

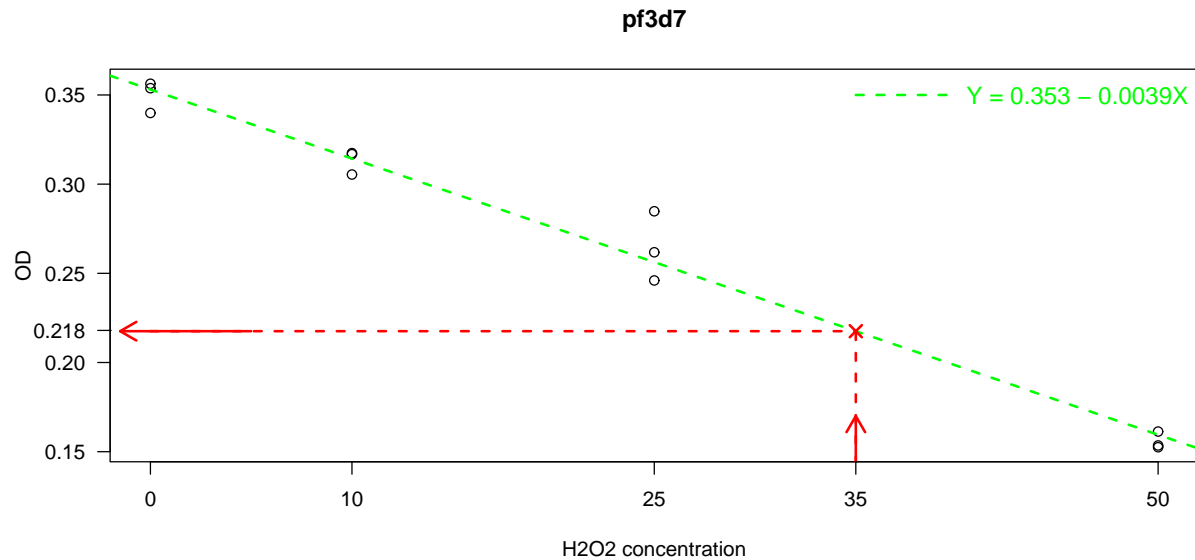
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# Estimating the mean response

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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

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

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

Then

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

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

where  $y$  is the true mean response.

# Why?

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

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

## Confidence intervals

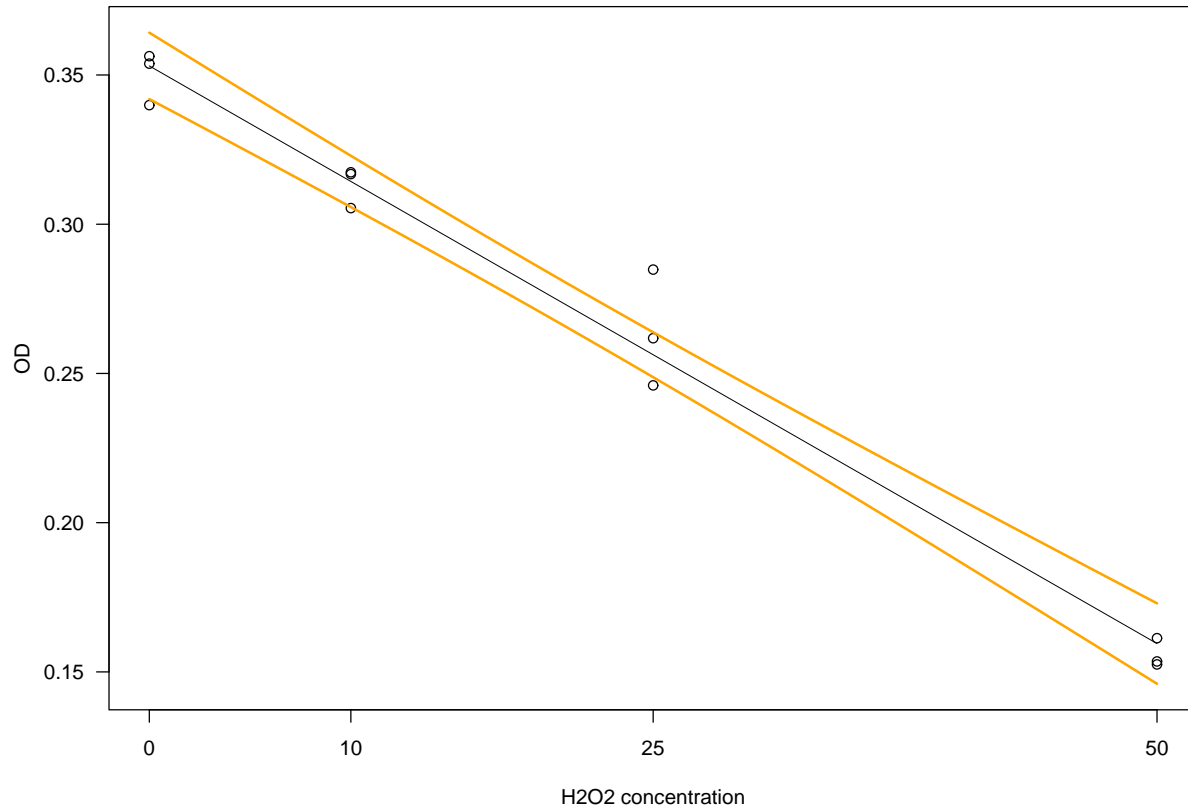
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Hence

