Phys 222 - class exercises report

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1 Lagrange Interpolation

Given an order n, to construct a curve between every 2 consecutive points, we want to evaluate this:

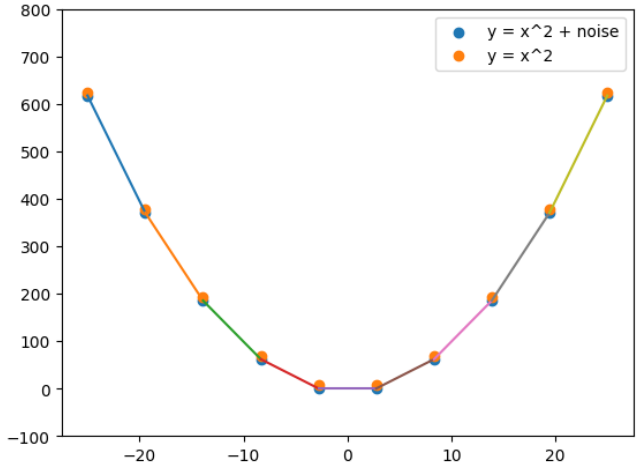
$$y = \sum_{j=0}^{n} f(x_j) \prod_{j=0}^{n} \frac{x - x_m}{x_j - x_m}$$

where $m \neq j$.

1.1 First order Lagrange interpolation.

code:

```
x = np.linspace(-25,25, 10)
noise = 1.5*np.random.randint(-10, 10)
y = x**2 + noise
y1 = x**2
plt.scatter(x, y, label = "y = x^2 + noise")
plt.scatter(x, y1, label = "y = x^2")
for i in range(0, len(x)-1):
    x1 = x[i]
    x2 = x[i+1]
    y1 = y[i]
    y2 = y[i+1]
    j = 1 # order
    i = np.linspace(x1,x2)
    p = y1 * ((i - x2)/(x1 - x2)) + y2 *((i-x1)/(x2-x1))
    plt.plot(i,p)
plt.ylim(-100, 800)
plt.legend()
plt.show()
```



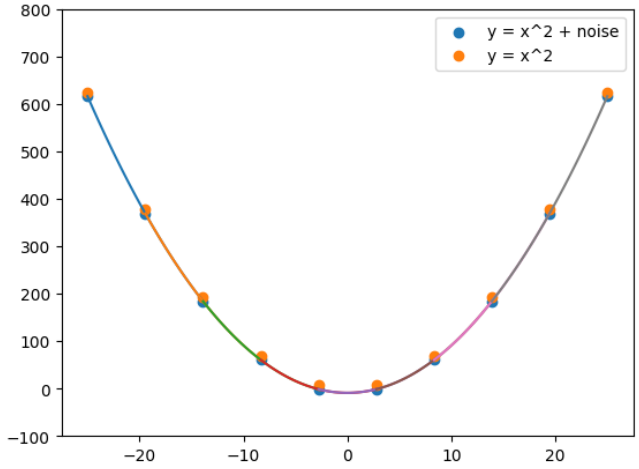
notes.

Each line passes by 2 consecutive data points and the collection of the lines forms an approximation, a bad one, of the function.

1.2 Second order Lagrange interpolation.

code:

```
x = np.linspace(-25,25, 10)
noise = 1.5*np.random.randint(-10, 10)
y = x**2 + noise
y1 = x**2
plt.scatter(x, y, label = "y = x^2 + noise")
plt.scatter(x, y1, label = "y = x^2")
for i in range(0, len(x)-2):
    x1 = x[i]
    x2 = x[i+1]
    x3 = x[i+2]
    y1 = y[i]
    y2 = y[i+1]
    y3 = y[i+2]
    j = 2 # order
    i = np.linspace(x1, x3)
    p = y1 * ((i - x2)/(x1 - x2))*((i-x3)/(x1-x3)) +
y2 *((i-x1)/(x2-x1))*((i-x3)/(x2-x3)) +
y3*((i-x2)/(x3-x2))*((i-x1)/(x3-x1))
    plt.plot(i,p)
plt.ylim(-100,800)
plt.legend()
plt.show()
```



