Parte 02 - Deslocamento temporal da função de onda

a equação da função de onda completa:

$$i\hbar\frac{\partial\Psi}{\partial t} = \text{op } H\Psi$$

O opH é um operador de evolução temporal. Pode,ele, também assumir, a seguinte identidade matemática:

$$\text{op } U(\Delta t) = e^{\frac{-i\text{ op } H}{\hbar}}$$

Resultando, portanto, na solução, descrita abaixo:

$$\Psi(x, t+\Delta t) = e^{\frac{-i\text{ op } H\Delta t}{\hbar}} \cdot \Psi(x,t)$$

Podendo tratar o expoente de um operador, por meio de uma série infinita, tem-se:

$$e^{\frac{-i\text{ op } H\Delta t}{\hbar}} = \sum_n \frac{\left(\frac{-i\text{ op } H\Delta t}{\hbar}\right)^n}{n!}$$

In [156…

```
#Bibliotecas

import matplotlib.animation as animation
from IPython.display import HTML
import matplotlib.pyplot as plt
import scipy.fftpack as fft
import scipy.linalg as scl
import numpy as np
import math
%matplotlib widget
%matplotlib inline
```

O Halmitoniano no espaço:

$x_n = x_0 + n\Delta x$, com $\Delta x = \frac{(x_N - x_0)}{N}$

Os valores de entrada:

In [160…

```
hbar = 1
m = 1
N = 2**11
```

```
L = 200.0
step_low = 0.
step_high= 1.
V0 = 10.
```

Definição do espaço:

In [162…

```
n = np.arange(N)
x0 = -L/2.
xN = L/2.
Delta_x = (xN - x0)/N
print("Delta_x = ",Delta_x)

x = x0 + n*Delta_x
```

```
Delta_x =  0.09765625
```

Definição do potencial:

In [164…

```
V = np.zeros(N)
for i in range(N):
    if x[i]>= step_low and x[i]<= step_high:
        V[i]= V0
```

Configuração do Hamiltoniano para a função `V`, multiplicação com a matriz inversa:

In [166…

```
Mdd = 1./(Delta_x**2)*(np.diag(np.ones(N-1),-1)
                       - 2* np.diag(np.ones(N),0)
                       + np.diag(np.ones(N-1),1))
H = -(hbar*hbar)/(2.0*m)*Mdd + np.diag(V)

En,psiT = np.linalg.eigh(H)   # autovalores e os autovetores.
psi = np.transpose(psiT)      # Tomamos a transposta de psiT para os vetores de fun
                              # que podem ser acessados como psi[n]
```

Intervalo temporal

In [168…

```
dt_max = 2/np.max(En)      # Critério de estabilidade.
dt = 0.001
if dt > dt_max:
    print("ATENÇÃO: dt está na região instável!")
```

Função de onda inicial

In [170…

```
g_x0=-10.
g_k0=6.
g_sig=2.
```

Definição de um Gaussiano no espaço K, com $p = \hbar k$, um momento k_0, e o espaço x, $\psi(x,0) = \left(\frac{2L}{\pi}\right)^{1/4} \cdot e^{-Lx^2}$:

In [172…
```
def psi0(x,g_x0,g_k0,g_sig):
    _Norm_x=np.sqrt(Delta_x/g_sig)/(np.pi**0.25)

    return(_Norm_x*np.exp(-(x-g_x0)**2/(2.*g_sig*g_sig)+1j*g_k0*x))

psi_t0 = psi0(x,g_x0,g_k0,g_sig)
```

In [173…
```
# H é Hermitiano?
print("Verifique se H é realmente Hermitiano : ",np.array_equal(H.conj().T,H))
```

```
Verifique se H é realmente Hermitiano :  True
```

In [174…
```
Ut_mat = np.diag(np.ones(N,dtype="complex128"),0)

print("Criação de uma matriz U(dt = {})".format(dt))
for n in range(1,3):
    # Realiza a soma. Como se trata de matrizes, o processo irá demorar se N for gr
    Ut_mat += np.linalg.matrix_power((-1j*dt*H/hbar),n)/math.factorial(n)
```

```
Criação de uma matriz U(dt = 0.001)
```

In [175…
```
p = Ut_mat.dot(psi_t0)

print("O quanto a normalização muda por etapa? Desde {} até {}".format(np.linalg.no
print("Nº de etapas em que a norma está errada por um fator 2 : ",1/(np.linalg.norm
```

```
O quanto a normalização muda por etapa? Desde 1.0 até 1.0000000127814086
Nº de etapas em que a norma está errada por um fator 2 :  78238637.96537858
```

teste do movimento gaussiano:

In [177…
```
psi_t0 = psi0(x,g_x0,g_k0,g_sig)
psi_t1 = psi_t0
psi_tu = []

for t in range(3500):
    psi_t1 = Ut_mat.dot(psi_t1)
    if t>0 and t%500==0:
        psi_tu.append( (t,psi_t1))
psi_tu.append( (t,psi_t1))
```

Teste e verificação de coerência dos resultados:

$< E >$ = estado esperado da energia;

$< x >$ = estado esperado da posição

In [179…
```
print("Normalização : ",np.linalg.norm(psi_tu[-1][1]))

vev_E0=float(np.real(np.sum(np.conjugate(psi_t0)*H.dot(psi_t0))))
vev_x0=float(np.real(np.sum(np.conjugate(psi_t0)*x*psi_t0)))
```