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

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

pf3d7 - 95% confidence limits for the mean response



## Prediction

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

There are two sources of uncertainty:

- (a) the mean response
- (b) the natural variation  $\sigma^2$

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

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

# Prediction intervals

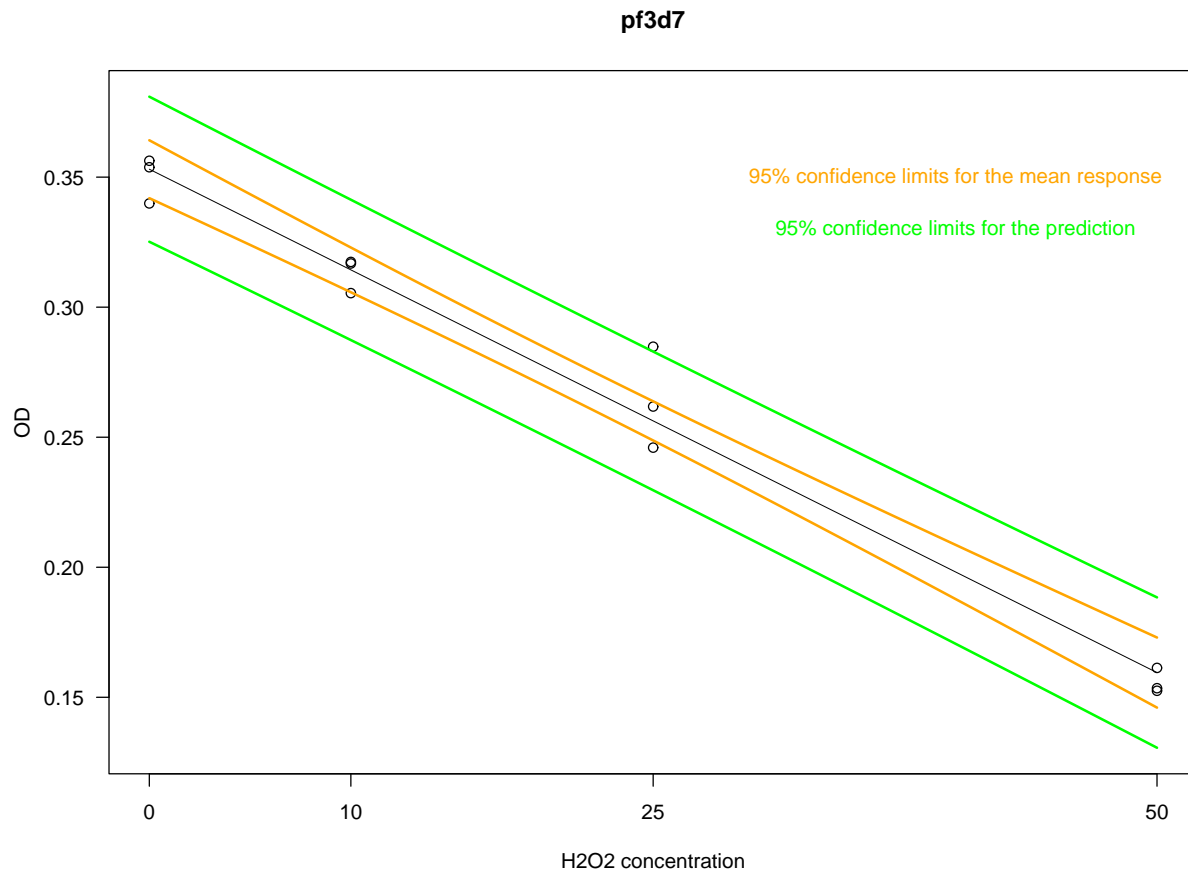
Hence

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

