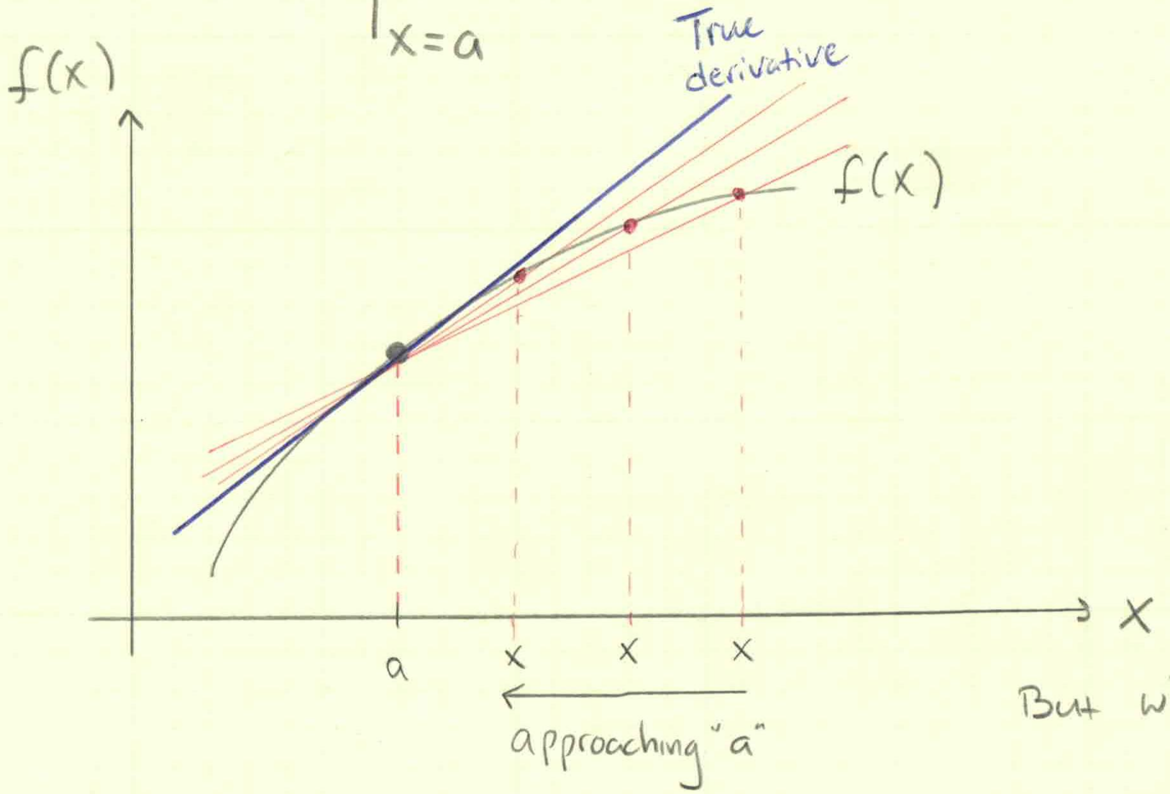
Derivative of a function:

$$\left.\frac{d\, f(x)}{dx}\right|_{x=a} = f'(a) = \lim_{x\to a} \frac{f(x) - f(a)}{x-a}$$ definition



examples:

$f(x) = 2x^3 - 4x^2 - 4x - 20$

$f'(x) = 6x^2 - 8x - 4$

$f(x) = \sin(x)$

$f'(x) = \cos(x)$

Analytical soln s

But what if:

$f(x) =$ long complex expression

or $f(x)$: f: -5.87, -4.23, -2.55, -0.89 ...
x: 0, 0.2, 0.4, 0.6 ...

or function [fofx] = fun(x)
(lots of code)

end

Use Numerical Differentiation.

(+) Very flexible. Applies in many cases

(−) Can perform poorly on very oscillatory or noisy functions

(−) Round-off & numerical errors

Alternative, when possible:

Symbolic Differentiation

Automatic Differentiation

Two Approaches: Find numerical Approximate of derivative at x_i

(A) Finite Difference Approximation

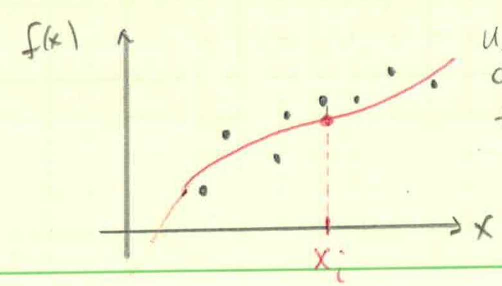
Find slope using $f(x_i)$ & neighboring values (e.g. $f(x_{i-1})$, $f(x_{i+1})$...).

Forward Difference, Backward Difference, Central Difference.

(B) Approximate points w/ analytic expression (i.e. Curve-fit),

Then take derivative of that.

