

Supplementary material

Detection limits of chemical sensors: applications and misapplications

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Derivation of equation (11)

Starting from eq (10)

$$\begin{aligned}
 x_C^2 &= \frac{t^2 s_y^2}{r^2} \left(\frac{1}{k} + \frac{x_{LOD}^2 n}{D} + \frac{\sum x_i^2}{D} - \frac{2x_{LOD} \sum x_i}{D} \right) \\
 0 &= \frac{t^2 s_y^2}{r^2} \left(+x_C^2 \left(\frac{n}{D} - \frac{r^2}{t^2 s_y^2} \right) - x_{LOD} \frac{2\sum x_i}{D} + \frac{1}{k} + \frac{\sum x_i^2}{D} \right) \\
 0 &= x_C^2 \left(n - \frac{Dr^2}{t^2 s_y^2} \right) - x_C 2\sum x_i + \frac{D}{k} + \sum x_i^2 \\
 x_{C,1,2} &= \frac{1}{2 \left(n - \frac{Dr^2}{t^2 s_y^2} \right)} \left(2\sum x_i \pm \sqrt{\left(2\sum x_i \right)^2 - 4 \left(n - \frac{Dr^2}{t^2 s_y^2} \right) \left(\frac{D}{k} + \sum x_i^2 \right)} \right) \\
 x_{C,1,2} &= \frac{t^2 s_y^2}{nt^2 s_y^2 - Dr^2} \left(\sum x_i \pm \sqrt{\left(\sum x_i \right)^2 - n \frac{D}{k} + \frac{D^2 r^2}{kt^2 s_y^2} - n \sum x_i^2 + \frac{Dr^2}{t^2 s_y^2} \sum x_i^2} \right)
 \end{aligned}$$

With eq (6)

$$D = n \sum x_i^2 - \left(\sum x_i \right)^2$$

We insert...

$$x_{C,1,2} = \frac{t^2 s_y^2}{nt^2 s_y^2 - Dr^2} \left(\sum x_i \pm \sqrt{-n \frac{D}{k} + \frac{D^2 r^2}{kt^2 s_y^2} + \frac{Dr^2}{t^2 s_y^2} \sum x_i^2 - D} \right)$$

... and rearrange

$$x_{C,1,2} = \frac{ts_y}{nt^2 s_y^2 - Dr^2} \left(ts_y \sum x_i \pm \sqrt{\frac{D^2 r^2}{k} + Dr^2 \sum x_i^2 - n \frac{D}{k} t^2 s_y^2 - Dt^2 s_y^2} \right)$$

With $x_{LOD} = 2 x_C$ we obtain equation (11)

$$x_{LOD} = \frac{2ts_y}{nt^2 s_y^2 - Dr^2} \left(ts_y \sum x_i \pm \sqrt{\frac{D^2 r^2}{k} + Dr^2 \sum x_i^2 - n \frac{D}{k} t^2 s_y^2 - Dt^2 s_y^2} \right) \quad (11)$$

This has to be compared to the equation (4.19) in the article by Currie and Svehla [reference 4] which can be rearranged to give equation (14)

$$x_{LOD} = \frac{2t \sqrt{s_a^2 + s_y^2}}{b} \frac{1 - \frac{\sum x_i}{\sqrt{n \sum x_i^2}} \frac{s_a}{\sqrt{s_a^2 + s_y^2}} t \frac{s_b}{b}}{1 - t^2 \frac{s_b^2}{b^2}} \quad (14)$$

After rewriting equation (14) we obtain

$$x_{LOD} = \frac{\frac{2t \sqrt{s_a^2 + s_y^2}}{b} - \frac{2t \sqrt{s_a^2 + s_y^2}}{b} \frac{\sum x_i}{\sqrt{n \sum x_i^2}} \frac{s_a}{\sqrt{s_a^2 + s_y^2}} t \frac{s_b}{b}}{1 - t^2 \frac{s_b^2}{b^2}}$$

$$x_{LOD} = \frac{2tb \sqrt{s_a^2 + s_y^2} - 2t^2 \frac{\sum x_i}{\sqrt{n \sum x_i^2}} s_a s_b}{b^2 - t^2 s_b^2}$$

The variable names are different from Harris (ref [6] of the main article) and the names used in the article and we identify:

- sensitivity: $b \rightarrow r$
- uncertainty of the sensitivity: $s_b \rightarrow s_r$
- uncertainty of the intercept: $s_a \rightarrow s_b$

We therefore rewrite using our names

$$x_{LOD} = \frac{2tr \sqrt{s_b^2 + s_y^2} - 2t^2 \frac{\sum x_i}{\sqrt{n \sum x_i^2}} s_b s_r}{r^2 - t^2 s_r^2}$$

Insertion of equations (7)...

$$s_r = s_y \sqrt{\frac{n}{D}}; \quad s_b = s_y \sqrt{\frac{\sum x_i^2}{D}} \quad (7)$$

...gives:

$$x_{LOD} = \frac{2tr \sqrt{s_b^2 + s_y^2} - 2t^2 \frac{\sum x_i}{\sqrt{n \sum x_i^2}} s_b s_r}{r^2 - t^2 s_r^2}$$

$$x_{LOD} = \frac{2tr \sqrt{s_y^2 \frac{\sum x_i^2}{D} + s_y^2} - 2t^2 \frac{\sum x_i}{\sqrt{n \sum x_i^2}} s_y \sqrt{\frac{\sum x_i^2}{D}} s_y \sqrt{\frac{n}{D}}}{r^2 - t^2 s_y^2 \frac{n}{D}}$$

$$x_{LOD} = \frac{2t r s_y \sqrt{\frac{\sum x_i^2}{D} + 1} - 2t^2 \sum x_i \frac{s_y}{D}}{r^2 - t^2 s_y^2 \frac{n}{D}}$$

$$x_{LOD} = \frac{2t r s_y \sqrt{D \sum x_i^2 + D^2} - 2t^2 s_y^2 \sum x_i}{D r^2 - t^2 s_y^2 n}$$

$$x_{LOD} = \frac{2t s_y}{D r^2 - t^2 s_y^2 n} \left(r \sqrt{D \sum x_i^2 + D^2} - t s_y \sum x_i \right)$$

And finally equation (15)

$$x_{LOD} = \frac{2t s_y}{n t^2 s_y^2 - D r^2} \left(t s_y \sum x_i - \sqrt{D r^2 \sum x_i^2 + r^2 D^2} \right) \quad (15)$$

This may be compared to eq (11) in the article

$$x_{LOD} = \frac{2t s_y}{n t^2 s_y^2 - D r^2} \left(t s_y \sum x_i \pm \sqrt{\frac{D^2 r^2}{k} + D r^2 \sum x_i^2 - n \frac{D}{k} t^2 s_y^2 - D t^2 s_y^2} \right) \quad (11)$$

The expressions are identical aside from the term

$$\Delta = -D t^2 s_y^2 (n/k + 1) \quad (16)$$

as was discussed in appendix I of the main article.