

# Overview

Intro to  
Comp. Phys.

James  
Farrell &  
Jure  
Dobnikar

Numerical  
Differenti-  
ation

Numerical  
Integration

Solving  
Equations

Stationary  
Points  
(one  
variable)

Stationary  
Points  
(many  
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Global Op-  
timisation

## 1 Numerical Differentiation

## 2 Numerical Integration

## 3 Solving Equations

## 4 Stationary Points (one variable)

## 5 Stationary Points (many variables)

## 6 Global Optimisation

# Difference Formulae

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The **Taylor expansion** of continuous and differentiable function of single variable,  $f(x)$ , around the point  $x + h$ , is given by,

$$\begin{aligned}f(x+h) &= f(x) + hf'(x) + \frac{1}{2!}h^2f''(x) + \frac{1}{3!}h^3f'''(x) + \dots \\&= \sum_{n=0}^{\infty} \frac{h^n}{n!} f^{(n)}(x)\end{aligned}$$

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We can **truncate** a Taylor expansion to arrive at **approximations of different orders**,

$$f(x + h) = f(x) + \mathcal{O}(h)$$

$$f(x + h) = f(x) + hf'(x) + \mathcal{O}(h^2)$$

$$f(x + h) = f(x) + hf'(x) + \frac{1}{2}h^2f''(x) + \mathcal{O}(h^3)$$

$$f(x + h) = f(x) + hf'(x) + \frac{1}{2}h^2f''(x) + \frac{1}{6}h^3f'''(x) + \mathcal{O}(h^4)$$

The approximations converge to the correct answer as  $h \rightarrow 0$ .

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Rearranging the **first-order** approximation yields a **first-order** approximation to the derivative,

$$f(x + h) = f(x) + hf'(x) + \mathcal{O}(h^2)$$

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$$f(x + h) = f(x) + hf'(x) + \mathcal{O}(h^2)$$

$$f'(x) = \frac{f(x + h) - f(x)}{h} + \mathcal{O}(h) \quad (1)$$

FIRST FORWARD DIFFERENCES

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Expanding  $f(x - h)$  instead, we get a different approximation with the same error characteristics,

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

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

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

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We can eliminate higher-order derivatives and get higher-order approximations by taking **linear combinations** of approximations at **different points**, giving us a **second-order approximation** to the derivative,

$$f(x + h) = f(x) + hf'(x) + \frac{1}{2}h^2f''(x) + \mathcal{O}(h^3)$$

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$$f(x - h) = f(x) - hf'(x) + \frac{1}{2}h^2f''(x) + \mathcal{O}(h^3)$$

$$\begin{aligned} f(x + h) - f(x - h) = & +f(x) + hf'(x) + \frac{1}{2}h^2f''(x) + \\ & - f(x) + hf'(x) - \frac{1}{2}h^2f''(x) + \mathcal{O}(h^3) \end{aligned}$$

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$$f(x + h) - f(x - h) = 2hf'(x) + \mathcal{O}(h^3)$$

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$$f'(x) = \frac{f(x + h) - f(x - h)}{2h} + \mathcal{O}(h^2) \quad (3)$$

FIRST CENTRAL DIFFERENCES

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$$f(x - h) = f(x) - hf'(x) + \frac{1}{2}h^2f''(x) + \mathcal{O}(h^3)$$

$$f'(x) = \frac{f(x + h) - f(x - h)}{2h} + \mathcal{O}(h^2) \quad (3)$$

## FIRST CENTRAL DIFFERENCES

Not only do the zeroth and second order terms of the Taylor series cancel, **ALL other even order terms** also cancel.

First central differences converges to the true value of  $f'(x)$  faster than first forward or first backward differences.

# Comparison of Forward, Backward, and Central Differences

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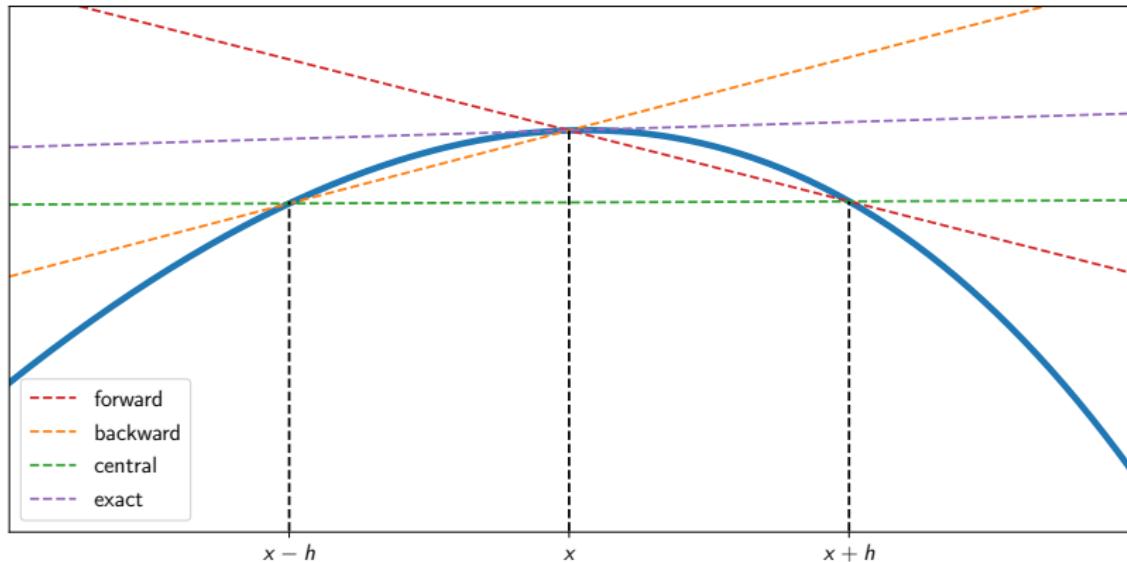


Figure 1: Comparison of the first forward, backward, and central differences methods for  $f(x) = x - x^2 + x^3 - x^4$  centred at the point  $x = 0.6$  with step size  $h = 0.1$ .

	forward	backward	central	exact
$f'(0.6)$	-0.135	0.139	0.002	0.016

Table 1:  $f'(0.6)$  at several levels of approximation.

Higher order derivatives can also be obtained in this way,

$$f(x + h) = f(x) + hf'(x) + \frac{1}{2}h^2f''(x) + \frac{1}{6}h^3f'''(x) + \mathcal{O}(h^4)$$

$$f(x - h) = f(x) - hf'(x) + \frac{1}{2}h^2f''(x) - \frac{1}{6}h^3f'''(x) + \mathcal{O}(h^4)$$

Higher order derivatives can also be obtained in this way,

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$$f(x-h) = f(x) - hf'(x) + \frac{1}{2}h^2f''(x) - \frac{1}{6}h^3f'''(x) + \mathcal{O}(h^4)$$

$$\begin{aligned} f(x+h) + f(x-h) = & +f(x) + hf'(x) + \frac{1}{2}h^2f''(x) + \frac{1}{6}h^3f'''(x) \\ & + f(x) - hf'(x) + \frac{1}{2}h^2f''(x) - \frac{1}{6}h^3f'''(x) + \mathcal{O}(h^4) \end{aligned}$$

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$$f(x - h) = f(x) - hf'(x) + \frac{1}{2}h^2f''(x) - \frac{1}{6}h^3f'''(x) + \mathcal{O}(h^4)$$

$$f(x + h) + f(x - h) = 2f(x) + h^2f''(x) + \mathcal{O}(h^4)$$

Higher order derivatives can also be obtained in this way,

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2f''(x) + \frac{1}{6}h^3f'''(x) + \mathcal{O}(h^4)$$
$$f(x-h) = f(x) - hf'(x) + \frac{1}{2}h^2f''(x) - \frac{1}{6}h^3f'''(x) + \mathcal{O}(h^4)$$

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \mathcal{O}(h^2) \quad (4)$$

### SECOND CENTRAL DIFFERENCES

We can construct approximations to **arbitrary order** by adding more and more combinations, e.g., this fourth-order approximation to the first derivative,

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2f''(x) + \frac{1}{6}h^3f'''(x) + \frac{1}{24}h^4f''''(x) + \mathcal{O}(h^5)$$

$$f(x-h) = f(x) - hf'(x) + \frac{1}{2}h^2f''(x) - \frac{1}{6}h^3f'''(x) + \frac{1}{24}h^4f''''(x) + \mathcal{O}(h^5)$$

$$f(x+2h) = f(x) + 2hf'(x) + 2h^2f''(x) + \frac{4}{3}h^3f'''(x) + \frac{2}{3}h^4f''''(x) + \mathcal{O}(h^5)$$

$$f(x-2h) = f(x) - 2hf'(x) + 2h^2f''(x) - \frac{4}{3}h^3f'''(x) + \frac{2}{3}h^4f''''(x) + \mathcal{O}(h^5)$$

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$$f(x+h) - f(x-h) = 2hf'(x) + \frac{1}{3}h^3f'''(x) + \mathcal{O}(h^5)$$

$$f(x+2h) - f(x-2h) = 4hf'(x) + \frac{8}{3}h^3f'''(x) + \mathcal{O}(h^5)$$

We can construct approximations to **arbitrary order** by adding more and more combinations, e.g., this fourth-order approximation to the first derivative,

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$$8(f(x+h) - f(x-h)) - (f(x+2h) - f(x-2h)) = 12hf'(x) + \mathcal{O}(h^5)$$

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$$f'(x) = \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h} + \mathcal{O}(h^4)$$

(5)

### FIVE POINT FORMULA

# Boundaries

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A solution for **boundary points** with the same error order as first central differences can be obtained by taking differences of  $f(x + h), f(x + 2h)$ ,

$$f(x + h) = f(x) + hf'(x) + \frac{1}{2}h^2f''(x) + \mathcal{O}(h^3)$$

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$$f(x + 2h) = f(x) + 2hf'(x) + 2h^2f''(x) + \mathcal{O}(h^3)$$

$$f(x + 2h) - 4f(x + h) = -3f(x) - 2hf'(x) + \mathcal{O}(h^3)$$

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$$f(x + 2h) = f(x) + 2hf'(x) + 2h^2f''(x) + \mathcal{O}(h^3)$$

$$f'(x) = \frac{4f(x + h) - 3f(x) - f(x + 2h)}{2h} + \mathcal{O}(h^2) \quad (6)$$

which expression approximates the derivative at  $x$  using only  $x$  and points to the right of  $x$ .

# Non-uniform grids

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It is easy enough to modify the second central difference equations to incorporate non-uniform spacings  $a, b$ ,

$$b^2 f(x+a) = b^2 f(x) + ab^2 f'(x) + \frac{1}{2}a^2 b^2 f''(x) + a^3 b^2 f'''(x) + \mathcal{O}(a^4)$$

$$a^2 f(x-b) = a^2 f(x) - ba^2 f'(x) + \frac{1}{2}b^2 a^2 f''(x) - b^3 a^2 f'''(x) + \mathcal{O}(b^4),$$

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rearranging,

$$f'(x) = \frac{b^2 f(x+a) - a^2 f(x-b) + (b^2 - a^2) f(x)}{ab(b+a)} + \mathcal{O}(h^2) \quad (7)$$

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rearranging,

$$f'(x) = \frac{b^2 f(x+a) - a^2 f(x-b) + (b^2 - a^2) f(x)}{ab(b+a)} + \mathcal{O}(h^2) \quad (7)$$

Notice that, with uneven spacings, only the second order terms in the Taylor series cancel—other, higher-order even terms remain.

# Richardson Extrapolation

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Say we can express a problem in the form,

$$A = A(h) + Kh^k + K' h^{k+1} + K'' h^{k+2} + \dots$$

where  $h, k, A(h)$  are known, and the constants  $K^n$  are in general not known.

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$$A = A(h) + Kh^k + K' h^{k+1} + K'' h^{k+2} + \dots$$

where  $h, k, A(h)$  are known, and the constants  $K^n$  are in general not known.

Truncating at  $k$ th order in  $h$ , we get,

$$A = A(h) + Kh^k + \mathcal{O}(h^{k+1}).$$

# Richardson Extrapolation

Intro to  
Comp. Phys.

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Stationary  
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Global Op-  
timisation

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Truncating at  $k$ th order in  $h$ , we get,

$$A = A(h) + Kh^k + \mathcal{O}(h^{k+1}).$$

How can we improve the error characteristics of this expression?

# Richardson Extrapolation

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Once again, we take **linear combinations** to eliminate the lowest-order unknown term,

$$A = A(h) + Kh^k + \mathcal{O}(h^{k+1})$$

$$A = A\left(\frac{h}{2}\right) + K\left(\frac{h}{2}\right)^k + \mathcal{O}(h^{k+1})$$

# Richardson Extrapolation

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Global Op-  
timisation

Once again, we take **linear combinations** to eliminate the lowest-order unknown term,

$$A = A(h) + Kh^k + \mathcal{O}(h^{k+1})$$

$$A = A\left(\frac{h}{2}\right) + \frac{1}{2^k} K(h)^k + \mathcal{O}(h^{k+1})$$

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Global Op-  
timisation

Once again, we take **linear combinations** to eliminate the lowest-order unknown term,

$$A = A(h) + Kh^k + \mathcal{O}(h^{k+1})$$

$$2^k A = 2^k A\left(\frac{h}{2}\right) + K(h)^k + \mathcal{O}(h^{k+1})$$

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Global Op-  
timisation

Once again, we take **linear combinations** to eliminate the lowest-order unknown term,

$$A = A(h) + Kh^k + \mathcal{O}(h^{k+1})$$

$$(2^k - 1) A = 2^k A\left(\frac{h}{2}\right) - A(h) + K(h)^k - K(h)^k + \mathcal{O}(h^{k+1})$$

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Once again, we take **linear combinations** to eliminate the lowest-order unknown term,

$$A = A(h) + Kh^k + \mathcal{O}(h^{k+1})$$

$$A = \frac{2^k A\left(\frac{h}{2}\right) - A(h)}{2^k - 1} + \mathcal{O}(h^{k+1})$$

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Once again, we take **linear combinations** to eliminate the lowest-order unknown term,

$$A = A(h) + Kh^k + \mathcal{O}(h^{k+1})$$

$$A = B(h) + \mathcal{O}(h^{k+1}) \tag{8}$$

$$B(h) = \frac{2^k A\left(\frac{h}{2}\right) - A(h)}{2^k - 1} \tag{9}$$

RICHARDSON EXTRAPOLATION

# Richardson Extrapolation: Example

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$$A = B(h) + \mathcal{O}(h^{k+1})$$
$$B(h) = \frac{2^k A\left(\frac{h}{2}\right) - A(h)}{2^k - 1}$$

let

$$A(h) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h)$$

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$$A = B(h) + \mathcal{O}(h^{k+1})$$
$$B(h) = \frac{2^k A\left(\frac{h}{2}\right) - A(h)}{2^k - 1}$$

let

$$A(h) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h)$$

then  $k = 1$  and

$$B(h) = 2A\left(\frac{h}{2}\right) - A(h)$$

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$$A = B(h) + \mathcal{O}(h^{k+1})$$
$$B(h) = \frac{2^k A\left(\frac{h}{2}\right) - A(h)}{2^k - 1}$$

let

$$A(h) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h)$$

substituting,

$$B(h) = 2 \frac{\frac{f(x+h/2) - f(x)}{\frac{h}{2}} - \frac{f(x+h) - f(x)}{h}}{2}$$

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$$A = B(h) + \mathcal{O}(h^{k+1})$$
$$B(h) = \frac{2^k A\left(\frac{h}{2}\right) - A(h)}{2^k - 1}$$

let

$$A(h) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h)$$

rearranging,

$$B(h) = \frac{4f(x+h/2) - 3f(x) - f(x+h)}{h}$$

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$$A = B(h) + \mathcal{O}(h^{k+1})$$
$$B(h) = \frac{2^k A\left(\frac{h}{2}\right) - A(h)}{2^k - 1}$$

let

$$A(h) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h)$$

setting  $h \rightarrow 2h$ ,

$$B(2h) = \frac{4f(x+h) - 3f(x) - f(x+2h)}{2h}$$

which you should remember from equation 6.

# Catastrophic Cancellation

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All of the difference methods suffer from catastrophic cancellation.

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

# Catastrophic Cancellation

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Global Op-  
timisation

All of the difference methods suffer from catastrophic cancellation.

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

On a computer, the **effective** value of  $h$  in the expression  $x - h$  is not the same as the  $h$  in the denominator.

$$x - (x - h) \neq h$$

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On a computer, the **effective** value of  $h$  in the expression  $x - h$  **is not the same** as the  $h$  in the denominator.

$$x - (x - h) \neq h$$

The **absolute** error in  $h$  is always the same, but the **relative** error increases as  $h$  decreases,

$$\epsilon = \left| \frac{(x - (x - h)) - h}{h} \right|$$

# Catastrophic Cancellation

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Global Op-  
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The **absolute** error in  $h$  is always the same, but the **relative** error increases as  $h$  decreases,

$$\epsilon = \left| \frac{(x - (x - h)) - h}{h} \right|$$

Remember, float addition is **NOT associative**, so the parentheses are meaningful.

# Complex Differences

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Global Op-  
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We can avoid this problem by taking an **imaginary step**,

$$f(x + ih) = f(x) + i h f'(x) - \frac{h^2}{2} f''(x) - i \frac{h^3}{6} f'''(x) + \mathcal{O}(h^4)$$

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$$\Im[f(x + ih)] = h f'(x) - \frac{h^3}{6} f'''(x) + \mathcal{O}(h^5)$$

# Complex Differences

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$$f(x + ih) = f(x) + ihf'(x) - \frac{h^2}{2}f''(x) - i\frac{h^3}{6}f'''(x) + \mathcal{O}(h^4)$$

$$f'(x) = \frac{\Im[f(x + ih)]}{h} + \frac{h^2}{6}f'''(x) + \mathcal{O}(h^4)$$

# Complex Differences

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$$f(x + ih) = f(x) + i h f'(x) - \frac{h^2}{2} f''(x) - i \frac{h^3}{6} f'''(x) + \mathcal{O}(h^4)$$

$$f'(x) = \frac{\Im[f(x + ih)]}{h} + \mathcal{O}(h^2) \quad (10)$$

FIRST COMPLEX DIFFERENCES

# Complex Differences

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We can avoid this problem by taking an **imaginary step**,

$$f(x + ih) = f(x) + i h f'(x) - \frac{h^2}{2} f''(x) - i \frac{h^3}{6} f'''(x) + \mathcal{O}(h^4)$$

$$f'(x) = \frac{\Im[f(x + ih)]}{h} + \mathcal{O}(h^2) \quad (10)$$

## FIRST COMPLEX DIFFERENCES

Addition of a real and imaginary float **does not incur precision loss!**

# Overview

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## 1 Numerical Differentiation

## 2 Numerical Integration

## 3 Solving Equations

## 4 Stationary Points (one variable)

## 5 Stationary Points (many variables)

## 6 Global Optimisation

# Numerical Integration

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A wealth of methods exist for approximating integrals with no closed form (or any other integral, for that matter).

$$\int_a^b \sqrt{1 - x^4} dx$$

$$\int_a^b \frac{1}{\log x} dx$$

$$\int_a^b \exp(-x^2) dx$$

$$\int_a^b \frac{\sin x}{x} dx$$

# Numerical Integration

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$$\int_a^b \sqrt{1 - x^4} dx$$

$$\int_a^b \exp(-x^2) dx$$

$$\int_a^b \frac{1}{\log x} dx$$

$$\int_a^b \frac{\sin x}{x} dx$$

We will look at **two** classes of approximations,

**NEWTON-COTES** and **GAUSSIAN QUADRATURE**

which both work by cutting up the integral into **slices**,

$$\int_a^b f(x) dx = \int_a^{a+h} f(x) dx + \dots + \int_{b-h}^b f(x) dx$$

small intervals on which  $f$  varies **smoothly**.

# From Taylor series

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Idea: integrate a Taylor expansion, then truncate the integral.

$$\int_a^b f(x) dx = \int_{-h}^h f(x_0 + y) dy$$

where  $h = (b - a)/2$ ,  $x_0 = (a + b)/2$ .

# From Taylor series

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$$\int_a^b f(x) dx = \int_{-h}^h f(x_0 + y) dy$$

where  $h = (b - a)/2$ ,  $x_0 = (a + b)/2$ .

$$\int_{-h}^h f(x_0 + y) dy = \int_{-h}^h \sum_{n=0}^{\infty} \frac{f^n(x_0)}{n!} y^n dy$$

# From Taylor series

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Idea: integrate a Taylor expansion, then truncate the integral.

$$\int_a^b f(x) dx = \int_{-h}^h f(x_0 + y) dy$$

where  $h = (b - a)/2$ ,  $x_0 = (a + b)/2$ .

$$\int_{-h}^h f(x_0 + y) dy = \sum_{n=0}^{\infty} \frac{f^n(x_0)}{n!} \int_{-h}^h y^n dy \quad (11)$$

$$= \sum_{n=0}^{\infty} \frac{f^n(x_0)}{n!} \left[ \frac{y^{n+1}}{n+1} \right]_{-h}^h \quad (12)$$

$$= \sum_{n=0}^{\infty} \frac{f^n(x_0)}{(n+1)!} (h^{n+1} - (-h)^{n+1}) \quad (13)$$

$$= \sum_{n=0}^{\infty} \frac{f^{2n}(x_0)}{(2n+1)!} 2h^{n+1} \quad (14)$$

# First order

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$$\int_{-h}^h f(x_0 + y) dy = \sum_{n=0}^{\infty} \frac{f^{2n}(x_0)}{(2n+1)!} 2h^{n+1}$$

# First order

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$$\int_{-h}^h f(x_0 + y) dy = \sum_{n=0}^{\infty} \frac{f^{2n}(x_0)}{(2n+1)!} 2h^{n+1}$$

Expanding to first order,

$$\int_{-h}^h f(x_0 + y) dy = 2hf(x_0) + \mathcal{O}(h^3)$$

# First order

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$$\int_{-h}^h f(x_0 + y) dy = \sum_{n=0}^{\infty} \frac{f^{2n}(x_0)}{(2n+1)!} 2h^{n+1}$$

Expanding to first order,

$$\int_{-h}^h f(x_0 + y) dy = 2hf(x_0) + \mathcal{O}(h^3)$$

$$\int_a^b f(x) dx \approx 2hf\left(\frac{a+b}{2}\right)$$
$$h = (b-a)/2$$

(15)

MIDPOINT RULE

# Second order

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$$\int_{-h}^h f(x_0 + y) dy = \sum_{n=0}^{\infty} \frac{f^{2n}(x_0)}{(2n+1)!} 2h^{n+1}$$

# Second order

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$$\int_{-h}^h f(x_0 + y) dy = \sum_{n=0}^{\infty} \frac{f^{2n}(x_0)}{(2n+1)!} 2h^{n+1}$$

Expanding to second order,

$$\int_{-h}^h f(x_0 + y) dy = 2hf(x_0) + \frac{f''(x_0)}{3} h^3 + \mathcal{O}(h^5)$$

# Second order

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$$\int_{-h}^h f(x_0 + y) dy = \sum_{n=0}^{\infty} \frac{f^{2n}(x_0)}{(2n+1)!} 2h^{n+1}$$

Expanding to second order,

$$\int_{-h}^h f(x_0 + y) dy = 2hf(x_0) + \frac{f''(x_0)}{3} h^3 + \mathcal{O}(h^5)$$

But!

$$f''(x_0) = \frac{f(x_0 - h) - 2f(x_0) + f(x_0 + h)}{h^2} + \mathcal{O}(h^2)$$

# Second order

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$$\int_{-h}^h f(x_0 + y) dy = \sum_{n=0}^{\infty} \frac{f^{2n}(x_0)}{(2n+1)!} 2h^{n+1}$$

Expanding to second order,

$$\int_{-h}^h f(x_0 + y) dy = 2hf(x_0) + \frac{f''(x_0)}{3} h^3 + \mathcal{O}(h^5)$$

But!

$$f''(x_0) = \frac{f(x_0 - h) - 2f(x_0) + f(x_0 + h)}{h^2} + \mathcal{O}(h^2)$$

$$\int_{-h}^h f(x_0 + y) dy = 2hf(x_0) + \frac{h^3}{3} \left[ \frac{f(x_0 - h) - 2f(x_0) + f(x_0 + h)}{h^2} + \mathcal{O}(h^2) \right] + \mathcal{O}(h^5)$$

# Second order

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timisation

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$$f''(x_0) = \frac{f(x_0 - h) - 2f(x_0) + f(x_0 + h)}{h^2} + \mathcal{O}(h^2)$$

$$\begin{aligned} \int_{-h}^h f(x_0 + y) dy &= 2hf(x_0) + \frac{h^3}{3} \left[ \frac{f(x_0 - h) - 2f(x_0) + f(x_0 + h)}{h^2} + \mathcal{O}(h^2) \right] + \mathcal{O}(h^5) \\ &= \frac{h}{3} [f(x_0 - h) + 4f(x_0) + f(x_0 + h)] + \mathcal{O}(h^5) \end{aligned}$$

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Global Op-  
timisation

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$$\boxed{\int_a^b f(x) dx \approx \frac{h}{3} \left[ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]} \quad (16)$$
$$h = (b-a)/2$$

SIMPSON'S RULE

# Summing up: composite rules

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- The midpoint rule and Simpson's rule allow us to approximate the integral over a single interval.

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Global Op-  
timisation

- The midpoint rule and Simpson's rule allow us to approximate the integral over a **single interval**.
- The approximation **improves** as the interval becomes **smaller** (proportional to  $h^3$  for the midpoint rule,  $h^5$  for Simpsons' rule).

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Global Op-  
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- We can take **higher-order expansions** to get formulae with better **asymptotic errors**...

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Global Op-  
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- The approximation **improves** as the interval becomes **smaller** (proportional to  $h^3$  for the midpoint rule,  $h^5$  for Simpsons' rule).
- We can take **higher-order expansions** to get formulae with better **asymptotic errors**...
- ...or **sum up** the approximations for many intervals to get smaller errors for each small interval.

# Summing up: composite rules

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Global Op-  
timisation

Take the midpoint rule as an example. If the approximation is made as a sum over many intervals,

$$\int_a^b f(x) dx = \sum_{i=0}^{n-1} [2hf(a + ih) + \mathcal{O}(h^3)] ; \quad h = \frac{b-a}{2n}$$

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$$= \left[ \sum_{i=0}^{n-1} 2hf(a + ih) \right] + n\mathcal{O}(h^3)$$

# Summing up: composite rules

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# Summing up: composite rules

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$$h = \frac{b-a}{2n}$$

COMPOSITE MIDPOINT RULE

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# Summing up: composite rules

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$$h = \frac{b-a}{2n}$$

## COMPOSITE MIDPOINT RULE

Notice the leading error term **goes down** one order of  $h$ .

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Global Op-  
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- When we derived equation 16, Simpson's rule for the integral of a function on an interval, we **truncated** a Taylor expansion of an integral and substituted an **approximation for a second derivative**.

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- When we derived equation 16, Simpson's rule for the integral of a function on an interval, we **truncated** a Taylor expansion of an integral and substituted an **approximation for a second derivative**.
- The result was a **linear combination of function values** on the interval.

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- Idea: approximate the integral as a weighted sum of function values at  $m$  evenly-spaced points on the interval,

$$A = \int_a^b f(x) dx \approx \sum_{i=1}^m w_i f(x_i) = \sum_{i=1}^m w_i f_i$$

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- Q. How do we choose the weights?

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- Q. How do we choose the weights?
- A. Choose the weights so that integrals of polynomials up to a given order are exact.

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- Q. How do we choose the weights?
- A. Choose the weights so that integrals of polynomials up to a given order are exact.
- Q. Why is that appealing?

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Global Op-  
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- Q. How do we choose the weights?
- A. Choose the weights so that integrals of polynomials up to a given order are exact.
- Q. Why is that appealing?
- A. The Taylor expansion of a function about a point is an infinite order polynomial; close to the point, the function and its integral are approximated well by a few low-order monomials.

