

# **Week 9: Numerical differentiation and application to solving the heat equation**

**Finite differencing, pseudospectral methods and their application to the heat equation**

**Dr K Clough, Topics in Scientific computing, Autumn term 2023**

# Lagrange polynomials use collocation at points

- Degree  $n$  Lagrange polynomials agree exactly with a function  $f(x)$  at  $n+1$  distinct points,  $(x_0, f(x_0)), (x_1, f(x_1)) \dots (x_{n+1}, f(x_{n+1}))$
- First we construct the basis functions

$$L_k(x) = \prod_{i=0, i \neq k}^n \frac{(x - x_i)}{(x_k - x_i)}$$

What does the numerator and denominator achieve here?

- Then their weights are the values of the functions at each point, so that the Lagrange interpolant is:

$$P_n(x) = \sum_{k=0}^n L_k(x) f(x_k)$$

# Plan for today

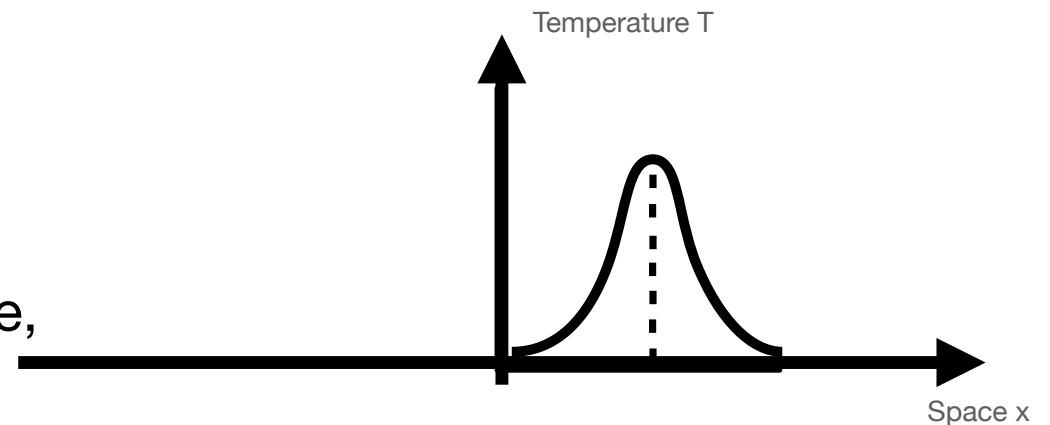
1. Motivation - solution of the heat equation
2. Revision of last week's interpolation content
3. Numerical differentiation - finite differencing
4. Numerical differentiation - pseudospectral methods
5. Application - solution of the heat equation

# Motivation: solving the heat equation

- The heat equation

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

- Tell me your initial temperature profile, and I can tell you how it changes over time
- Cannot usually just write down  $T = f(x,t)$  except in very simple cases



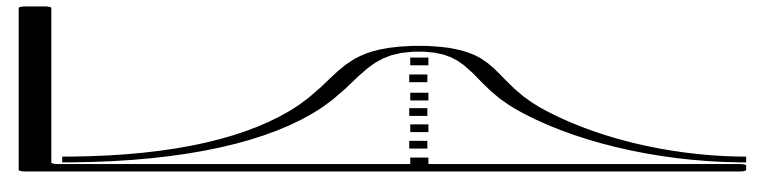
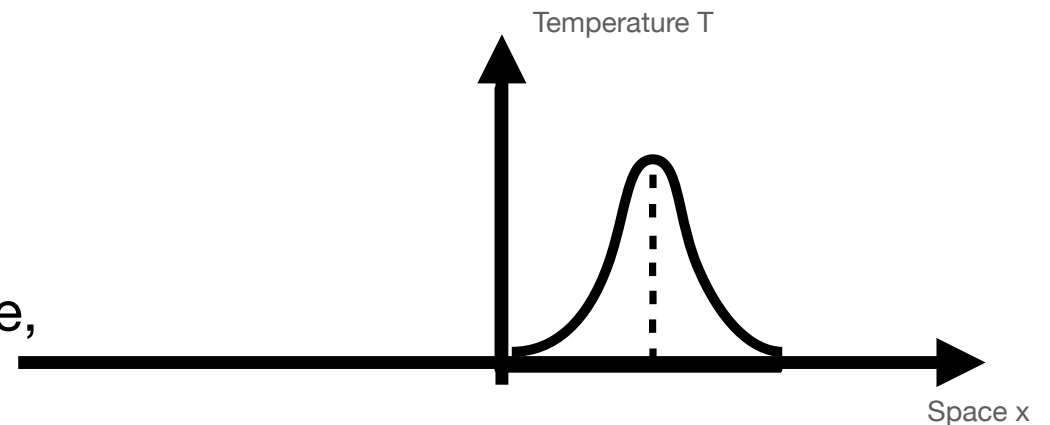
How does T change over time?

# Motivation: solving the heat equation

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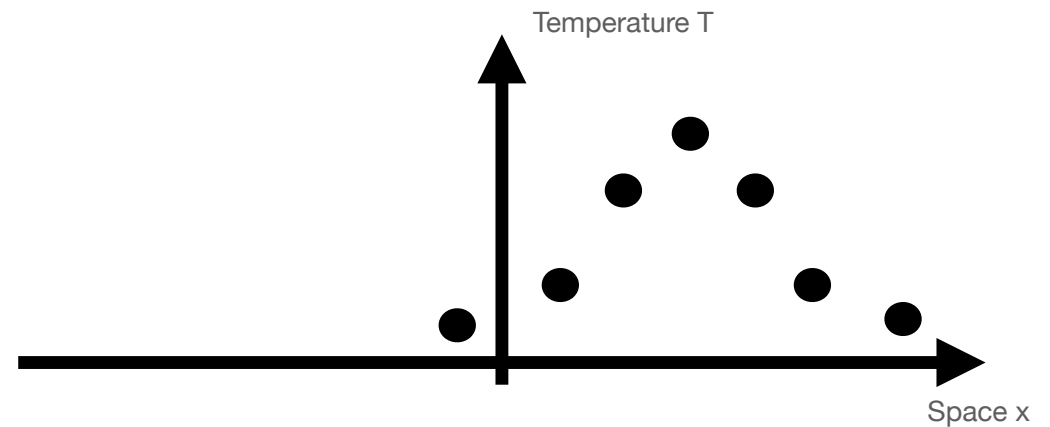
The temperature profile spreads out - the value decreases at a maximum where the second derivative is negative

# Motivation: solving the heat equation

- The heat equation

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

- How to find the spatial derivative of  $T$  if it is represented as a series of points?



# Plan for today

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- First we construct the basis functions

$$L_k(x) = \prod_{i=0, i \neq k}^n \frac{(x - x_i)}{(x_k - x_i)}$$

*Numerator - functions to be zero at all of the points other than  $x_k$  - denominator - function is normalised so it has value 1 at  $x_k$*

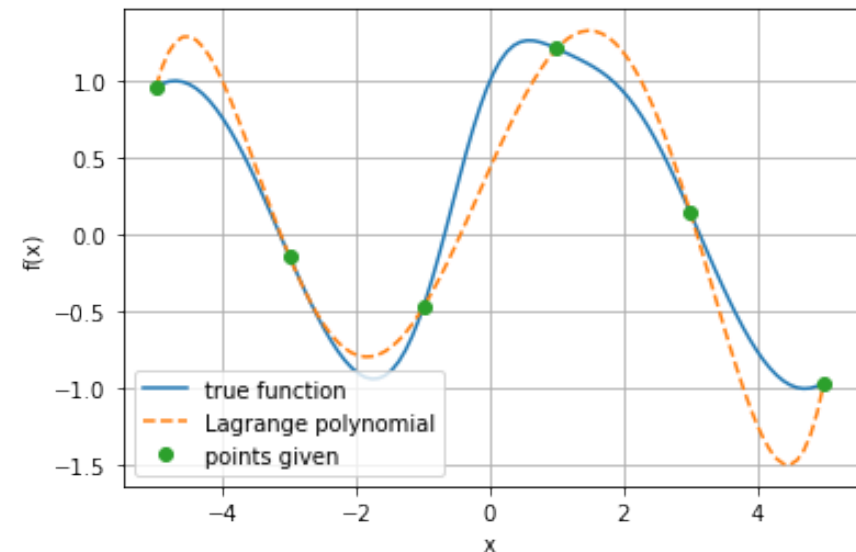
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# Lagrange polynomials use collocation at points

- Can use a python function `scipy.interpolate.lagrange()` to construct using higher number of points

Is a higher number of points always better?

