Skewed Temperature Response Functions

1/30/15

$$R(T) = \alpha T^n \left(1 - \left(\frac{T - T_{opt}}{\sigma}\right)^2\right) \quad (\underline{\text{Power Laws}})$$

$$0 = \frac{\partial R}{\partial T} = \frac{\partial}{\partial T}\left[\alpha\left[T^n - \frac{T^{n+2}}{\sigma^2} + \frac{2T^{n+1}T_{opt}}{\sigma^2} - \frac{T_{opt}^2 T^n}{\sigma^2}\right]\right]$$

$$= \cancel{\alpha}\left[nT^{n-1} - (n+2)\frac{T^{n+1}}{\sigma^2} + \frac{2(n+1)T^n T_{opt}}{\sigma^2} - \frac{nT_{opt}^2 T^{n-1}}{\sigma^2}\right]$$

$$= \frac{n}{\sigma^2} T_{opt}^2 - \left(\frac{2(n+1)T_{pk}}{\sigma^2}\right) T_{opt} + \left(-n + \frac{(n+2)}{\sigma^2} T_{pk}^2\right)$$

$$T_{opt} = \frac{+\frac{2(n+1)T_{pk}}{\sigma^2} \pm \sqrt{\left(-\frac{2(n+1)T_{pk}}{\sigma^2}\right)^2 - 4\left(-n + \frac{(n+2)}{\sigma^2}T_{pk}^2\right)\frac{n}{\sigma^2}}}{2\,\frac{n}{\sigma^2}}$$

$$= \left(\frac{n+1}{n}\right) T_{pk} \pm \sqrt{\left[\frac{(n+1)}{n} T_{pk}\right]^2 - \frac{\sigma^2}{n}\left(-n + \frac{(n+2)}{\sigma^2} T_{pk}^2\right)}$$

$$= T_{pk}\left[\frac{n+1}{n} \pm \sqrt{\underbrace{\left(\frac{n+1}{n}\right)^2 + \frac{\sigma^2}{T_{pk}^2} - \frac{(n+2)}{n}}_{= \frac{\cancel{n^2} + \cancel{2n} + 1 - \cancel{n^2} - \cancel{2n}}{n^2} + \frac{\sigma^2}{T_{pk}^2} = \frac{1}{n^2} + \frac{\sigma^2}{T_{pk}^2}}}\right]$$

$$\Rightarrow \boxed{T_{opt} = \frac{T_{pk}}{n}\left[n+1 \pm \sqrt{1 + \left(\frac{n\sigma}{T_{pk}}\right)^2}\right]}$$

If $\left(\frac{n\sigma}{T_{pk}}\right)^2 \gg 1$,

choose "−" sign because actual peak is <u>higher</u> than Topt parameter

$$T_{opt} \sim \frac{T_{pk}}{n}\left[n+1 - \frac{n\sigma}{T_{pk}}\right] = T_{pk}\frac{(n+1)}{n} - \sigma \underset{\text{for } n \gg 1}{\sim} T_{pk} - \sigma$$

If $\left(\frac{n\sigma}{T_{pk}}\right)^2 \ll 1$

$$T_{opt} \sim T_{pk}\left(\frac{n+1}{n}\right) \underset{\text{for } n \gg 1}{\sim} T_{pk}$$

$$\Rightarrow \boxed{R(T)} = \alpha T^n \left(1 - \left(\frac{T - T^*_{pk} + \sigma}{\sigma} \right)^2 \right)$$

$$= \alpha T^n \left(\cancel{1} - \left(\frac{T - T^*_{pk}}{\sigma} \right)^2 - \cancel{\left(\frac{\sigma}{\sigma} \right)^2} - \frac{2}{\sigma^2} (T - T^*_{pk}) \sigma \right)$$

$$= \alpha T^n \frac{(T^*_{pk} - T)}{\sigma} \left[2 - \frac{(T^*_{pk} - T)}{\sigma} \right]$$

$$\boxed{= \alpha T^n \frac{\left(T_{pk} \left(\frac{n+1}{n} \right) - T \right)}{\sigma} \left[2 - \frac{\left(T_{pk} \left(\frac{n+1}{n} \right) - T \right)}{\sigma} \right]}$$

