1 An example of using envelope functions

The radial part of the Woods-Saxon distribution is given by

$$P_r(x) = \frac{x^2}{1 + e^{x - X_A}} \tag{1}$$

The envelope function is

1. Region I ($0 \leq x < x_1$)

$$P_I(x) = x^2 \tag{2}$$

2. Region II ($x_1 \leq x < x_2$)

$$P_{II}(x) = P_{\max} \tag{3}$$

3. Region III ($x \geq x_2$)

$$P_{III}(x) = x(x+2)e^{-x+X_A} \tag{4}$$

The boundary between regions I and II are determined by

$$x_1^2 = P_{\max} \tag{5}$$

or

$$x_1 = \sqrt{P_{\max}} \tag{6}$$

The boundary between regions II and III are determined by

$$P_{\max} = x_2(x_2+2)e^{-x_2+X_A} \tag{7}$$

which is best solved numerically. But first, we need to get $P_{\max}$.

1.1 Get $P_{\max}$

To get $P_{\max}$, we first take the derivate to get

$$\frac{dP_r}{dx} = \frac{xe^{X_A}\left(2e^{X_A} - e^x(x-2)\right)}{\left(e^x + e^{X_A}\right)^2} \tag{8}$$

To solve $dP_r/dx = 0$, we need to find a solution of

$$e^x(x-2) = 2e^{X_A} \tag{9}$$

This can be manipulated into

$$(x-2)e^{(x-2)} = 2e^{X_A-2} \tag{10}$$

So the solution is

$$x_c = W(2e^{X_A-2}) + 2 \tag{11}$$

where $W(x)$ is the Lambert function which solves $y = xe^x$. We get

$$P_{\max} = \frac{x_c^2}{1+e^{x_c - X_A}} \tag{12}$$

1.2 Integral of P_{env} and its inverse

The integral of the envelope function is

1. Region I:

$$z_I = \int_0^x P_I(x) = \frac{x^3}{3} \tag{13}$$

Or

$$x = (3z_I)^{1/3} \tag{14}$$

with

$$0 \leq z_I < z_1 \tag{15}$$

where $z_1 = \frac{x_1^3}{3}$

2. Region II:

$$z_{II} = z_1 + \int_{x_1}^x dx\, P_{\max} = z_1 + P_{\max}(x - x_1) \tag{16}$$

or

$$x = x_1 + \frac{z_{II} - z_1}{P_{\max}} \tag{17}$$

with

$$z_1 \leq z_{II} < z_2 \tag{18}$$

where $z_2 = z_1 + P_{\max}(x_2 - x_1)$.

3. Region III:

$$
\begin{aligned}
z_{III} &= z_2 + \int_{x_2}^{x} dx'\, x'(x'+2)e^{-x'+X_A} \\
&= z_2 + (2+x_2)^2 e^{-x_2+X_A} - (2+x)^2 e^{-x+X_A} \\
&= z_3 - (2+x)^2 e^{-x+X_A}
\end{aligned} \tag{19}
$$

where $z_3 = z_2 + (2+x_2)^2 e^{-x_2+X_A}$ and

$$z_2 \le z_{III} < z_3 \tag{20}$$

To solve for x, rewrite this as

$$(2+x)^2 e^{-x-2} \;=\; (z_3 - z_{III})e^{-X_A-2} \tag{21}$$

which becomes

$$-\frac{2+x}{2} e^{-(x+2)/2} \;=\; -\frac{1}{2}\left(z_3 - z_{III}\right)^{1/2} e^{-(X_A+2)/2} \tag{22}$$

The solution is

$$x = -2(W_{-1}(Z) + 1) \tag{23}$$

where

$$Z = -\frac{1}{2}\left(z_3 - z_{III}\right)^{1/2} e^{-(X_A+2)/2} \tag{24}$$

The Lambert function of a negative argument is double-valued. It turns out that what we need is actually the second branch value (W_{-1}).

To generate random number according to the envelope function,

1. Generate a uniform random number z between 0 and z_3.

2. If $0 \le z < z_1$, then

$$x = (3z)^{1/3} \tag{25}$$

3. Else if $z_1 \leq z < z_2$, then

$$x = x_1 + \frac{z - z_1}{P_{\mathrm{max}}} \tag{26}$$

4. Else

$$x = -2(W_{-1}(Z) + 1) \tag{27}$$

   where $Z = -\left(z_3 - z\right)^{1/2} e^{-(X_A+2)/2}$

5. Generate another random number y.

6. Form a ratio

$$r = \frac{P_r(x)}{P_{\mathrm{env}}(x)} \tag{28}$$

7. If $y < r$, accept x.

8. Else reject x and go back to 1.