Finite Difference Method

Motivation

For a given smooth function $f(x)$, we want to calculate the derivative $f'(x)$ at a given value of x.

Suppose we don't know how to compute the analytical expression for $f'(x)$, or it is computationally very expensive. However you do know how to evaluate the function value:

```python
def f(x):
    # do stuff here
    feval = ...
    return feval
```

We know that:

$$f'(x) = \lim_{h \to 0} \left(\frac{f(x+h) - f(x)}{h} \right)$$

Can we just use $f'(x) \approx \frac{f(x+h)-f(x)}{h}$ as an approximation? How do we choose h? Can we get estimate the error of our approximation?

Finite difference method

For a differentiable function $f: \mathcal{R} \rightarrow \mathcal{R}$, the derivative is defined as:

$$f'(x) = \lim_{h \to 0} \left(\frac{f(x+h) - f(x)}{h} \right)$$

Taylor Series centered at x, where $\bar{x} = x + h$

$$f(x+h) = f(x) + f'(x)\,h + f''(x)\frac{h^2}{2} + f'''(x)\frac{h^3}{6} + \cdots$$

$$f(x+h) = f(x) + f'(x)\,h + O(h^2)$$

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

We define the **Forward Finite Difference** as:

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

Therefore, the **truncation error** of the forward finite difference approximation is bounded by:

$$|f'(x) - df(x)| \leq M h$$

In a similar way, we can write:

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

And define the **Backward Finite Difference** as:

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

And subtracting the two Taylor approximations

$$f(x+h) = \cancel{f(x)} + f'(x)\,h + \cancel{f''(x)\frac{h^2}{2}} + f'''(x)\frac{h^3}{6} + \cdots$$

$$f(x-h) = \cancel{f(x)} - f'(x)\,h + \cancel{f''(x)\frac{h^2}{2}} - f'''(x)\frac{h^3}{6} + \cdots$$

$$f(x+h) - f(x-h) = 2f'(x)\,h + f'''(x)\frac{h^3}{6} + O(h^5) \qquad \div h$$

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

And define the **Central Finite Difference** as:

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

How accurate is the finite difference approximation? How many function evaluations (in additional to $f(x)$)?

$\boxed{f(x)}$

Forward Finite Difference:

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

Truncation error: $O(h)$

Cost: 1 function evaluation

Backward Finite Difference:

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

Truncation error: $O(h)$

Cost: 1 function evaluation

Central Finite Difference:

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

Truncation error: $O(h^2)$

Cost: 2 function evaluation2

Our typical trade-off issue! We can get **better accuracy** with Central Finite Difference with the (possible) **increased computational** cost.

How small should the value of *h*?