T_{pk} = peak

σ = breadth

n = skewness control [could even try $n = \frac{T_{pk} - T_{min}}{T_{max} - T_{pk}}$]

α = height of response

Response Functions

Another Alternative with Exponential, like Q_{10},

$$R(T) = \alpha e^{sT}\left(1 - \left(\frac{T - T_{opt}}{\sigma}\right)^2\right)$$

$$0 = \frac{\partial R}{\partial T} = \cancel{\alpha e^{sT}} s\left(1 - \left(\frac{T - T_{opt}}{\sigma}\right)^2\right) - 2\cancel{\alpha e^{sT}}\left(\frac{T - T_{opt}}{\sigma^2}\right)$$

$$\Rightarrow 0 = s\sigma^2 - sT^2 - sT_{opt}^2 + 2TT_{opt}s - 2T + 2T_{opt}$$

$$= sT_{opt}^2 + (-2T_{pk}s - 2)T_{opt} + (-s\sigma^2 + sT_{pk}^2 + 2T_{pk})$$

$$= T_{opt}^2 - 2\left(T_{pk} + \frac{1}{s}\right)T_{opt} + \left(T_{pk}^2 + \frac{2T_{pk}}{s} - \sigma^2\right)$$

$$\Rightarrow T_{opt} = \frac{+2\left(T_{pk} + \frac{1}{s}\right) \pm \sqrt{\left(2\left(T_{pk} + \frac{1}{s}\right)\right)^2 - 4 \cdot 1 \cdot \left(T_{pk}^2 + \frac{2T_{pk}}{s} - \sigma^2\right)}}{2}$$

$$= T_{pk} + \frac{1}{s} \pm \sqrt{\left(T_{pk} + \frac{1}{s}\right)^2 - \left(T_{pk}^2 + \frac{2T_{pk}}{s} - \sigma^2\right)}$$

$$\cancel{T_{pk}^2} + \cancel{\frac{2T_{pk}}{s}} + \left(\frac{1}{s}\right)^2 - \cancel{T_{pk}^2} - \cancel{\frac{2T_{pk}}{s}} + \sigma^2$$

$$= T_{pk} + \frac{1}{s} \pm \left(\frac{1}{s}\sqrt{1 + (s\sigma)^2}\right)$$

If $s\sigma \gg 1$,

$$T_{opt} \sim T_{pk} + \frac{1}{s} \pm \frac{1}{\cancel{s}}\cancel{s}\sigma$$

If $s\sigma \ll 1$,

$$T_{opt} \sim T_{pk}.$$

$T_{pk} \approx T_{opt} - \frac{1}{s} + \sigma$, so $\boxed{T_{opt} \sim T_{pk} + \frac{1}{s} - \sigma}$

to shift up

$$\frac{\left[\left(T-\left(T_{pk}+\frac{1}{s}\right)\right)+\sigma\right]^2}{\sigma^2}$$

$$\|$$

Thus,

$$R(T)=\alpha e^{sT}\left(1-\frac{\left(T-\left(T_{pk}+\frac{1}{s}-\sigma\right)\right)^2}{\sigma^2}\right)$$

$$=\alpha e^{sT}\left(\cancel{1}-\frac{\left(T-\left(T_{pk}+\frac{1}{s}\right)\right)^2}{\sigma^2}-\cancel{\frac{\sigma^2}{\sigma^2}}\cancel{-2\left(T-\left(T_{pk}+\frac{1}{s}\right)\right)\sigma}\;\frac{2\left(T-\left(T_{pk}+\frac{1}{s}\right)\right)}{\sigma}\right]$$

Similar to before except $T_{pk}^{*}=T_{pk}+\frac{1}{s}$ instead of $T_{pk}\left(\frac{n+1}{n}\right)$.