# Deriving Newton-Cotes Weights

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For  $m$  evenly-spaced points, we get exact results for order- $(n-1)$  polynomials by solving  $m$  equations:

$$f(x) = 1 \implies \int_{x_1}^{x_m} 1 dx = x_m - x_1 = \sum_{i=1}^m w_i \cdot 1;$$

$$f(x) = x \implies \int_{x_1}^{x_m} x dx = \frac{1}{2} (x_m^2 - x_1^2) = \sum_{i=1}^m w_i x_i;$$

⋮

⋮

$$f(x) = x^{m-1} \implies \int_{x_1}^{x_m} x^{m-1} dx = \frac{1}{m} (x_m^m - x_1^m) = \sum_{i=1}^m w_i x_i^{m-1}.$$

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Global Op-  
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Solving for a single weight,

$$x_2 - x_1 = \sum_{i=1}^{m=1} w_i f_i$$

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Solving for a single weight,

$$x_2 - x_1 = w_1 \cdot 1$$

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Solving for a single weight,

$$x_2 - x_1 = w_1 \cdot 1$$

$$\implies w_1 = x_2 - x_1$$

# Deriving Newton-Cotes Weights

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Global Op-  
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Solving for a single weight,

$$x_2 - x_1 = w_1 \cdot 1$$

$$\implies w_1 = x_2 - x_1$$

$$\boxed{\int_{x_1}^{x_2} f(x) dx \approx hf_1}$$
$$h = x_2 - x_1$$

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RECTANGLE RULE

# Deriving Newton-Cotes Weights

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Global Op-  
timisation

Solving for two weights,

$$x_2 - x_1 = w_1 \cdot 1 + w_2 \cdot 1$$

$$\frac{1}{2} (x_2^2 - x_1^2) = w_1 x_1 + w_2 x_2$$

by symmetry,

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Global Op-  
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Solving for two weights,

$$x_2 - x_1 = w_1 \cdot 1 + w_2 \cdot 1$$

$$\frac{1}{2} (x_2^2 - x_1^2) = w_1 x_1 + w_2 x_2$$

by symmetry,

$$w_1 = w_2$$

$$\implies 2w_1 = x_2 - x_1$$

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Solving for two weights,

$$x_2 - x_1 = w_1 \cdot 1 + w_2 \cdot 1$$

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by symmetry,

$$w_1 = w_2 = \frac{1}{2} (x_2 - x_1)$$

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Global Op-  
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Solving for two weights,

$$x_2 - x_1 = w_1 \cdot 1 + w_2 \cdot 1$$

$$\frac{1}{2} (x_2^2 - x_1^2) = w_1 x_1 + w_2 x_2$$

by symmetry,

$$w_1 = w_2 = \frac{1}{2} (x_2 - x_1)$$

$$\boxed{\int_{x_1}^{x_2} f(x) dx \approx \frac{h}{2} (f_1 + f_2)}$$
$$h = x_2 - x_1$$

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TRAPEZIUM RULE

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Global Op-  
timisation

Solving for three weights,

$$x_3 - x_1 = w_1 \cdot 1 + w_2 \cdot 1 + w_3 \cdot 1$$

$$\frac{1}{2} (x_3^2 - x_1^2) = w_1 x_1 + w_2 x_2 + w_3 x_3$$

$$\frac{1}{3} (x_3^3 - x_1^3) = w_1 x_1^2 + w_2 x_2^2 + w_3 x_3^2$$

By symmetry,  $w_1 = w_3$ ; we also require the  $x_i$  to be evenly-spaced, so can write

$$x_1 = x_2 - h; x_3 = x_2 + h;$$

Substituting and rearranging,

# Deriving Newton-Cotes Weights

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Solving for three weights,

$$x_3 - x_1 = w_1 \cdot 1 + w_2 \cdot 1 + w_3 \cdot 1$$

$$\frac{1}{2} (x_3^2 - x_1^2) = w_1 x_1 + w_2 x_2 + w_3 x_3$$

$$\frac{1}{3} (x_3^3 - x_1^3) = w_1 x_1^2 + w_2 x_2^2 + w_3 x_3^2$$

By symmetry,  $w_1 = w_3$ ; we also require the  $x_i$  to be evenly-spaced, so can write

$$x_1 = x_2 - h; x_3 = x_2 + h;$$

Substituting and rearranging,

$$2h = 2w_1 + w_2$$

$$2hx_2 = 2w_1 x_2 + w_2 x_2$$

$$2hx_2^2 + \frac{2}{3}h^3 = 2w_1 (x_2^2 + h^2) + w_2 x_2^2$$

# Deriving Newton-Cotes Weights

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James  
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Jure  
Dobnikar

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Numerical  
Integration

Solving  
Equations

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Points  
(one  
variable)

Stationary  
Points  
(many  
variables)

Global Op-  
timisation

Solving for three weights,

$$x_3 - x_1 = w_1 \cdot 1 + w_2 \cdot 1 + w_3 \cdot 1$$

$$\frac{1}{2} (x_3^2 - x_1^2) = w_1 x_1 + w_2 x_2 + w_3 x_3$$

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$$x_1 = x_2 - h; x_3 = x_2 + h;$$

Substituting and rearranging,

$$\implies w_1 = \frac{1}{3}h = w_3; \quad w_2 = \frac{4}{3}h.$$

# Deriving Newton-Cotes Weights

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$$x_1 = x_2 - h; x_3 = x_2 + h;$$

Substituting and rearranging,

$$\boxed{\int_{x_1}^{x_3} f(x) dx \approx \frac{h}{3} (f_1 + 4f_2 + f_3)}$$
$$2h = x_3 - x_1$$

SIMPSON'S RULE

# Error in the Trapezium Rule

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Global Op-  
timisation

Compare the trapzeum rule,

$$\int_{-h}^h f(x+y) dy \approx h [f(x-h) + f(x+h)] = A_{\text{est}}$$

with the exact integral,

$$\int_{-h}^h f(x+y) dy = 2hf(x) + \frac{f''(x)}{3}h^3 + \mathcal{O}(h^5) = A_{\text{exact}}$$

# Error in the Trapezium Rule

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Q. What is the error in the trapezium rule approximation?

# Error in the Trapezium Rule

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$$A_{\text{exact}} - A_{\text{est}} = 2hf(x) + \frac{f''(x)}{3}h^3 - h[f(x-h) + f(x+h)] + \mathcal{O}(h^5)$$

# Error in the Trapezium Rule

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but, from the central differences formula,

$$-h^3 f''(x) = 2hf(x) - h[f(x-h) + f(x+h)] + \mathcal{O}(h^5)$$

# Error in the Trapezium Rule

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$$-h^3 f''(x) = 2hf(x) - h[f(x-h) + f(x+h)] + \mathcal{O}(h^5)$$

so,

$$A_{\text{exact}} - A_{\text{est}} = -\frac{2f''(x)}{3}h^3$$

# Romberg's method

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Global Op-  
timisation

- applying **Richardson extrapolation** to the trapezium rule yields Simpson's rule...

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Global Op-  
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- applying **Richardson extrapolation** to the trapezium rule yields Simpson's rule...
- applying Richardson extrapolation to Simpson's rule yields **Boole's rule**, a Newton–Cotes formula that is exact to fifth order.

# Romberg's method

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- ...doesn't lead to a Newton–Cotes formula.

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- at high orders, the Newton–Cotes formulae containing large weights of different signs, leading to loss of precision

# Romberg's method

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- applying Richardson extrapolation to Boole's rule...
- ...doesn't lead to a Newton–Cotes formula.
- at high orders, the Newton–Cotes formulae containing large weights of different signs, leading to loss of precision
- the formulae that come from Richardson extrapolation, Romberg's methods, are relatively stable

# Gaussian Quadrature

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Global Op-  
timisation

In deriving the weights for the Newton-Cotes formulae, our goal was to make an  $m$ -point approximation to the integral

$$\int_{x_1}^{x_m} f(x) dx$$

that was exact for order- $(m - 1)$  polynomials.

# Gaussian Quadrature

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By **fixing the integration limits to  $(-1, 1)$** , we can make the approximation **exact for all odd monomials**,

$$\int_{-1}^1 x^n = 0 \quad \text{for all odd } n$$

# Gaussian Quadrature

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If a change of coordinates that gives these limits is possible, then

## GAUSSIAN QUADRATURE

gives an  $m$ -point approximation exact for **order- $(2m - 1)$  polynomials**.

# Deriving Gaussian Quadrature nodes and weights

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Global Op-  
timisation

For two points, in this context called **nodes**,  $x_1, x_2$ ;  $x_1 < x_2$  somewhere on the interval  $(-1, 1)$ , we have **four equations with four unknowns**,

$$f(x) = 1 \rightarrow A = \int_{-1}^1 dx = 2 = w_1 + w_2$$

$$f(x) = x \rightarrow A = \int_{-1}^1 x dx = 0 = w_1 x_1 + w_2 x_2$$

$$f(x) = x^2 \rightarrow A = \int_{-1}^1 x^2 dx = \frac{2}{3} = w_1 x_1^2 + w_2 x_2^2$$

$$f(x) = x^3 \rightarrow A = \int_{-1}^1 x^3 dx = 0 = w_1 x_1^3 + w_2 x_2^3$$

# Deriving Gaussian Quadrature nodes and weights

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$$f(x) = x^3 \rightarrow A = \int_{-1}^1 x^3 dx = 0 = w_1 x_1^3 + w_2 x_2^3$$

Solving, we find,

$$x_2 = -x_1 = \frac{1}{\sqrt{3}}; \quad w_1 = w_2 = 1.$$

# Deriving Gaussian Quadrature nodes and weights

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$$\boxed{\int_{-1}^1 f(x) dx \approx f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)}$$

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GAUSSIAN QUADRATURE ON TWO NODES

# Coordinate transformation

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Global Op-  
timisation

In the general case of limits  $[a, b]$ , we must first apply the coordinate transformation,

$$\begin{aligned} t &= \frac{b-a}{2}x + \frac{b+a}{2} \\ \int_a^b f(t) dt &= \int_{-1}^1 f\left(\frac{b-a}{2}x + \frac{b+a}{2}\right) \frac{b-a}{2} dx \\ &= \int_{-1}^1 g(x) dx \end{aligned} \tag{22}$$

# Coordinate transformation

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The approximate expression for the integral becomes,

$$\int_a^b f(t) dt \approx \frac{b-a}{2} \sum_{i=1}^n w_i f\left(\frac{b-a}{2}x_i + \frac{b+a}{2}\right) \tag{23}$$

# Newton–Cotes vs. Gaussian quadrature

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Global Op-  
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- Gaussian quadrature is more accurate with fewer points, incurring **less computational effort...**

# Newton–Cotes vs. Gaussian quadrature

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Global Op-  
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- Gaussian quadrature is more accurate with fewer points, incurring **less computational effort**...
- ...but requires the function to be sampled at **specific points**, which is generally **not possible** with **experimental** data.

# Newton–Cotes vs. Gaussian quadrature

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- Gaussian quadrature is more accurate with fewer points, incurring **less computational effort**...
- ...but requires the function to be sampled at **specific points**, which is generally **not possible** with **experimental** data.
- Newton–Cotes methods can be generalised to work with **non-uniform data points**, making Simpson's method a good choice from integrating experimental data.

# Overview

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## 1 Numerical Differentiation

## 2 Numerical Integration

## 3 Solving Equations

## 4 Stationary Points (one variable)

## 5 Stationary Points (many variables)

## 6 Global Optimisation

# Solving Equations

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Solving any equation

$$f(x) = g(x)$$

# Solving Equations

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Solving any equation

$$f(x) = g(x)$$

can be recast as a **root-finding exercise**

$$f(x) - g(x) = 0.$$

# Solving Equations

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Solving any equation

$$f(x) = g(x)$$

can be recast as a **root-finding exercise**

$$f(x) - g(x) = 0.$$

Sometimes **closed-form** solutions exist, e.g. for polynomials with degree  $\leq 4$

$$ax^2 + bx + c = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

# Solving Equations

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Sometimes **closed-form** solutions exist, e.g. for polynomials with degree  $\leq 4$

$$ax^2 + bx + c = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

but for most equations, including almost all polynomials degree  $\geq 5$ , **no closed-form solution exists**

$$x^5 - x - 1 = 0 \implies x = 1.1673\dots$$

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Solving any equation

$$f(x) = g(x)$$

can be recast as a **root-finding exercise**

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Q. How do we solve such equations?

A. Make a **guess**, and try to **improve** it.

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Consider that deceptively difficult quintic,

$$x^5 - x - 1 = 0$$

which has a solution when  $x = \xi$

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We can rearrange to express  $x$  as a **slowly-varying** function of  $x$ ,

$$x = \phi(x) = \sqrt[5]{x + 1}$$

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## REARRANGEMENT METHOD

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At the **solution** to the quintic,  $\phi$  is equal to  $x$ ,

$$\phi(\xi) = \xi$$

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## REARRANGEMENT METHOD

At the **solution** to the quintic,  $\phi$  is equal to  $x$ ,

$$\phi(\xi) = \xi$$

but at other points  $x_i$  there is an **error**,  $\epsilon_i$ ,

$$\phi(x_i) = \xi + \epsilon_i$$

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Idea:

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Idea:

- 1 start with some guess,  $x_0$ ;

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Idea:

- 1 start with some guess,  $x_0$ ;
- 2 compute a new guess,  $x_1 = \phi(x_0)$ , and hope its closer to  $\xi$ ;

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Problem: how do we know if the sequence  $x_0, x_1, \dots, x_k, x_{k+1}$  converges to  $\xi$ ?

$$\lim_{k \rightarrow \infty} \phi(x_k) = \xi$$

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In order for this sequence to converge, we require the **absolute error**

$$|\epsilon_k| = |\xi - x_k|$$

to decrease after each iteration.

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Starting with,

$$\xi + \epsilon_{k+1} = x_{k+1} = \phi(x_k) = \phi(\xi + \epsilon_k),$$

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Starting with,

$$\xi + \epsilon_{k+1} = x_{k+1} = \phi(x_k) = \phi(\xi + \epsilon_k),$$

we expand the right-most term as a Taylor series,

$$\xi + \epsilon_{k+1} = \phi(\xi) + \epsilon_k \phi'(\xi) + \mathcal{O}(\epsilon_k^2)$$

$$\epsilon_{k+1} = \epsilon_k \phi'(\xi) + \mathcal{O}(\epsilon_k^2)$$

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therefore a **necessary** (but not sufficient) condition for the sequence to converge to  $\xi$  is

$$\|\phi'(\xi)\| < 1$$

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How quickly does  $\phi(x)$  converge to  $\xi$ ?

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How quickly does  $\phi(x)$  converge to  $\xi$ ?

In general we can write,

$$\lim_{k \rightarrow \infty} \frac{|\epsilon_{k+1}|}{|\epsilon_k|^q} = \mu$$

Q-CONVERGENCE

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Q-CONVERGENCE

where  $q$  is the order of convergence and  $\mu$  is the rate of convergence

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In the example,

$$\epsilon_{k+1} = \epsilon_k \phi'(\xi) + \mathcal{O}(\epsilon_k^2)$$

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$$\lim_{k \rightarrow \infty} \frac{|\epsilon_{k+1}|}{|\epsilon_k|} = |\phi'(\xi)|$$

$$q = 1 \text{ and } \mu = |\phi'(\xi)|$$

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$$\epsilon_{k+1} = \epsilon_k \phi'(\xi) + \mathcal{O}(\epsilon_k^2)$$

$$\lim_{k \rightarrow \infty} \frac{|\epsilon_{k+1}|}{|\epsilon_k|} = |\phi'(\xi)|$$

$q = 1$  and  $\mu = |\phi'(\xi)|$

we say that the sequence converges linearly to  $\xi$  with rate  $|\phi'(\xi)|$ .

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If  $\phi'$  vanishes at the solution, but  $\phi''$  is finite and non-zero,

$$\xi + \epsilon_{k+1} = \phi(\xi) + \epsilon_k \phi'(\xi) + \frac{1}{2} \epsilon_k^2 \phi''(\xi) + \mathcal{O}(\epsilon_k^3)$$

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$$\frac{\epsilon_{k+1}}{\epsilon_k^2} = \frac{1}{2} \phi''(\xi) + \mathcal{O}(\epsilon_k)$$

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$$\lim_{k \rightarrow \infty} \frac{|\epsilon_{k+1}|}{|\epsilon_k|^2} = \frac{1}{2} \phi''(\xi)$$

$q = 2$ ,  $\mu = \frac{1}{2} \phi''(\xi)$ , and the sequence converges quadratically to the limit  $\xi$ .

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$q = 2$ ,  $\mu = \frac{1}{2} \phi''(\xi)$ , and the sequence converges quadratically to the limit  $\xi$ .

A heuristic to estimate  $q$  is given by,

$$q \approx \frac{\log \left| \frac{x_{k+1} - x_k}{x_k - x_{k-1}} \right|}{\log \left| \frac{x_k - x_{k-1}}{x_{k-1} - x_{k-2}} \right|} \quad (25)$$

Q-CONVERGENCE RATE ESTIMATE

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Q. Does the quintic sequence converge?

$$x^5 - x - 1 = 0$$

$$x_{k+1} = \phi(x_k) = \sqrt[5]{x_k + 1}$$

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$$\xi + \epsilon_{k+1} = \phi(\xi) + \epsilon_k \phi'(\xi) + \mathcal{O}(\epsilon_k^2)$$

# Solving the Quintic

Intro to  
Comp. Phys.

James  
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Jure  
Dobnikar

Numerical  
Differenti-  
ation

Numerical  
Integration

Solving  
Equations

Stationary  
Points  
(one  
variable)

Stationary  
Points  
(many  
variables)

Global Op-  
timisation

Q. Does the quintic sequence converge?

$$x^5 - x - 1 = 0$$

$$x_{k+1} = \phi(x_k) = \sqrt[5]{x_k + 1}$$

$$\phi'(x) = \frac{1}{5} \frac{\phi(x)}{x_k + 1}$$

$$\xi + \epsilon_{k+1} = \phi(\xi) + \epsilon_k \frac{1}{5} \frac{\phi(\xi)}{\xi + 1} + \mathcal{O}(\epsilon_k^2)$$

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# Solving the Quintic

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# Solving the Quintic

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$$\lim_{k \rightarrow \infty} \frac{|\epsilon_{k+1}|}{|\epsilon_k|} = \left| \frac{1}{5} \frac{\xi}{\xi + 1} \right|$$

# Solving the Quintic

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A.  $q = 1, \mu \approx 0.11 < 0$

# Solving the Quintic

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A.  $q = 1, \mu \approx 0.11 < 0$

the sequence **converges** to the solution for **all** starting values  $x_k$ .

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Global Op-  
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- 1 find an interval  $(a, b)$  that contains a zero;

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Global Op-  
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- 1 find an interval  $(a, b)$  that contains a zero;
- 2 find  $c = (a + b)/2$ ;

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Global Op-  
timisation

- 1 find an interval  $(a, b)$  that contains a zero;
- 2 find  $c = (a + b)/2$ ;
- 3 set  $(a, b) \leftarrow (a, c)$  or  $(a, b) \leftarrow (c, b)$  such that  $(a, b)$  still contains a zero

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Global Op-  
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- 4 continue until  $|a - b| < \delta$

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Global Op-  
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- 4 continue until  $|a - b| < \delta$

$$a_{k+1}, b_{k+1} = \phi(a_k, b_k) = \begin{cases} \left(a_k, \frac{a_k+b_k}{2}\right) & \text{if } f\left(\frac{a_k+b_k}{2}\right) > 0; \\ \left(\frac{a_k+b_k}{2}, b_k\right) & \text{if } f\left(\frac{a_k+b_k}{2}\right) < 0. \end{cases} \quad (26)$$

BISECTION UPDATE

# Bisection

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Numerical  
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tion

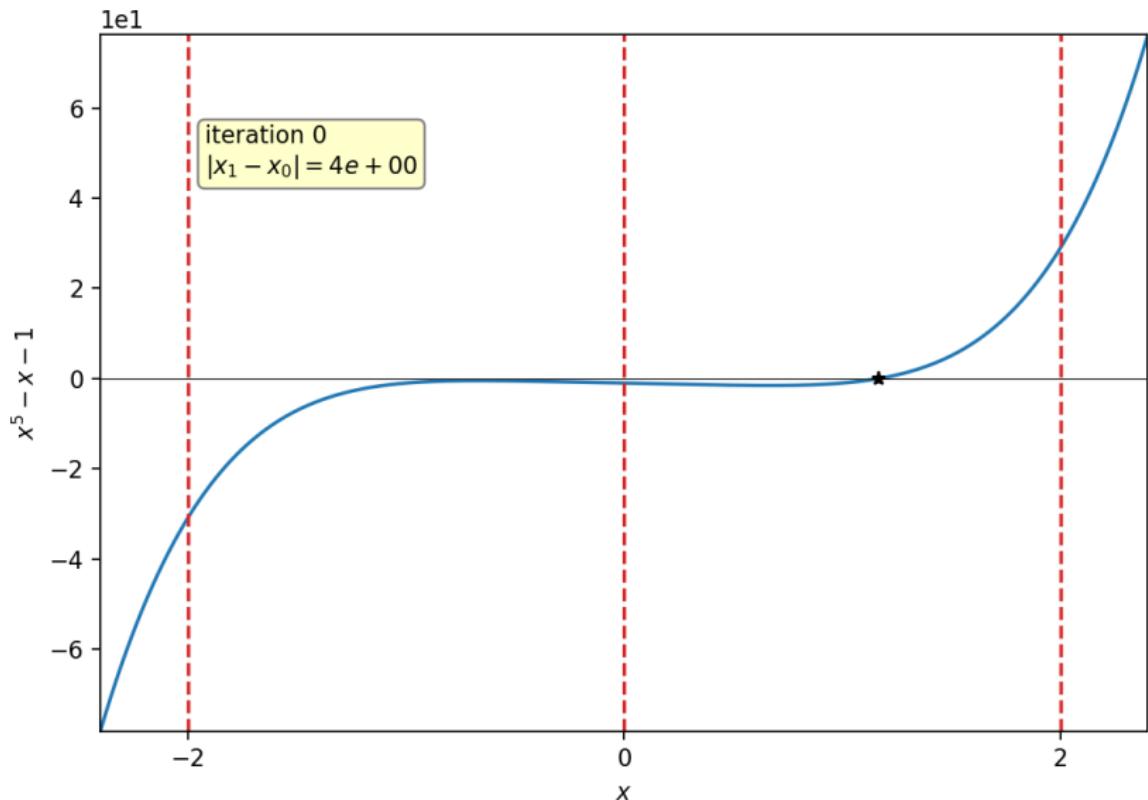
Numerical  
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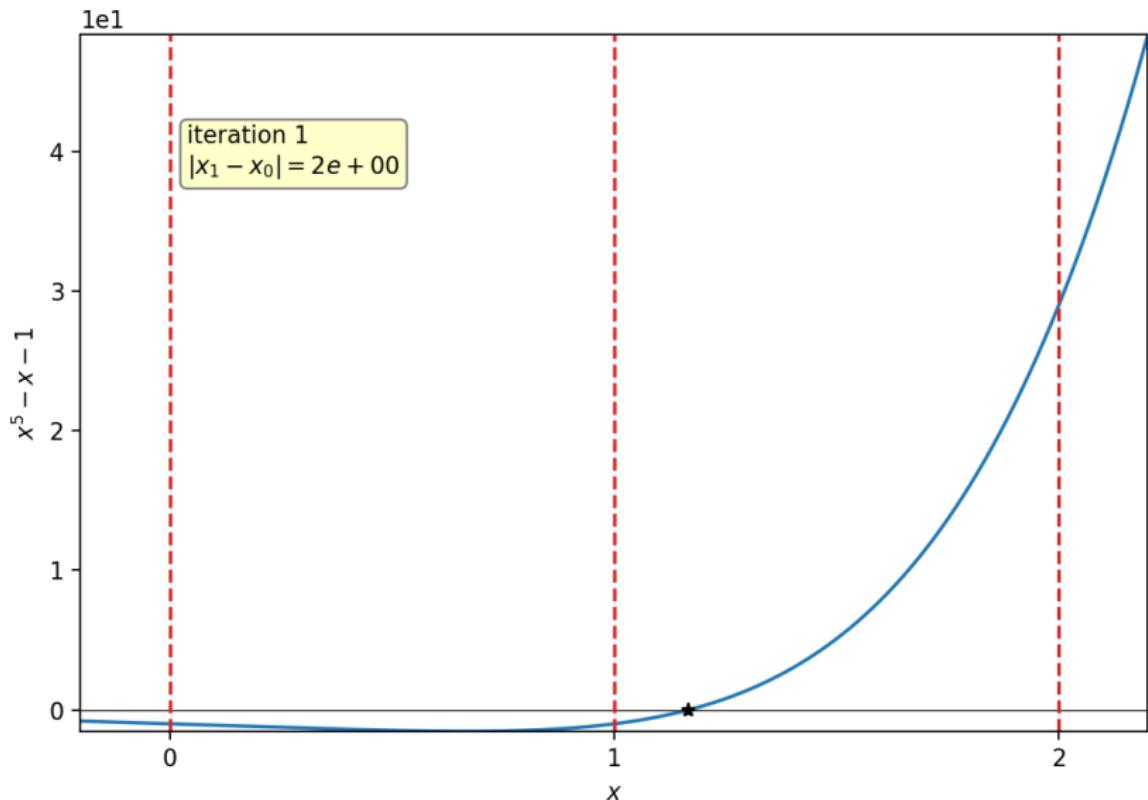
Numerical  
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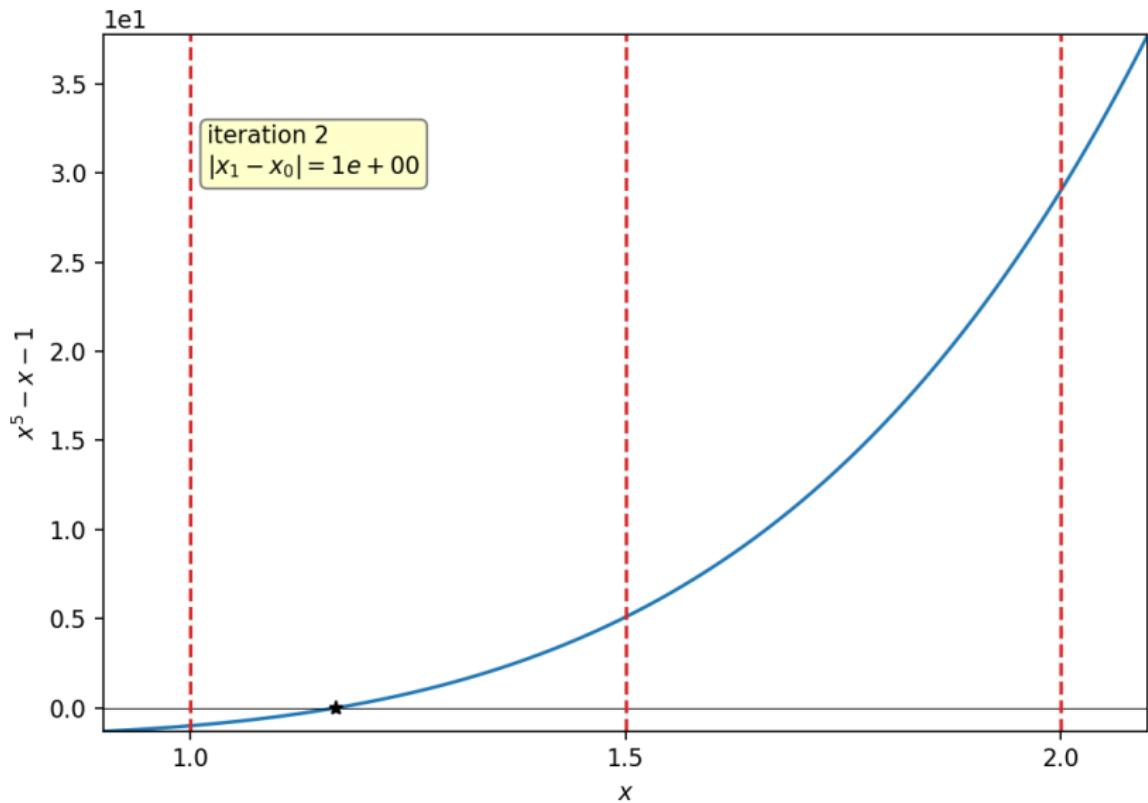
Numerical  
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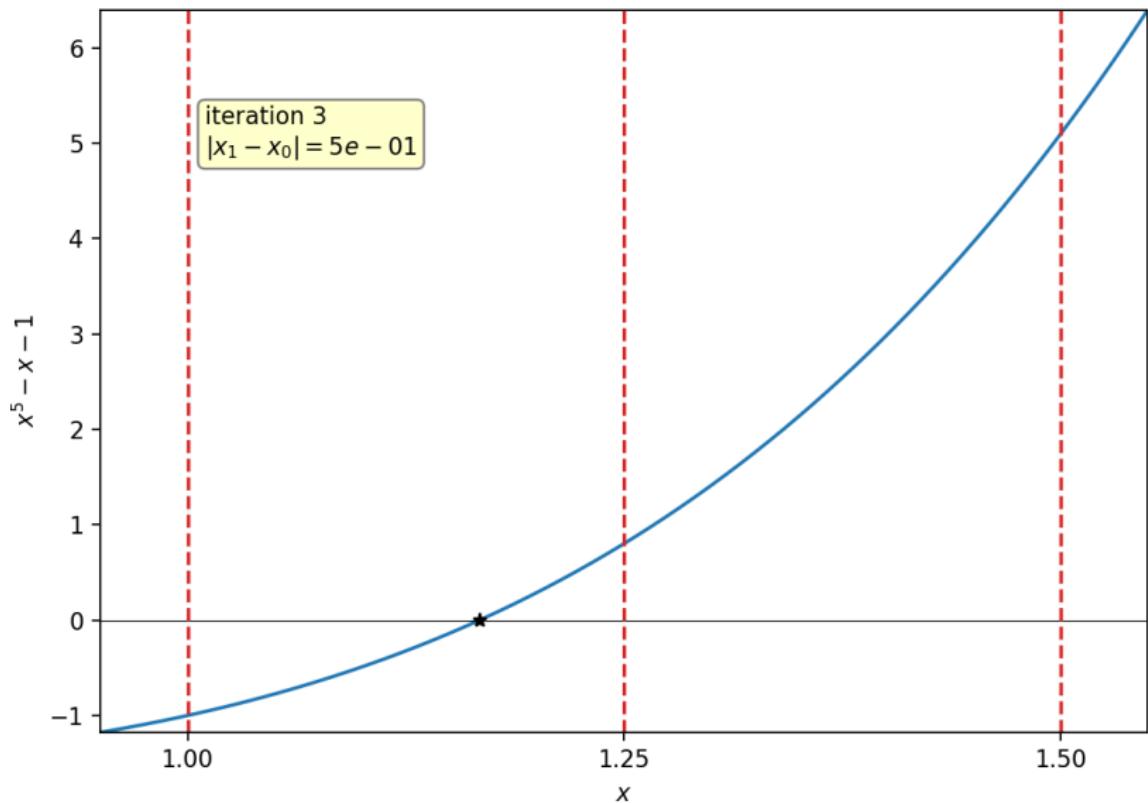
Numerical  
Integration