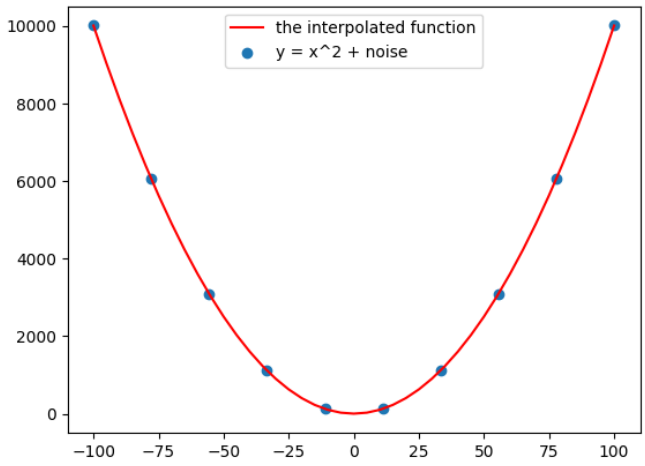
notes.

Looping over my data points and using 3 points at a time in the Lagrange polynomials gave me a decent, almost perfect, approximation of the function.

1.3 Defining the order as the number of data points - 1.

code:

```
x = np.linspace(-100,100, 10)
y = x**2 + 1.5*np.random.randint(-20,20)
y1 = x**2
j = len(x) - 1 # order
x_given_int = []
y_we_seek_int = []
for i in np.arange(x[0], x[len(x)-1], 5):
    x_given = i
    x_given_int.append(x_given)
    y_we_seek = 0
    for i in range(j+1):
        p =1
        for j in range(j+1):
            if j != i:
                p *= ((x_given - x[j])/(x[i] - x[j]))
        y_we_seek += y[i]*p
    y_we_seek_int.append(y_we_seek)
plt.plot(x_given_int, y_we_seek_int, color = "r", label = "the interpolated function")
plt.scatter(x,y, label = "y = x^2 + noise")
plt.scatter(x,y1, label = "y = x^2")
plt.legend()
plt.show()
```



notes.

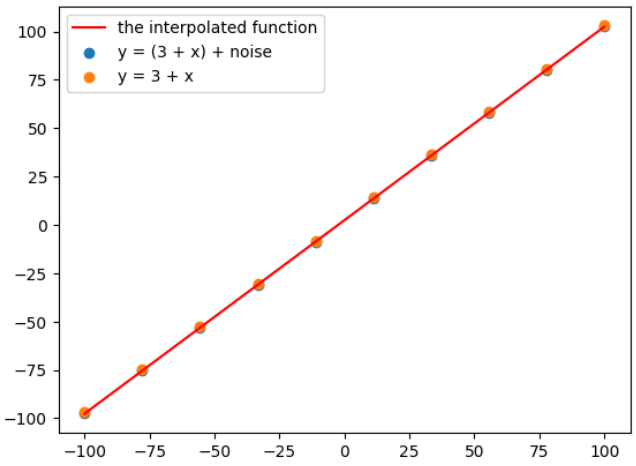
I figured here to go to the highest order which is equal to the number of my data points - 1 and fill the points between each 2 consecutive data points. I stored the "given x" points in an array that represents points between 2 consecutive data points and the corresponding "expected y" points that I got from the interpolation and then plotted the function.

1.4 Trying the above on a linear function.

code:

```
x = np.linspace(-100,100, 10)
y = 3 + x + 0.2*np.random.randint(-20,20)
y1 = 3 + x
j = len(x) - 1 # order
x_given_int = []
y_we_seek_int = []
for i in np.arange(x[0], x[len(x)-1], 5):
    x_given = i
    x_given_int.append(x_given)

    y_we_seek = 0
    for i in range(j+1):
        p =1
        for j in range(j+1):
            if j != i:
                p *= ((x_given - x[j])/(x[i] - x[j]))
        y_we_seek += y[i]*p
    y_we_seek_int.append(y_we_seek)
plt.plot(x_given_int, y_we_seek_int, color = "r", label = "the interpolated function")
plt.scatter(x,y, label = "y = (3 + x) + noise")
plt.scatter(x,y1, label = "y = 3 + x")
plt.legend()
plt.show()
```



notes.

I wanted to see if higher orders also work on simple linear functions.

