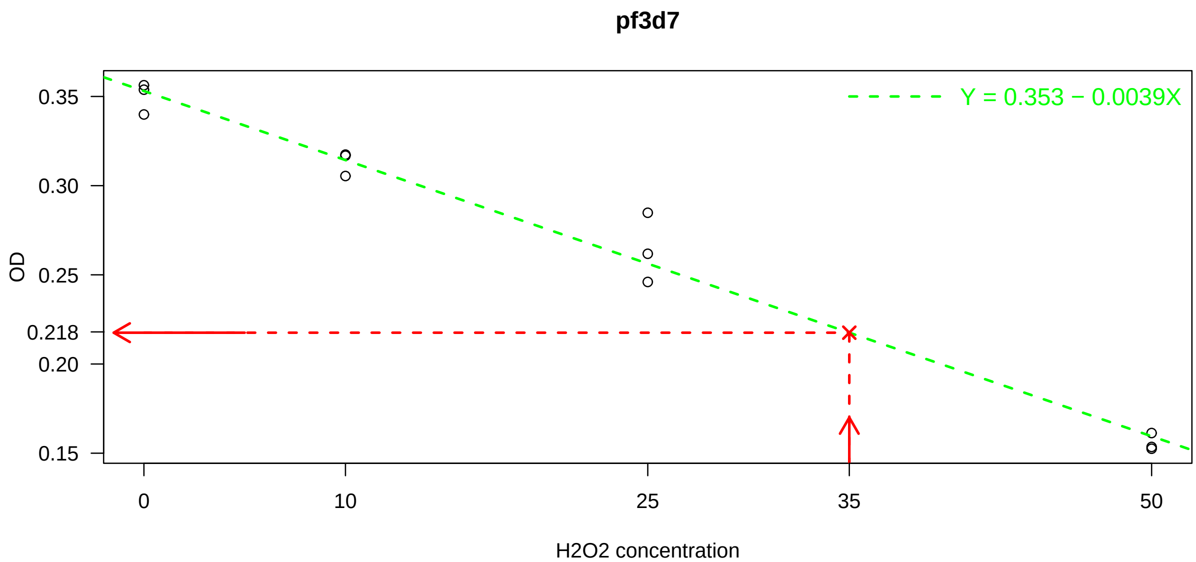
Estimating the mean response



We can use the regression results to predict the expected response for a new concentration of hydrogen peroxide. But what is its variability?

Variability of the mean response

Let $\hat{y}$ be the predicted mean for some x, i. e.

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$$

Then

$$E(\hat{y}) = \beta_0 + \beta_1 x$$

$$\mathrm{var}(\hat{y}) = \sigma^2 \left(\frac{1}{n} + \frac{(x - \bar{x})^2}{SXX} \right)$$

where y is the true mean response.

Why?

$$
\begin{aligned}
E(\hat{y}) &= E(\hat{\beta}_0 + \hat{\beta}_1 x) \\
&= E(\hat{\beta}_0) + x\, E(\hat{\beta}_1) \\
&= \beta_0 + x\, \beta_1
\end{aligned}
$$

