

Convolution of a Gaussian with an exponential (and its application in programs halflife.c/nanofit.f)

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1 Derivation of the convolution

The convolution of a normalised (unit area) Gaussian and an exponential is derived below (special thanks to Dr. Dave Forest (University of Birmingham) for the maths in Section 1.

Taking a Gaussian function, $G(x)$, of full-width at half maximum (FWHM) of $2\sigma\sqrt{2\ln(2)} = 2.35\sigma$ (see Section 2),

$$G(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2}} \quad (1)$$

The exponential function is defined with decay constant, λ , as,

$$F(x) = e^{-\lambda x} \quad (2)$$

The convolution is given by,

$$\begin{aligned} I(y) &= F(x) * G(x) \equiv \frac{1}{\sigma\sqrt{2\pi}} \int_0^\infty e^{-\lambda x} e^{-\frac{(y-x)^2}{2\sigma^2}} dx \\ &= \frac{1}{\sigma\sqrt{2\pi}} \int_0^\infty e^{-\frac{(x^2 + 2\sigma^2\lambda x - 2xy + y^2)}{2\sigma^2}} dx \end{aligned} \quad (3)$$

Now use the transformation,

$$z = \frac{1}{\sqrt{2}\sigma} (x - (y - \sigma^2\lambda)) \quad (4)$$

This yields:

$$\begin{aligned} &dx = \sqrt{2}\sigma dz \\ \Rightarrow \text{ at } x = \infty, z = \infty \text{ and at } x = 0, z &= \frac{-(y - \sigma^2\lambda)}{\sqrt{2}\sigma} \\ z^2 &= \frac{(x^2 + y^2 + \sigma^4\lambda^2 - 2xy + 2\sigma^2\lambda x - 2y\sigma^2\lambda)}{2\sigma^2} \\ \Rightarrow \frac{(x^2 + 2\sigma^2\lambda x - 2xy + y^2)}{2\sigma^2} &= z^2 + \lambda \left(y - \frac{\sigma^2\lambda}{2} \right) \end{aligned} \quad (5)$$

The results from Eqns. 5 above, can be substituted into Eqn. 3, leading to,

$$I(y) = \frac{1}{\sqrt{\pi}} e^{-\lambda \left(y - \frac{\sigma^2\lambda}{2} \right)} \int_{\frac{-(y - \sigma^2\lambda)}{\sqrt{2}\sigma}}^\infty e^{-z^2} dz \quad (6)$$

The error function, $\text{erf}(x)$, can be introduced as follows:

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-z^2} dz \quad (7)$$

and corresponds to the area under the Gaussian curve between $-x$ and x . However, $\text{erf}(x)$ is defined for all values of x and is an odd function, such that $\text{erf}(-x) = -\text{erf}(x)$. See Fig. 1. Correspondingly, the complementary error function, $\text{erfc}(x)$, is the area outside of $-x$ and x implying,

$$\text{erfc}(x) = 1 - \text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-z^2} dz \quad (8)$$

Figure 1: A plot of the error function, $\text{erf}(x)$.

Using the above result (Eqn. 8) in Eqn. 6 leads to,

$$\begin{aligned} I(y) &= \frac{1}{\sqrt{\pi}} e^{-\lambda(y - \frac{\sigma^2 \lambda}{2})} \left\{ \frac{\sqrt{\pi}}{2} \text{erfc} \left(\frac{-(y - \sigma^2 \lambda)}{\sqrt{2}\sigma} \right) \right\} \\ &= \frac{1}{2} e^{-\lambda(y - \frac{\sigma^2 \lambda}{2})} \left[1 - \text{erf} \left(\frac{-(y - \sigma^2 \lambda)}{\sqrt{2}\sigma} \right) \right] \end{aligned} \quad (9)$$

The final result for the convolution is, therefore,

$$\boxed{I(y) = \frac{1}{2} e^{-\lambda(y - \frac{\sigma^2 \lambda}{2})} \left[1 + \text{erf} \left(\frac{(y - \sigma^2 \lambda)}{\sqrt{2}\sigma} \right) \right]} \quad (10)$$

For a non-zero offset for the Gaussian centroid, y is replaced by $y - k$, where k is the offset.

2 Gaussian FWHM

The FWHM is defined as the distance between two points either side of the Gaussian centroid at which the height falls to half of the height at the centroid, *i.e.*

$$FWHM = 2|x - y| \quad (11)$$

where the centroid lies at x and the Gaussian fall to half the centroid height at y , Such that,

$$\begin{aligned}
[G(x) - G(y)] &= [G(x) - \frac{G(x)}{2}] = \frac{1}{2}G(x) \\
\Rightarrow \frac{1}{\sigma\sqrt{2\pi}} \left[e^{\frac{-x^2}{2\sigma^2}} - e^{\frac{-y^2}{2\sigma^2}} \right] &= \frac{1}{2\sigma\sqrt{2\pi}} e^{\frac{-x^2}{2\sigma^2}} \\
\Rightarrow \frac{1}{2} e^{\frac{-x^2}{2\sigma^2}} - e^{\frac{-y^2}{2\sigma^2}} &= 1 \\
\Rightarrow e^{\frac{-x^2}{2\sigma^2}} &= 2e^{\frac{-y^2}{2\sigma^2}} \\
\Rightarrow \frac{(y^2 - x^2)}{2\sigma^2} &= \ln(2) \\
(y^2 - x^2) &= (y - x)(y + x) = |y - x|^2 = 2\sigma^2 \ln(2)
\end{aligned} \tag{12}$$