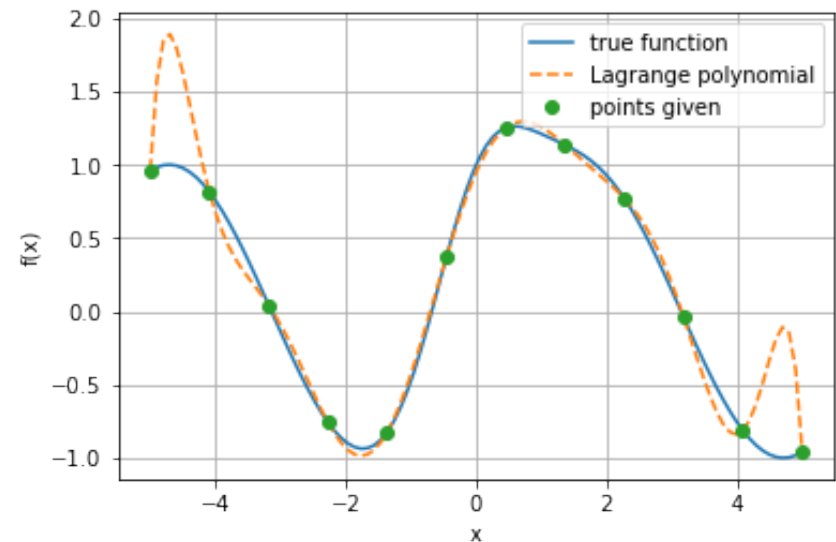


# Lagrange polynomials use collocation at points

- More points improved the fit at the interior, but with regular intervals it tends to lead to spurious oscillations at the edges of the interval

-> “Runge’s phenomenon”

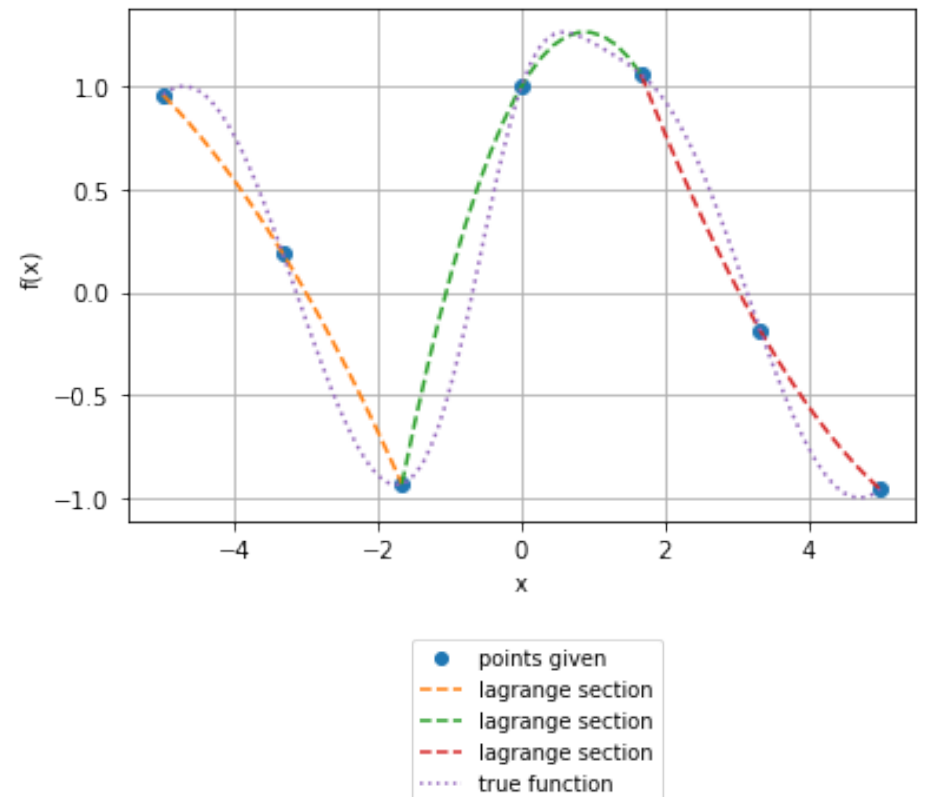
How can we do better?



# Strategy 1: composite collocation

1. We could try to divide the interval up into smaller sections and fit lower order Lagrange polynomials to each part in turn - this is a **composite collocation** method.

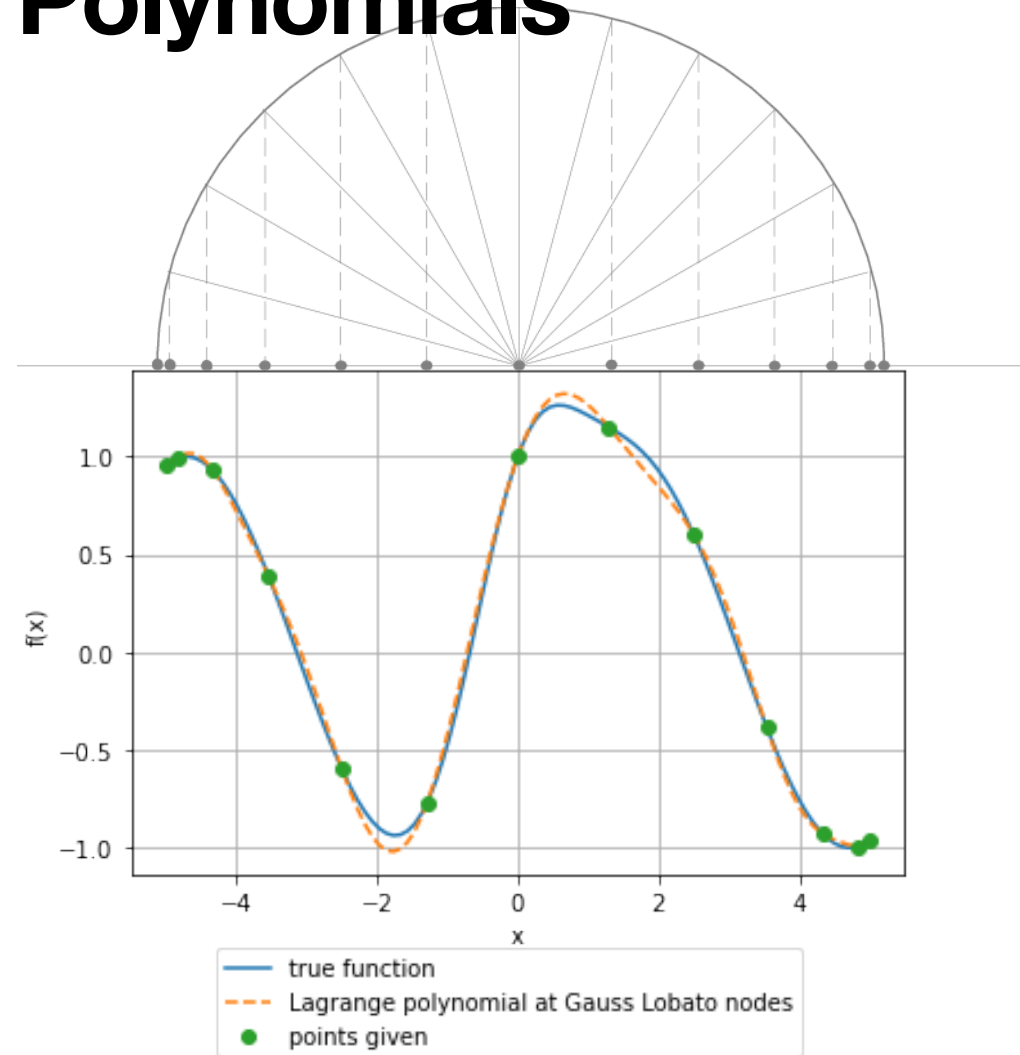
This approach gives rise to the idea of ***finite differencing*** for finding derivatives.



# Strategy 2 - Chebyshev Polynomials

2. If we locate the points not evenly, but at the zeros of the Chebyshev polynomials, we get an exponentially convergent fit and eliminate Runge's phenomenon

This approach gives rise to the idea of ***pseudospectral*** methods for finding derivatives.

