

Interval Bound Hills with Zero Derivative

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1 An interval sigmoid with exact tails

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

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

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 gaussian with the following boundary condition:

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

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

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

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 $m(s, U, L)$.

$$\bar{G}(s, L, U, b, \sigma) = m(s, U, L) + \left(\frac{1}{2}\sqrt{\pi}\sigma - m(s, U, L) \right) u\left(\frac{s-L}{b\sigma}\right) + \\ \left(\frac{1}{2}\sqrt{\pi}\sigma - m(s, U, L) \right) u\left(\frac{U-s}{b\sigma}\right) \quad (4)$$

$$m(s, U, L) = \frac{\sqrt{\pi}}{2}\sigma \left[\operatorname{erf}\left(\frac{s-L}{\sigma}\right) + \operatorname{erf}\left(\frac{U-s}{\sigma}\right) \right] \quad (5)$$

5 1D Derivatives

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