Rejection method for sampling the Maxwell flux distribution

Maxwell distribution

This is the Maxwell flux distribution with $x = \frac{v}{v_T}$, v : velocity, v_T : thermal velocity

```
f@x_D := 2  Exp@-x^2D  x^3
```

with a maximum at xm

```
Solve@D@f@xD, xD « 0, xD
```

```
98x → 0<, 8x → 0<, 9x → - $ 3/2 =, 9x → $ 3/2 ==
```

```
xm = %@@4, 1, 2DD
```

```
$ 3/2
```

and value at xm

```
f@xmD
```

```
3 "###
  3/2
---------
  e^(3/2)
```

Comparison Function

As comparison function we will use the Lorentz distribution

```
fl@x_, xo_, s_D := 1 ê Hπ  sL  1 ê H1 + Hx − xoL^2 ê s^2L;
TraditionalForm@fl@x, xo, σDD
```

```
                1
p I Hx-xoL2 + 1M s
    s2
```

which has a cumulative distribution

```
Integrate@fl@x, xo, sD, xD
```

```
ArcTan@ x-xo D
         s
      π
```

that can be inverted

```
Solve@% « z, xD
```

```
88x → xo + s Tan@π zD<<
```

Matching the two functions

To match the maxima of f and fl we require that xo=xm and

```
ao = f@xmD ê fl@xm, xm, sD
```

```
3 "π s
Ą3ê2
```

Thus our comparison function so far is

```
Simplify@ao  fl@x, xm, sDD
```

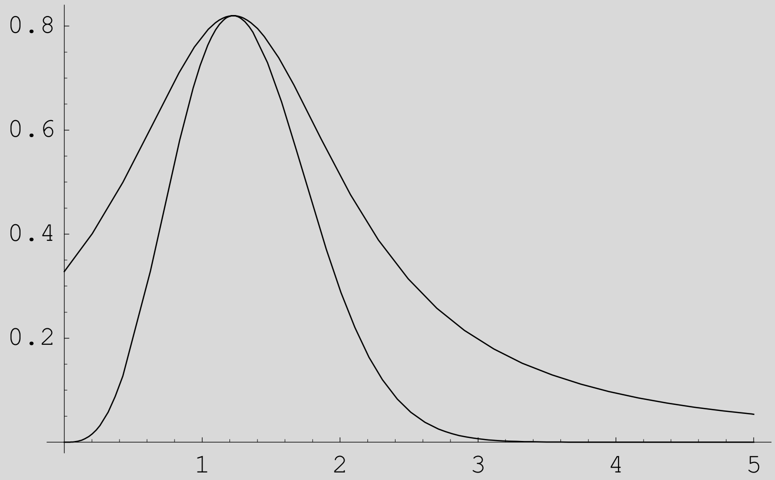
```
        3 "
Ą3ê2 J1 + J "  −xN
            s      N
```

$$fc[x\_, s\_] := \frac{3\sqrt{\frac{3}{2}}}{\pi^{3/2}\left(1+\frac{\left(\sqrt{\frac{3}{2}}-x\right)^2}{s^2}\right)}$$

We have now the freedom to choose s. Examples:

First guess: s=1

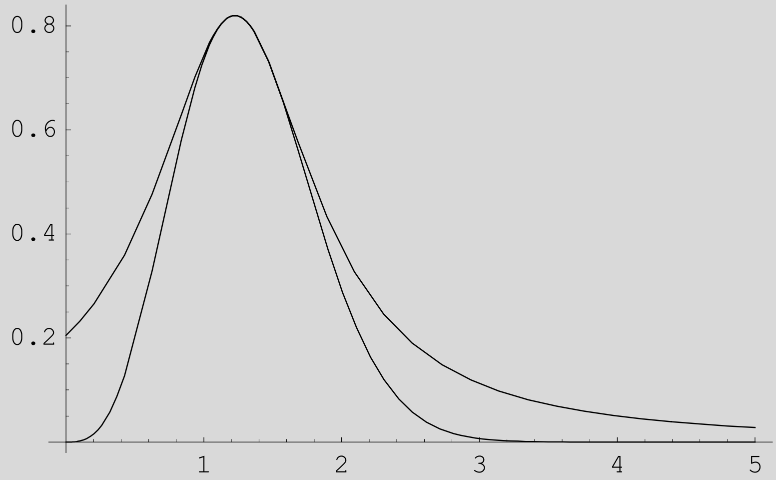
```
Plot[{f[x], fc[x, 1]}, {x, 0, 5}]
```




```
- Graphics -
```