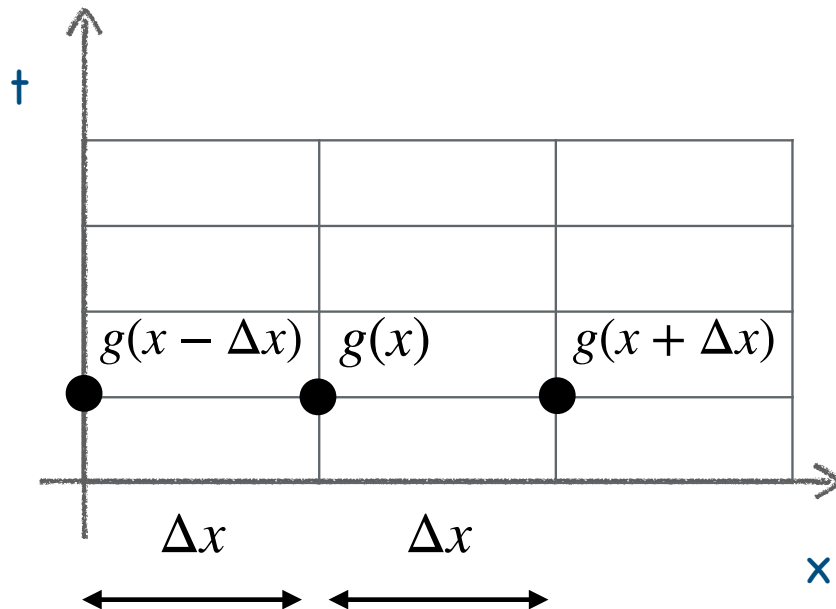


# Plan for today

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2. ~~Revision of last week's interpolation content~~
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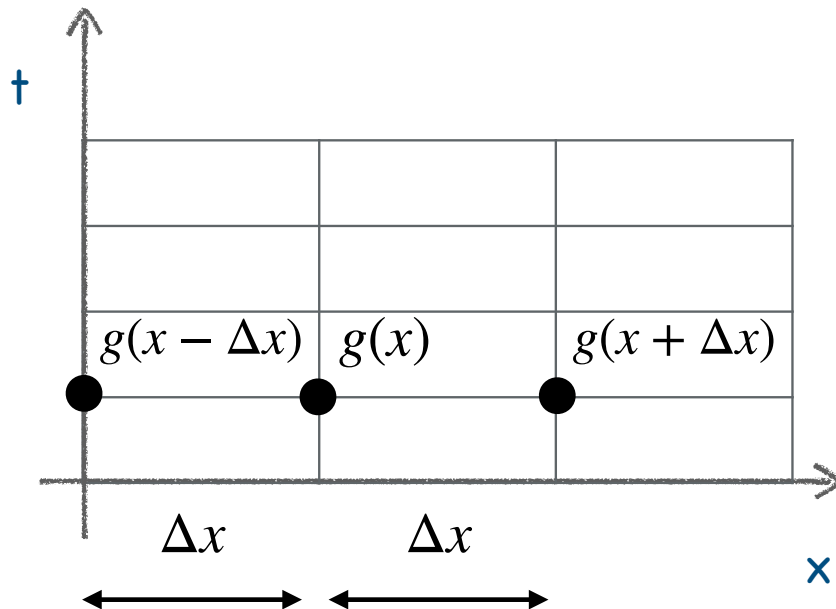
# Numerical differentiation - finite differencing

How do I find the first derivative at the central point?



# Numerical differentiation - finite differencing

How do I find the first derivative at the central point?

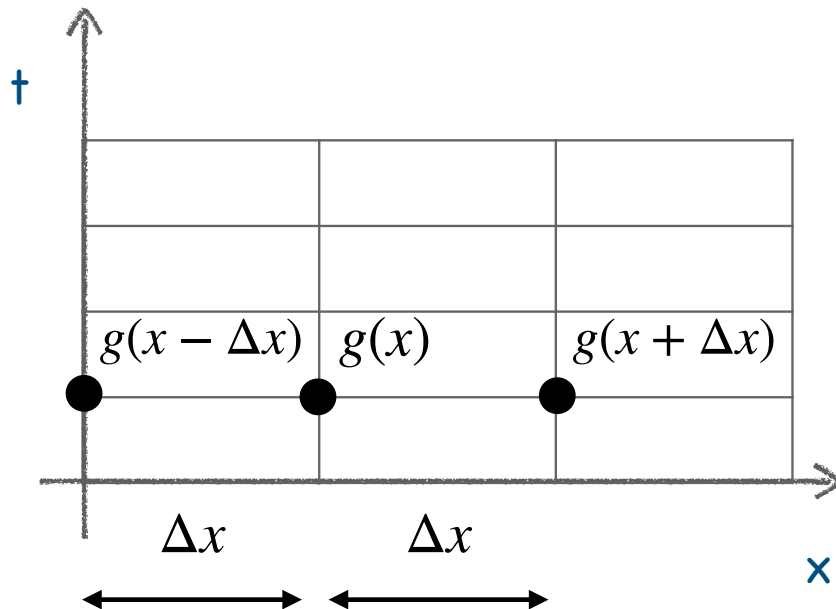


$$\frac{\partial g}{\partial x} \approx \frac{g(x + \Delta x) - g(x - \Delta x)}{2\Delta x}$$



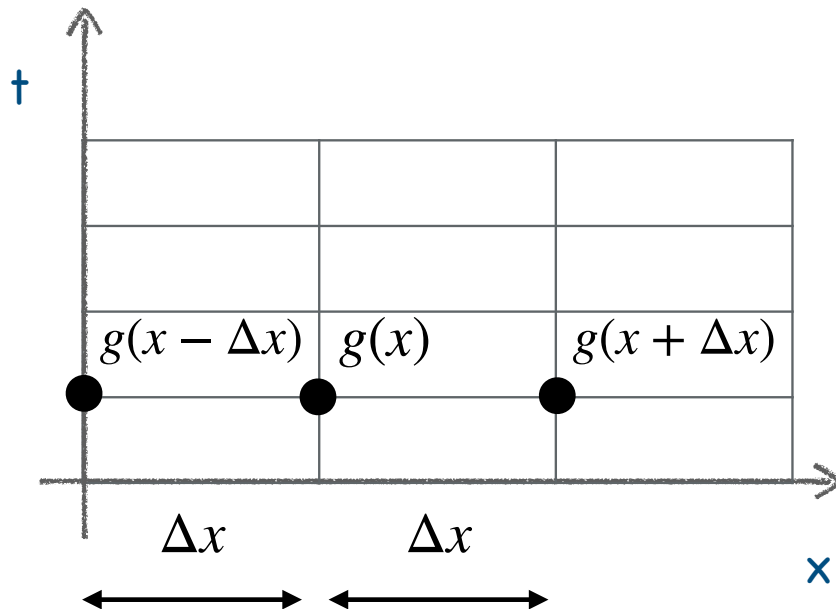
# Numerical differentiation - finite differencing

How do I find the second derivative at the central point?



# Numerical differentiation - finite differencing

How do I find the second derivative at the central point?



$$\begin{aligned}\frac{\partial^2 g}{\partial x^2} &\approx \frac{\frac{g(x + \Delta x) - g(x)}{\Delta x} - \frac{g(x) - g(x - \Delta x)}{\Delta x}}{\Delta x} \\ &\approx \frac{g(x + \Delta x) - 2g(x) + g(x - \Delta x)}{\Delta x^2}\end{aligned}$$

# Finite differencing - stencil representation

We can see *finite differencing* as the convolution of a stencil with the current state vector.

