Optimization

Find local minimum of $f(x)$

Brent's Method → bracketing

Newton's Method : find $f'(x)=0$

let x_n be a tentative value near the minimum x^*

Taylor Series

$$f'(x) = f'(x_n) + f''(x_n)(x-x_n) + \frac{1}{2} f'''(x_n)(x-x_n)^2 + H.O.T.$$

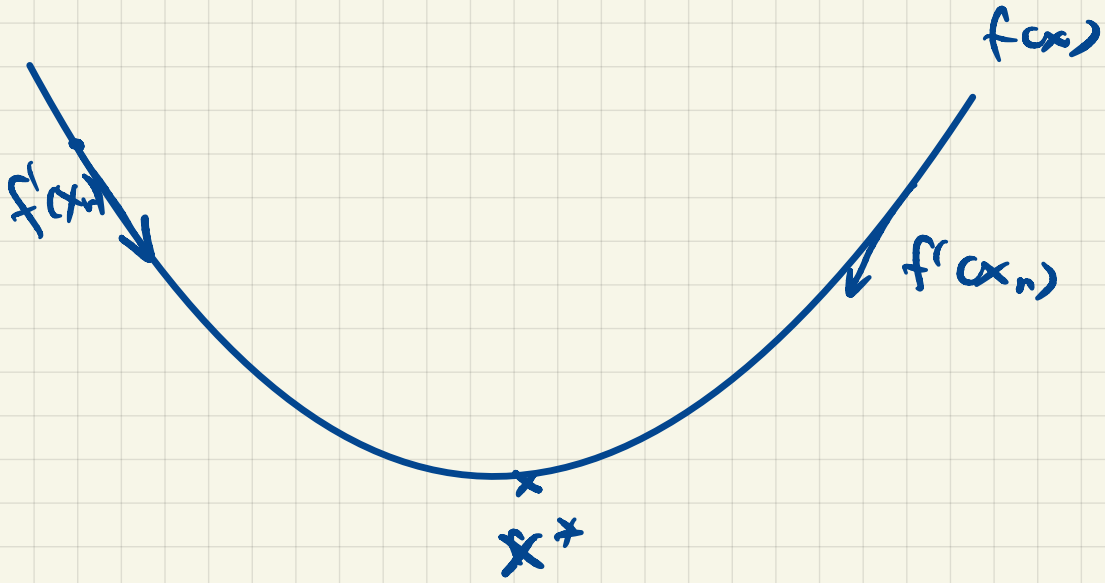
$$\Rightarrow \hat{f}'(x) = f'(x_n) + f''(x_n)(x-x_n) = 0$$

$$\Rightarrow \boxed{x_{n+1} = x_n - \frac{f'(x_n)}{f''(x_n)}}$$

① might diverge ⇒ $f''(x_n) \sim 0$

② might oscillate

Steepest Gradient Descent

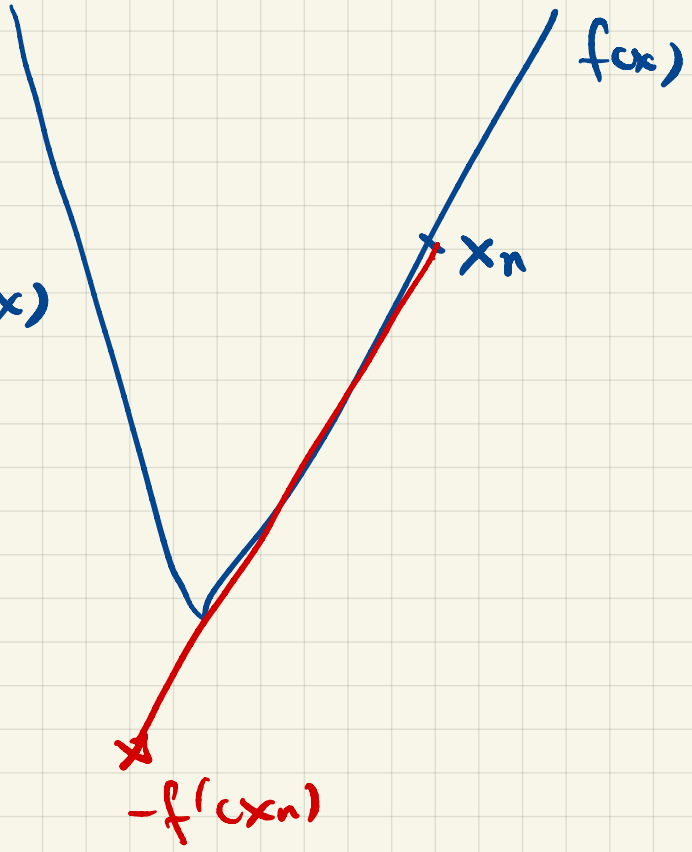


$$x_{n+1} = x_n - \alpha_n f'(x_n)$$

need damping

need damping

because the behavior of f(x) is unclear



Multivariable Minimization

Minimize $f(\underline{x})$ (a scalar) w/ $\underline{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$

ex) minimize $f(x_1, x_2) = \sin(x_1)\cos(x_2)$

Minimum occurs where

$$\nabla f(\underline{x}^*) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Taylor Series for $\underline{x}_n$ near minimum, $\underline{x}^*$

$$\nabla f(\underline{x}) = \nabla f(\underline{x}_n) + \underline{\underline{H}}(\underline{x}_n)(\underline{x} - \underline{x}_n) + \text{H.O.T.}$$

