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Class: Machine Learning

Elements of Local Optimisation

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Learning outcomes

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- Describe the difference between zero, first, and second-order optimisation methods.
- Apply gradient descent to a given objective function.
- Choose an appropriate step size for gradient descent.

Goal

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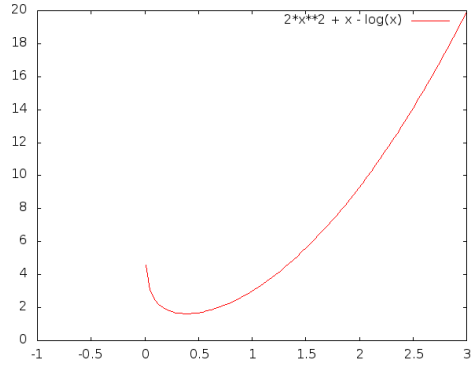
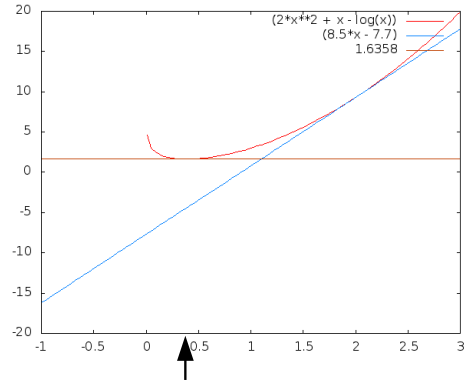
Find the minimum point of a given function:





The minimum is at 0.39

Optimisation is the field that studies how to find the minimum (or maximum) of a function.

Stationary points (minimum, maximum, and saddle points) have an important property: the derivative of the function in those points is always 0.

Local Methods

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Local methods move from the current point along a given direction by a certain step, until a local minimum is found. Different methods determine the direction and the step differently.

There are in general infinitely many directions, some will improve the current point (go down) others will make the current solution worse (of higher value, by going up).

The best possible direction is the direction of steepest descent, which is the anti-gradient (the gradient is the direction of steepest ascent).

Gradient descent

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First order: gradient descent

$$x_{t+1} = x_t - \eta \nabla f(x_t)$$

step parameter

Second order: Newton's method

$$f(x_n + \Delta x) \approx f(x_n) + f'(x_n)\Delta x + \frac{1}{2} f''(x_n)\Delta x^2$$

Taylor's expansion

$$\frac{\partial}{\partial \Delta x} f(x_n + \Delta x) = f'(x_n) + f''(x_n)\Delta x = 0$$

Optimal step

$$\Delta x = \frac{-f'(x_n)}{f''(x_n)}$$

Many dimensions: $x_{t+1} = x_t - H^{-1}|_{x_n} \nabla f$

Question

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The current point is <1,0>, compute the next point following gradient descent on the function $f(x,y) = x^3 + 2y^2 - y$ with step size 0.1.

Question

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We want to compute: $x_{t+1} = \langle 1,0 \rangle - 0.1 \nabla f(x_t)$

$\nabla f = \langle 3x^2, 4y - 1 \rangle$ Evaluated in <1,0> is <3,-1>

$$x_{t+1} = \langle 1,0 \rangle - 0.1 \cdot \langle 3, -1 \rangle = \langle 0.7, 0.1 \rangle$$

$f(1,0) = 1$

Our solution has improved!

$f(0.7, 0.1) = 0.263$

In 3D

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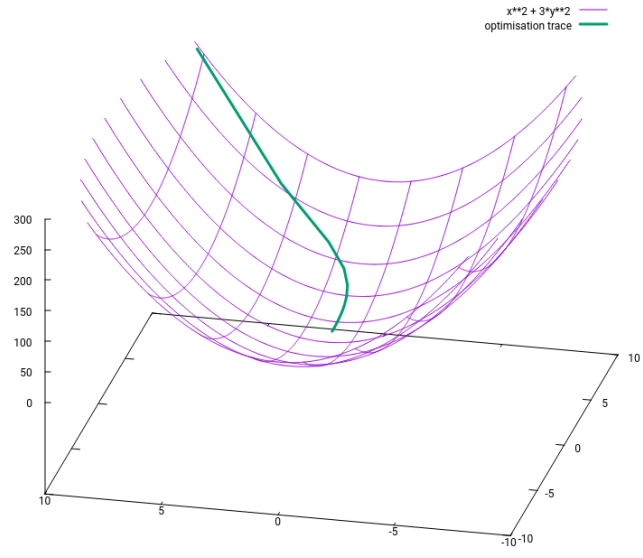

Step size: 0.1

The step size determines how much the algorithm will move the point along the gradient. In first-order methods it is usually chosen as a small constant <= 0.1.