2 Aitken - Neville Interpolation

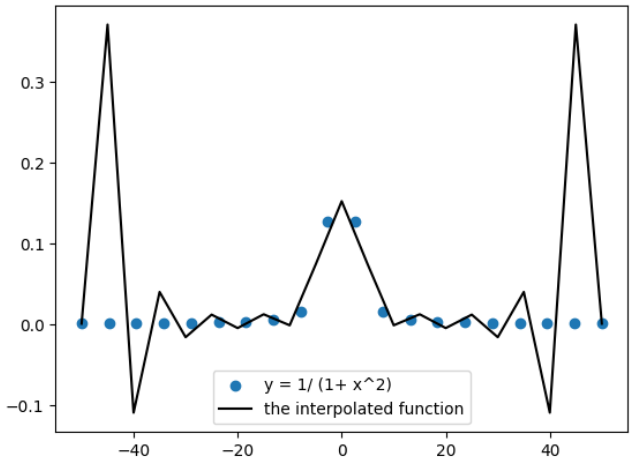
Using the Lagrange polynomials in a recursive way.

2.1 For y = $\frac{1}{1+x^2}$

code:

```
x = np.linspace(-50,50, 20)
y = 1 / (1 + x**2)
def AN(x, x_given, y, initial, final):
     if initial == final:
         ans = y[final]
     else:
        ans =
        (x_given-x[final])/(x[initial] - x[final]) *
        AN(x,x_given, y,initial, final -1 ) +
        (x_given-x[initial])/(x[final] - x[initial]) *
        AN(x,x_given,y, initial +1, final)
     return ans
x_given = 0
x_given_int = []
y_expected = []
for i in np.arange(x[0], x[len(x) - 1] + 1, 5):
        x_given = i
        x_given_int.append(x_given)
        y_expected.append(AN(x, x_given, y, 0, 19))
plt.scatter(x,y, label = "y = 1/ (1+ x^2)")
plt.plot(x_given_int, y_expected, color = "k", label = "the interpolated function")
plt.legend()
```

```
plt.show()
```



notes.

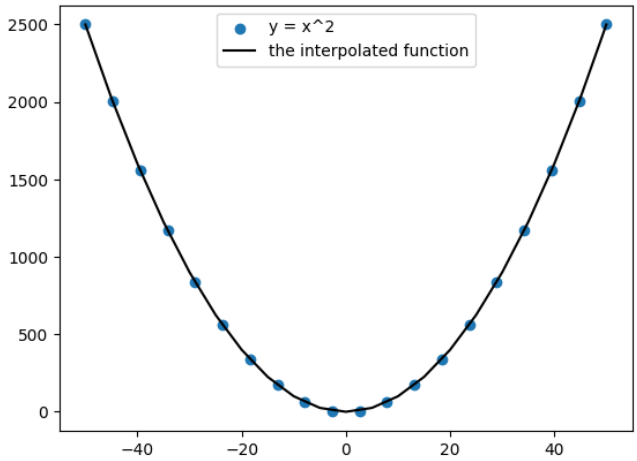
I took the order to be equal to the number of my data points - 1. The interpolated function seems to be a good approximation of the original function but only in a small interval around x = 0, on the edges, we notice unwanted oscillations with big magnitude.

2.2 For $y = x^2$

code:

```
x = np.linspace(-50,50, 20)
y = x**2 + 0.2
def AN(x, x_given, y, initial, final):
     if initial == final:
         ans = y[final]
     else:
        ans =
        (x_given-x[final])/(x[initial] - x[final]) *
        AN(x,x_given, y,initial, final -1 ) +
        (x_given-x[initial])/(x[final] - x[initial]) *
        AN(x,x_given,y, initial +1, final)
     return ans
x_given = 0
x_given_int = []
y_expected = []
for i in np.arange(x[0], x[len(x) - 1] + 1, 5):
        x_given = i
        x_given_int.append(x_given)
        y_expected.append(AN(x, x_given, y, 0, 19))
plt.scatter(x,y, label = "y = x^2")
plt.plot(x_given_int, y_expected, color = "k", label = "the interpolated function")
```

```
plt.legend()
plt.show()
```