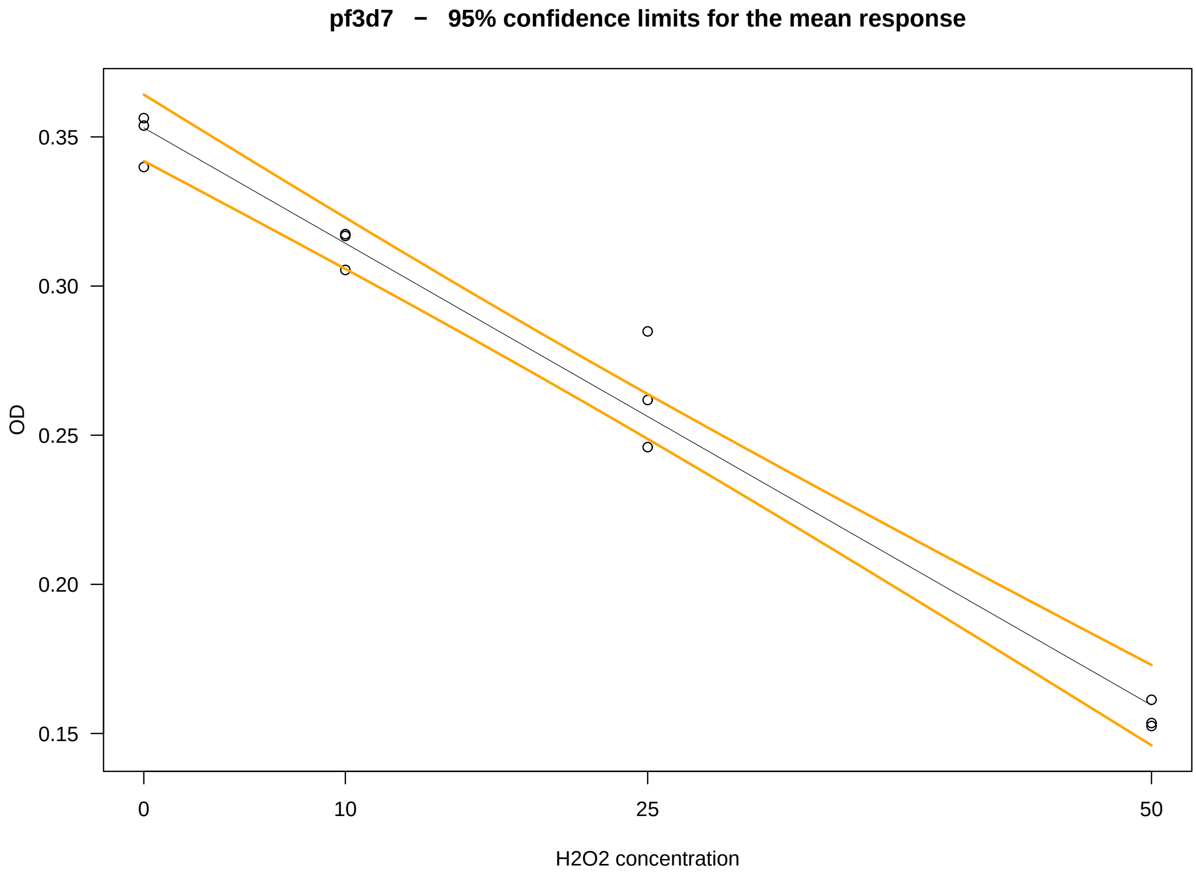
$$
\begin{aligned}
\mathrm{var}(\hat{y}) &= \mathrm{var}(\hat{\beta}_0 + \hat{\beta}_1 x) \\
&= \mathrm{var}(\hat{\beta}_0) + \mathrm{var}(\hat{\beta}_1 x) + 2\,\mathrm{cov}(\hat{\beta}_0, \hat{\beta}_1 x) \\
&= \mathrm{var}(\hat{\beta}_0) + x^2\, \mathrm{var}(\hat{\beta}_1) + 2\, x\, \mathrm{cov}(\hat{\beta}_0, \hat{\beta}_1) \\
&= \sigma^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{SXX} \right) + \sigma^2 \left(\frac{x^2}{SXX} \right) - \frac{2\, x\, \bar{x}\, \sigma^2}{SXX} \\
&= \sigma^2 \left[\frac{1}{n} + \frac{(x - \bar{x})^2}{SXX} \right]
\end{aligned}
$$

Confidence intervals

Hence

$$
\hat{y} \pm t_{(1-\frac{\alpha}{2}),n-2} \times \hat{\sigma} \times \sqrt{\frac{1}{n} + \frac{(x-\bar{x})^2}{SXX}}
$$

is a $(1 - \alpha)\times 100\%$ confidence interval for the mean response given x.



Prediction

Now assume that we want to calculate an interval for the predicted response $y^\star$ for a value of x.

