Optimum Design

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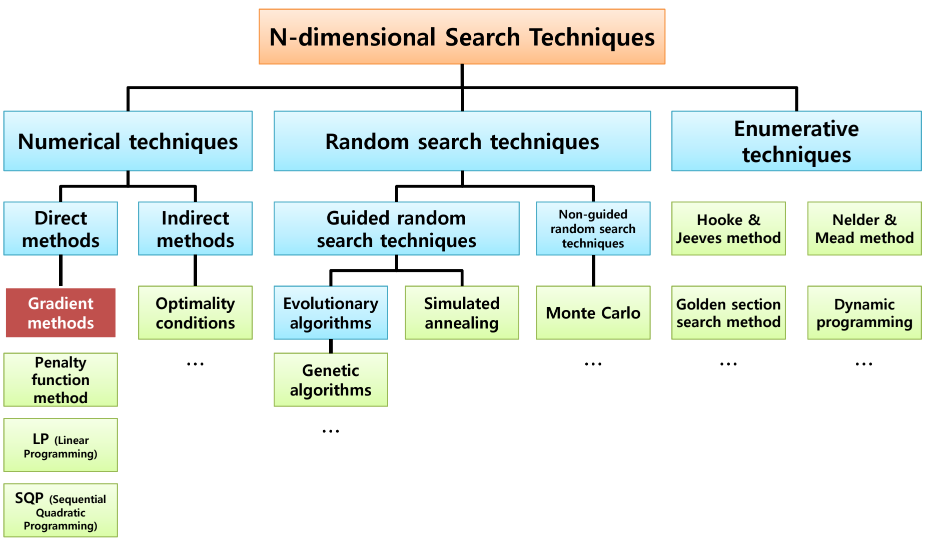
Classes of Search Techniques



Iterative Search for Optimum in Direct Methods

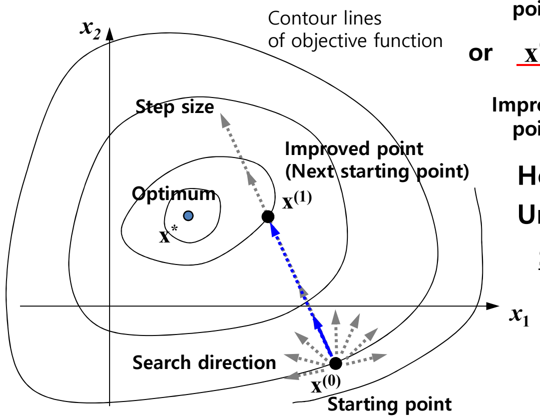
To find optimum is to improve the starting point continuously by determining the search direction and step size.

$$\underbrace{\mathbf{x}^{(k+1)}}_{\text{Improved point}} = \underbrace{\mathbf{x}^{(k)}}_{\text{Starting point}} + \underbrace{\alpha_k}_{\text{Step size}} \underbrace{\mathbf{d}^{(k)}}_{\text{Search direction}}$$

or

$$\underbrace{\mathbf{x}^{(k+1)}}_{\text{Improved point}} = \underbrace{\mathbf{x}^{(k)}}_{\text{Starting point}} + \underbrace{\mathbf{d}^{(k)}}_{\text{Design change}}$$

Ex) Minimize the objective function



How long should we do?
Until no improvement is made.

<u>**Stopping criteria**</u>

$\left|\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}\right| \le \underbrace{\varepsilon}_{\text{Convergence tolerance}}$ **or**

$\left|\mathbf{d}^{(k+1)} - \mathbf{d}^{(k)}\right| \le \varepsilon$ **or**

$\left|f(\mathbf{x}^{(k+1)}) - f(\mathbf{x}^{(k)})\right| \le \varepsilon$

Iterative Search for Optimum in Indirect Methods

To find optimum is to solve some equations, called optimality conditions, which should be satisfied at the optimum.

<u>**Necessary condition for $\mathbf{x} = \mathbf{x}^*$ to be a maximum or minimum**</u>

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

This method does not need any iterative search.

Thus, it does not need the starting point.

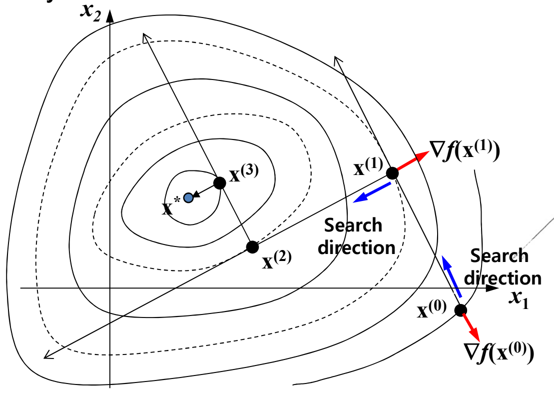
The necessary is to construct equations for optimality conditions from the problem, and then to solve the equations with a suitable method.

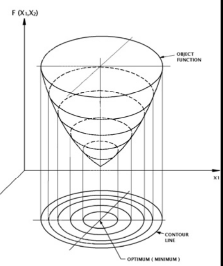
1. Steepest Descent Method (1/6)

- **Step 1: The search direction (d) is taken as the negative of the gradient of the objective function (f) at current iteration since the objective function decreases mostly rapidly toward that direction.**
  The direction of gradient vector of f, $\nabla f(\mathbf{x})$, is the direction of maximum increase of f at $\mathbf{x}$.

$$\text{Search direction} \quad \mathbf{d} = -\mathbf{c} \equiv -\nabla f(\mathbf{x})$$

- **Step 2: Iterate successively to find the optimum design point.**
  Ex) Minimize the objective function





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1. Steepest Descent Method (2/6): Example

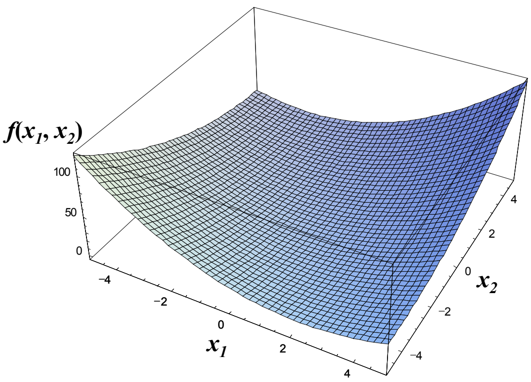
☑ **By using the steepest descent method, find the minimum design point for the following function of 2-variables.**

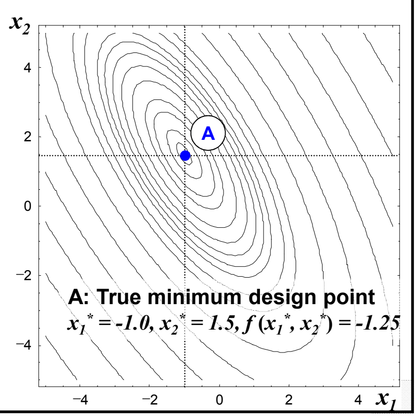
Given: Starting design point $\mathbf{x}^{(0)} = (0, 0)$, convergence tolerance $\varepsilon = 0.001$

Find: $\mathbf{x}^{(1)}$, $\mathbf{x}^{(2)}$

Minimize $f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$

➡ **Optimization problem with two unknown variables**





1. Steepest Descent Method (3/6): Example

Minimize $f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$ **Starting design point** $\mathbf{x}^{(0)}$ = (0, 0)

$$\nabla f(\mathbf{x}) = \nabla f(x_1, x_2) = \begin{pmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{pmatrix}$$

■ **1st Iteration: Find** $\mathbf{x}^{(1)}$

$$\nabla f(\mathbf{x}^{(0)}) = \nabla f\begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} - \alpha^{(0)} \nabla f(\mathbf{x}^{(0)})$$

$$= \begin{pmatrix} 0 \\ 0 \end{pmatrix} - \alpha \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} -\alpha \\ \alpha \end{pmatrix}$$ Replacing $\alpha^{(0)}$ to α for convenience

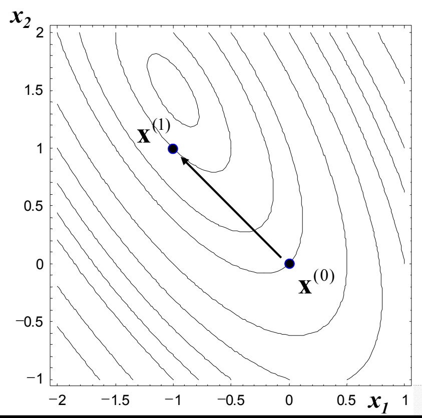
Substituting $\mathbf{x}^{(1)} = (-\alpha, \alpha)$ into the objective function

$$f(\mathbf{x}^{(1)}) = -\alpha - \alpha + 2\alpha^2 - 2\alpha^2 + \alpha^2$$
$$= \alpha^2 - 2\alpha$$

To minimize $f(\mathbf{x}^{(1)})$,

$$\boxed{\frac{df(\mathbf{x}^{(1)})}{d\alpha}} = 2\alpha - 2 = 0 \;\rightarrow\; \alpha = 1.0 \qquad \therefore \mathbf{x}^{(1)} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

How can we differentiate f with respect to α?