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Stationary  
Points  
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Points  
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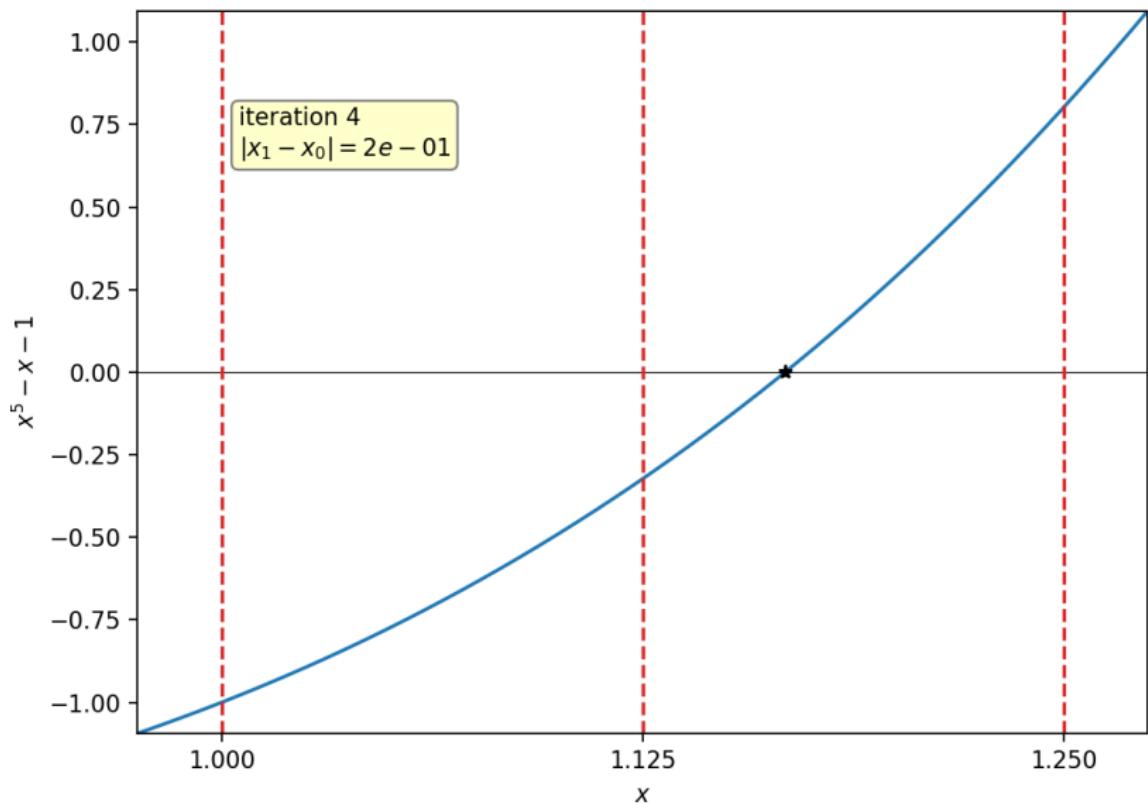
Numerical  
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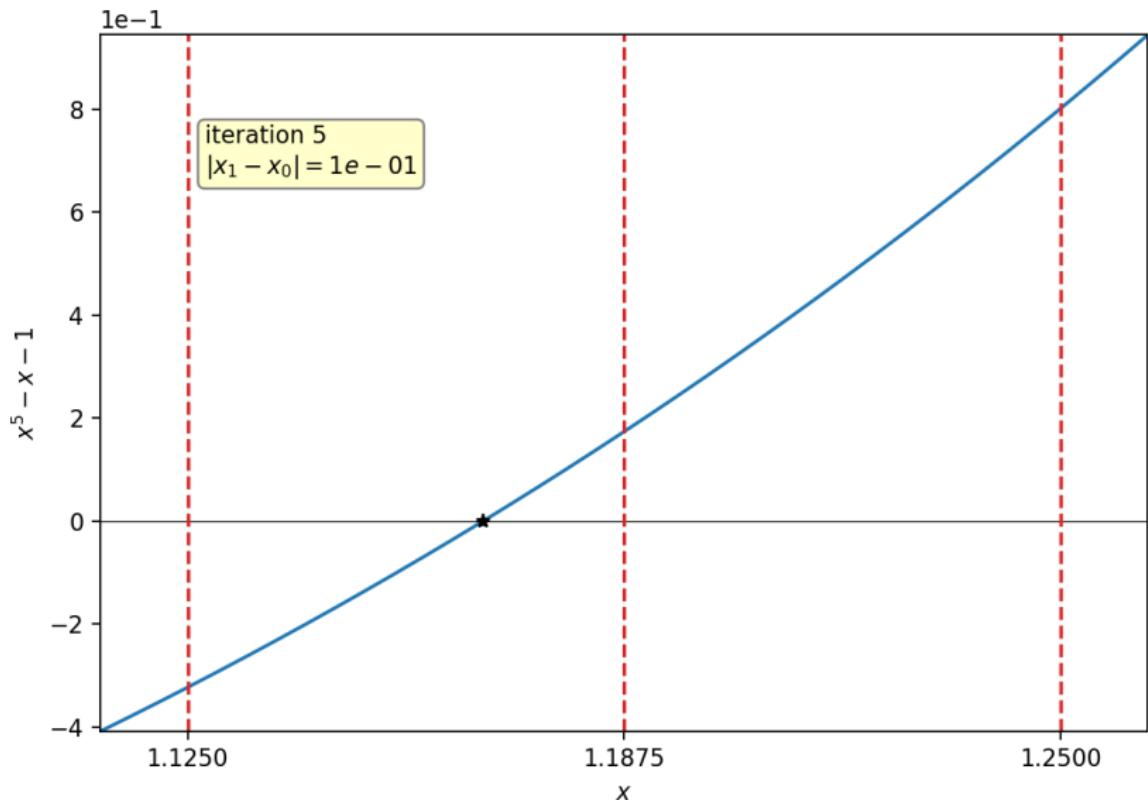
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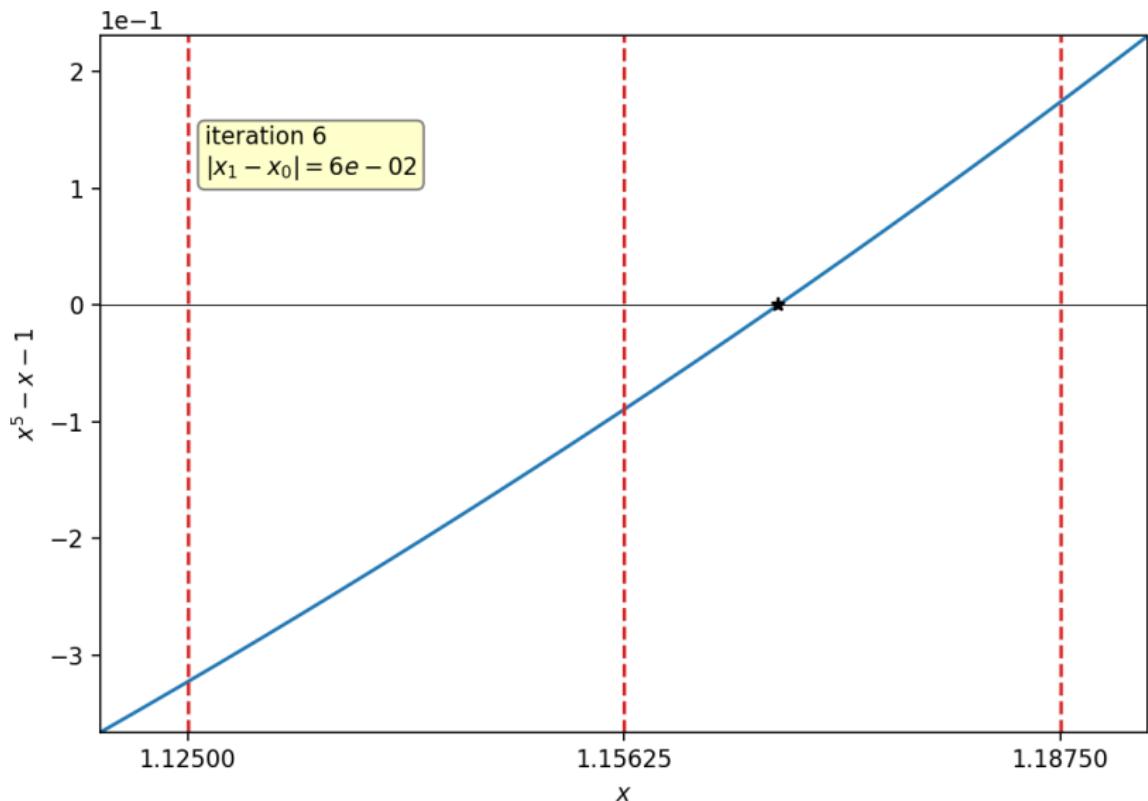
Numerical  
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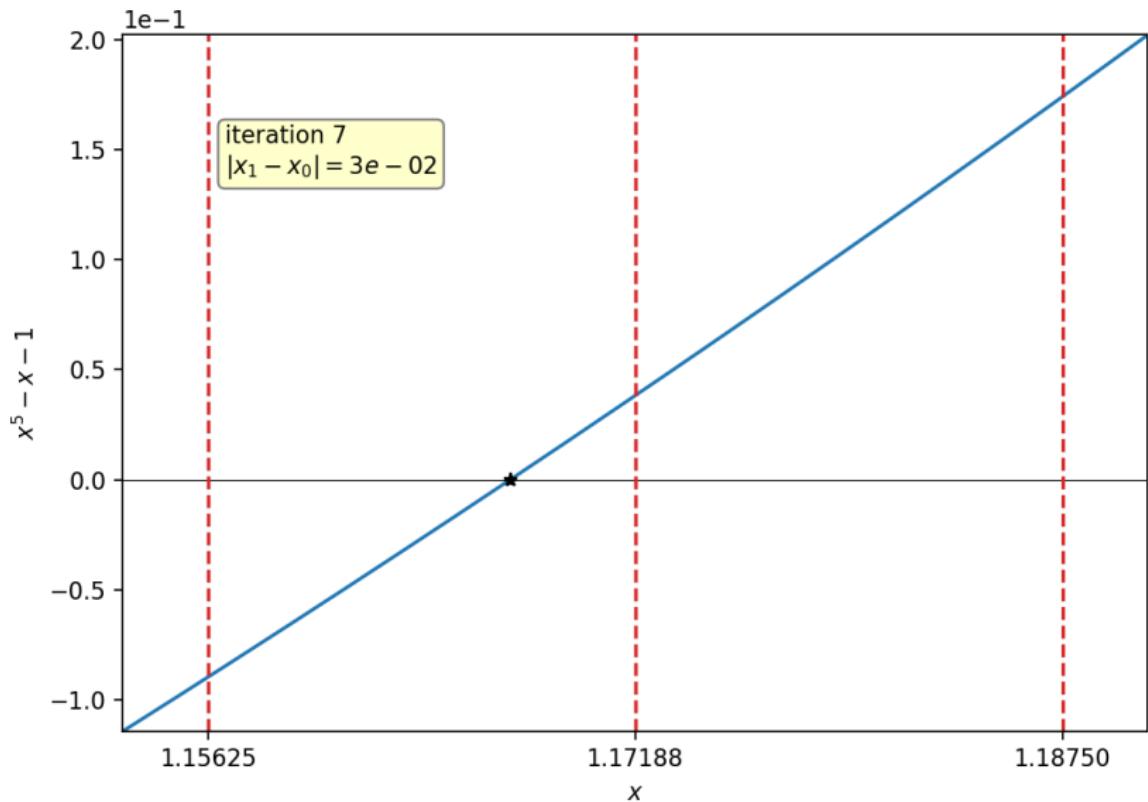
Numerical  
Integration

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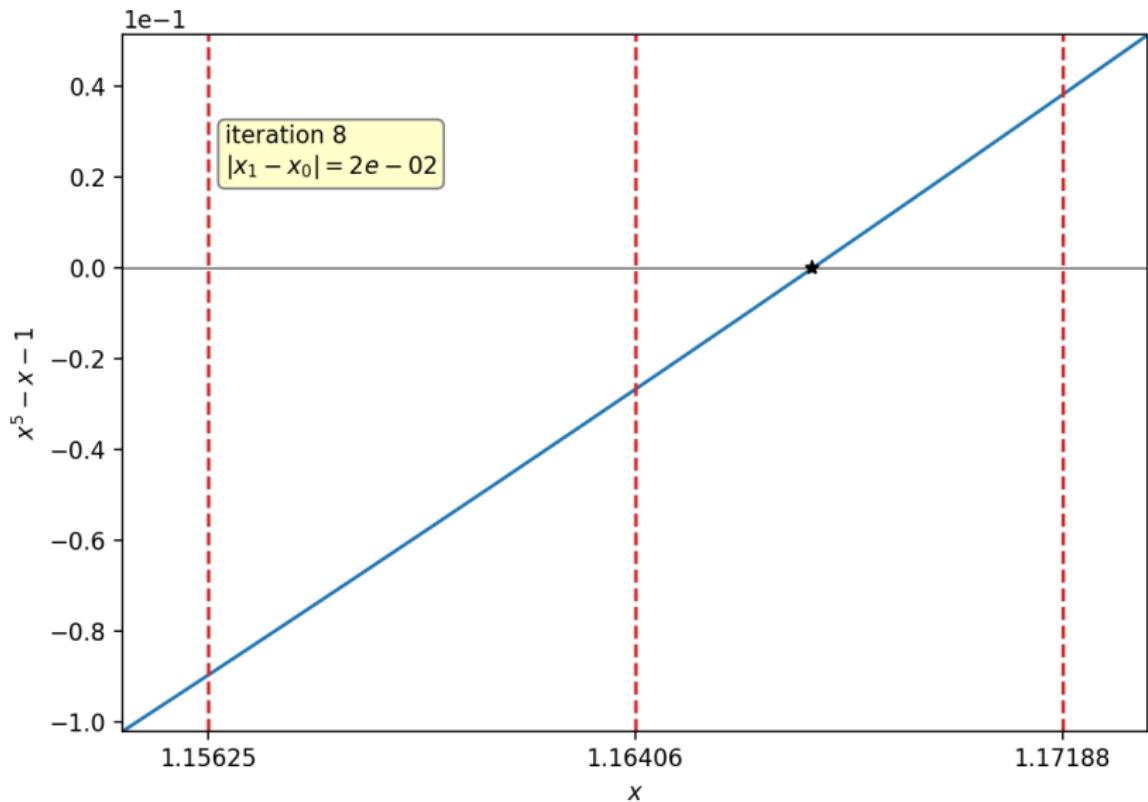
Numerical  
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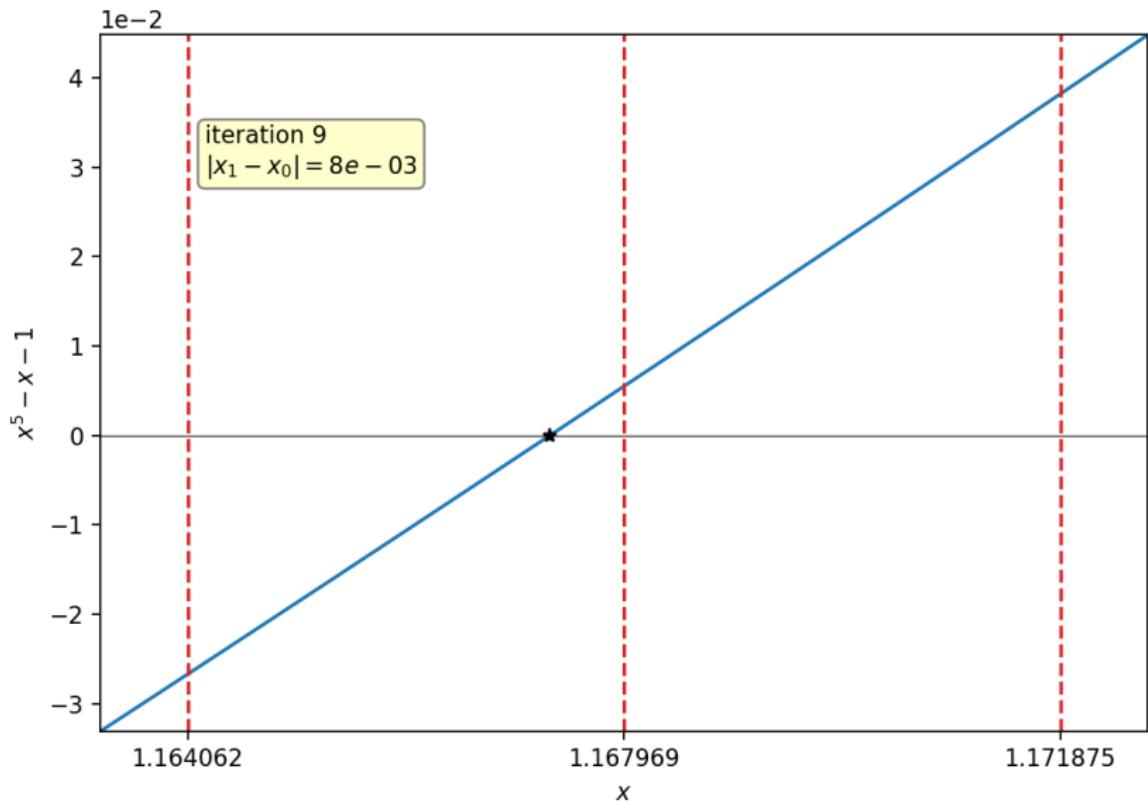
Numerical  
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Global Op-  
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- 1 choose an interval  $(x_0, x_1)$ , ideally containing a zero;

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Global Op-  
timisation

- 1 choose an interval  $(x_0, x_1)$ , ideally containing a zero;
- 2 find the secant line that passes through  $(x_0, f_0), (x_1, f_1)$

$$y = \frac{f_1 - f_0}{x_1 - x_0}(x - x_1) + f_1$$

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Global Op-  
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- 3 find the zero of the secant line,  $x_2$

$$x_2 = x_1 - f_1 \frac{x_1 - x_0}{f_1 - f_0}$$

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Global Op-  
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- 4  $(x_0, x_1) \leftarrow (x_1, x_2)$

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Global Op-  
timisation

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- 5 continue until  $|x_0 - x_1| < \delta$

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Global Op-  
timisation

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- 5 continue until  $|x_0 - x_1| < \delta$

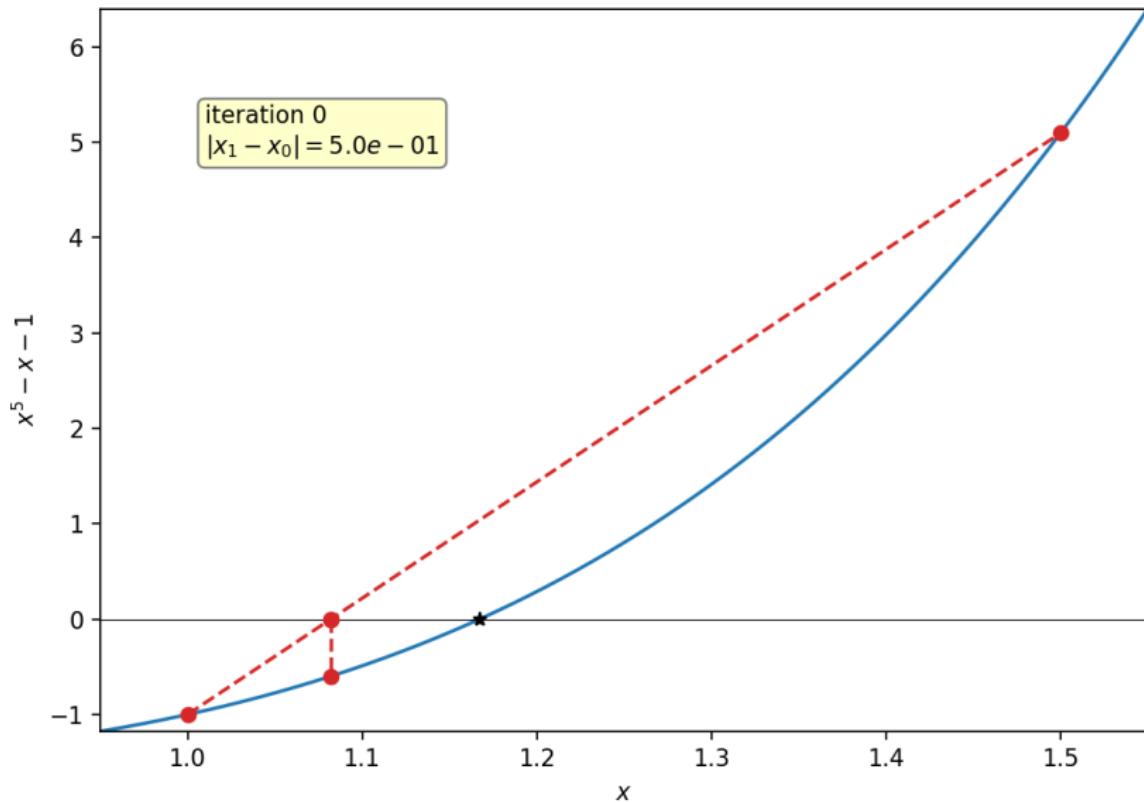
$$(x_{k+1}, x_{k+2}) = \left( x_{k+1}, \left\{ x_{k+1} - f_{k+1} \frac{x_{k+1} - x_k}{f_{k+1} - f_k} \right\} \right)$$

(27)

SECANT UPDATE

# Secant Method

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Numerical Integration  
Solving Equations  
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Stationary Points (many variables)  
Global Optimisation



# Secant Method

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Differentia-  
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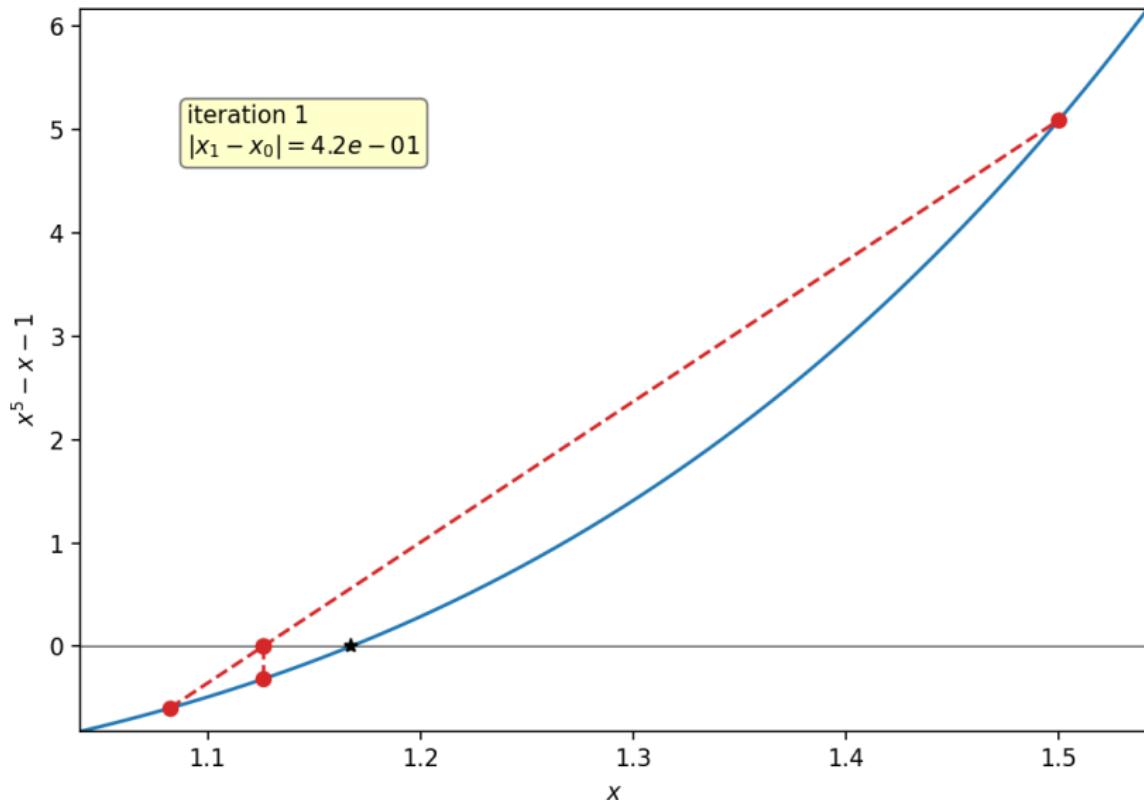
Numerical  
Integration

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variable)

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Points  
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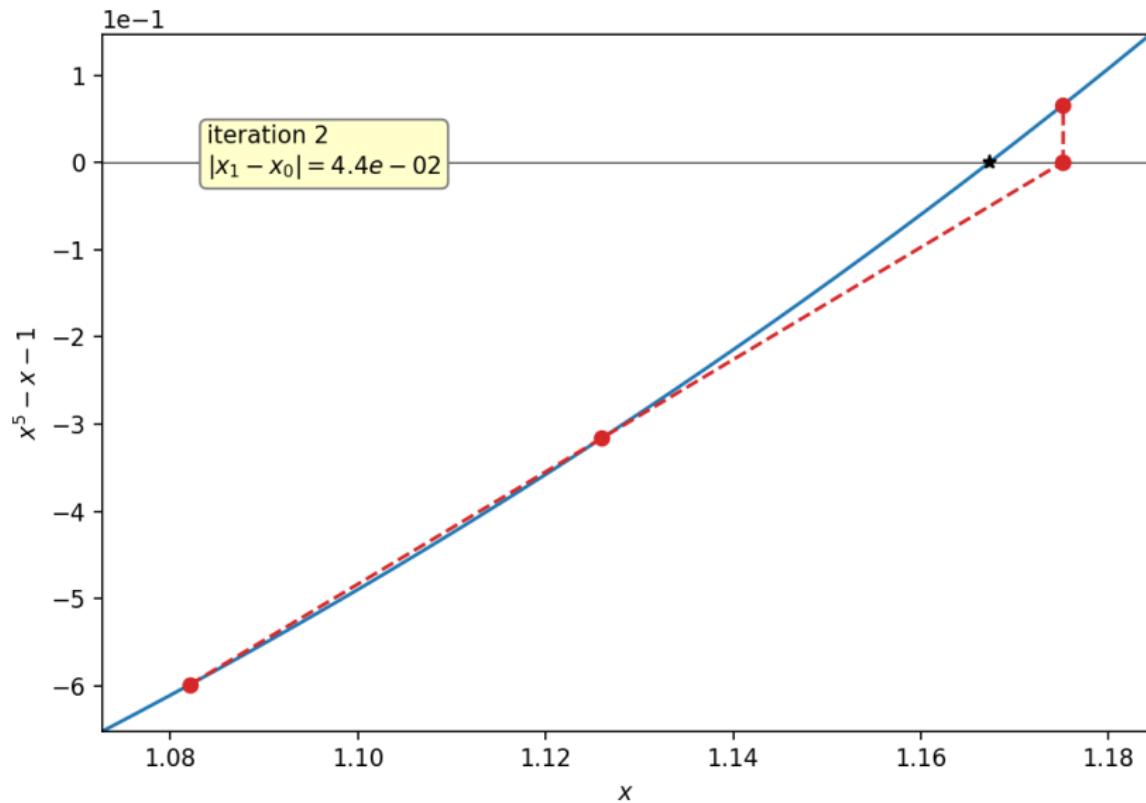
Numerical  
Integration

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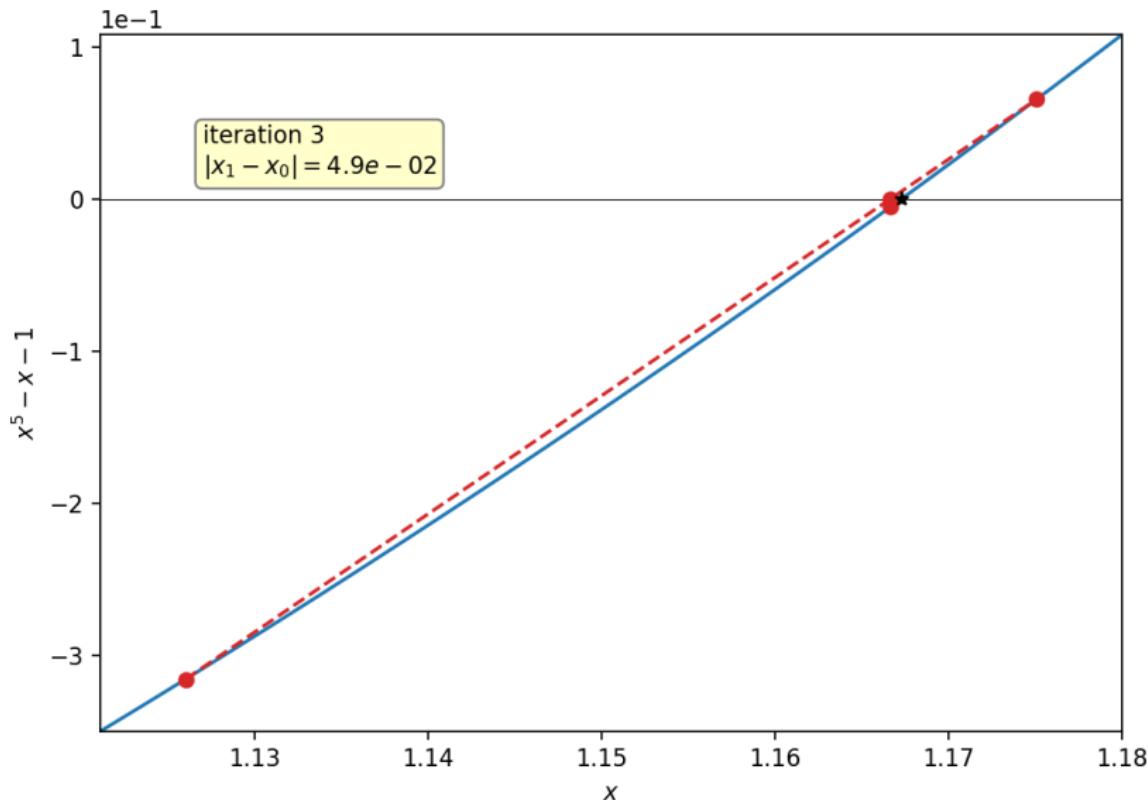
Numerical  
Integration

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Equations

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variables)

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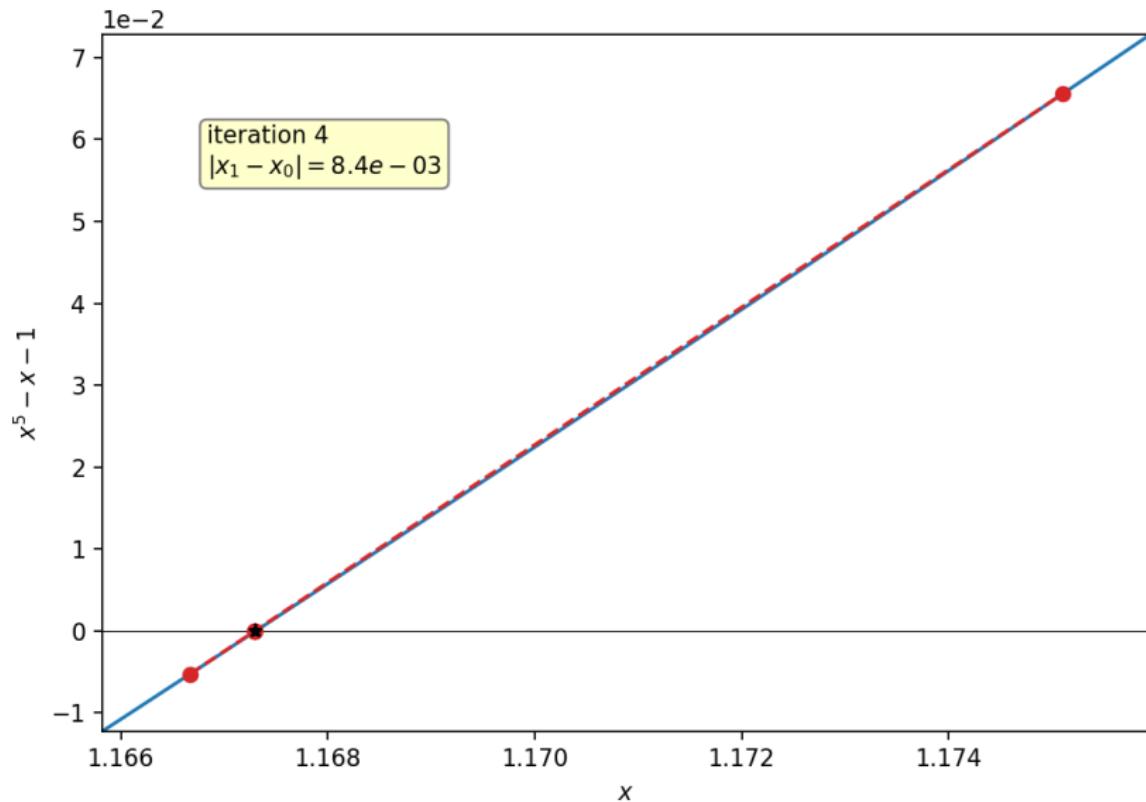
Numerical  
Integration

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Stationary  
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(one  
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Stationary  
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variables)

