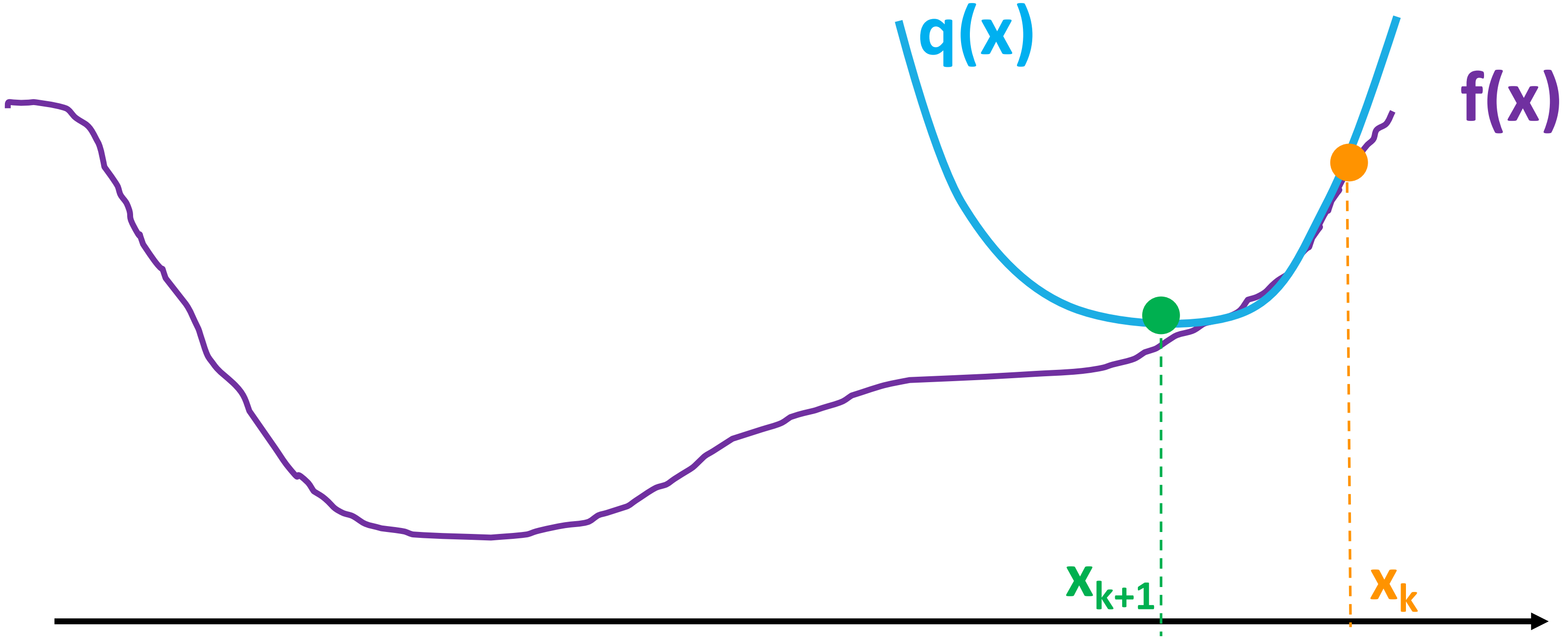
- Approximation methods are often used
  - conjugate gradient method
  - quasi-newton method

Newton’s Method



Newton's Method

$$\min_x f(x) \qquad x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)} \qquad x_{k+1} = x_k - H^{-1}.\nabla f$$



Terminology

The *gradient* ∇f of a multivariable function is a vector consisting of the function's partial derivatives:

$$\nabla f(x_1, x_2) = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2} \right)$$

The *Hessian matrix* $H(f)$ of a function $f(x)$ is the square matrix of second-order partial derivatives of $f(x)$:

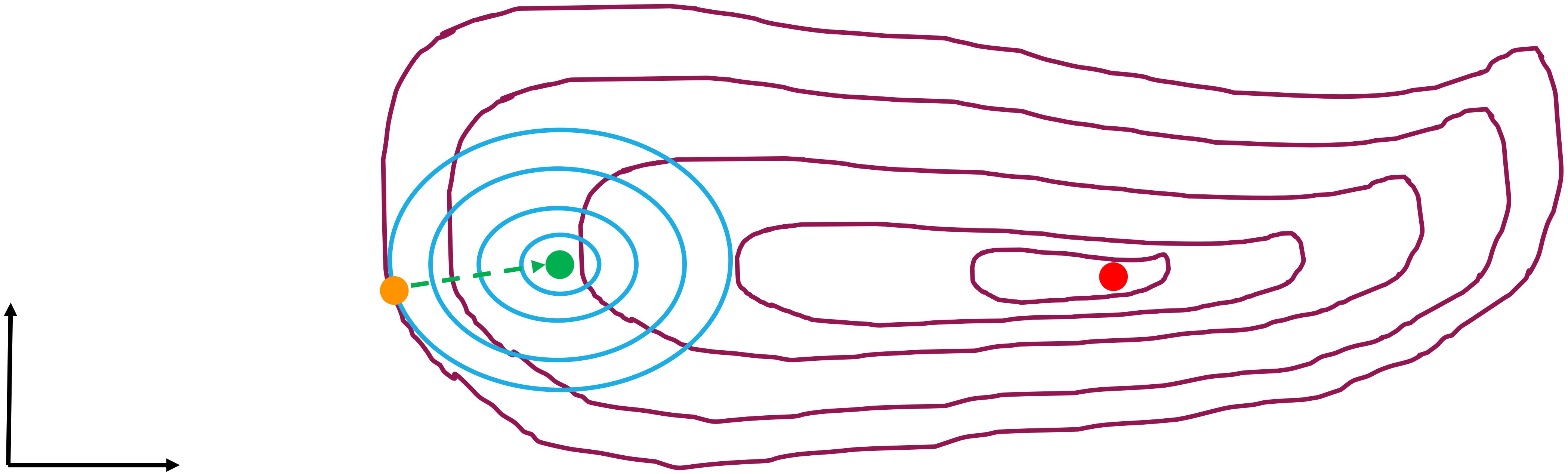
$$H(f(x_1, x_2)) = \begin{pmatrix} \frac{\partial f}{\partial x_1^2} & \frac{\partial f}{\partial x_1 \partial x_2} \\ \frac{\partial f}{\partial x_1 \partial x_2} & \frac{\partial f}{\partial x_2^2} \end{pmatrix}$$