$\underline{\underline{H}}(\underline{x})$: Hessian Matrix of $f(\underline{x})$

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

$$\underline{\underline{H}}(\underline{x}) = \underline{\underline{H}}^T(\underline{x})$$

To first order

$$\nabla \hat{f}(\underline{x}) = \nabla f(\underline{x}_n) + \underline{\underline{H}}(\underline{x}_n)(\underline{x} - \underline{x}_n)$$

$$\nabla \hat{f}(\underline{x}_{n+1}) = 0$$

$$\Rightarrow \underline{x}_{n+1} = \underline{x}_n - \underline{\underline{H}}_n^{-1} \nabla f(\underline{x}_n)$$

① Solve $\underline{H}_n \underline{\delta}_n = -\nabla f_n$

$\underline{\delta}_n = (\underline{x}_{n+1} - \underline{x}_n)$

② Update $\underline{x}_{n+1} = \underline{x}_n + \alpha_n \underline{\delta}_n$

Note:

① $\underline{H}_n$ changes every iteration

② Need to solve a linear system each iteration

③ $\underline{H}_n$ might be expensive or unknown

Quasi-Newton Method

Idea: Find a $\underline{\underline{B}}_n \approx \underline{\underline{H}}_n$ where

$\underline{\underline{B}}_n$ is cheap to compute and

solving $\underline{\underline{B}}_n \underline{s}_n = -\nabla \underline{f}_n$ is also cheap

Need: A sequence $\underline{\underline{B}}_0, \underline{\underline{B}}_1, \underline{\underline{B}}_2 \ldots$

1) How to choose $\underline{\underline{B}}_0$?

2) How does $\underline{\underline{B}}_n$ update based on $\underline{\underline{B}}_{n-1}, \underline{\underline{B}}_{n-2}, \ldots$

General Quasi-Newton Algorithm

let x_0 & $\underline{\underline{B}}_0$ be known

$n=0$

until converge

Solve $\underline{\underline{B}}_n \underline{s}_n = -\nabla \underline{f}_n$

$\underline{x}_{n+1} = \underline{x}_n + \alpha_n \underline{s}_n$ via line search

$\underline{y}_n = \nabla f(x_{n+1}) - \nabla f(x_n)$

$= \nabla (f(x_{n+1}) - f(x_n))$

$\underline{B}_{n+1}$ = function of $\underline{B}_n$, $\underline{\delta}_n$, $\underline{y}_n$

Choice for $\underline{B}_0$

Let $\underline{\hat{s}}_0 = -\nabla f(\underline{x}_0)$

$$\underline{y}_0 = \nabla(f(\underline{x} + \hat{\underline{\delta}}_0) - f(\underline{x}))$$

$$\underline{B}_0 = \frac{\underline{y}_0^T \underline{y}_0}{\underline{y}_0^T \underline{\delta}_0} \underline{\underline{I}}$$

$$\underline{B}_0^{-1} = \frac{\underline{y}_0^T \underline{\delta}_0}{\underline{y}_0^T \underline{y}_0} \underline{\underline{I}}$$

Then iteration, $\underline{\delta}_0 = -\frac{\underline{y}_0^T \underline{\delta}_0}{\underline{y}_0^T \underline{y}_0} \nabla f_0$

Many Choices for B_n

- DFP method Davidson - Fletcher - Powell

$$B_{n+1} = \left(I - \frac{y_n \delta_n^T}{y_n^T y_n} \right) B_n \left(I - \frac{\delta_n y_n^T}{y_n^T y_n} \right) + \frac{y_n y_n^T}{y_n^T y_n}$$

$$B_{n+1}^{-1} = B_n^{-1} + \frac{\delta_n \delta_n^T}{\delta_n^T y_n} - B_n^{-1} \left(\frac{y_n y_n^T}{y_n^T B_n^{-1} y_n} \right) B_n^{-1}$$

- BFGS method Broyden - Fletcher - Goldfarb - Shanno

$$B_{n+1} = B_n + \frac{y_n y_n^T}{y_n^T \delta_n} - B_n \left(\frac{\delta_n \delta_n^T}{\delta_n^T B_n \delta_n} \right) B_n^T$$

$$B_{n+1}^{-1} = \left(I - \frac{\delta_n y_n^T}{y_n^T y_n} \right) B_n^{-1} \left(I - \frac{y_n \delta_n^T}{y_n^T \delta_n} \right)$$

$$+ \frac{\underline{\delta}_n \underline{y}_n^T}{\underline{y}_n^T \underline{\delta}_n}$$

