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A note on the matrices X and G

Both X and G are based on standard samples. They do not involve the test samples.

Suppose on one micro-plate, there are $n\_{s}$ unique standard samples with known concentrations denoted by $x\_{Standard, 1}$, $x\_{Standard, 2}$, …, $x\_{Standard, n\_{s}}$, respectively. For the *l*th ($l=1,…, n\_{s}$) standard sample, there are $m\_{l}$ replicate measurements. Then the total number of replicated standard samples is $N\_{s}=\sum\_{l=1}^{n\_{s}}m\_{l}$.

The matrix $X$ is an $N\_{s}×4$ gradient matrix with columns being $\left(∂Q\left(x | b\right)/∂b\right)^{T}$ $b=\hat{b}$, and rows corresponding to each of the $N\_{s} $standard samples. The first $m\_{1}$ rows of the gradient matrix $X$ are identical, each row being $\left(∂Q\left(x\_{Standard, 1} | b\right)/∂b\right)^{T}$ with $b=\hat{b}$, thus denoted by being $\left(∂Q\left(x\_{Standard, 1} | \hat{b}\right)/∂b\right)^{T}$. The rows ($m\_{1}+1$) to $(m\_{1}+m\_{2})$ are also identical, each row being $\left(∂Q\left(x\_{Standard, 2} | \hat{b}\right)/∂b\right)^{T}$, and so on.

The matrix $G$ is a $N\_{s}×N\_{s}$ diagonal matrix with the first $m\_{1}$ diagonal elements equal to $\left(Q\left(x\_{Standard, 1} | \hat{b}\right)\right)\_{ }^{2\hat{θ}}$, the ($m\_{1}+1$)th to $(m\_{1}+m\_{2})$th diagonal element equal to $\left(Q\left(x\_{Standard, 2} | \hat{b}\right)\right)\_{ }^{2\hat{θ}}$, and so on.

For example, on one plate, there are 20 standard samples with unique known concentrations, each with two replicates. In this example, $n\_{s}=20$ and $m\_{l}=2$ for all $l=1,…, n\_{s}$. Therefore, the total number of replicated standard samples is $N\_{s}=40. $ The matrix $X$ is a $40×4$ matrix in the following form

$$X=\left(\begin{array}{c}\genfrac{}{}{0pt}{}{\frac{∂Q\left(x\_{Standard, 1}| \hat{b}\right)}{∂b\_{1}}, \frac{∂Q\left(x\_{Standard, 1}| \hat{b}\right)}{∂b\_{2}}, \frac{∂Q\left(x\_{Standard, 1}|\hat{b}\right)}{∂b\_{3}}, \frac{∂Q\left(x\_{Standard, 1}| \hat{b}\right)}{∂b\_{4}}}{\frac{∂Q\left(x\_{Standard, 1}| \hat{b}\right)}{∂b\_{1}}, \frac{∂Q\left(x\_{Standard, 1}| \hat{b}\right)}{∂b\_{2}}, \frac{∂Q\left(x\_{Standard, 1}| \hat{b}\right)}{∂b\_{3}}, \frac{∂Q\left(x\_{Standard, 1}| \hat{b}\right)}{∂b\_{4}}}\\ \genfrac{}{}{0pt}{}{\frac{∂Q\left(x\_{Standard, 2}| \hat{b}\right)}{∂b\_{1}}, \frac{∂Q\left(x\_{Standard, 2}| \hat{b}\right)}{∂b\_{2}}, \frac{∂Q\left(x\_{Standard, 2}| \hat{b}\right)}{∂b\_{3}}, \frac{∂Q\left(x\_{Standard, 2}| \hat{b}\right)}{∂b\_{4}}}{\frac{∂Q\left(x\_{Standard, 2}| \hat{b}\right)}{∂b\_{1}}, \frac{∂Q\left(x\_{Standard, 2}| \hat{b}\right)}{∂b\_{2}}, \frac{∂Q\left(x\_{Standard, 2}| \hat{b}\right)}{∂b\_{3}}, \frac{∂Q\left(x\_{Standard, 2}| \hat{b}\right)}{∂b\_{4}}}\\. \\.\\.\\\genfrac{}{}{0pt}{}{\frac{∂Q\left(x\_{Standard, 20}| \hat{b}\right)}{∂b\_{1}}, \frac{∂Q\left(x\_{Standard, 20}| \hat{b}\right)}{∂b\_{2}}, \frac{∂Q\left(x\_{Standard, 20}| \hat{b}\right)}{∂b\_{3}}, \frac{∂Q\left(x\_{Standard, 20}| \hat{b}\right)}{∂b\_{4}}}{\frac{∂Q\left(x\_{Standard, 20}| \hat{b}\right)}{∂b\_{1}}, \frac{∂Q\left(x\_{Standard, 20}| \hat{b}\right)}{∂b\_{2}}, \frac{∂Q\left(x\_{Standard, 20}| \hat{b}\right)}{∂b\_{3}}, \frac{∂Q\left(x\_{Standard, 20}| \hat{b}\right)}{∂b\_{4}}}\end{array}\right)\_{ }$$

where $b\_{1}$ to $b\_{4}$ are the parameters of the four-parameter logistic model that $b=\left(b\_{1}, b\_{2}, b\_{3}, b\_{4}\right)^{T}$.

And the matrix $G$ is a $40×40$ diagonal matrix in the following form

$$G=diag\left\{\left(Q\left(x\_{Standard, 1} | \hat{b}\right)\right)\_{ }^{2\hat{θ}},\left(Q\left(x\_{Standard, 1} | \hat{b}\right)\right)\_{ }^{2\hat{θ}},\left(Q\left(x\_{Standard, 2} | \hat{b}\right)\right)\_{ }^{2\hat{θ}},\right.$$

$\left.\left(Q\left(x\_{Standard, 2} | \hat{b}\right)\right)\_{ }^{2\hat{θ}},…, \left(Q\left(x\_{Standard, 20} | \hat{b}\right)\right)\_{ }^{2\hat{θ}},\left(Q\left(x\_{Standard, 20} | \hat{b}\right)\right)\_{ }^{2\hat{θ}}\right\}$.