betaFIT: A software for fitting points to functions

EXTENDEND MORSE OSCILLATOR

Consider the EMO function:

$$V(r) = \mathfrak{D}_e \left(1 - \exp\left(-\beta(r)\left(r - r_e\right)\right)\right)^2 + V_e. \tag{1}$$

If we know $V(r)$, $\mathfrak{D}_e$ and r_e, then we can obtain a corresponding function $\beta(r)$. However, similar to the equation $4 = x^2$ having two real-number solutions, for each value of r, there can be more than one real number $\beta(r)$ that satisfies Eq. 1. To find the possible values of $\beta(r)$, we can start with the following rearrangement:

$$\frac{V(r) - V_e}{\mathfrak{D}_e} = \left(1 - \exp\left(-\beta(r)\left(r - r_e\right)\right)\right)^2. \tag{2}$$

$V(r) \geq V_e$ for all r, because V_e is defined as the minimum value of $V(r)$. Also, $\mathfrak{D}_e > 0$ for bound potentials, so the left side cannot be negative. We can then proceed as follows:

$$\begin{aligned} 4 &= x^2 \\ \pm\sqrt{4} &= x \end{aligned} \qquad\qquad \begin{aligned} \tfrac{V(r)-V_e}{\mathfrak{D}_e} &= \left(1 - \exp\left(-\beta(r)\left(r - r_e\right)\right)\right)^2 \\ \pm\sqrt{\tfrac{V(r)-V_e}{\mathfrak{D}_e}} &= 1 - \exp\left(-\beta(r)\left(r - r_e\right)\right). \end{aligned}$$

The $+\sqrt{4}$ in the equation above corresponds to $x > 0$ and the $-\sqrt{4}$ corresponds to $x < 0$, and similarly we have:

$$+\sqrt{\frac{V(r) - V_e}{\mathfrak{D}_e}} = 1 - \exp\left(-\beta(r)(r - r_e)\right), \quad 1 - \exp\left(-\beta(r)\left(r - r_e\right)\right) > 0 \tag{3}$$

$$-\sqrt{\frac{V(r) - V_e}{\mathfrak{D}_e}} = 1 - \exp\left(-\beta(r)(r - r_e)\right), \quad 1 - \exp\left(-\beta(r)\left(r - r_e\right)\right) < 0, \tag{4}$$

and after considering the behavior of the exp function more carefully we have:

$$+\sqrt{\frac{V(r) - V_e}{\mathfrak{D}_e}} = 1 - \exp\left(-\beta(r)\left(r - r_e\right)\right), \quad \beta(r)(r - r_e) > 0 \tag{5}$$

$$-\sqrt{\frac{V(r) - V_e}{\mathfrak{D}_e}} = 1 - \exp\left(-\beta(r)\left(r - r_e\right)\right), \quad \beta(r)(r - r_e) < 0. \tag{6}$$

Rearranging, we get:

$$\beta(r)\left(r - r_e\right) = -\ln\left(1 - \sqrt{\frac{V - V_e}{\mathfrak{D}_e}}\right), \quad \beta(r)(r - r_e) > 0 \tag{7}$$

$$\beta(r)\left(r - r_e\right) = -\ln\left(1 + \sqrt{\frac{V - V_e}{\mathfrak{D}_e}}\right), \quad \beta(r)(r - r_e) < 0. \tag{8}$$

We also know that $\ln(\cdot) > 0$ for arguments greater than 1, and $\ln(\cdot) < 0$ for arguments smaller than 1, and that $\sqrt{\frac{V-V_e}{\mathfrak{D}_e}} > 0$, we can conclude the following, which completely agrees with what we derived above:

$$\ln\left(1-\sqrt{\frac{V-V_e}{\mathfrak{D}_e}}\right) < 0 \tag{9}$$

$$\ln\left(1-\sqrt{\frac{V-V_e}{\mathfrak{D}_e}}\right) > 0. \tag{10}$$

Rearranging again yields:

$$\beta(r) = \frac{\ln\left(1-\sqrt{\frac{V-V_e}{\mathfrak{D}_e}}\right)}{r_e - r}, \quad \beta(r)(r-r_e) > 0 \tag{11}$$

$$\beta(r) = \frac{\ln\left(1+\sqrt{\frac{V-V_e}{\mathfrak{D}_e}}\right)}{r_e - r}, \quad \beta(r)(r-r_e) < 0. \tag{12}$$