Example

$$f(x+h) = e^{x+h} - 2$$

$f(x) = e^x - 2$

$f'(x) = e^x$

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

We want to obtain an approximation for $f'(1)$

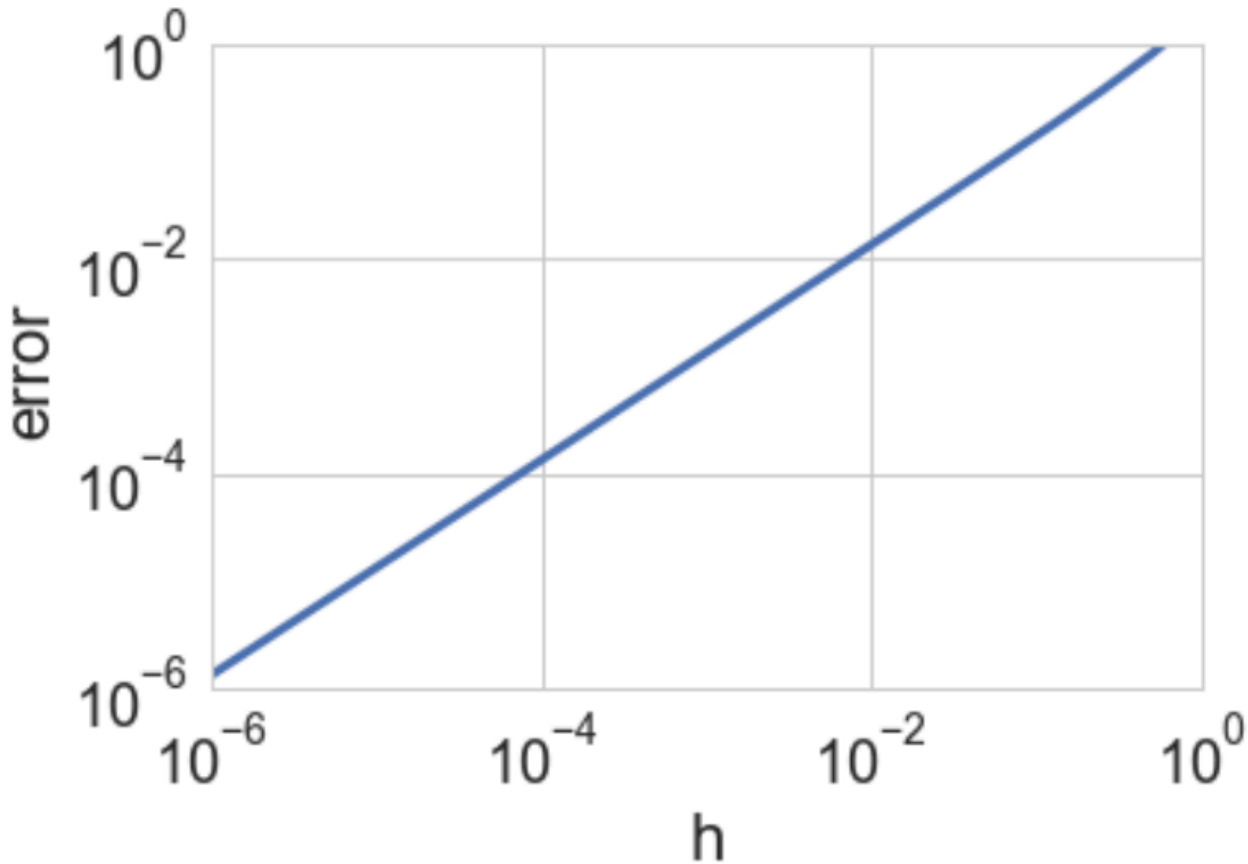
$$dfapprox = \frac{(e^{x+h} - 2) - (e^x - 2)}{h}$$