1. Steepest Descent Method (4/6): Example

Minimize $f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$ **Starting design point** $\mathbf{x}^{(0)}$ = (0, 0)

■ **2nd Iteration: Find** $\mathbf{x}^{(2)}$

$$\nabla f(\mathbf{x}^{(1)}) = \nabla f\begin{pmatrix} -1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{pmatrix} = \begin{pmatrix} -1 \\ -1 \end{pmatrix}$$

$$\mathbf{x}^{(2)} = \mathbf{x}^{(1)} - \alpha^{(1)} \nabla f(\mathbf{x}^{(1)})$$

$$= \begin{pmatrix} -1 \\ 1 \end{pmatrix} - \alpha \begin{pmatrix} -1 \\ -1 \end{pmatrix} = \begin{pmatrix} -1 + \alpha \\ 1 + \alpha \end{pmatrix}$$ Replacing $\alpha^{(1)}$ to α for convenience

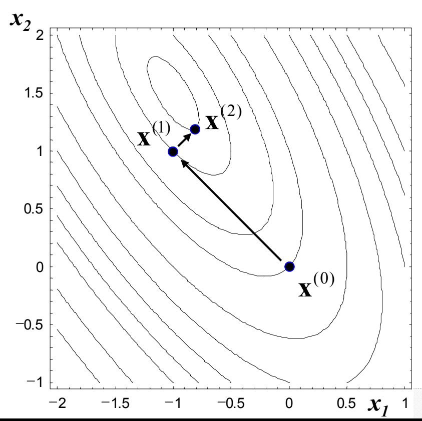
Substituting $\mathbf{x}^{(2)} = (-1 + \alpha, 1 + \alpha)$ into the objective function

$$f(\mathbf{x}^{(2)}) = 5\alpha^2 - 2\alpha - 1$$

To minimize $f(\mathbf{x}^{(2)})$,

$$\frac{df(\mathbf{x}^{(2)})}{d\alpha} = 10\alpha - 2 = 0 \;\rightarrow\; \alpha = 0.2$$

$$\therefore \mathbf{x}^{(2)} = \begin{pmatrix} -0.8 \\ 1.2 \end{pmatrix}$$



1. Steepest Descent Method (5/6): Example

Minimize $f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$ **Starting design point $\mathbf{x}^{(0)}$ = (0, 0)**

- **3rd Iteration: Find $\mathbf{x}^{(3)}$**

$$\nabla f(\mathbf{x}^{(2)}) = \nabla f\begin{pmatrix} -0.8 \\ 1.2 \end{pmatrix} = \begin{pmatrix} 1+4x_1+2x_2 \\ -1+2x_1+2x_2 \end{pmatrix} = \begin{pmatrix} 0.2 \\ -0.2 \end{pmatrix}$$

$$\mathbf{x}^{(3)} = \mathbf{x}^{(2)} - \alpha^{(2)}\nabla f(\mathbf{x}^{(2)})$$

$$= \begin{pmatrix} -0.8 \\ 1.2 \end{pmatrix} - \alpha\begin{pmatrix} 0.2 \\ -0.2 \end{pmatrix} = \begin{pmatrix} -0.8-0.2\alpha \\ 1.2+0.2\alpha \end{pmatrix}$$ Replacing $\alpha^{(1)}$ to α for convenience

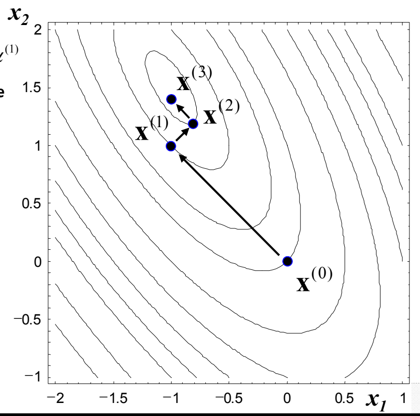
Substituting $\mathbf{x}^{(3)} = (-0.8-0.2\alpha, 1.2+0.2\alpha)$ **into the objective function**

$$f(\mathbf{x}^{(3)}) = 0.04\alpha^2 - 0.08\alpha - 1.2$$

To minimize $f(\mathbf{x}^{(3)})$,

$$\frac{df(\mathbf{x}^{(3)})}{d\alpha} = 0.08\alpha - 0.08 = 0 \ \rightarrow \ \alpha = 1.0$$

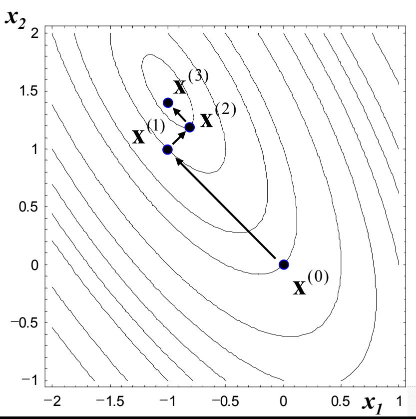
$$\therefore \mathbf{x}^{(3)} = \begin{pmatrix} -1 \\ 1.4 \end{pmatrix}$$



1. Steepest Descent Method (6/6): Example

Minimize $f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$ **Starting design point $\mathbf{x}^{(0)}$ = (0, 0)**

- **4th Iteration: Find the minimum design point.**
  To obtain the minimum design point, we have to iterate.
  If $\left|\mathrm{x}^{(k+1)} - \mathrm{x}^{(k)}\right| \le \varepsilon$, **then stop the iterative process because $\mathbf{x}^{(k+1)}$ can be assumed as the minimum design point.**



2. Conjugate Gradient Method (1/5)

☑ This method requires only a simple modification to the steepest descent method and dramatically improves the convergence rate of the optimization process.

☑ The current steepest descent direction is modified by adding a scaled direction used in the previous iteration.

- Step 1: Estimate a starting design point as $\mathbf{x}^{(0)}$. Set the iteration counter $k = 0$. Also, specify a tolerance ε for stopping criterion. Calculate

$$\mathbf{d}^{(0)} = -\mathbf{c}^{(0)} \equiv -\nabla f(\mathbf{x}^{(0)})$$

Check stopping criterion. If $\left\|\mathbf{c}^{(0)}\right\| < \varepsilon$, then stop. Otherwise, go to Step 4.

It is noted that Step 1 of the conjugate gradient method and steepest descent method is the same.

2. Conjugate Gradient Method (2/5)

- Step 2: Compute the gradient of the objective function as $\mathbf{c}^{(k)} = \nabla f(\mathbf{x}^{(k)})$. If $\left\|\mathbf{c}^{(k)}\right\| < \varepsilon$, then stop; otherwise continue.

- Step 3: Calculate the new search direction as

$$\boxed{\mathbf{d}^{(k)} = -\mathbf{c}^{(k)} + \beta_k \mathbf{d}^{(k-1)}} \longrightarrow \text{Previous search direction}$$

$$\beta_k = \left(\left\|\mathbf{c}^{(k)}\right\| / \left\|\mathbf{c}^{(k-1)}\right\|\right)^2$$

The current search direction is calculated by adding a scaled direction used in the previous iteration.

- Step 4: Compute a step size $\alpha = \alpha_k$ to minimize $f(\mathbf{x}^{(k)}+\alpha\mathbf{d}^{(k)})$.

- Step 5: Change the design point as follows, then set $k = k+1$ and go to Step 2.

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k \mathbf{d}^{(k)}$$

2. Conjugate Gradient Method (3/5): Example

Minimize $f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$ **Starting design point $\mathbf{x}^{(0)}$ = (0, 0)**

$$\nabla f(\mathbf{x}) = \nabla f(x_1, x_2) = \begin{pmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{pmatrix}$$

☑ **1st Iteration: Find $\mathbf{x}^{(1)}$**

$$\mathbf{d}^{(0)} = -\mathbf{c}^{(0)} = -\nabla f\left(\mathbf{x}^{(0)}\right) = -\nabla f\begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$= -\begin{pmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{pmatrix} = -\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \alpha_0 \mathbf{d}^{(0)}$$

$$= \begin{pmatrix} 0 \\ 0 \end{pmatrix} + \alpha \begin{pmatrix} -1 \\ 1 \end{pmatrix} = \begin{pmatrix} -\alpha \\ \alpha \end{pmatrix}$$

Replacing α_0 to α for convenience

Substituting $\mathbf{x}^{(1)} = (-\alpha, \alpha)$ into the objective function

$$f(\mathbf{x}^{(1)}) = -\alpha - \alpha + 2\alpha^2 - 2\alpha^2 + \alpha^2$$

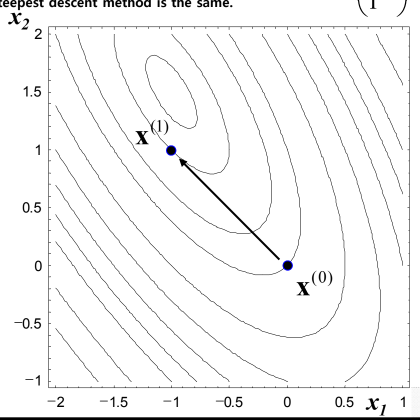
$$= \alpha^2 - 2\alpha$$

To minimize $f(\mathbf{x}^{(1)})$,

$$\frac{df(\mathbf{x}^{(1)})}{d\alpha} = 2\alpha - 2 = 0 \;\rightarrow\; \alpha = 1.0$$

$$\therefore \mathbf{x}^{(1)} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

Note: Step 1 of the conjugate gradient method and steepest descent method is the same.