$$\Rightarrow \boxed{R(T)}=\alpha e^{sT}\left[\frac{2\left(\left(T_{pk}+\frac{1}{s}\right)-T\right)}{\sigma}-\frac{\left(T-\left(T_{pk}+\frac{1}{s}\right)\right)^2}{\sigma^2}\right]$$

$$\boxed{=\alpha e^{sT}\left[\frac{\left(T_{pk}+\frac{1}{s}\right)-T}{\sigma}\right]\left[2-\frac{\left[\left(T_{pk}+\frac{1}{s}\right)-T\right]}{\sigma}\right]}$$

T_{pk} = peak

σ = breadth

s = skewness control [could even be $s=\frac{T_{pk}-T_{min}}{T_{max}-T_{pk}}$]

α = height of response

Response Functions

2/4/16

Another Alternative with Exponential, like Boltzmann,

$$R(T) = \alpha e^{-\frac{E}{kT}}\left(1 - \left(\frac{T - T_{opt}}{\sigma}\right)^2\right)$$

$$0 = \frac{\partial R}{\partial T} = \cancel{\alpha} e^{-\frac{E}{kT}}\left(\frac{-E}{kT^2}\right)\left(1-\left(\frac{T-T_{opt}}{\sigma}\right)^2\right) - 2\cancel{\alpha}e^{-\frac{E}{kT}}\left(\frac{T-T_{opt}}{\sigma^2}\right)$$

$$\Rightarrow 0 = -\frac{E\sigma^2}{kT^2} + \frac{E}{k\cancel{T^2}}\cancel{T^2} + \frac{E}{kT^2}T_{opt}^2 - 2TT_{opt}\frac{E}{kT^2} - 2T + 2T_{opt}$$

$$= \frac{E}{kT^2}T_{opt}^2 + \left(2 - 2\cancel{T}\frac{E}{kT^{\cancel{2}}}\right)T_{opt} + \left(\frac{E}{k} - 2T - \frac{E\sigma^2}{kT^2}\right)$$

$$\Rightarrow T_{opt} = \frac{-\cancel{2}\left(1-\frac{E}{kT}\right) \pm \sqrt{\cancel{4}\left(1-\frac{E}{kT}\right)^2 - \cancel{4}\frac{E}{kT^2}\left(\frac{E}{k} - 2T - \frac{E\sigma^2}{kT^2}\right)}}{\cancel{2}\left(\frac{E}{kT^2}\right)}$$

$$= -\frac{kT^2}{E} + T \pm \underbrace{\sqrt{\left(\frac{kT^2}{E}-T\right)^2 - \frac{kT^2}{E}\left(\frac{E}{k} - 2T - \frac{E\sigma^2}{kT^2}\right)}}_{\left(\frac{kT^2}{E}\right)^2 + \cancel{T^2} - 2\frac{kT^3}{E} - \cancel{T^2} + \cancel{2\frac{kT^3}{E}} + \sigma^2}$$

$$= T - \frac{kT^2}{E} \pm \frac{kT^2}{E}\sqrt{1 + \left(\frac{E\sigma}{kT^2}\right)^2}$$

If $\frac{E\sigma}{kT} \gg 1$,

$$\boxed{T_{opt} \sim T_{pk} - \frac{kT^2}{E} \pm \left(\frac{kT^2}{\cancel{E}}\right)\left(\frac{\cancel{E}\sigma}{kT^2}\right) = T_{pk}\left(1 - \frac{kT_{pk}}{E}\right) \pm \sigma \sim T_{pk}\left(1-\frac{kT_{pk}}{E}\right) - \sigma}$$

to shift down from peak.

If $\frac{E\sigma}{kT} \ll 1$, $T_{opt} \sim T_{pk} - \frac{kT^2}{E} \pm \frac{kT^2}{E} \sim T_{pk}$.