Newton's Method

$$\min_x f(x)$$

$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}$$

$$x_{k+1} = x_k - H^{-1}.\nabla f$$



Newton's Method

$Let\ f(x)\colon \mathcal{R}^n \rightarrow \mathcal{R}$ *be sufficiently smooth*

Taylor's approximation: For close to point 'a' $f(x) \approx f(a) + g^T(x-a) + \frac{1}{2}\underbrace{(x-a)^T H(x-a)}_{x^T Hx - 2a^T Hx + a^T Ha} + h.o.t.$

$g = \nabla f(a) \qquad H = \nabla^2 f(a)$

$$q(x) = \frac{1}{2}x^T Hx + b^T x + c \qquad \textit{where} \qquad b = g - Ha$$

$$\nabla q = 0 \Rightarrow Hx + b = 0 \Rightarrow x = -H^{-1}b = -H^{-1}g + a = a - H^{-1}g$$

$$x = a - H^{-1}g \Longrightarrow x_{k+1} = x_k - H^{-1}.\nabla f$$

Newton's Method

$\nabla q = 0 \Rightarrow Hx + b$

For minima

$\nabla^2 q > 0$

$\nabla^2 q = H$

Minima if H is PSD

1) Initialize: x_0

2) Iterate: $x_{k+1} = x_k - H^{-1}.g$

$g = \nabla f(x_k) \quad H = \nabla^2 f(x_k)$

1) H may fail to be PSD
2) H may not be invertible.
3) Difficult to compute H in practice through numerical methods

Recall: Non-linear least squares

$$f(x) = \sum_{j=1}^{N} \left(r_j(x)\right)^2 = \|r(x)\|_2^2$$

The j-th component of the vector r(x) is the residual

$$r_j(x) = y_j - \widehat{y_j}$$

$$r(x) = (r_1(x), r_2(x), \dots, r_N(x))^T$$

Non-linear least squares

The *Jacobian* $J(x)$ is a matrix of all $\nabla r_j(x)$:

$$J(x) = \left[\frac{\partial r_j}{\partial x_i}\right]_{j=1,\dots,N;\, i=1,\dots,n} = \begin{bmatrix} \nabla r_1(x)^T \\ \nabla r_2(x)^T \\ \vdots \\ \nabla r_N(x)^T \end{bmatrix}$$

Non-linear least squares

$$\nabla f(x) = \sum_{j=1}^{N} r_j(x) \nabla r_j(x) = J(x)^T r(x)$$

$$\nabla^2 f(x) = \sum_{j=1}^{N} \nabla r_j(x) \nabla r_j(x)^T + \sum_{j=1}^{N} r_j(x) \nabla^2 r_j(x)$$