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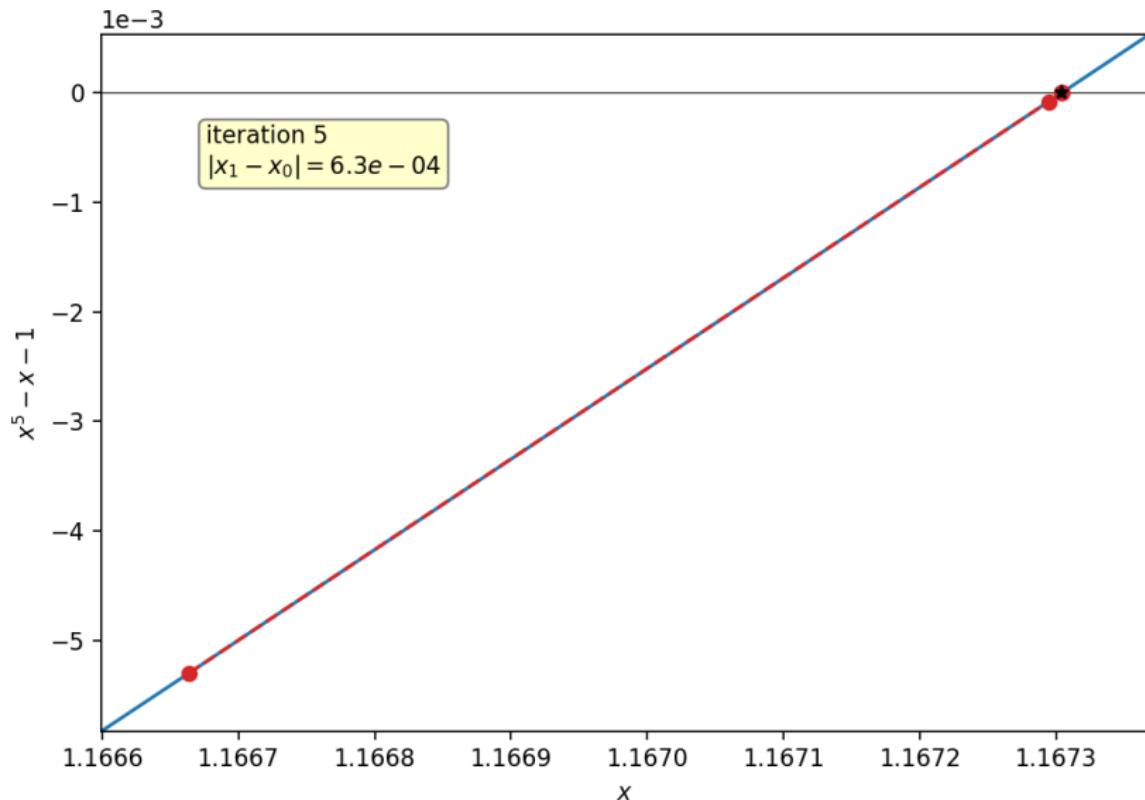
Numerical  
Integration

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Equations

Stationary  
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(one  
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Stationary  
Points  
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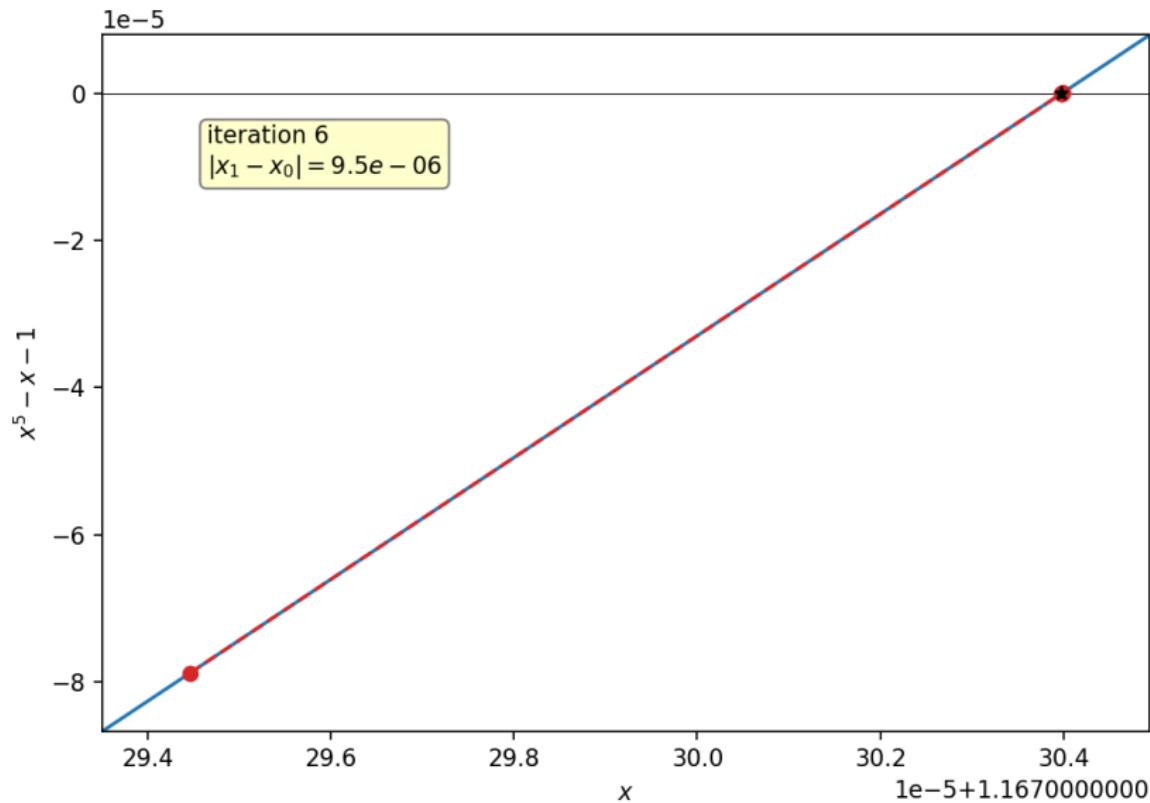
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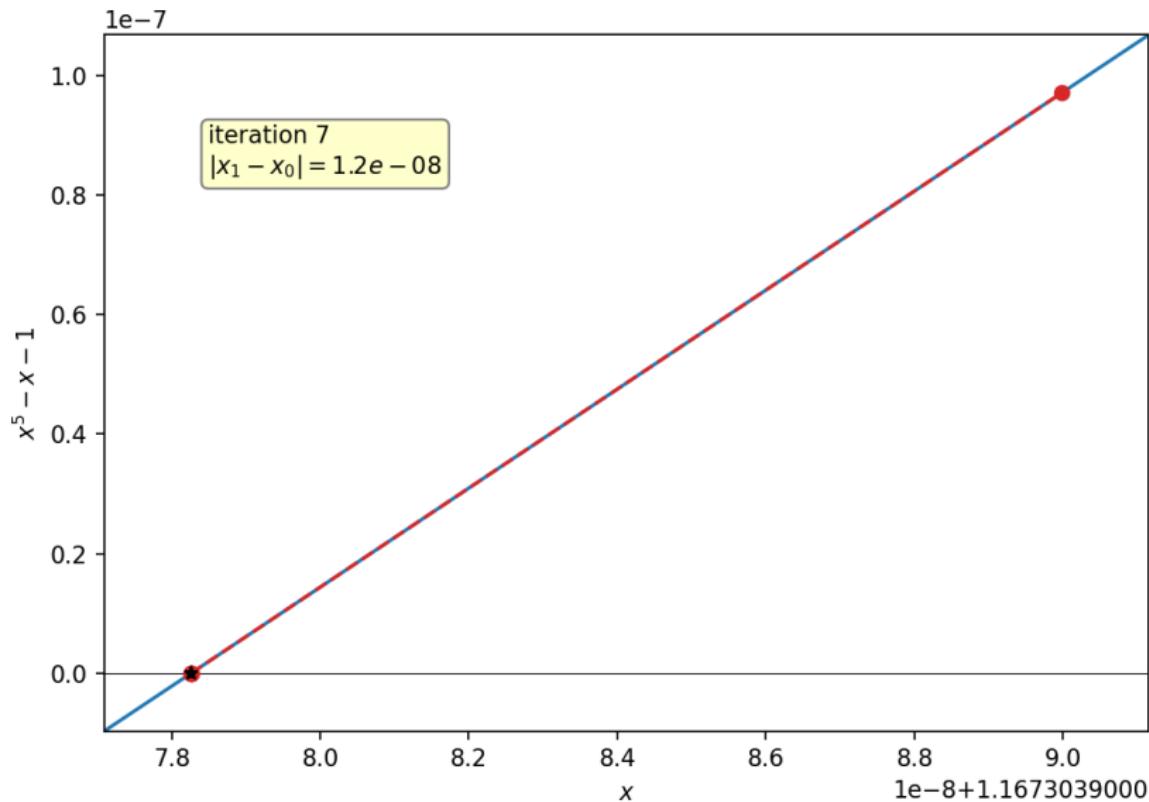
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# Newton–Raphson

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Stationary  
Points  
(many  
variables)

Global Op-  
timisation

- 1 choose a point  $x_0$ , ideally near a zero;

# Newton–Raphson

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Numerical  
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- 1 choose a point  $x_0$ , ideally near a zero;
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$$y = f'_0(x - x_0) + f_0$$

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$$x_1 = x_0 - \frac{f_0}{f'_0}$$

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$$x_{k+1} = x_k - \frac{f_k}{f'_k}$$

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NEWTON–RAPHSON UPDATE

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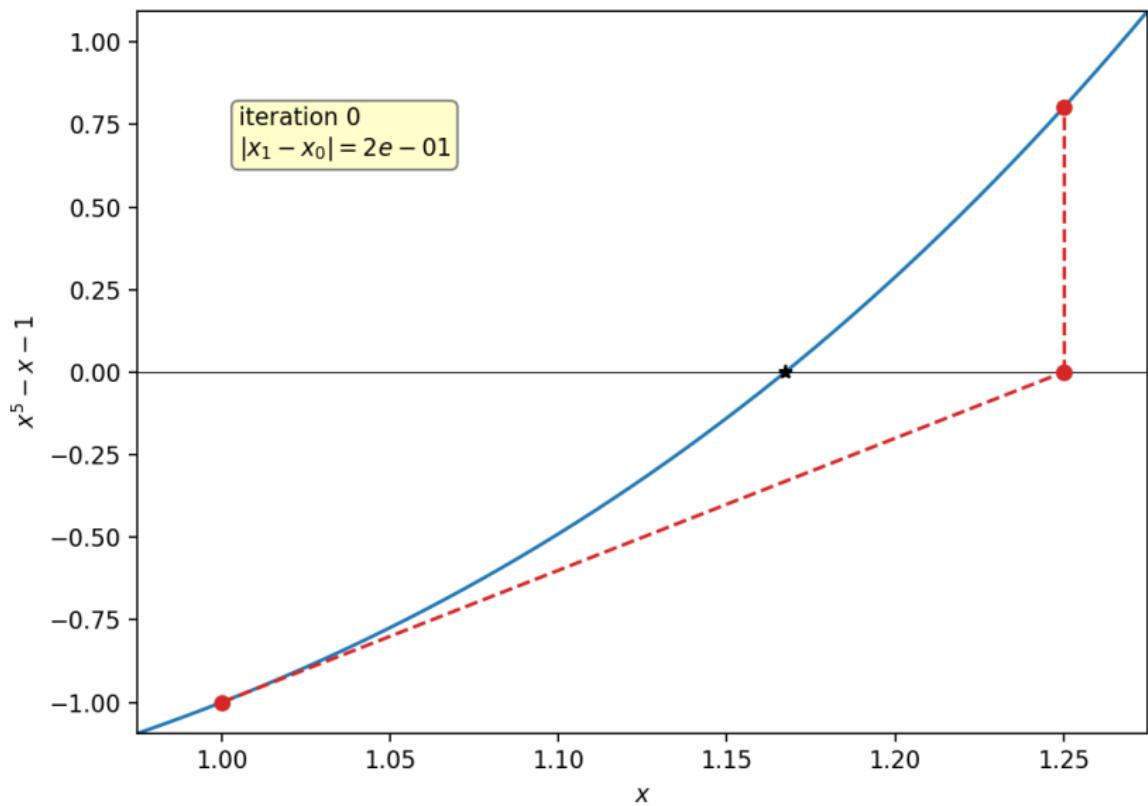
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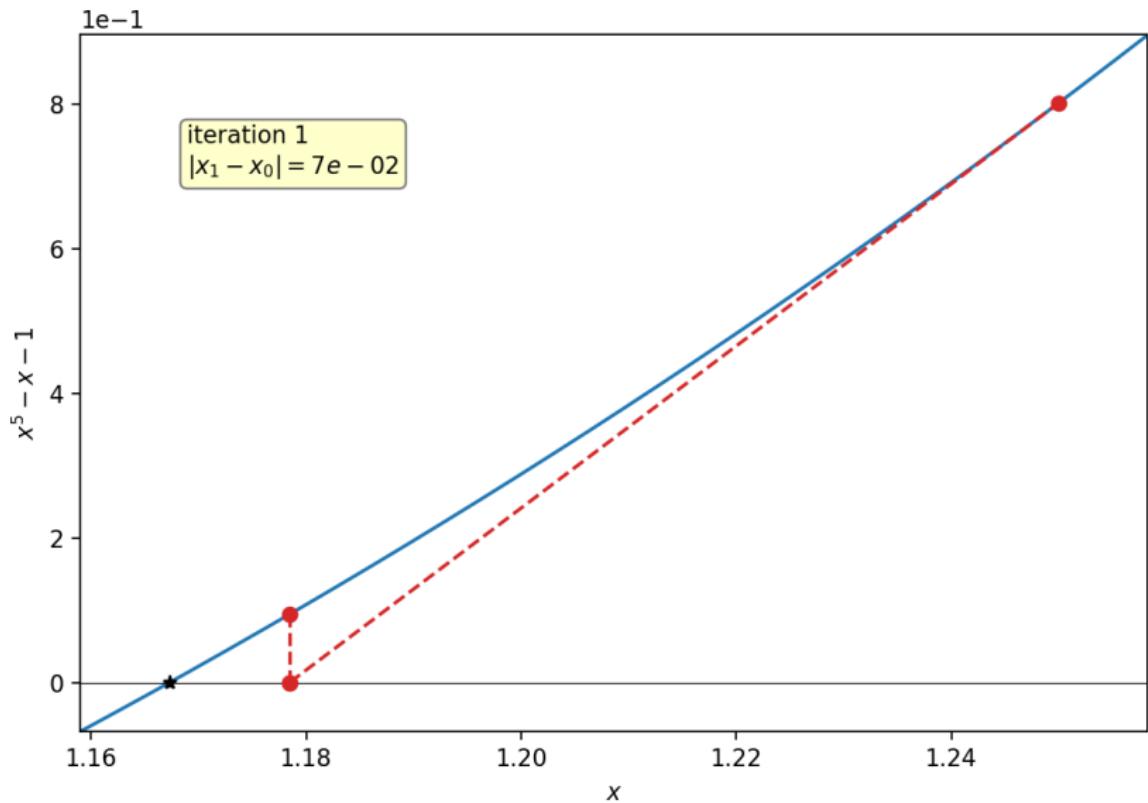
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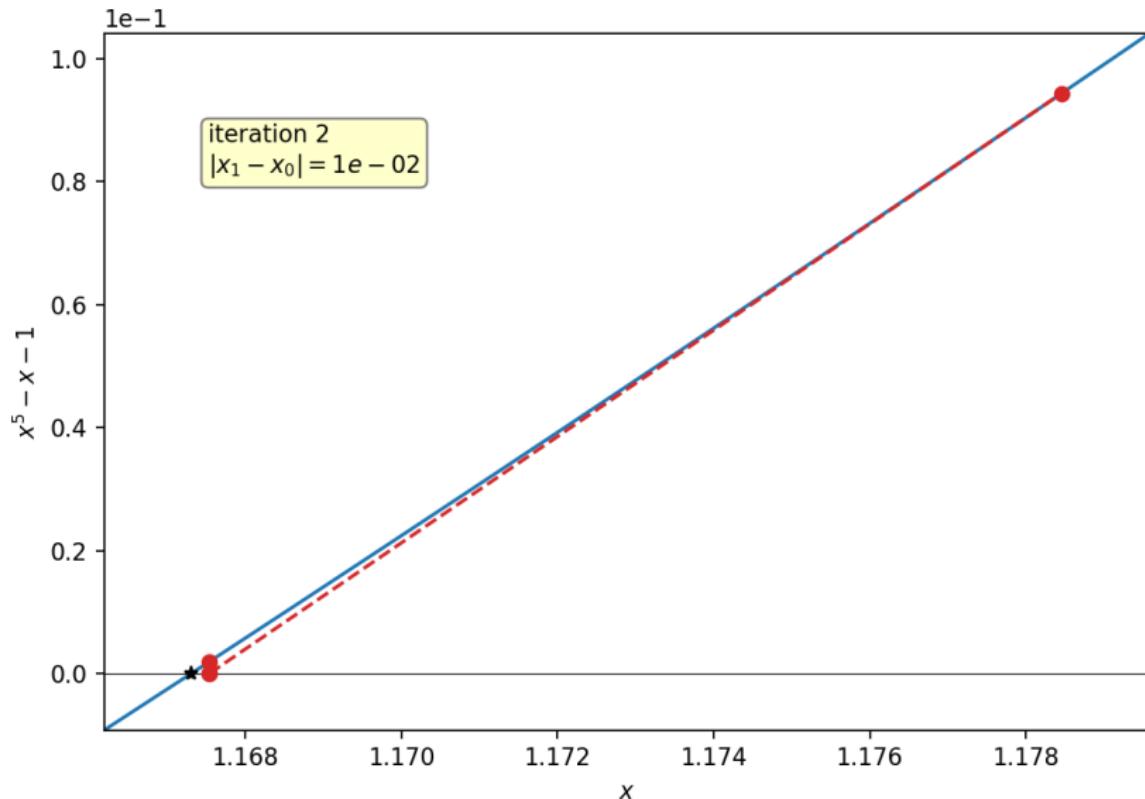
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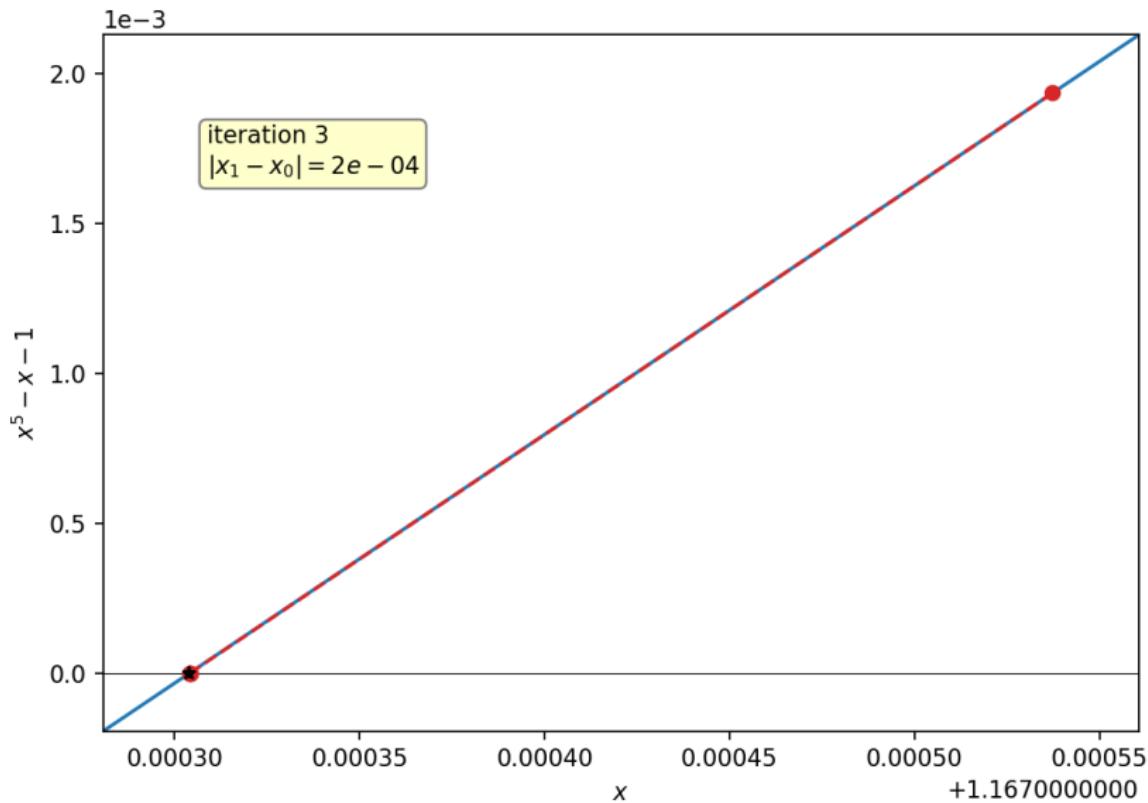
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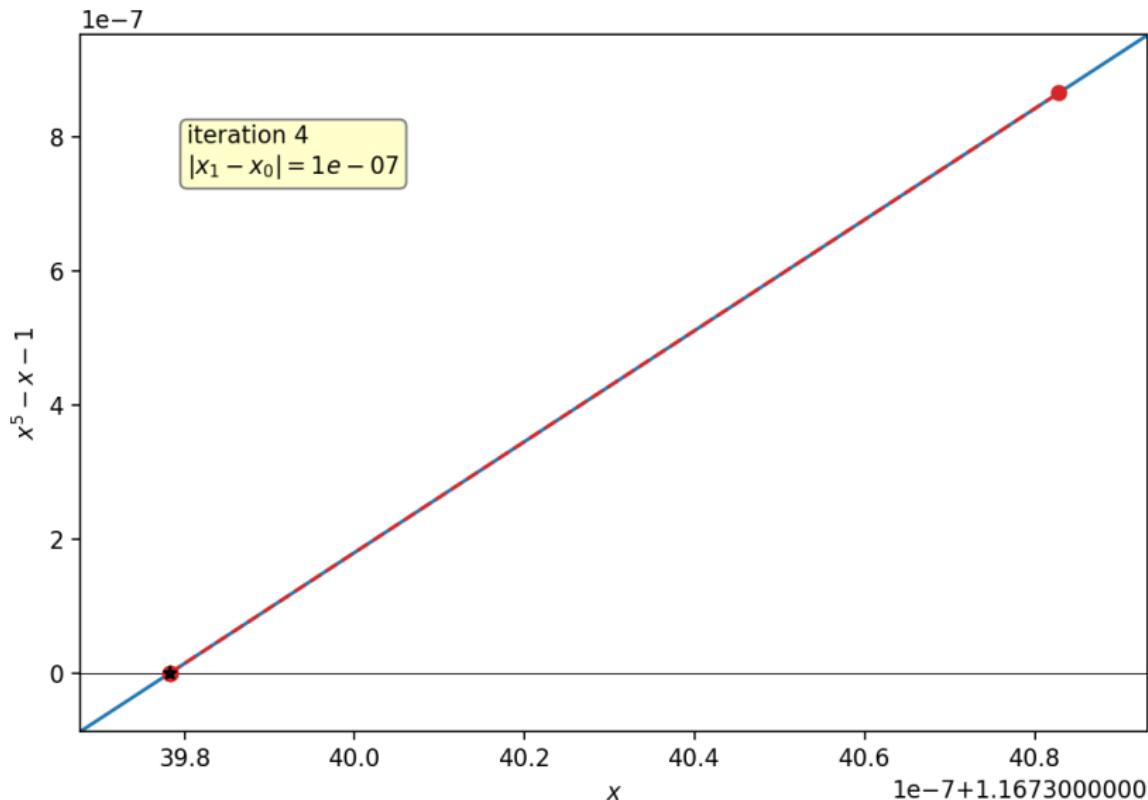
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# Inverse Quadratic Interpolation

- 1 choose three non-collinear points  $(x_0, x_1, x_2)$ , ideally near a zero;

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$$f^{-1}(y) = \sum_{i=0}^2 x_i \prod_{i \neq j} \frac{y - f_j}{f_i - f_j}$$

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- 3 find the zero of that quadratic function,  $x_3$

$$x_3 = f^{-1}(0) = \sum_{i=0}^2 x_i \prod_{i \neq j} \frac{f_j}{f_i - f_j}$$

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# Inverse Quadratic Interpolation

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$$\begin{aligned} x_{k+1} &= \frac{f_{k-1} f_k}{(f_{k-2} - f_{k-1})(f_{k-2} - f_k)} x_{k-2} \\ &+ \frac{f_{k-2} f_k}{(f_{k-1} - f_{k-2})(f_{k-1} - f_k)} x_{k-1} \\ &+ \frac{f_{k-2} f_{k-1}}{(f_k - f_{k-2})(f_k - f_{k-1})} x_k \end{aligned}$$