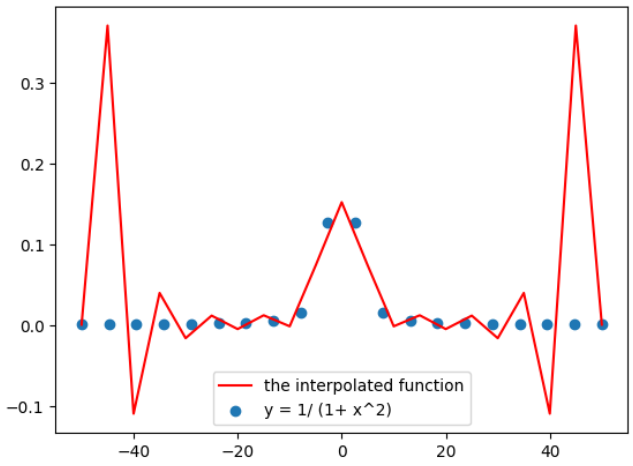
notes.

To make sure that the Aitken Neville code works, I used it on the data points that I used Lagrange interpolation on. The interpolated function is a perfect approximation for this function meaning the unwanted oscillations don't always occur (at least not for simple functions) and my code works fine.

2.3 Trying Lagrange interpolation on $y = \frac{1}{1+x^2}$

code:

```
x = np.linspace(-50,50, 20)
y = 1 / (1+x**2)
j = len(x) - 1 # order
x_given_int = []
y_we_seek_int = []
for i in np.arange(x[0], x[len(x)-1] +1, 5):
    x_given = i
    x_given_int.append(x_given)
    y_we_seek = 0
    for i in range(j+1):
        p =1
        for j in range(j+1):
            if j != i:
                p *= ((x_given - x[j])/(x[i] - x[j]))
        y_we_seek += y[i]*p
    y_we_seek_int.append(y_we_seek)
plt.plot(x_given_int, y_we_seek_int, color = "r", label = "the interpolated function")
plt.scatter(x,y, label = "y = 1/ (1+ x^2)")
plt.legend()
plt.show()
```



notes.

I tried the Lagrange Interpolation on $y = \frac{1}{1+x^2}$ to make sure the oscillations were not an error in the Aitken Neville code. The results were exactly like in the Aitken Neville case. Meaning the higher order polynomials may lead to "over fitting".

3 Splines Interpolation

3.1 Quadratic splines.

Given n+1 data points, we can derive n equations of the curves between each 2 consecutive points which gives us 2 evaluations, so we end up with 2n equations with 3n unknowns. We impose continuity conditions on these equations at the inner points (we want our fit to be smooth) which gives us n-1 equations. And, finally, we fix the first variable ($a_1 = 0$) such that the first curve would be linear.
We then solve for the 3n-1 equations to find the coefficients of the curves between each 2 consecutive data points:

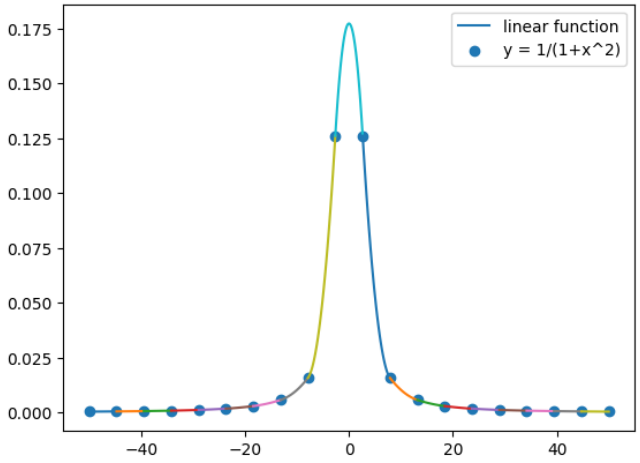
$$a_i x_{i-1}^2 + b_i x_{i_-1} + c_i = y_{i_-1} \quad \forall i \in [1, n]$$
$$a_i x_i^2 + b_i x_i + c_i = y_i \quad \forall i \in [1, n]$$
$$2a_i x_i - 2a_{i+1} xi + b_i - b_{i+1} = 0 \quad \forall i \in [1, n-1]$$