A smaller step makes the algorithm slower, but a step that's too large will make it bounce between solutions indefinitely, or even overshoot (example in next slide).

In 3D

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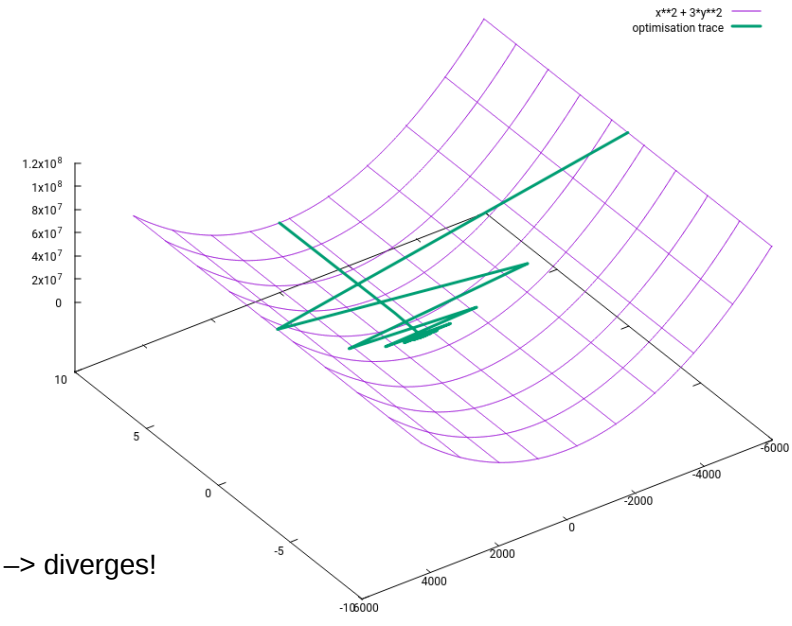

Step size: 0.14 –> diverges!

Local Minima

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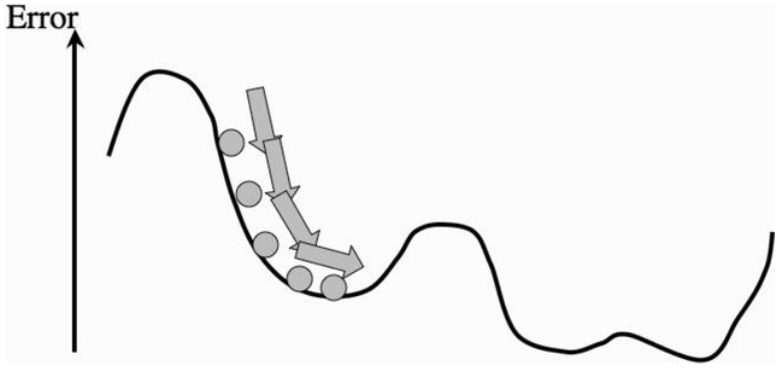

Local methods stop when the gradient is close to zero, which means that they are close to a stationary point.

There is no guarantee that such a point is the *global* minimum. Local methods will, in general, converge to a *local* minimum of the objective function.

A local minimum is a point such that all the points around it have a higher value of the objective function.

Conclusion

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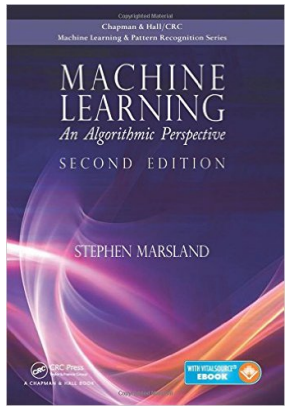

Sections 9.0, 9.1