There are two sources of uncertainty:

(a) the mean response

(b) the natural variation σ^2

The variance of $\hat{y}^\star$ is

$$\text{var}(\hat{y}^\star) = \sigma^2 + \sigma^2\left(\frac{1}{n} + \frac{(x-\bar{x})^2}{SXX}\right) = \sigma^2\left(1 + \frac{1}{n} + \frac{(x-\bar{x})^2}{SXX}\right)$$

Prediction intervals

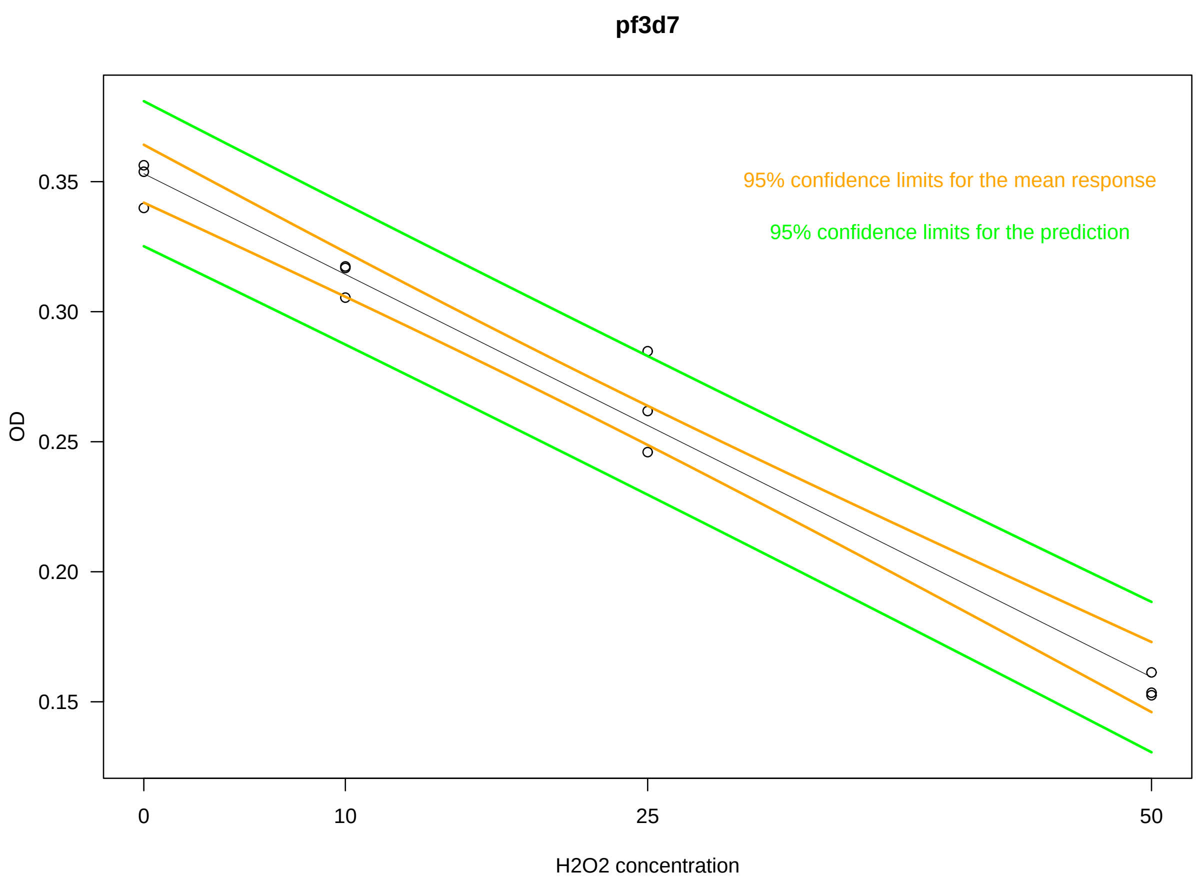
Hence

$$\hat{y}^{\star} \pm t_{(1-\frac{\alpha}{2}),n-2} \times \hat{\sigma} \times \sqrt{1 + \frac{1}{n} + \frac{(x-\bar{x})^2}{SXX}}$$