Line Search / Backtracking

$$\underline{x}_{n+1} = \underline{x}_n + \alpha_n \underline{\delta}_n$$

Newton: $\underline{\delta}_n = - \underline{J}_n^{-1} \underline{f}_n$

Gradient Descent: $\underline{\delta}_n = - \nabla f(\underline{x}_n)$

Minimization: $\underline{\delta}_n = - \underline{\underline{H}}_n^{-1} \nabla f(\underline{x}_n)$

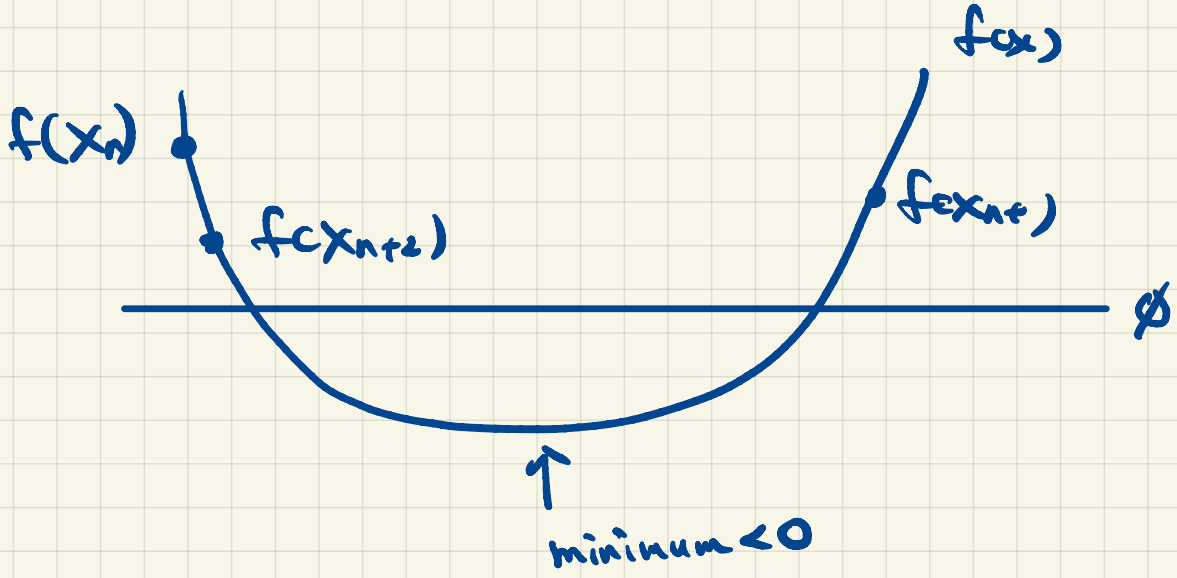
In all cases,

$$\boxed{f(\underline{x}_n + \alpha_n \underline{\delta}_n) < f(\underline{x}_n)}$$ minimization

$$\| f(\underline{x}_n + \alpha_n \underline{\delta}_n) \| < \| f(\underline{x}_n) \|$$

Focus on $f(x)$

It is not sufficient to simply require $\boxed{}$



Wolfe Conditions.

① $f(\underline{x}_n + \alpha_n \underline{\delta}_n) \leq f(\underline{x}_n) + c_1 \alpha_n (\nabla f_n)^T \delta_n$

for some $c_1 \in [0, 1]$

This requires sufficient progress towards the sol.

$c_1 \sim 10^{-4}$ small

(2) To avoid small α_n, require

$$(\nabla f(\underline{x}_n + \alpha_n \underline{s}_n))^T \underline{s}_n \geq c_2 (\nabla f_n)^T \underline{s}_n$$

for $c_2 \in (c_1, 1)$

Thus $0 < c_1 < c_2 < 1$

It can be shown that if $f: \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable, $\underline{s}_n$ is a descent direction at $\underline{x}_n$ and if range of α_n that satisfy the wolfe condition.

$$\alpha_n = \frac{\overbrace{(\underline{x}_n - \underline{x}_{n-1})^T}^{\underline{s}_{n-1}} \overbrace{(\nabla(f(x_n) - f(x_{n-1}))}^{y_{n-1}}}{\| \nabla f(x_n) - \nabla f(x_{n-1}) \|_2^2}$$

Optimization

Find local minimum of $f(x)$

Brent's Method → bracketing

Newton's Method: find $f'(x)=0$

let x_n be a tentative value near the minimum x^*.