$\Delta x = 0.5$   
↔

|               |   |     |   |     |   |     |
|---------------|---|-----|---|-----|---|-----|
| Position x    | 0 | 0.5 | 1 | 1.5 | 2 | 2.5 |
| Temperature T | 0 | 1   | 3 | 2   | 1 | 0   |

↑

|    |   |   |
|----|---|---|
| -1 | 0 | 1 |
|----|---|---|

*First derivative stencil*

$$\frac{\partial g}{\partial x} \approx \frac{g(x + \Delta x) - g(x - \Delta x)}{2\Delta x}$$

|       |  |  |  |  |  |  |
|-------|--|--|--|--|--|--|
| dT/dx |  |  |  |  |  |  |
|-------|--|--|--|--|--|--|

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|    |   |   |
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|       |  |  |   |  |  |  |
|-------|--|--|---|--|--|--|
| dT/dx |  |  | 1 |  |  |  |
|-------|--|--|---|--|--|--|

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|    |   |   |
|----|---|---|
| -1 | 0 | 1 |
|----|---|---|



*First derivative stencil*

$$\frac{\partial g}{\partial x} \approx \frac{g(x + \Delta x) - g(x - \Delta x)}{2\Delta x}$$

|       |  |  |   |  |  |  |
|-------|--|--|---|--|--|--|
| dT/dx |  |  | 1 |  |  |  |
|-------|--|--|---|--|--|--|

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|    |   |   |
|----|---|---|
| -1 | 0 | 1 |
|----|---|---|



*First derivative stencil*

$$\frac{\partial g}{\partial x} \approx \frac{g(x + \Delta x) - g(x - \Delta x)}{2\Delta x}$$


|       |  |   |   |  |  |  |
|-------|--|---|---|--|--|--|
| dT/dx |  | 3 | 1 |  |  |  |
|-------|--|---|---|--|--|--|

# Finite differencing - stencil representation

We can see *finite differencing* as the convolution of a stencil with the current state vector.

|               |   |     |   |     |   |     |
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| Position x    | 0 | 0.5 | 1 | 1.5 | 2 | 2.5 |
| Temperature T | 0 | 1   | 3 | 2   | 1 | 0   |

|    |   |   |
|----|---|---|
| -1 | 0 | 1 |
|----|---|---|




|       |  |   |   |    |  |  |
|-------|--|---|---|----|--|--|
| dT/dx |  | 3 | 1 | -2 |  |  |
|-------|--|---|---|----|--|--|

# Finite differencing - stencil representation

We can see *finite differencing* as the convolution of a stencil with the current state vector.

|               |   |     |   |     |   |     |
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| Temperature T | 0 | 1   | 3 | 2   | 1 | 0   |

|    |   |   |
|----|---|---|
| -1 | 0 | 1 |
|----|---|---|



|       |  |   |   |    |    |  |
|-------|--|---|---|----|----|--|
| dT/dx |  | 3 | 1 | -2 | -2 |  |
|-------|--|---|---|----|----|--|

What about the end points?




# Finite differencing - stencil representation

We can see *finite differencing* as the convolution of a stencil with the current state vector.

|               |   |     |   |     |   |     |
|---------------|---|-----|---|-----|---|-----|
| Position x    | 0 | 0.5 | 1 | 1.5 | 2 | 2.5 |
| Temperature T | 0 | 1   | 3 | 2   | 1 | 0   |

*Use one sided stencil - doesn't  
have to be centralised*

|    |   |
|----|---|
| -2 | 2 |
|----|---|



|       |  |   |   |    |    |    |
|-------|--|---|---|----|----|----|
| dT/dx |  | 3 | 1 | -2 | -2 | -2 |
|-------|--|---|---|----|----|----|

# Finite differencing - stencil representation

We can see *finite differencing* as the convolution of a stencil with the current state vector.

|               |   |     |   |     |   |     |
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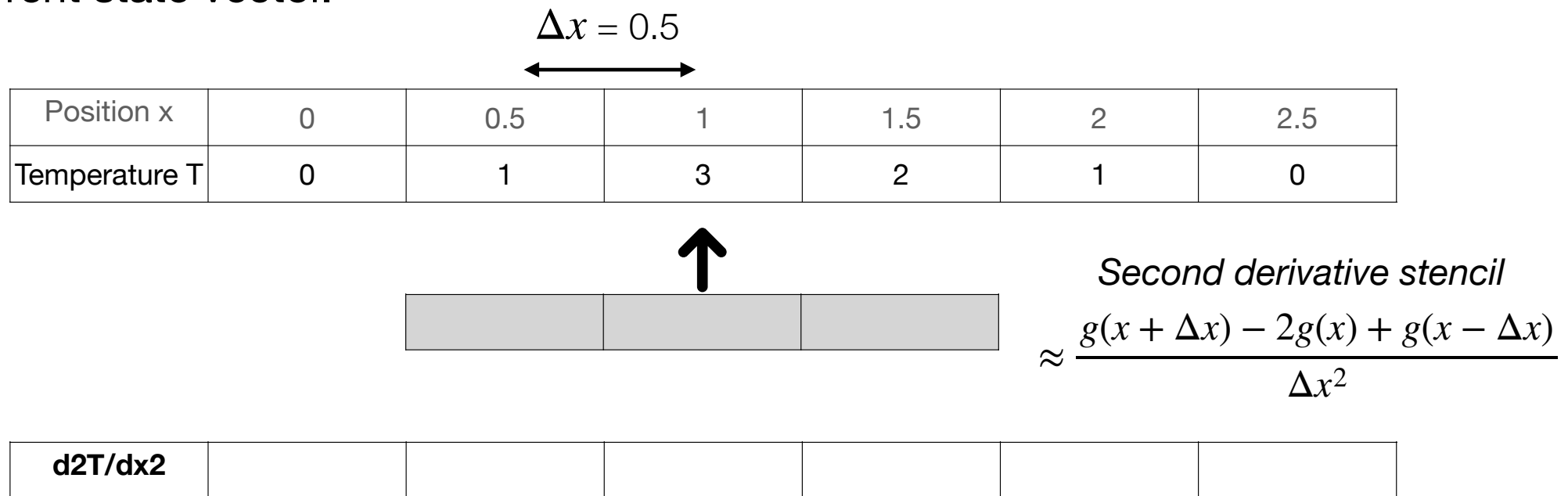
OR use a **boundary condition** -  
some knowledge about the function  
- e.g. maybe its derivative goes to zero here



|       |  |   |   |    |    |   |
|-------|--|---|---|----|----|---|
| dT/dx |  | 3 | 1 | -2 | -2 | 0 |
|-------|--|---|---|----|----|---|

# Finite differencing - stencil representation

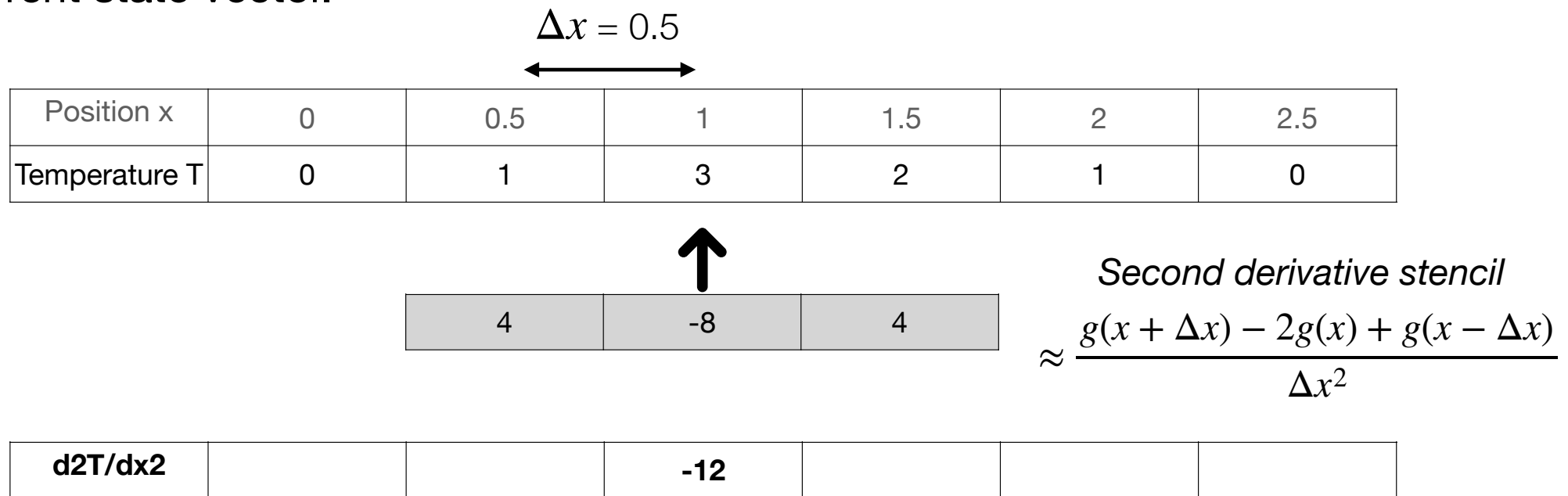
We can see *finite differencing* as the convolution of a stencil with the current state vector.