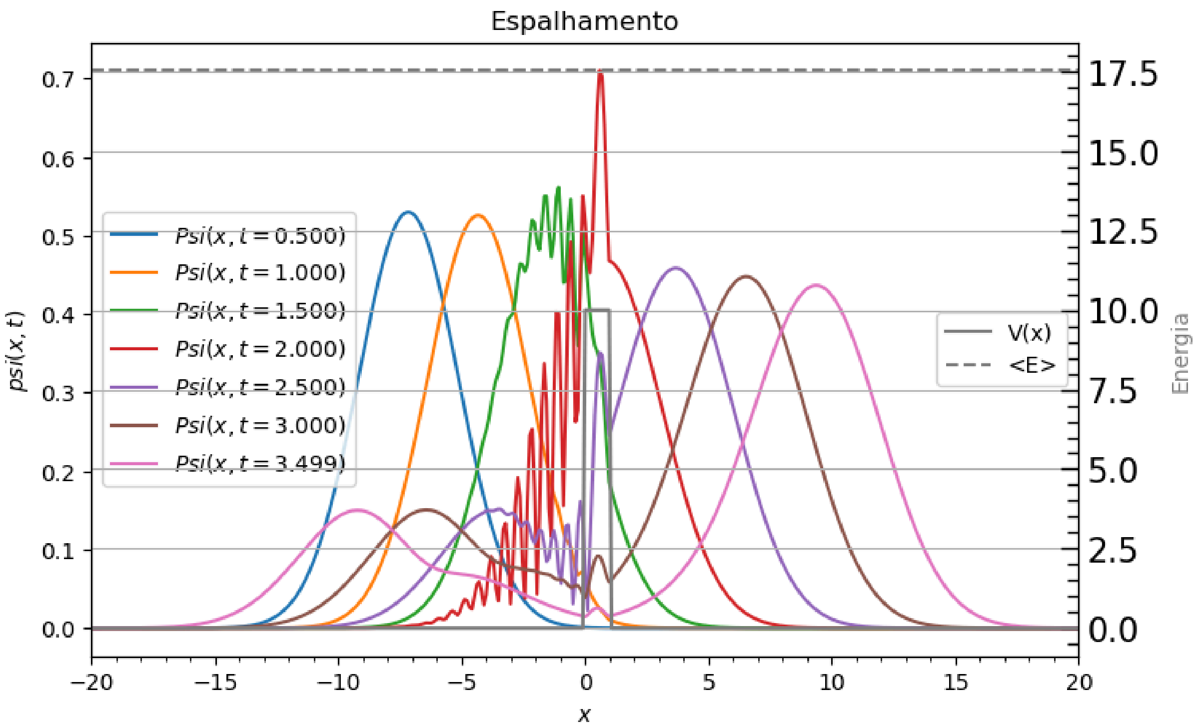
```python
print("<E_(t = 0)> = {:8.4f}  <x_(t = 0)> = {:8.4f}".format(vev_E0,vev_x0))

for t,p in psi_tu:
    norm = np.linalg.norm(p)
    vev_E1 = float(np.real(np.sum(np.conjugate(p)*H.dot(p))))
    vev_x1 = float(np.real(np.sum(np.conjugate(p)*x*p)))
    print("dt = {:7.1f}  norm = {:8.5f}  <E> = {:8.4f}  <x_(dt)> = {:8.4g}".format(
```

```
Normalização :  1.000044736361259
<E_(t = 0)> =  17.5429  <x_(t = 0)> = -10.0000
dt =   500.0  norm =  1.00001  <E> =  17.5432  <x_(dt)> =   -7.164
dt =  1000.0  norm =  1.00001  <E> =  17.5434  <x_(dt)> =   -4.335
dt =  1500.0  norm =  1.00002  <E> =  17.5436  <x_(dt)> =    -1.55
dt =  2000.0  norm =  1.00003  <E> =  17.5439  <x_(dt)> =   0.8044
dt =  2500.0  norm =  1.00003  <E> =  17.5441  <x_(dt)> =     2.91
dt =  3000.0  norm =  1.00004  <E> =  17.5443  <x_(dt)> =    5.103
dt =  3499.0  norm =  1.00004  <E> =  17.5446  <x_(dt)> =    7.305
```

Dos dados obtidos, resulta:

In [181…

```
def opt_plot():
    plt.minorticks_on()
    plt.tick_params(axis='both',which='minor', direction = "in",
                    top = True,right = True, length=5,width=1,
                    labelsize=15)
    plt.tick_params(axis='both',which='major', direction = "in",
                    top = True,right = True, length=8,width=1,
                    labelsize=15)



plt.figure(figsize=(8,5))

if vev_E0>max(V):
    plt.title('Espalhamento')
else:
    plt.title('Tunelamento')
plt.ylabel('$psi(x,t)$')
plt.xlabel('$x$')
# plt.plot(x,np.abs(psi_t0)/np.sqrt(Delta_x),label="$\Psi(x,t=0)$")

for t,p in psi_tu:

    plt.plot(x,np.abs(p)/np.sqrt(Delta_x),label="$Psi(x,t={:6.3f})$".format(t*dt))
    plt.legend(loc = 'center left')

ax1 = plt.twinx()
plt.plot(x,V,color="grey",label="V(x)")
plt.plot([x[0],x[N-1]],[vev_E0,vev_E0],color="grey",linestyle="--",label="<E>")
plt.ylabel("Energia",color="grey")
plt.xlim(g_x0-5*g_sig,-g_x0+5*g_sig)
plt.legend(loc='best')
plt.grid()
opt_plot()

plt.savefig('Estado deslocado.png')
```



In [182…

```
%time Ut_05s = np.linalg.matrix_power(Ut_mat,int(0.5/dt) )
```

```
CPU times: total: 7min 6s
Wall time: 2min
```

Repetição de tarefa

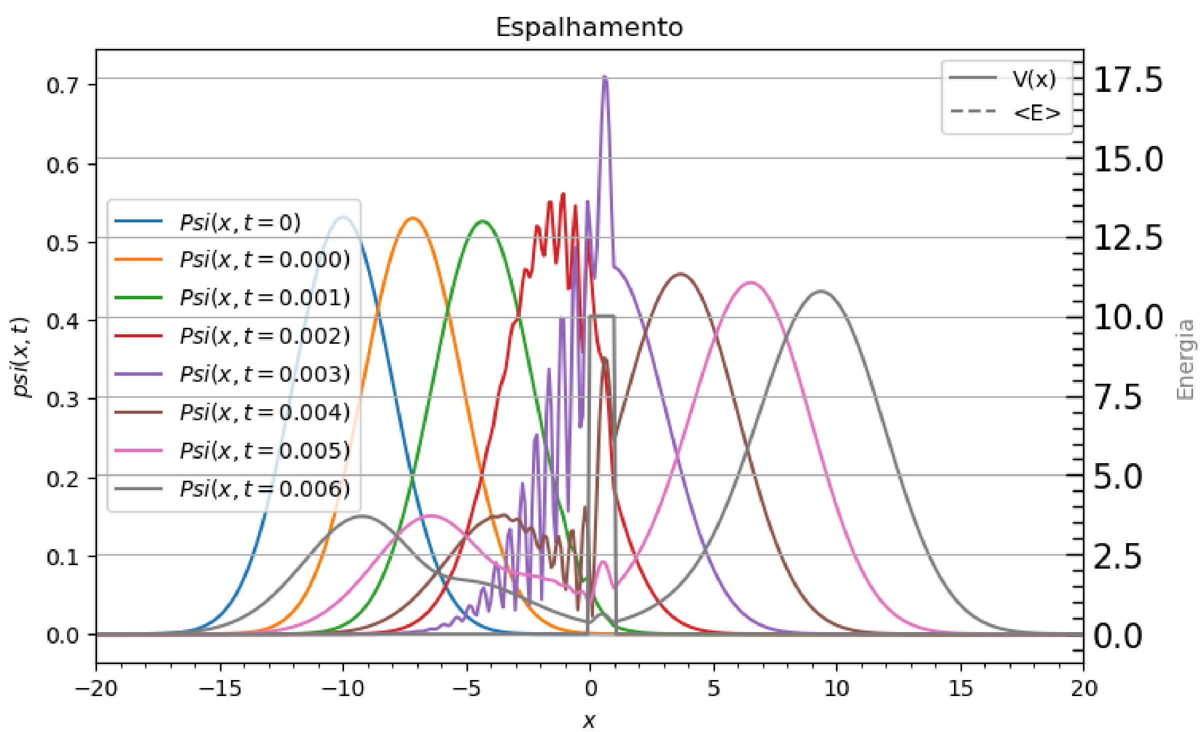
In [184…

```
psi_t0 = psi0(x,g_x0,g_k0,g_sig)
psi_t1 = psi_t0
psi_tu05 = []

for t in range(7):
    psi_t1 = Ut_05s.dot(psi_t1)
    psi_tu05.append( (t,psi_t1))
    # psi_tu.append( (t,psi_t1))
print("Start")
v1=[]
v2=[]
tm=[]
count=0
for t,p in psi_tu05:
    norm = np.linalg.norm(p)
    vev_E1 = float(np.real(np.sum(np.conjugate(p)*H.dot(p))))
    vev_x1 = float(np.real(np.sum(np.conjugate(p)*x*p)))
    v1.append(vev_E1)

    v2.append(vev_x1)
    tm.append(count)
    count=count+1
    print("dt = {:7.1f}  norm = {:8.5f}  <E> = {:8.4f}  <x_(dt)> = {:8.4g}".format(
```

```
Start
dt =     0.0  norm =  1.00001  <E> =  17.5432  <x_(dt)> =    -7.17
dt =     1.0  norm =  1.00001  <E> =  17.5434  <x_(dt)> =    -4.34
dt =     2.0  norm =  1.00002  <E> =  17.5436  <x_(dt)> =   -1.555
dt =     3.0  norm =  1.00003  <E> =  17.5439  <x_(dt)> =   0.8002
dt =     4.0  norm =  1.00003  <E> =  17.5441  <x_(dt)> =    2.905
dt =     5.0  norm =  1.00004  <E> =  17.5443  <x_(dt)> =    5.099
dt =     6.0  norm =  1.00004  <E> =  17.5446  <x_(dt)> =    7.305
```

