1.3. MATHEMATICAL DEFINITIONS AND PREREQUISITES

Gradient of a differentiable function f: $\mathbb{R}^n \rightarrow \mathbb{R}$

$$g(\mathbf{x}) = \nabla f(\mathbf{x}) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

Hessian matrix of a twice differentiable function f: $\mathbb{R}^n \rightarrow \mathbb{R}$

$$H(x) = \nabla^2 f(\mathbf{x}) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_1 \partial x_2} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial^2 f}{\partial x_1 \partial x_n} & \frac{\partial^2 f}{\partial x_2 \partial x_n} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{pmatrix}$$

For a quadratic function $f(\mathbf{x}) = ½\, \mathbf{x}^T\mathbf{Q}\mathbf{x} + \mathbf{c}^T\mathbf{x} + d$

$\nabla f(\mathbf{x}) = \mathbf{Q}\mathbf{x} + \mathbf{c}$
$\nabla^2 f(\mathbf{x}) = \mathbf{Q}$.

Order notation: A univariate function f(x) is said to be f *order* h^p, written $f(h)=O(h^p)$, if there exits a finite number M>0 such that as |h| approaches zero

$$|f(h)| \leq M|h^p|.$$

TAYLOR'S FORMULA FOR UNIVARIATE FUNCTIONS

Let f: $\mathbb{R} \rightarrow \mathbb{R}$ be r times continuously differentiable i.e. f has continuos derivatives of order 1 through r. Then there exists a scalar $\theta \in [0, 1]$ such that

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \cdots + \frac{1}{(r-1)!}h^{r-1}f^{(r-1)}(x) + \frac{1}{r!}h^r f^{(r)}(x+\theta h)$$

or

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \cdots + \frac{1}{(r-1)!}h^{r-1}f^{(r-1)}(x) + O(h^r)$$

Names: Taylor's formula, Taylor expansion, Taylor series, Taylor's polynomial.

We shall be interested only in the first three terms in this expansion.

A special case: Taylor's polynomial of second order for a multivariate function

Let f: $\mathbb{R}^n \rightarrow \mathbb{R}$ be at least twice continuously differentiable function and let **x** be a given point in $\mathbb{R}^n$, **p** a unit vector in $\mathbb{R}^n$ and h a scalar.

Then there exists a scalar θ ∈ [0, 1] such that

$$f(\boldsymbol{x}+h\boldsymbol{p}) = f(\boldsymbol{x}) + h\boldsymbol{p}^T\nabla f(\boldsymbol{x}) + \frac{1}{2}h^2\boldsymbol{p}^T\nabla^2 f(\boldsymbol{x})\boldsymbol{p} + O(h^3)$$

FINITE DIFFERENCE APPROXIMATIONS TO DERIVATIVES

Taylor's formula gives

1) *the forward difference approximation* for derivative f'(x):

$$\frac{f(x+h) - f(x)}{h} = f'(x) + O(h)$$

2) *the central-difference approximation* for derivative f'(x):

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + O(h^2)$$

RATE OF CONVERGENCE OF ITERATIVE SEQUENCES

Let us assume that the sequence $\{\mathbf{x}_k\}$ converges to $\mathbf{x}^*$, i.e. $\lim_{k\to\infty} \|\boldsymbol{x}_k - \boldsymbol{x}^*\| = 0$.

The sequence $\{\mathbf{x}_k\}$ *converges with order r* when there is a constant c and integer N such that

$|\mathbf{x}_{k+1} - \mathbf{x}^*| \leq c\, |\mathbf{x}_k - \mathbf{x}^*|^r$ when $k \geq N$

or

$$0 \leq \lim_{k\to\infty} \frac{\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\|}{\|\boldsymbol{x}_k - \boldsymbol{x}^*\|^r} < \infty$$

When the asymptotic error constant

$$\gamma = \lim_{k\to\infty} \frac{\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\|}{\|\boldsymbol{x}_k - \boldsymbol{x}^*\|} = 0,$$

the convergence is *superlinear*.

Linear convergence: r = 1
Quadratic convergence: r = 2
Superlinear convergence: r > 1