$$= J(x)^T J(x) + \sum_{j=1}^{N} r_j(x) \nabla^2 r_j(x)$$

Gauss-Newton Method

Use the approximation $\nabla^2 f_k \approx J_k^T J_k$

J_k must have full rank

Requires accurate initial guess

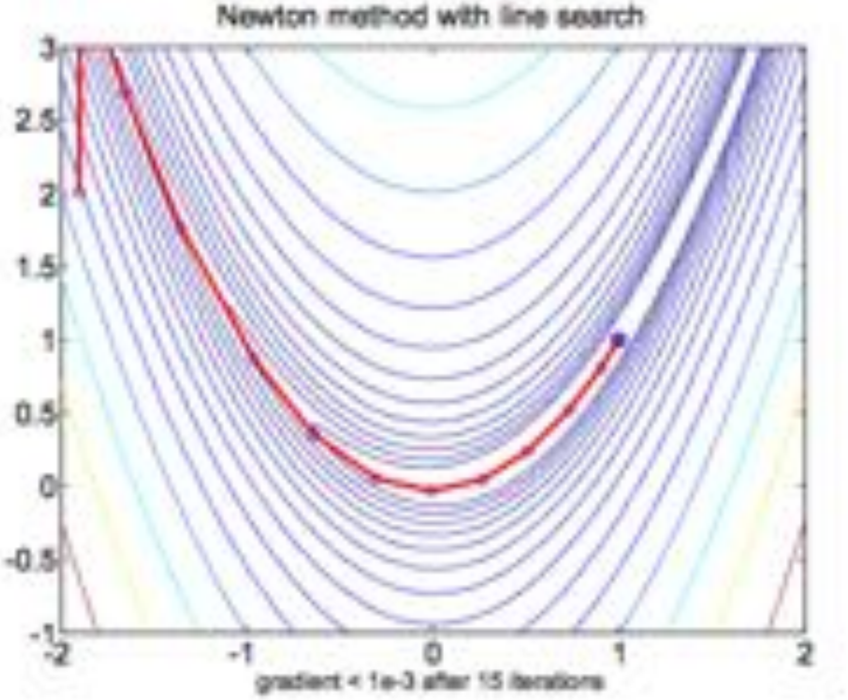
Fast convergence close to solution

$$J(x)^T J(x) + \sum_{j=1}^{N} r_j(x) \nabla^2 r_j(x)$$

Residuals are small when close to the optimal

Comparison

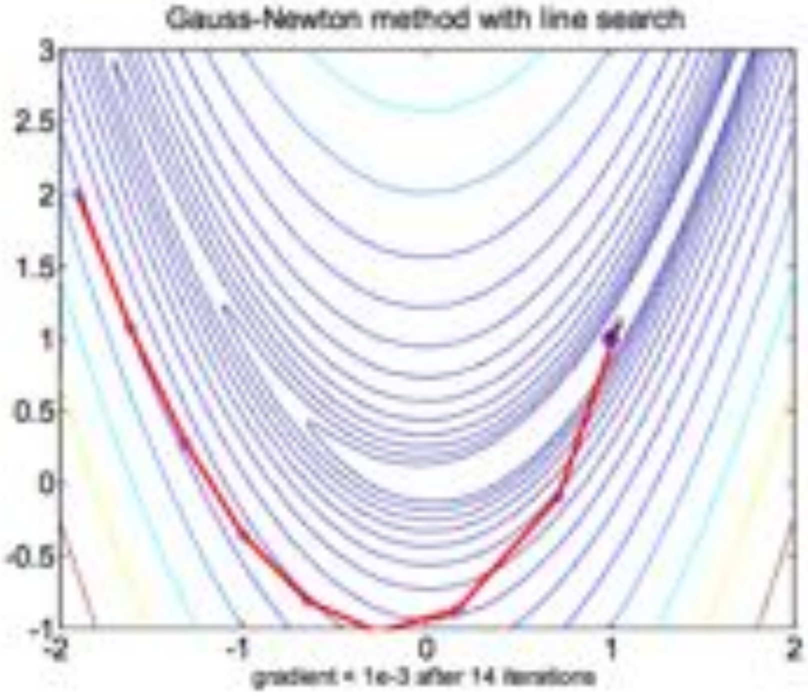
Newton



• requires computing Hessian (i.e. n^2 second derivatives)

• exact solution if quadratic

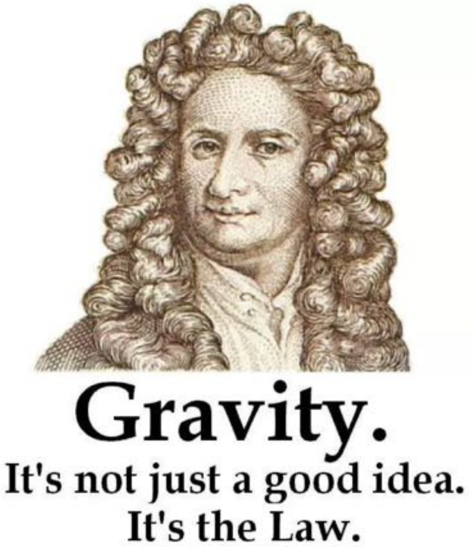
Gauss-Newton

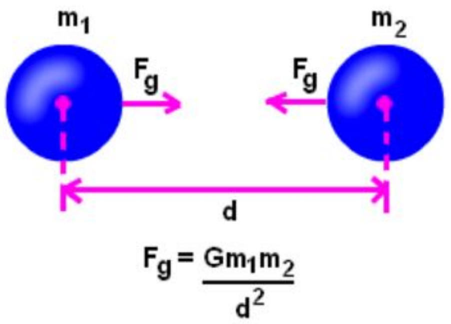


• approximates Hessian by Jacobian product

• requires only n first derivatives

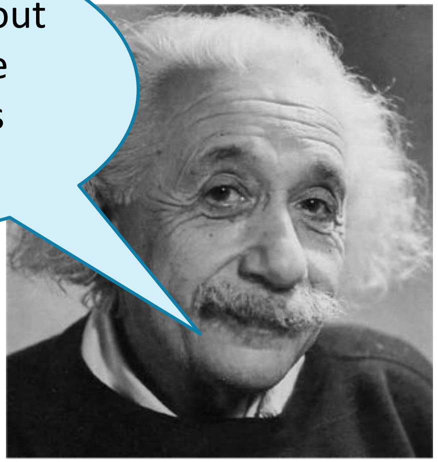
Lets talk about curvatures..