2. Conjugate Gradient Method (4/5): Example

Minimize $f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$

■ **2nd Iteration: Find $\mathbf{x}^{(2)}$**

Compute the gradient of the objective function as

$$\mathbf{c}^{(1)} = \nabla f\left(\mathbf{x}^{(1)}\right)$$

$$= \nabla f\begin{pmatrix} -1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{pmatrix} = \begin{pmatrix} -1 \\ -1 \end{pmatrix}$$

Calculate the new search direction as

$$\mathbf{d}^{(1)} = -\mathbf{c}^{(1)} + \beta_1 \mathbf{d}^{(0)} = -\mathbf{c}^{(1)} + \frac{\left\|\nabla f\left(\mathbf{x}^{(1)}\right)\right\|^2}{\left\|\nabla f\left(\mathbf{x}^{(0)}\right)\right\|^2}\mathbf{d}^{(0)}$$

$$= -\begin{pmatrix} -1 \\ -1 \end{pmatrix} + \frac{2}{2}\begin{pmatrix} -1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 2 \end{pmatrix}$$

$$\mathbf{x}^{(1)} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$\mathbf{d}^{(0)} = -\nabla f\left(\mathbf{x}^{(0)}\right) = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$\mathbf{d}^{(k)} = -\mathbf{c}^{(k)} + \beta_k \mathbf{d}^{(k-1)}$$

$$\beta_k = (\|\mathbf{c}^{(k)}\| / \|\mathbf{c}^{(k-1)}\|)^2$$

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k \mathbf{d}^{(k)}$$

2. Conjugate Gradient Method (5/5): Example

Minimize $f(x_1,x_2)=x_1-x_2+2x_1^2+2x_1x_2+x_2^2$

$$\mathbf{x}^{(k+1)}=\mathbf{x}^{(k)}+\alpha_k\mathbf{d}^{(k)}$$

$$\mathbf{x}^{(1)}=\begin{pmatrix}-1\\1\end{pmatrix}\quad \mathbf{d}^{(1)}=\begin{pmatrix}0\\2\end{pmatrix}$$

$$\nabla f(\mathbf{x})=\nabla f(x_1,x_2)=\begin{pmatrix}1+4x_1+2x_2\\-1+2x_1+2x_2\end{pmatrix}$$

$$\mathbf{x}^{(2)}=\mathbf{x}^{(1)}+\alpha_1\mathbf{d}^{(1)}$$

$$=\begin{pmatrix}-1\\1\end{pmatrix}+\alpha\begin{pmatrix}0\\2\end{pmatrix}=\begin{pmatrix}-1\\1+2\alpha\end{pmatrix}$$

Replacing α_1 to α for convenience

Substituting $\mathbf{x}^{(2)}=(-1,1+2\alpha)$ into the objective function

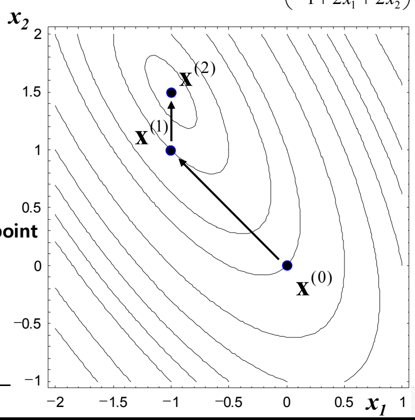
$$f(\mathbf{x}^{(2)})=4\alpha^2-2\alpha-1$$

To minimize $f(\mathbf{x}^{(1)})$,

$$\frac{df(\mathbf{x}^{(2)})}{d\alpha}=8\alpha-2=0\ \rightarrow\ \alpha=0.25$$

$$\therefore \mathbf{x}^{(2)}=\begin{pmatrix}-1\\1.5\end{pmatrix}$$

→Minimum design point



Check stopping criterion.

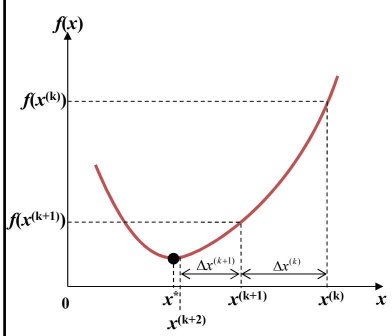
$$\mathbf{c}^{(2)}=\nabla f\left(\mathbf{x}^{(2)}\right)=\nabla f\begin{pmatrix}-1\\1.5\end{pmatrix}=\begin{pmatrix}0\\0\end{pmatrix}$$

$$\left\|\mathbf{c}^{(2)}\right\|=0<\varepsilon\quad \rightarrow \textbf{Stop!}$$

3. Newton's Method (1/9)

Given: $f(x)$

Find: x^* which minimizes $f(x)$



Assume that $f(x)$ has minimum at $x^{(k+1)}=x^{(k)}+\Delta x^{(k)}$.

Consider the quadratic approximation of the function $f(x)$ at $x=x^{(k)}$ using the second-order Taylor expansion.

$$f(x^{(k)}+\Delta x^{(k)})=f(x^{(k)})+\frac{df(x^{(k)})}{dx}\Delta x^{(k)}+\frac{1}{2}\frac{d^2f(x^{(k)})}{dx^2}\left(\Delta x^{(k)}\right)^2+\cancel{O\left(\left(\Delta x^{(k)}\right)^3\right)}$$

In this equation, $x^{(k)}$ is a constant and $\Delta x^{(k)}$ is a variable. So, the following equation is a quadratic function in terms of $\Delta x^{(k)}$.

$$f(x^{(k)}+\Delta x^{(k)})=f(x^{(k)})+\frac{df(x^{(k)})}{dx}\Delta x^{(k)}+\frac{1}{2}\frac{d^2f(x^{(k)})}{dx^2}\left(\Delta x^{(k)}\right)^2$$

Differentiate this equation with respect to $\Delta x^{(k)}$.

$$\frac{df(x^{(k)}+\Delta x^{(k)})}{d\Delta x^{(k)}}=\frac{df(x^{(k)})}{dx}+\frac{d^2f(x^{(k)})}{dx^2}\Delta x^{(k)}=0 \rightarrow$$ The necessary condition for minimization of this function

Calculate the small change $\Delta x^{(k)}$ in design.

$$\Delta x^{(k)}=\left(-\frac{df(x^{(k)})}{dx}\right)\Big/\left(\frac{d^2f(x^{(k)})}{dx^2}\right)$$

Is $|\Delta x^{(k)}|<\varepsilon$?

NO → $k=k+1$

YES → Set $x^*=x^{(k+1)}$ and stop the iteration.

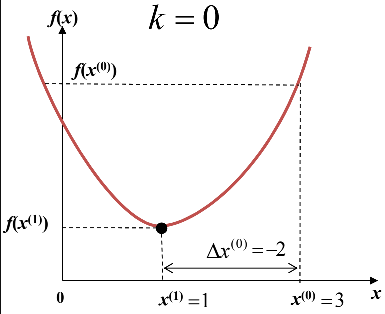
3. Newton's Method (2/9): Example

Given: $f(x) = x^2 - 2x + 2$

Starting design point $x^{(0)} = 3$

Find: x^* **which minimizes** $f(x)$

$k = 0$



Assume that $f(x)$ has minimum at $x^{(1)} = x^{(0)} + \Delta x^{(0)}$.

Consider the quadratic approximation of the function $f(x)$ at $x = x^{(0)}$ using the second-order Taylor expansion.

$$f(x^{(0)} + \Delta x^{(0)}) = f(x^{(0)}) + \frac{df(x^{(0)})}{dx}\Delta x^{(0)} + \frac{1}{2}\frac{d^2 f(x^{(0)})}{dx^2}\left(\Delta x^{(0)}\right)^2$$

In this equation, $x^{(0)}$ is a constant and $\Delta x^{(0)}$ is a variable. So, the following equation is a quadratic function in terms of $\Delta x^{(0)}$.

$$f(x^{(0)} + \Delta x^{(0)}) = f(x^{(0)}) + \frac{df(x^{(0)})}{dx}\Delta x^{(0)} + \frac{1}{2}\frac{d^2 f(x^{(0)})}{dx^2}\left(\Delta x^{(0)}\right)^2$$

Differentiate this equation with respect to $\Delta x^{(0)}$.

$$\frac{df(x^{(0)} + \Delta x^{(0)})}{d\Delta x^{(0)}} = \frac{df(x^{(0)})}{dx} + \frac{d^2 f(x^{(0)})}{dx^2}\Delta x^{(0)} = 0 \rightarrow$$ The necessary condition for minimization of this function

Calculate the small change $\Delta x^{(0)}$ in design.

$$\Delta x^{(0)} = \left(-\frac{df(x^{(0)})}{dx}\right) \Big/ \left(\frac{d^2 f(x^{(0)})}{dx^2}\right)$$

$$= (-2x+2)_{x=3} / (2)_{x=3} = -2$$

Is $|\Delta x^{(0)}| < \varepsilon$?