What is the second derivative stencil?

# Finite differencing - stencil representation

We can see *finite differencing* as the convolution of a stencil with the current state vector.



# Finite differencing - matrix representation

We can also represent this convolution in matrix form:

|               |   |     |   |     |   |     |
|---------------|---|-----|---|-----|---|-----|
| Position x    | 0 | 0.5 | 1 | 1.5 | 2 | 2.5 |
| Temperature T | 0 | 1   | 3 | 2   | 1 | 0   |

**$DT/dx$**

**=**

***Matrix D***

***T***

|    |
|----|
| 2  |
| 3  |
| 1  |
| -2 |
| -2 |
| -2 |

**=**

|    |    |    |    |    |   |
|----|----|----|----|----|---|
| -2 | 2  |    |    |    |   |
| -1 | 0  | 1  |    |    |   |
|    | -1 | 0  | 1  |    |   |
|    |    | -1 | 0  | 1  |   |
|    |    |    | -1 | 0  | 1 |
|    |    |    |    | -2 | 2 |

•

|   |
|---|
| 0 |
| 1 |
| 3 |
| 2 |
| 1 |
| 0 |

*All blank entries zero*

# Finite differencing - relation to Lagrange polynomials

Using the Lagrange polynomials helps us to have general method for constructing the stencils.

This is important to answer the questions:

- How do I know the order of accuracy of my method?
- How many points should I use?
- What if I don't have evenly spaced points?

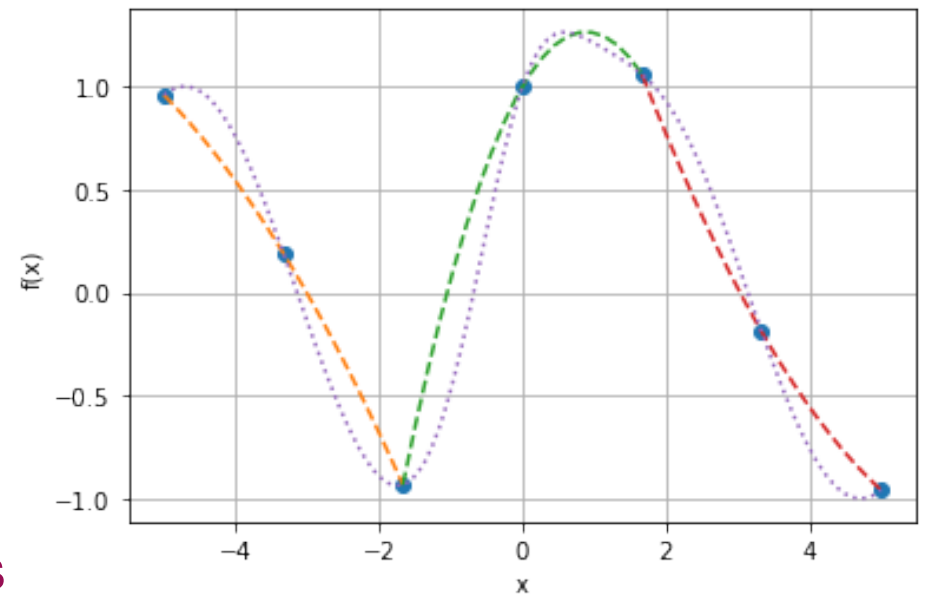
# How many points?

We will fit a polynomial of order  $n-1$  to the  $n$  points we want to use in the stencil.

One can show that the truncation error is of order  $O(\Delta x^{(n-1)})$

What is the minimum number of points for a second derivative stencil?

What is the accuracy of the stencil with this number of points?

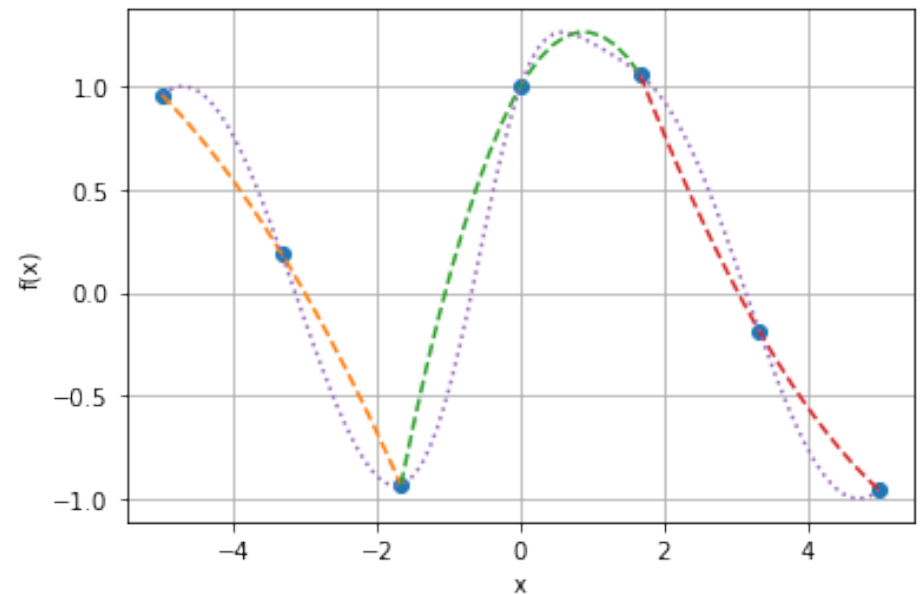


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One can show that the truncation error is of order  $O(\Delta x^{(n-1)})$

*Need at least 3 points to capture a 2nd order derivative, and the approximation has error of  $O(\Delta x^2)$*





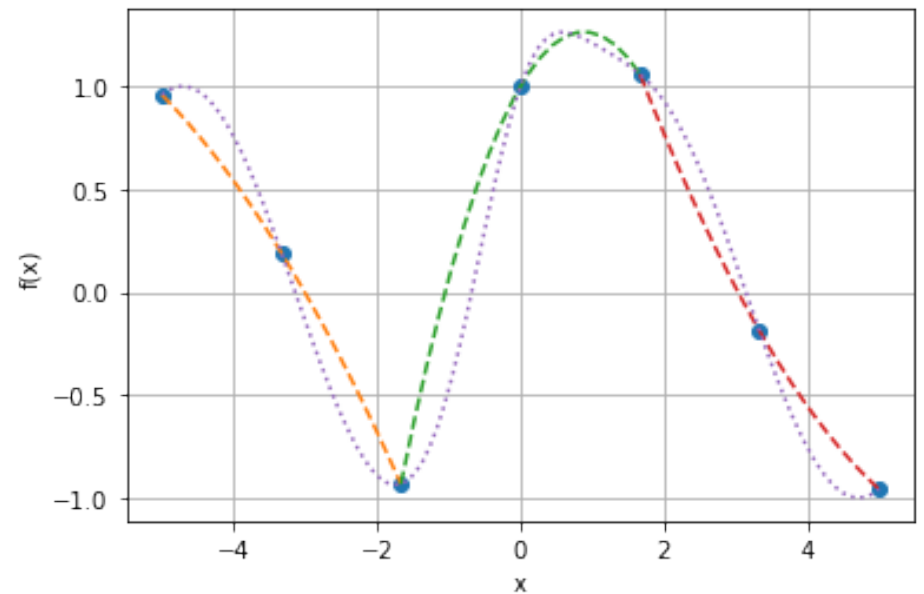
# Finite differencing - relation to Lagrange polynomials

We fit a polynomial of order  $N-1$  to the  $N$  points we want to use in the stencil.