code:

```
x = np.linspace(-50,50, 20)
y = 1 / (1+ x**2)
n = len(x) - 1
x_matrix = np.zeros((3*n, 3*n))
y_matrix = np.zeros((3*n - 1, 1))
# fill 2n rows:
for i in range(0, 2*n -1, 2):
    row1 = []
    row2 = []
    for j in range(i - int(i/2)):
```

```
            row1.append(0)
            row1.append(0)
            row1.append(0)
            row2.append(0)
            row2.append(0)
            row2.append(0)
        row1.append(x[i-int(i/2)]**2)
        row1.append(x[i - int(i/2)])
        row1.append(1)
        row2.append(x[i-int(i/2) + 1 ]**2)
        row2.append(x[i-int(i/2) + 1])
        row2.append(1)
        if len(row1) < 3*n:
            for o in range(3*n - len(row1)):
                row1.append(0)
                row2.append(0)
        x_matrix[i] = row1
        x_matrix[i+1] = row2
    # fill n -1 rows:
    for i in range(1, n):
        row = []
        for j in range(1, i):
            row.append(0)
            row.append(0)
            row.append(0)
        row.append(2*x[i])
        row.append(1)
        row.append(0)
        row.append(- 2* x[i])
        row.append(-1)
        if len(row) < 3*n:
            for o in range(3*n - len(row)):
                row.append(0)
        x_matrix[2*n - 1 + i] = row
    # last row of zeros
    # fill y matrix:
    y_matrix[0] = y[0]
    y_matrix[2*n - 1] = y[len(y) -1]
    for i in range(1, 2*n -1, 2):
        y_matrix[i] = y[i + 1 - int((i+1)/2)]
        y_matrix[i+1] = y[i + 1 - int((i+1)/2)]
    x_matrix = np.delete(x_matrix, obj = 0, axis = 1)
    x_matrix = np.delete(x_matrix, obj = 3*n - 1, axis = 0)
    unknown_matrix = np.linalg.solve(x_matrix, y_matrix)
    # a1 = 0
    i = np.linspace(x[0], x[1])
    j = unknown_matrix[0]*i + unknown_matrix[1]
    plt.plot(i,j, label = "linear function")
    for i in range(1, n):
```

```
        o = np.linspace(x[i], x[i+1])
        l = unknown_matrix[3*i - 1] * o**2 +
        unknown_matrix[3*i] * o + unknown_matrix[3*i + 1]
        plt.plot(o,l)
plt.scatter(x,y, label = "y = 1/(1+x^2) + noise")
plt.legend()
plt.show()
```



notes.

I constructed a 5×5 matrix by hand and noticed a pattern that I used in the code to construct any $3n \times 3n$ matrix (the x matrix). then I removed the first column and last row. Did the same for the y matrix then solved for the unknown matrix. I then plotted the linear function relating the first 2 points (I set $a_1 = 0$) and looped over each 2 consecutive points to plot the second order functions. (i want to try cubic and n order spline)

4 L2 Optimization using Vandermonde matrix

Given n+1 data points and a polynomial of order m:

$$P_m(x) = \sum_{i=0}^{m} a_i x^i$$

We introduce the sum of the square of the deviations:

$$\chi^2 = \sum_{i=0}^{n} \left[p_m(x_i) - f(x_i)\right]^2$$

We want to find the coefficients that would minimize the deviations of a global fit approximation $p_m(x)$ of the initial function $f(x)$. To do that, we set the derivatives of χ^2 wrt the coefficients to be 0:

$$\frac{\partial \chi^2}{\partial a_i} = 0$$

Alternatively, we set the Valindrome matrix which is a (nb of points $\times$ order) matrix :

$$V = \begin{pmatrix} x_0^n & x_0^{n-1} & ... & x_0 & 1 \\ x_1^n & x_1^{n-1} & ... & x_1 & 1 \\ . & . & . & . & . \\ . & . & . & . & . \end{pmatrix}$$