NO

$k = k + 1$

$= 0 + 1 = 1$

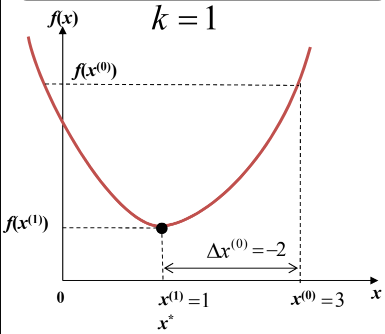
3. Newton's Method (3/9): Example

Given: $f(x) = x^2 - 2x + 2$

Starting design point $x^{(0)} = 3$

Find: x^* **which minimizes** $f(x)$

$k = 1$



Assume that $f(x)$ has minimum at $x^{(2)} = x^{(1)} + \Delta x^{(1)}$.

Consider the quadratic approximation of the function $f(x)$ at $x = x^{(1)}$ using the second-order Taylor expansion.

$$f(x^{(1)} + \Delta x^{(1)}) = f(x^{(1)}) + \frac{df(x^{(1)})}{dx}\Delta x^{(1)} + \frac{1}{2}\frac{d^2 f(x^{(1)})}{dx^2}\left(\Delta x^{(1)}\right)^2$$

In this equation, $x^{(1)}$ is a constant and $\Delta x^{(1)}$ is a variable. So, the following equation is a quadratic function in terms of $\Delta x^{(1)}$.

$$f(x^{(1)} + \Delta x^{(1)}) = f(x^{(1)}) + \frac{df(x^{(1)})}{dx}\Delta x^{(1)} + \frac{1}{2}\frac{d^2 f(x^{(1)})}{dx^2}\left(\Delta x^{(1)}\right)^2$$

Differentiate this equation with respect to $\Delta x^{(1)}$.

$$\frac{df(x^{(1)} + \Delta x^{(1)})}{d\Delta x^{(1)}} = \frac{df(x^{(1)})}{dx} + \frac{d^2 f(x^{(1)})}{dx^2}\Delta x^{(1)} = 0 \rightarrow$$ The necessary condition for minimization of this function

Calculate the small change $\Delta x^{(1)}$ in design.

$$\Delta x^{(1)} = \left(-\frac{df(x^{(1)})}{dx}\right) \Big/ \left(\frac{d^2 f(x^{(1)})}{dx^2}\right)$$

$$= (-2x+2)_{x=1} / (2)_{x=1} = 0$$

Is $|\Delta x^{(1)}| < \varepsilon$?

YES

Set $x^* = x^{(1)}$ and stop the iteration.

Is it possible to find the x* which minimizes a cubic function at once?

3. Newton's Method (4/9): Example

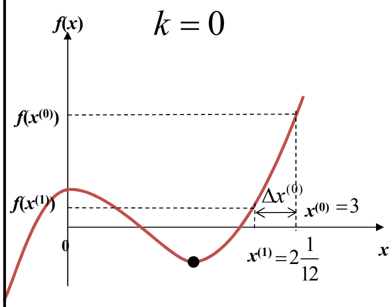
Is it possible to find the x* which minimizes a cubic function at once?

Given: $f(x) = x^3 - 3x^2 + 2x$

Starting design point $x^{(0)} = 3$

Find: x^* which minimizes $f(x)$

$k = 0$



Assume that $f(x)$ has minimum at $x^{(1)} = x^{(0)} + \Delta x^{(0)}$.

Consider the quadratic approximation of the function $f(x)$ at $x = x^{(0)}$ using the second-order Taylor expansion.

$$f(x^{(0)} + \Delta x^{(0)}) = f(x^{(0)}) + \frac{df(x^{(0)})}{dx}\Delta x^{(0)} + \frac{1}{2}\frac{d^2 f(x^{(0)})}{dx^2}(\Delta x^{(0)})^2 + \cancel{O((\Delta x^{(0)})^3)}$$

In this equation, $x^{(0)}$ is a constant and $\Delta x^{(0)}$ is a variable. So, the following equation is a quadratic function in terms of $\Delta x^{(0)}$.

$$f(x^{(0)} + \Delta x^{(0)}) = f(x^{(0)}) + \frac{df(x^{(0)})}{dx}\Delta x^{(0)} + \frac{1}{2}\frac{d^2 f(x^{(0)})}{dx^2}(\Delta x^{(0)})^2$$

Differentiate this equation with respect to $\Delta x^{(0)}$.

$$\frac{df(x^{(0)} + \Delta x^{(0)})}{d\Delta x^{(0)}} = \frac{df(x^{(0)})}{dx} + \frac{d^2 f(x^{(0)})}{dx^2}\Delta x^{(0)} = 0 \rightarrow$$ The necessary condition for minimization of this function

Calculate the small change $\Delta x^{(0)}$ in design.

$$\Delta x^{(0)} = \left(-\frac{df(x^{(0)})}{dx}\right) \Big/ \left(\frac{d^2 f(x^{(0)})}{dx^2}\right)$$

$$= \left(-3x^2 + 6x - 2\right)_{x=3} / \left(6x - 6\right)_{x=3} = -\frac{11}{12}$$

Is $|\Delta x^{(0)}| < \varepsilon$?

NO

$k = k + 1$
$= 0 + 1 = 1$

3. Newton's Method (5/9): Example

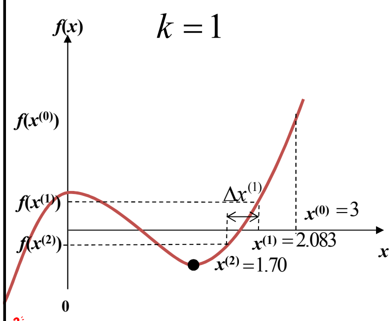
Is it possible to find the x* which minimizes a cubic function at once?

Given: $f(x) = x^3 - 3x^2 + 2x$

Starting design point $x^{(0)} = 3$

Find: x^* which minimizes $f(x)$

$k = 1$



Assume that $f(x)$ has minimum at $x^{(2)} = x^{(1)} + \Delta x^{(1)}$.

Consider the quadratic approximation of the function $f(x)$ at $x = x^{(1)}$ using the second-order Taylor expansion.

$$f(x^{(1)} + \Delta x^{(1)}) = f(x^{(1)}) + \frac{df(x^{(1)})}{dx}\Delta x^{(1)} + \frac{1}{2}\frac{d^2 f(x^{(1)})}{dx^2}(\Delta x^{(1)})^2 + \cancel{O((\Delta x^{(1)})^3)}$$

In this equation, $x^{(1)}$ is a constant and $\Delta x^{(1)}$ is a variable. So, the following equation is a quadratic function in terms of $\Delta x^{(1)}$.

$$f(x^{(1)} + \Delta x^{(1)}) = f(x^{(1)}) + \frac{df(x^{(1)})}{dx}\Delta x^{(1)} + \frac{1}{2}\frac{d^2 f(x^{(1)})}{dx^2}(\Delta x^{(1)})^2$$

Differentiate this equation with respect to $\Delta x^{(1)}$.

$$\frac{df(x^{(1)} + \Delta x^{(1)})}{d\Delta x^{(1)}} = \frac{df(x^{(1)})}{dx} + \frac{d^2 f(x^{(1)})}{dx^2}\Delta x^{(1)} = 0 \rightarrow$$ The necessary condition for minimization of this function

Calculate the small change $\Delta x^{(1)}$ in design.

$$\Delta x^{(1)} = \left(-\frac{df(x^{(1)})}{dx}\right) \Big/ \left(\frac{d^2 f(x^{(1)})}{dx^2}\right)$$

$$= \left(-3x^2 + 6x - 2\right)_{x=\frac{25}{12}} / \left(6x - 6\right)_{x=\frac{25}{12}} = -0.388$$

Is $|\Delta x^{(1)}| < \varepsilon$?

NO

$k = k + 1$
$= 1 + 1 = 2$

Why is it not possible to find the x* which minimizes a cubic function at once?

⇨ Since the second-order Taylor expansion is just an approximation for $f(x)$ at the point $x^{(0)}$ or $x^{(1)}$, $x^{(1)}$ or $x^{(2)}$ will probably not be the precise minimum design point of $f(x)$.

3. Newton's Method (6/9): Example of Function of Two Variables

Minimize $f(\mathbf{x}) = f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$, Starting design point $\mathbf{x}^{(0)}$ = (0, 0)

$$\nabla f(\mathbf{x}) = \nabla f(x_1, x_2) = \begin{pmatrix} f_{x_1} \\ f_{x_2} \end{pmatrix} = \begin{pmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{pmatrix}, \quad \mathbf{H}(\mathbf{x}) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_1 \partial x_2} & \frac{\partial^2 f}{\partial x_2^2} \end{pmatrix} = \begin{pmatrix} 4 & 2 \\ 2 & 2 \end{pmatrix}$$

- **1st Iteration: Find $\mathbf{x}^{(1)}$**

Assume that $f(x)$ has minimum at $\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \Delta\mathbf{x}^{(0)}$.