In [185…

```python
plt.figure(figsize=(8,5))

if vev_E0>max(V):
    plt.title('Espalhamento')
else:
    plt.title('Tunelamento')
plt.ylabel('$psi(x,t)$')
plt.xlabel('$x$')
line, = plt.plot(x,np.abs(psi_t0)/np.sqrt(Delta_x),label="$Psi(x,t=0)$")

for t,p in psi_tu05:
    plt.plot(x,np.abs(p)/np.sqrt(Delta_x),label="$Psi(x,t={:6.3f})$".format(t*dt))
    plt.legend(loc='center left')

ax1 = plt.twinx()
plt.plot(x,V,color="grey",label="V(x)")
plt.plot([x[0],x[6]],[vev_E0,vev_E0],color="grey",linestyle="--",label="<E>")
plt.ylabel("Energia",color="grey")
plt.xlim(g_x0-5*g_sig,-g_x0+5*g_sig)
plt.legend(loc='best')
plt.grid()
opt_plot()

plt.savefig('Estado deslocado - Pré-computados.png')
```



Parte 3 - A Regressão Simbólica

In [187…

```
from sklearn.utils import check_random_state, shuffle
from gplearn.genetic import SymbolicRegressor
from sklearn.ensemble import RandomForestRegressor
from sklearn.tree import DecisionTreeRegressor
from sklearn.utils.random import check_random_state
from mpl_toolkits.mplot3d import Axes3D
from IPython.display import Image
import pydot
import graphviz
from sympy import *
import pandas as pd
```

Definição dos Operadores

In [189…

```
converter = {
    'sub': lambda x, y : x - y,
     'div': lambda x, y : x/y,
    'mul': lambda x, y : x*y,
    'add': lambda x, y : x + y,
    'neg': lambda x    : -x,
    'pow': lambda x, y : x**y,
    'sin': lambda x    : sin(x),
    'cos': lambda x    : cos(x),
    'inv': lambda x: 1/x,
    'sqrt': lambda x: x**0.5,
    'pow3': lambda x: x**3
}
```

Interpretação Probabilística Gaussiana da Distribuição Normal

$$N(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \cdot e^{-\frac{1}{2}\frac{(x-\mu)}{\sigma}^2}$$

:

In [191…

```
m1=[]
md=[]
count=0
tem=0
df=pd.DataFrame()
df2=pd.DataFrame()
xix=[]
df['v1']=v1
df2['v2']=v2

for i in v2:
    m1.append(i)
    tem=i-vev_x0
    md.append(tem**2)
```

```
df['m1']=md
df2['t']=tm



dp=2.83/3
A = [float(i) for i in m1]
for i in A:
    xix=np.linspace(-(3.*dp),(3.*dp),40)
    y=0.39*(2.76**(-0.5*(xix**2)))
```

A amostra acima, resulta:

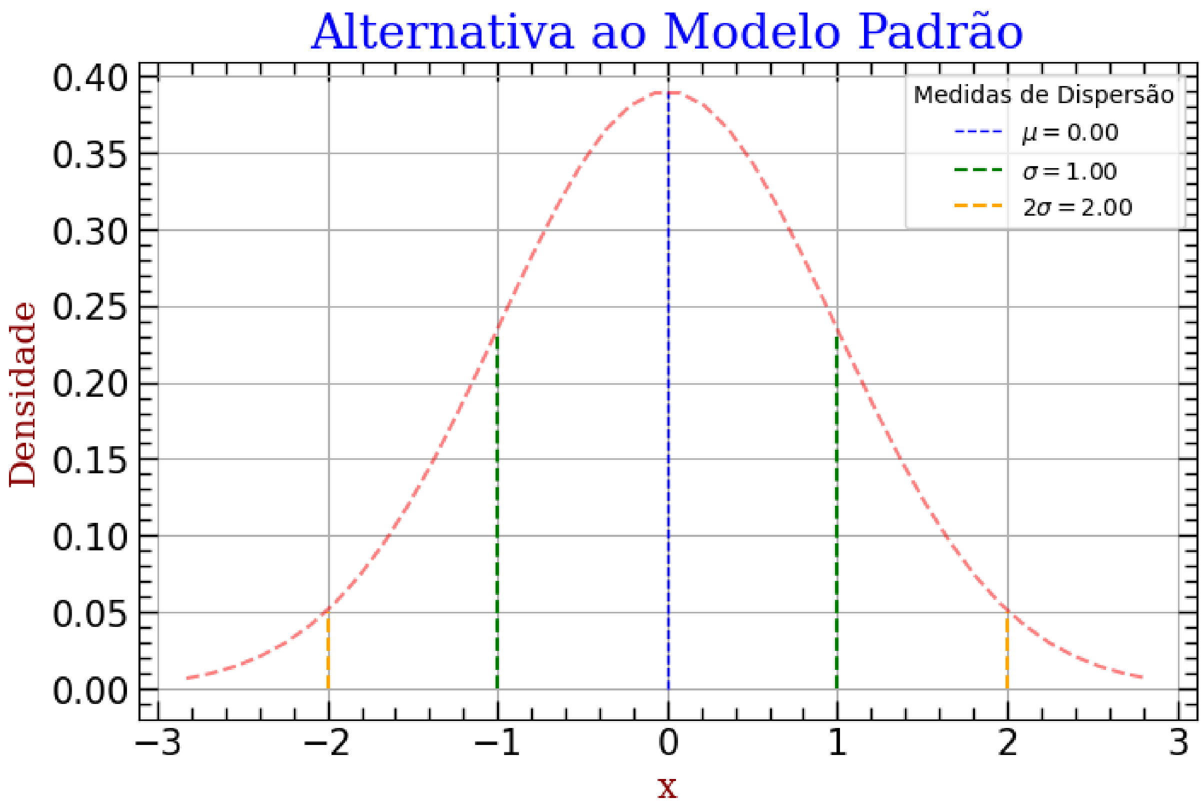
In [193…

```
def opt_plot():
    plt.minorticks_on()
    plt.tick_params(axis='both',which='minor', direction = "in",
                    top = True,right = True, length=5,width=1,
                    labelsize=15)
    plt.tick_params(axis='both',which='major', direction = "in",
                    top = True,right = True, length=8,width=1,
                    labelsize=15)
plt.figure(figsize=(8,5))

textstr = '\n'.join((
    r'$\mu=%.2f$' % (0, ),
    ))

textstr02 = '\n'.join((
    r'$\sigma=%.2f$' % (1, ),
))

textstr03 = '\n'.join((
    r'$\sigma=%.2f$' % (2, ),
))

textstr04 = '\n'.join((
    r'$\sigma=%.2f$' % (1, ),
    r'$\mu=%.2f$' % (0, ),
))

plt.vlines(0, 0, 0.39, linestyle='dashed', color='b', linewidth=1, label=str(textst
plt.vlines(1, 0, 0.23, linestyle='dashed', color='green', linewidth=1.5, label= str
plt.vlines(-1, 0, 0.23, linestyle='dashed', color='green', linewidth=1.5) # vlines(
plt.vlines(2, 0, 0.05, linestyle='dashed', color='orange', linewidth=1.5, label= '2
plt.vlines(-2, 0, 0.05, linestyle='dashed', color='orange', linewidth=1.5) # vlines

font1 = {'family':'serif','color':'blue','size':20}
font2 = {'family':'serif','color':'darkred','size':15}

plt.title("Alternativa ao Modelo Padrão", fontdict = font1)
plt.xlabel("x", fontdict = font2)
plt.ylabel("Densidade", fontdict = font2)

plt.legend(title='Medidas de Dispersão')
plt.grid()
```

```
opt_plot()
plt.plot(xix,y ,'r--', alpha=0.5, label= textstr04)
```