Thus,

$$R(T) = \alpha e^{-\frac{E}{kT}}\left(1 - \frac{\left(T - T_{pk}\left(1-\frac{kT_{pk}}{E}\right) + \sigma\right)^2}{\sigma^2}\right)$$

$$= \alpha e^{-\frac{E}{kT}}\left(\cancel{1} - \frac{\left(T - T_{pk}\left(1-\frac{kT_{pk}}{E}\right)\right)^2}{\sigma^2} - \cancel{\frac{\sigma^2}{\sigma^2}} - \frac{2\left(T - \left(T_{pk}\left(1-\frac{kT_{pk}}{E}\right)\right)\right)}{\sigma}\right)$$

Similar to before except $T_{pk}^* = T_{pk}\left(1-\frac{kT_{pk}}{E}\right)$ instead of $T_{pk}+\frac{1}{s}$ or $T_{pk}\left(\frac{n+1}{n}\right)$

$$\boxed{R(T)} = \alpha e^{-\frac{E}{kT}}\left[2\frac{\left(T_{pk}\left(1-\frac{kT_{pk}}{E}\right) - T\right)}{\sigma} - \frac{\left(T - \left(T_{pk}\left(1-\frac{kT_{pk}}{E}\right)\right)\right)^2}{\sigma^2}\right]$$

$$\boxed{= \alpha e^{-\frac{E}{kT}}\frac{\left(T_{pk}\left(1-\frac{kT_{pk}}{E}\right) - T\right)}{\sigma}\left[2 - \frac{\left(T_{pk}\left(1-\frac{kT_{pk}}{E}\right) - T\right)}{\sigma}\right]}$$

T_{pk} = peak

α = height of response

σ = breadth

$\beta \equiv \frac{E}{k}$ = skewness control

Peak Temperature for Johnson-Lewin Model

$$0 = \frac{\partial R}{\partial T} = \frac{-S_1 \cancel{\alpha} e^{-\frac{S_1}{T}}}{\cancel{1+\left(\frac{S_1}{S_2-S_1}\right)e^{-S_2\left(\frac{1}{T}-\frac{1}{T_{opt}}\right)}}}$$

$$- \frac{\alpha \cancel{e^{-\frac{S_1}{T}}} \left(\frac{S_1}{S_2-S_1}\right)\left(\frac{S_2}{T^2}\right) e^{-S_2\left(\frac{1}{T}-\frac{1}{T_{opt}}\right)}}{\left(1+\left(\frac{S_1}{S_2-S_1}\right)e^{-S_2\left(\frac{1}{T}-\frac{1}{T_{opt}}\right)}\right)^{\cancel{2}}}$$

$$0 = S_1 + \left(\frac{S_1^2}{S_2-S_1}\right)e^{-S_2\left(\frac{1}{T}-\frac{1}{T_{opt}}\right)} + \left(\frac{S_1 S_2}{S_2-S_1}\right)\frac{1}{T^2}e^{-S_2\left(\frac{1}{T}-\frac{1}{T_{opt}}\right)}$$

$$\Rightarrow -S_1 e^{S_2\left(\frac{1}{T}-\frac{1}{T_{opt}}\right)} = \frac{S_1(S_1+S_2)}{S_2-S_1}$$

$$\Rightarrow e^{S_2\left(\frac{1}{T}-\frac{1}{T_{opt}}\right)} = -\frac{S_1+S_2}{S_2-S_1} = \frac{S_1+S_2}{S_1-S_2}$$

$$\Rightarrow \frac{1}{T_{pk}} - \frac{1}{T_{opt}} = \frac{1}{S_2}\ln\left(\frac{S_1+S_2}{S_1-S_2}\right)$$

$$\Rightarrow \boxed{\frac{1}{T_{opt}} = \frac{1}{T_{pk}} - \frac{1}{S_2}\ln\left(\frac{S_1+S_2}{S_1-S_2}\right)}$$

$$\Rightarrow \boxed{R(T)} = \frac{\alpha e^{-\frac{S_1}{T}}}{1+\frac{S_1}{S_2-S_1}e^{-\frac{S_2}{T}+S_2\left(\frac{1}{T_{pk}}-\frac{1}{S_2}\ln\left(\frac{S_1+S_2}{S_1-S_2}\right)\right)}} = \frac{\alpha e^{-\frac{S_1}{T}}}{1+\frac{S_1}{S_2-S_1}e^{-\ln\left(\frac{S_1+S_2}{S_2-S_1}\right)}e^{-S_2\left(\frac{1}{T}-\frac{1}{T_{pk}}\right)}}$$