Consider the quadratic approximation of the function $f(\mathbf{x})$ at $\mathbf{x} = \mathbf{x}^{(0)}$ using the second-order Taylor expansion.

$$f(\mathbf{x}^{(0)} + \Delta\mathbf{x}^{(0)}) = f(\mathbf{x}^{(0)}) + \nabla f(\mathbf{x}^{(0)})^T \Delta\mathbf{x}^{(0)} + \frac{1}{2}(\Delta\mathbf{x}^{(0)})^T \mathbf{H}(\mathbf{x}^{(0)}) \Delta\mathbf{x}^{(0)}$$

How?

In this equation, $\mathbf{x}^{(0)}$ is a constant and $\Delta\mathbf{x}^{(0)}$ is a variable. So, the following equation is a quadratic function in terms of $\Delta\mathbf{x}^{(0)}$.

$$f(\mathbf{x}^{(0)} + \Delta\mathbf{x}^{(0)}) = f(\mathbf{x}^{(0)}) + \nabla f(\mathbf{x}^{(0)})^T \Delta\mathbf{x}^{(0)} + \frac{1}{2}(\Delta\mathbf{x}^{(0)})^T \mathbf{H}(\mathbf{x}^{(0)}) \Delta\mathbf{x}^{(0)}$$

3. Newton's Method (7/9): Example of Function of Two Variables

Minimize $f(\mathbf{x}) = f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$, Starting design point $\mathbf{x}^{(0)}$ = (0, 0)

- **1st Iteration: Find $\mathbf{x}^{(1)}$**

$$f(\mathbf{x}^{(0)} + \Delta\mathbf{x}^{(0)}) = f(\mathbf{x}^{(0)}) + \nabla f(\mathbf{x}^{(0)})^T \Delta\mathbf{x}^{(0)} + \frac{1}{2}(\Delta\mathbf{x}^{(0)})^T \mathbf{H}(\mathbf{x}^{(0)}) \Delta\mathbf{x}^{(0)}$$

How?

$$\nabla f(\mathbf{x}) = \nabla f(x_1, x_2) = \begin{pmatrix} f_{x_1} \\ f_{x_2} \end{pmatrix} = \begin{pmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{pmatrix}$$

Differentiate this equation with respect to $\Delta\mathbf{x}^{(0)}$.

$$\frac{\partial f(\mathbf{x}^{(0)} + \Delta\mathbf{x}^{(0)})}{\partial(\Delta\mathbf{x}^{(0)})} = \nabla f(\mathbf{x}^{(0)}) + \mathbf{H}(\mathbf{x}^{(0)}) \Delta\mathbf{x}^{(0)} = 0 \longrightarrow$$

The necessary condition for minimization of function $f(x_1, x_2)$

Calculate the small change $\Delta\mathbf{x}^{(0)}$ in design.

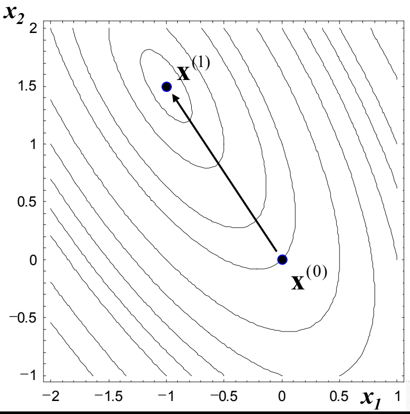
$$\mathbf{H}(\mathbf{x}^{(0)}) \Delta\mathbf{x}^{(0)} = -\nabla f(\mathbf{x}^{(0)})$$

$$\Delta\mathbf{x}^{(k)} = -[\mathbf{H}(\mathbf{x}^{(k)})]^{-1} \nabla f(\mathbf{x}^{(k)})$$

$$\downarrow \quad \left(-\nabla f(\mathbf{x}^{(0)}) = \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \ \mathbf{H}(\mathbf{x}^{(0)}) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_1 \partial x_2} & \frac{\partial^2 f}{\partial x_2^2} \end{pmatrix} = \begin{pmatrix} 4 & 2 \\ 2 & 2 \end{pmatrix} \right)$$

$$\begin{pmatrix} \Delta x_1^{(0)} \\ \Delta x_2^{(0)} \end{pmatrix} = \begin{pmatrix} 4 & 2 \\ 2 & 2 \end{pmatrix}^{-1} \begin{pmatrix} -1 \\ 1 \end{pmatrix} \rightarrow \begin{pmatrix} \Delta x_1^{(0)} \\ \Delta x_2^{(0)} \end{pmatrix} = \begin{pmatrix} -1 \\ 1.5 \end{pmatrix}$$

$$\therefore x^{(1)} = x^{(0)} + \Delta\mathbf{x}^{(0)} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} + \begin{pmatrix} -1 \\ 1.5 \end{pmatrix} = \begin{pmatrix} -1 \\ 1.5 \end{pmatrix}$$



3. Newton's Method (8/9): Example of Function of Two Variables

Minimize $f(\mathbf{x}) = f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$, Starting design point $\mathbf{x}^{(0)}$ = (0, 0)

■ 2nd Iteration: Find $\mathbf{x}^{(2)}$ $\qquad x^{(1)} = \begin{pmatrix} -1 \\ 1.5 \end{pmatrix}$

In the same way as 1st Iteration,

Assume that $f(x)$ has minimum at $\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + \Delta\mathbf{x}^{(1)}$.

Consider the quadratic approximation of the function $f(\mathbf{x})$ at $\mathbf{x} = \mathbf{x}^{(1)}$ using the second-order Taylor expansion.

$$f(\mathbf{x}^{(1)} + \Delta\mathbf{x}^{(1)}) = f(\mathbf{x}^{(1)}) + \nabla f(\mathbf{x}^{(1)})^T \Delta\mathbf{x}^{(1)} + \frac{1}{2}(\Delta\mathbf{x}^{(1)})^T \mathbf{H}(\mathbf{x}^{(1)})\Delta\mathbf{x}^{(1)}$$

In this equation, $\mathbf{x}^{(1)}$ is a constant and $\Delta\mathbf{x}^{(1)}$ is a variable. So, the following equation is a quadratic function in terms of $\Delta\mathbf{x}^{(1)}$.

$$f(\mathbf{x}^{(1)} + \Delta\mathbf{x}^{(1)}) = f(\mathbf{x}^{(1)}) + \nabla f(\mathbf{x}^{(1)})^T \Delta\mathbf{x}^{(1)} + \frac{1}{2}(\Delta\mathbf{x}^{(1)})^T \mathbf{H}(\mathbf{x}^{(1)})\Delta\mathbf{x}^{(1)}$$

Differentiate this equation with respect to $\Delta\mathbf{x}^{(1)}$.

$$\frac{\partial f(\mathbf{x}^{(1)} + \Delta\mathbf{x}^{(1)})}{\partial(\Delta\mathbf{x}^{(1)})} = \nabla f(\mathbf{x}^{(1)}) + \mathbf{H}(\mathbf{x}^{(1)})\Delta\mathbf{x}^{(1)} = 0 \longrightarrow$$

The necessary condition for minimization of function $f(x_1, x_2)$

3. Newton's Method (9/9): Example of Function of Two Variables

Minimize $f(\mathbf{x}) = f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$, Starting design point $\mathbf{x}^{(0)}$ = (0, 0)

■ 2nd Iteration: Find $\mathbf{x}^{(2)}$ $\qquad x^{(1)} = \begin{pmatrix} -1 \\ 1.5 \end{pmatrix}$

$$\nabla f(\mathbf{x}) = \nabla f(x_1, x_2) = \begin{pmatrix} f_{x_1} \\ f_{x_2} \end{pmatrix} = \begin{pmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{pmatrix}$$

Calculate the small change $\Delta\mathbf{x}^{(1)}$ in design.

$$\mathbf{H}(\mathbf{x}^{(1)})\Delta\mathbf{x}^{(1)} = -\nabla f(\mathbf{x}^{(1)})$$

$$\Delta\mathbf{x}^{(k)} = -[\mathbf{H}(\mathbf{x}^{(k)})]^{-1}\nabla f(\mathbf{x}^{(k)})$$

$$\downarrow \left(-\nabla f(\mathbf{x}^{(1)}) = \begin{pmatrix} 0 \\ 0 \end{pmatrix},\ \mathbf{H}(\mathbf{x}^{(1)}) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_1 \partial x_2} & \frac{\partial^2 f}{\partial x_2^2} \end{pmatrix} = \begin{pmatrix} 4 & 2 \\ 2 & 2 \end{pmatrix} \right)$$

$$\begin{pmatrix} \Delta\mathbf{x}_1^{(1)} \\ \Delta\mathbf{x}_2^{(1)} \end{pmatrix} = \begin{pmatrix} 4 & 2 \\ 2 & 2 \end{pmatrix}^{-1} \begin{pmatrix} 0 \\ 0 \end{pmatrix} \rightarrow \begin{pmatrix} \Delta\mathbf{x}_1^{(1)} \\ \Delta\mathbf{x}_2^{(1)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

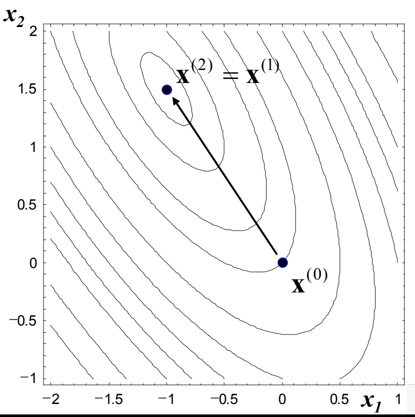
$$\therefore x^{(2)} = x^{(1)} + \Delta\mathbf{x}^{(1)} = \begin{pmatrix} -1 \\ 1.5 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} -1 \\ 1.5 \end{pmatrix}$$

→Optimal design point

Check stopping criterion.

$$\left|\Delta\mathbf{x}^{(1)}\right| = 0 < \varepsilon$$

→Stop!