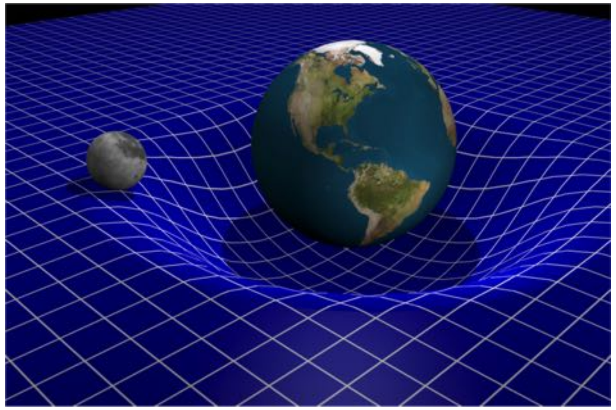




Newton does not have a good track record of accounting for curvatures

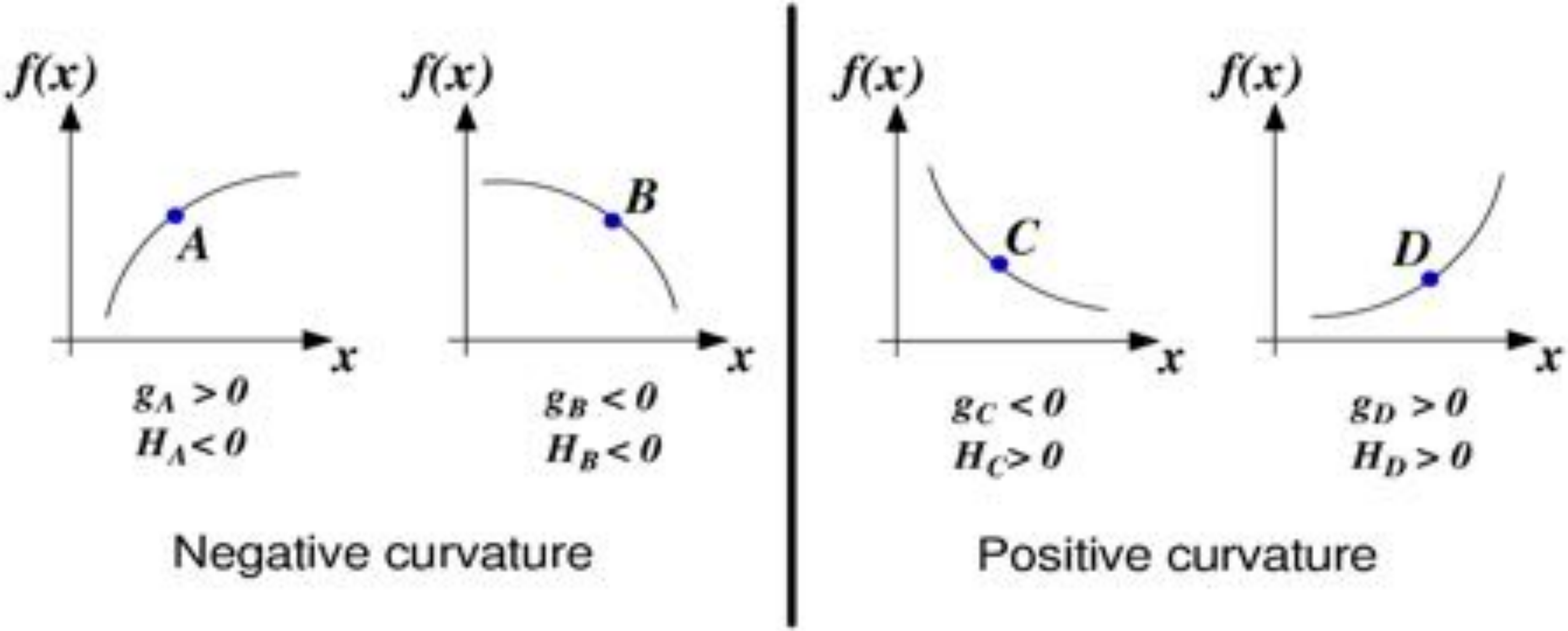
Nope, its about space-time curvatures dude.





Are you serious right now ! Lets see you try to invent calculus..

Newton’s method cannot use negative curvature



Newton's method cannot use negative curvature

- We can progress if we use a positive definite approximation of the Hessian matrix of f(x). $x_{k+1} = x_k \ - \ H^{-1}. g$
- One possibility is to approximate *H* by the identity matrix I (always PD)
  - This will be the same as steepest descent: $x_{k+1} = x_k \ - \Delta g$
  - Too slow, + convergence issues
- Instead use $\widetilde{H} = H_k + \lambda I$
  - High value of λ == steepest (gradient) descent.
  - Low value == Newton or Gauss Newton method

Levenberg-Marquardt Method

- Mixture of Gauss-Newton and Gradient descent.
- Acts like Gauss-Newton when close to the minimum (quadratic region)
- Gradient descent when improvement is difficult.
- Depends on a parameter λ which
  1. Controls the mixture of Gauss-Newton and Gradient Descent
  2. Controls the step-length.

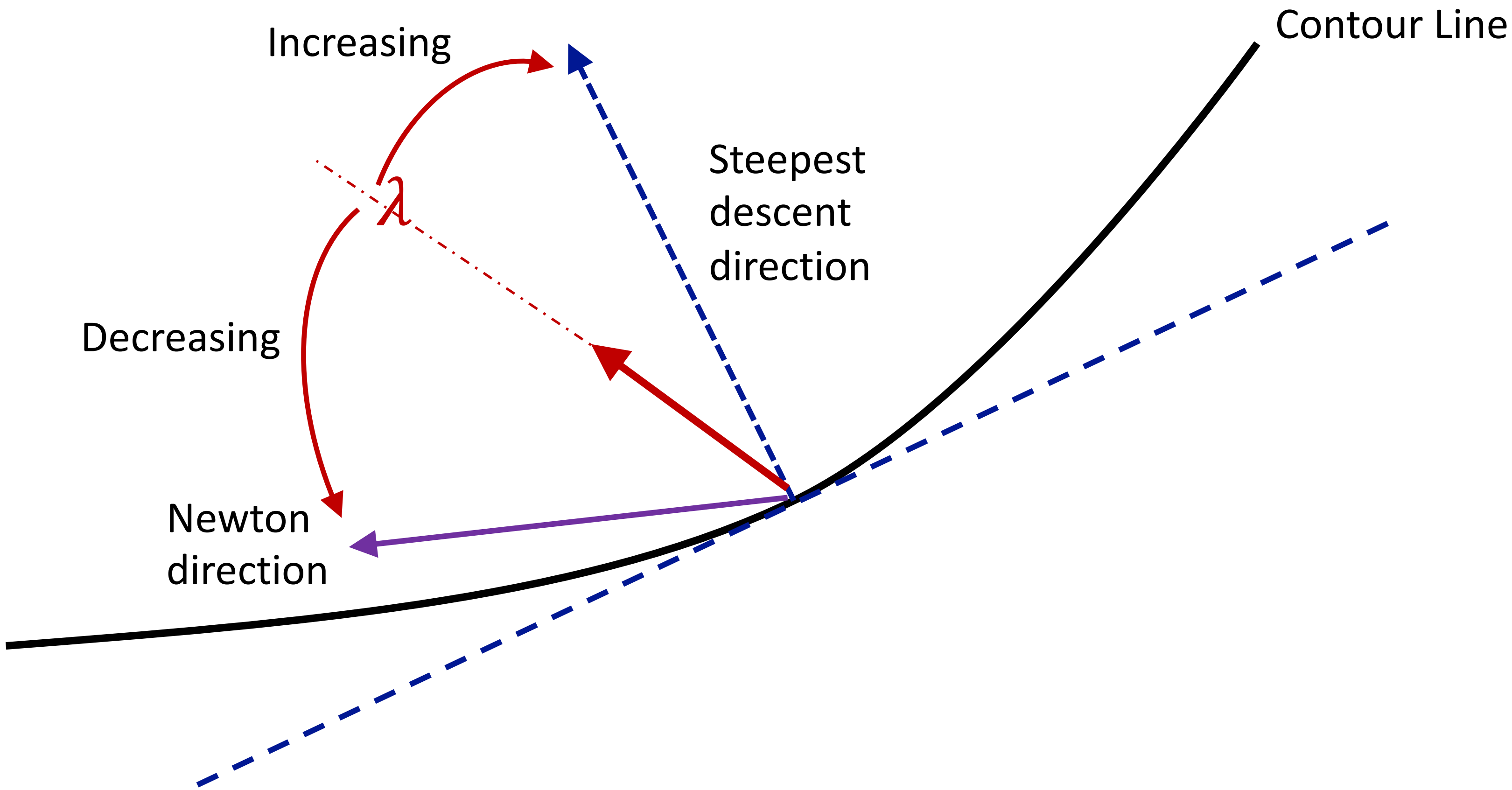


Illustration of Levenberg-Marquardt gradient descent

Levenberg-Marquardt Method

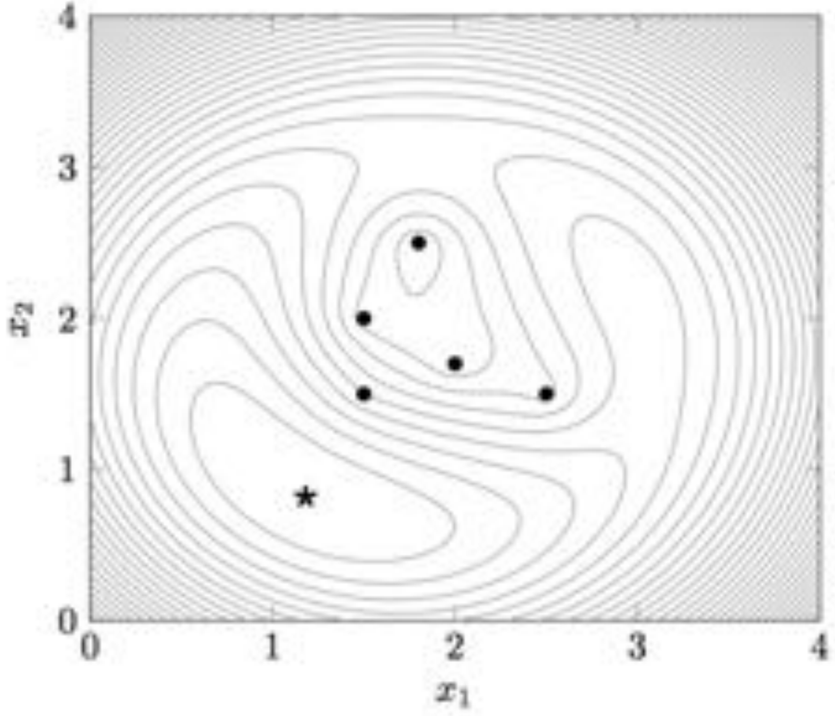
1) Adapt the value of λ during the optimization.

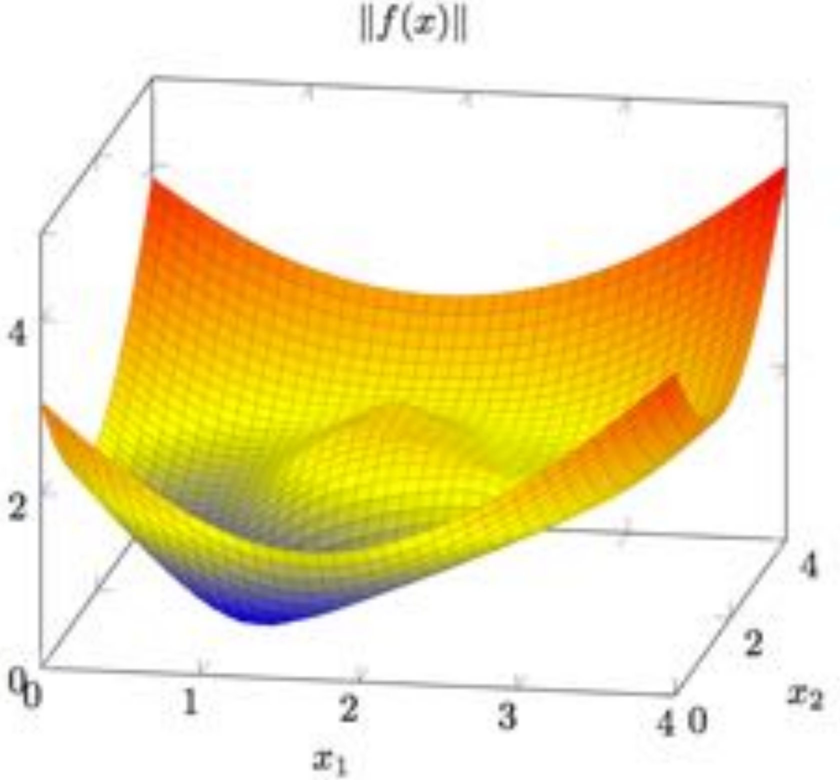
2) If the iteration was successful ($F(x_{k+1}) < F(x_k)$)
   a) Decrease λ and try to use as much curvature information as possible.

3) If the previous iteration was unsuccessful ($F(x_{k+1}) > F(x_k)$)
   a) Increase λ and use only basic gradient information.

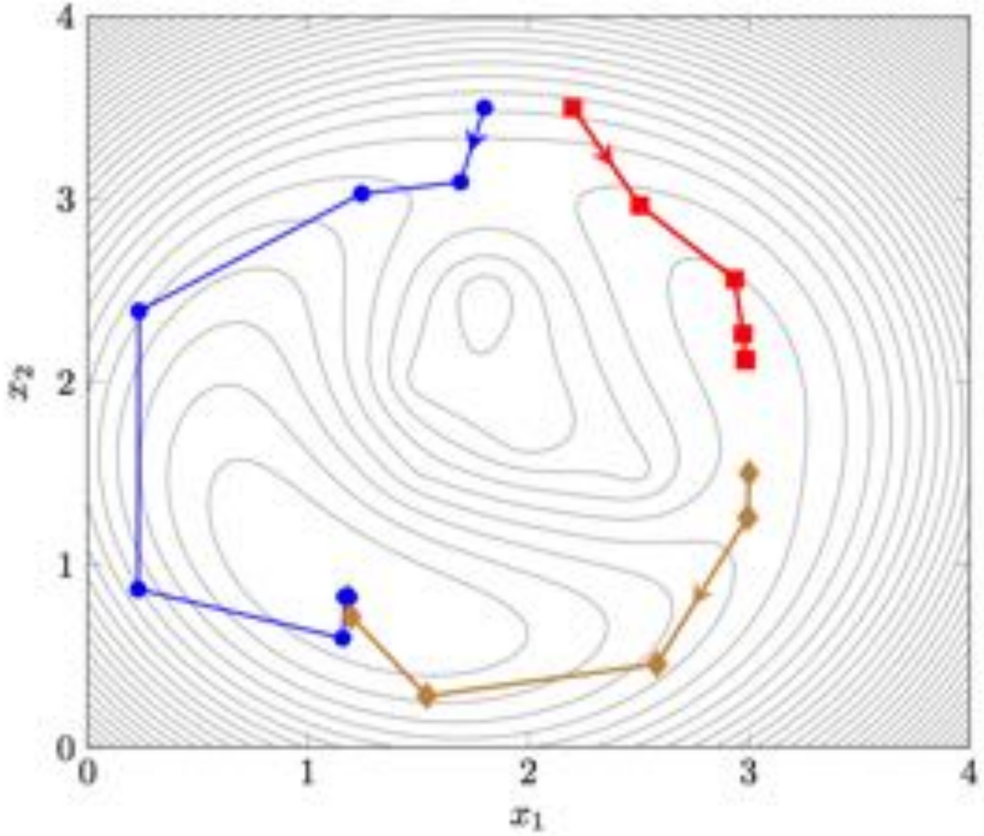
4) Trust Region Algorithm

Levenberg-Marquardt Method

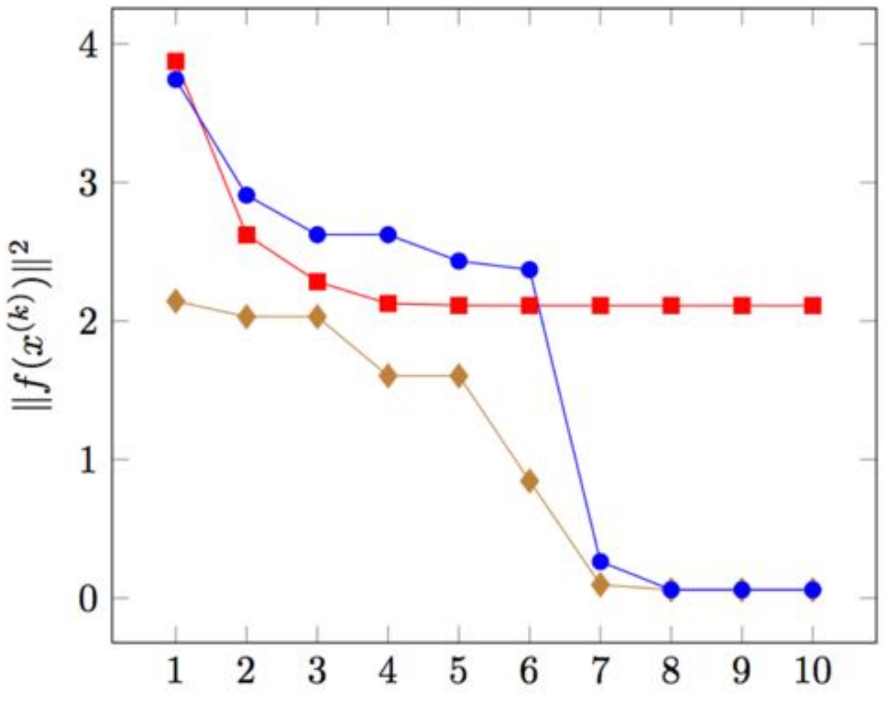


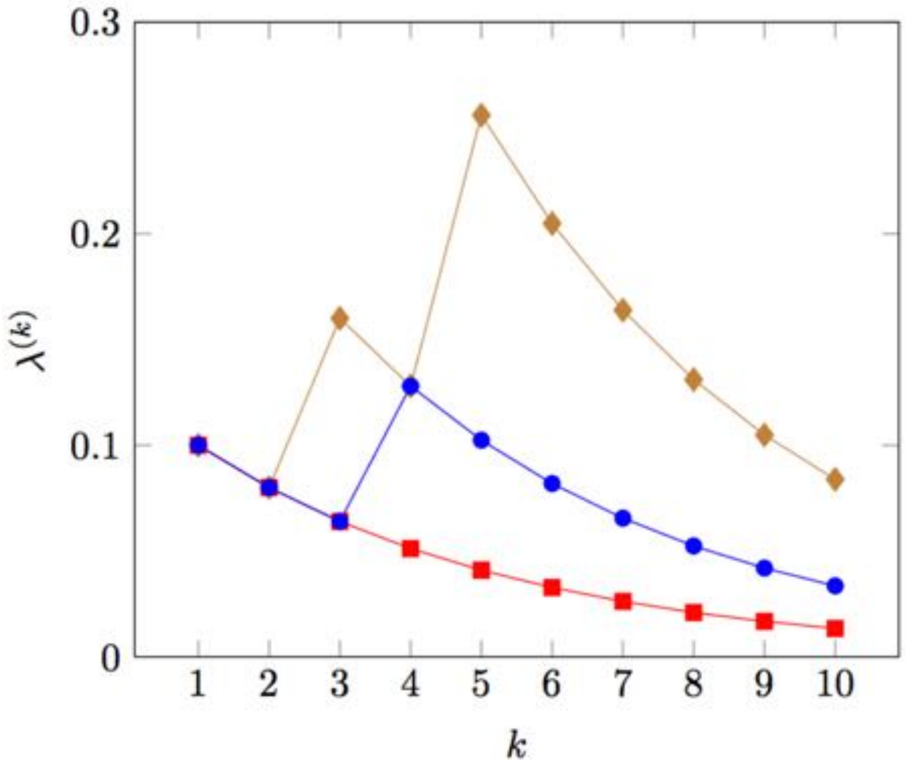


Levenberg-Marquardt from 3 initial points



Levenberg-Marquardt from 3 initial points





Stopping Criteria

Criterion 1: reach the number of iteration specified by the user

$$K > k_{max}$$

Stopping Criteria

Criterion 1: reach the number of iteration specified by the user

$$K > k_{max}$$

Criterion 2: when the current function value is smaller than a user-specified threshold

$$F(x_k) < \sigma_{user}$$

Stopping Criteria

Criterion 1: reach the number of iteration specified by the user

$$K > k_{max}$$

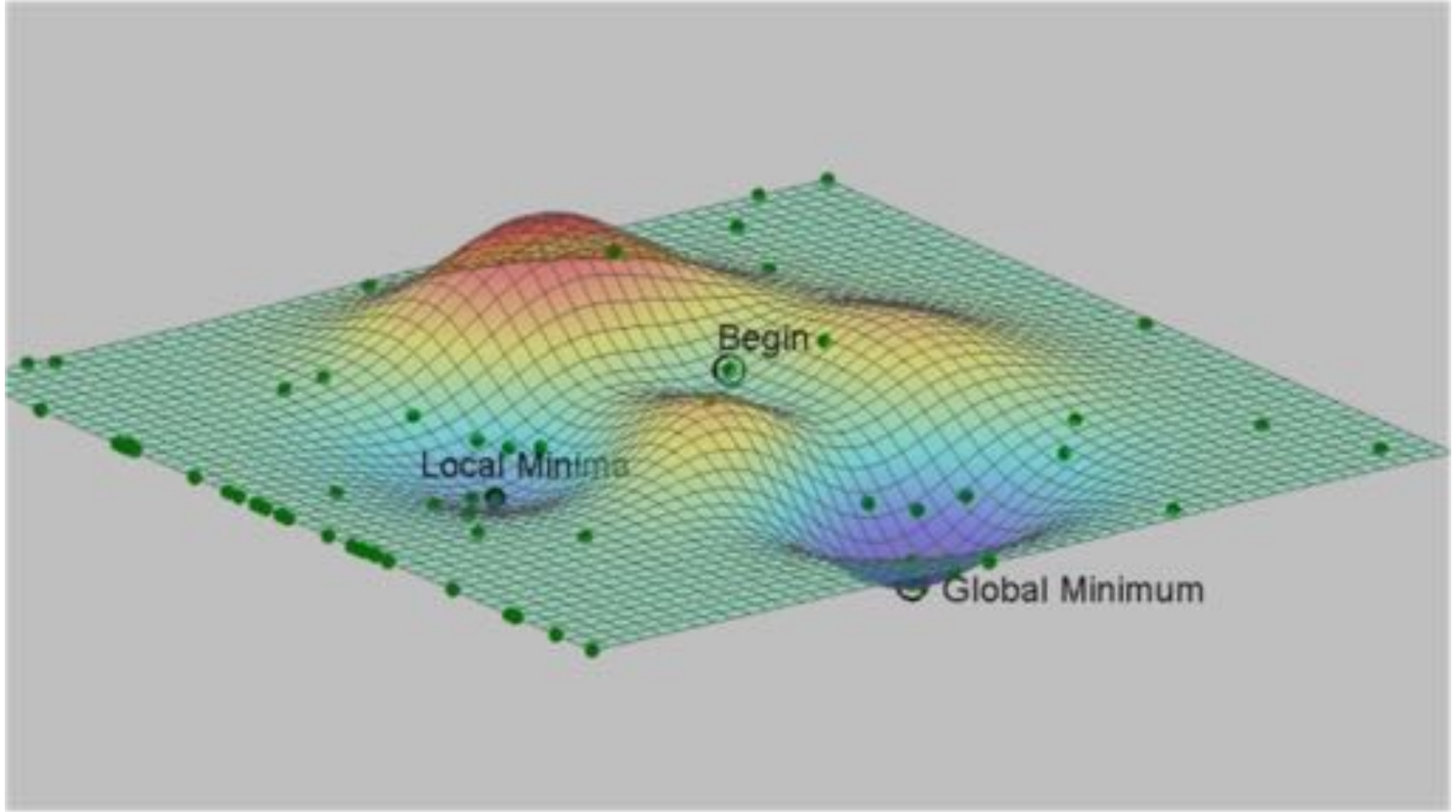
Criterion 2: when the current function value is smaller than a user-specified threshold

$$F(x_k) < \sigma_{user}$$

Criterion 3: when the change of function value is smaller than a user specified threshold

$$||F(x_k) - F(x_{k-1})|| < \varepsilon_{user}$$

Multi-start search



- Several points as initial guesses for regression and the regression is performed for each point.

1) Choose randomly..
2) Choose within some neighborhood of nominal values.

