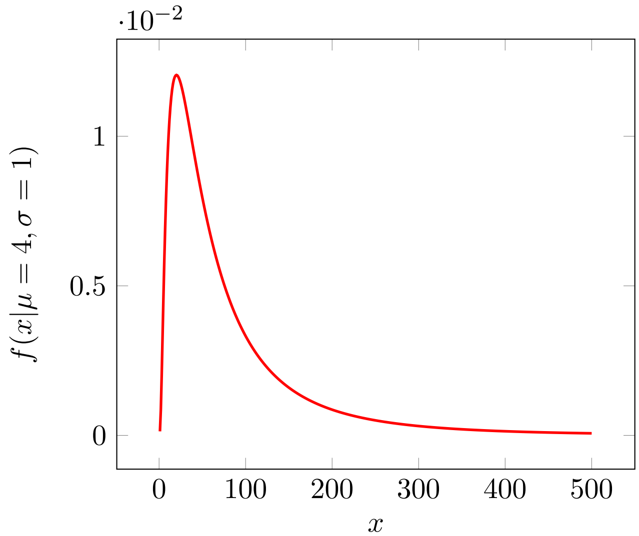
Matrícula (First-name Last-name) **CK0030: Homework 01**

Exercise 1. Consider the Lognormal function $f(x|\mu, \sigma)$ with parameters μ and σ and $x \in (0, \infty)$

$$f(x|\mu,\sigma) = \underbrace{\frac{1}{\sqrt{2\pi\sigma^2}}}_{a} \underbrace{\frac{1}{x}}_{b} \exp\Big\{ - \underbrace{\frac{1}{2\sigma^2}}_{c} \big[\underbrace{\log(x) - \mu}_{d}\big]^2 \Big\} = a(\sigma)b(x)\exp\big[- c(\sigma)d(x|\mu)^2\big]. \qquad (1)$$



The piece of code below was developed to evaluate the Lognormal at $x = 100$, for $\mu = 4$ and $\sigma = 1$

```
from math import sqrt, pi, exp, log

mu = 4
sigma = 1
x = 100

a = 1/sqrt(2*pi*sigma**2)
b = 1/x.
c = 1/2*sigma**2
d = (log(x)-mu)**2

f = a*b*exp(-c*d**2)

print '%.16f' % f
```

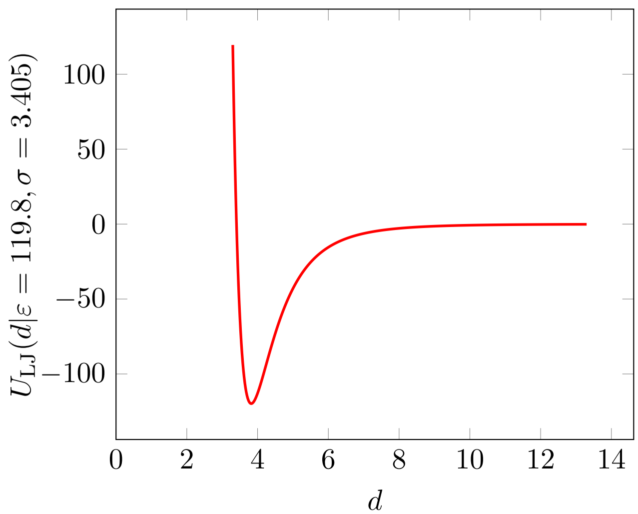
When executed to calculate $f(x = 100|\mu = 4, \sigma = 1)$, the printed result is `0.0000000000000000`.

The result seems wrong (see plot), explain why and show how to fix the code accordingly. Write a program `my_lognorm.py` (or a code snippet in a notebook) with a working version of the code.

Exercise 2. The Lennard-Jones potential is a simple pair-wise potential between two identical particles that is often used to describe Van der Walls forces between rare-gas atoms

$$U_{\mathrm{LJ}}(d|\varepsilon,\sigma) = 4\varepsilon\Big[\big(\sigma/d\big)^{12} - \big(\sigma/d\big)^{6}\Big], \tag{2}$$

ε denotes the depth of the potential well, σ is the finite distance at which the inter-particle potential is zero and d denotes the distance between the particles.



Write a program `my_lj.py` (or a code snippet in a notebook) for evaluating the function $U_{\mathrm{LJ}}(d|\varepsilon,\sigma)$ at $d \in \{0, 1, 2, 3, 4, 8, 16\}$, when the function parameters are $\varepsilon = 119.8$ [energy] and $\sigma = 3.405$ [nm].

[*Hint*]: To verify the correctness of the obtained results, you could use the plot of the function.