This function that fits all the points is just an order  $N$  polynomial, whose coefficients are combinations of the function values at each point and the points themselves

e.g. for 3 points separated by a distance  $dx$ :

$$T = (-f_1(x - x_2)(dx - x + x_2) + 2f_2(dx - x + x_2)(dx + x - x_2) + f_3(x - x_2)(dx + x - x_2)) / (2dx^2)$$



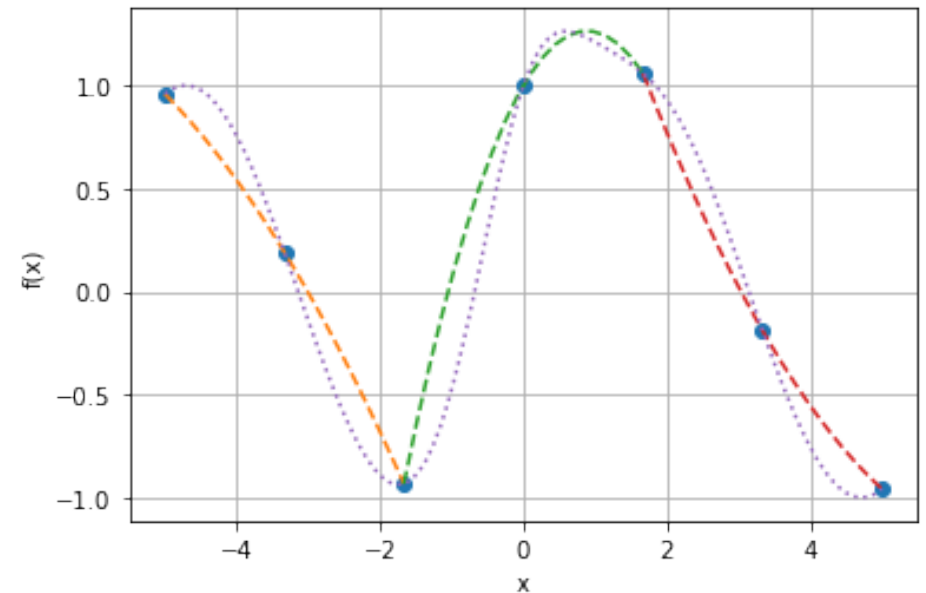
# Finite differencing - relation to Lagrange polynomials

We can take the derivative of this polynomial

$$\frac{dT}{dx} = (-dx f_1/2 + dx f_3/2 + xf_1 - x_2 f_1 - 2xf_2 + 2f_2 x_2 + xf_3 - x_2 f_3)/dx^2 + O(dx^2)$$

And evaluate it at  $x = x_2$

$$\left. \frac{dT}{dx} \right|_{x=x_2} = \frac{(f_3 - f_1)}{2dx} + O(dx^2)$$

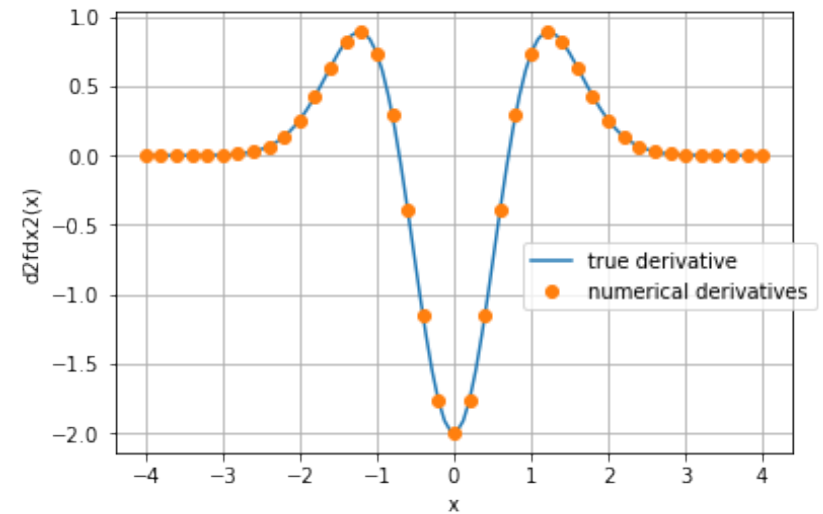


# Finite differencing - relation to Lagrange polynomials

This will give us a stencil for the function values to apply at  $x_2$

$$\left. \frac{dT}{dx} \right|_{x=x_2} = \frac{(f_3 - f_1)}{2dx} + O(dx^2)$$

|                |       |               |
|----------------|-------|---------------|
| $f_1$          | $f_2$ | $f_3$         |
| $\uparrow$     |       |               |
| $-1/(2 \, dx)$ | 0     | $1/(2 \, dx)$ |



# Finite differencing - general number of points

The MIT finite difference calculator is a useful resource for working out the stencil for a general collection of **equally spaced** points, up to any derivative order.

For non equally spaced points thing get a lot more complicated, and may also depend on the position.

## Finite Difference Coefficients Calculator

What is this?

Locations of Sampled Points

-2,-1,0,1,2

Derivative Order

2

Finite Difference Equation

$$\frac{\partial^{(2)} f}{\partial x^{(2)}} \approx \frac{-1f(x-2h) + 16f(x-h) - 30f(x+0h) + 16f(x+1h) - 1f(x+2h)}{12h^2}$$

Python Code

```
f_xx = (-1*f[i-2]+16*f[i-1]-30*f[i+0]+16*f[i+1]-1*f[i+2])/(12*1.0*h**2)
```

How does it work?

How can I cite this tool?

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3. ~~Numerical differentiation – finite differencing~~
4. Numerical differentiation - pseudospectral methods
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# Numerical differentiation - pseudospectral method

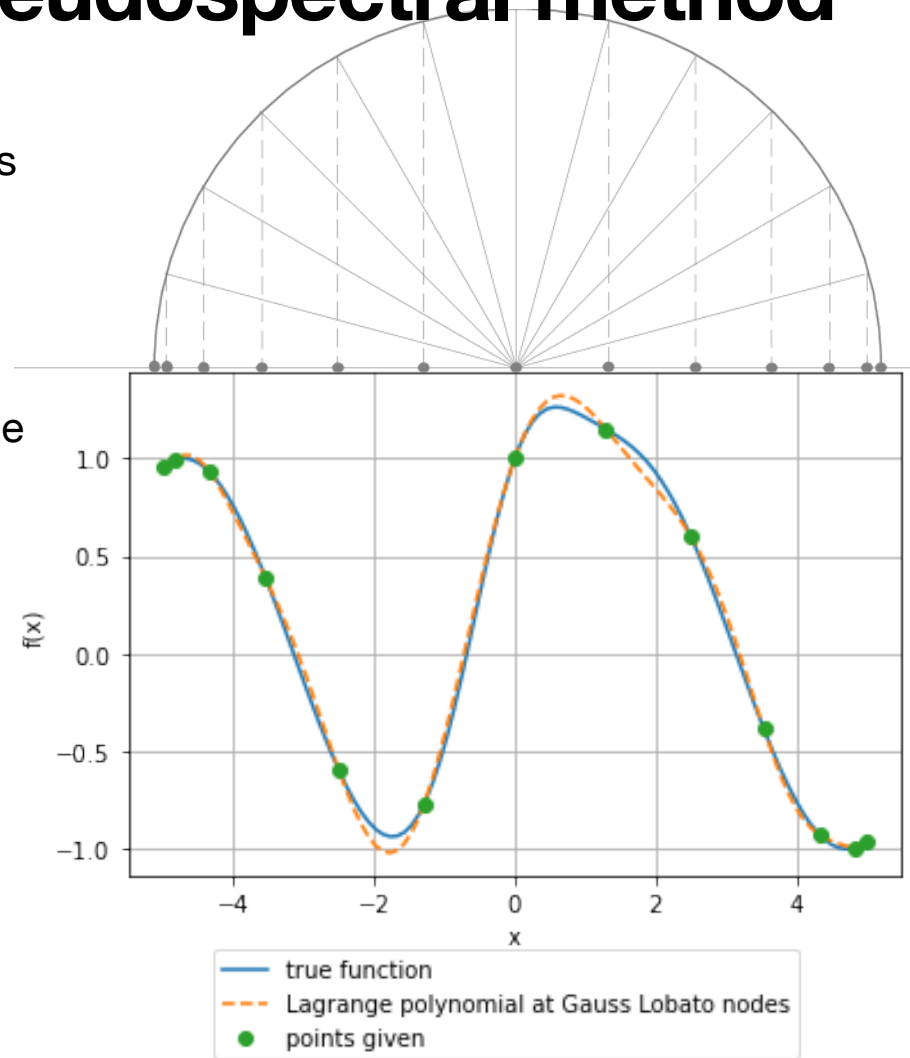
We can apply the same Lagrange method to find the stencils for the Chebyshev polynomials used in the Pseudospectral method.