Taylor Series

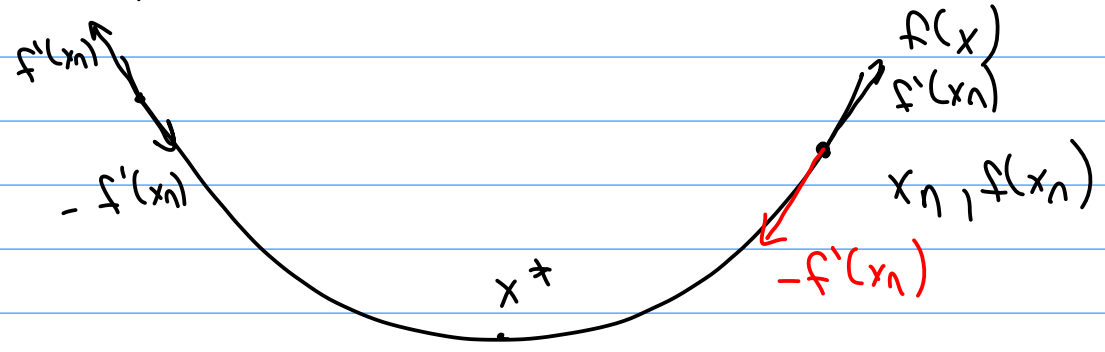
$$f'(x) = f'(x_n) + f''(x_n)(x-x_n) + \tfrac{1}{2} f'''(x_n)(x-x_n)^2 + \text{H.O.T.}$$

$$\hat{f}'(x) = f'(x_n) + f''(x_n)(x-x_n) = 0$$

$$\Rightarrow x_{n+1} = x_n - \frac{f'(x_n)}{f''(x_n)}$$

1) might diverge if $f''(x_n) \to 0$
2) might oscillate

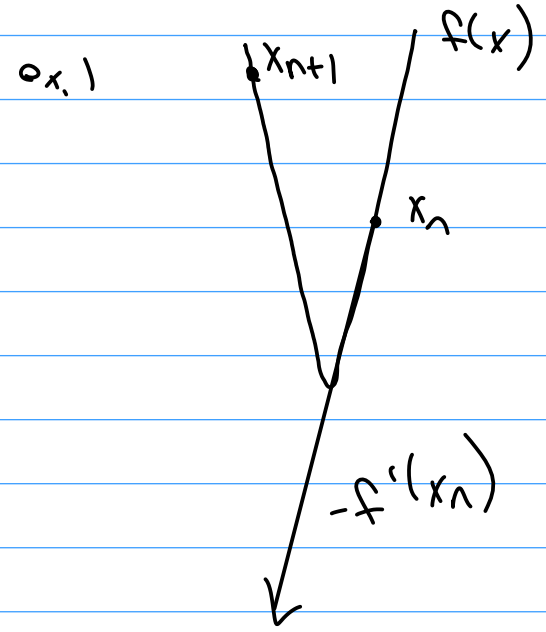
Steepest Gradient Descent



$$x_{n+1} = x_n - \alpha_n f'(x_n)$$

↑ will need damping

You need damping as you do not know how $f'(x)$ behaves



Multivariable Minimization

Minimize $f(\underline{x})$ w/ $\underline{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$

↑ A scalar

ex.1) minimize $f(x_1, x_2) = \sin(x_1)\cos(x_2)$

Minimum occurs where

$$\nabla f(\underline{x}^*) = \begin{bmatrix} \partial f/\partial x_1 \\ \partial f/\partial x_2 \\ \vdots \\ \partial f/\partial x_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Taylor Series for $\underline{x}_n$ near minimum, $\underline{x}^*$

$$\nabla f(\underline{x}) \approx \nabla f(\underline{x}_n) + \underline{H}(\underline{x}_n)(\underline{x} - \underline{x}_n) + \cancel{H.O.T.}$$

$\underline{H}(\underline{x})$ = Hessian Matrix of $f(\underline{x})$

$$= \begin{bmatrix} \partial^2 f/\partial x_1^2 & \partial^2 f/\partial x_1 \partial x_2 & \cdots & \partial^2 f/\partial x_1 \partial x_n \\ \partial^2 f/\partial x_2 \partial x_1 & \partial^2 f/\partial x_2^2 & \cdots & \partial^2 f/\partial x_2 \partial x_n \\ \vdots & & & \\ \partial f/\partial x_n \partial x_1 & \cdots & & \partial^2 f/\partial x_n^2 \end{bmatrix}$$

$$\underline{H}(\underline{x}) = \underline{H}^T(\underline{x})$$

To first-order, $\hat{\nabla f}(\underline{x}) = \nabla f(\underline{x}_n) + \underline{H}(\underline{x}_n)(\underline{x} - \underline{x}_n)$

$$\hat{\nabla f}(\underline{x}_{n+1}) = \underline{0}$$

$$\Rightarrow \underline{x}_{n+1} = \underline{x}_n - \underline{H}_n^{-1} \nabla f(\underline{x}_n)$$

