

Mathematical notation of calibration models

The linear glucose calibration model uses a 1st order polynomial of the glucose concentration x to describe the location parameter of a Student- t distribution. The scale parameter was modeled as a 1st order polynomial function of the location and the distributions degree of freedom ν was estimated as a constant.

$$\begin{aligned}
 A_{360 \text{ nm}} &\sim \text{Student-}t(\text{loc}, \text{scale}, \nu) \\
 &\text{with} \\
 \text{loc} &= \mu_0 + \mu_1 x \\
 \text{scale} &= \text{loc} \cdot \text{scale}_1 + \text{scale}_0 \\
 \mu_0, \mu_1, \text{scale}_0, \text{scale}_1 &\in \mathbb{R} \\
 \nu &\in \mathbb{R} > 0
 \end{aligned} \tag{1}$$

In comparison to the linear version in Eq 1, the logistic glucose calibration model in Eq 2 uses the asymmetric logistic function (S1 File) to describe the location parameter.

$$\begin{aligned}
 A_{360 \text{ nm}} &\sim \text{Student-}t(\text{loc}, \text{scale}, \nu) \\
 &\text{with} \\
 s_0 &= -L_L + L_U \\
 s_1 &= e^c + 1 \\
 s_2 &= e^{-c} \\
 s_3 &= s_1^{s_1 s_2} \\
 \text{loc} &= L_L + s_0 \left(e^{s_3 \left(\frac{S(I_x - x)}{s_0} + \frac{c}{s_3} \right)} + 1 \right)^{-s_2} \\
 \text{scale} &= \text{loc} \cdot \text{scale}_1 + \text{scale}_0 \\
 L_L, L_U, I_x, S, c, \text{scale}_0, \text{scale}_1 &\in \mathbb{R} \\
 \nu &\in \mathbb{R} > 0
 \end{aligned} \tag{2}$$

Similar to the logistic glucose calibration model (Eq 2), the biomass calibration model in Eq 3 uses an asymmetric logistic function, but first applies a base-10 logarithm to the biomass concentration x . Due to the base-10 logarithm, the intercept and slope parameters ($I_{\log_{10}(x)}$, $S_{\log_{10}}$) of the biomass calibration model refer to the log scale.

backscatter \sim Student- t (loc, scale, ν)

with

$$s_0 = -L_L + L_U$$

$$s_1 = e^c + 1$$

$$s_2 = e^{-c}$$

$$s_3 = s_1^{s_1 s_2}$$

$$\text{loc} = L_L + s_0 \left(e^{s_3 \left(\frac{S_{\log_{10}}(I_{\log_{10}(x)} - \log_{10}(x)})}{s_0} + \frac{c}{s_3} \right)} + 1 \right)^{-s_2} \quad (3)$$

$$\text{scale} = \text{loc} \cdot \text{scale}_1 + \text{scale}_0$$

$$L_L, L_U, I_{\log_{10}(x)}, S_{\log_{10}}, c, \text{scale}_0, \text{scale}_1 \in \mathbb{R}$$

$$\nu \in \mathbb{R} > 0$$