We can now :

- choose to use ***only*** Eq. 11 with the consequence that $\beta(r)$ will be negative in the inner wall of the potential well, then will switch signs at r_e; or we can
- choose to use ***only*** Eq. 12 with the consequence that $\beta(r)$ will be positive in the inner wall of the potential well, then will switch signs at r_e; or we can
- choose $\beta(r)$ to be always positive, with the consequence that we would have to switch at r_e from using Eq. 12 in the inner wall to using Eq. 11 in the outer wall; or (among maybe other choices?) we can just
- choose either Eq. 12 or Eq. 11 for each individual value of r depending on which choice gives us a smaller residual, but with the consequence that $\beta(r)$ will often be switching signs.

LINEAR REGRESSION

Remember that:

$$\beta(r) \equiv \beta_0 x(r)^0 + \beta_1 x(r)^1 + \beta_2 x(r)^2 \cdots \beta_N x(r)^N, \tag{13}$$

$$x(r) \equiv \frac{r^p - r_e^p}{r^p + r_e^p}, \tag{14}$$

for some value of p that is larger than 1. We now have the following formula (with the $\pm$ chosen in whatever of the above described ways that we wish to choose):

$$\frac{\ln\left(1\pm\sqrt{\frac{V(r)-V_e}{\mathfrak{D}_e}}\right)}{r_e - r} = \beta(r) \equiv \beta_0 x(r)^0 + \beta_1 x(r)^1 + \beta_2 x(r)^2 \cdots \beta_N x(r)^N \tag{15}$$

By defining the LHS to be $y(r)$ we can write the last equation in a way that resembles the classic linear regression formula:

$$y(r) = \vec{x}(r)^{\mathrm{T}}\vec{\beta} + \varepsilon(r), \tag{16}$$

in which,

$$\vec{\beta} \equiv \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_N \end{pmatrix}, \vec{x} \equiv \begin{pmatrix} x(r)^0 \\ x(r)^1 \\ x(r)^2 \\ \vdots \\ x(r)^N \end{pmatrix}. \tag{17}$$

If we know $V(r)$ at N_V different values of r, then we can define the following vectors:

$$\vec{y} \equiv \begin{pmatrix} y(r_0) \\ y(r_1) \\ y(r_3) \\ \vdots \\ y(r_{N_v}) \end{pmatrix}, \vec{\epsilon} \equiv \begin{pmatrix} \epsilon(r_0) \\ \epsilon(r_1) \\ \epsilon(r_3) \\ \vdots \\ \epsilon(r_{N_v}) \end{pmatrix}, \tag{18}$$

and the following matrix:

$$\mathrm{X} \equiv \begin{pmatrix} x(r_0)^0 & x(r_0)^1 & x(r_0)^2 & \cdots & x(r_0)^N \\ x(r_1)^0 & x(r_1)^1 & x(r_1)^2 & \cdots & x(r_1)^N \\ x(r_2)^0 & x(r_2)^1 & x(r_2)^2 & \cdots & x(r_2)^N \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x(r_{N_V})^0 & x(r_{N_V})^1 & x(r_{N_V})^2 & \cdots & x(r_{N_V})^N \end{pmatrix}. \tag{19}$$

We now have the following desired equation:

$$\vec{y} = X\vec{\beta}, \tag{20}$$

with the following solution (with \ being the "backslash operator" which is readily available in MATLAB, Octave or Julia):

$$\vec{\beta} = X \backslash \vec{y} \tag{21}$$