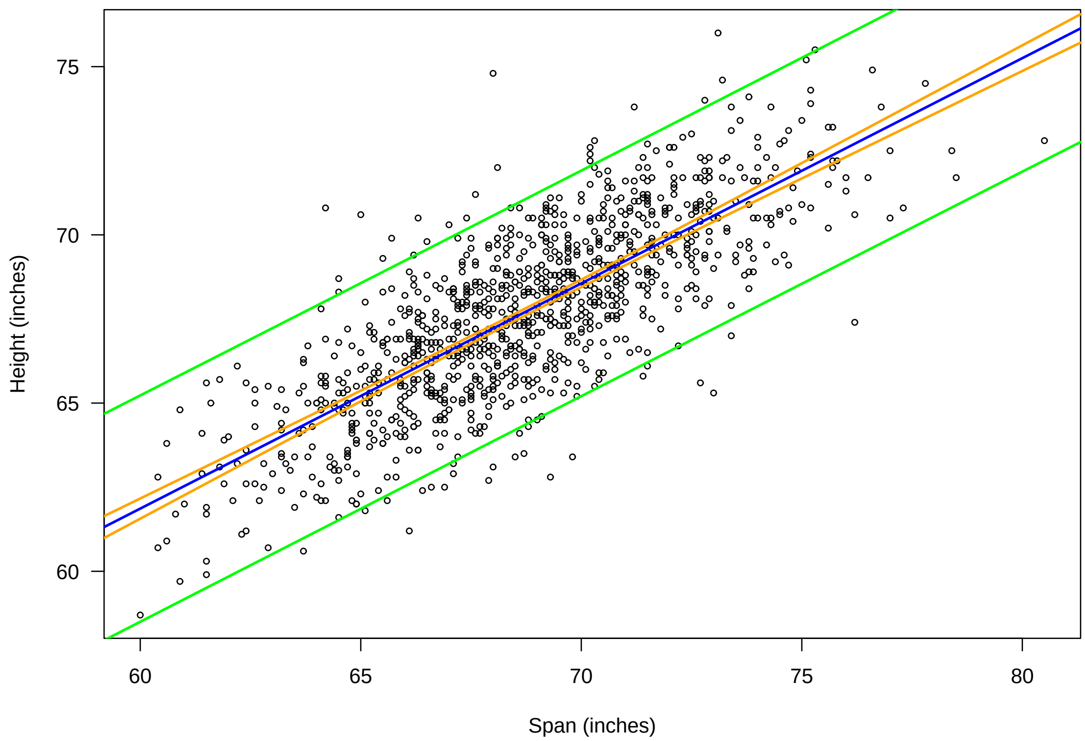
is a $(1-\alpha)\times 100\%$ prediction interval for the predicted response given x.

Note: When n is very large, we get just

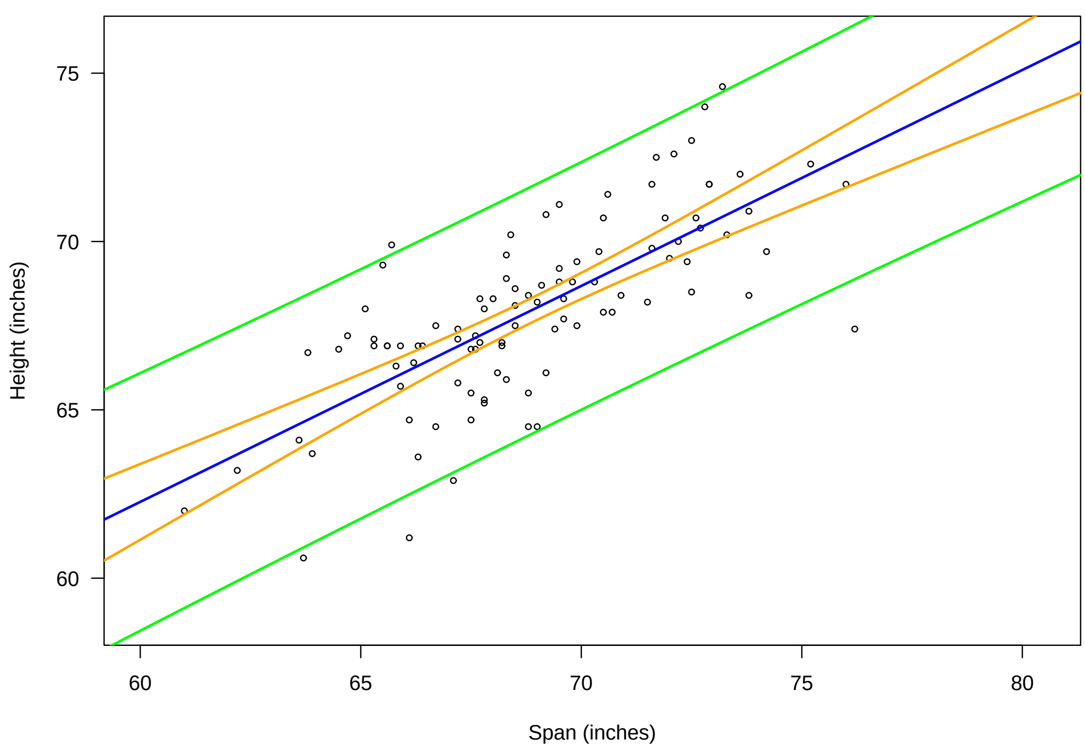
$$\hat{y}^{\star} \pm t_{(1-\frac{\alpha}{2}),n-2} \times \hat{\sigma}$$



