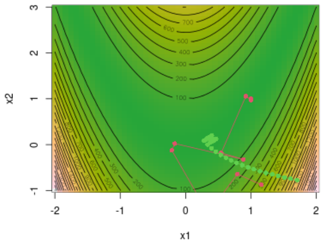
Optimization in Machine Learning

Second order methods
Newton-Raphson



Learning goals

- Newton-Raphson
- Limitations

FROM FIRST TO SECOND ORDER METHODS

- So far: **First order methods**
  $\Rightarrow$ *Gradient* information, i.e., first derivatives

- Now: **Second order methods**
  $\Rightarrow$ *Hessian* information, i.e., second derivatives

NEWTON-RAPHSON

Assumption: $f \in \mathcal{C}^2$

Aim: Find stationary point $\mathbf{x}^*$, i.e., $\nabla f(\mathbf{x}^*) = \mathbf{0}$

Idea: Find root of first order Taylor approximation of $\nabla f(\mathbf{x})$:

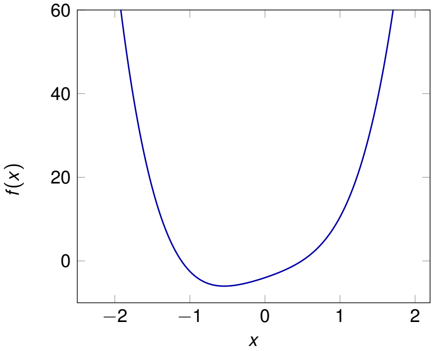
NEWTON-RAPHSON / 2

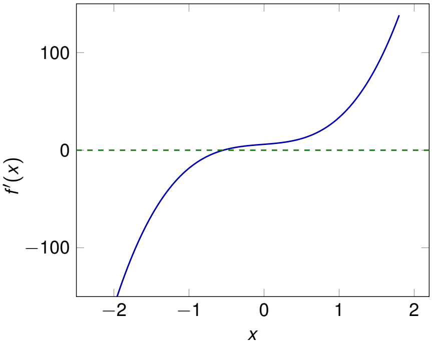
Extrema:

$$f(x) = 5 \cdot x^4 + \frac{1}{2}x^3 + 3x^2 + 6x - 4$$

Condition:

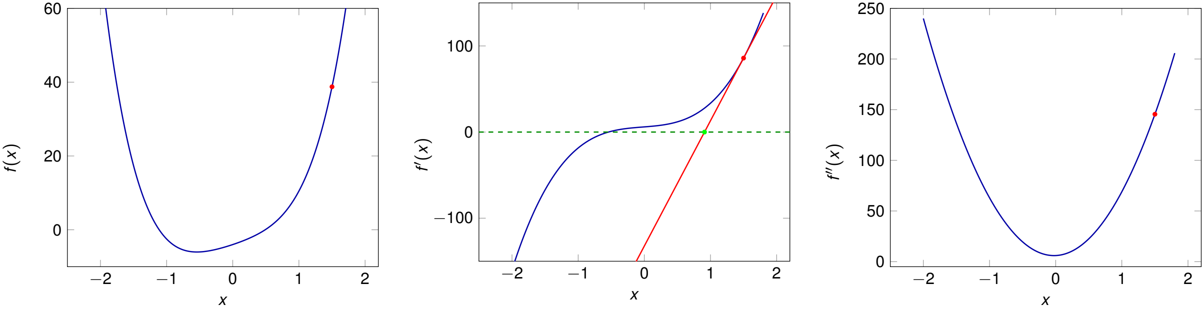
$$f'(x) = 20 \cdot x^3 + \frac{3}{2}x^2 + 6x + 6 = 0$$





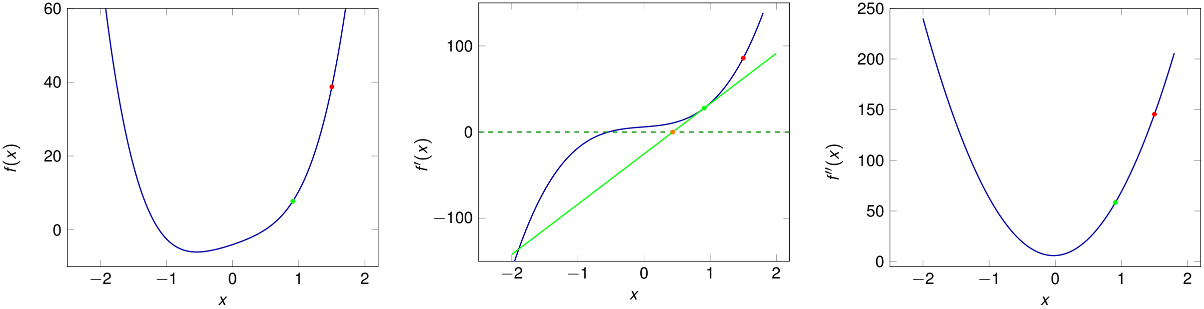
NEWTON-RAPHSON / 3

Iteration 1



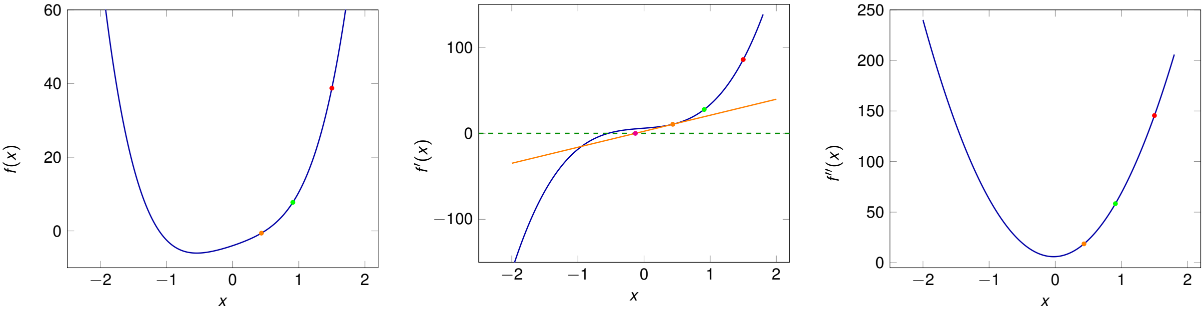
NEWTON-RAPHSON / 4

Iteration 2



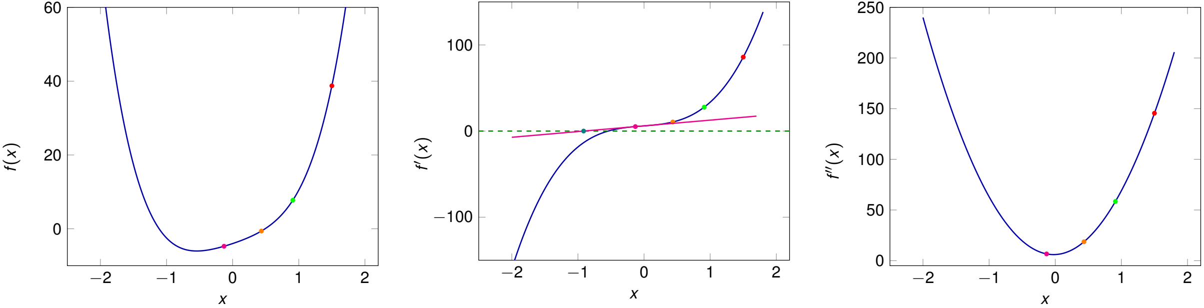
NEWTON-RAPHSON / 5

Iteration 3



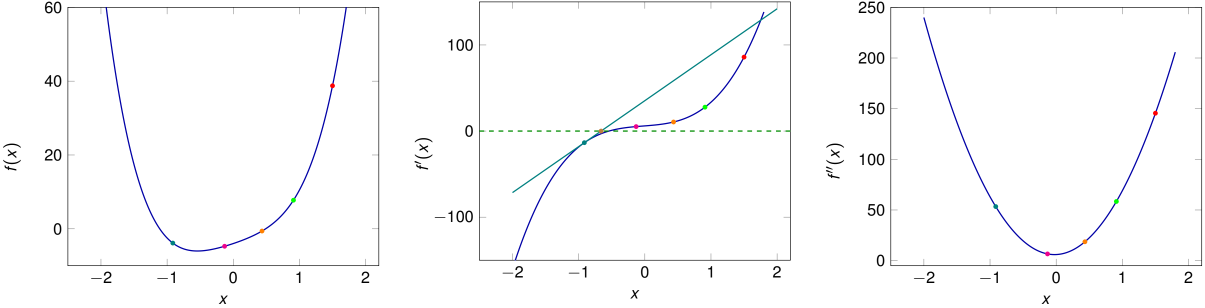
NEWTON-RAPHSON / 6

Iteration 4



NEWTON-RAPHSON / 7

Iteration 5



NEWTON-RAPHSON / 8

$$\nabla f(\mathbf{x}) \approx \nabla f(\mathbf{x}^{[t]}) + \nabla^2 f(\mathbf{x}^{[t]})(\mathbf{x} - \mathbf{x}^{[t]}) = \mathbf{0}$$

$$\nabla^2 f(\mathbf{x}^{[t]})(\mathbf{x} - \mathbf{x}^{[t]}) = -\nabla f(\mathbf{x}^{[t]})$$

$$\mathbf{x}^{[t+1]} = \mathbf{x}^{[t]} - \left(\nabla^2 f(\mathbf{x}^{[t]})\right)^{-1} \nabla f(\mathbf{x}^{[t]})$$

Update scheme:

$$\mathbf{x}^{[t+1]} = \mathbf{x}^{[t]} + \mathbf{d}^{[t]}$$

with $\mathbf{d}^{[t]} = -\left(\nabla^2 f(\mathbf{x}^{[t]})\right)^{-1} \nabla f(\mathbf{x}^{[t]})$

NEWTON-RAPHSON / 9

Note: In practice, we get $\mathbf{d}^{[t]}$ by solving the linear system

$$\nabla^2 f(\mathbf{x}^{[t]})\mathbf{d}^{[t]} = -\nabla f(\mathbf{x}^{[t]})$$

with direct (matrix decompositions) or iterative methods.

Relaxed/Damped Newton-Raphson: Use step size $\alpha > 0$ with

$$\mathbf{x}^{[t+1]} = \mathbf{x}^{[t]} + \alpha\mathbf{d}^{[t]}$$

to satisfy Wolfe conditions (or just Armijo rule)

ANALYTICAL EXAMPLE WITH QUADRATIC FORM

$$f(x_1, x_2) = x_1^2 + \frac{x_2^2}{2}$$

Update direction: $\mathbf{d}^{[t]} = -\left(\nabla^2 f(x_1^{[t]}, x_2^{[t]})\right)^{-1} \nabla f(x_1^{[t]}, x_2^{[t]})$

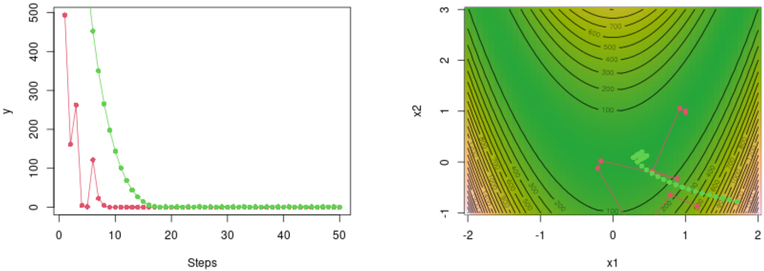
$$\nabla f(x_1, x_2) = \begin{pmatrix} 2x_1 \\ x_2 \end{pmatrix}, \quad \nabla^2 f(x_1, x_2) = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}$$

First step:

$$\begin{aligned} \begin{pmatrix} x_1^{[1]} \\ x_2^{[1]} \end{pmatrix} &= \begin{pmatrix} x_1^{[0]} \\ x_2^{[0]} \end{pmatrix} + \mathbf{d}^{[0]} = \begin{pmatrix} x_1^{[0]} \\ x_2^{[0]} \end{pmatrix} - \begin{pmatrix} 1/2 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 2x_1^{[0]} \\ x_2^{[0]} \end{pmatrix} \\ &= \begin{pmatrix} x_1^{[0]} \\ x_2^{[0]} \end{pmatrix} + \begin{pmatrix} -x_1^{[0]} \\ -x_2^{[0]} \end{pmatrix} = \mathbf{0} \end{aligned}$$

Note: Newton-Raphson only needs one iteration for quadratic forms

NEWTON-RAPHSON VS. GD ON BRANIN FUNCTION



Red: Newton-Raphson. Green: Gradient descent.
Newton-Raphson has much better convergence speed here.

DISCUSSION

Advantage:

- For f sufficiently smooth:

Newton-Raphson converges *locally* quadratically
(i.e., for starting points close enough to stationary point)

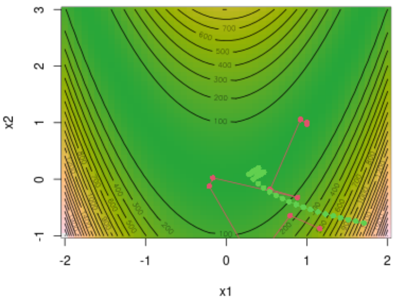
Disadvantage:

- For “bad” starting points:

Newton-Raphson may diverge

LIMITATIONS

Problem 1: In general, $\mathbf{d}^{[t]}$ is not a descent direction



But: If Hessian is positive definite, $\mathbf{d}^{[t]}$ is descent direction:

$$\nabla f(\mathbf{x}^{[t]})^\top \mathbf{d}^{[t]} = -\nabla f(\mathbf{x}^{[t]})^\top \left(\nabla^2 f(\mathbf{x}^{[t]})\right)^{-1} \nabla f(\mathbf{x}^{[t]}) < 0$$

Near minimum, Hessian is positive definite. For initial steps, Hessian is often not positive definite and Newton-Raphson may give non-descending update directions

LIMITATIONS / 2

Problem 2: Hessian can be **computationally expensive** to calculate, since descent direction $\mathbf{d}^{[t]}$ is the solution of the linear system

$$\nabla^2 f(\mathbf{x}^{[t]})\mathbf{d}^{[t]} = -\nabla f(\mathbf{x}^{[t]}).$$

Aim: Find quasi-second order methods not relying on exact Hessians

- Quasi-Newton method
- Gauss-Newton algorithm (for least squares)