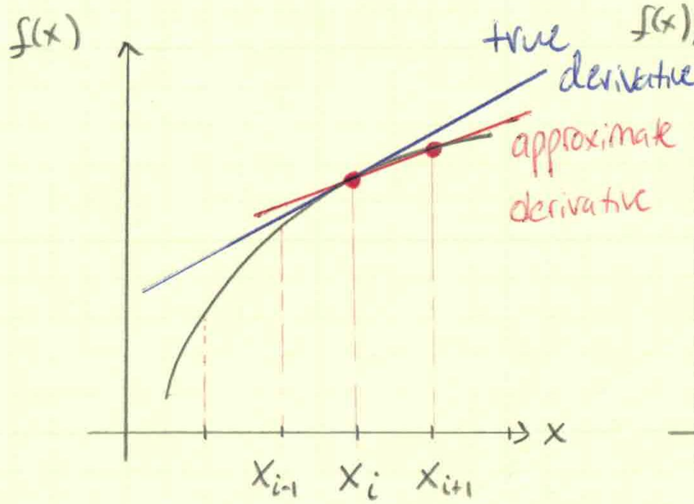
e.g using low-order polynomial.

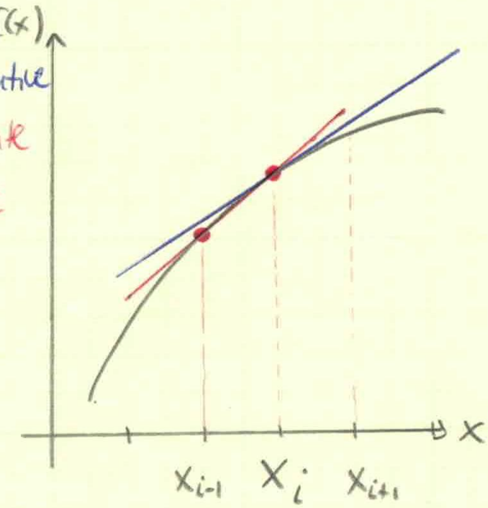


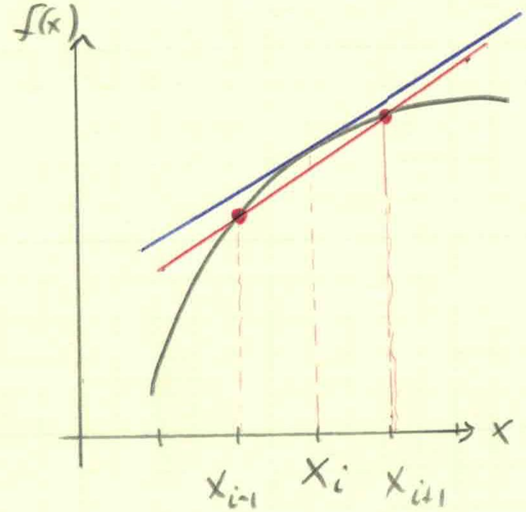
Use 3rd order polynomial to fit data.

⇒ take derivative at x_i

Finite Difference Approximation







$$\left.\frac{df}{dx}\right|_{x=x_i} \qquad \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} \qquad \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} \qquad \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}}$$

Forward Finite Difference

Backward Finite Difference

Central Finite Difference

How good are the approximations?

A: Derive them (and others) using Taylor Series Expansion.

Two Point Fwd-Difference

Where. $\Delta x = (x_{i+1} - x_i)$

Approximate $f(x_{i+1})$ by expanding about x_i

notice!

$$f(x_{i+1}) = f(x_i) + f'(x_i)\cdot\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 + \frac{f'''(x_i)}{3!}(\Delta x)^3 + \dots$$

Solve for $f'(x_i)$

$$f'(x_i)\Delta x = f(x_{i+1}) - f(x_i) - \frac{f''(x_i)}{2!}(\Delta x)^2 - \frac{f'''(x_i)}{3!}(\Delta x)^3 - \dots$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{\Delta x} \underbrace{- \frac{f''(x_i)}{2!}(\Delta x) - \frac{f'''(x_i)}{3!}(\Delta x)^2 - \dots}_{O(\Delta x)}$$

Thus: $$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} + O(\Delta x)$$

The error is on the order of Δx. Smaller Δx leads to better approximation... until other effects take over!

Two Point Bwd Difference

Approximate $f(x_{i-1})$ by expanding about x_i

notice!

Follow same approach. Error is $O(\Delta x)$ again.

Two Point Central Difference

Take the two earlier Taylor series expansions:

$$f(x_{i+1}) = \ldots$$

$$f(x_{i-1}) = \ldots$$

and difference them. Then solve for $f'(x_i)$.

The error is now $O((\Delta x)^2)$!

This derivation method can be extended to 3+ points to improve the approximations

⇒ See Table 8.4 for summary.