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IQR UPDATE

# Inverse Quadratic Interpolation

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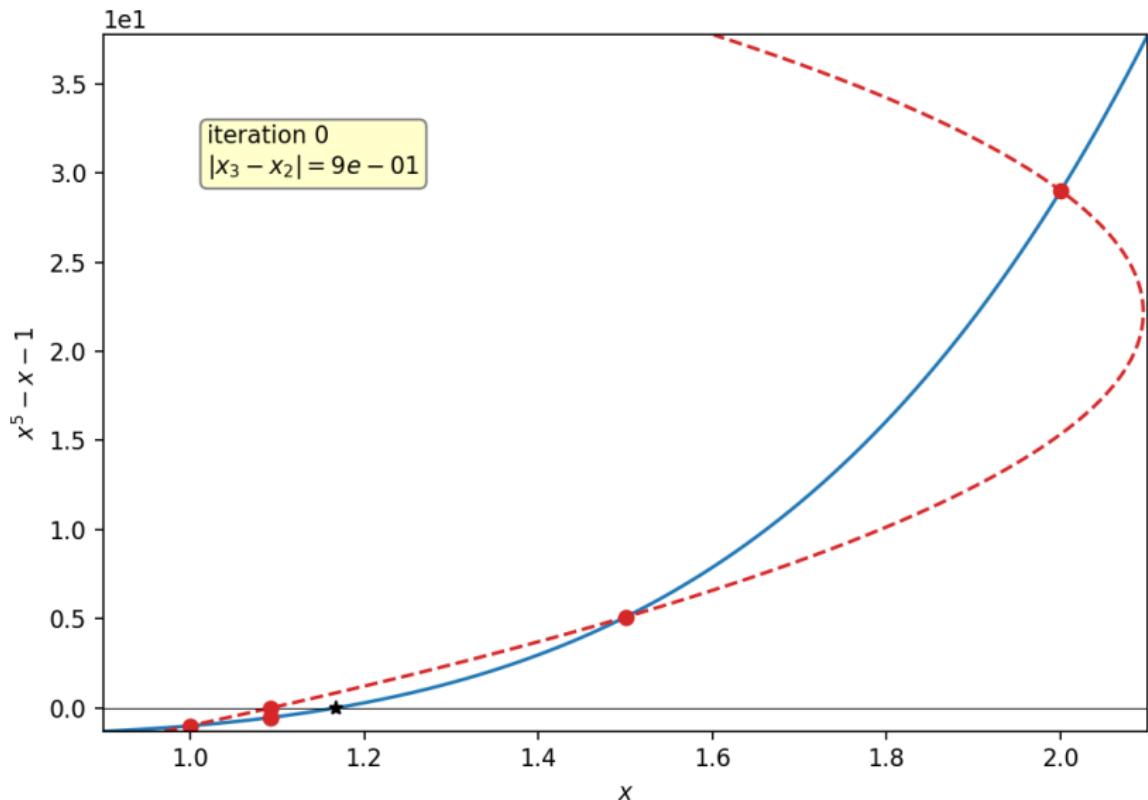
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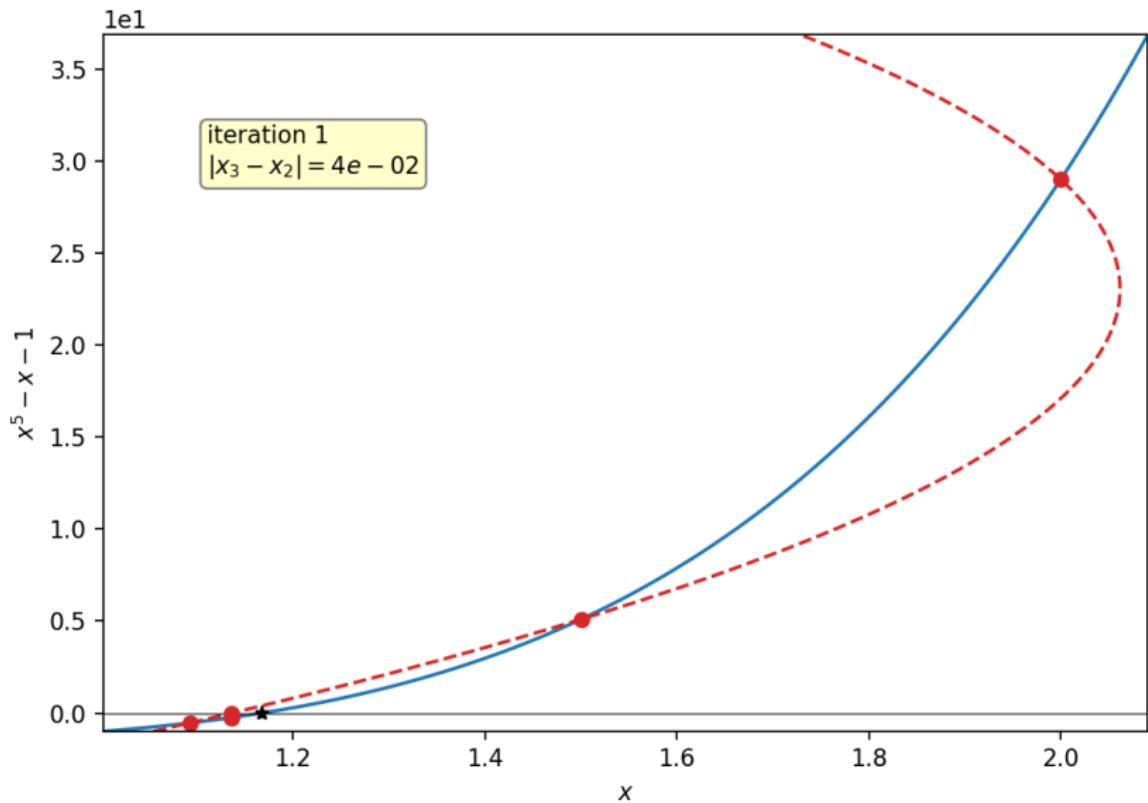
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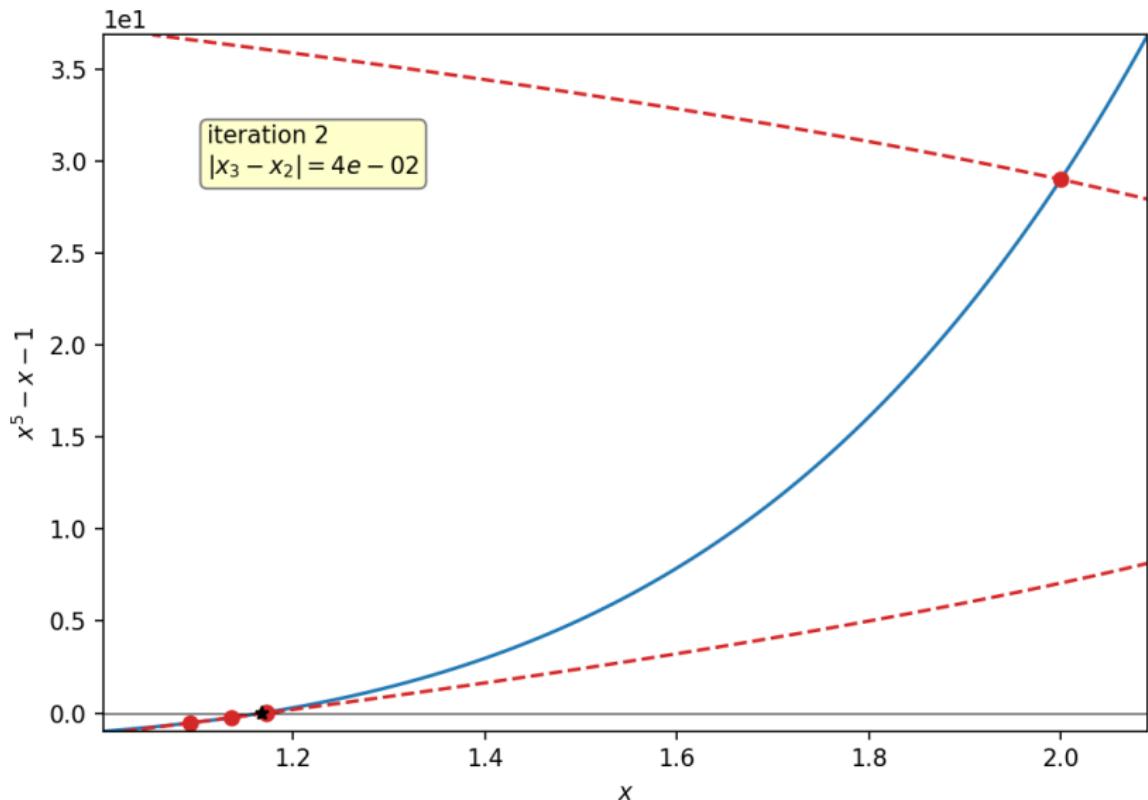
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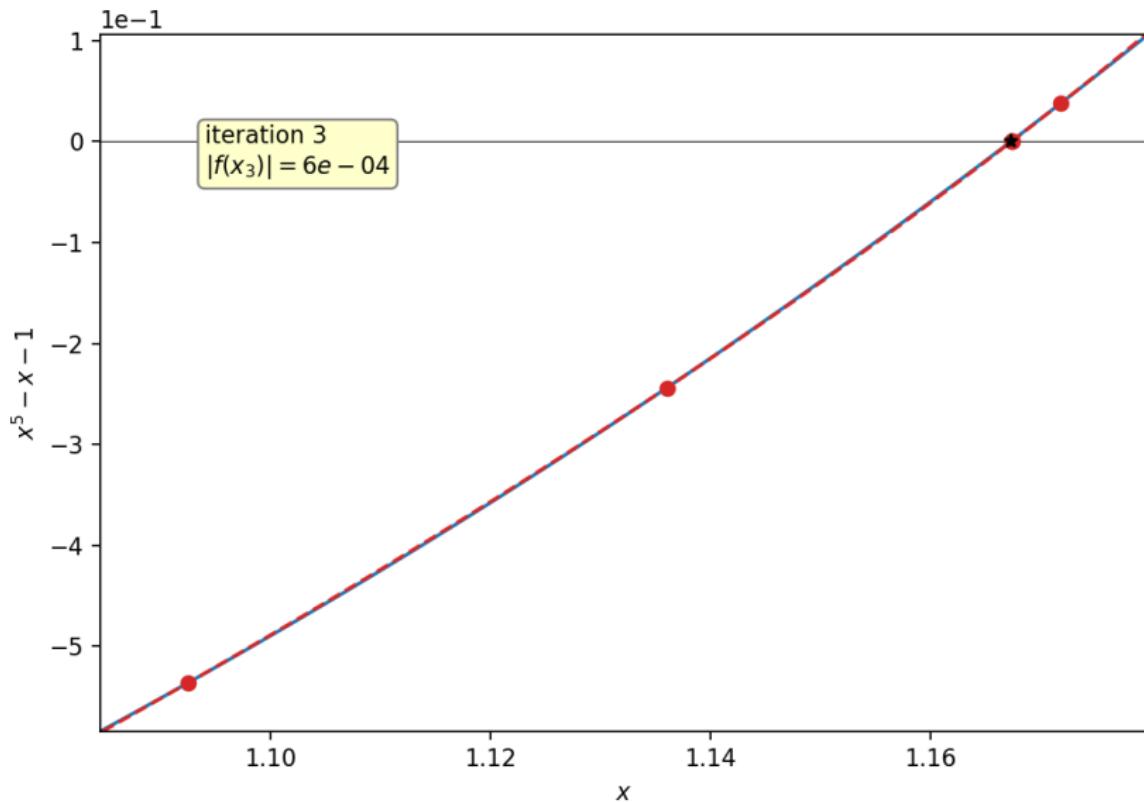
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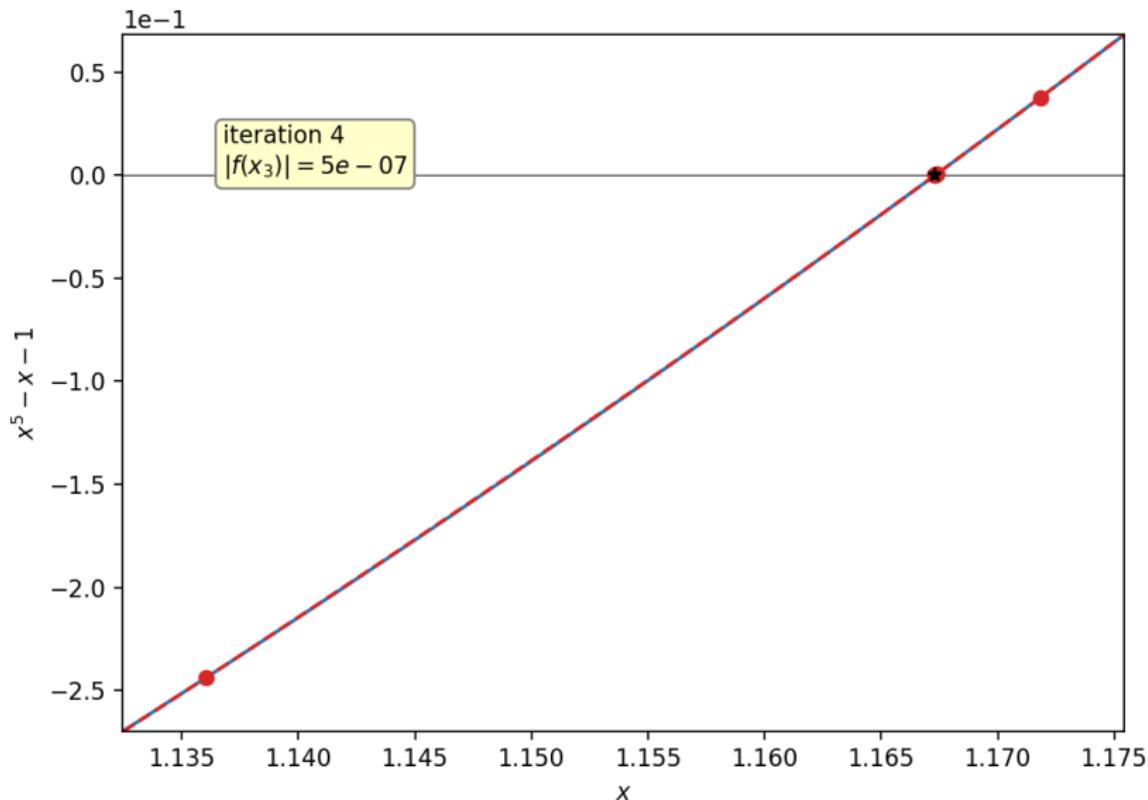
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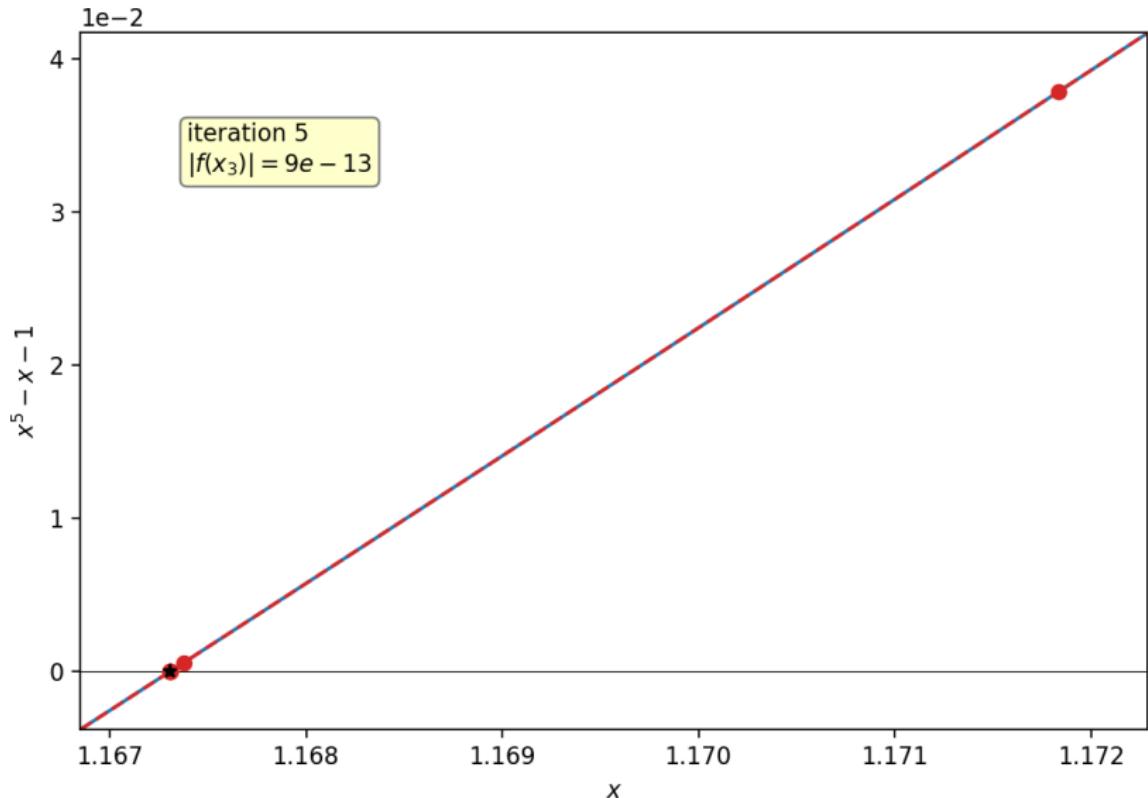
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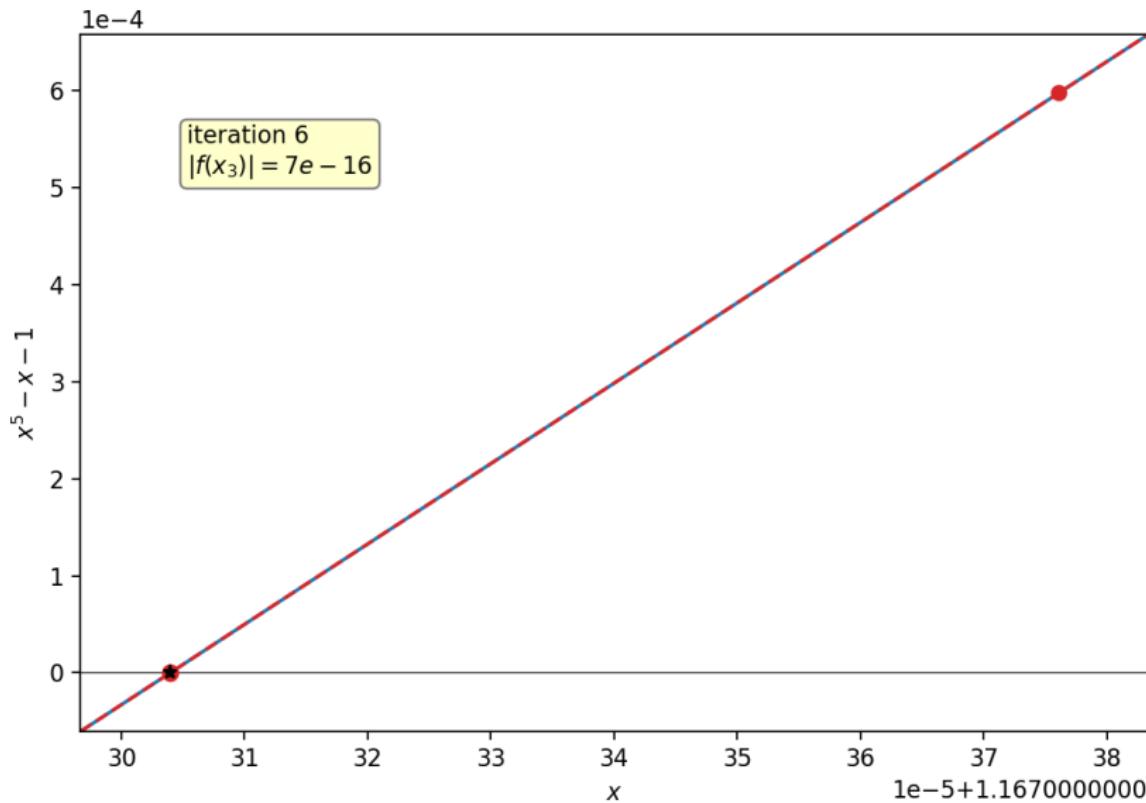
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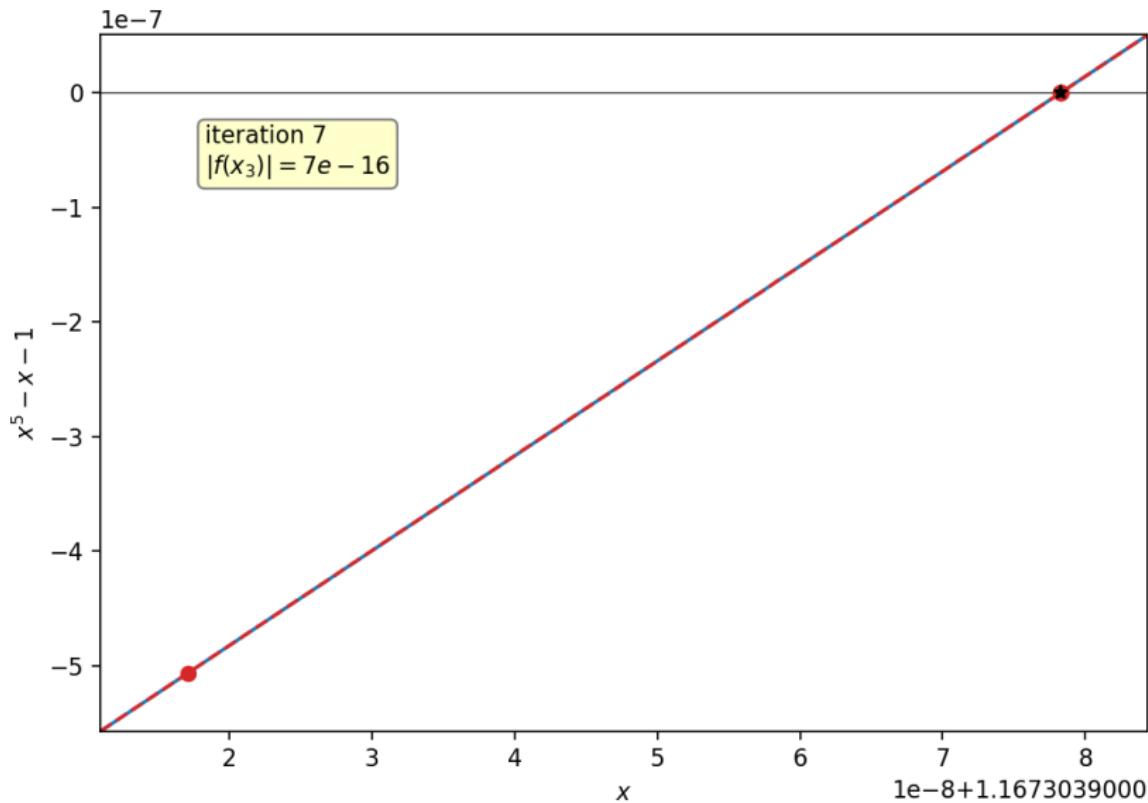
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# Homework

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## Pathological Cases

Implement the five root-finding methods we have studied, and use them to find the roots of,

1  $x^5 - x - 1 = 0;$

2  $16x^4 - 8x + 3 = 0;$

3  $x^3 - 2x^2 - 11x + 12 = (x - 4)(x - 1)(x + 3) = 0,$

for a range of starting values (plot the curves to get an idea of what a sensible range of values might be). What do you notice? Do all of the methods find all of the roots? Estimate the order of convergence using the formula given above. Is the order of convergence always the theoretical maximum?

# Cycles

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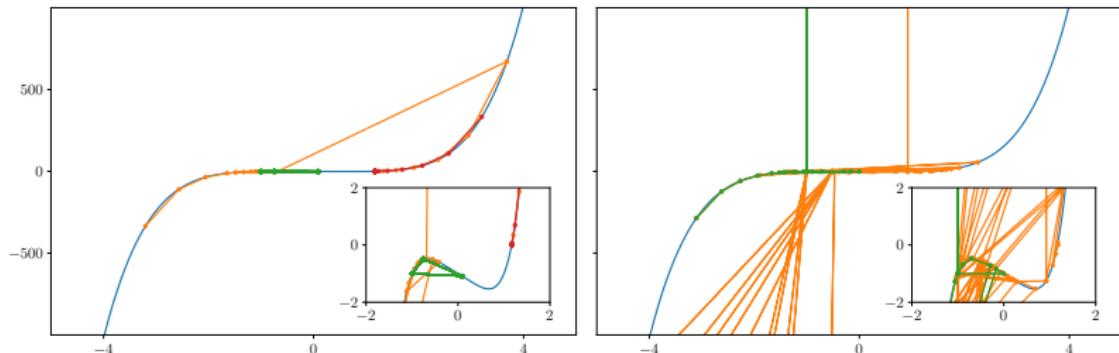
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Left: NR root finding with  $x_0 = -4, 0, 4$ .

Right: Secant root finding with  $(x_0, x_1) = (-4.5, -3.5)$  and  $\delta = 10^{-8}, 10^{-12}$ .

# Convergence

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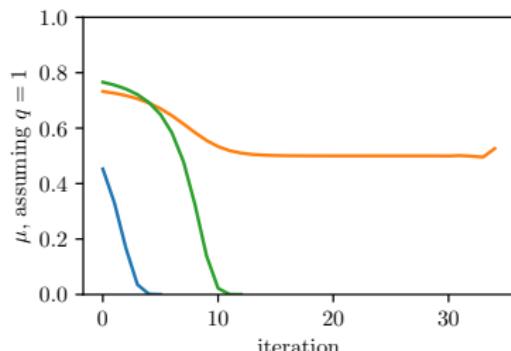
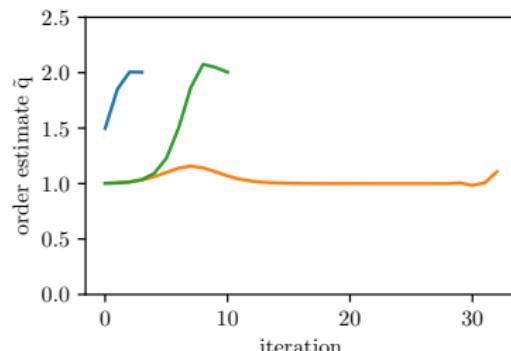
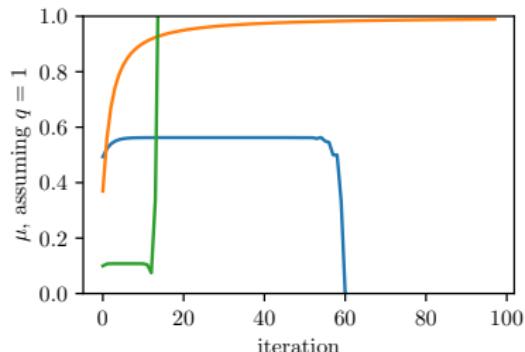
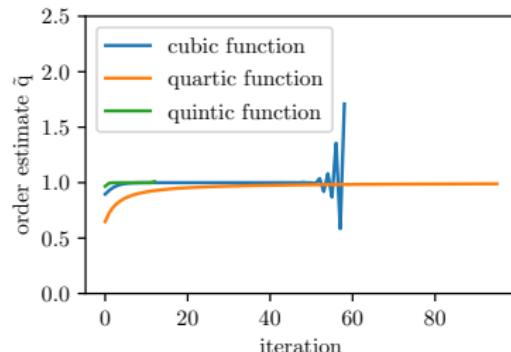
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Upper: rearrangement; lower: NR.

# Which Root?

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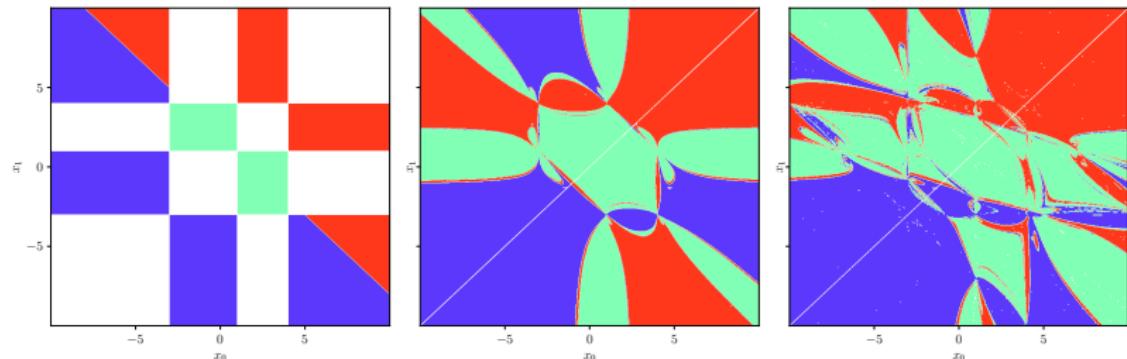
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L-R: bisection, secant, IQR methods applied to the cubic.

blue, green, and red indicate convergence to the roots -3, 1, and 4, respectively.

# Solving equations: Review

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$$\lim_{k \rightarrow \infty} \frac{|\epsilon_{k+1}|}{|\epsilon_k|^q} = \mu$$

Q-CONVERGENCE

$$q \approx \frac{\log \left| \frac{x_{k+1} - x_k}{x_k - x_{k-1}} \right|}{\log \left| \frac{x_k - x_{k-1}}{x_{k-1} - x_{k-2}} \right|}$$

Q-CONVERGENCE RATE ESTIMATE

# Solving equations: Review

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$$x_{k+1} = x_k - \frac{f_k}{f'_k}$$

NEWTON-RAPHSON UPDATE

$$(x_{k+1}, x_{k+2}) = \left( x_{k+1}, \left\{ x_{k+1} - f_{k+1} \frac{x_{k+1} - x_k}{f_{k+1} - f_k} \right\} \right)$$

SECANT UPDATE

# Solving equations: Review

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$$a_{k+1}, b_{k+1} = \phi(a_k, b_k) = \begin{cases} \left(a_k, \frac{a_k+b_k}{2}\right) & \text{if } f\left(\frac{a_k+b_k}{2}\right) > 0; \\ \left(\frac{a_k+b_k}{2}, b_k\right) & \text{if } f\left(\frac{a_k+b_k}{2}\right) < 0. \end{cases}$$

## BISECTION UPDATE

$$\begin{aligned} x_{k+1} = & \frac{f_{k-1}f_k}{(f_{k-2} - f_{k-1})(f_{k-2} - f_k)} x_{k-2} \\ & + \frac{f_{k-2}f_k}{(f_{k-1} - f_{k-2})(f_{k-1} - f_k)} x_{k-1} \\ & + \frac{f_{k-2}f_{k-1}}{(f_k - f_{k-2})(f_k - f_{k-1})} x_k \end{aligned}$$

## IQR UPDATE

# Overview

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## 1 Numerical Differentiation

## 2 Numerical Integration

## 3 Solving Equations

## 4 Stationary Points (one variable)

## 5 Stationary Points (many variables)

## 6 Global Optimisation

# Finding Stationary Points

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the problem of finding a **stationary point** of a function is the same as finding a **zero of the first derivative** of that function

# Finding Stationary Points

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ation

Numerical  
Integration

Solving  
Equations

Stationary  
Points  
(one  
variable)

Stationary  
Points  
(many  
variables)

Global Op-  
timisation

the problem of finding a **stationary point** of a function is the same as finding a **zero of the first derivative** of that function

the methods we will study are very **similar to root-finding methods**

# Finding Stationary Points

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Global Op-  
timisation

the problem of finding a **stationary point** of a function is the same as finding a **zero of the first derivative** of that function

the methods we will study are very **similar to root-finding methods**

special care must be taken if we are only looking for **minima or maxima**

# Golden Section Search

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Global Op-  
timisation

- 1 choose two points  $(a, b)$  that bracket a minimum;

# Golden Section Search

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Global Op-  
timisation

- 1 choose two points  $(a, b)$  that bracket a minimum;
- 2 choose two probe points  $(c, d)$  on the bracket;

# Golden Section Search

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Global Op-  
timisation

- 1 choose **two** points  $(a, b)$  that **bracket** a minimum;
- 2 choose two **probe points**  $(c, d)$  on the bracket;
- 3 proceed with whichever interval  $(a, d)$  or  $(c, b)$  brackets the minimum;

# Golden Section Search

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# Golden Section Search

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Q. We want a reliable, efficient method; how should we choose the points  $(c, d)$ ?

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Q. We want a **reliable, efficient** method; how should we choose the points  $(c, d)$ ?

A1. Such that  $(a, d)$  and  $(c, b)$  have the same width (**reliable**),

$$c = b - \frac{b-a}{x}; \quad d = a + \frac{b-a}{x}$$

# Golden Section Search

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$$c = b - \frac{b-a}{x}; \quad d = a + \frac{b-a}{x}$$

A2. and such  $c$  is a probe point on  $(a, d)$ , and that  $d$  is a probe point on  $(c, b)$  (**efficient**),

$$\frac{b-a}{d-a} = \frac{d-a}{c-a}$$

# Golden Section Search

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$$\frac{b-a}{d-a} = \frac{d-a}{c-a}$$

the conditions are satisfied when

$$x = \frac{\sqrt{5}+1}{2},$$

**the golden ratio**, hence the name, “golden section search.”

# Golden Section Search

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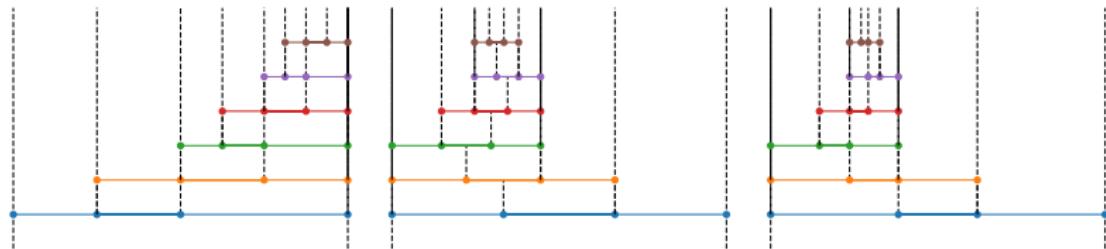
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- Uneven intervals (left), even, but suboptimal intervals (centre), and golden section search (right)

# Golden Section Search

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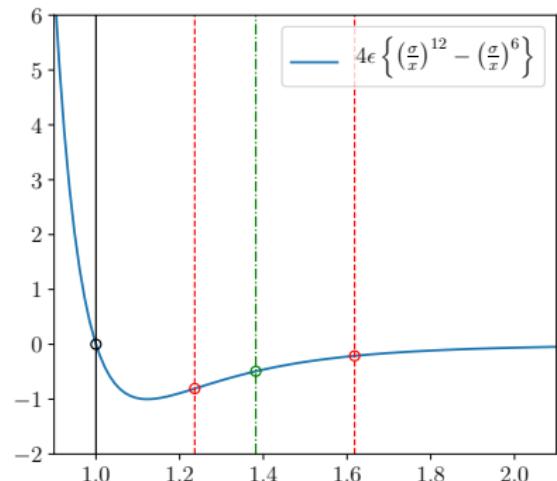
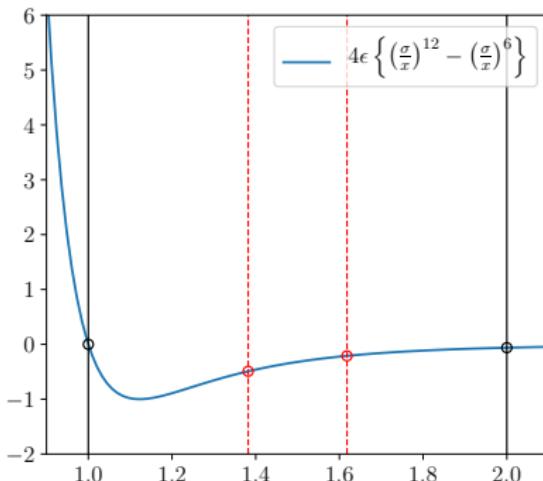
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- One iteration of the golden section search applied to the Lennard-Jones potential.