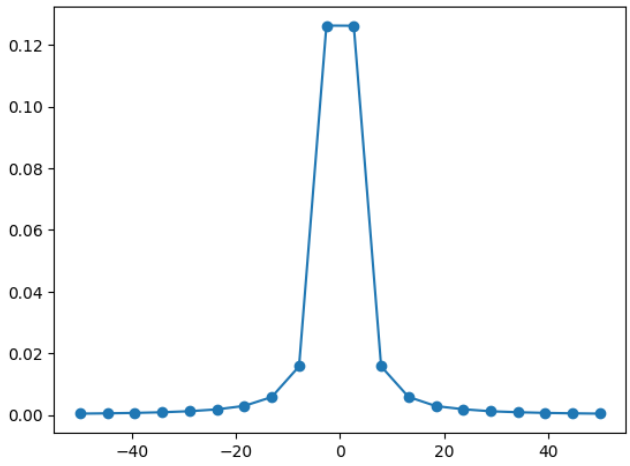
We want to solve this system:

$$\begin{pmatrix} x_0^n & x_0^{n-1} & ... & x_0 & 1 \\ x_1^n & x_1^{n-1} & ... & x_1 & 1 \\ . & . & . & . & . \\ . & . & . & . & . \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ . \\ . \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ . \\ . \end{pmatrix}$$

The solution would be $A = (V^T V)^{-1} V^T y$. And then we plug in the coefficients we found in the global fit.

code:

```
x = np.linspace(-50,50,20)
y = 1/(1+x**2)
n = len(x)
order = 18
v = np.zeros((n, order+1))
for i in range(n):
    row = []
    for j in range(order+1):
        row.append(x[i])
    v[i] = row
exp = []
for i in range(order, -1, -1):
    exp.append(i)
v = v ** exp
v_new = np.transpose(v) @ v
y_matrix = np.transpose(v) @ y
coef_matrix = np.linalg.solve(v_new, y_matrix)
p = 0
for i in range(order+1):
    p += coef_matrix[len(coef_matrix) - (i+1)]* x**i
plt.plot(x, p)
plt.scatter(x,y)
plt.show()
```



notes.

The optimal order of the global fit polynomial is dependent on the number of my data points, at least for complex functions like $y = \frac{1}{1+x^2}$. However, for less complex functions like $y = x^2$, order 2 is perfect (which is expected).

5 Testing vs Training errors

(still working on it)

6 Approximating Derivatives

We start with a Taylor series expansion of our function about a point x_0 (the point at which we want to find the derivative):

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \frac{f'''(x_0)}{3!}(x - x_0)^3 + O(h^4)$$

Approximating the first derivative

First try: we cut the series at the first order and we get

$$f'(x_0) = \frac{f(x) - f(x_0)}{h} + O(h)$$

where $h = x - x_0$ represents the distance from x to the nearest point on its left or right. This 1st order approximation requires 1 extra data point (x) only.

Second try: we cut the series at the second order and we introduce

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x) + O(h^3)$$

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2}f''(x) + O(h^3)$$

subtracting them, we get

$$f(x_0+h)-f(x_0-h)=2hf'(x_0)+O(h^3)$$

and hence

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

For this 2nd order approximation, we need 2 points at an equal distance h from x_0 (x_0+h and x_0-h).

Third try: we cut the series at the third order and we introduce

$$f(x_0+2h)=f(x_0)+2hf'(x_0)+\frac{4h^2}{2}f''(x)+\frac{8h^3}{6}+O(h^4)$$

$$f(x_0-2h)=f(x_0)-2hf'(x_0)+\frac{4h^2}{2}f''(x)-\frac{8h^3}{6}f'''(x_0)+O(h^4)$$

subtracting them we get

$$f(x_0+2h)-f(x_0-2h)=4hf'(x_0)+\frac{8h^3}{3}f'''(x_0)+O(h^5)$$

to find the $f'''(x_0)$ term, we return to

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

hence

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

replacing, we get

$$f(x_0+2h)-f(x_0-2h)=4hf'(x_0)+8f(x_0+h)-8f(x_0-h)-16hf'(x_0)+O(h^5)$$

and finally

$$f'(x_0)=\frac{f(x_0-2h)-f(x_0+2h)-8f(x_0-h)+8f(x_0+h)}{12h}+O(h^4)$$

For this 4th order approximation, we need 4 points at equal distances from x_0 (x_0+h, x_0-h, x_0+2h and x_0-2h).

