

# betaFIT: A software for fitting points to functions

## EXTENDEND MORSE OSCILLATOR

Consider the EMO function:

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

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:

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

$V(r) \geq V_e$  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:

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

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

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

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

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

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

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

Rearranging, we get:

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

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

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:

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

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

Rearranging again yields:

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

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

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:

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

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

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):

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

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

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

in which,

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

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

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

and the following matrix:

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

We now have the following desired equation:

$$\vec{y} = X\vec{\beta}, \quad (20)$$

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

$$\vec{\beta} = X\backslash\vec{y} \quad (21)$$