# Golden Section Search

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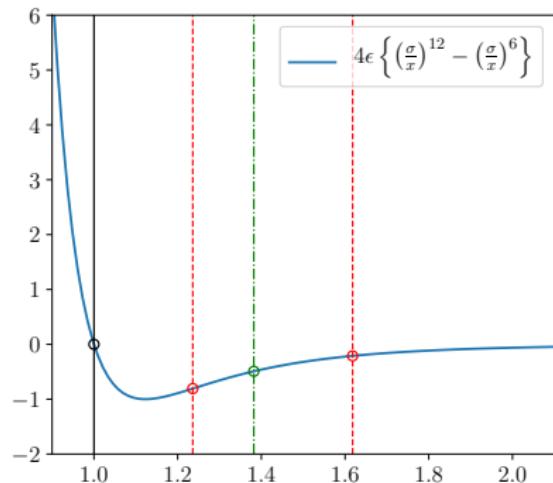
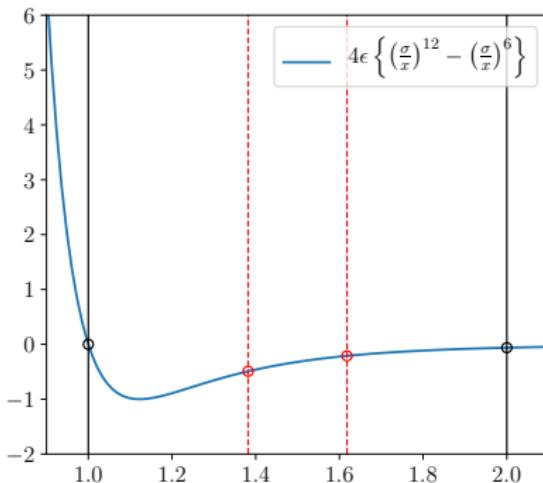
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- One iteration of the golden section search applied to the Lennard-Jones potential.
- The “c” point in the first bracket is **reused** as the “d” point in the second bracket.

# Successive parabolic interpolation

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Global Op-  
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- 1 choose three points  $(a, b, c)$  that need not bracket a stationary point;

# Successive parabolic interpolation

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Global Op-  
timisation

- 1 choose three points  $(a, b, c)$  that need not bracket a stationary point;
- 2 find the unique parabola to the curve passing through those points,

$$p(x) = \frac{(x - b)(x - c)}{(a - b)(a - c)} f_a + \frac{(x - a)(x - c)}{(b - a)(b - c)} f_b + \frac{(x - a)(x - b)}{(c - a)(c - b)} f_c$$

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- 3 find the unique stationary point of the parabola,

$$d = \frac{1}{2} \frac{a^2 (f_c - f_b) + b^2 (f_a - f_c) + c^2 (f_b - f_a)}{a(f_c - f_b) + b(f_a - f_c) + c(f_b - f_a)}$$

# Successive parabolic interpolation

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- 4  $(a, b, c) \leftarrow (b, c, d)$

# Successive parabolic interpolation

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- 4  $(a, b, c) \leftarrow (b, c, d)$
- 5 continue until  $|c - b| < \delta$

# Successive parabolic interpolation

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- 2 find the unique parabola to the curve passing through those points,

$$p(x) = \frac{(x - b)(x - c)}{(a - b)(a - c)} f_a + \frac{(x - a)(x - c)}{(b - a)(b - c)} f_b + \frac{(x - a)(x - b)}{(c - a)(c - b)} f_c$$

- 3 find the unique stationary point of the parabola,

$$d = \frac{1}{2} \frac{a^2 (f_c - f_b) + b^2 (f_a - f_c) + c^2 (f_b - f_a)}{a (f_c - f_b) + b (f_a - f_c) + c (f_b - f_a)}$$

- 4  $(a, b, c) \leftarrow (b, c, d)$
- 5 continue until  $|c - b| < \delta$
- 6 the order of convergence  $q \approx 1.324$

# Successive parabolic interpolation

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Global Op-  
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What if we only want to converge to minima?

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What if we only want to converge to minima?

- 1 find a bracket  $(a, c, b)$ ;

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What if we only want to converge to minima?

- 1 find a bracket  $(a, c, b)$ ;
- 2 find the new point  $d$ ;

# Successive parabolic interpolation

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What if we only want to converge to minima?

- 1 find a bracket  $(a, c, b)$ ;
- 2 find the new point  $d$ ;
- 3 update with the new, narrower bracket,

$$(a, c, b) \leftarrow \begin{cases} (a, d, c) & d < c, \quad f(d) < f(c) \\ (d, c, b) & d < c, \quad f(d) > f(c) \\ (c, d, b) & d > c, \quad f(d) < f(c) \\ (a, c, d) & d > c, \quad f(d) > f(c). \end{cases}$$

# Successive parabolic interpolation

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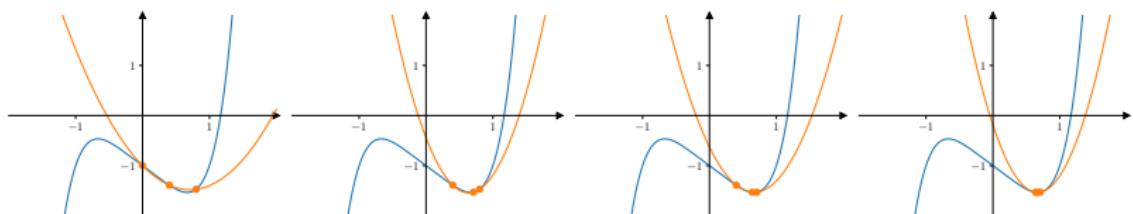
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- Successive parabolic interpolation applied to the quintic with  $(a, b, c) = (0.0, 0.4, 0.8)$ .

# Successive parabolic interpolation

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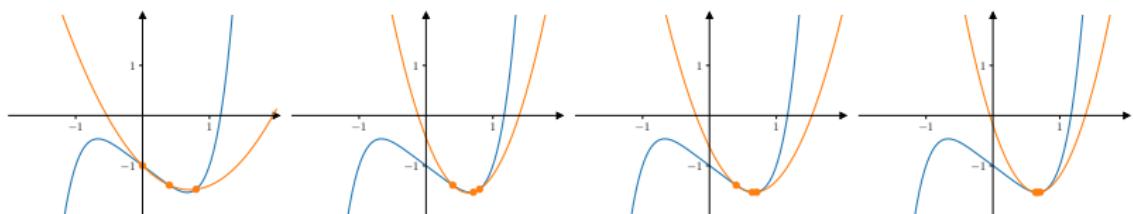
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Global Op-  
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- Successive parabolic interpolation applied to the quintic with  $(a, b, c) = (0.0, 0.4, 0.8)$ .
- What happens if you set  $(a, b, c) = (0.0, 0.5, 1.0)$ ?

# Newton–Raphson (again)

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Global Op-  
timisation

- 1 pick an initial guess  $x_0$  close to the stationary point;

# Newton–Raphson (again)

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Global Op-  
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- 1 pick an initial guess  $x_0$  close to the stationary point;
- 2 find the extremum of the parabola that at  $x_0$  has the **same function value, derivative, and curvature** as the objective function

# Newton–Raphson (again)

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- 3 i.e., solve for the extremum of a second-order Taylor expansion of the function,

$$f(\xi) = f(x_0 + \epsilon_0) = f_0 + \epsilon_0 f'_0 + \mathcal{O}(\epsilon_0^2)$$

# Newton–Raphson (again)

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$$f'(\xi) = f'(x_0 + \epsilon_0) = f'_0 + \epsilon_0 f''_0 + \mathcal{O}(\epsilon_0^2)$$

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$$0 = f'_0 + \epsilon_0 f''_0 + \mathcal{O}(\epsilon_k^2)$$

# Newton–Raphson (again)

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$$\epsilon_0 = -\frac{f'_0}{f''_0} + \mathcal{O}(\epsilon_k^2)$$

# Newton–Raphson (again)

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- 3 i.e., solve for the extremum of a second-order Taylor expansion of the function,

$$\epsilon_0 = -\frac{f'_0}{f''_0} + \mathcal{O}(\epsilon_k^2)$$

- 4 which point is,

$$x_1 = x_0 - \frac{f'_0}{f''_0}$$

# Newton–Raphson (again)

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- 4 which point is,

$$x_1 = x_0 - \frac{f'_0}{f''_0}$$

- 5  $x_0 \leftarrow x_1$

# Newton–Raphson (again)

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- 5  $x_0 \leftarrow x_1$
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# Newton–Raphson (again)

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Differentia-  
tion

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Integration

Solving  
Equations

Stationary  
Points  
(one  
variable)

Stationary  
Points  
(many  
variables)

Global Op-  
timisation

- to find only minima, take the absolute value of the second derivative in the update step,

$$x_1 = x_0 - \frac{f'_0}{|f''_0|}$$

# Newton–Raphson (again)

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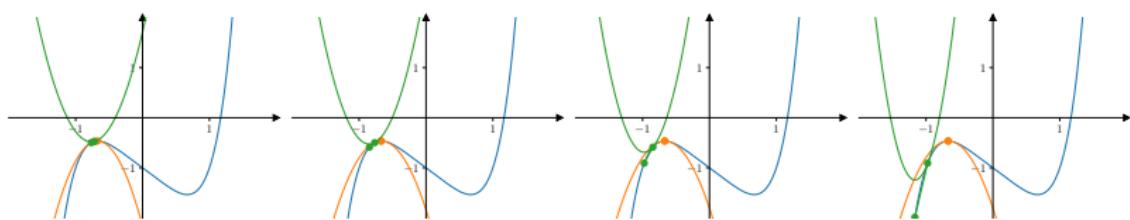
Stationary  
Points  
(one  
variable)

Stationary  
Points  
(many  
variables)

Global Op-  
timisation

- to find only minima, take the absolute value of the second derivative in the update step,

$$x_1 = x_0 - \frac{f'_0}{|f''_0|}$$



- Convergence to a minimum is not guaranteed...

# Secant Method (again)

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Global Op-  
timisation

- You may have noticed that the secant method for zeros is equivalent to the NR method for zeros with the derivative approximated by first backward differences

# Secant Method (again)

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Global Op-  
timisation

- You may have noticed that the secant method for zeros is equivalent to the NR method for zeros with the **derivative approximated by first backward differences**
- the secant method for stationary points works on a similar basis, with the **second derivative** term replaced by a **first backward differences** approximation of the first derivative...of the first derivative

# Gradient Descent (something new!)

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Global Op-  
timisation

- 1 pick an initial guess  $x_0$  close to the stationary point;

# Gradient Descent (something new!)

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Stationary  
Points  
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variables)

Global Op-  
timisation

- 1 pick an initial guess  $x_0$  close to the stationary point;
- 2 move a small amount in the direction that the function is decreasing,

$$x_1 = x_0 + \Delta x_0 = x_0 - \alpha p$$

( $\alpha$  is a small, positive, adjustable parameter, chosen to guarantee function decrease)

# Gradient Descent (something new!)

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- 3  $x_0 \leftarrow x_1$

# Gradient Descent (something new!)

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$$x_1 = x_0 + \Delta x_0 = x_0 - \alpha p$$

( $\alpha$  is a small, positive, adjustable parameter, chosen to guarantee function decrease)

- 3  $x_0 \leftarrow x_1$
- 4 continue until  $|x_1 - x_0| < \delta$

# Gradient Descent (something new!)

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- By construction, this method only finds minima

# Gradient Descent (something new!)

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$$x_1 = x_0 + \Delta x_0 = x_0 - \alpha p$$

( $\alpha$  is a small, positive, adjustable parameter, chosen to guarantee function decrease)

- 3  $x_0 \leftarrow x_1$
  - 4 continue until  $|x_1 - x_0| < \delta$
- By construction, this method only finds minima
  - to find maxima, a negative value of  $\alpha$  should be employed

# Homework

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## The gradient-descent (one dimensional)

Choosing the value of  $\alpha$  is a critical consideration: if  $\alpha$  is too small, convergence is slow; if  $\alpha$  is too large, then we risk jumping back and forth over the minimum, which also results in slow convergence.

- 1 devise a simple algorithm to choose  $\alpha$ ;
- 2 implement the gradient-descent method, using this algorithm.

# Backtracking line search

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Global Op-  
timisation

- consider the update

$$x_1 = x_0 - \alpha p$$

where  $\alpha$  is a **positive, adjustable parameter**, and  $p = f'(x) / |f'(x)|$  is either 1 or -1

# Backtracking line search

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- consider the update

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- start with a **linear approximation** to  $f$ ,

$$f(x_0 - \alpha p) = f(x_0) - \alpha p f'(x_0) + \mathcal{O}(\alpha^2)$$

# Backtracking line search

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- if  $f$  really was linear, then

$$f(x_0 - \alpha p) - f(x_0) = -\alpha p f'(x_0)$$

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- if  $f$  really was linear, then

$$f(x_0 - \alpha p) - f(x_0) = -\alpha p f'(x_0)$$

- so we say the function value has **decreased sufficiently** if

$$f(x_0 - \alpha p) \leq f(x_0) - \alpha c m \tag{30}$$

where  $m = p f'(x_0) = |f'(x_0)|$  and  $c \in (0, 1)$  is a **control parameter**

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- if condition 30 is not satisfied, update  $\alpha$  as  $\alpha \leftarrow \tau \alpha$  where  $\tau \in (0, 1)$  is another control parameter

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- continue until condition 30 is satisfied

# Backtracking line search

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Global Op-  
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where  $m = p f'(x_0) = |f'(x_0)|$  and  $c \in (0, 1)$  is a **control parameter**

- if condition 30 is not satisfied, update  $\alpha$  as  $\alpha \leftarrow \tau \alpha$  where  $\tau \in (0, 1)$  is another control parameter
- continue until condition 30 is satisfied
- typically,  $c = 0.5$ ,  $\tau = 0.5$

# Overview

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Global Op-  
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## 1 Numerical Differentiation

## 2 Numerical Integration

## 3 Solving Equations

## 4 Stationary Points (one variable)

## 5 Stationary Points (many variables)

## 6 Global Optimisation

# Nelder–Mead

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Global Op-  
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- think multivariable golden section: **only uses function values**

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Global Op-  
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- think multivariable golden section: **only uses function values**
- how to bracket a minimum?

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Global Op-  
timisation

- think multivariable golden section: **only uses function values**
- how to bracket a minimum?
- in 2D, we would need to find a region enclosed by a closed curve  $\mathcal{C}$ , and a probe point  $d$  inside the region such that for all points  $\forall c \in \mathcal{C}, f(d) < f(c)$ .

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- think multivariable golden section: **only uses function values**
- how to bracket a minimum?
- in 2D, we would need to find a region enclosed by a closed curve  $\mathcal{C}$ , and a probe point  $d$  inside the region such that for all points  $\forall c \in \mathcal{C}, f(d) < f(c)$ .
- in general, this approach is **not feasible**—in many dimensions, we can't reliably bracket a minimum, and there is **no algorithm** that is **guaranteed** to converge to a minimum.

# Nelder–Mead in one dimension

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Global Op-  
timisation

- Consider once more the one-dimensional problem, minimising  $f : \mathbb{R} \mapsto \mathbb{R}$ , but this time imagine we cannot bracket a minimum.

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Global Op-  
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- Consider once more the one-dimensional problem, minimising  $f : \mathbb{R} \mapsto \mathbb{R}$ , but this time imagine we cannot bracket a minimum.
- We begin with two points,  $(x_1, x_2)$  where the function values are  $(f_1, f_2)$  and  $f_1 < f_2$ .

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- We say that the point with the lowest function value is the **best** point, and the point with the highest function value is the **worst** point.

# Nelder–Mead in one dimension

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- We say that the point with the lowest function value is the **best** point, and the point with the highest function value is the **worst** point.
- How do we find a **better** point?

# Nelder–Mead in one dimension

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Global Op-  
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- Assume  $f$  is a decreasing function; then a better point is found by **reflecting** the worst point  $x_2$  through the best point  $x_1$  by some amount  $\alpha$ :

$$x_r = x_1 + \alpha(x_1 - x_2); \quad \alpha > 0. \quad (31)$$

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$$x_r = x_1 + \alpha(x_1 - x_2); \quad \alpha > 0. \quad (31)$$

- **IF**  $x_r$  is better than  $x_1$ , we can try to **expand** our options by choosing another point,

$$x_e = x_1 + \gamma(x_r - x_1); \quad \gamma > 1. \quad (32)$$

# Nelder–Mead in one dimension

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- **IF**  $x_r$  is better than  $x_1$ , we can try to **expand** our options by choosing another point,

$$x_e = x_1 + \gamma(x_r - x_1); \quad \gamma > 1. \quad (32)$$

- We then replace  $x_2$  with whichever of  $x_r$  and  $x_e$  is better.
- **ELSE**  $x_r$  is worse than the best point, then we **contract** the worst point toward the best point,

$$x_c = x_1 + \rho(x_2 - x_1); \quad 0 < \rho \leq 0.5. \quad (33)$$

# Nelder–Mead in one dimension

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- **ELSE**  $x_r$  is worse than the best point, then we **contract** the worst point toward the best point,

$$x_c = x_1 + \rho(x_2 - x_1); \quad 0 < \rho \leq 0.5. \quad (33)$$

- If  $x_c$  is better than  $x_2$ , we replace  $x_2$  with  $x_c$ ; otherwise, we **shrink** the interval further toward the best point,

$$x_2 = x_1 + \sigma(x_2 - x_1); \quad 0 < \sigma < 0.5. \quad (34)$$

# Nelder–Mead in many dimensions

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Global Op-  
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- In  $n$ -dimensions, we require  $n + 1$  points.

# Nelder–Mead in many dimensions

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Global Op-  
timisation

- In  $n$ -dimensions, we require  $n + 1$  points.
- in one dimension, the points must be **different**;

# Nelder–Mead in many dimensions

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- In  $n$ -dimensions, we require  $n + 1$  points.
- in one dimension, the points must be **different**;
- in two dimensions, the points must not be **collinear**;
- in three dimensions, the points must not be **coplanar**;
- in  $n$ -dimensions, we require  $n + 1$  points that are **affinely independent**—an  **$n$ -simplex**.

# Nelder–Mead in many dimensions

- reflect the worst point through the **centroid** of the best points,

$$x_o = \sum_{i=1}^n x_i. \quad (35)$$

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- reflect the worst point through the centroid of the best points,

$$x_o = \sum_{i=1}^n x_i. \quad (35)$$

- giving the reflected point,

$$x_r = x_o + \alpha (x_o - x_{n+1}). \quad (36)$$

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- ELSE IF the reflected point is the best point, we expand as before,

$$\mathbf{x}_e = \mathbf{x}_o + \gamma (\mathbf{x}_r - \mathbf{x}_o), \quad (37)$$

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- replacing worst point with the best of  $x_r$  and  $x_e$
- ELSE  $x_r$  is no better than the second-best point, so we contract the worst point toward the centroid,

$$x_c = x_o + \rho (x_{n+1} - x_o). \quad (38)$$

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$$\mathbf{x}_c = \mathbf{x}_o + \rho (\mathbf{x}_{n+1} - \mathbf{x}_o). \quad (38)$$

- if  $\mathbf{x}_c$  is better than the worst point, we replace the worst point with  $\mathbf{x}_c$ , and if not, we shrink all the points toward the best point,

$$\mathbf{x}_i = \mathbf{x}_1 + \sigma (\mathbf{x}_i - \mathbf{x}_1). \quad (39)$$

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$$\mathbf{x}_i = \mathbf{x}_1 + \sigma (\mathbf{x}_i - \mathbf{x}_1). \quad (39)$$

- At each iteration, we must relabel the vertices of the simplex so that  $f_i < f_{i+1}$ .

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- At each iteration, we must relabel the vertices of the simplex so that  $f_i < f_{i+1}$ .
- continue until the mean standard deviation of the coordinates  $\{\mathbf{x}_i\}$  of the simplex is less than some tolerance

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Global Op-  
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- Consider the system of equations,

$$\begin{aligned}2x + y - z &= 8; \\-3x - y + 2z &= -11; \\-2x + y + 2z &= -3,\end{aligned}$$

- we can summarise these equations in an **augmented matrix**

$$\left[ \begin{array}{ccc|c} 2 & 1 & -1 & 8 \\ -3 & -1 & 2 & -11 \\ -2 & 1 & 2 & -3 \end{array} \right]$$

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Global Op-  
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- Consider the system of equations,

$$\begin{aligned}2x + y - z &= 8; \\-3x - y + 2z &= -11; \\-2x + y + 2z &= -3,\end{aligned}$$

- $(R2) - \frac{3}{2}(R1)$ ,  $(R3) + (R1)$

$$\left[ \begin{array}{ccc|c} 2 & 1 & -1 & 8 \\ 0 & 0.5 & 0.5 & 1 \\ 0 & 2 & 1 & 5 \end{array} \right]$$

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Global Op-  
timisation

- Consider the system of equations,

$$\begin{aligned}2x + y - z &= 8; \\-3x - y + 2z &= -11; \\-2x + y + 2z &= -3,\end{aligned}$$

- $(R3) - 4(R2)$

$$\left[ \begin{array}{ccc|c} 2 & 1 & -1 & 8 \\ 0 & 0.5 & 0.5 & 1 \\ 0 & 0 & -1 & 1 \end{array} \right]$$

- at this point, we could solve by **back-substitution**
- we could also find the **determinant** of the original matrix as the product of the diagonal elements
- additionally, if the matrix is symmetric, the **signs of the eigenvalues** of the matrix are the same as the **signs of the diagonal elements**

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Global Op-  
timisation

- Consider the system of equations,

$$\begin{aligned}2x + y - z &= 8; \\-3x - y + 2z &= -11; \\-2x + y + 2z &= -3,\end{aligned}$$

- reflect in the antidiagonal

$$\left[ \begin{array}{ccc|c} -1 & 0 & 0 & 1 \\ 0.5 & 0.5 & 0 & 1 \\ -1 & 1 & 2 & 8 \end{array} \right]$$

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Global Op-  
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- Consider the system of equations,

$$\begin{aligned}2x + y - z &= 8; \\-3x - y + 2z &= -11; \\-2x + y + 2z &= -3,\end{aligned}$$

- $(R2) + \frac{1}{2}(R1)$ ,  $(R3) - (R1)$

$$\left[ \begin{array}{ccc|c} -1 & 0 & 0 & 1 \\ 0 & 0.5 & 0 & 1.5 \\ 0 & 1 & 2 & 7 \end{array} \right]$$

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Global Op-  
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- Consider the system of equations,

$$\begin{aligned}2x + y - z &= 8; \\-3x - y + 2z &= -11; \\-2x + y + 2z &= -3,\end{aligned}$$

- $(R3) - 2(R2)$

$$\left[ \begin{array}{ccc|c} -1 & 0 & 0 & 1 \\ 0 & 0.5 & 0 & 1.5 \\ 0 & 0 & 2 & 4 \end{array} \right]$$

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Global Op-  
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- Consider the system of equations,

$$\begin{aligned}2x + y - z &= 8; \\-3x - y + 2z &= -11; \\-2x + y + 2z &= -3,\end{aligned}$$

- divide through by the diagonal

$$\left[ \begin{array}{ccc|c} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & 3 \\ 0 & 0 & 1 & 2 \end{array} \right]$$

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- Consider the system of equations,

$$\begin{aligned}2x + y - z &= 8; \\-3x - y + 2z &= -11; \\-2x + y + 2z &= -3,\end{aligned}$$

- don't forget that we switched  $x$  and  $z$

$$\left[ \begin{array}{ccc|c} 1 & 0 & 0 & 2 \\ 0 & 1 & 0 & 3 \\ 0 & 0 & 1 & -1 \end{array} \right]$$

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- don't forget that we switched  $x$  and  $z$

$$\left[ \begin{array}{ccc|c} 1 & 0 & 0 & 2 \\ 0 & 1 & 0 & 3 \\ 0 & 0 & 1 & -1 \end{array} \right]$$

- the proof:

$$\begin{aligned}2(2) + (3) - (-1) &= 8 \\-3(2) - (3) + 2(-1) &= -11 \\-2(2) + (3) + 2(-1) &= -3\end{aligned}$$

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- solving for the **inverse** of a matrix amounts to applying the above procedure to

$$[\mathbf{A} \mid \mathbf{I}]$$

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- solving for the **inverse** of a matrix amounts to applying the above procedure to

$$[\mathbf{A} \mid \mathbf{I}]$$

- for example, our matrix,

$$\left[ \begin{array}{ccc|ccc} 2 & 1 & -1 & 1 & 0 & 0 \\ -3 & -1 & 2 & 0 & 1 & 0 \\ -2 & 1 & 2 & 0 & 0 & 1 \end{array} \right],$$

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- for example, our matrix,

$$\left[ \begin{array}{ccc|ccc} 2 & 1 & -1 & 1 & 0 & 0 \\ -3 & -1 & 2 & 0 & 1 & 0 \\ -2 & 1 & 2 & 0 & 0 & 1 \end{array} \right],$$

- reduces to,

$$\left[ \begin{array}{ccc|ccc} -1 & 0 & 0 & -5 & -4 & 1 \\ 0 & \frac{1}{2} & 0 & -1 & -1 & \frac{1}{2} \\ 0 & 0 & 2 & 8 & 6 & -2 \end{array} \right],$$

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- and finally solves to,

$$\left[ \begin{array}{ccc|ccc} 1 & 0 & 0 & 4 & 3 & -1 \\ 0 & 1 & 0 & -2 & -2 & 1 \\ 0 & 0 & 1 & 5 & 4 & -1 \end{array} \right].$$

# Non-linear equations—Newton's method—again (2)

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- Newton's method in many variables is derived in a similar way to single variable case

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Global Op-  
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- Newton's method in many variables is derived in a similar way to single variable case
- We start with the many variable Taylor expansion of a function at the stationary point,  $\xi$ ,

$$f(\xi) = f(\mathbf{x}_k + \boldsymbol{\epsilon}_k) = f(\mathbf{x}_k) + \nabla f(\mathbf{x}_k)^T \cdot \boldsymbol{\epsilon}_k + \mathcal{O}(|\boldsymbol{\epsilon}_k^2|)$$

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- Taking derivatives, and setting the derivative at the stationary point to zero,

$$\nabla f(\xi) = \mathbf{0} = \nabla f(\mathbf{x}_k) + \nabla^2 f(\mathbf{x}_k) \cdot \boldsymbol{\epsilon}_k + \mathcal{O}(|\boldsymbol{\epsilon}_k^2|)$$

# Non-linear equations—Newton's method—again (2)

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$$f(\xi) = f(\mathbf{x}_k + \boldsymbol{\epsilon}_k) = f(\mathbf{x}_k) + \nabla f(\mathbf{x}_k)^T \cdot \boldsymbol{\epsilon}_k + \mathcal{O}(|\boldsymbol{\epsilon}_k^2|)$$

- Taking derivatives, and setting the derivative at the stationary point to zero,

$$\nabla f(\xi) = \mathbf{0} = \nabla f(\mathbf{x}_k) + \nabla^2 f(\mathbf{x}_k) \cdot \boldsymbol{\epsilon}_k + \mathcal{O}(|\boldsymbol{\epsilon}_k^2|)$$

- rearranging,

$$\cdot \nabla^2 f(\mathbf{x}_k) \cdot \boldsymbol{\epsilon}_k = -\nabla f(\mathbf{x}_k) + \mathcal{O}(|\boldsymbol{\epsilon}_k^2|)$$

# Non-linear equations—Newton's method—again (2)

- truncating at second order in the error, we have a matrix equation of the form,

$$\mathbf{A}\mathbf{x} = \mathbf{b},$$

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- giving the many-variable Newton update,

$$\boxed{\mathbf{x}_{k+1} = \mathbf{x} - \nabla^2 f(\mathbf{x}_k)^{-1} \cdot \nabla f(\mathbf{x}_k)}$$

(40)

MANY-VARIABLE NEWTON-RAPHSON UPDATE

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## MANY-VARIABLE NEWTON-RAPHSON UPDATE

- we can compute the inverse of the matrix of second derivatives, the Hessian matrix, using the matrix methods outlined above.

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- in the one dimensional version, we take as the new point the **stationary point of a parabola**

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- in many dimensions we find the stationary point of a **quadratic form**,

$$f(\mathbf{x}) = \frac{1}{2} \mathbf{x}^T \mathbf{A} \mathbf{x} - \mathbf{b}^T \mathbf{x} + c$$

a linear combination of **orthogonal parabolas**

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- i.e., if the Hessian matrix is **positive definite**, i.e.,

$$\forall \mathbf{x} \neq \mathbf{0}, \quad \mathbf{x}^T \mathbf{A} \mathbf{x} > 0$$

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- this condition is true iff all of the **eigenvalues of the Hessian matrix are positive**

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- we can **shift the eigenvalues** of a symmetric matrix to positive values, while leaving the **eigenvectors unchanged**, by adding to it a multiple of the identity matrix,

$$\mathbf{B} = \mathbf{A} + \mu \mathbf{I}$$

where  $\mu + \lambda_{\min} > 0$ , and  $\lambda_{\min}$  is the **smallest (most negative) eigenvalue** of  $\mathbf{A}$

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Global Op-  
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- computing the Hessian and its inverse is expensive for large systems—we would like to compute it **infrequently or never...**

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$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{B}_k^{-1} \cdot \nabla f(\mathbf{x}_k)$$

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- and then **update the the approximate Hessian**,

$$\mathbf{B}_{k+1} = ??$$

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- and then **update the the approximate Hessian**,

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- how do we choose the update?

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- the one-dimensional secant equation (from first backward differences),

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

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- re-writing in the above terms, we get

$$\nabla^2 f(\mathbf{x}_{k+1}) \cdot (\mathbf{x}_{k+1} - \mathbf{x}_k) \approx \nabla f(\mathbf{x}_{k+1}) - \nabla f(\mathbf{x}_k)$$

- choose an update that is **consistent with the secant equation!**

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- choose an update that is **consistent with the secant equation!**
- but... there is no unique solution to the secant equation!