Span and height



With just 100 individuals



Regression for calibration

That prediction interval is for the case that the x's are known without error while

$$y = \beta_0 + \beta_1 x + \epsilon \quad \text{where } \epsilon = \text{ error}$$

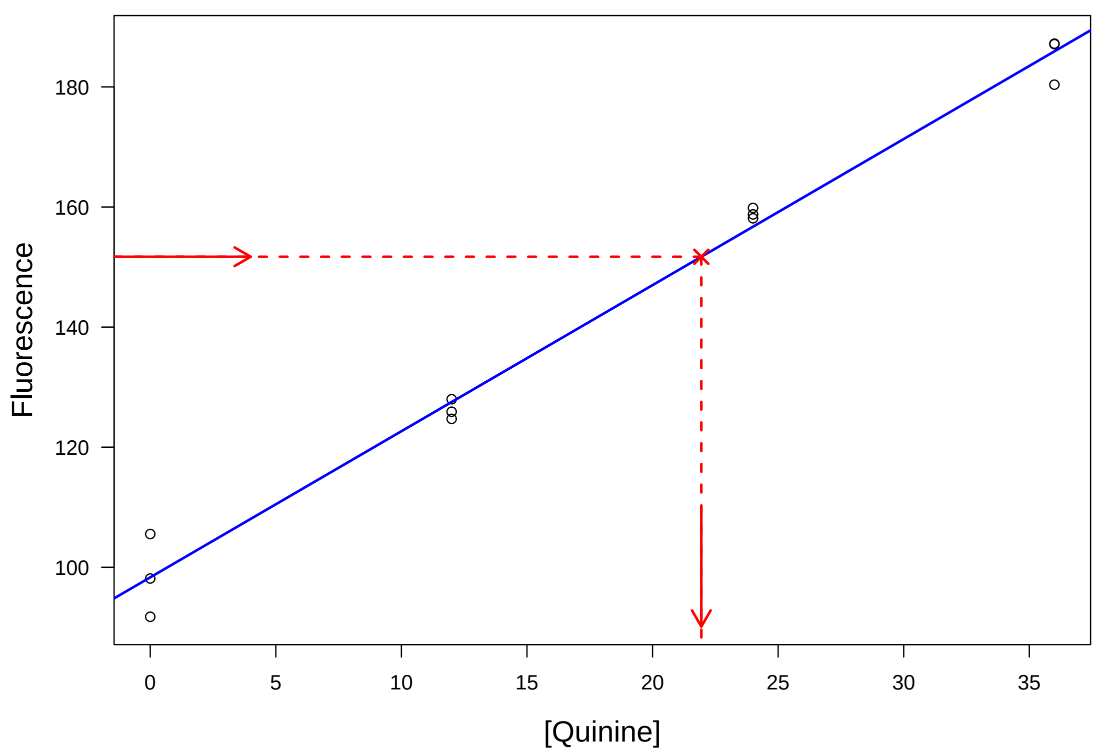
A more common situation:

We have a number of pairs (x,y) to get a calibration line/curve.
x's basically without error; y's have measurement error