Try to bring the functions more close by choosing a smaller s

```
PlotA9f@xD, fcAx, 1 ë è!!! 2 E=, 8x, 0, 5<E
```



```
¦ Graphics ¦
```

This is better.

To optimize the value of s we try to match the functions at another point x > xm

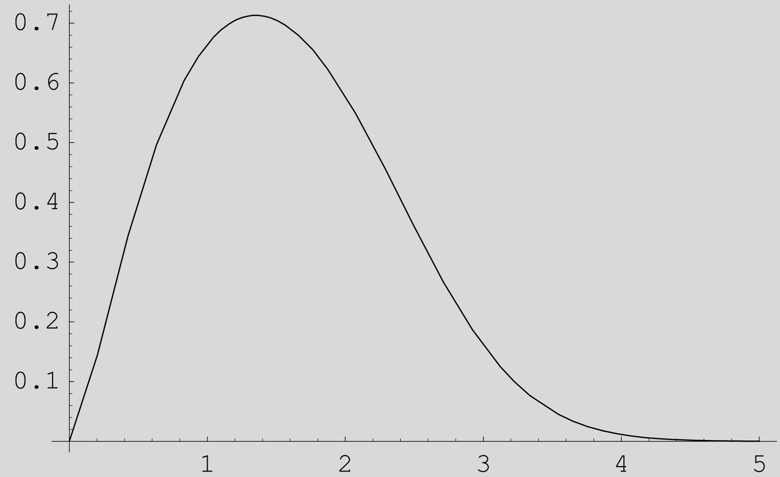
```
Solve@f@xD « fc@x, sD, sD

         è!!! "##############è!!!######################
         2    3 Ą3ê2 x3 − 2   6 Ą3ê2 x4 + 2 Ą3ê2 x5
99s → − ¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡ =,
                  "###è!!!############
                  3   6 Ąx2 − 4 Ą3ê2 x3

        è!!! "##############è!!!######################
        2    3 Ą3ê2 x3 − 2   6 Ą3ê2 x4 + 2 Ą3ê2 x5
 9s → ¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡ ==
                 "###è!!!############
                 3   6 Ąx2 − 4 Ą3ê2 x3
```

```
           è!!! "##############è!!!######################
           2    3 Ą3ê2 x3 − 2   6 Ą3ê2 x4 + 2 Ą3ê2 x5
g@x_D := ¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡¡
                    "###è!!!############
                    3   6 Ąx2 − 4 Ą3ê2 x3
```

```
Plot@g@xD, 8x, 0, 5<D
```




```
¦ Graphics ¦
```

Get the max of this function

```
S = D@g@xD, xD « 0
```

```
                  9 Ą^3ê2 x^2 - 8 è!!!6 Ą^3ê2 x^3 + 10 Ą^3ê2 x^4
iiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiii -
è!!!2 "3 è!!!6 Ą^x^2 - 4 Ą^3ê2 x^3  "3 Ą^3ê2 x^3 - 2 è!!!6 Ą^3ê2 x^4 + 2 Ą^3ê2 x^5

  I6 è!!!6 Ą^x^2 x - 12 Ą^3ê2 x^2M "3 Ą^3ê2 x^3 - 2 è!!!6 Ą^3ê2 x^4 + 2 Ą^3ê2 x^5
  iiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiiii == 0
              è!!!2 I3 è!!!6 Ą^x^2 - 4 Ą^3ê2 x^3M^3ê2
```

```
FindRoot@S, 8x, 1.5<D

8x → 1.35126<
```