Out[193…

```
[<matplotlib.lines.Line2D at 0x11c3e679d60>]
```



Criação e Calibração de um modelo Simbólico Regressor:

In [195…

```
function_set = ['add', 'sub', 'mul', 'div','cos','sin','neg','inv']
# Instanciação
est_gp = SymbolicRegressor(population_size=5000,
                           generations=20,function_set=function_set,
                           stopping_criteria=0.01,
                           p_crossover=0.7, p_subtree_mutation=0.1,
                           p_hoist_mutation=0.05, p_point_mutation=0.1,
                           max_samples=0.9, verbose=1,
                           parsimony_coefficient=0.01, random_state=0)
# Ajuste
est_gp.fit(xix.reshape(-1, 1),y)
```

```
     |  Population Average    |             Best Individual              |
---- ------------------------- ------------------------------------------ ----------
 Gen   Length          Fitness   Length          Fitness      OOB Fitness  Time Left
   0    15.94          8.42754       24         0.101256         0.141842      3.93m
   1     8.38          1.41838       10        0.0282817        0.0287366      4.66m
   2     4.25         0.913171       10        0.0275074        0.0357058      2.07m
   3     2.38         0.458598       10        0.0262319        0.0471853      1.69m
   4     2.34          69.5123       10        0.0262295        0.0472067      1.69m
   5     4.42          1.11605       11        0.0181481        0.0271488      2.21m
   6     6.21          1.40624       11        0.0183373        0.0356987      2.37m
   7     6.89          1.00531       11        0.0196629        0.0237683      1.42m
   8     7.20          0.86294       11        0.0185499        0.0337846      1.46m
   9     7.36         0.927227       12        0.0193277        0.0303689      1.27m
  10     7.54          1.14538       12        0.0202671        0.0219142      1.03m
  11     7.90          1.22699        8        0.0258667         0.038024      1.21m
  12     8.04          1.22625        8        0.0252462        0.0436084     57.18s
  13     7.96          1.29076        8        0.0249788        0.0460152      1.27m
  14     7.86          1.30819        8        0.0245602          0.04586      1.12m
  15     8.06          1.22489        8        0.0247419        0.0481478     46.88s
  16     7.99          1.55607        8        0.0246505          0.04897     36.24s
  17     7.92          1.26517       11        0.0241093        0.0259531     23.80s
  18     7.97          1.25025        8        0.0246505          0.04897      7.76s
  19     8.00           1.2177       10         0.023813        0.0384339      0.00s
```

Out[195…

```
SymbolicRegressor
div(0.333, sub(0.812, neg(mul(mul(0.696, X0), X0))))
```

Escore:

In [197…

```python
print('R2:',est_gp.score(xix.reshape(-1, 1),y))
next_e = sympify(str(est_gp._program), locals=converter)
y1=next_e
```

```
R2: 0.9502743138806782
```

Equação Proposta:

In [199…

```python
y1
```

Out[199…

$$\frac{0.333}{0.696X_0^2 + 0.812}$$

Soluções para o Poço de Potencial Infinito

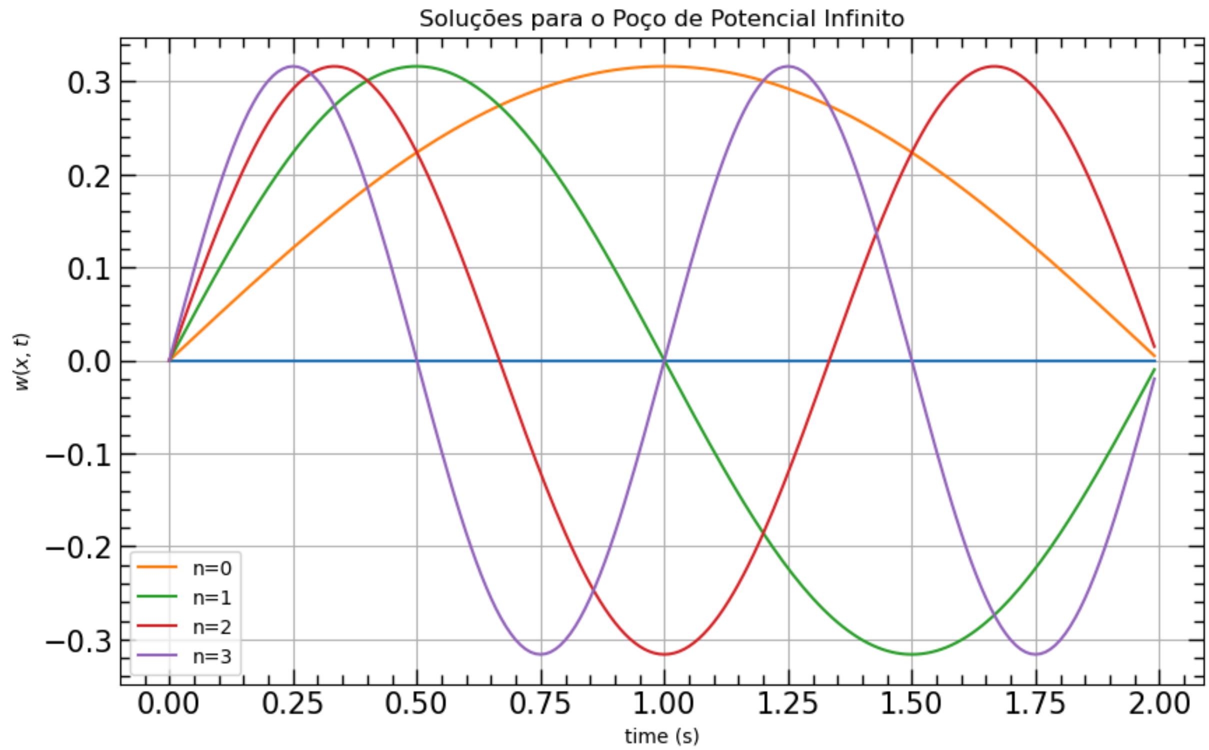
Solução da função de onda da posição

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

In [202…

```python
import matplotlib.pyplot as plt
import numpy as np
```

```python
def opt_plot():
    plt.minorticks_on()
    plt.tick_params(axis='both',which='minor', direction = "in",
                    top = True,right = True, length=5,width=1,
                    labelsize=15)
    plt.tick_params(axis='both',which='major', direction = "in",
                    top = True,right = True, length=8,width=1,
                    labelsize=15)


a=20
A=np.sqrt(2/a)
# Data for plotting
for i in range(5):
    t = np.arange(0.0, 2.0, 0.01)
    s = A*np.sin(0 * np.pi * t)
s1 = A*+np.sin(0.5 * np.pi * t)
s2 = A*np.sin(1.0 * np.pi * t)
s3 = A*np.sin(1.5 * np.pi * t )
s4 = A*np.sin(2.0 * np.pi * t)


fig, ax = plt.subplots(figsize=(10,6))


ax.plot(t, s)
ax.plot(t, s1,label='n=0')
ax.plot(t, s2,label='n=1')
ax.plot(t, s3,label='n=2')
ax.plot(t, s4,label='n=3')


ax.set(xlabel='time (s)', ylabel='$w(x,t)$',
       title="Soluções para o Poço de Potencial Infinito")
ax.grid()
opt_plot()

plt.legend()

fig.savefig("test.png")
plt.show()
```



Gera-se e ajusta-se,um modelo Simbólico Regressor para a solução da função de onda da Posição:

In [204…

```
est_gp.fit(t.reshape(-1, 1),s1)
```

	Population Average		Best Individual			
Gen	Length	Fitness	Length	Fitness	OOB Fitness	Time Left
0	15.94	10.9162	6	0.0305686	0.0286007	4.07m
1	8.25	1.36407	9	0.0238001	0.0246281	2.44m
2	5.03	0.916274	9	0.0248264	0.0153917	3.08m
3	2.76	0.458664	7	0.0265144	0.031241	1.97m
4	2.38	16.2677	7	0.026512	0.0312625	2.16m
5	5.04	0.628504	6	0.0142702	0.0251	1.99m
6	6.00	1.07399	6	0.0145615	0.0224778	1.42m
7	6.08	0.645816	6	0.0137287	0.0299735	2.52m
8	6.07	0.686379	6	0.013608	0.0310599	2.07m
9	6.19	0.767054	6	0.0124938	0.0410876	2.18m
10	6.10	0.799589	6	0.0129802	0.0367098	1.99m
11	6.08	0.641764	6	0.013121	0.0354423	1.06m
12	6.19	0.677095	6	0.0122761	0.0430471	2.23m
13	6.17	0.895997	6	0.012991	0.0366123	1.28m
14	6.06	0.736398	6	0.0132391	0.03438	41.61s
15	6.18	0.696137	6	0.0133269	0.0335893	35.80s
16	6.17	0.844118	6	0.0132413	0.0343599	24.23s
17	6.09	0.700994	6	0.0128263	0.0380947	12.49s
18	6.16	0.612862	6	0.0130871	0.0357479	8.11s
19	6.17	0.633526	6	0.0125276	0.0407834	0.00s

Out[204…

```
▾ SymbolicRegressor
add(mul(-0.517, X0), sin(X0))
```

Escore

In [206…

```
print('R2:',est_gp.score(t.reshape(-1, 1),s1))
next_e = sympify(str(est_gp._program), locals=converter)
y2=next_e
```

```
R2: 0.9048979343134357
```

Equação Proposta

In [208…

```
y2
```

Out[208…

$-0.517X_0 + \sin(X_0)$

Solução para o espectro energético

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

Verificando os níveis de energia:

In [210…

```
import numpy as np
a=1
h=1
m=1
En=0
Enn=[]
for i in range(7):
    En=((i**2)*(h**2)*(np.pi**2))/(2*m*a*a)
    Enn.append(En)

for i in range(7):
    n = i+1
    print("E[{}] = {:9.4f}".format(n,Enn[i],n, n*n*np.pi**2*h*h/(2*m*a*a)))
```

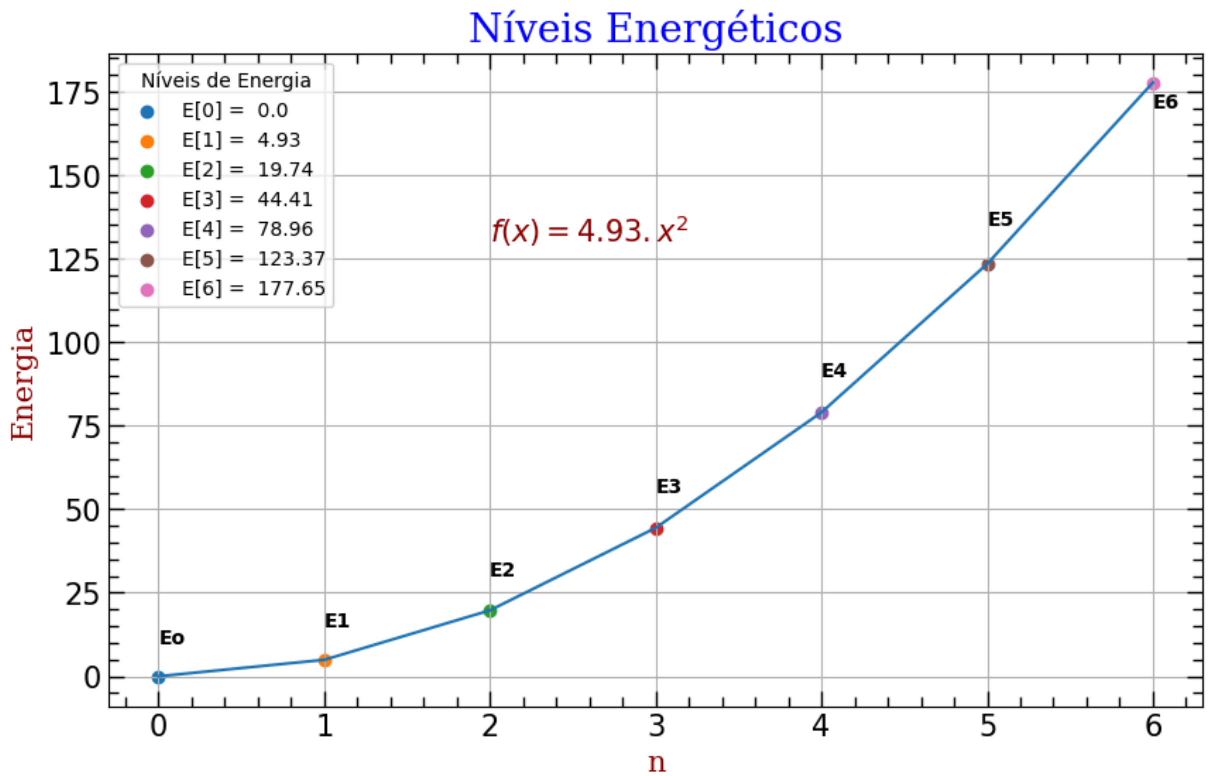
```
E[1] =    0.0000
E[2] =    4.9348
E[3] =   19.7392
E[4] =   44.4132
E[5] =   78.9568
E[6] =  123.3701
E[7] =  177.6529
```

