

Molecular Statistics, Week 2



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Week 2, Overview

- Week 1 problems
- Functions
- Debugging
- Double loop



Week 1 problems

What was the hardest part of week 1?

```
pos_x = [random.random() for i in range(n_particles)]  
  
for i in range(n_particles):  
    print pos_x[i]
```



Functions

$$y(x) = x^2$$

```
def square(x):  
    y = x**2  
    return y
```

```
print square(5.0)
```



Create a Gaussian function

$$g(x) = a \exp\left(-\frac{(x-b)^2}{(2c^2)}\right) + d$$

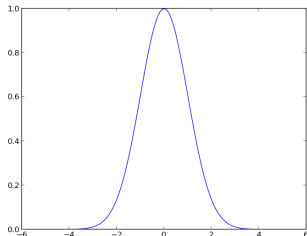
with the following constants

$$a = 1.0$$

$$b = 0.0$$

$$c = 1.0$$

$$d = 0.0$$



Gaussian Function

```
def gaussian(x):  
  
    a = 1.0  
    b = 0.0  
    c = 1.0  
    d = 0.0  
  
    g = a*np.exp( -(x-b)**2 / (2*c**2) ) + d  
  
    return g
```

```
print gaussian(0.0)
```



Gaussian Function

Multiple parameters

```
def gaussian(x, a):  
  
    b = 0.0  
    c = 1.0  
    d = 0.0  
  
    g = a*np.exp( -(x-b)**2 / (2*c**2) ) + d  
  
    return g
```

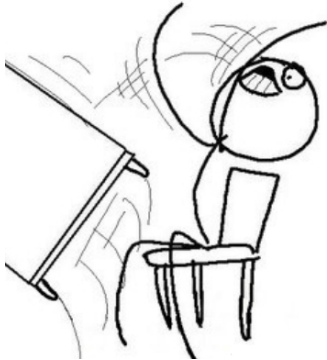
```
print gaussian(0.0, 1.0)
```



Debugging

Typical errors:

- Indentation error
- Out of bounds
- Object not callable
- Invalid syntax



Exercise Week 2

```
import random

...

def initialize_particles(n_particles):
    """ Initialize particles , positions and velocities
    """
    return pos_x , pos_y , vel_x , vel_y

...

n_particles = 40
n_steps = 10000
```