The complication is that the order of the polynomial is now  $N-1$  where  $N$  is the number of points. Now all the values of the function at every point are used in the stencil, not just the neighbouring ones, and the grid spacing is not equal so the factors don't cancel nicely.

|                   |                    |           |
|-------------------|--------------------|-----------|
| $f_1$             | $f_2$              | $f_3$     |
| $3x_3^2 + x_2x_1$ | $3x_1x_3 + 2x_1^2$ | $2x_2x_1$ |

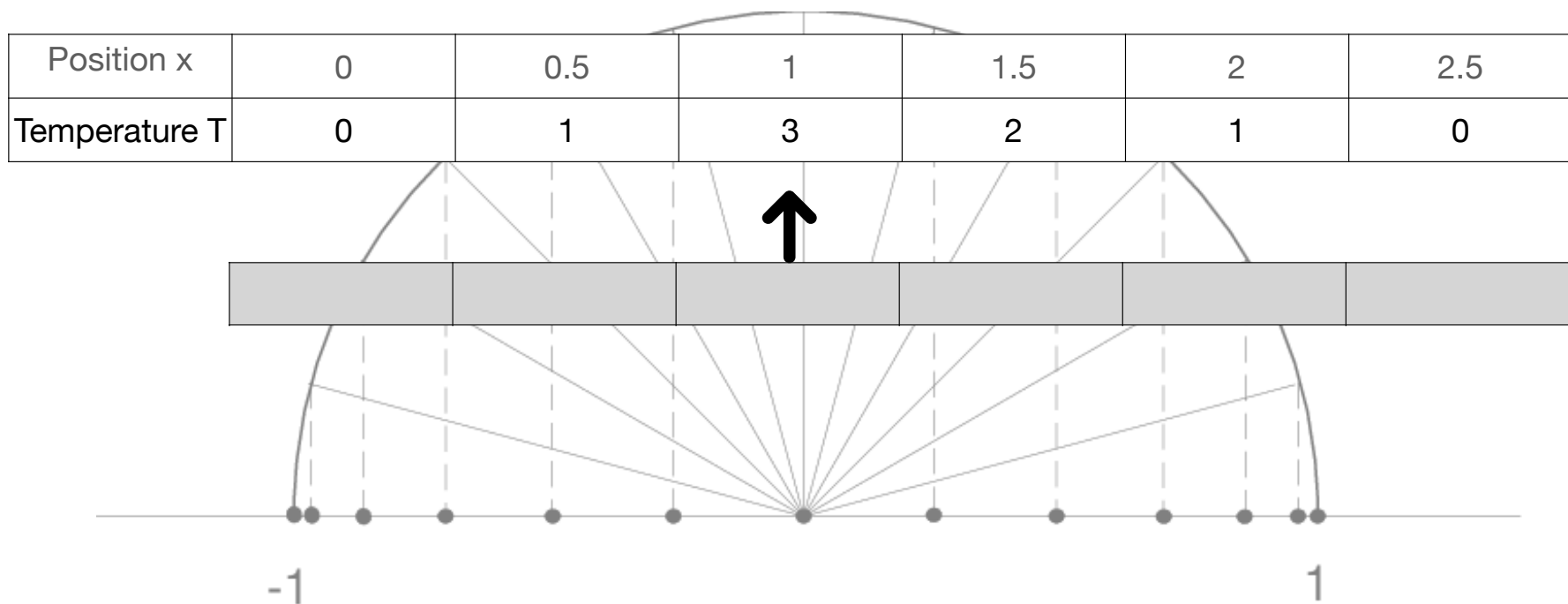


*Made up complicated looking stencil*



# Pseudospectral method - stencil representation

Now the stencil includes all the points in the grid, and is a bit more complicated to work out, but the principle is the same!



# Pseudospectral methods - matrix representation

The simplest thing is to represent the derivatives in matrix form:

|               |   |     |   |     |   |     |
|---------------|---|-----|---|-----|---|-----|
| Position x    | 0 | 0.5 | 1 | 1.5 | 2 | 2.5 |
| Temperature T | 0 | 1   | 3 | 2   | 1 | 0   |

$DT/dx$ 

|    |
|----|
| 2  |
| 3  |
| 1  |
| -2 |
| -2 |
| -2 |

=

Chebyshev Spectral Differentiation

**Theorem 8.4.** Let  $N \geq 1$  be any integer. The first-order spectral differentiation matrix  $D_N$  has entries

$$(D_N)_{00} = \frac{2N^2+1}{6}, \quad (D_N)_{NN} = -\frac{2N^2+1}{6},$$

$$(D_N)_{jj} = \frac{-x_j}{2(1-x_j^2)} \quad \text{for } 1 \leq j \leq N-1,$$

$$(D_N)_{ij} = \frac{c_i}{c_j} \frac{(-1)^{i+j}}{x_i-x_j} \quad \text{for } i \neq j.$$

Trefethen 1994

•

|   |
|---|
| 0 |
| 1 |
| 3 |
| 2 |
| 1 |
| 0 |

Matrix D

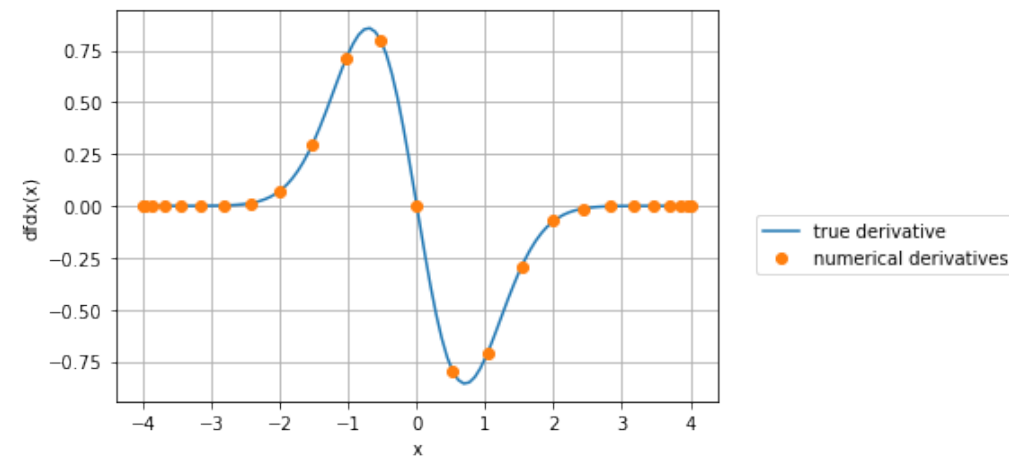
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# Pseudospectral methods - matrix representation

In the tutorial (and the coursework) this matrix will be provided to you, but you need to know how to use it.

```
def get_pseudospectral_first_derivative_matrix(N) :  
    indices = np.arange(N+1)  
    u_i = np.cos(np.pi * indices / N)  
    c_i = np.ones_like(indices)  
    c_i[0] = 2.0  
    c_i[N] = 2.0  
  
    D_matrix = np.zeros([N+1,N+1])  
  
    for idx_i in indices :  
        for idx_j in indices :  
            if (idx_i == 0 and idx_j == 0) :  
                D_matrix[idx_i,idx_j] = (2.0 * N * N + 1.0)/6.0  
  
            elif (idx_i == N and idx_j == N) :  
                D_matrix[idx_i,idx_j] = -(2.0 * N * N + 1.0)/6.0  
  
            elif (idx_i == idx_j) :  
                D_matrix[idx_i,idx_j] = - u_i[idx_i] / 2.0 / (1.0 - u_i[idx_i] * u_i[idx_i])  
  
            else :  
                D_matrix[idx_i,idx_j] = (c_i[idx_i] / c_i[idx_j] * (-1)**(idx_i+idx_j)  
                    / (u_i[idx_i] - u_i[idx_j]))  
  
    # Fix numerical errors when function flat  
    for idx_i in indices :  
        D_matrix[idx_i,idx_i] = 0  
        for idx_j in indices :  
            if (idx_j != idx_i) :  
                D_matrix[idx_i,idx_i] += -D_matrix[idx_i,idx_j]  
  
    return D_matrix
```