Write as:

1) Solve $\underline{H}_n \underline{d}_n = -\nabla f_n$
2) Update: $\underline{x}_{n+1} = \underline{x}_n + \alpha_n \underline{d}_n$

Notes:
- $\underline{H}_n$ changes every iteration
- Need to solve a linear system each iteration
- $\underline{H}_n$ might be expensive or unknown

Quasi-Newton Methods

Idea: Find a $\underline{B}_n \approx \underline{H}_n$ where
$\underline{B}_n$ is cheap to compute &
solving $\underline{B}_n \underline{\delta}_n = -\nabla f_n$ is also cheap

Need: A sequence $\underline{B}_0, \underline{B}_1, \underline{B}_2$, etc.
1) How to chose $\underline{B}_0$?
2) How does $\underline{B}_n$ depend on $\underline{B}_{n-1}$, $\underline{B}_{n-2}$, solution, etc.

General Quasi-Newton Algorithm
let $\underline{x}_0$ & $\underline{B}_0$ be known
$n=0$
until converged
Solve $\underline{B}_n \underline{\delta}_n = -\nabla f_n$
$\underline{x}_{n+1} = \underline{x}_n + \alpha_n \underline{\delta}_n$ via line search
$\underline{\gamma}_n = \nabla f(\underline{x}_{n+1}) - \nabla f(\underline{x}_n) = \nabla (f(\underline{x}_{n+1}) - f(\underline{x}_n))$
$\underline{B}_{n+1} =$ function of $\underline{B}_n, \underline{\delta}_n, \underline{\gamma}_n$

Simple choice for $\underline{B}_0$

let $\hat{\underline{\delta}}_0 = -\nabla f(\underline{x}_0)$ $\quad \underline{\gamma}_0 = \nabla (f(\underline{x} + \hat{\underline{\delta}}_0) - f(\underline{x}_0))$

$$\underline{B}_0 = \frac{\underline{\gamma}_0^T \underline{\gamma}_0}{\underline{\gamma}_0^T \underline{\delta}_0} \underline{I} \qquad \underline{B}_0^{-1} = \frac{\underline{\gamma}_0^T \hat{\underline{\delta}}_0}{\underline{\gamma}_0^T \underline{\gamma}_0} \underline{I}$$

Thus, in iteration $\underline{\delta}_0 = -\frac{\underline{\gamma}_0^T \hat{\underline{\delta}}_0}{\underline{\gamma}_0^T \underline{\gamma}_0} \nabla f_0$

Many choices for $\underline{B}_n$

- Davidon - Fletcher - Powell (DFP) Method

$$\underline{B}_{n+1} = \left(\underline{I} - \frac{\underline{y}_n \underline{\delta}_n^T}{\underline{y}_n^T \underline{\delta}_n} \right) \underline{B}_n \left(\underline{I} - \frac{\underline{\delta}_n \underline{y}_n^T}{\underline{y}_n^T \underline{\delta}_n} \right) + \frac{\underline{y}_n \underline{y}_n^T}{\underline{y}_n^T \underline{y}_n}$$

$$\underline{B}_{n+1}^{-1} = \underline{B}_n^{-1} + \frac{\underline{\delta}_n \underline{\delta}_n^T}{\underline{\delta}_n^T \underline{y}_n} - \underline{B}_n^{-1} \left(\frac{\underline{y}_n \underline{y}_n^T}{\underline{y}_n^T \underline{B}_n^{-1} \underline{y}_n} \right) \underline{B}_n^{-1}$$

Given $\underline{B}_0^{-1}$, $\underline{B}_1^{-1}$ is known,
Given $\underline{B}_1^{-1}$, $\underline{B}_2^{-1}$ is known, etc.

- Broyden - Fletcher - Goldfarb - Shanno (BFGS)

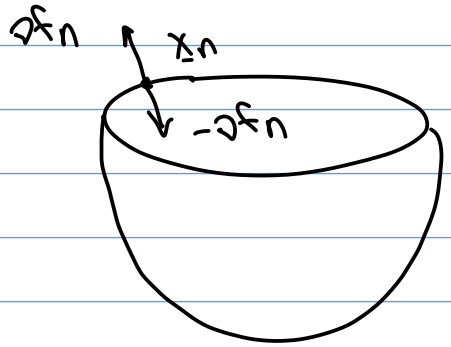
Based on outer products:

$$\underline{B}_{n+1} = \underline{B}_n + \frac{\underline{y}_n \underline{y}_n^T}{\underline{y}_n^T \underline{\delta}_n} - \underline{B}_n \left(\frac{\underline{\delta}_n \underline{\delta}_n^T}{\underline{\delta}_n^T \underline{B}_n \underline{\delta}_n} \right) \underline{B}_n^T$$

$$\underline{B}_{n+1}^{-1} = \left(\underline{I} - \frac{\underline{\delta}_n \underline{y}_n^T}{\underline{y}_n^T \underline{y}_n} \right) \underline{B}_n^{-1} \left(\underline{I} - \frac{\underline{y}_n \underline{\delta}_n^T}{\underline{y}_n^T \underline{\delta}_n} \right) + \frac{\underline{\delta}_n \underline{y}_n^T}{\underline{y}_n^T \underline{\delta}_n}$$