Gráfico da Energia Quantizada:

In [212…

```
def opt_plot():
    plt.minorticks_on()
    plt.tick_params(axis='both',which='minor', direction = "in",
```

```
                    top = True,right = True, length=5,width=1,
                    labelsize=15)
    plt.tick_params(axis='both',which='major', direction = "in",
                    top = True,right = True, length=8,width=1,
                    labelsize=15)

plt.figure(figsize=(10, 6))
plt.plot(Enn)
plt.text(x=0.0, y=10, s="Eo", weight="bold")
plt.text(x=1.0, y=15, s="E1", weight="bold")
plt.text(x=2.0, y=30, s="E2", weight="bold")
plt.text(x=3.0, y=55, s="E3", weight="bold")
plt.text(x=4.0, y=90, s="E4", weight="bold")
plt.text(x=5.0, y=135, s="E5", weight="bold")
plt.text(x=6.0, y=170, s="E6", weight="bold")

for i in range(7):
    En=((i**2)*(h**2)*(np.pi**2))/(2*m*a*a)

    plt.scatter(i,En, marker='o',label="E["+str(i)+"] =  "+str(round(Enn[i],2)))

font1 = {'family':'serif','color':'blue','size':20}
font2 = {'family':'serif','color':'darkred','size':15}

plt.title("Níveis Energéticos", fontdict = font1)
plt.xlabel("n", fontdict = font2)
plt.ylabel("Energia", fontdict = font2)
plt.text(x=2.0, y=130, s=r'$f(x) = 4.93.{x^2}$',fontdict = font2)

plt.legend(title='Níveis de Energia')
opt_plot()

plt.grid()
```



Para:

In [214…

```
l_count=np.linspace(0,6,7)
E_df=np.array([l_count,Enn])
E_df02=E_df.T
E_df02
y_E=4.93*E_df[:,0]**2
```

Obtem-se o seguinte modelo:

In [216…

```
function_set = ['add', 'sub', 'mul', 'div','cos','sin','neg','inv']
# Instanciação
est_gp = SymbolicRegressor(population_size=5000,
                           generations=20,function_set=function_set,
                           stopping_criteria=0.01,
                           p_crossover=0.7, p_subtree_mutation=0.1,
                           p_hoist_mutation=0.05, p_point_mutation=0.1,
                           max_samples=0.9, verbose=1,
                           parsimony_coefficient=0.01, random_state=0)
# Ajuste
est_gp.fit(E_df,y_E)
```

```
    |   Population Average    |             Best Individual              |
---- ------------------------- ------------------------------------------ ----------
 Gen   Length          Fitness   Length          Fitness      OOB Fitness  Time Left
   0    10.86      1.23511e+07       14                0                0      2.13m
```

Out[216…

SymbolicRegressor

neg(neg(div(mul(inv(X0), mul(X1, -0.362)), sub(cos(X2), sin(0.200)))))

Cujo Escore é:

In [218…

```
next_e = sympify(str(est_gp._program), locals=converter)
y3=next_e
```

com a proposta de equação:

In [220…

```
y3
```

Out[220…

$$-\frac{0.362X_1}{X_0\left(\cos\left(X_2\right)-0.198669330795061\right)}$$

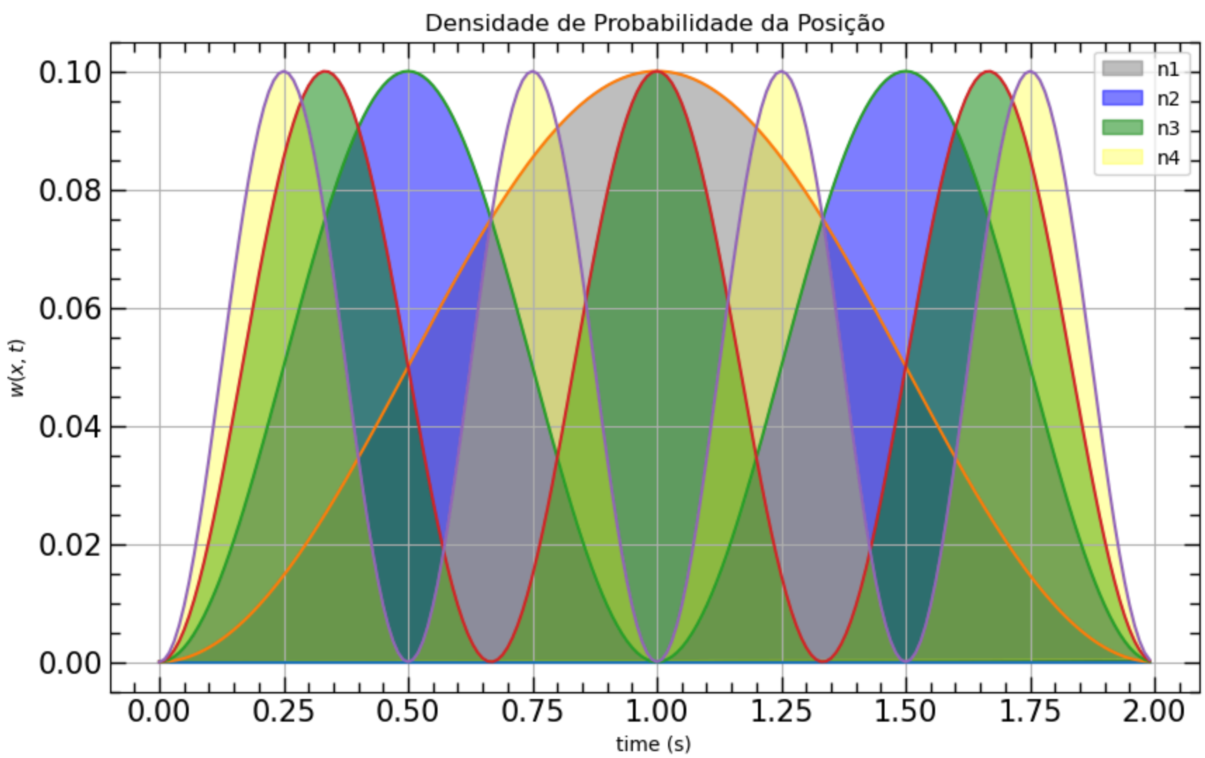
Densidade de Probabilidade da posição

$$|\psi_n(x)|^2=\frac{2}{a}\sin^2(n\pi x)$$

In [222…

```
import matplotlib.pyplot as plt
import numpy as np

def opt_plot():
    plt.minorticks_on()
    plt.tick_params(axis='both',which='minor', direction = "in",
                    top = True,right = True, length=5,width=1,
                    labelsize=15)
    plt.tick_params(axis='both',which='major', direction = "in",
                    top = True,right = True, length=8,width=1,
                    labelsize=15)

val_esp=[-7.17,-4.344,-1.555,0.8002,2.905,5.095 ,7.305]

a=20
A=(2/a)
# Data for plotting
t = np.arange(0.0, 2.0, 0.01)
x=np.arange(0.0,2.0,0.01)


s = A*(np.sin((0 * np.pi * x)))**2

s1 = A*(np.sin((0.5 * np.pi * abs(x))))**2
s2 = A*(np.sin((1.0 * np.pi * x)))**2
s3 = A*(np.sin((1.5 * np.pi * x)))**2
s4 = A*(np.sin((2.0 * np.pi * x)))**2


fig, ax = plt.subplots(figsize=(10,6))
```

```python
ax.plot(x, s)

ax.plot(x, s1)
ax.fill(x,s1,color='grey', alpha=0.5, label='n1')
ax.plot(x, s2)
ax.fill(x,s2,color='blue', alpha=0.5, label='n2')
ax.plot(x, s3)
ax.fill(x,s3,color='green', alpha=0.5, label='n3')
ax.plot(x, s4)
ax.fill(x,s4,color='yellow', alpha=0.3, label='n4')



ax.set(xlabel='time (s)', ylabel='$w(x,t)$',
       title="Densidade de Probabilidade da Posição")
ax.grid()
ax.legend()
opt_plot()

fig.savefig("test.png")
plt.show()
```



Relaciona-se os valores médios esperados, da funçao de onda, com a função normal gaussiana:

In [224…

```python
val_esp=np.array([-7.17,-4.344,-1.555,0.8002,2.905,5.095 ,7.305])
niveis=[0,1,2,3,4,5,6]
arr_value=np.array([[niveis],[val_esp]])
x_arr = val_esp
print(x_arr)
y_arr=0.399*(2.76**(-0.5*x_arr[:]**2))
```

```
[-7.17   -4.344  -1.555   0.8002  2.905   5.095   7.305 ]
```

para então, modular:

In [226…

```python
function_set = ['add', 'sub', 'mul', 'div','cos','sin','neg','inv']
# Instanciação
est_gp = SymbolicRegressor(population_size=5000,
                           generations=20,function_set=function_set,
                           stopping_criteria=0.01,
                           p_crossover=0.7, p_subtree_mutation=0.1,
                           p_hoist_mutation=0.05, p_point_mutation=0.1,
                           max_samples=0.9, verbose=1,
                           parsimony_coefficient=0.01, random_state=0)
# Ajuste
est_gp.fit(x_arr.reshape(-1,1),y_arr)
```

```
    |   Population Average    |             Best Individual              |
---- ------------------------- ----------------------------------------- ----------
 Gen   Length          Fitness   Length          Fitness      OOB Fitness  Time Left
   0    15.94          24.2581        9        0.0150923         0.125521      2.42m
   1     9.25          3.10342       29         0.001741         0.390678      2.71m
```

Out[226…

```
SymbolicRegressor

sin(mul(cos(sub(sin(add(0.782, 0.138)), sin(sub(0.773, X0)))), div(cos(inv
(cos(X0))), sub(sin(add(-0.483, 0.614)), mul(mul(X0, X0), add(X0, X0))))))
```

Escore:

In [228…

```python
print('R2:',est_gp.score(x_arr.reshape(-1,1),y_arr))
next_e = sympify(str(est_gp._program), locals=converter)
y2_arr=next_e
```

```
R2: -1.099778938698206
```

Equaçao:

In [230…

```python
y2_arr
```

Out[230…

$$\sin\left(\frac{\cos\left(\sin\left(X_0 - 0.773\right) + 0.795601620036366\right)\cos\left(\frac{1}{\cos\left(X_0\right)}\right)}{0.130625639531083 - 2X_0^3}\right)$$

O desvio padrão da posição:

$$\Delta xn = \sqrt{< x^2 n > - < xn >^2} = a\sqrt{\frac{1}{12} - \frac{1}{2\pi^2 n^2}}$$

In [232…

```python
import pandas as pd
xx0=-10
val_esp=[-7.17,-4.344,-1.555,0.8002,2.905,5.095 ,7.305]
a=val_esp[6]-val_esp[0]
```

```
x_quadrado=0
dp=[]
n=1
desp=0
j=-10

c=0
dsp=[]
for i in val_esp:
    if (j<0 and i>0):
        c=np.abs(j)+i
    else:
        c=np.abs(j)-np.abs(i)
        c=np.abs(c)
    dsp.append(c)
    j=i
dsp
er_count=0
err=[]
med_ex=2.86
for i in dsp:
    er_count=med_ex-i
    err.append(er_count)
err
dpp=pd.DataFrame()
dpp['DesvioP']=dsp
dpp['ErrDesvioP']=err

dpp
```

Out[232...

	DesvioP	ErrDesvioP
0	2.8300	0.0300
1	2.8260	0.0340
2	2.7890	0.0710
3	2.3552	0.5048
4	2.1048	0.7552
5	2.1900	0.6700
6	2.2100	0.6500

Podemos encontrar, também, o desvio padrão do momento

$$e^{\frac{-i \operatorname{op} H\Delta t}{\hbar}} = \sum_n \frac{\left(\frac{-i \operatorname{op} H\Delta t}{\hbar}\right)^n}{n!}$$

$$\Delta Kn =< K^2 n > - < Kn >^2 = \frac{n\hbar}{a}$$

In [234…

```
import numpy as np
a=20

h=1
dpm=0
dmp=[]
for i in range(7):
    a=np.abs(a)
    dpm=(i*np.pi)/a
    dmp.append(dpm)
```

O Princípio da Incerteza

$$\Delta x.\Delta p > \frac{\hbar}{2}$$

In [236…

```
desvf=pd.DataFrame()
desvf["dp"]=dpp.DesvioP
desvf["dmp"]=dmp
j=0
incerteza=[]
form=[]
f=r'$\Delta x.\Delta p $'
g=r'$\Delta x $'
h=r'$\Delta p $'
c=0
gord=dpp.DesvioP
hord=dmp
for i in dpp.DesvioP:
   j=dmp[c]*i
   incerteza.append(j)
   form.append(f)


   c=c+1
desvf02=pd.DataFrame()
desvf02[g]=gord
desvf02[h]=hord
desvf02["lesquerdo"]=form
desvf02["incerteza"]=incerteza
desvf02
```

Out[236...