Truncation error

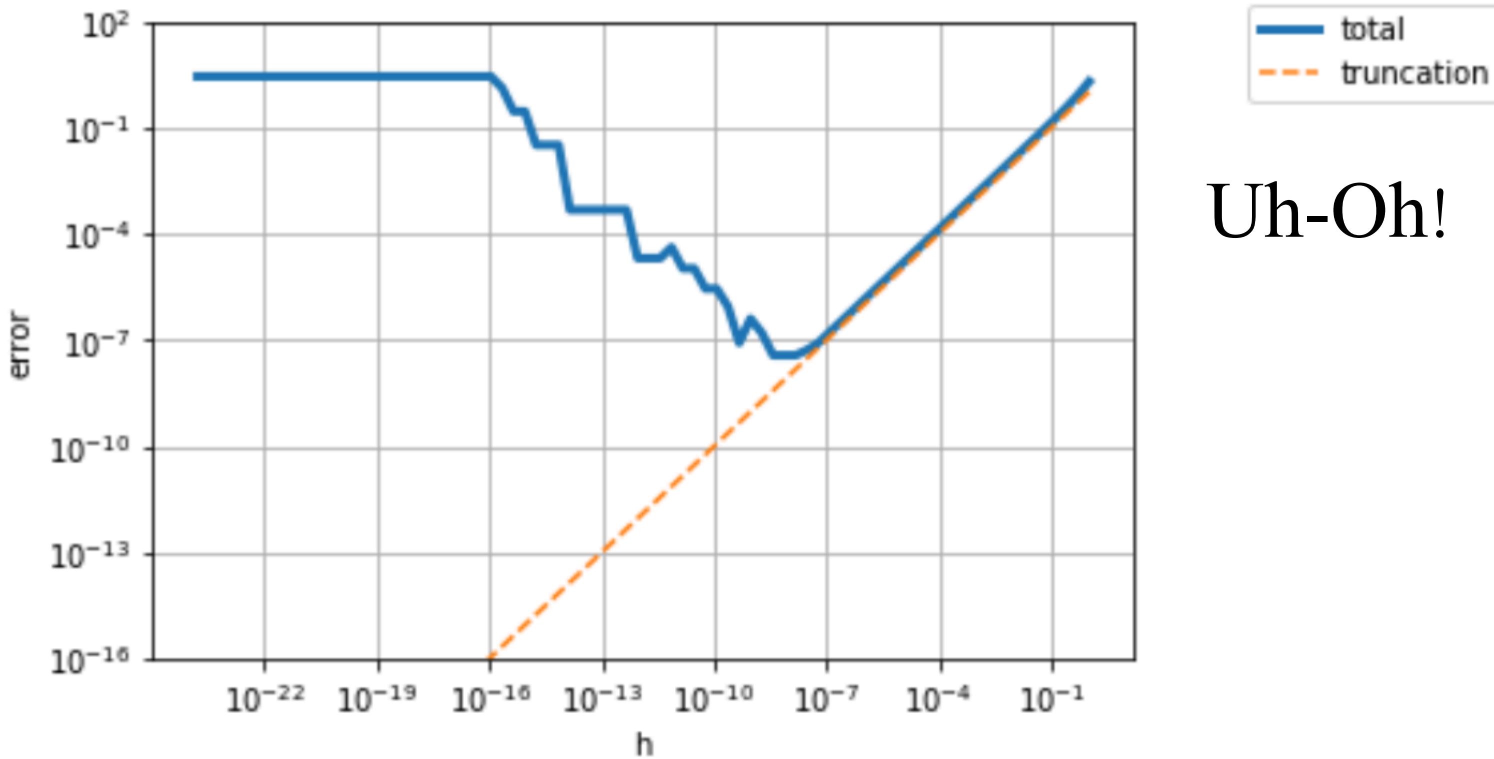
$$error(h) = abs(f'(x) - dfapprox)$$

h	$error$
1.000000E+00	1.952492E+00
5.000000E-01	8.085327E-01
2.500000E-01	3.699627E-01
1.250000E-01	1.771983E-01
6.250000E-02	8.674402E-02
3.125000E-02	4.291906E-02
1.562500E-02	2.134762E-02
7.812500E-03	1.064599E-02
3.906250E-03	5.316064E-03
1.953125E-03	2.656301E-03
9.765625E-04	1.327718E-03
4.882812E-04	6.637511E-04