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Global Op-  
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- if we want to do minimisation, we require that  $\mathbf{B}_k$  be **symmetric and positive definite**
- similarly, the updated matrix  $\mathbf{B}_{k+1}$  must also be **symmetric and positive definite**

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- taking  $\mathbf{B}_{k+1} \approx \nabla^2 f(\mathbf{x}_{k+1})$ ,  $\mathbf{s}_k = \mathbf{x}_{k+1} - \mathbf{x}_k$  and  $\mathbf{y}_k = \nabla f(\mathbf{x}_{k+1}) - \nabla f(\mathbf{x}_k)$ , the secant equation is expressed as,

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- this matrix is in general **non-symmetric**

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- the added term is a symmetric, positive semi-definite rank-two matrix

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- we require,

$$\mathbf{B}_{k+1} \mathbf{s}_k = \mathbf{y}_k$$

- choosing  $\mathbf{u} = \mathbf{y}_k$  and  $\mathbf{v} = \mathbf{B}_k \mathbf{s}_k$ , and solving for  $\alpha, \beta$ , we get

$$\alpha = \frac{1}{\mathbf{y}_k^T \mathbf{s}_k}; \quad \beta = -\frac{1}{\mathbf{s}_k^T \mathbf{B}_k \mathbf{s}_k},$$

# Broyden–Fletcher–Goldfarb–Shanno (BFGS) method

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- one solution is Broyden–Fletcher–Goldfarb–Shanno (BFGS) method
- assume the update is of the form,

$$\mathbf{B}_{k+1} = \mathbf{B}_k + \alpha \mathbf{u} \mathbf{u}^T + \beta \mathbf{v} \mathbf{v}^T$$

- the added term is a **symmetric, positive semi-definite** rank-two matrix
- we require,

$$\mathbf{B}_{k+1} \mathbf{s}_k = \mathbf{y}_k$$

- choosing  $\mathbf{u} = \mathbf{y}_k$  and  $\mathbf{v} = \mathbf{B}_k \mathbf{s}_k$ , and solving for  $\alpha, \beta$ , we get

$$\alpha = \frac{1}{\mathbf{y}_k^T \mathbf{s}_k}; \quad \beta = -\frac{1}{\mathbf{s}_k^T \mathbf{B}_k \mathbf{s}_k},$$

- so the update to  $\mathbf{B}$  is,

$$\mathbf{B}_{k+1} = \mathbf{B}_k + \frac{\mathbf{y}_k \mathbf{y}_k^T}{\mathbf{y}_k^T \mathbf{s}_k} - \frac{\mathbf{B}_k \mathbf{s}_k \mathbf{s}_k^T \mathbf{B}_k^T}{\mathbf{s}_k^T \mathbf{B}_k \mathbf{s}_k}$$

(verify this for yourselves)

# Broyden–Fletcher–Goldfarb–Shanno (BFGS) method

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- collecting these ideas together, recalling that  $\mathbf{s}_k = \mathbf{x}_{k+1} - \mathbf{x}_k$ , and  $\mathbf{y}_k = \nabla f(\mathbf{x}_{k+1}) - \nabla f(\mathbf{x}_k)$ ,

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{B}_k^{-1} \cdot \nabla f(\mathbf{x}_k) \quad (41)$$

$$\mathbf{B}_{k+1} = \mathbf{B}_k + \frac{\mathbf{y}_k \mathbf{y}_k^T}{\mathbf{y}_k^T \mathbf{s}_k} - \frac{\mathbf{B}_k \mathbf{s}_k \mathbf{s}_k^T \mathbf{B}_k^T}{\mathbf{s}_k^T \mathbf{B}_k \mathbf{s}_k}. \quad (42)$$

BFGS UPDATES

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- however, since we only need the **inverse** of  $\mathbf{B}$ , we can rewrite the update using the **Sherman–Morrison formula**,

$$\mathbf{B}_{k+1}^{-1} = \left( \mathbf{I} - \frac{\mathbf{s}_k \mathbf{y}_k^T}{\mathbf{y}_k^T \mathbf{s}_k} \right) \mathbf{B}_k^{-1} \left( \mathbf{I} - \frac{\mathbf{y}_k \mathbf{s}_k^T}{\mathbf{y}_k^T \mathbf{s}_k} \right) + \frac{\mathbf{s}_k \mathbf{s}_k^T}{\mathbf{y}_k^T \mathbf{s}_k} \quad (43)$$

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- as  $\mathbf{B}_k^{-1}$  is symmetric, and both  $\mathbf{y}_k^T \mathbf{B}_k^{-1} \mathbf{y}_k$  and  $\mathbf{s}_k^T \mathbf{y}_k$  are scalars, we can write

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{B}_k^{-1} \cdot \nabla f(\mathbf{x}_k) \quad (44)$$

$$\mathbf{B}_{k+1}^{-1} = \mathbf{B}_k^{-1} + \frac{(\mathbf{s}_k^T \mathbf{y}_k + \mathbf{y}_k^T \mathbf{B}_k^{-1} \mathbf{y}_k)(\mathbf{s}_k \mathbf{s}_k^T)}{(\mathbf{s}_k^T \mathbf{y}_k)^2} - \frac{\mathbf{B}_k^{-1} \mathbf{y}_k \mathbf{s}_k^T + \mathbf{s}_k \mathbf{y}_k^T \mathbf{B}_k^{-1}}{\mathbf{s}_k^T \mathbf{y}_k} \quad (45)$$

## BFGS UPDATES (IMPROVED)

and we never need to invert a matrix ever again.

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- we can use the real Hessian matrix as a starting guess, but it is often sufficient to start with the **identity matrix**...

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## BFGS UPDATES (IMPROVED)

and we never need to invert a matrix ever again.

- we can use the real Hessian matrix as a starting guess, but it is often sufficient to start with the **identity matrix**...
- ...at the first iteration, the update behaves like **gradient descent**, but in favourable circumstances, the approximate Hessian quickly approaches the values of the real Hessian

# Non-linear equations—Gradient Descent—again

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- we can easily generalise the gradient-descent update to the many-variable case

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- we can easily generalise the gradient-descent update to the many-variable case
- our update shall be

$$\boxed{\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha \mathbf{p}} \quad (46)$$

## GRADIENT DESCENT UPDATE

where  $\alpha$  is a **small, positive, adjustable parameter**, and  $\mathbf{p}$  is a unit vector chosen as a **direction of function decrease**

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- expanding the function around the new point,

$$f(\mathbf{x}_{k+1}) = f(\mathbf{x}_k) - \alpha \nabla f(\mathbf{x}_k)^T \mathbf{p} + \mathcal{O}(\alpha^2)$$

- we find that, **if the function were linear**, the function value would decrease by an amount,

$$\begin{aligned} f(\mathbf{x}_{k+1}) - f(\mathbf{x}_k) &= -\alpha \nabla f(\mathbf{x}_k)^T \mathbf{p} \\ &= -\alpha m \end{aligned}$$

where  $m = f(\mathbf{x}_k)^T \mathbf{p}$

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- as a condition for choosing  $\alpha$ , we say that the function value has decreased **by a sufficient amount** if it decreases by some amount,

$$f(\mathbf{x}_{k+1}) - f(\mathbf{x}_k) < -\alpha cm \quad (47)$$

## ARMIJO–GOLDSTEIN CONDITION

where  $0 < c < 1$  is a **control parameter** (non-adjustable)

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$$\alpha \leftarrow \tau \alpha$$

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- this method is known as a **backtracking line search**, because we start far from the original point with relatively large  $\alpha$ , and backtrack, decreasing  $\alpha$  until the condition is satisfied.

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- this method is known as a **backtracking line search**, because we start far from the original point with relatively large  $\alpha$ , and backtrack, decreasing  $\alpha$  until the condition is satisfied.
- in practice, the Newton and BFGS updates aren't always used directly—we use those equations to find a **suitable search direction**, then use a **line search** to find a **suitable step size**

# First-order saddles—eigenvector following

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- sometimes we want to find stationary points that are **not minima or maxima**—they are generally harder to converge to

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- the idea is to, starting at a point with Hessian index 1, **maximise** parallel to the negative eigenvector while **minimising** in all orthogonal directions

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- we did this in the one variable case of Newton's method by taking the absolute value of the second derivative
- to do so, we find the relevant eigenvector  $\mathbf{v}_{\min}$  and take a small step in the direction the function is **increasing**, using, *e.g.*, a line search...
- then minimise in the direction obtained by **projecting the eigenvector out of the gradient vector**, using *e.g.*, BFGS,

$$\boxed{\nabla f_{\perp} = \nabla f - (\nabla f^T \cdot \mathbf{v}_{\min}) \mathbf{v}_{\min}} \quad (48)$$

EIGENVECTOR FOLLOWING PROJECTED GRADIENT

# Eigenvalues and eigenvectors—Rayleigh–Ritz ratio

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- how do we find this crucial eigenvector?

# Eigenvalues and eigenvectors—Rayleigh–Ritz ratio

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- how do we find this crucial eigenvector?
- or large systems, inverting the Hessian to find its eigenvectors can become a bottleneck; to avoid this problem, we can make use of the Rayleigh–Ritz ratio,

$$\lambda(\mathbf{v}) = \frac{\mathbf{v}^T \mathbf{H}(x) \mathbf{v}}{\mathbf{v}^T \mathbf{v}} \quad (49)$$

$$\nabla \lambda(\mathbf{v}) = \frac{(\mathbf{v}^T \mathbf{v})(\mathbf{H}\mathbf{v} + \mathbf{H}^T \mathbf{v}) - 2(\mathbf{v}^T \mathbf{H}\mathbf{v})\mathbf{v}}{(\mathbf{v}^T \mathbf{v})^2} \quad (50)$$

## RAYLEIGH–RITZ RATIO & GRADIENT THEREOF

# Eigenvalues and eigenvectors—Rayleigh–Ritz ratio

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## RAYLEIGH–RITZ RATIO & GRADIENT THEREOF

- $\lambda(\mathbf{v})$  has a unique minimum when  $\mathbf{v} \parallel \mathbf{v}_{\min}$

# Eigenvalues and eigenvectors—Rayleigh–Ritz ratio

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## RAYLEIGH–RITZ RATIO & GRADIENT THEREOF

- $\lambda(\mathbf{v})$  has a unique minimum when  $\mathbf{v} \parallel \mathbf{v}_{\min}$
- we can search for the minimum with gradient descent, BFGS...

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$$\lambda(\mathbf{v}) = \frac{\mathbf{v}^T \mathbf{H}(x) \mathbf{v}}{\mathbf{v}^T \mathbf{v}} \quad (49)$$

$$\nabla \lambda(\mathbf{v}) = \frac{(\mathbf{v}^T \mathbf{v})(\mathbf{H}\mathbf{v} + \mathbf{H}^T \mathbf{v}) - 2(\mathbf{v}^T \mathbf{H}\mathbf{v})\mathbf{v}}{(\mathbf{v}^T \mathbf{v})^2} \quad (50)$$

## RAYLEIGH–RITZ RATIO & GRADIENT THEREOF

- $\lambda(\mathbf{v})$  has a unique minimum when  $\mathbf{v} \parallel \mathbf{v}_{\min}$
- we can search for the minimum with gradient descent, BFGS...
- we can also use **approximate Hessian matrices** if exact ones are not available

# Overview

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Stationary  
Points  
(many  
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Global Op-  
timisation

## 1 Numerical Differentiation

## 2 Numerical Integration

## 3 Solving Equations

## 4 Stationary Points (one variable)

## 5 Stationary Points (many variables)

## 6 Global Optimisation

# Global optimisation—motivation

- Global optimisation is the field dedicated to discovering the global optimum of a system, i.e., the least minimum or greatest maximum of some cost function on some domain (the search space), e.g.,

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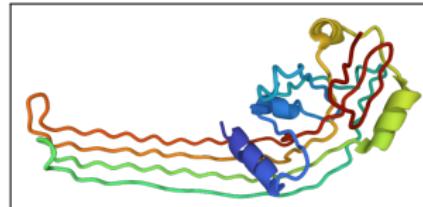
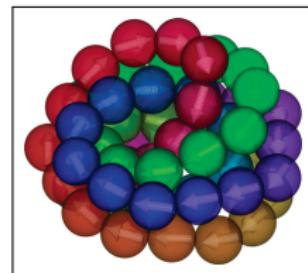
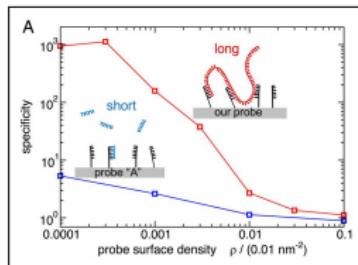
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Global Op-  
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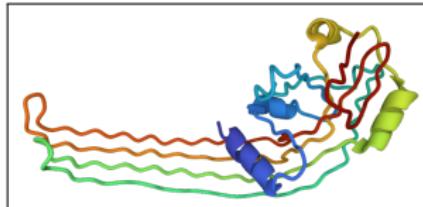
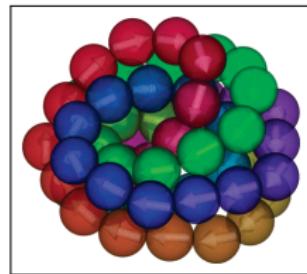
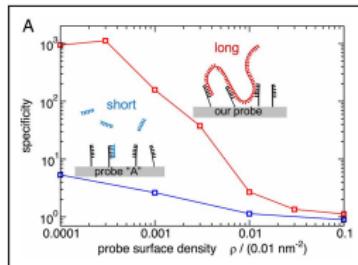
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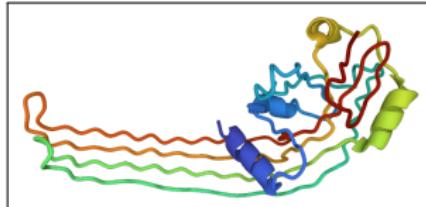
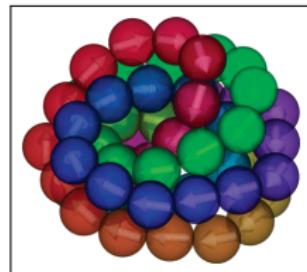
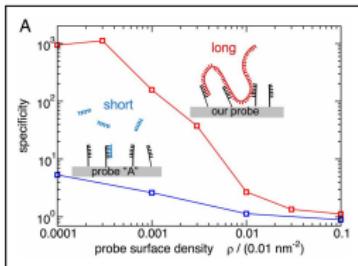
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Global Op-  
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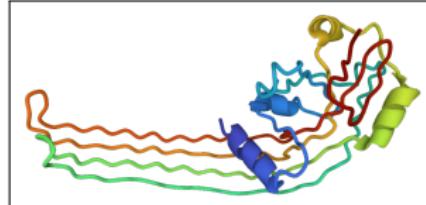
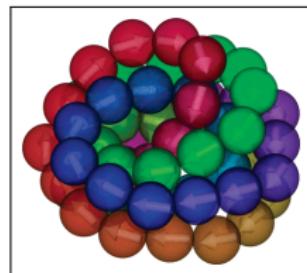
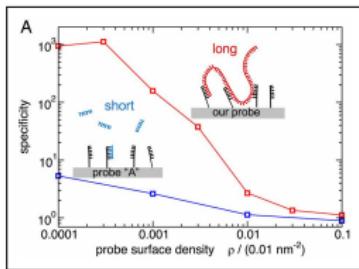
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- the short strand of DNA that binds most strongly/sensitively to a bacterial genome... (the search space is the strand sequence space)
- the lowest-energy arrangement of interacting particles in space... (the search space is the configuration space)
- the structure of the native state of a protein... (the search space is the space of protein conformations)



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Global Op-  
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  - maximising the **profit of a business**
  - maximising the **performance of a microchip**

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  - maximising the **profit of a business**
  - maximising the **performance of a microchip**
  - maximising the **structural integrity of a building** / minimising the **risk of catastrophic failure**

# Global optimisation—energy landscapes

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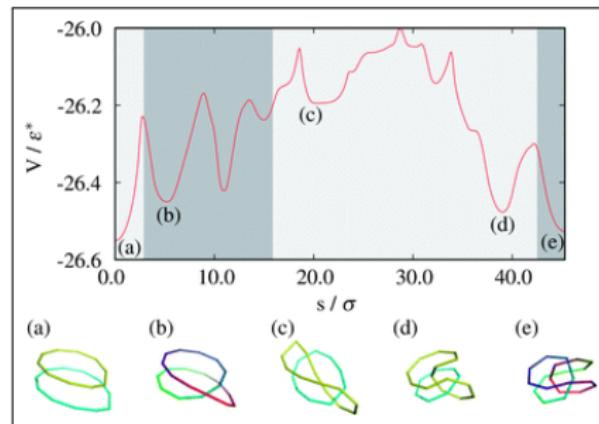
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Global Op-  
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- global (and local) optimisation are central to the theory of **energy landscapes**



# Global optimisation—energy landscapes

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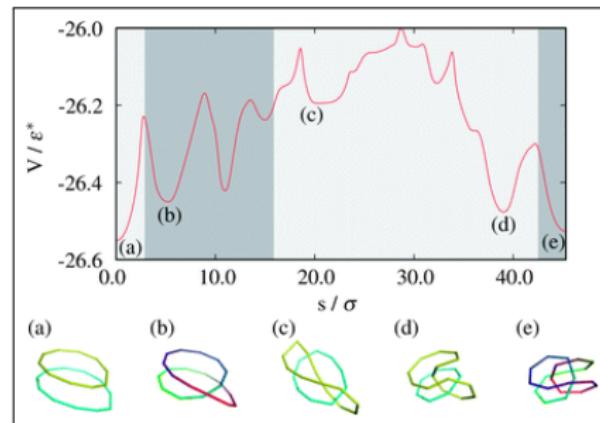
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Global Op-  
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- global (and local) optimisation are central to the theory of **energy landscapes**
- at **finite temperature**, a physical system spends most of its time near to **local minima (inherent structures)** on the potential energy surface (PES)



# Global optimisation—energy landscapes

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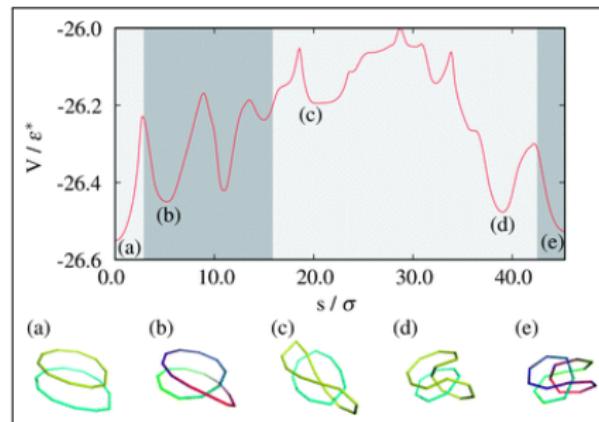
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Global Op-  
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- global (and local) optimisation are central to the theory of **energy landscapes**
- at **finite temperature**, a physical system spends most of its time near to **local minima (inherent structures)** on the potential energy surface (PES)
- the most **physically relevant pathways** to get from one minimum to another go *via* **index one saddles (transition states)**



# Global optimisation—energy landscapes

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- at **low temperatures**, the properties of a system are well-described by the properties of **relatively few (energy) minima**

# Global optimisation—energy landscapes

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# Global optimisation—energy landscapes

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- at **lower temperatures** still, and at thermodynamic equilibrium, the most important feature on the PES is the **global (energy) minimum**
- so far we have studied methods to locate both minima and index one saddles; this lecture concerns ways of finding global minima

# Global optimisation—methods

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Global Op-  
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- global optimisation methods fall into three main categories
- **deterministic methods guarantee** a solution will be found, e.g., linear programming problems;

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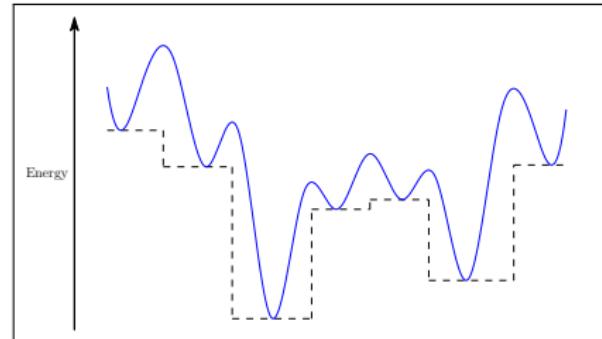
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  - basin-hopping, a stochastic technique widely applied in the physical sciences to find ground-state structures;
  - and genetic (or evolutionary) algorithms, a class of heuristic methods which draw inspiration from natural selection and genetics.
- although these methods both find applications outside of the physical sciences, our discussion will be geared toward solving physical problems

# A stochastic method—Basin-hopping



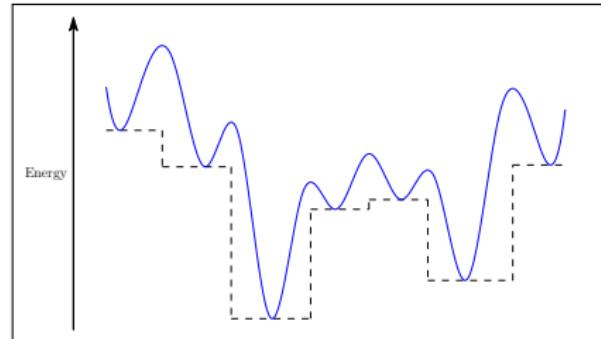
- basic idea: map every point on the surface to the closest minimum

$$\tilde{f}(\mathbf{x}) = f(\tilde{\mathbf{x}}) = \min \{f(\mathbf{x})\} \quad (51)$$

## BASIN-HOPPING TRANSFORMATION

where  $\min \{f(\mathbf{x})\}$  is defined as the energy at the local minimum with coordinates  $\tilde{\mathbf{r}}$ , obtained from a local minimisation of the potential energy in coordinate space (i.e. a quench), starting from  $\mathbf{r}$

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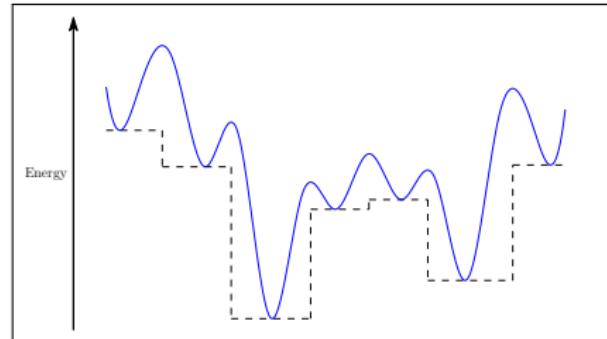
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- the surface is partitioned into disjoint sets of basins of attraction, each containing a local minimum and all points that quench to it.

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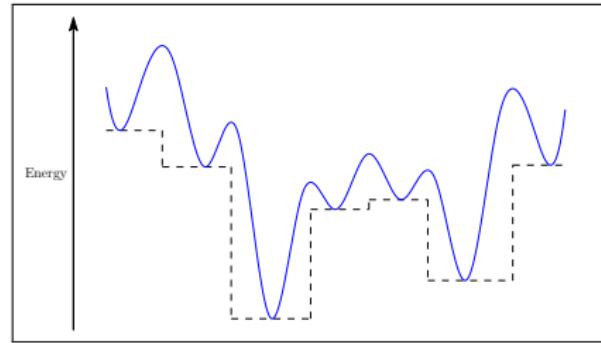
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- the surface is partitioned into disjoint sets of basins of attraction, each containing a local minimum and all points that quench to it.
- the transformation removes barriers between minima, allow more efficient exploration of the surface compared with MD, MC...

# A stochastic method—Basin-hopping



- the basic BH scheme proceeds as follows:

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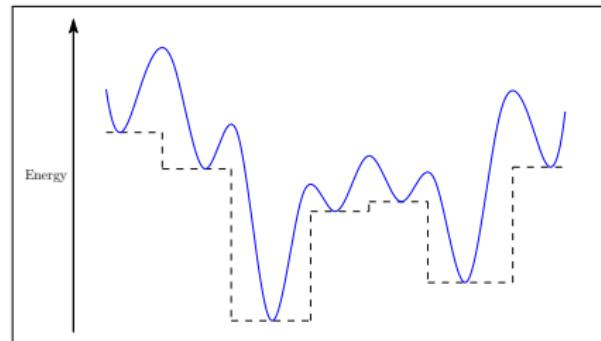
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# A stochastic method—Basin-hopping



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  - 1 start from a point  $x_k$ ;

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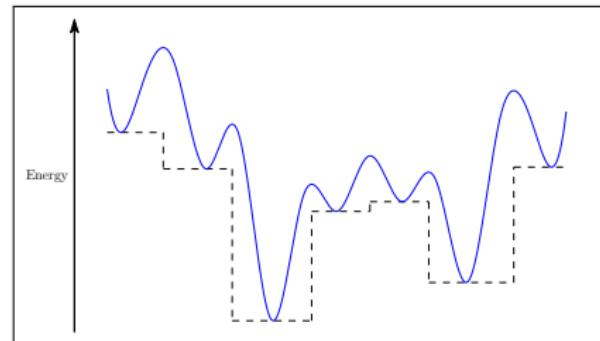
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# A stochastic method—Basin-hopping



- the basic BH scheme proceeds as follows:

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- 2 move the point with a perturbation,  $x_p = P(x_k)$ ;

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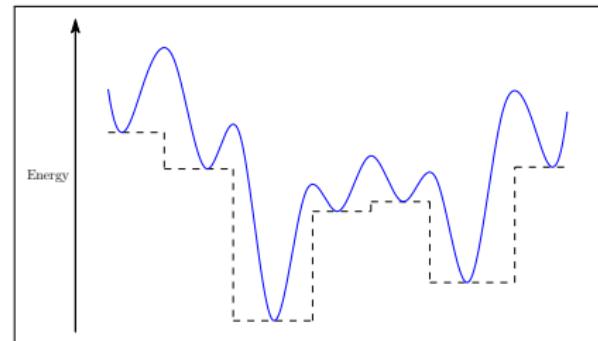
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# A stochastic method—Basin-hopping



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- 2 move the point with a perturbation,  $x_p = P(x_k)$ ;
- 3 minimise to the local minimum near the perturbed point,  $x_n = \min \{f(x)\}$

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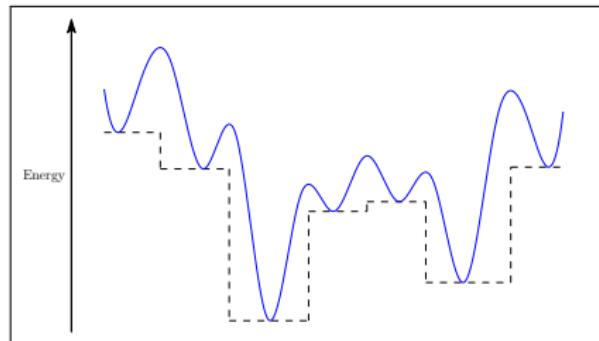
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- 3 minimise to the local minimum near the perturbed point,  $x_n = \min \{f(x)\}$
- 4 then set  $x_{k+1}$  according to the Metropolis criterion,

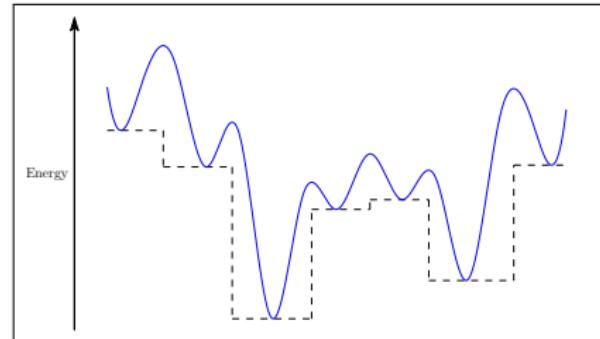
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(52)

## METROPOLIS CRITERION

where  $\beta$  is a control parameter, usually written as  $\beta = 1/kT$ , where  $k$  is Boltzmann's constant and  $T$  is the temperature parameter.

# A stochastic method—Basin-hopping



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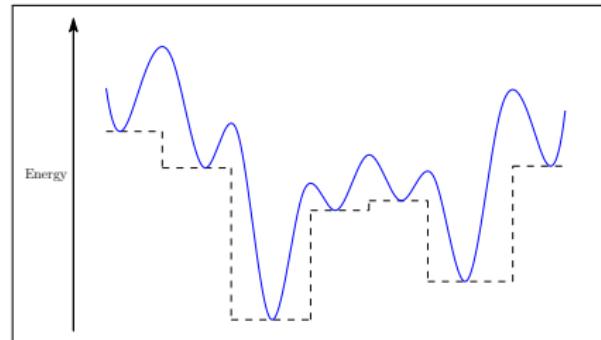
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Global Op-  
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# A stochastic method—Basin-hopping



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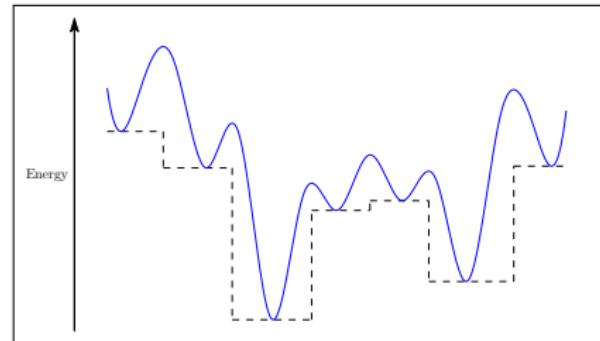
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# A stochastic method—Basin-hopping

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- when using a deterministic method, the solution can be found, and be shown to be the solution

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# A stochastic method—Basin-hopping

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- so when do we **terminate** a basin-hopping run?
- one protocol is to stop if many independent basin-hopping runs have **converged upon a common best solution**
- the success of such an approach depends sensitively on the **initial conditions**

# Basin-hopping—tuning the parameters

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wherein  $T \propto \frac{1}{\beta}$

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# Basin-hopping—tuning the parameters

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- how do we choose the perturbation?

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  - for physical problems, the choice is dependent on the **energy scales** of the system
- how do we choose the perturbation? this is a much more interesting question!

# Choosing the perturbation—simple translations

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Global Op-  
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- imagine you are tasked with finding the global energy minimum of  $N$  Lennard-Jones particles

# Choosing the perturbation—simple translations

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- imagine you are tasked with finding the global energy minimum of  $N$  Lennard-Jones particles (not so difficult to imagine)

# Choosing the perturbation—simple translations

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Global Op-  
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- imagine you are tasked with finding the global energy minimum of  $N$  Lennard-Jones particles
- a simple approach to perturbing the coordinates is to **translate** one or more particles by some **random amount** in some **random direction**,

$$P(\mathbf{x}) = \mathbf{x} + \boldsymbol{\xi}$$

# Choosing the perturbation—simple translations

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$$P(\mathbf{x}) = \mathbf{x} + \boldsymbol{\xi}$$

- the **magnitude** of  $\boldsymbol{\xi}$  is a critical consideration
  - choose  $x_i$  **too large**, and most of the steps will be **rejected**, because the energies of the new configurations will be too high
  - choose  $x_i$  **too small**, and we will **never escape** the original basin!