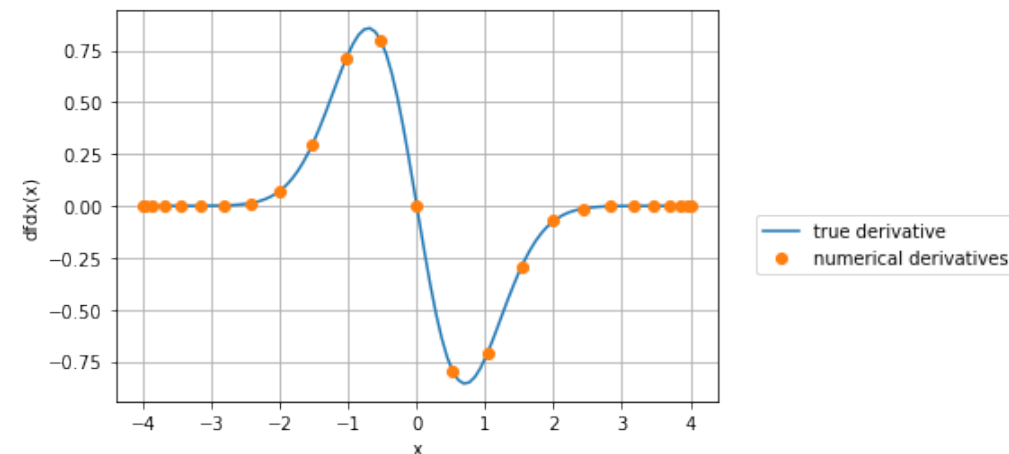
# Pseudospectral methods - matrix representation

The main thing to remember is that the matrix is specific to the number of points used. It also needs to be **rescaled** if the interval is not  $[-1, 1]$ .

```
# Testing the first derivatives
N = 24
a = -4
b = 4

# Find the Gauss Lobato nodes
indices = np.arange(N+1)
u_points = np.cos(np.pi * indices / N)
x_points = (b - a)/2.0 * u_points + (a + b)/2.0
y_points = get_y_test_function(x_points)

D_matrix = get_pseudospectral_first_derivative_matrix(N)
# Rescale from interval [-1, 1] to [a, b]
dydx = 2.0/(b - a) * np.dot(D_matrix, y_points)
```



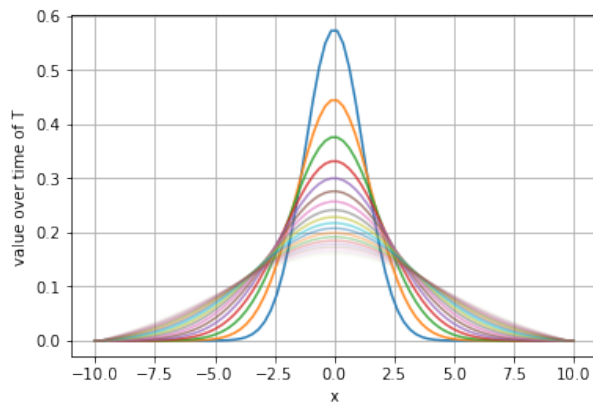
# Plan for today

1. ~~Motivation – solution of the heat equation~~
2. ~~Revision of last week's interpolation content~~
3. ~~Numerical differentiation – finite differencing~~
4. ~~Numerical differentiation – pseudospectral methods~~
5. Application - solution of the heat equation

# Application: solving the heat equation

- In the tutorial you will solve the heat equation using `solve_ivp()`

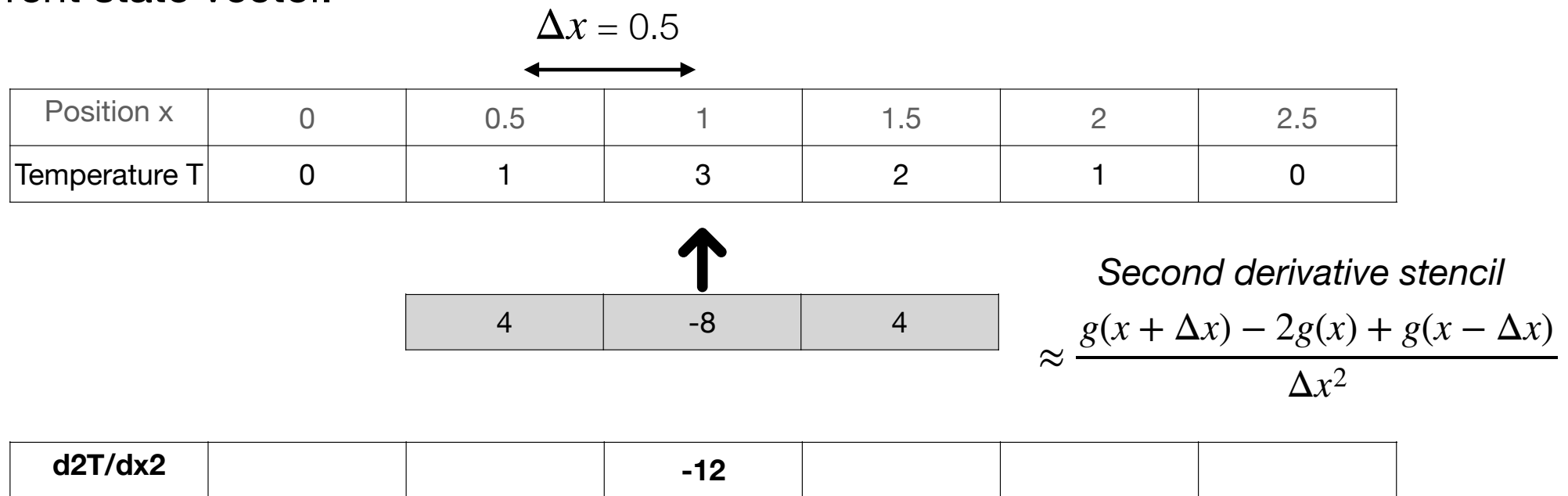
$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$



```
def calculate_dydt(self, t, current_state) :  
  
    # Just for readability  
    dTdt = np.zeros_like(current_state)  
  
    # Now actually work out the time derivatives  
    dTdt[:] = self.alpha * np.dot(self.D2_matrix, current_state)  
  
    # Zero the derivatives at the end for stability  
    # (especially important in the pseudospectral method)  
    dTdt[0] = 0.0  
    dTdt[1] = 0.0  
    dTdt[self.N_grid-1] = 0.0  
    dTdt[self.N_grid-2] = 0.0  
  
    return dTdt
```

# Derivatives - stencil representation

We can see *finite differencing* as the convolution of a stencil with the current state vector.



# Derivatives - matrix representation

Here we are using the matrix representation to calculate the time derivative

|               |   |     |   |     |   |     |
|---------------|---|-----|---|-----|---|-----|
| Position x    | 0 | 0.5 | 1 | 1.5 | 2 | 2.5 |
| Temperature T | 0 | 1   | 3 | 2   | 1 | 0   |

**$D2Tdx2$**        **$=$**        **$Matrix\ D^2$**        **$\bullet$**        **$T$**

|    |
|----|
| 2  |
| 3  |
| 1  |
| -2 |
| -2 |
| -2 |

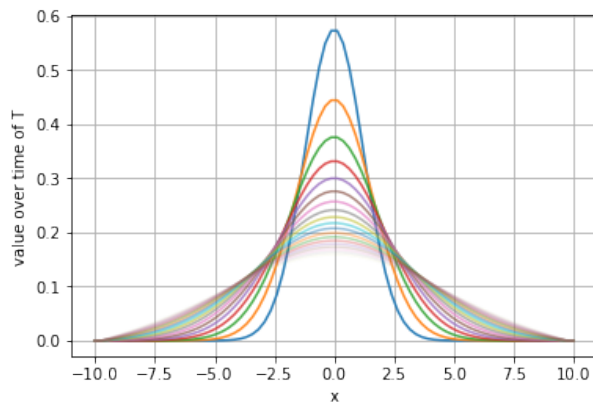
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| X | X |   |   |   |   |
| X | X | X |   |   |   |
|   | X | X | X |   |   |
|   |   | X | X | X |   |
|   |   |   | X | X | X |
|   |   |   |   | X | X |

|   |
|---|
| 0 |
| 1 |
| 3 |
| 2 |
| 1 |
| 0 |

# Application: solving the heat equation

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$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$



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