2.441406E-04	3.318485E-04
1.220703E-04	1.659175E-04
6.103516E-05	8.295707E-05
3.051758E-05	4.147811E-05
1.525879E-05	2.073897E-05
7.629395E-06	1.036945E-05
3.814697E-06	5.184779E-06
1.907349E-06	2.592443E-06

Example



Should we just keep decreasing the perturbation h, in order to approach the limit $h \to 0$ and obtain a better approximation for the derivative?



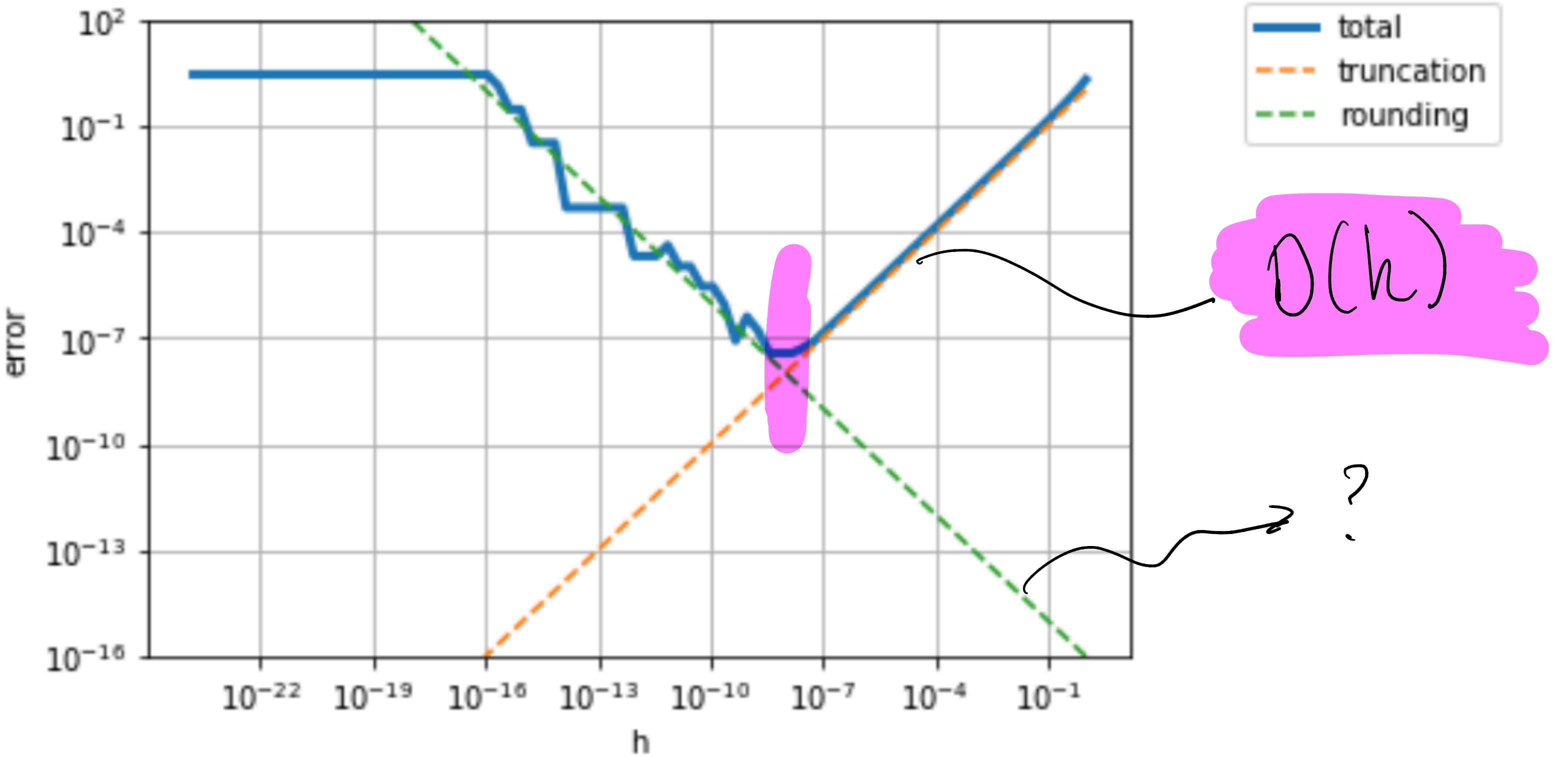
Uh-Oh!