3. Modified Newton's Method (1/3)

☑ In this method, we treat $\Delta\mathbf{x}^{(k)} = -[\mathbf{H}(\mathbf{x}^{(k)})]^{-1}\nabla f(\mathbf{x}^{(k)})$ of the Newton's method as the search direction and use any of the one dimensional search methods to calculate the step size in the search direction.

- Step 1: Estimate a starting design point $\mathbf{x}^{(0)}$.
  Set iteration counter $k = 0$. Specify a tolerance ε for the stopping criterion.

- Step 2: Calculate $c_i^{(k)} = \partial f(\mathbf{x}^{(k)})/\partial x_i$ for $i = 1$ to n. If $\|\mathbf{c}^{(k)}\| < \varepsilon$, then stop the iterative process. Otherwise, continue.

- Step 3: Calculate the Hessian matrix $\mathbf{H}^{(k)}$ at current design point $\mathbf{x}^{(k)}$.

$$\mathbf{H}(\mathbf{x}^{(k)}) = \left[\frac{\partial^2 f}{\partial x_i \partial x_j}\right], \quad i = 1,\cdots,n; \; j = 1,\cdots,n$$

3. Modified Newton's Method (2/3)

- Step 4: Calculate the search direction as follows:

$$\boxed{\mathbf{d}^{(k)} = \Delta\mathbf{x}^{(k)} = -\mathbf{H}^{-1}\mathbf{c}^{(k)}}$$

When $f(\mathbf{x}^* + \Delta\mathbf{x}) = f(\mathbf{x}^*) + \mathbf{c}^T\Delta\mathbf{x} + \frac{1}{2}\Delta\mathbf{x}^T\mathbf{H}(\mathbf{x}^*)\,\Delta\mathbf{x}$,
the necessary condition for minimization of this function is as follows:

$$df(\Delta\mathbf{x})/d\Delta\mathbf{x} = \mathbf{c} + \mathbf{H}(\mathbf{x}^*)\Delta\mathbf{x} = 0$$

$$\Rightarrow \mathbf{H}(\mathbf{x}^*)\,\Delta\mathbf{x} = -\mathbf{c} \Rightarrow \; \Delta\mathbf{x} = -\mathbf{H}(\mathbf{x}^*)^{-1}\mathbf{c}$$

- Step 5: Update the design point as $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha\mathbf{d}^{(k)}$, where α is calculated to minimize $f(\mathbf{x}^{(k)} + \alpha\mathbf{d}^{(k)})$. Any one dimensional search method may be used to calculate α.

- Step 6: Set $k = k+1$ and go to Step 2.

3. Modified Newton's Method (3/3)
- Disadvantages of the Newton's Method

The Newton's method is not very useful in practice, due to following features of the method:

1. It requires the storing of the $n \times n$ matrix $\mathbf{H}(\mathbf{x}^{(k)})$.
2. It becomes very difficult and sometimes, impossible to compute the elements of the matrix $\mathbf{H}(\mathbf{x}^{(k)})$.
3. It requires the inversion of the matrix $\mathbf{H}(\mathbf{x}^{(k)})$ at each iteration.
4. It requires the evaluation of the quantity $\mathbf{H}(\mathbf{x}^{(k)})^{-1}\nabla f(\mathbf{x}^{(k)})$ at each iteration.

4. Davidon-Fletcher-Powell (DFP) Method (1/6)

☑ This method builds an approximation for the inverse of the Hessian matrix of $f(\mathbf{x})$ using only the first derivatives.

- Step 1: Estimate a starting design point $\mathbf{x}^{(0)}$.
  Choose a symmetric positive definite $n \times n$ matrix $\mathbf{A}^{(0)}$ as an approximation for the inverse of the Hessian matrix of the objective function. In the absence of more information, $\mathbf{A}^{(0)} = \mathbf{I}$ may be chosen. Also, specify a tolerance ε for the stopping criterion. Set $k = 0$ and compute the gradient vector as $\mathbf{d}^{(0)} = -\mathbf{c}^{(0)} \equiv -\nabla f(\mathbf{x}^{(0)})$.

- Step 2: Calculate the norm of the gradient vector as $\left\|\mathbf{c}^{(k)}\right\|$.
  If $\left\|\mathbf{c}^{(k)}\right\| < \varepsilon$, then stop the iterative process. Otherwise, continue.
  It is noted that Step 1 and 2 of this method and the steepest descent method are the same.

4. Davidon-Fletcher-Powell (DFP) Method (2/6)

- Step 3: Calculate the search direction as follows:

$$\boxed{\mathbf{d}^{(k)} = -\mathbf{A}^{(k)}\mathbf{c}^{(k)}}$$

Newton's method

$$\Delta\mathbf{x}^{(k)} = -[\mathbf{H}(\mathbf{x}^{(k)})]^{-1}\nabla f(\mathbf{x}^{(k)})$$
$$\therefore \mathbf{d}^{(k)} = -(\mathbf{H}^{(k)})^{-1}\mathbf{c}^{(k)}$$

Here, the matrix $\mathbf{A}$ is used as an estimate for the inverse of the Hessian matrix $\mathbf{H}^{-1}$ of the objective function.

- Step 4: Compute optimum step size $\alpha = \alpha_k$ to minimize $f(\mathbf{x}^{(k)} + \alpha\mathbf{d}^{(k)})$.

- Step 5: Update the design point as $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k\mathbf{d}^{(k)}$.

4. Davidon-Fletcher-Powell (DFP) Method (3/6)

- Step 6: Update the matrix $\mathbf{A}^{(k)}$ - approximation for the inverse of the Hessian matrix of the objective function - as follows:

$$\mathbf{A}^{(k+1)} = \mathbf{A}^{(k)} + \mathbf{B}^{(k)} + \mathbf{C}^{(k)} \quad ; \ n \times n \text{ matrix}$$

where, the correction matrices $\mathbf{B}^{(k)}$ and $\mathbf{C}^{(k)}$ are calculated as below.

$$\mathbf{B}^{(k)} = \frac{\mathbf{s}^{(k)}\mathbf{s}^{(k)^T}}{\mathbf{s}^{(k)^T}\mathbf{y}^{(k)}} \quad ; \ n \times n \ \text{ matrix} \qquad \mathbf{C}^{(k)} = \frac{-\mathbf{z}^{(k)}\mathbf{z}^{(k)^T}}{\mathbf{y}^{(k)^T}\mathbf{z}^{(k)}} \quad ; \ n \times n \ \text{ matrix}$$

$$\mathbf{s}^{(k)} = \alpha_k\mathbf{d}^{(k)} \quad : \ n \times 1 \ \text{ matrix}$$
$$\mathbf{y}^{(k)} = \mathbf{c}^{(k+1)} - \mathbf{c}^{(k)} \quad : \ n \times 1 \ \text{ matrix}$$
$$\mathbf{c}^{(k+1)} = \nabla f(\mathbf{x}^{(k+1)}) \quad : \ n \times 1 \ \text{ matrix}$$
$$\mathbf{z}^{(k)} = \mathbf{A}^{(k)}\mathbf{y}^{(k)} \quad : \ [n \times n][n \times 1] = [n \times 1] \ \text{ matrix}$$

$\mathbf{d}^{(k)}$: search direction
$\alpha^{(k)}$: optimum step size

- Step 7: Set $k = k+1$ and go to Step 2.

