# Interval Bound Hills with Zero Derivative

Andrew White

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## 1 An interval sigmoid with exact tails

To achive a sigmoid on an interval with exactly zero tails, I'd like to find 3rd degree polynomial with the following properties:

$$\begin{array}{ll} f(0) = 1 & f'(0) = 0 \\ f(1) = 0 & f'(1) = 0 \end{array}$$

This polynomial will work:

$$u(x) = 2x^3 - 3x^2 + 1 \tag{1}$$

## 2 Gaussian with Boundary Condition

The hills will be added at $x$ and $s$ is the resulting bias. I'd like a guassian with the following boundary condition:

$$\frac{\partial}{\partial x} e^{-(x-s)^2/\sigma^2} h(s,x) = 0$$

$$\frac{\partial h(s,x)}{\partial s} = \frac{2(s-x)}{\sigma} h(s,x)$$

$$h(s,x) = e^{(x-s)^2/\sigma^2}$$

Therefore, the function should be

$$e^{-(x-s)^2/\sigma^2} \left[ e^{(x-s)^2/\sigma^2} u(s) + (1 - u(s)) \right]$$

Adding an additional constraint on $G(s,x) = C(x)$ is, we have the following equation for a single boundary:

$$G(s,x) = e^{-(x-s)^2/\sigma^2} + \left( C(x) - e^{-(x-s)^2/\sigma^2} \right) u(s) \tag{2}$$

## 3 Gaussian with 2 Boundary Conditions

$$G(s,x) = e^{-(x-s)^2/\sigma^2} + \left(e^{-(x-L)^2/\sigma^2} - e^{-(x-s)^2/\sigma^2}\right) u\left(\frac{s-L}{b\sigma}\right)$$
$$+ \left(e^{-(U-x)^2/\sigma^2} - e^{-(x-s)^2/\sigma^2}\right) u\left(\frac{U-s}{b\sigma}\right) \tag{3}$$

## 4 Boundary Corrected Gaussian with Zero Derivatives in 1D

Now we must calculate the correction, just like in McGovern-De Pablo Hills

$$\int G(s,x)dx = A$$

All the exponential terms are corrected just like normal McGovern-De Pablo equations. The ones that do not depend on $s$ are, presuming the bounds are far greater than $2b\sigma$, just half the integral of the exponential. I'll indicate the McGovern De-Pablo correction as $m(s,U,L)$.

$$\bar{G}(s,L,U,b,\sigma) = m(s,U,L) + \left(\frac{1}{2}\sqrt{\pi}\sigma\,\mathrm{erf}\left(\frac{U-L}{\sigma}\right) - m(s,U,L)\right) u\left(\frac{s-L}{b\sigma}\right) +$$
$$\left(\frac{1}{2}\sqrt{\pi}\sigma\,\mathrm{erf}\left(\frac{U-L}{\sigma}\right) - m(s,U,L)\right) u\left(\frac{U-s}{b\sigma}\right) \tag{4}$$
$$m(s,U,L) = \frac{\sqrt{\pi}}{2}\sigma\left[\mathrm{erf}\left(\frac{s-L}{\sigma}\right) + \mathrm{erf}\left(\frac{U-s}{\sigma}\right)\right] \tag{5}$$

## 5 1D Derivatives

$$\frac{\partial G}{\partial s} = \frac{2(s-x)}{\sigma^2}e^{-(x-s)^2/\sigma^2} +$$
$$\left(e^{-(x-L)^2/\sigma^2} - e^{-(x-s)^2/\sigma^2}\right)\frac{\partial u}{\partial x}\left(\frac{s-L}{b\sigma}\right)\frac{1}{b\sigma} - \frac{2(s-x)}{\sigma^2}e^{-(x-s)^2/\sigma^2}u\left(\frac{s-L}{b\sigma}\right) -$$
$$\left(e^{-(U-x)^2/\sigma^2} - e^{-(x-s)^2/\sigma^2}\right)\frac{\partial u}{\partial x}\left(\frac{U-s}{b\sigma}\right)\frac{1}{b\sigma} - \frac{2(s-x)}{\sigma^2}e^{-(x-s)^2/\sigma^2}u\left(\frac{U-s}{b\sigma}\right)$$
$$\frac{\partial \bar{G}}{\partial s} = \frac{\partial m(s,U,L)}{\partial s} + \left(\frac{1}{2}\sqrt{\pi}\sigma\,\mathrm{erf}\left(\frac{U-L}{\sigma}\right) - m(s,U,L)\right)\frac{\partial u}{\partial x}\left(\frac{s-L}{b\sigma}\right)\frac{1}{b\sigma} - \frac{\partial m(s,U,L)}{\partial s}u\left(\frac{s-L}{b\sigma}\right) -$$
$$\left(\frac{1}{2}\sqrt{\pi}\sigma\,\mathrm{erf}\left(\frac{U-L}{\sigma}\right) - m(s,U,L)\right)\frac{\partial u}{\partial x}\left(\frac{U-s}{b\sigma}\right)\frac{1}{b\sigma} - \frac{\partial m(s,U,L)}{\partial s}u\left(\frac{U-s}{b\sigma}\right)$$
$$\frac{\partial G/\bar{G}}{\partial s} = \frac{\frac{\partial G}{\partial s}\bar{G} - \frac{\partial \bar{G}}{\partial s}G}{\bar{G}^2}$$

## 6 Hard Boundaries..?

For a hard boundary, we desire

$$\frac{\partial}{\partial x} e^{-(x-s)^2/\sigma^2} h(s, x) = \infty$$