What happened here?

$$f(x) = e^x - 2, \qquad f'(x) = e^x \to f'(1) \approx 2.7$$

Forward Finite Difference

$$df(1) = \frac{f(1+h) - f(1)}{h} \longrightarrow \text{Cancelation!}$$

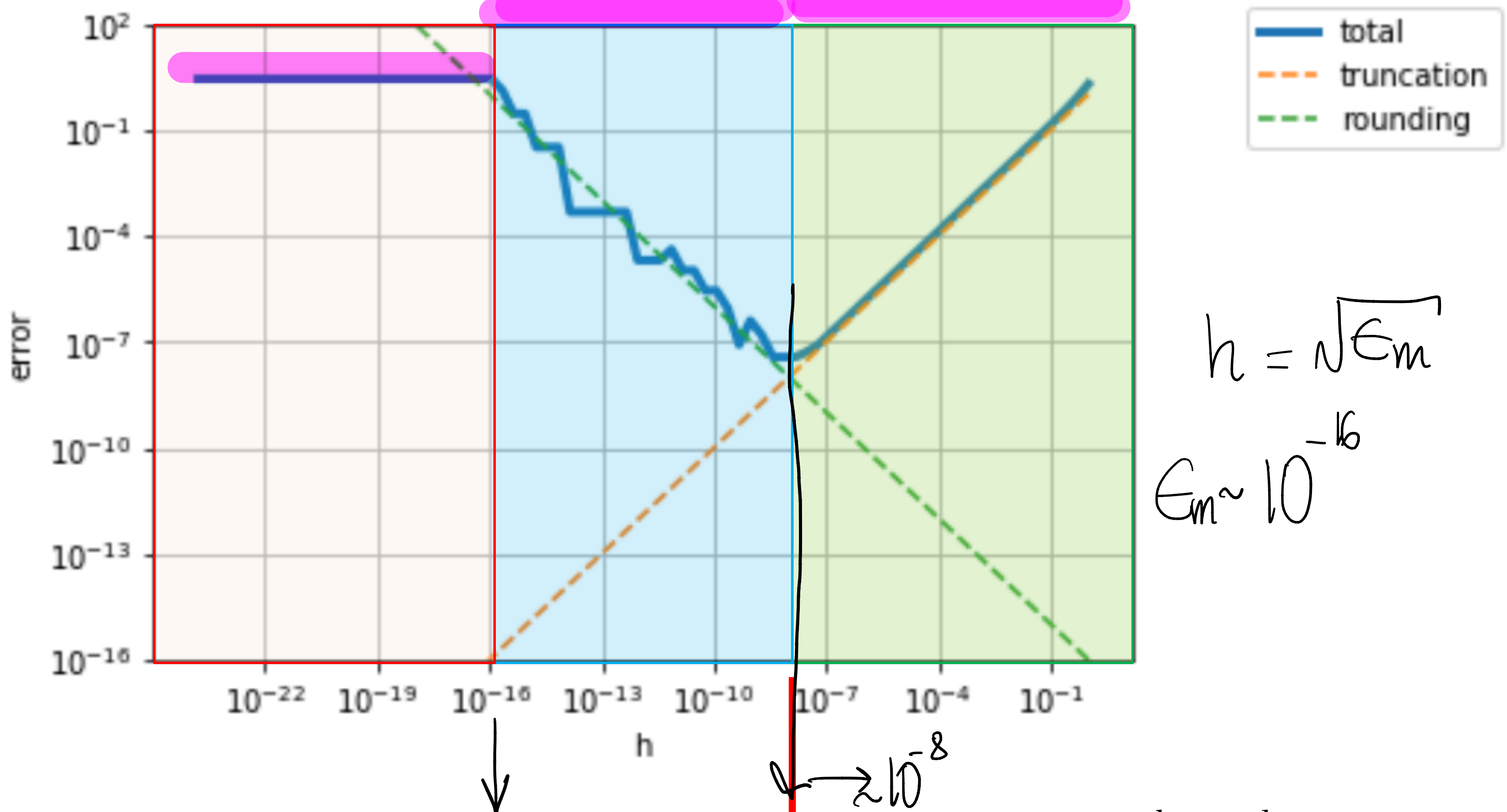


When computing the finite difference approximation, we have two competing source of errors: Truncation errors and **Rounding errors**

$$\underline{df(x)} = \frac{f(x+h) - f(x)}{h} \leq \frac{\epsilon_m \, |f(x)|}{h}$$

$\epsilon_m |x|$

Loss of accuracy
due to rounding



Truncation error: $error \sim M\, h$

Optimal "h"

Minimize the total error

$$error \sim \frac{\epsilon_m |f(x)|}{h} + Mh$$

Gives

$$h = \sqrt{\epsilon_m |f(x)|/M}$$

Rounding error: $error \sim \dfrac{\epsilon_m |f(x)|}{h}$

Finite Difference Method

Review: $f: \mathbb{R} \to \mathbb{R}$

$$\underline{\underline{df}} = \frac{f(x+h) - f(x)}{h} \longleftrightarrow f'(x)$$

$$f: \mathbb{R}^n \to \mathbb{R} \qquad f(\underset{\sim}{x}) = f(x_1, x_2, x_3, \dots x_n)$$

$$\nabla f(\underset{\sim}{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix} \longrightarrow (\nabla f)_{FD} = \begin{bmatrix} ? \\ \\ \\ \end{bmatrix}$$

gradient

$$\boxed{(\underset{\sim}{\nabla f}) = \begin{bmatrix} \frac{f(\underset{\sim}{x} + h\underset{\sim}{\delta_1}) - f(\underset{\sim}{x})}{h} \\ \frac{f(\underset{\sim}{x} + h\underset{\sim}{\delta_2}) - f(\underset{\sim}{x})}{h} \\ \vdots \\ \frac{f(\underset{\sim}{x} + h\underset{\sim}{\delta_n}) - f(\underset{\sim}{x})}{h} \end{bmatrix}}$$

$$\underset{\sim}{\delta_1} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \qquad \underset{\sim}{\delta_2} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{bmatrix}$$

$$\underset{\sim}{\delta_i} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \leftarrow i$$

$$f(x_1, x_2) = 2x_1 + x_1^2 x_2 + x_2^3$$

$$\nabla f = \begin{bmatrix} \dfrac{\partial f}{\partial x_1} \\[2em] \dfrac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2 + 2x_1 x_2 \\[2em] x_1^2 + 3x_2^2 \end{bmatrix} \rightarrow \nabla f(1.3, 4.9) = \begin{bmatrix} 14.74 \\ 73.72 \end{bmatrix} //$$

$$(\overline{\nabla f})_{FD} = \begin{bmatrix} \dfrac{f(\underline{x} + h\underline{\delta_1}) - f(\underline{x})}{h} \\[2em] \dfrac{f(\underline{x} + h\underline{\delta_2}) - f(\underline{x})}{h} \end{bmatrix}$$

$$f : \mathbb{R}^n \longrightarrow \mathbb{R}^m$$

$$\underset{\sim}{f}(\underset{\sim}{x}) = \begin{bmatrix} f_1(x_1, x_2, \dots, x_n) \\ f_2(x_1, x_2, \dots, x_n) \\ \vdots \\ f_m(x_1, x_2, \dots, x_n) \end{bmatrix} \qquad \frac{\partial f_i}{\partial x_j}$$

$$\frac{\partial f}{\partial x_1}$$

$$\underset{\sim}{J} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$