4. Davidon-Fletcher-Powell (DFP) Method (4/6): Example

Minimize $f(\mathbf{x}) = f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2,$ **Starting design point $\mathbf{x}^{(0)}$ = (0, 0)**

$$\nabla f(\mathbf{x}) = \nabla f(x_1, x_2) = \begin{pmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{pmatrix}$$

■ **1st Iteration: Find $\mathbf{x}^{(1)}$**

$$\mathbf{x}^{(0)} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \ \mathbf{A}^{(0)} = \mathbf{I}$$

$$\mathbf{c}^{(0)} = \nabla f(\mathbf{x}^{(0)}) = \begin{pmatrix} 1+4\cdot 0+2\cdot 0 \\ -1+2\cdot 0+2\cdot 0 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Check stopping criterion.

$$\left\| \mathbf{c}^{(0)} \right\| = \sqrt{1^2 + (-1)^2} = \sqrt{2} > \varepsilon$$

$$\mathbf{d}^{(0)} = -\mathbf{A}^{(0)}\mathbf{c}^{(0)} = -\mathbf{I}\,\mathbf{c}^{(0)} = -\mathbf{c}^{(0)} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \alpha_0 \mathbf{d}^{(0)}$$

$$= \begin{pmatrix} 0 \\ 0 \end{pmatrix} + \alpha \begin{pmatrix} -1 \\ 1 \end{pmatrix} = \begin{pmatrix} -\alpha \\ \alpha \end{pmatrix}$$

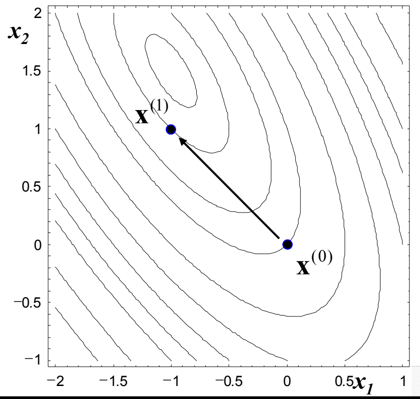
Replacing α_0 to α for convenience

Substitute $\mathbf{x}^{(1)} = (-\alpha, \alpha)$ into the objective function

$$f(\mathbf{x}^{(1)}) = \alpha^2 - 2\alpha$$

To minimize $f(\mathbf{x}^{(1)})$,

$$\frac{df(\mathbf{x}^{(1)})}{d\alpha} = 2\alpha - 2 = 0 \ \rightarrow \ \alpha = 1.0 \qquad \therefore \mathbf{x}^{(1)} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$



4. Davidon-Fletcher-Powell (DFP) Method (5/6): Example

$$\nabla f(\mathbf{x}) = \nabla f(x_1, x_2) = \begin{pmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{pmatrix}$$

Minimize $f(\mathbf{x}) = f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2,$ **Starting design point $\mathbf{x}^{(0)}$ = (0, 0)**

■ **2nd Iteration: Find $\mathbf{x}^{(2)}$**

Update the matrix $\mathbf{A}^{(1)}$ - approximation for the inverse of the Hessian matrix of the objective function - as follows:

$$\mathbf{A}^{(1)} = \mathbf{A}^{(0)} + \mathbf{B}^{(0)} + \mathbf{C}^{(0)}$$

$$\mathbf{B}^{(0)} = \frac{\mathbf{s}^{(0)}\mathbf{s}^{(0)^T}}{\mathbf{s}^{(0)^T}\mathbf{y}^{(0)}}$$

$$\mathbf{s}^{(0)} = \alpha\mathbf{d}^{(0)} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$\mathbf{c}^{(0)} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad \mathbf{c}^{(1)} = \begin{pmatrix} -1 \\ -1 \end{pmatrix}$$

$$\mathbf{y}^{(0)} = \mathbf{c}^{(1)} - \mathbf{c}^{(0)} = \begin{pmatrix} -2 \\ 0 \end{pmatrix}$$

$$\mathbf{s}^{(0)}\mathbf{s}^{(0)^T} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

$$\mathbf{s}^{(0)^T}\mathbf{y}^{(0)} = 2$$

$$= \begin{pmatrix} 0.5 & -0.5 \\ -0.5 & 0.5 \end{pmatrix}$$

$$\mathbf{C}^{(0)} = \frac{-\mathbf{z}^{(0)}\mathbf{z}^{(0)T}}{\mathbf{y}^{(0)^T}\mathbf{z}^{(0)}}$$

$$\mathbf{A}^{(0)} = \mathbf{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\mathbf{z}^{(0)} = \mathbf{A}^{(0)}\mathbf{y}^{(0)} = \begin{pmatrix} -2 \\ 0 \end{pmatrix}$$

$$\mathbf{y}^{(0)^T}\mathbf{z}^{(0)} = 4$$

$$\mathbf{z}^{(0)}\mathbf{z}^{(0)^T} = \begin{pmatrix} 4 & 0 \\ 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} -1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\mathbf{A}^{(1)} = \mathbf{A}^{(0)} + \mathbf{B}^{(0)} + \mathbf{C}^{(0)}$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0.5 & -0.5 \\ -0.5 & 0.5 \end{pmatrix} + \begin{pmatrix} -1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0.5 & -0.5 \\ -0.5 & 1.5 \end{pmatrix}$$

4. Davidon-Fletcher-Powell (DFP) Method (6/6): Example

$\nabla f(\mathbf{x}) = \nabla f(x_1, x_2) = \begin{pmatrix} 1+4x_1+2x_2 \\ -1+2x_1+2x_2 \end{pmatrix}$

Minimize $f(\mathbf{x}) = f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$, Starting design point $\mathbf{x}^{(0)}$ = (0, 0)

■ 2nd Iteration: Find $\mathbf{x}^{(2)}$

Check stopping criterion.

$$\left\|\mathbf{c}^{(1)}\right\| = \sqrt{2} > \varepsilon$$

$$\mathbf{d}^{(1)} = -\mathbf{A}^{(1)}\mathbf{c}^{(1)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + \alpha_1 \mathbf{d}^{(1)}$$

$$= \begin{pmatrix} -1 \\ 1 \end{pmatrix} + \alpha \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 \\ 1+\alpha \end{pmatrix}$$

Replacing α_1 to α for convenience

Substitute $\mathbf{x}^{(2)} = (-1, 1+\alpha)$ into the objective function

$$f(\mathbf{x}^{(2)}) = \alpha^2 - \alpha - 1$$

To minimize $f(\mathbf{x}^{(2)})$,

$$\frac{df(\mathbf{x}^{(2)})}{d\alpha} = 2\alpha - 1 = 0 \quad \rightarrow \quad \alpha = 0.5$$

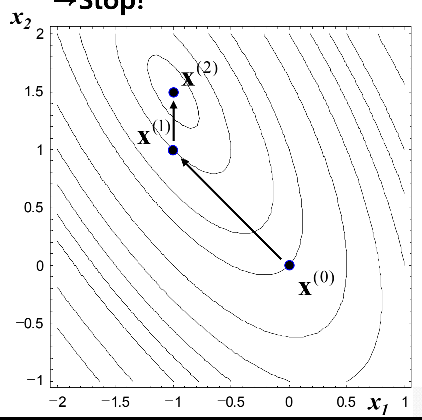
$$\therefore \mathbf{x}^{(2)} = \begin{pmatrix} -1 \\ 1.5 \end{pmatrix}$$ →Optimal design point

$$\mathbf{c}^{(2)} = \nabla f(\mathbf{x}^{(2)}) = \begin{pmatrix} 1+4\cdot(-1)+2\cdot 1.5 \\ -1+2\cdot(-1)+2\cdot 1.5 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Check stopping criterion.

$$\left\|\mathbf{c}^{(2)}\right\| = 0 \le \varepsilon$$

→Stop!



5. Broyden-Fletcher-Goldfarb-Shanno (BFGS) Method (1/6)

☑ This method updates the Hessian matrix rather than its inverse at every iteration.

- Step 1: Estimate a starting design point $\mathbf{x}^{(0)}$.
  Choose a symmetric positive definite $n \times n$ matrix $\tilde{\mathbf{H}}^{(0)}$ as an approximation for the Hessian matrix of the objective function.
  In the absence of more information, let $\tilde{\mathbf{H}}^{(0)} = \mathbf{I}$. Specify a tolerance ε for the stopping criterion. Set $k = 0$, and compute the gradient vector as $\mathbf{c}^{(0)} = \nabla f(\mathbf{x}^{(0)})$.

- Step 2: Calculate the norm of the gradient vector as $\left\|\mathbf{c}^{(k)}\right\|$.
  If $\left\|\mathbf{c}^{(k)}\right\| < \varepsilon$, then stop the iterative process. Otherwise, continue.
  It is noted that Step 1 and 2 of this method and the steepest descent method are the same.

5. Broyden-Fletcher-Goldfarb-Shanno (BFGS) Method (2/6)

- Step 3: Solve the linear system of the following equation to obtain the search direction.

$$\boxed{\mathbf{d}^{(k)} = -(\tilde{\mathbf{H}}^{(k)})^{-1}\mathbf{c}^{(k)}}$$

Newton's method

$$\Delta\mathbf{x}^{(k)} = -[\mathbf{H}(\mathbf{x}^{(k)})]^{-1}\nabla f(\mathbf{x}^{(k)})$$
$$\therefore \mathbf{d}^{(k)} = -(\mathbf{H}^{(k)})^{-1}\mathbf{c}^{(k)}$$

This equation looks like $\mathbf{d}^{(k)} = -(\mathbf{H}^{(k)})^{-1}\mathbf{c}^{(k)}$ of the Newton's method, but $\tilde{\mathbf{H}}^{(k)}$ is an approximated Hessian matrix $\mathbf{H}^{(k)}$, comprised of the first order derivatives.

- Step 4: Compute optimum step size $\alpha = \alpha_k$ to minimize $f(\mathbf{x}^{(k)} + \alpha\mathbf{d}^{(k)})$.

- Step 5: Update the design point as $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k\mathbf{d}^{(k)}$.