Multidimensional Gradient Descent

A 2D convex function $f(x_1, x_2)$



$$\Rightarrow \quad \underline{x}_{n+1} = \underline{x}_n - \alpha_n \nabla f(\underline{x}_n)$$

Line Search / Backtracking

Many methods written as $\underline{x}_{n+1} = \underline{x}_n + \alpha_n \underline{d}_n$

Newton: $\underline{d}_n = -\underline{J}_n^{-1} \underline{f}_n$

Gradient Descent: $\underline{d}_n = -\nabla f(\underline{x}_n)$

Minimization: $\underline{d}_n = -\underline{H}_n^{-1} \nabla f(\underline{x}_n)$

In all cases you want

$f(\underline{x}_n + \alpha_n \underline{d}_n) < f(\underline{x}_n)$ minimization

or

$\|\underline{f}(\underline{x}_n + \alpha \underline{d}_n)\| < \|\underline{f}(\underline{x}_n)\|$ root finding

Focus on $f(\underline{x})$ (or $f(\underline{x}) = \|g(\underline{x})\|$)

It is not sufficient to simply require $f(\underline{x}_n + \alpha_n \underline{d}_n) < f(\underline{x}_n)$ ←

ex) Some minimization problem has $f(\underline{x}_n) = \underline{5}$

minimum is never achieved.

Wolfe Conditions

Require that

1) $f(\underline{x}_n + \alpha_n \underline{p}_n) \leq f(\underline{x}_n) + c_1 \alpha_n (\nabla f_n)^T \underline{p}_n$
for some $c_1 \in (0, 1)$

This requires sufficient progress towards the solution.

In practice c_1 is small, say $c_1 \approx 10^{-4}$

2) To avoid small α_n require that

$$(\nabla f(\underline{x}_n + \alpha_n \underline{p}_n))^T \underline{p}_n \geq c_2 (\nabla f_n)^T \underline{p}_n$$

for some $c_2 \in (c_1, 1)$

Thus $0 < c_1 < c_2 < 1$

It can be shown that if $f: \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable, $\underline{p}_n$ is a descent direction at $\underline{x}_n$, and if $0 < c_1 < c_2 < 1$ there exists a range of α_n that satisfy the Wolfe conditions

One method for α_n:

$$\alpha_n = \frac{(\underbrace{\underline{x}_n - \underline{x}_{n-1}}_{\underline{s}_{n-1}})^T (\underbrace{\nabla f(\underline{x}_n) - \nabla f(\underline{x}_{n-1})}_{\underline{y}_{n-1}})}{\| \nabla f(\underline{x}_n) - \nabla f(\underline{x}_{n-1}) \|_2^2}$$

Another method

Define $\phi(\alpha) = f(\underline{x}_n + \alpha \underline{s}_n)$ (known) $\quad \phi(0) = f(\underline{x}_n)$

$\phi'(\alpha) = \underline{s}_n \cdot \nabla f(\underline{x}_n + \alpha \underline{s}_n) \quad \phi'(0) = \underline{s}_n \cdot \nabla f(\underline{x}_n)$

Wolfe Condition #1: $\phi(\alpha) \leq \phi(0) + c_1 \alpha \phi'(0)$

General Idea: choose α_0, say $\alpha_0 = 1$ (full step)

If $\phi(\alpha_0) \leq \phi(0) + c_1 \alpha_0 \phi'(0)$ use α_0

If not satisfied select $\alpha \in (0, \alpha_0)$

Currently given: $\phi(0), \phi'(0), \phi(\alpha_0)$

Form an interpolant

$$\hat{\phi}(\alpha) = \left(\frac{\phi(\alpha_0) - \phi(0) - \alpha_0 \phi'(0)}{\alpha_0^2} \right) \alpha^2 + \phi'(0)\alpha + \phi(0)$$

Find minimum of $\hat{\phi}(\alpha)$

$$\alpha_1 = \frac{-\phi'(0)\,\alpha_0^2}{2\left[\phi(\alpha_0) - \phi(0) - \phi'(0)\,\alpha_0\right]}$$

If $\phi(\alpha_1) \leq \phi(0) + c_1 \alpha_1 \phi(0)$ use α_1

If not form a cubic polynomial w/
$\phi(0), \phi'(0), \phi(\alpha_0), \phi(\alpha_1)$