Tao: We can, of course, make the accuracy even higher by including more points, but in many cases this is not good practice. For real problems, the derivatives at points close to the boundaries are important and need to be calculated accurately. The errors in the derivatives of the boundary points will accumulate in other points when the scheme is used to integrate an equation. The more points involved in the expressions of the derivatives, the more difficulties we encounter in obtaining accurate derivatives at the boundaries. Another way to increase the accuracy is by decreasing the interval h.

Approximating the second derivative

1D Grid:

We use $f(x_0+h)+f(x_0-h)=2f(x_0)=h^2f''(x_0)+O(h^4)$, and we find

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

which we can represent in a matrix form

$$\nabla^2=\begin{pmatrix} . & . & . & . & . & . & . & . & . \\ 0 & 0 & \cdots & 1 & -2 & 1 & 0 & 0 & \cdots \\ 0 & 0 & \cdots & 0 & 1 & -2 & 1 & 0 & \cdots \\ 0 & 0 & \cdots & 0 & 0 & 1 & -2 & 1 & \cdots \\ . & . & . & . & . & . & . & . & . \end{pmatrix}\begin{pmatrix} . \\ f(x_0+h) \\ f(x_0) \\ f(x_0-h) \\ . \end{pmatrix}=-D+A$$

where D is a diagonal matrix called the degree matrix. And A denotes the equally spaced neighbor points. For our purposes, the Laplacian is used in the diffusion equation to describe how information diffuses in a network:

$$\frac{\partial C}{\partial t}=D\nabla^2C$$

To use this logic, we have to abandon the notion of the Euclidean distance and define a new meaning for "distance" in each context. For instance, if we want to study a Facebook network that includes 3 elements/users {R,S,G}, we can use a matrix notation to deduce the "distance" between each 2:

$$\begin{array}{c} \\ R \\ S \\ G \end{array}\begin{array}{c} \begin{array}{ccc} R & S & G \end{array} \\ \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \end{array}$$

where 1 represents a connection on Facebook (they follow each other). The "distance" between R and G is of magnitude 1 since they are directly connected. And the "distance" between R and S is of magnitude 2 since R is connected to G and G is connected to S.
Back to the diffusion equation, it is a linear heat equation (linear evolution equation) whose solution is dependent on the eigenvalues of the Laplacian matrix and is of the form $\mathbf{C}(t)=e^{\lambda t}\mathbf{v}$.

Solution to the diffusion equtaion

I will be discussing this problem (for fun).
To solve a linear heat equation of the form $\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}$, we start with the elementary scalar ODE $\frac{\partial u}{\partial t}=\lambda u$ where λ is a scalar. We know the solution is of the form $u(t)=ce^{\lambda t}$.
Applying this logic in the case when we have $\frac{\partial \mathbf{u}}{\partial t}=A\mathbf{u}$ where A is an $n\times n$ matrix (the Laplacian matrix), we suggest (by analogy with the previous case) the ansatz $\mathbf{u}(t)=e^{\lambda t}\mathbf{v}$. Differentiating wrt time, we get the condition $A\mathbf{v}=\lambda\mathbf{v}$ which is an eigenvalue problem that has a nonzero solution $\mathbf{v}\neq 0$ if and only if λ is an eigenvalue of A and $\mathbf{v}$ a corresponding eigenvector.
Note that if ∇^2 has 2 eigenvalues, the physical meaning of the largest one is the speed of diffusion and the smallest one is the relaxation time (time needed for the information to reach the whole network).

2D Grid:

For higher dimensions, specifically working with 2 dimensions here, the formula for the second derivative becomes

$$f''(x_0, y_0) = \frac{f(x_0 + h, y_0) - 4f(x_0, y_0) + f(x_0 - h, y_0) + f(x_0, y_0 + h) + f(x_0, y_0 - h)}{h^2}$$

which now requires 4 neighboring points (2 to the left and right of x_0 and 2 above and below x_0). In general, the number of the required neighboring points for the second derivative is equal to 2^d where d is the number of dimensions.

Boundaries Problem

How to evaluate the derivatives at the boundary point?
For the first derivative, we can only use the first order approximation and use the point right before/after the boundary point. But if we want more precision or we want to calculate the second derivative (we need 2 neighboring points minimum), we manipulate the topology of the grid. we could fold the 1D grid (line) into a circle and we could fold the 2D grid in a way that it forms a torus.