5. Broyden-Fletcher-Goldfarb-Shanno (BFGS) Method (3/6)

- Step 6: Update the matrix $\tilde{\mathbf{H}}^{(k)}$ - approximation for the Hessian matrix of the objective function - as follows:

$$\tilde{\mathbf{H}}^{(k+1)} = \tilde{\mathbf{H}}^{(k)} + \mathbf{D}^{(k)} + \mathbf{E}^{(k)} \quad : \quad n \times n \text{ matrix}$$

where, the correction matrices $\mathbf{D}^{(k)}$ and $\mathbf{E}^{(k)}$ are given as below.

$$\mathbf{D}^{(k)} = \frac{\mathbf{y}^{(k)}\mathbf{y}^{(k)^T}}{\mathbf{y}^{(k)^T}\mathbf{s}^{(k)}}; \qquad \mathbf{E}^{(k)} = \frac{\mathbf{c}^{(k)}\mathbf{c}^{(k)^T}}{\mathbf{c}^{(k)^T}\mathbf{d}^{(k)}};$$

$\mathbf{s}^{(k)} = \alpha_k\mathbf{d}^{(k)}$: change in design

$\mathbf{y}^{(k)} = \mathbf{c}^{(k+1)} - \mathbf{c}^{(k)}$: change in gradient

$\mathbf{c}^{(k+1)} = \nabla f(\mathbf{x}^{(k+1)})$

$\mathbf{d}^{(k)}$: search direction

$\alpha^{(k)}$: optimum step size

- Step 7: Set $k = k+1$ and go to Step 2.

5. Broyden-Fletcher-Goldfarb-Shanno (BFGS) Method (4/6): Example

Minimize $f(\mathbf{x}) = f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$, **Starting design point $\mathbf{x}^{(0)}$ = (0, 0)**

$$\nabla f(\mathbf{x}) = \nabla f(x_1, x_2) = \begin{pmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{pmatrix}$$

■ **1st Iteration: Find $\mathbf{x}^{(1)}$**

$$\mathbf{x}^{(0)} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \tilde{\mathbf{H}}^{(0)} = \mathbf{I}$$

$$\mathbf{c}^{(0)} = \nabla f(\mathbf{x}^{(0)}) = \begin{pmatrix} 1 + 4 \cdot 0 + 2 \cdot 0 \\ -1 + 2 \cdot 0 + 2 \cdot 0 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Check stopping criterion.

$$\left\| \mathbf{c}^{(0)} \right\| = \sqrt{1^2 + (-1)^2} = \sqrt{2} > \varepsilon$$

$$\mathbf{d}^{(0)} = -(\tilde{\mathbf{H}}^{(0)})^{-1}\mathbf{c}^{(0)} = -\mathbf{I}\,\mathbf{c}^{(0)} = -\mathbf{c}^{(0)} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \alpha_0 \mathbf{d}^{(0)}$$

$$= \begin{pmatrix} 0 \\ 0 \end{pmatrix} + \alpha \begin{pmatrix} -1 \\ 1 \end{pmatrix} = \begin{pmatrix} -\alpha \\ \alpha \end{pmatrix}$$

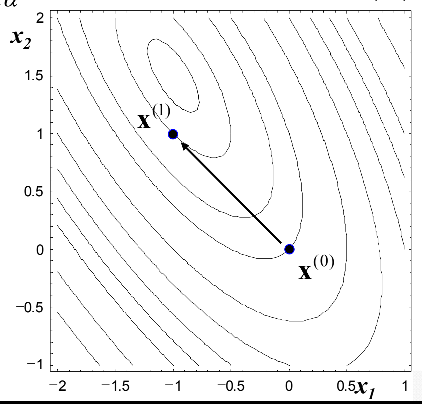
Replacing α_0 to α for convenience

Substitute $\mathbf{x}^{(1)} = (-\alpha, \alpha)$ into the objective function

$$f(\mathbf{x}^{(1)}) = \alpha^2 - 2\alpha$$

To minimize $f(\mathbf{x}^{(1)})$,

$$\frac{df(\mathbf{x}^{(1)})}{d\alpha} = 2\alpha - 2 = 0 \;\rightarrow\; \alpha = 1.0 \qquad \therefore \mathbf{x}^{(1)} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$



$\nabla f(\mathbf{x}) = \nabla f(x_1, x_2) = \begin{pmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{pmatrix}$

5. Broyden-Fletcher-Goldfarb-Shanno (BFGS) Method (5/6): Example

Minimize $f(\mathbf{x}) = f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$, **Starting design point $\mathbf{x}^{(0)}$ = (0, 0)**

■ **2nd Iteration: Find $\mathbf{x}^{(2)}$**

Update the matrix $\tilde{\mathbf{H}}^{(0)}$ - approximation for the Hessian matrix of the objective function - as follows:

$$\tilde{\mathbf{H}}^{(1)} = \tilde{\mathbf{H}}^{(0)} + \mathbf{D}^{(0)} + \mathbf{E}^{(0)}$$

$$\mathbf{D}^{(0)} = \frac{\mathbf{y}^{(0)}\mathbf{y}^{(0)^T}}{\mathbf{y}^{(0)^T}\mathbf{s}^{(0)}}$$

$$\mathbf{s}^{(0)} = \alpha \mathbf{d}^{(0)} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$\mathbf{c}^{(0)} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad \mathbf{c}^{(1)} = \begin{pmatrix} -1 \\ -1 \end{pmatrix}$$

$$\mathbf{y}^{(0)} = \mathbf{c}^{(1)} - \mathbf{c}^{(0)} = \begin{pmatrix} -2 \\ 0 \end{pmatrix}$$

$$\mathbf{y}^{(0)}\mathbf{y}^{(0)^T} = \begin{pmatrix} 4 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\mathbf{y}^{(0)^T}\mathbf{s}^{(0)} = 2$$

$$= \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\mathbf{E}^{(0)} = \frac{-\mathbf{c}^{(0)}\mathbf{c}^{(0)T}}{\mathbf{c}^{(0)^T}\mathbf{d}^{(0)}}$$

$$\mathbf{c}^{(0)} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad \mathbf{d}^{(0)} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$\mathbf{c}^{(0)}\mathbf{c}^{(0)^T} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

$$\mathbf{c}^{(0)^T}\mathbf{d}^{(0)} = -2$$

$$= \begin{pmatrix} -0.5 & 0.5 \\ 0.5 & -0.5 \end{pmatrix}$$

$$\tilde{\mathbf{H}}^{(1)} = \tilde{\mathbf{H}}^{(0)} + \mathbf{D}^{(0)} + \mathbf{E}^{(0)}$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} -0.5 & 0.5 \\ 0.5 & -0.5 \end{pmatrix}$$

$$= \begin{pmatrix} 2.5 & 0.5 \\ 0.5 & 0.5 \end{pmatrix}$$

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5. Broyden-Fletcher-Goldfarb-Shanno (BFGS) Method (6/6): Example

$\nabla f(\mathbf{x}) = \nabla f(x_1, x_2) = \begin{pmatrix} 1+4x_1+2x_2 \\ -1+2x_1+2x_2 \end{pmatrix}$

Minimize $f(\mathbf{x}) = f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$, **Starting design point $\mathbf{x}^{(0)}$ = (0, 0)**

■ 2nd Iteration: Find $\mathbf{x}^{(2)}$

Check stopping criterion.

$$\left\|\mathbf{c}^{(1)}\right\| = \sqrt{2} > \varepsilon$$

$$\tilde{\mathbf{H}}^{(1)}\mathbf{d}^{(1)} = -\mathbf{c}^{(1)} \quad \mathbf{d}^{(1)} = -(\tilde{\mathbf{H}}^{(1)})^{-1}\mathbf{c}^{(1)}$$

$$\tilde{\mathbf{H}}^{(1)} = \begin{pmatrix} 2.5 & 0.5 \\ 0.5 & 0.5 \end{pmatrix}, \quad \mathbf{d}^{(1)} = \begin{pmatrix} 0 \\ 2 \end{pmatrix} \quad \mathbf{c}^{(1)} = \begin{pmatrix} -1 \\ -1 \end{pmatrix}$$

$$\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + \alpha_1\mathbf{d}^{(1)}$$

$$= \begin{pmatrix} -1 \\ 1 \end{pmatrix} + \alpha\begin{pmatrix} 0 \\ 2 \end{pmatrix} = \begin{pmatrix} -1 \\ 1+2\alpha \end{pmatrix}$$

Replacing α_1 to α for convenience

Substitute $\mathbf{x}^{(2)} = (-1, 1+2\alpha)$ **into the objective function**

$$f(\mathbf{x}^{(2)}) = 4\alpha^2 - 2\alpha - 1$$

To minimize $f(\mathbf{x}^{(2)})$,

$$\frac{df(\mathbf{x}^{(2)})}{d\alpha} = 8\alpha - 2 = 0 \;\rightarrow\; \alpha = 0.25$$

$$\therefore \mathbf{x}^{(2)} = \begin{pmatrix} -1 \\ 1.5 \end{pmatrix}$$

→Optimal design point

$$\mathbf{c}^{(2)} = \nabla f(\mathbf{x}^{(2)}) = \begin{pmatrix} 1+4\cdot(-1)+2\cdot 1.5 \\ -1+2\cdot(-1)+2\cdot 1.5 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Check stopping criterion.

$$\left\|\mathbf{c}^{(2)}\right\| = 0 \le \varepsilon$$

→Stop!