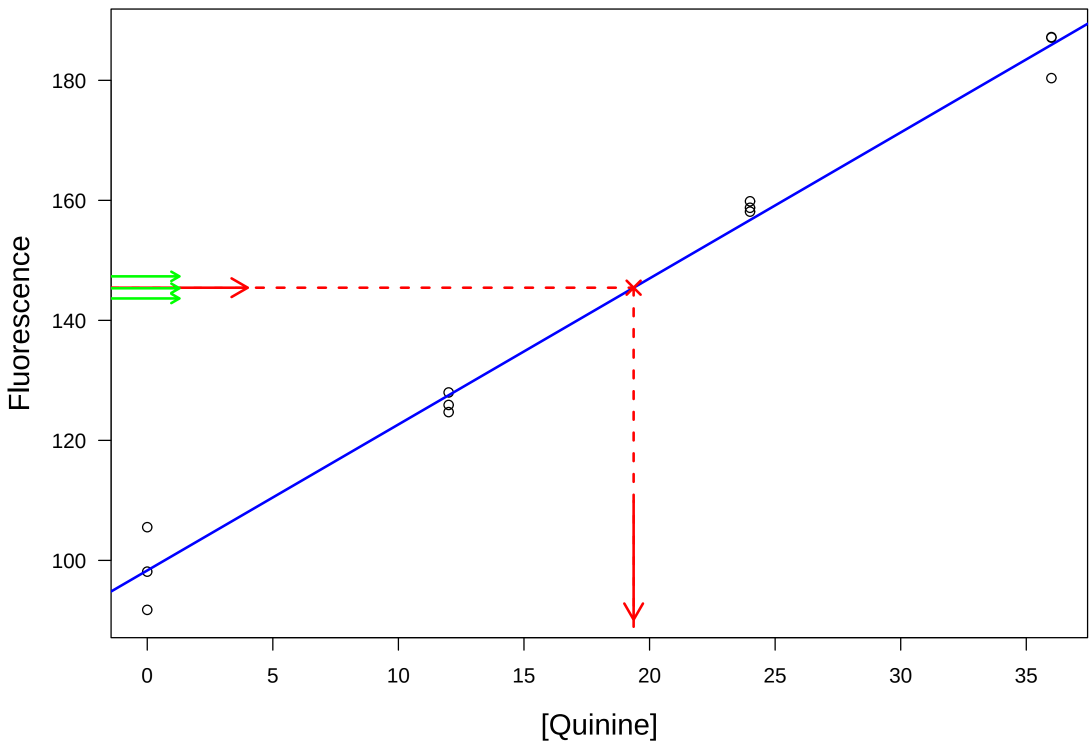
We obtain a new value, $y^\star$, and want to estimate the corresponding $x^\star$.

$$y^\star = \beta_0 + \beta_1 x^\star + \epsilon$$

Example



Another example



Regression for calibration

Data: (x_i, y_i) for $i = 1, \ldots, n$

with $y_i = \beta_0 + \beta_1 x_i + \epsilon_i$, $\epsilon_i \sim$ iid Normal$(0, \sigma)$

$y_j^\star$ for $j = 1, \ldots, m$

with $y_j^\star = \beta_0 + \beta_1 x^\star + \epsilon_j^\star$, $\epsilon_j^\star \sim$ iid Normal$(0, \sigma)$

for some $x^\star$

Goal: Estimate $x^\star$ and give a 95% confidence interval.

The estimate: Obtain $\hat\beta_0$ and $\hat\beta_1$ by regressing the y_i on the x_i.

Let $\hat{x}^\star = (\bar{y}^\star - \hat\beta_0)/\hat\beta_1$ where $\bar{y}^\star = \sum_j y_j^\star / m$

95% CI for $\hat{x}^\star$

Let T denote the 97.5th percentile of the t distr'n with n–2 d.f.

Let $g = T \,/\, [|\hat\beta_1| \,/\, (\hat\sigma / \sqrt{SXX})] \quad = \quad (T\,\hat\sigma) \,/\, (|\hat\beta_1|\,\sqrt{SXX})$

If $g \geq 1$, we would fail to reject $H_0 : \beta_1 = 0$!