$$= \frac{\alpha e^{-\frac{S_1}{T}}}{1+\frac{S_1}{S_2-S_1}\frac{S_1-S_2}{S_1+S_2}e^{-S_2\left(\frac{1}{T}-\frac{1}{T_{pk}}\right)}} = \boxed{\frac{\alpha e^{-\frac{S_1}{T}}}{1-\frac{S_1}{S_1+S_2}e^{-S_2\left(\frac{1}{T}-\frac{1}{T_{pk}}\right)}}}$$

Peak Temperature for β function

$$0 = \frac{\partial PDF\beta(a,b)}{\partial T} = \frac{c}{\beta(a,b)} \frac{\partial}{\partial T}\left[\left(\frac{T-s}{\sigma}\right)^{a-1} - \left(\frac{T-s}{\sigma}\right)^{a+b-2}\right]$$

$$= (a-1)\frac{(T-s)^{a-2}}{\sigma^{a-1}} - \frac{(a+b-2)}{\sigma^{a+b-2}}(T-s)^{a+b-3}$$

$$\Rightarrow 0 = \sigma^{b-1}(a-1) - (a+b-2)(T-s)^{b-1}$$

$$\Rightarrow (T_{pk}-s)^{b-1} = \frac{(a-1)\sigma^{b-1}}{(a+b-2)}$$

$$\Rightarrow \boxed{T_{pk} = \left[\frac{(a-1)\sigma^{b-1}}{a+b-2}\right]^{\frac{1}{b+1}} + s}$$

$$\boxed{= \left[\frac{a-1}{a+b-2}\right]^{\frac{1}{b-1}}\sigma + s}$$

$a+b = \frac{1}{\alpha}$, $a = \frac{\gamma}{\alpha}$, $b = \frac{1-\gamma}{\alpha}$, so

$$\boxed{T_{pk}} = \left[\frac{\frac{\gamma}{\alpha}-1}{\frac{1}{\alpha}-2}\right]^{\frac{1}{\left(\frac{1-\gamma}{\alpha}\right)-1}} \sigma + s = \boxed{\left[\frac{\gamma-\alpha}{1-2\alpha}\right]^{\frac{\alpha}{1-\gamma-\alpha}}\sigma + S}$$

or

$$\boxed{S = T_{pk} - \left[\frac{\gamma-\alpha}{1-2\alpha}\right]^{\frac{\alpha}{1-\gamma-\alpha}}}$$

Hence,

$$\frac{T-S}{\sigma} = \frac{T - T_{pk} + \left[\frac{\gamma-\alpha}{1-2\alpha}\right]^{\frac{\alpha}{1-\gamma-\alpha}}\sigma}{\sigma}$$

$$= \left(\frac{T-T_{pk}}{\sigma}\right) + \left[\frac{\gamma-\alpha}{1-2\alpha}\right]^{\frac{\alpha}{1-\gamma-\alpha}}$$

$$\boxed{\Rightarrow R(T) = C\,\frac{\left[\frac{(T-T_{pk})}{\sigma} + \left(\frac{\gamma-\alpha}{1-2\alpha}\right)^{\frac{\alpha}{1-\gamma-\alpha}}\right]^{a-1}\left[1-\left\{\frac{(T-T_{pk})}{\sigma} + \left(\frac{\gamma-\alpha}{1-2\alpha}\right)^{\frac{\alpha}{1-\gamma-\alpha}}\right]^{b-1}\Gamma(a+b)}{\Gamma(a)\Gamma(b)}}$$

5 parameters

γ = skew
α = breadth
C = height of response
T_{pk} = peak
σ = Tolerance $\Leftarrow$ seems like this should be computable from function and not a free parameter