Chapter 2

Numerical Methods

Numerical methods are used to solve non-linear algebraic equations.

Direct Substitution method (or "fixed point" method)

Consider first one equation and one unknown.

Example:

① write $f(x)=0$ as $g(x)=x$

$f(x)=0 \longrightarrow f(x)+x=x \longrightarrow g(x)=x$

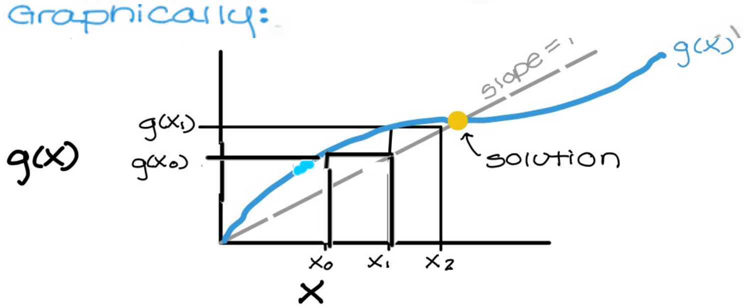
② Guess an initial x (ie., x_0)

This number is the iteration number

③ Evaluate $g(x)$

④ use $g(x)$ as the next guess for x

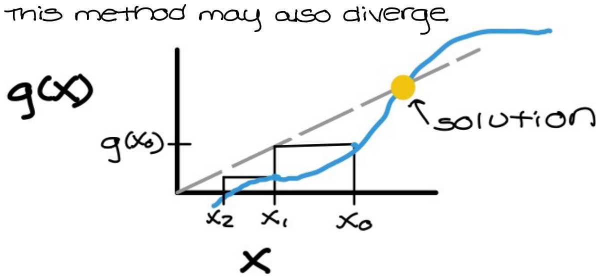
Graphically:



Wegstein acceleration method:

$$x_{i+1} = (1-q)x_i + q\,g(x_i)$$

This method may also diverge



Diverges if the slope is > 1.

Extension to multivariable System

Solve:

$$\underbrace{\begin{pmatrix} f_1(x_1, x_2, \dots) \\ f_2(x_1, x_2, \dots) \\ \vdots \end{pmatrix}}_{\text{vector of functions}} = \underbrace{\begin{pmatrix} 0 \\ 0 \\ \vdots \end{pmatrix}}_{\text{vector of numbers}}$$

x_n

subscript denotes the variable number for a multi-variable system.

Rewrite as:

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} g_1(x_1, x_2, \dots) \\ g_2(x_1, x_2, \dots) \\ \vdots \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \end{pmatrix} + \begin{pmatrix} f_1(x_1, x_2, \dots) \\ f_2(x_1, x_2, \dots) \\ \vdots \end{pmatrix}$$

and proceed as before...

$$\begin{pmatrix} x_{1,0} \\ x_{2,0} \\ \vdots \end{pmatrix} \Rightarrow \begin{pmatrix} g_1(x_{1,0}, x_{2,0}, \dots) \\ g_2(x_{1,0}, x_{2,0}, \dots) \\ \vdots \end{pmatrix} \Rightarrow \begin{pmatrix} x_{1,1} \\ x_{2,1} \\ \vdots \end{pmatrix} \Rightarrow \text{etc...}$$

$x_{n,m}$ ↳ The 2nd subscript denotes the iteration number.

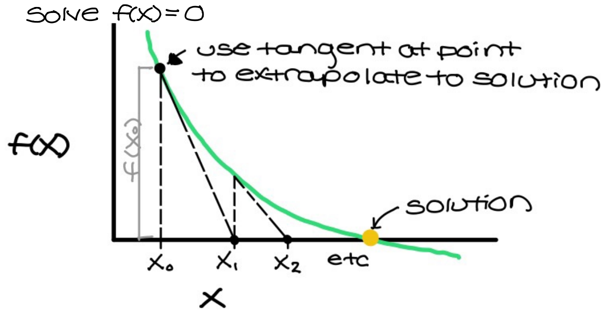
Wegstein method:

$$\begin{pmatrix} x_{1,i+1} \\ x_{2,i+1} \\ \vdots \end{pmatrix} = (1-q)\begin{pmatrix} x_{1,i} \\ x_{2,i} \\ \vdots \end{pmatrix} + q\begin{pmatrix} g_1(x_{1,i} \dots) \\ g_2(x_{1,i} \dots) \\ \vdots \end{pmatrix}$$

* This method may fail if $\frac{\partial g_i}{\partial x_j}$ is large.