# Choosing the perturbation—orientational displacements

- now imagine you are tasked with finding the global energy minimum of  $N$  Stockmayer particles—that is, Lennard-Jones particles with **dipoles** slapped on top

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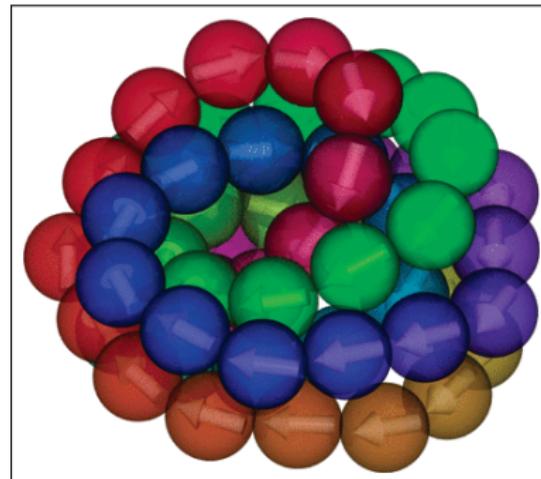
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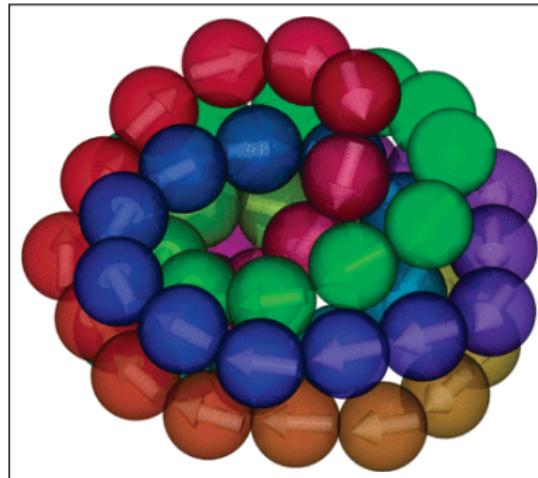
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# Choosing the perturbation—orientational displacements

- now imagine you are tasked with finding the global energy minimum of  $N$  Stockmayer particles—that is, Lennard-Jones particles with **dipoles** slapped on top
- this time we have both translational and **orientational** degrees of freedom to consider



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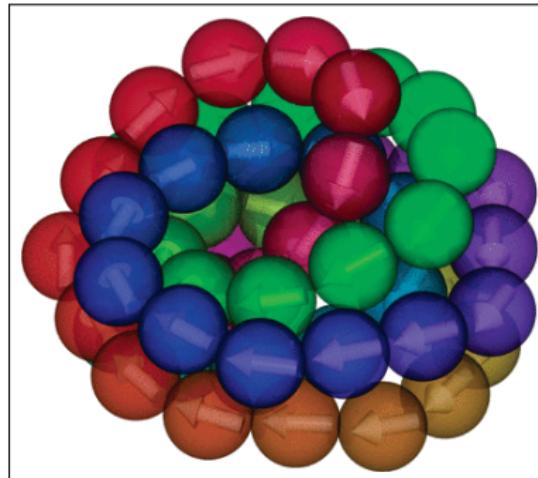
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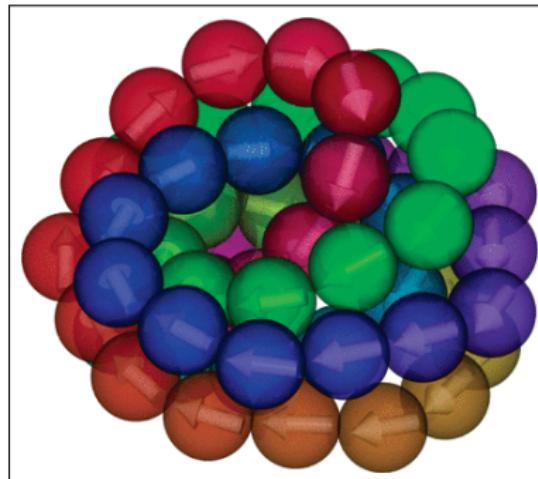
# Choosing the perturbation—orientational displacements

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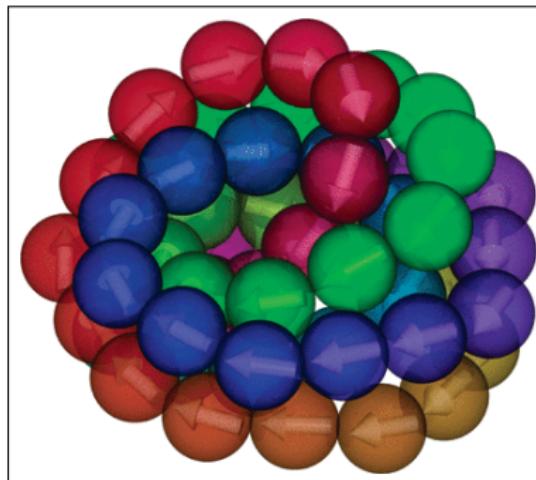
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- applying **orientational moves** such as **random rotations** to one or more dipoles is a plausible perturbation
- depending on the system, it may be best to apply translational and orientational moves together, separately, or even **hierarchically**...
- ...i.e., the translational perturbation could be a translation followed by a short basin-hopping run with orientational perturbations



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# Choosing the perturbation—surface moves

- imagine trying to optimise a **very large** LJ cluster

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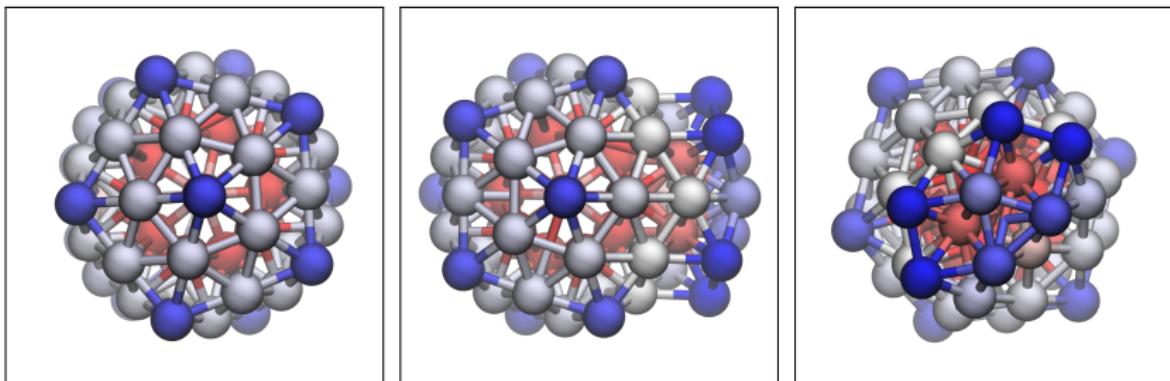
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Global minimum of 62 LJ particles. Red particles have low energy, blue particles have high energy.

# Choosing the perturbation—surface moves

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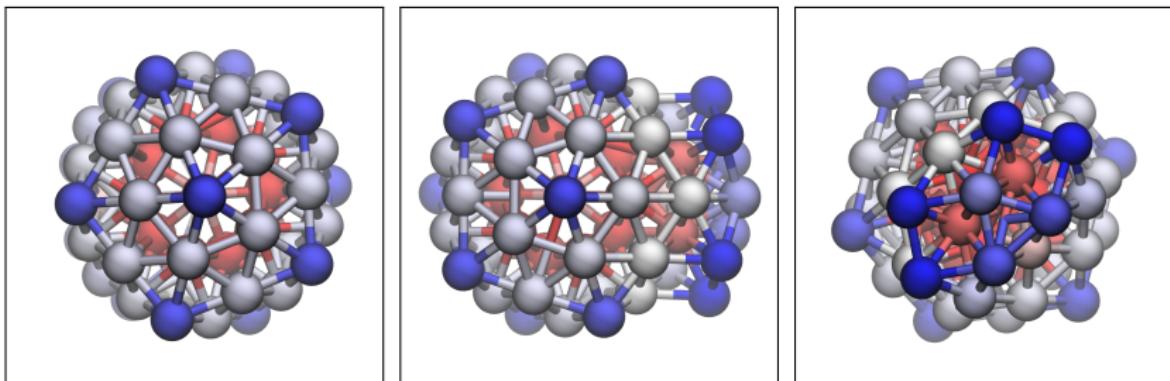
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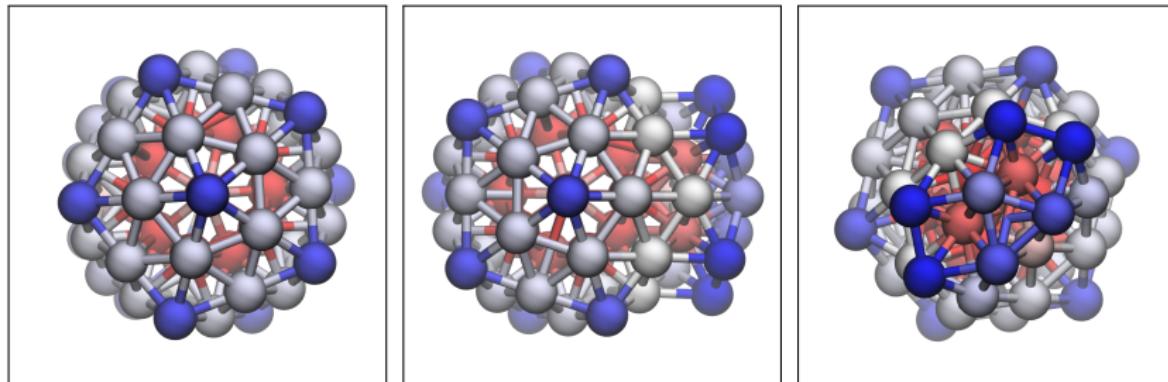
- imagine trying to optimise a **very large** LJ cluster
- particles in the **core** of the cluster are highly-coordinated and low in energy



Global minimum of 62 LJ particles. Red particles have low energy, blue particles have high energy.

# Choosing the perturbation—surface moves

- imagine trying to optimise a **very large** LJ cluster
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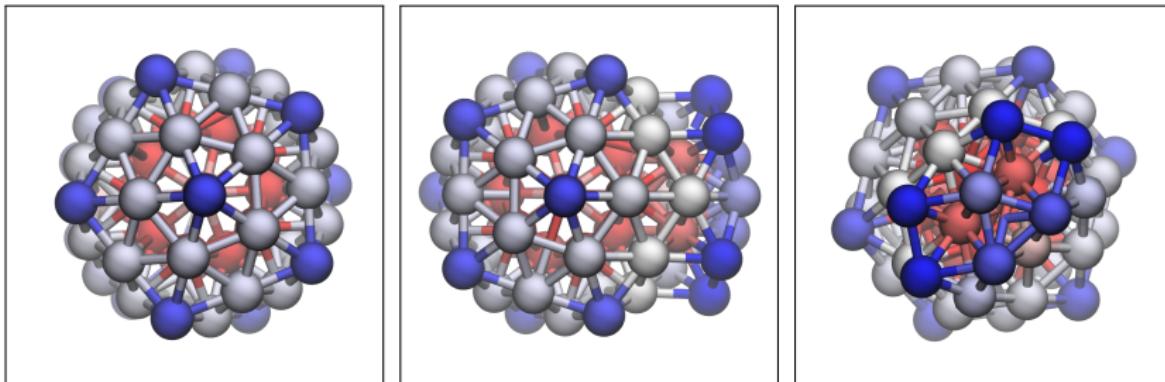
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Global Op-  
timisation

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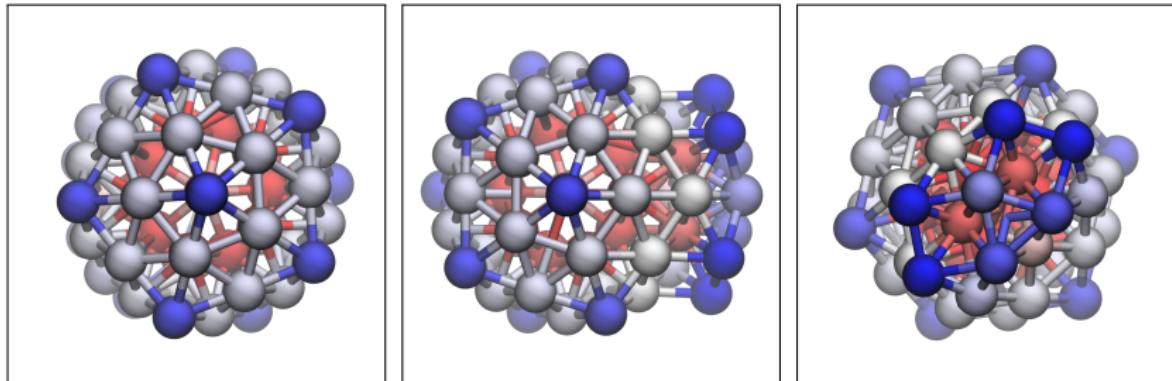
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# Choosing the perturbation—surface moves

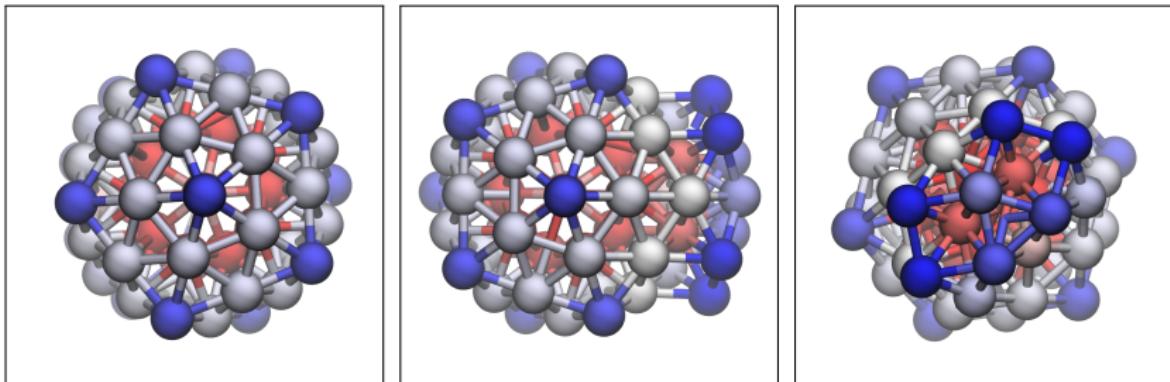
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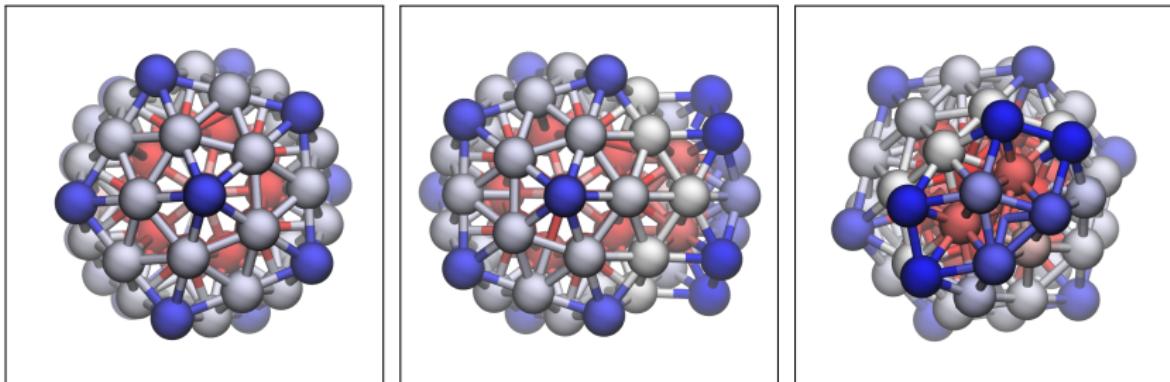
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# Choosing the perturbation—symmetry-based moves

- can we do **better than randomly** relocating the surface particles?

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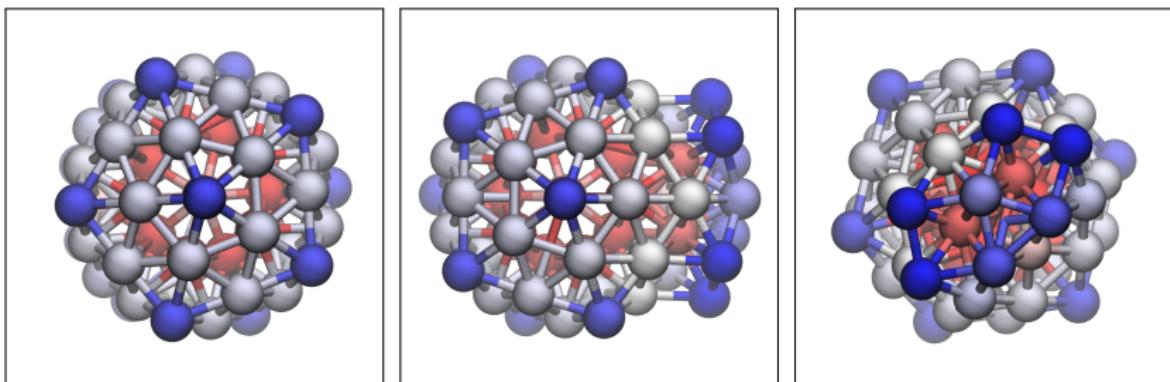
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# Choosing the perturbation—symmetry-based moves

- can we do **better than random**ly relocating the surface particles?
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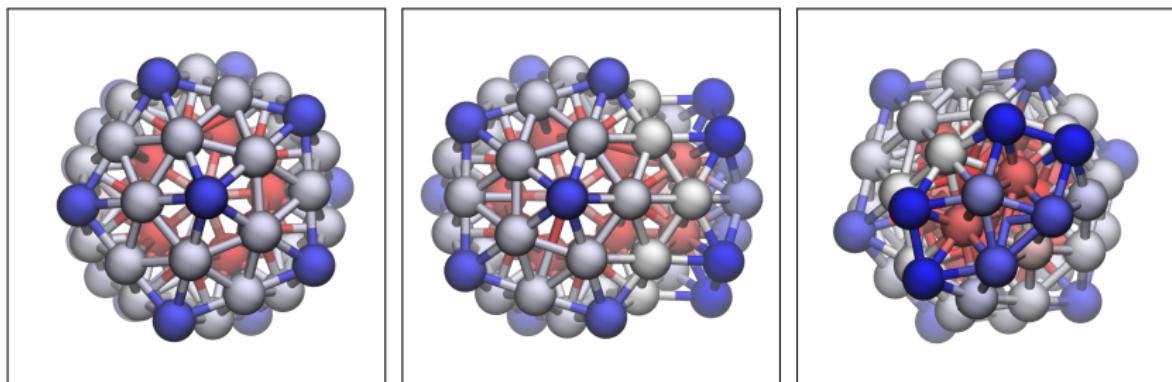
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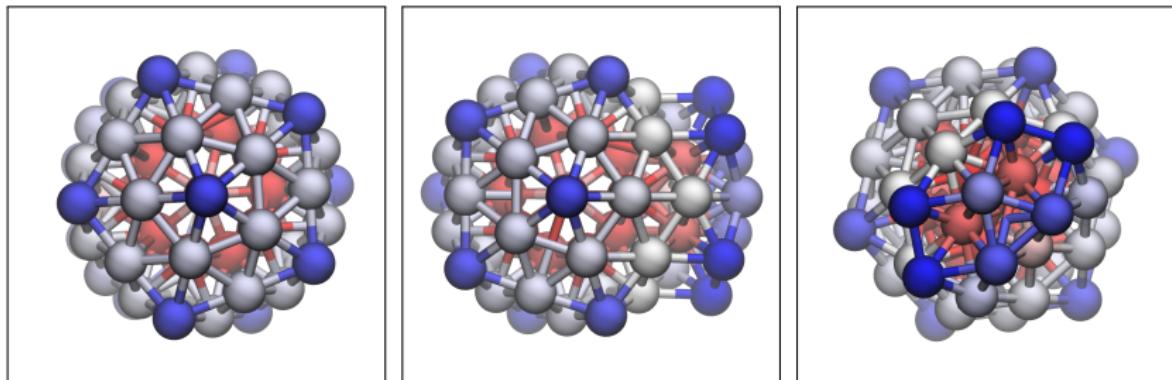
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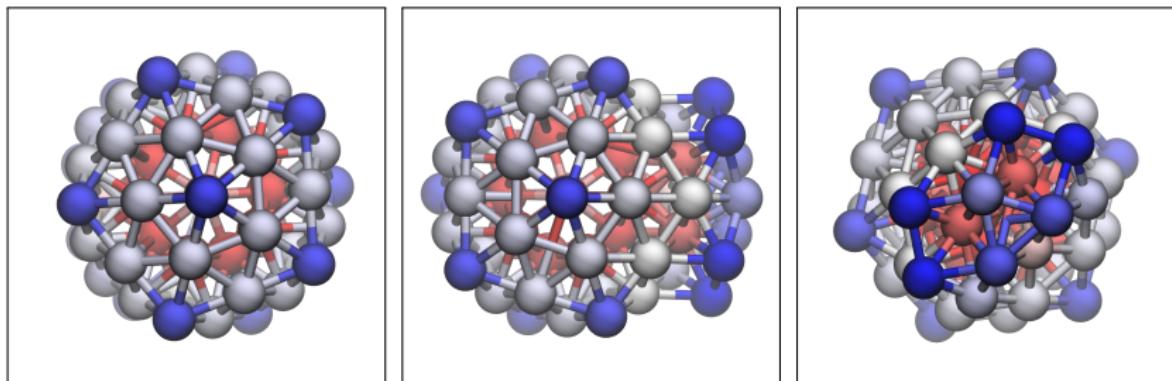
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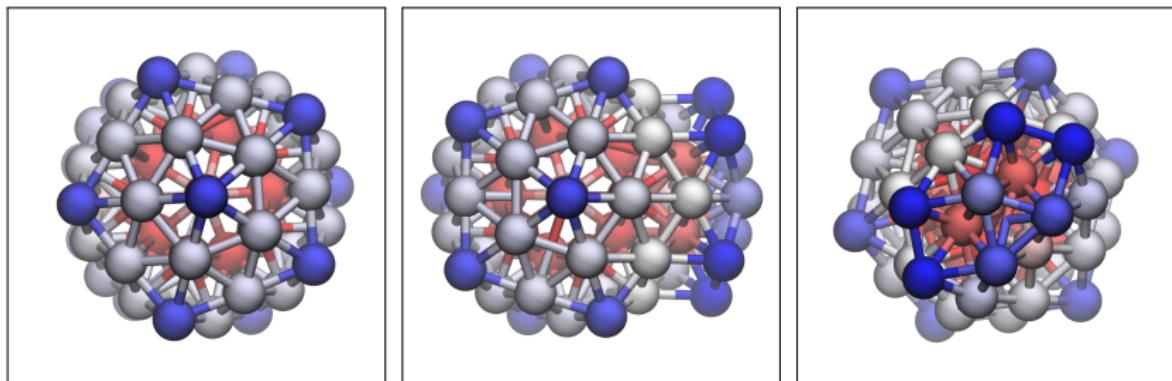
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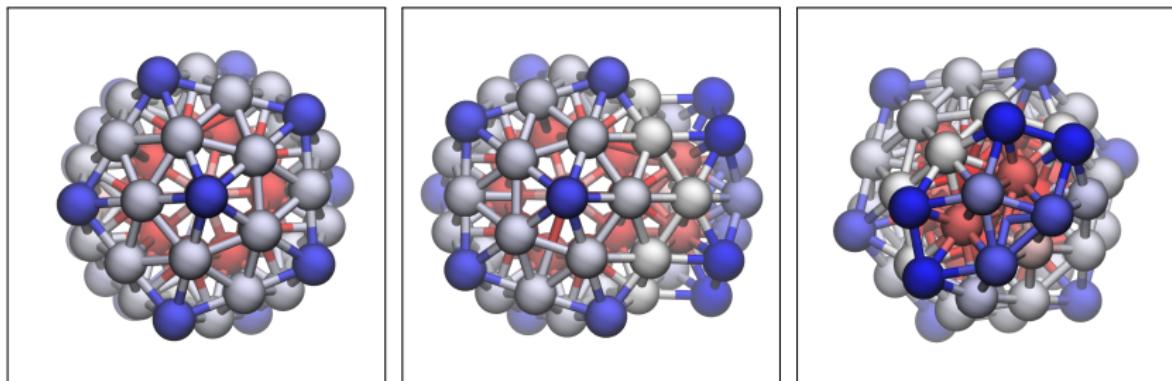
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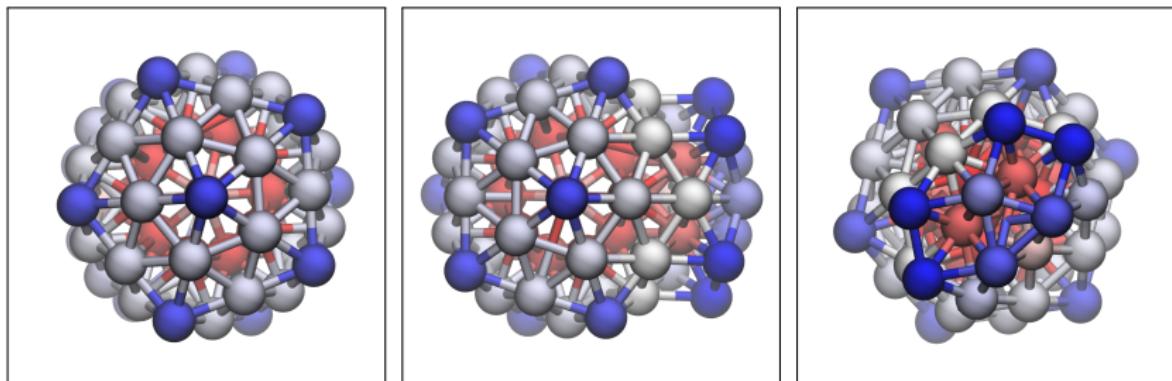
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  - 1 identify a **symmetrical core**, and generate symmetry positions on the surface
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  - 3 choose the permutation with the lowest energy
- even though the global minimum of 98 Lennard-Jones particles has only  $C_s$  symmetry, this method reduces the time taken to find that global minimum by **a factor of 70** compared to translational moves



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# Choosing the perturbation—molecular dynamics

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- the perturbation can also be a **short molecular dynamics trajectory**

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- the perturbation can also be a **short molecular dynamics trajectory**
- this approach is useful for **complex molecules** such as proteins, polynucleotides (DNA, RNA), and other biomolecules, for which a random displacement may result in **physically unreasonable structures**, e.g., inversion around a chiral centre.

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# Choosing the perturbation—molecular dynamics

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- ...but differs from the example basin-hopping method outlined above in that it does not use the Metropolis criterion, but a **threshold** for the accept/reject part
- a step is accepted if the energy increases by less than some threshold energy  $E_{\text{diff}}$ , which is adjusted on-the-fly to give an average acceptance probability of 0.5.

# Choosing the perturbation—more complicated ideas

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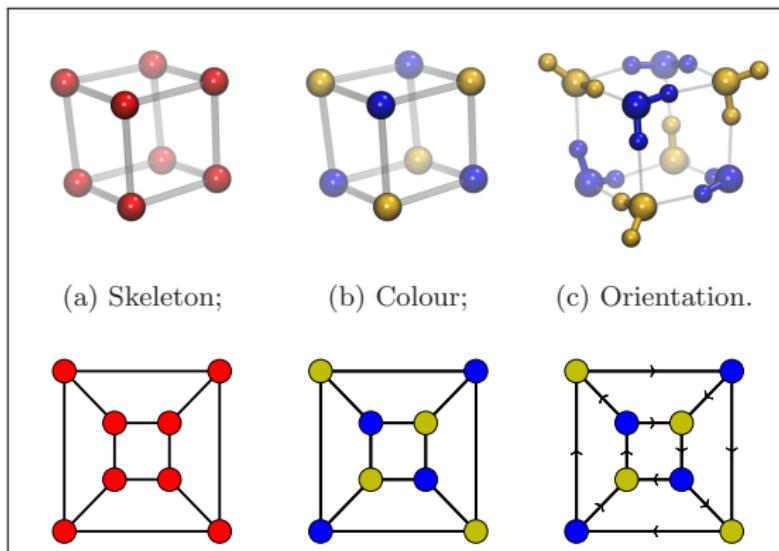
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Global Op-  
timisation

- we can use **system-specific** information to design perturbations for specific systems
- take **water clusters** as an example
- water clusters have horrifically complex energy landscapes due to the complex interplay of translational and orientational degrees of freedom
- **hierarchical schemes** have been developed which directly modify the **hydrogen-bond topology** of a water cluster...
- ...allowing relatively **large steps** in the search space with relatively **high acceptance probabilities**



# Modifying the landscape—flooding

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- ...decreasing the probability that those basins will be visited again during the simulation
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- ...so the basins can be revisited, but will quickly be escaped as the **local temperature is high**

# Heuristic methods—genetic algorithms

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Global Op-  
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- **genetic algorithms**, or evolutionary algorithms, are a class of techniques that use **ideas from evolution** to find the solution that optimises a cost function, *i.e.*, the individual most suited to his environment

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- the coordinates  $x$  are encoded as a **binary string**, the **chromosome**; the encoded forms of each  $x_i$  constitute **genes**

$$x = \{x_1, x_2, \dots, x_n\} \rightarrow \{\{11010101\}, \{11101110\}, \dots, \{00110101\}\}$$

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- genetic algorithms can be applied to both **discrete and continuous problems**
- they employ analogues of **competition/selection**, **mating/crossover**, and **mutation**

# A basic genetic algorithm

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Global Op-  
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- the first step is to initialise a fixed number,  $n_r$ , of chromosomes to compose the gene pool of the first generation
- subsequent generations are produced by iterating the following three steps:

# A basic genetic algorithm

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Global Op-  
timisation

- the first step is to initialise a fixed number,  $n_r$ , of chromosomes to compose the gene pool of the first generation
- subsequent generations are produced by iterating the following three steps:
  - select from the gene pool the  $n_g = n_r/2$  chromosomes that will survive into the next generation;

# A basic genetic algorithm

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  - 3 introduce random mutations into the chromosomes of some of the population

# A basic genetic algorithm—selection

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- selection is done in such a way that the **fittest chromosomes**, those which represent **relatively optimal solutions** to the cost function, are more likely to proceed to the next generation, and those least fit, more likely to be discarded

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  - **liberal selection** (choosing chromosomes at random) is like basin-hopping with a high temperature, resulting in a **random search**

# A basic genetic algorithm—crossover

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- **crossover** operations are the first of two ways that a genetic algorithm **explores new regions of the solution space**

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- in a process analogous sexual reproduction, pairs of chromosomes are chosen from the gene pool and mixed together in some way to produce new, different chromosomes, representing new elements of the solution space

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- one type of crossover scheme is the single-point crossover, wherein two chromosomes are cut in half, and two new chromosomes are created by splicing opposite halves together...

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- ...e.g., if the crossover point was taken to be the centre of the arrays, parents

$$y_1 = \{01010101\} \quad \& \quad y_2 = \{11001100\}$$

would produce offspring

$$w_3 = \{01011100\} \quad \& \quad w_4 = \{11000101\}$$

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- as with in the selection step, there are many possibilities for choosing pairs of parents in the crossover step

# A basic genetic algorithm—mutation

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- using crossover operations **alone**, the gene pool can get **stuck in a local minimum**, comprising chromosomes that represent **very similar solutions**
- **mutation** operations add some extra diversity into the gene pool by **randomly flipping bits** in some of the chromosomes
- the probability of flipping a bit,  $p_f$ , is a **control parameter**, and works similarly to step size parameter in basin hopping:
  - choose  $p_f$  **too low**, and the search **doesn't go anywhere**;
  - choose  $p_f$  **too high**, and the resulting chromosomes will have a **random (likely relatively poor) fitness**, and will be **rejected** at the selection stage.

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- thanks for listening

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- thanks for listening
- I hope something we've discussed turns out to be useful