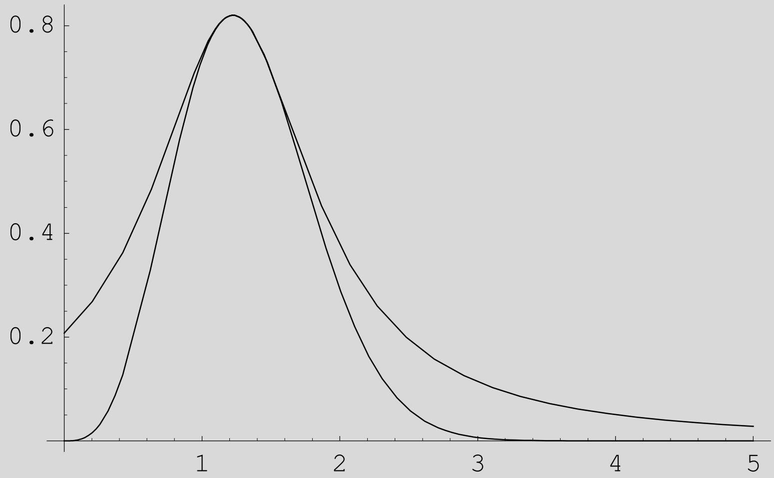
This is our optimal s:

```
so = g@%@@1, 2DDD

0.713127
```

This is how it looks like:

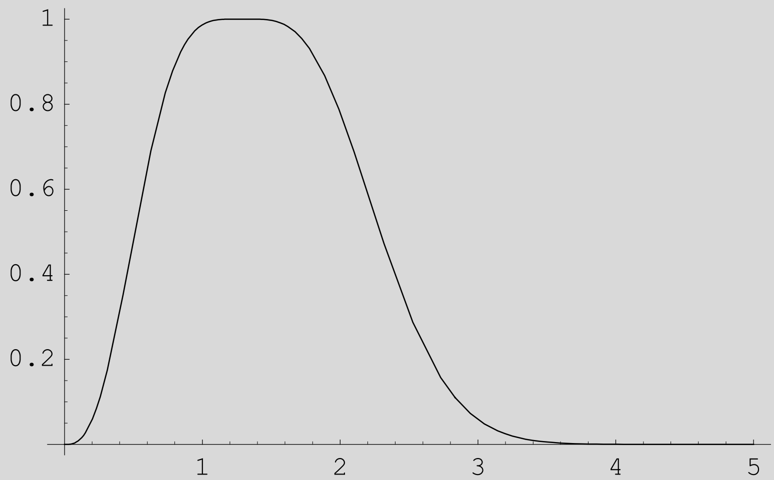
```
Plot@8f@xD, fc@x, soD<, 8x, 0, 5<, PlotRange → AllD
```



¦ Graphics ¦

Check that our fuction is everywhere above f[x]

```
Plot@8f@xD ê fc@x, soD<, 8x, 0, 5<, PlotRange → AllD
```



¦ Graphics ¦

Ratio of distribution to comparison function

```
Simplify@f@xD ê fc@x, soDD
```

Ą$^{-x^2}$ x^3 H9.63504 − 11.7502 x + 4.79701 x^2L

Algorithm

1. Take *a* uniform variate U_1

2. Tranform to *a* Lorentz distribution variate *x* with

```
x -> xm + so  Tan@π  U1D

x → $ 3/2 + 0.713127 Tan@π U1D
```

3. If x <= 0 recejct it and start again from step 1.

4. Compute the ratio R

```
R -> Simplify@f@xD ê fc@x, soDD

R → Ą^(-x^2) x^3 H9.63504 − 11.7502 x + 4.79701 x^2L
```

5. Take a second uniform variate U_2

6. If U_2 > R reject x and start again from step 1. Else return x.