Newton's method

Solve $f(x) = 0$



First step:

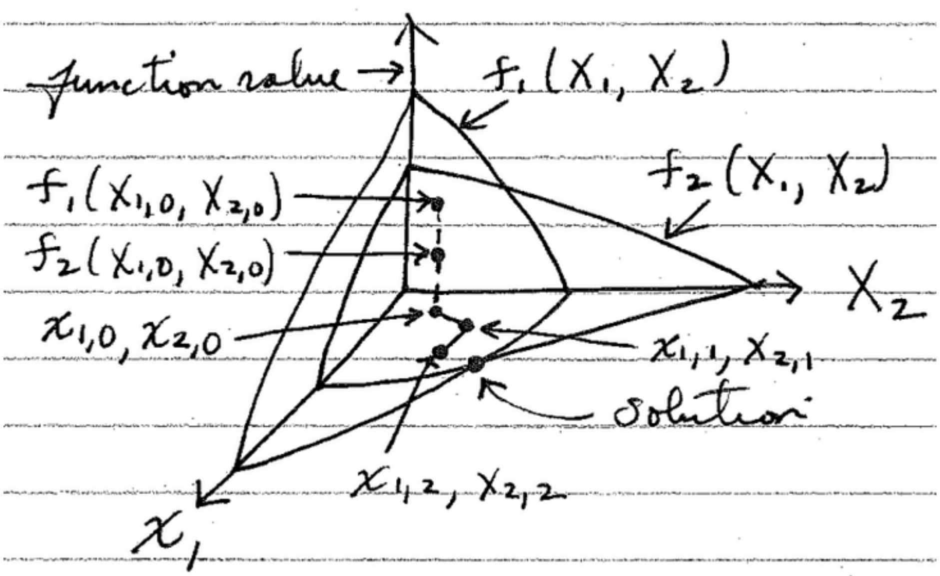
$$\left.\frac{df(x)}{dx}\right|_{x_0} = f'(x_0) = \frac{-f(x_0)}{x_1 - x_0} \Rightarrow x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

more generally: $x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$

multivariable Newton's method

$f_1(x_1, x_2) = 0$

$f_2(x_1, x_2) = 0$



If f_1 and f_2 are linear functions (i.e., surfaces are flat planes) then the solution is given by solving the following linear set of equations.

$$\underbrace{\begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix}_{(x_{1,0},\, x_{2,0})}}_{\text{Jacobian matrix}} \begin{pmatrix} x_{1,1} - x_{1,0} \\ x_{2,1} - x_{2,0} \end{pmatrix} = -\begin{pmatrix} f_1 \\ f_2 \end{pmatrix}_{(x_{1,0},\, x_{2,0})}$$

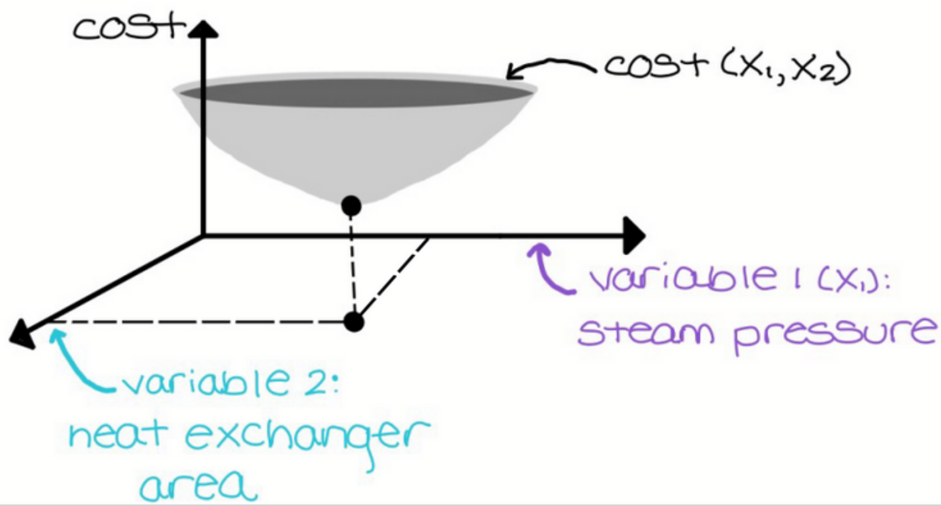
multidimensional analog of previous equation

subscript denotes evaluation at this point

To generalize, replace 0 by i and 1 by $i+1$.

Optimization methods

Example: design of a heat exchanger



At the minimum of the function:

$$\frac{\partial cost}{\partial x_1} = \frac{\partial cost}{\partial x_2} = 0$$

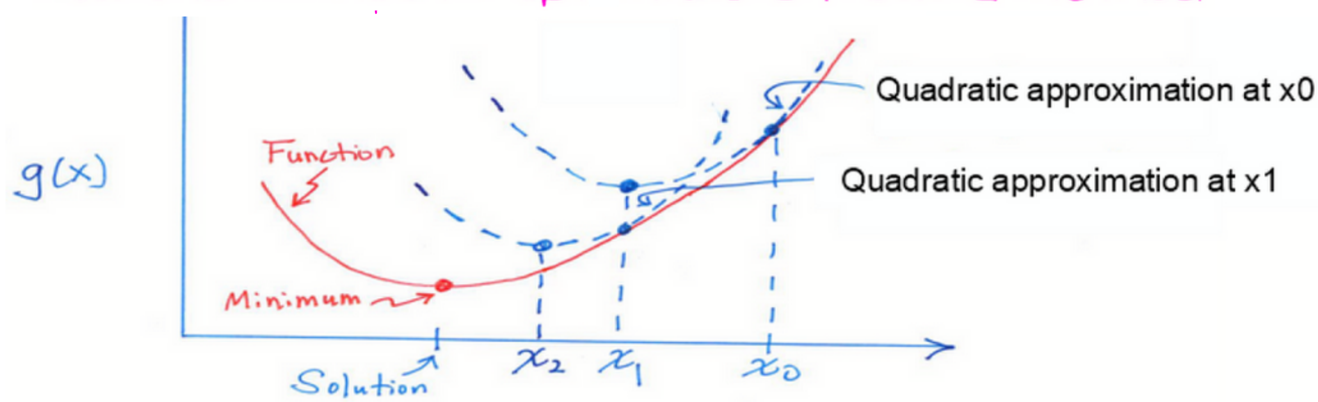
Note: Optimization can also be used to solve systems of equations $\rightarrow$

Solve: $f_1(x_1, x_2) = 0$ and $f_2(x_1, x_2) = 0$.

Let $g(x_1, x_2) = f_1^2(x_1, x_2) + f_2^2(x_1, x_2)$

The minimum of g, which is zero, is also where $f_1 = f_2 = 0$.

Newton's method for optimization: basic method



Taylor series expansion of g(x) about x_0:

$$g(x) \approx g(x_0) + \underbrace{\left.\frac{\partial g}{\partial x}\right|_{x_0}}_{g'(x_0)} (x - x_0) + \frac{1}{2} \underbrace{\left.\frac{\partial^2 g}{\partial x^2}\right|_{x_0}}_{g''(x_0)} (x - x_0)^2$$

Need the point where $\frac{dg}{dx} = 0$ $\longrightarrow$ Take the derivative of both sides of the above equation to yield: $0 = \frac{dg(x)}{dx} = g'(x_0) + g''(x_0)(x - x_0)$

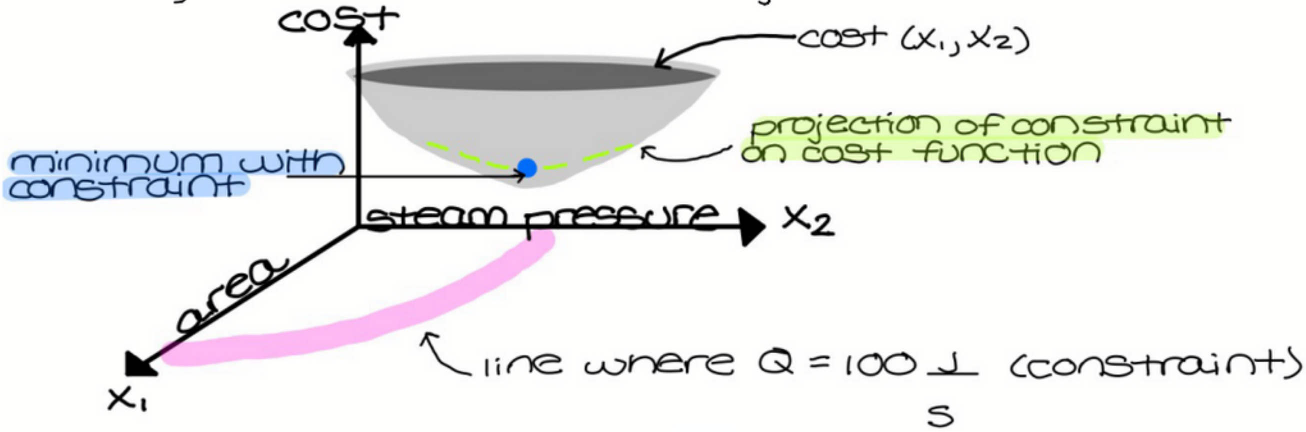
Solve for x: $\underset{x_1}{x} = x_0 - \frac{g'(x_0)}{g''(x_0)}$ more generally: $x_{i+1} = x_i - \frac{g'(x_i)}{g''(x_i)}$

* can also be generalized to a multivariable system.

Constrained Optimization

minimize $g(x_1, x_2)$ but where $f(x_1, x_2) = 0$

Looking back at the heat exchanger example:



Penalty function method:

$$h(x_1, x_2; \lambda) = g(x_1, x_2) + \lambda \left[f(x_1, x_2)\right]^2$$

λ is a parameter

Set λ to a "large" number

Perform an unconstrained optimization on $h(x_1, x_2)$ after setting λ to a large number.

Lagrange multiplier method

Lagrange function

$$h(x_1, x_2, \lambda) = g(x_1, x_2) + \lambda f(x_1, x_2)$$

Find the values of x_1, x_2 and λ that satisfy the following 3 nonlinear algebraic equations:

This is also the solution of the original constrained optimization problem.

$$\vec{\nabla} g(x_1, x_2) = \lambda \vec{\nabla} f(x_1, x_2)$$

$$f(x_1, x_2) = 0$$

where $\vec{\nabla} = \vec{i} \frac{\partial}{\partial x_1} + \vec{j} \frac{\partial}{\partial x_2}$

The above equations can be written as:

$$\vec{\nabla}_{x_1, x_2, \lambda} h(x_1, x_2, \lambda) = 0$$

Solving systems of ODEs using Eulers method

one independent variable

consider the equations $z(t)$ and $w(t)$ that satisfy the equations:

$$\frac{dz}{dt} = f_1(z,w,t) \quad \text{and} \quad \frac{dw}{dt} = f_2(z,w,t)$$

with initial conditions: $z(0)=z_0$ and $w(0)=w_0$.

From Eulers formula (finite difference approximation):

$$\frac{dz}{dt} = \frac{z(t+\Delta t) - z(t)}{\Delta t} = f_1\,(z(t), w(t), t)$$

$$\frac{dw}{dt} = \frac{w(t+\Delta t) - w(t)}{\Delta t} = f_2\,(z(t), w(t), t)$$

solving for $z(t+\Delta t)$ and $w(t+\Delta t)$:

$$z(t+\Delta t) = z(t) + f_1\,(z(t), w(t), t)\Delta t$$

$$w(t+\Delta t) = w(t) + f_2\,(z(t), w(t), t)\Delta t$$