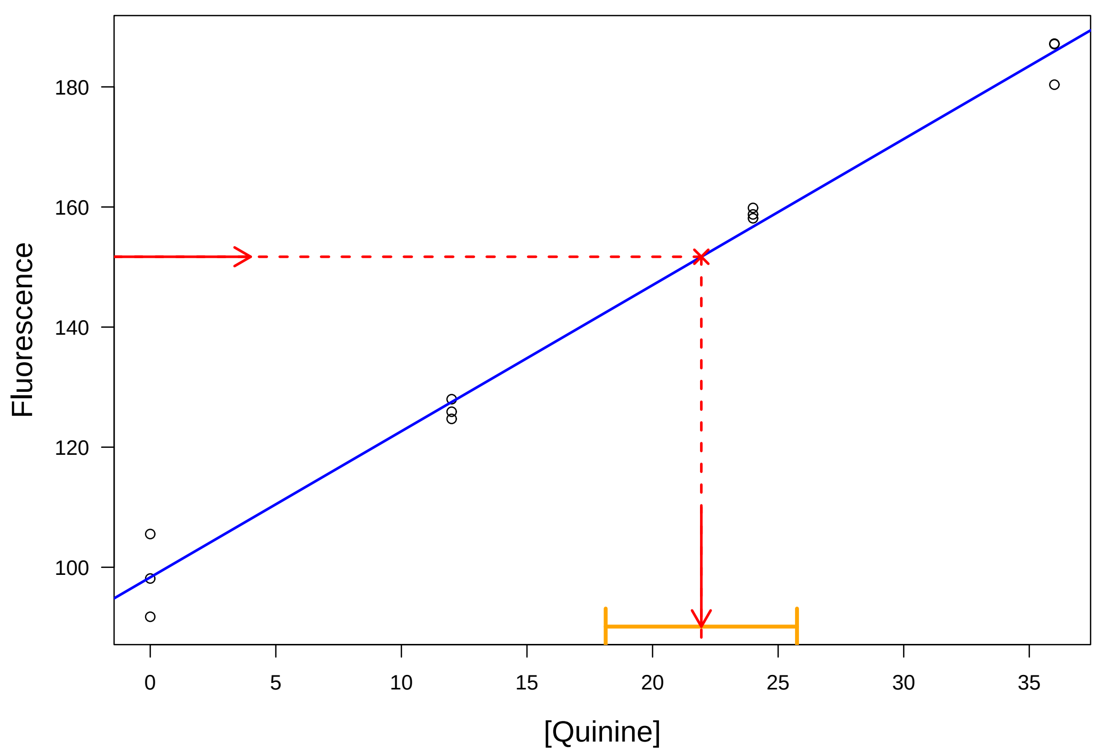
In this case, the 95% CI for $\hat{x}^\star$ is $(-\infty, \infty)$.

If $g < 1$, our 95% CI is the following:

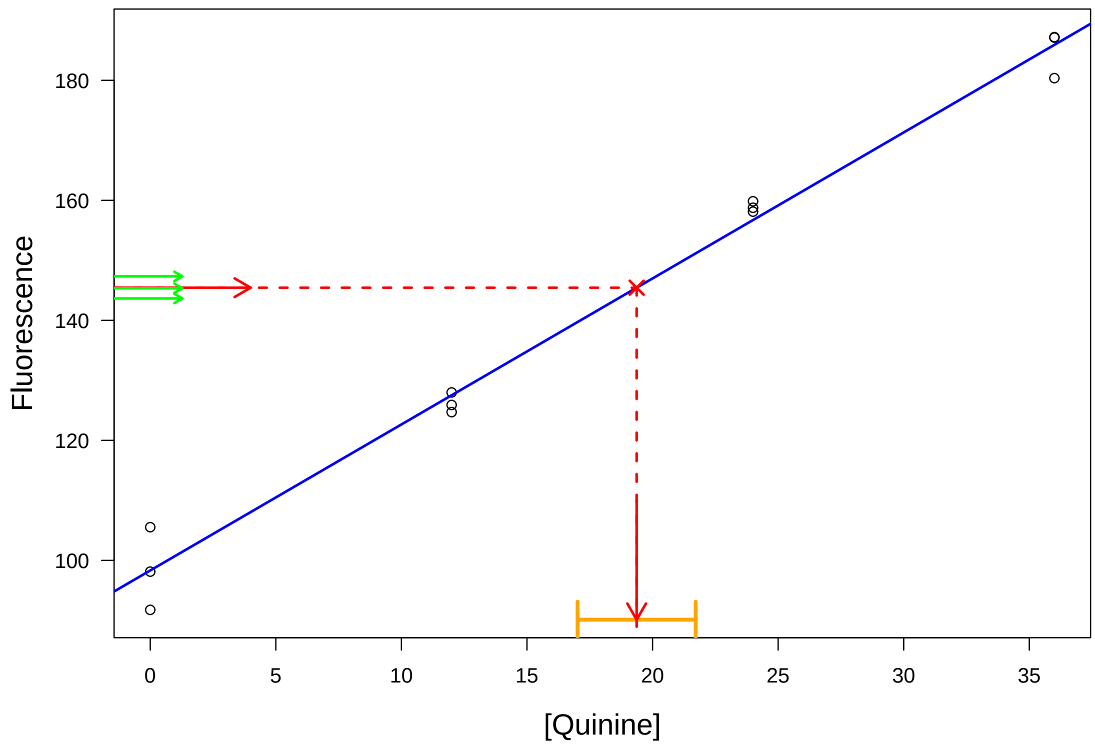
$$\hat{x}^\star \pm \frac{(\hat{x}^\star - \bar{x})\, g^2 + (T\,\hat\sigma \,/\, |\hat\beta_1|) \sqrt{(\hat{x}^\star - \bar{x})^2/SXX + (1 - g^2)\,(\frac{1}{m} + \frac{1}{n})}}{1 - g^2}$$