NLLS in Matlab

nlinfit

Nonlinear regression

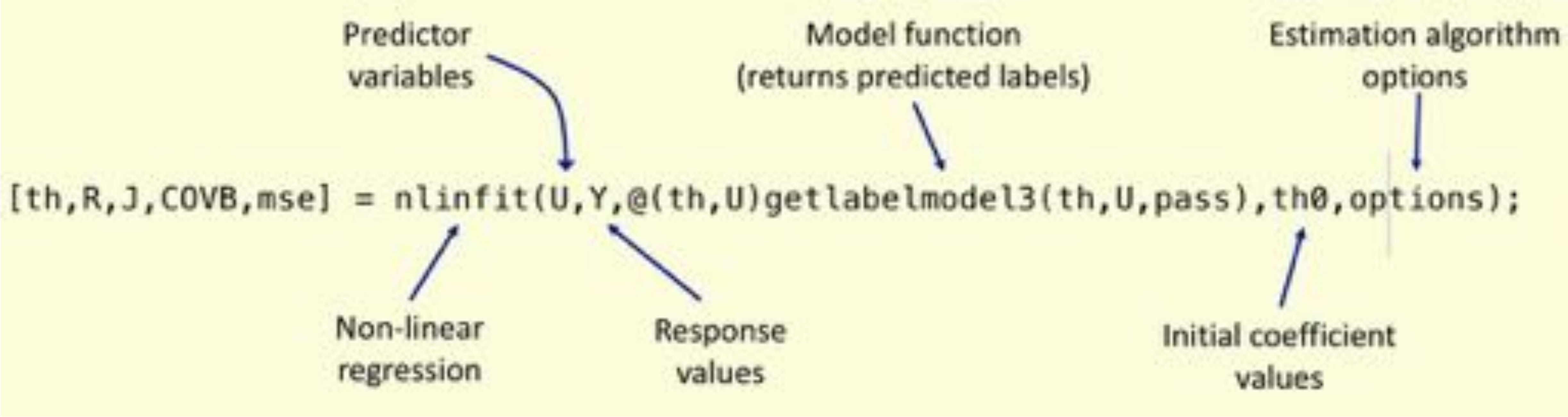
lsqnonlin

Solve nonlinear least-squares (nonlinear data-fitting) problems

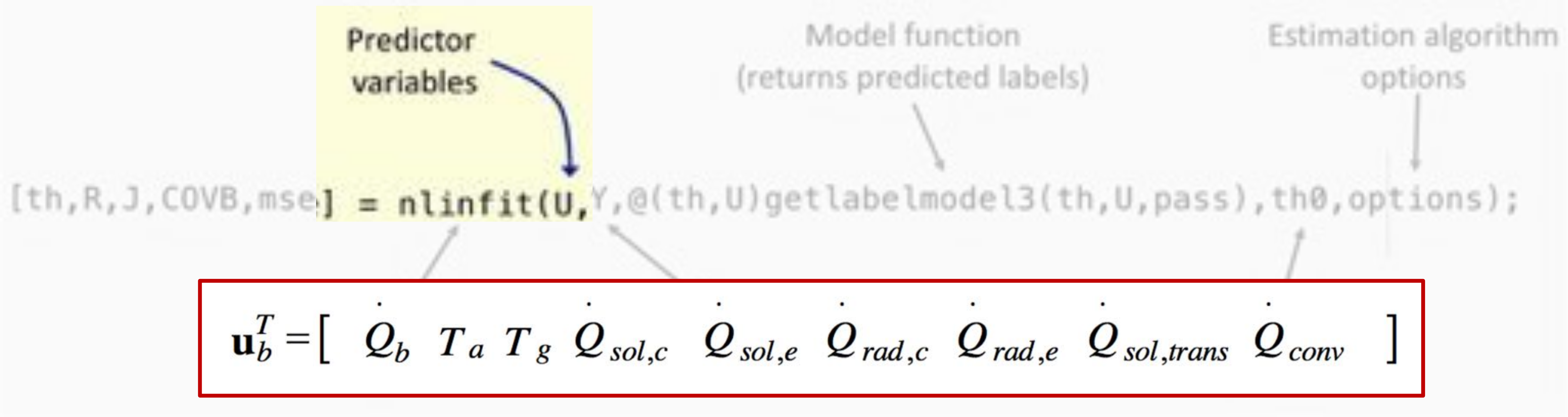
lsqcurvefit

Solve nonlinear curve-fitting (data-fitting) problems in least-squares sense

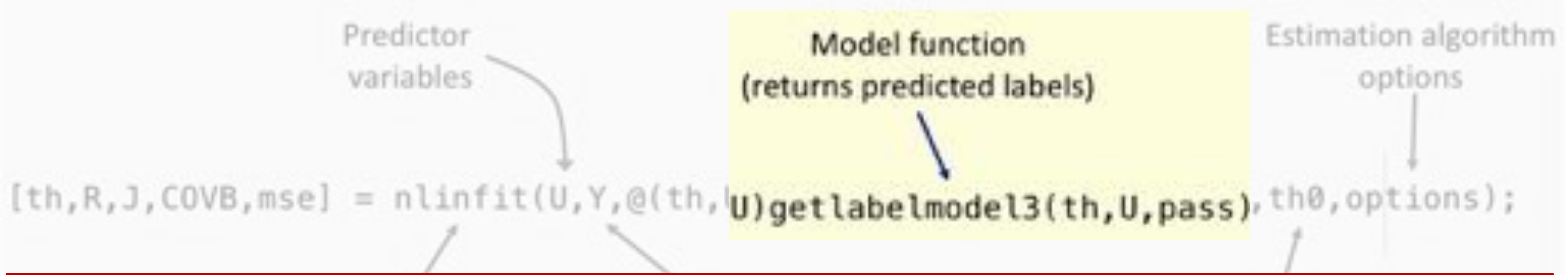
Example: nlinfit



Example: nlinfit



Example: nlinfit



$$\begin{pmatrix} y(0) \\ y(1) \\ \vdots \\ y(N-1) \end{pmatrix} = \mathcal{O}\, x(0) + \mathcal{T} \begin{pmatrix} u(0) \\ u(1) \\ \vdots \\ u(N-1) \end{pmatrix} \qquad \mathcal{O} = \begin{pmatrix} C_\theta \\ C_\theta A_\theta \\ \vdots \\ C_\theta A_\theta^{N-1} \end{pmatrix} \qquad \mathcal{T} = \begin{pmatrix} D_\theta & 0 & \dots & \\ C_\theta B_\theta & D_\theta & 0 & \dots \\ \vdots & \vdots & \vdots & \\ C_\theta A_\theta^{N-2} B_\theta & C_\theta A_\theta^{N-3} B_\theta & \dots C_\theta B_\theta & D_\theta \end{pmatrix}$$

Example: nlinfit

$$\theta_1 = [C_{e1}\ C_{i1}\ C_{c1}\ C_{g1}\ R_{e1}\ R_{e2}\ R_{i1}\ R_{i2}\ R_{c1}\ R_{c2}\ R_{g1}\ R_{g1}\ R_{g2}\ C_{e2}\ C_{i2}\ C_{c2}\ C_{g2}\ R_{e3}\ R_{i3}\ R_{c3}\ R_{g3}\ ]$$