$\tilde{\phi}(\alpha) = a\alpha^3 + b\alpha^2 + c\alpha + d$

Solve $\tilde{\phi}(\alpha_2) = 0$

$$\alpha_2 = \frac{-b + \sqrt{b^2 - 3a\phi'(0)}}{3a}$$

$$\begin{bmatrix} a \\ b \end{bmatrix} = \frac{1}{\alpha_0^2 \alpha_1^2 (\alpha_1 - \alpha_0)} \begin{bmatrix} \alpha_0^2 & -\alpha_1^2 \\ -\alpha_0^3 & \alpha_1^3 \end{bmatrix} \begin{bmatrix} \phi(\alpha_1) - \phi(0) - \phi'(0)\alpha_1 \\ \phi(\alpha_0) - \phi(0) - \phi'(0)\alpha_0 \end{bmatrix}$$

check if $\phi(\alpha_2) \leq \phi(0) + c_1 \alpha_2 \phi'(0)$
If not true repeat $\phi(0), \phi'(0), \phi(\alpha_{k-1}), \phi(\alpha_{k-2})$

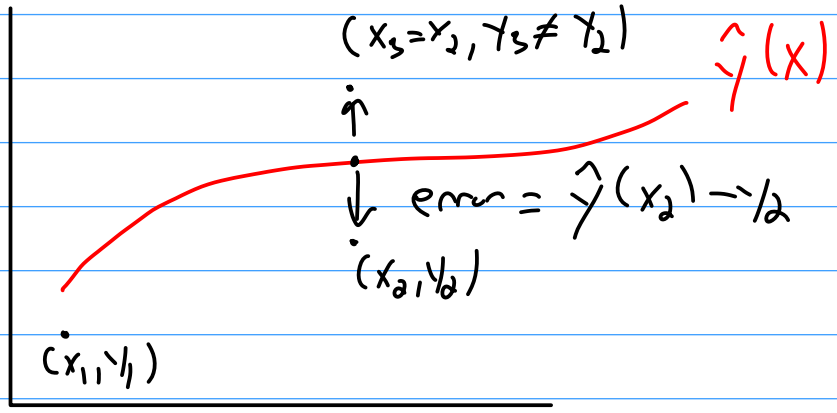
Sequence of
$\alpha_0 > \alpha_1 > \alpha_2 > \cdots > \alpha_{k-1} > \alpha_k > \cdots > 0$

If any $\alpha_k - \alpha_{k-1} < \varepsilon$ or $\alpha_k << \alpha_{k-1}$
or $\alpha_k = \frac{1}{2}\alpha_{k-1}$

See "Numerical Optimization" by
Nocedal & Wright

Regression : Curve fitting

Regression → fit an equation to a set of Data but do not require that it pass through the Data,



Goal: minimize the error

Define the error @ point (x_i, y_i) as

$$r_i = y_i - \hat{y}(x_i, \underline{a})$$

$\underline{a}$ = list of coefficients in the model equation

ex.) $\hat{y}(x, \underline{a}) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$
example of linear regression

ex.) $\hat{y}(x, \underline{a}) = a_0 \sin(x) + a_1 \sin(2x) + a_2 \cos(x) + a_3 \cos(2x)$
Linear regression

ex.) $\hat{y}(x, \underline{a}) = \dfrac{a_1 x}{a_2 + x}$ Nonlinear regression

ex 1) $\hat{y}(x, \underline{a}) = a_0 \sin(a_1 x) + a_2 \cos(a_2 x)$

non-linear regression

For both, need to minimize $\|\underline{r}\|_2$

$$\underline{r} = \begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_n \end{bmatrix} = \begin{bmatrix} y_1 - \hat{y}(x_1, \underline{a}) \\ y_2 - \hat{y}(x_2, \underline{a}) \\ \vdots \\ y_n - \hat{y}(x_n, \underline{a}) \end{bmatrix}$$ for n-data points

For Linear regression:

$$\hat{y}(x, \underline{a}) = a_1 f_1(x) + a_2 f_2(x) + \cdots + a_p f_p(x)$$

$$\begin{aligned} \hat{y}(x_1, \underline{a}) &= a_1 f_1(x_1) + a_2 f_2(x_1) + \cdots + a_p f_p(x_1) = y_1 \\ \hat{y}(x_2, \underline{a}) &= a_1 f_1(x_2) + \cdots + a_p f_p(x_2) = y_2 \\ &\vdots \\ \hat{y}(x_n, \underline{a}) &= a_1 f_1(x_n) + \cdots + a_p f_p(x_n) = y_n \end{aligned}$$

$$\Downarrow$$

$$\begin{bmatrix} f_1(x_1) & f_2(x_1) & \cdots & f_p(x_1) \\ f_2(x_1) & \cdots & & f_p(x_2) \\ \vdots & & & \vdots \\ f_p(x_1) & & & f_p(x_n) \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_p \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix}$$

$\underline{F}$ ($n \times p$) $\underline{a}$ ($p \times 1$) $\underline{y}$ ($n \times 1$)

n = # of data points; p = # of functions

In general $n > p \Rightarrow$ minimize $\|\underline{r}\|_2$

The Normal Equations minimize $\|r\|_2$

Given $F\underline{q} = \underline{y}$, the solution to

$F^T F \hat{\underline{q}} = F^T \underline{y}$ minimizes

$\|F\hat{\underline{q}} - \underline{y}\|_2$

Also called the least squares solution

$\hat{\underline{q}} = (F^T F)^{-1} F^T \underline{y}$ is unique

Never actually form the Normal Equation, why?