For very large n, this reduces to $\quad \hat{x}^\star \pm (T\,\hat\sigma) \,/\, (|\hat\beta_1|\sqrt{m})$

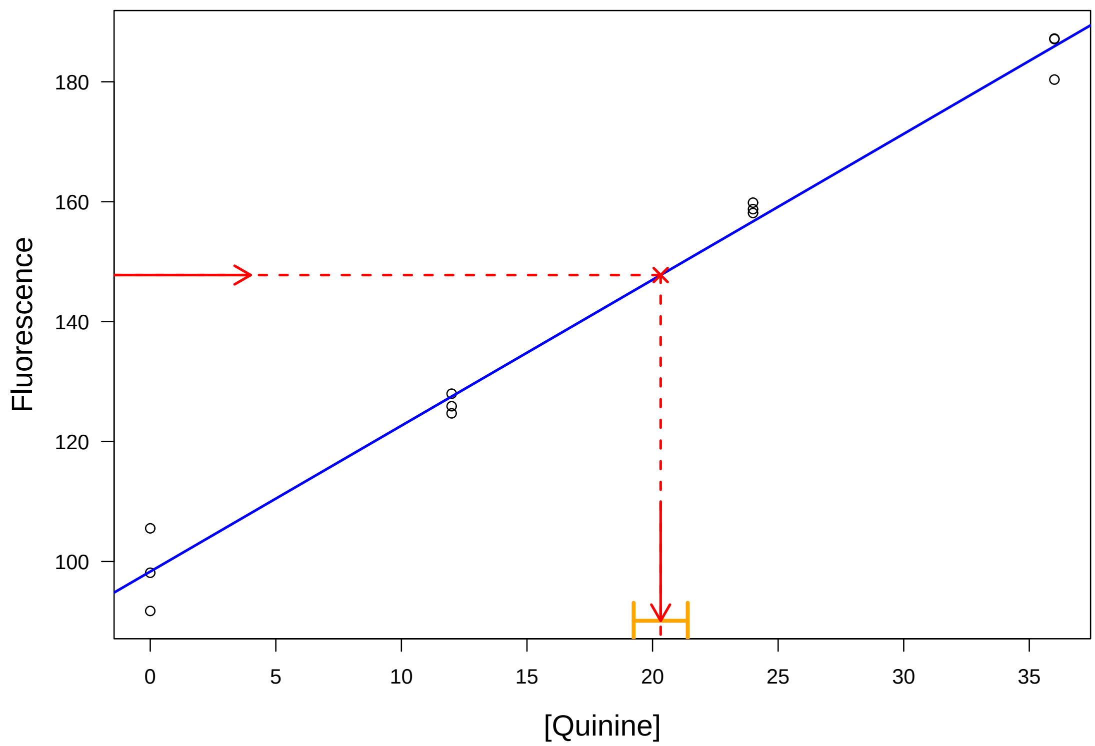
Example



Another example



Infinite m



Infinite n