Therefore,

$$FWHM = 2\sigma\sqrt{2\ln(2)} = 2.35\sigma \tag{13}$$

3 Programs halflife.c/nanofit.f

In the eval function/subroutine the function is written as the instructions:

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x1 = x - pars(3)
ep = (0.5*pars(2))/(pars(1))
xsq = (x1/pars(2)) + ep
xt = x1/pars(1)
ep = ep*ep
e = xt + ep - xsq*xsq
fit = 0.5*erfpol(xsq)*exp(e)
e = xt + ep
fit = exp(e) - fit
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where, $\text{pars}(1) = -\tau = -1/\lambda$, $\text{pars}(2) = \sqrt{2}\sigma$, $\text{pars}(3) = \text{centroid of Gaussian} = \text{offset}$, k . Firstly, the equations from the code can be rewritten using the standard notation and ignoring k . Proceeding stepwise:

$$x1 = x - \text{pars}(3) \rightarrow x1 = y \tag{14}$$

$$\text{ep} = (0.5*\text{pars}(2))/(\text{pars}(1)) \rightarrow \text{ep} = \frac{-\lambda\sqrt{2}\sigma}{2} \tag{15}$$

$$\left(\Rightarrow \text{ep}^2 = \frac{\lambda^2\sigma^2}{2} \right) \tag{16}$$

$$\text{xsq} = (x1/\text{pars}(2)) + \text{ep} \rightarrow \text{xsq} = \frac{y}{\sqrt{2}\sigma} - \frac{\lambda\sqrt{2}\sigma}{2} \tag{17}$$

$$\left(\Rightarrow \text{xsq}^2 = \frac{y^2}{2\sigma^2} + \frac{\lambda^2\sigma^2}{2} - y\lambda \right) \tag{18}$$

$$\mathbf{xt} = \mathbf{x1}/\mathbf{pars}(1) \rightarrow \mathbf{xt} = -y\lambda \quad (19)$$

In the following, remember that the preceding line in the code sets \mathbf{ep} to \mathbf{ep}^2

$$\begin{aligned} \mathbf{e} = \mathbf{xt} + \mathbf{ep} - \mathbf{xsq*xsq} &\rightarrow \mathbf{e} = -y\lambda + \frac{\lambda^2\sigma^2}{2} - \frac{y^2}{2\sigma^2} - \frac{\lambda^2\sigma^2}{2} + y\lambda \\ &\mathbf{e} = -\frac{y^2}{2\sigma^2} \end{aligned} \quad (20)$$

The function $\text{erfpol}(x)$ [1], returns $[e^{x^2} \text{erfc}(|x|)]$

$$\begin{aligned} \mathbf{fit} &= 0.5*\text{erfpol}(\mathbf{xsq})*\exp(\mathbf{e}) \rightarrow \\ \mathbf{fit}_1 &= \frac{1}{2}e^{\left(\frac{y^2}{2\sigma^2} + \frac{\lambda^2\sigma^2}{2} - y\lambda\right)} e^{-\frac{y^2}{2\sigma^2}} \text{erfc}\left(\left|\frac{y}{\sqrt{2}\sigma} - \frac{\lambda\sqrt{2}\sigma}{2}\right|\right) \end{aligned} \quad (21)$$

$$\mathbf{fit}_1 = \frac{1}{2}e^{-\lambda\left(y - \frac{\sigma^2\lambda}{2}\right)} \text{erfc}\left(\left|\frac{y - \lambda\sigma^2}{\sqrt{2}\sigma}\right|\right) \quad (22)$$

Continuing down the code

$$\mathbf{e} = \mathbf{xt} + \mathbf{ep} \rightarrow \mathbf{e} = -y\lambda + \frac{\sigma^2\lambda^2}{2} = -\lambda\left(y - \frac{\sigma^2\lambda}{2}\right) \quad (23)$$

$$\begin{aligned} \mathbf{fit} = \exp(\mathbf{e}) - \mathbf{fit} &\rightarrow \mathbf{fit}_2 = e^{-\lambda\left(y - \frac{\sigma^2\lambda}{2}\right)} - \frac{1}{2}e^{-\lambda\left(\frac{y - \sigma^2\lambda}{2}\right)} \text{erfc}\left(\left|\frac{y - \sigma^2\lambda}{\sqrt{2}\sigma}\right|\right) \\ \mathbf{fit}_2 &= \frac{1}{2}e^{-\lambda\left(y - \frac{\sigma^2\lambda}{2}\right)} \left[2 - \text{erfc}\left(\left|\frac{y - \sigma^2\lambda}{\sqrt{2}\sigma}\right|\right)\right] \end{aligned} \quad (24)$$

However, substituting from Section 1, Eqn. 8 yields, $2 - \text{erfc}(x) = 1 + (1 - \text{erfc}(x)) = 1 + \text{erf}(x)$. This gives the final result of

$$\mathbf{fit}_2 = \frac{1}{2}e^{-\lambda\left(y - \frac{\sigma^2\lambda}{2}\right)} \left[1 + \text{erf}\left(\left|\frac{y - \sigma^2\lambda}{\sqrt{2}\sigma}\right|\right)\right] \quad (25)$$

This exactly matches the earlier result of Eqn. 10.

References

- [1] C. Hastings, *Approximations for Digital Computers*, Princeton University Press, Princeton, New Jersey (1955).