Condition Number

$$\kappa(A^T) = \kappa(A)$$
$$\kappa(AB) = \kappa(A)\kappa(B)$$
$$\kappa(A^T A) = \kappa(A^T)\kappa(A) = (\kappa(A))^2$$

But, other methods can find the least squares solution (QR, SVD, etc.)

In Matlab: Backslash $q = F \backslash y$

Nonlinear: No simple linear system

Define a objective function $S(\underline{q}) = \|r\|_2^2$

$$S(\underline{a}) = \sum_{i=1}^{n} r_i^2$$ Use any minimization method.

look at Gauss-Newton

(The information below has been expanded on past that presented in lecture)

$$\underline{a}_{k+1} = \underline{a}_k - \underline{H}_k \underline{g}_k$$

$$\underline{g}_k = \nabla S(\underline{a}_k) \rightarrow \quad g_j = \frac{\partial S}{\partial a_j}$$

$\underline{H}_k$ = Hessian of S @ $\underline{a}_k$

$$\Rightarrow H_{jk} = \frac{\partial^2 S}{\partial a_j \partial a_k} = \frac{d}{da_k}\left(\frac{dS}{da_j}\right) = \frac{dg_j}{da_k}$$

$$S(\underline{a}) = \sum_{i=1}^{n} (y_i - \hat{y}(x_i, \underline{a}_k))^2 = \sum_{i=1}^{n} r_i^2$$

$$g_j = \frac{d}{da_j}\left(\sum_{i=1}^{n} r_i^2\right) = 2\sum_{i=1}^{n} r_i \frac{\partial r_i}{\partial a_j} = 2\sum_{i=1}^{n} r_i J_{ij}$$ ↑ Jacobian of $r(\underline{a})$

$$\Rightarrow \underline{g} = 2\,\underline{r}^T \underline{J}$$

$$H_{jk} = 2\sum_{i=1}^{n}\left(\underbrace{\frac{\partial r_i}{\partial a_j}\frac{\partial r_i}{\partial a_k}}_{\text{1st-order}} + \underbrace{r_i \frac{\partial^2 r_i}{\partial a_j \partial a_k}}_{\text{2nd-order}}\right)$$

neglect 2nd-order part

Thus $H_{jk} \approx 2 \sum_{i=1}^{n} \frac{\partial r_i}{\partial a_j} \frac{\partial r_i}{\partial a_k} = 2 \sum_{i=1}^{n} J_{ij} J_{ik}$

$\Rightarrow \underline{H} = 2 \underline{J}^T \underline{J}$

$\Rightarrow \underline{a}_{k+1} = \underline{a}_k - \underline{H}_k^{-1} \underline{g}_k \approx \underline{a}_k - \frac{1}{2}(\underline{J}_k^T \underline{J}_k)^{-1} (2 \underline{J}_k^T \underline{r}_k)$

$\underline{a}_{k+1} = \underline{a}_k - (\underline{J}_k^T \underline{J}_k)(\underline{J}_k^T \underline{r}_k)$

Define $\underline{\delta}_k = \underline{a}_{k+1} - \underline{a}_k$

$\Rightarrow \underline{\delta}_k = -(\underline{J}_k^T \underline{J}_k)^{-1} (\underline{J}_k^T \underline{r}_k)$

$\underline{J}_k^T \underline{J}_k \underline{\delta}_k = -\underline{J}_k^T \underline{r}_k$ ← normal equations for $\underline{J} \underline{\delta}_k = -\underline{r}_k$!

Thus, solve $\underline{J}_k \underline{\delta}_k = -\underline{r}_k$ in least-squares sense, then $\underline{a}_{k+1} = \underline{a}_k + \alpha_k \underline{\delta}_k$

Advantage: No Hessian!

Disadvantage: Only converges if

$$\left| r_i \frac{\partial^2 r_i}{\partial a_j \partial a_k} \right| \ll \left| \frac{\partial r_i}{\partial a_j} \frac{\partial r_i}{\partial a_k} \right|$$

↑ Part that is ignored

↑ Part that is kept

Typically valid if $\|\underline{\alpha}\|$ is initially small or if $\hat{y}(x, \underline{\alpha})$ is mildly non-linear (no large oscillations).