Introduction to Engineering Optimization (ME6806)

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Module 4

Multi-variable Optimization Algorithms

Outlines

- **Optimality Criteria**
- **Direct Search Methods**
    - Nelder and Mead (Simplex Search)
    - Hook and Jeeves (Pattern Search)
    - Powell's Method (The Conjugated Direction Search)
- **Gradient Based Methods**
    - Steepest Descent (Cauchy's) Method
    - **Newton's Method**
    - Modified Newton's Method
    - Marquardt's Method
    - Conjugate Gradient Method
    - Quasi-Newton Method
    - Trust Regions
    - Gradient-Based Algorithm
    - Numerical Gradient Approximations

Newton's Method

Consider the quadratic approximation of the function *f*(**x**), at $X = X_i$ using the Taylor's series expansion,

$$f(\mathbf{X}) = f(\mathbf{X}_i) + \nabla f_i^{\mathrm{T}}(\mathbf{X} - \mathbf{X}_i) + \frac{1}{2}(\mathbf{X} - \mathbf{X}_i)^{\mathrm{T}}[J_i](\mathbf{X} - \mathbf{X}_i)$$

where $[J_i] = [J]|_{Xi}$ is the matrix of second partial derivatives (Hessian matrix) of ***f*** evaluated at the point X_i.

$$\mathbf{X}_{i+1} = \mathbf{X}_i - [J_i]^{-1} \nabla f_i$$

Newton's Method

Let the quadratic function be given by

$$f(\mathbf{X}) = \frac{1}{2}\mathbf{X}^{\mathrm{T}}[A]\mathbf{X} + \mathbf{B}^{\mathrm{T}}\mathbf{X} + C$$

The minimum of $f(\mathbf{X})$ is given by

$$\nabla f = [A]\mathbf{X} + \mathbf{B} = \mathbf{0}$$

or

$$\mathbf{X}^* = -[A]^{-1}\mathbf{B}$$

$$\mathbf{X}_{i+1} = \mathbf{X}_i - [A]^{-1}([A]\mathbf{X}_i + \mathbf{B}) \qquad (\mathrm{E}_1)$$

where $\mathbf{X}_i$ is the starting point for the ith iteration. Thus Eq. (E_1) gives the exact solution

$$\mathbf{X}_{i+1} = \mathbf{X}^* = -[A]^{-1}\mathbf{B}$$

Newton's Method - Example

Minimize $f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$ by taking the starting point as $\mathbf{X}_1 = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix}$.

To find $\mathbf{X}_2$, we require $[J_1]^{-1}$, where

$$[J_1] = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x_1^2} & \dfrac{\partial^2 f}{\partial x_1 \partial x_2} \\ \dfrac{\partial^2 f}{\partial x_2 \partial x_1} & \dfrac{\partial^2 f}{\partial x_2^2} \end{bmatrix}_{\mathbf{X}_1} = \begin{bmatrix} 4 & 2 \\ 2 & 2 \end{bmatrix}$$

Therefore,

$$[J_1]^{-1} = \frac{1}{4} \begin{bmatrix} +2 & -2 \\ -2 & 4 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & 1 \end{bmatrix}$$

Newton's Method - Example

As

$$\mathbf{g}_1 = \begin{Bmatrix} \partial f/\partial x_1 \\ \partial f/\partial x_2 \end{Bmatrix}_{\mathbf{X}_1} = \begin{Bmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{Bmatrix}_{(0,0)} = \begin{Bmatrix} 1 \\ -1 \end{Bmatrix}$$

$$\mathbf{X}_2 = \mathbf{X}_1 - [J_1]^{-1}\mathbf{g}_1 = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} - \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & 1 \end{bmatrix} \begin{Bmatrix} 1 \\ -1 \end{Bmatrix} = \begin{Bmatrix} -1 \\ \frac{3}{2} \end{Bmatrix}$$

To see whether or not $\mathbf{X}_2$ is the optimum point, we evaluate

$$\mathbf{g}_2 = \begin{Bmatrix} \partial f/\partial x_1 \\ \partial f/\partial x_2 \end{Bmatrix}_{\mathbf{X}_2} = \begin{Bmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{Bmatrix}_{(-1,3/2)} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix}$$

As $\mathbf{g}_2 = \mathbf{0}$, $\mathbf{X}_2$ is the optimum point. Thus the method has converged in one iteration for this quadratic function.