	Δx	Δp	Iesquerdo	incerteza
0	2.8300	0.000000	$\Delta x.\Delta p$	0.000000
1	2.8260	0.157080	$\Delta x.\Delta p$	0.443907
2	2.7890	0.314159	$\Delta x.\Delta p$	0.876190
3	2.3552	0.471239	$\Delta x.\Delta p$	1.109862
4	2.1048	0.628319	$\Delta x.\Delta p$	1.322485
5	2.1900	0.785398	$\Delta x.\Delta p$	1.720022
6	2.2100	0.942478	$\Delta x.\Delta p$	2.082876

Regressão Simbólica entre os Δx e Δp, como variáveis independentes.

In [238...

```
from array import array
pr_in=[]
mul=0
co=0
for i in dp:
    mul=dmp[co]*i
    pr_in.append(mul)
    co=co+1
pr_in
l=np.linspace(-20,20,7)
est_gp.fit(desvf,l)
```

```
    |    Population Average    |             Best Individual              |
---- ------------------------- ------------------------------------------ ----------
 Gen   Length          Fitness   Length          Fitness      OOB Fitness  Time Left
   0    14.12          17.3358       61          4.58152          2.20469      3.45m
   1    13.19          12.2287       63          2.01855          16.5301      2.28m
   2    22.91          12.5299       68          1.48236          19.5784      3.20m
   3    45.90          11.1265       67          1.35883          16.5595      3.00m
   4    57.10          8.42914       74           1.2534          16.1118      2.97m
   5    56.64          8.65533      103         0.940835          17.0272      2.68m
   6    55.98          8.42966       74         0.897443          18.0636      3.05m
   7    55.51          8.75305       89         0.915222          18.4083      2.35m
   8    54.16          8.32359       57          0.83206          5.84937      2.04m
   9    54.13          8.69014       59         0.601793          5.16499      1.84m
  10    51.85           8.2424       59         0.601793          5.16499      1.64m
  11    50.01          8.74759       70         0.566704          2.36483      1.42m
  12    48.89          8.13448       63         0.433342          38.7046      1.45m
  13    51.54          7.87202       75         0.439702           1.6471      1.06m
  14    55.80          7.78783       74         0.409549           1.6472     59.38s
  15    62.10          7.10821       63         0.414798          1.55232     56.88s
  16    65.83           8.2369       79         0.343407          1.43067     37.18s
  17    66.11          7.72361       78         0.387547          1.80321     24.98s
  18    64.58          7.55171       78         0.274171          1.35523     13.50s
  19    63.97          7.15509       77         0.328465            1.395      0.00s
```

Out[238...

SymbolicRegressor

```
sub(sub(sub(mul(neg(div(X0, X0)), add(neg(X1), div(X0, X1))), inv(add(neg
(-0.046), div(-0.094, X1)))), mul(add(neg(div(add(neg(X1), add(neg(X1), ne
g(X1))), X0)), sin(X1)), neg(sin(X1)))), div(sin(sub(sub(sub(mul(neg(div(X
0, X0)), add(neg(sub(X1, -0.041)), div(X0, X1))), inv(add(neg(-0.046), div
(-0.094, X1)))), sin(0.355)), div(sin(div(-0.094, X1)), sub(X1, -0.04
1)))), sub(X1, -0.041)))
```

Escore:

In [240...

```python
print('R2:',est_gp.score(desvf,l))
next_e = sympify(str(est_gp._program), locals=converter)
y4=next_e
```

```
R2: 0.9974758366230793
```

Equação Proposta:

In [242...

```python
print(y4)
```

```
-X0/X1 + X1 + (sin(X1) + 3*X1/X0)*sin(X1) + sin(X0/X1 - X1 + 0.306590365235784 - sin
(0.094/X1)/(X1 + 0.041) + 1/(0.046 - 0.094/X1))/(X1 + 0.041) - 1/(0.046 - 0.094/X1)
```

Regressão Simbólica entre os Δx e Δp, como um produto entre ambas.

In [244...

```python
deltax=np.linspace(2.1,2.83,100)
deltap=np.linspace(0.15,0.94,100)
delta_dp=pd.DataFrame()
delta_dp['deltax']=deltax
delta_dp['deltap']=deltap
c=0
mult=[]
for i in deltax:
   j=deltap[c]*i
   mult.append(j)

   c=c+1
c_inf=0
mult_inf=[]
mult_sup=[]
for i in mult:
    if i<0.5:
        mult_inf.append(i)
        c_inf=c_inf+1
    else:
        mult_sup.append(i)
```

In [245...

```python
est_gp.fit(delta_dp,mult)
```

```
    |   Population Average    |             Best Individual              |
---- ------------------------- ----------------------------------------- ----------
 Gen   Length          Fitness   Length          Fitness      OOB Fitness  Time Left
   0    14.12          9.75688        5                0                0      2.22m
```

Out[245…

```
▾ SymbolicRegressor
mul(neg(X0), neg(X1))
```

Escore:

In [247…

```
print('R2:',est_gp.score(delta_dp,mult))
next_e = sympify(str(est_gp._program), locals=converter)
y5=next_e
```

```
R2: 1.0
```

Equação

In [249…

```
print(y5)
```

```
X0*X1
```

As Equações Sugeridas:

In [251…

```
print('As Equações Sugeridas:')
print('____________')
print('')
print('I - y1(X0) =', y1)
print('-------')
print('II - y2(X0) =', y2)
print('-------')
print('III - y3(X0,X1,X2) =', y3)
print('-------')
print('IV - y2_arr(X0) = ',y2_arr)
print('-------')
print('V - y4(X0,X1) = ', y4)
print('-------')
print('VI - y5(X0,X1) = ', y5)
print('-------')
```

```
As Equações Sugeridas:
_____________

I - y1(X0) = 0.333/(0.696*X0**2 + 0.812)
-------
II - y2(X0) = -0.517*X0 + sin(X0)
-------
III - y3(X0,X1,X2) = -0.362*X1/(X0*(cos(X2) - 0.198669330795061))
-------
IV - y2_arr(X0) =  sin(cos(sin(X0 - 0.773) + 0.795601620036366)*cos(1/cos(X0))/(0.13
0625639531083 - 2*X0**3))
-------
V - y4(X0,X1) =  -X0/X1 + X1 + (sin(X1) + 3*X1/X0)*sin(X1) + sin(X0/X1 - X1 + 0.3065
90365235784 - sin(0.094/X1)/(X1 + 0.041) + 1/(0.046 - 0.094/X1))/(X1 + 0.041) - 1/
(0.046 - 0.094/X1)
-------
VI - y5(X0,X1) =  X0*X1
-------
```

In [ ]:

In [ ]:

In [ ]: