$$V(r) \quad V^*(r) \quad V(r)$$

$$x_0 = 0 \quad x_1 \quad x_2 \quad x_3 = 3$$

## Quadratic potential

$$V(r) = k (r - a)^2$$

· Generate data

$${k = 1, k^* = 1, a = 1, a^* = 1.2}$$
  
 ${x_1 = 0.933, x_2 = 2.067}$ 

• Estimate positions and parameters

Guess -> 
$$\{k = 0.9, k^* = 1.1, a = 1.1, a^* = 1.1\}$$

10<sup>-10</sup>
10<sup>-20</sup>
10<sup>-25</sup>
10<sup>-30</sup>
0 2000 4000 6000 8000 10000

Iterations

## Output parameter set

$$\{k = 0.89, k^* = 1.1, a = 1.02, a^* = 1.2\}$$

## Lennard Jones potential

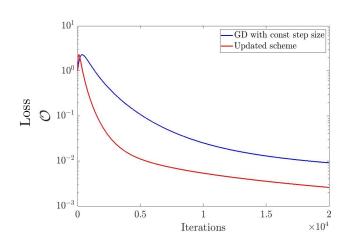
$$V(r) = \frac{A}{r^{12}} - \frac{B}{r^6}$$

Generate data

$${A = 1, A^* = 1.1, B = 2, B^* = 2}$$
  
 ${x_1 = 0.985, x_2 = 1.984}$ 

Estimate positions and parameters

Guess -> 
$$\{A=0.9, A^*=1.2, B=2.2, B^*=2.1\}$$



Output parameter set

$${A = 1.8, A^* = 1.92, B = 2.1, B^* = 1.75}$$