Example problems:

1) Numerical calculation of gradient of a function & its comparison with analytical value.

lets say. $f : \mathbb{R}^2 \longrightarrow \mathbb{R}$.

$$f(x_1, x_2) = 12.069\, x_1^2 + 21.504\, x_2^2 - 1.7321\, x_1 - x_2.$$

We need to find its gradient "numerically".

Step I: Analytical gradient

$$\nabla f = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{pmatrix} = \begin{pmatrix} 24.138\, x_1 - 1.7321 \\ 43.008\, x_2 - 1 \end{pmatrix}$$

~~Numerical gradient~~ given a pt $\underline{x}_0 = \begin{pmatrix} 5 \\ 6 \end{pmatrix}$

$$\nabla f \Big|_{\underline{x}_0} = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{pmatrix}\Bigg|_{@\, \underline{x}_0} = \begin{pmatrix} 1.1896 \times 10^2 \\ 2.5705 \times 10^2 \end{pmatrix}$$

$$\underline{x}_0 = \begin{pmatrix} 5 \\ 6 \end{pmatrix}.$$

Numerical gradient calculation:

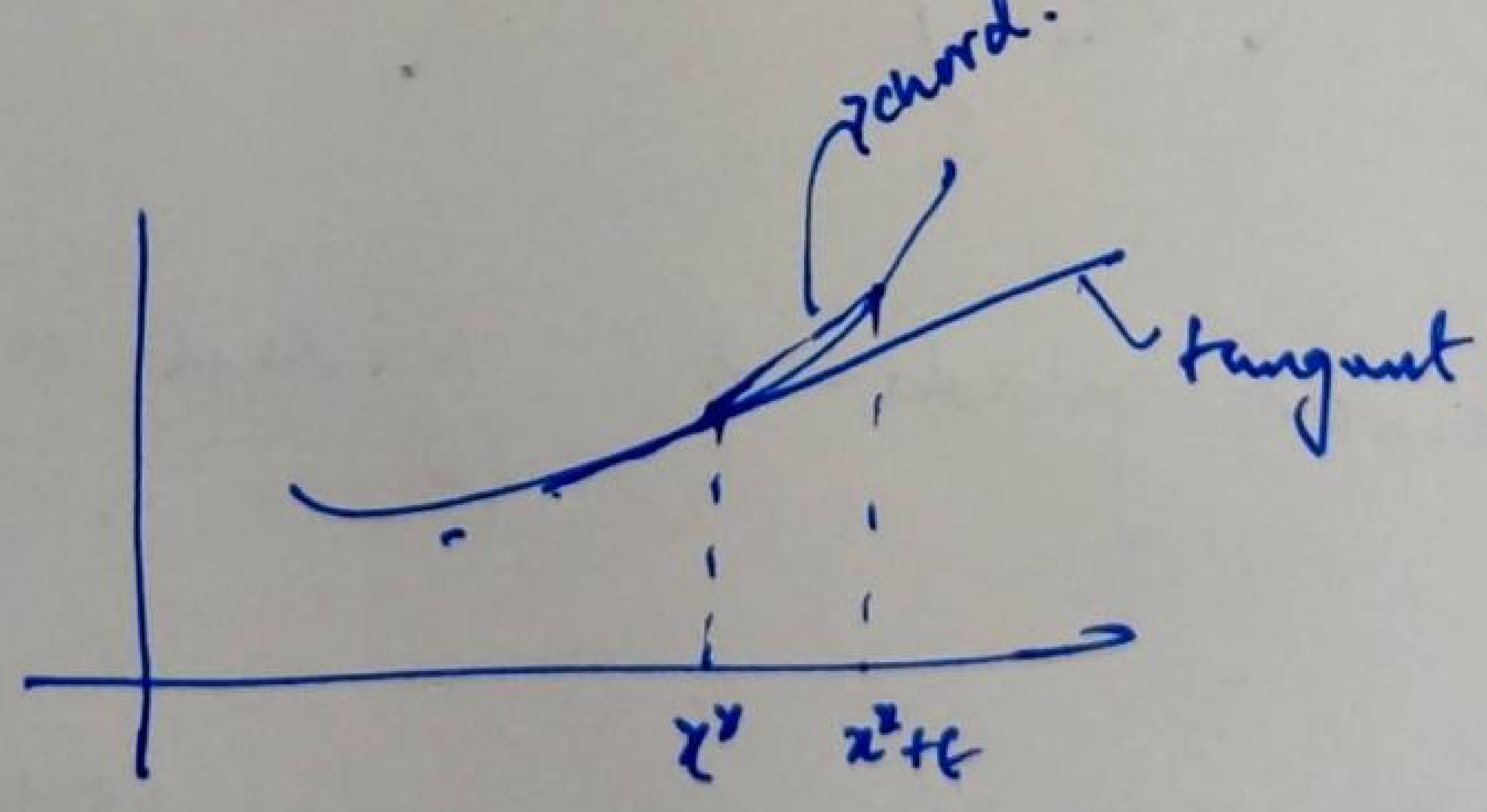
Step I: estimate the ϵ (divided difference param)

- each variable is purterbed oncye with ϵ and the derivatives calculated.

- a) Too small a choice of ϵ leads to a very loss of significance error, since two very nearly equal quantities will be substracted from each other.

b) Small ϵ is also recommended in probs where there is noise in the function evaluation, as occurs when using a nonlinear iterative simulation code to evaluate f

- Too large an ϵ results in a large trucation error, graphicall it is the error arising due to the mismatch betn the "chord" and "tangent" at the point.



Thumb rule.

$$\epsilon = \max{}^{m}\left(\epsilon_{min},\ 0.01\,x_i^0\right)$$ works wel.

Step II : A) Using ~~central~~ forward difference

$$\frac{\partial f}{\partial x_i} = \frac{f(x_1^0, x_2^0, \dots x_i^0 + \epsilon, \dots) - f(x_1^0, x_2^0, \dots x_n^0)}{\epsilon}$$

for $\forall \; i = 1, 2, \dots n$.

B) Using. Backward difference.

$$\frac{\partial f}{\partial x_i} = \frac{f(x_1^0, x_2^0, \dots x_i^0 - \epsilon, x_{i+1}^0, \dots x_n^0) - f(\underline{x}^0)}{\epsilon} \quad \forall \; i = 1, 2, \dots n$$

C) Using Central difference.

$$\frac{\partial f}{\partial x_i} = \frac{f(x_1^0, x_2^0, \dots x_i + 0.5\epsilon, \dots x_n) - f(x_1^0, x_2^0, \dots x_i - 0.5\epsilon, \dots x_n)}{\epsilon}.$$

Choosing $\epsilon = 0.01 \, \text{abs}(x_i^0)$

$\nabla f(\underline{x}^0)$ Forward difference	$\nabla f(\underline{x}^0)$ Backward ~~Central~~ diff	$\nabla f(\underline{x}^0)$ Central ~~Backward~~ diff
$\begin{pmatrix} 1.1956 \times 10^2 \\ 2.5834 \times 10^2 \end{pmatrix}$	$\begin{pmatrix} 1.1835 \times 10^2 \\ 2.5576 \times 10^2 \end{pmatrix}$	$\begin{pmatrix} 1.1896 \times 10^2 \\ 2.5705 \times 10^2 \end{pmatrix}$.

Problem 2: ~~Numerical evaluation of Hessian matrix.~~

Assignment: 1

1) Try to plot error in (For the prob discussed).

   a) Forward diff approximation

   b) Backward diff "

   c) Central diff ".

as you change the value of "ϵ", check the convergence. Plot them on the same curve.

2) Take a function.

   a) $$f = \frac{4x_2^2 - x_1x_2}{10000(x_2x_1^3 - x_1^4)} \quad @ \quad \underset{\sim}{x}^0 = \begin{pmatrix} 0.5 \\ 1.5 \end{pmatrix}$$

Find its gradient using Forward diff, Backward & central diff.

Plot the error & ~~converg~~ show convergence graphically.

Clearly show the graph label, title etc.