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

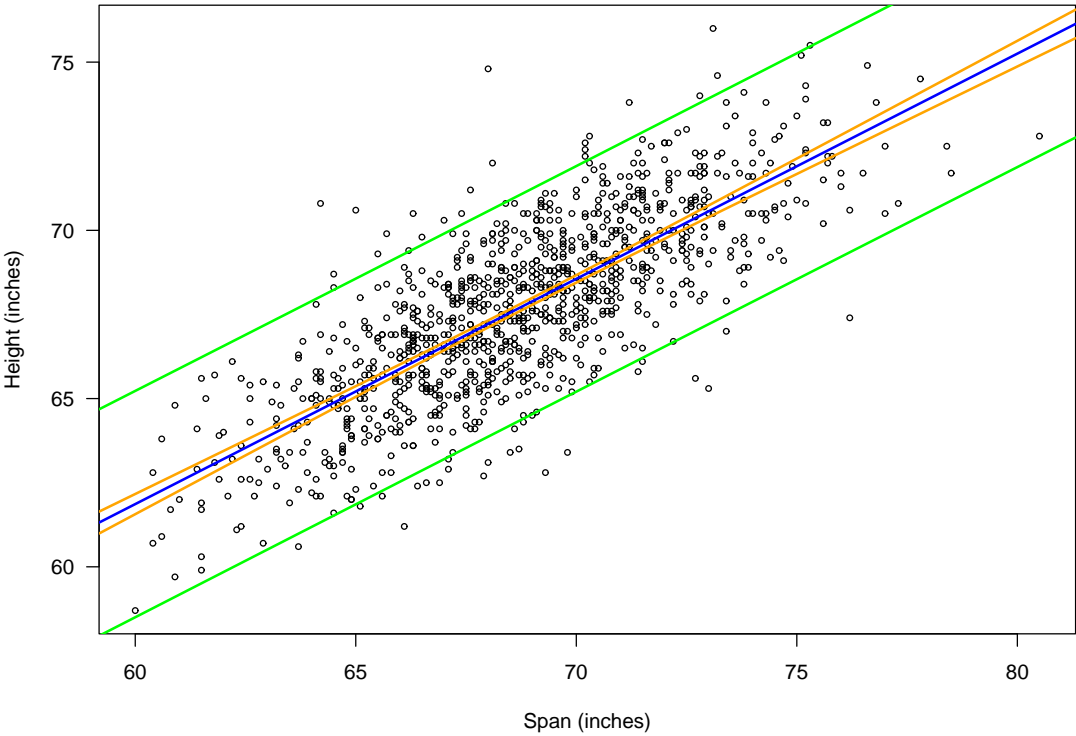
Note: When  $n$  is very large, we get just

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



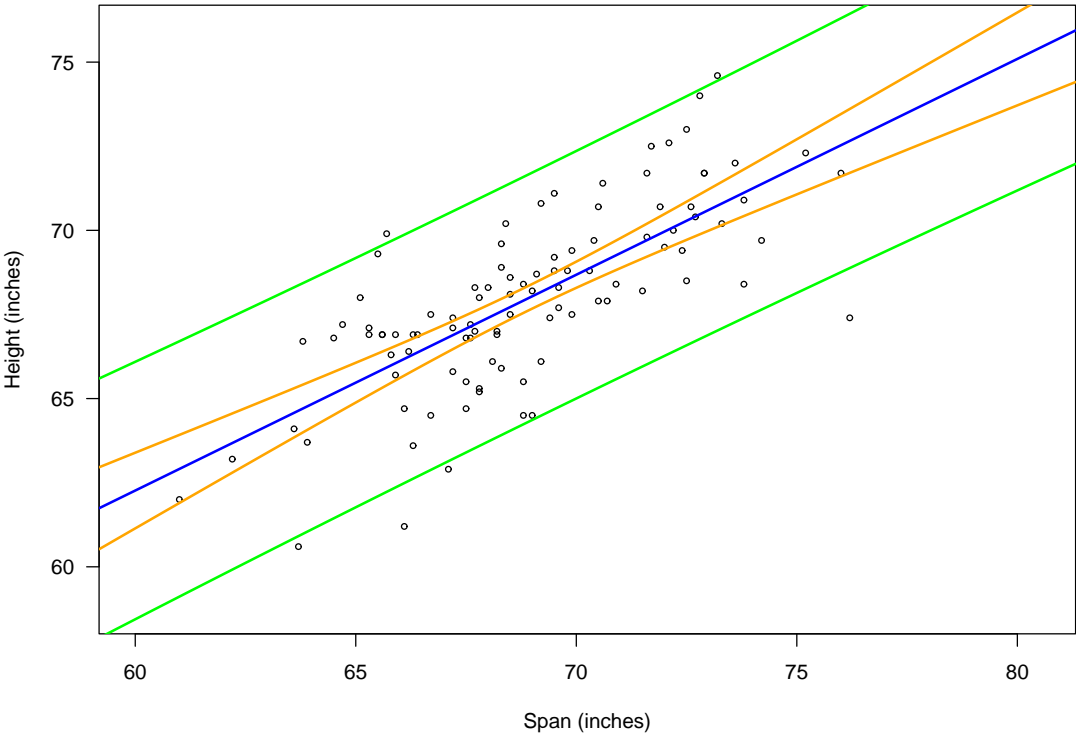
# Span and height

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## With just 100 individuals

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# Regression for calibration

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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:

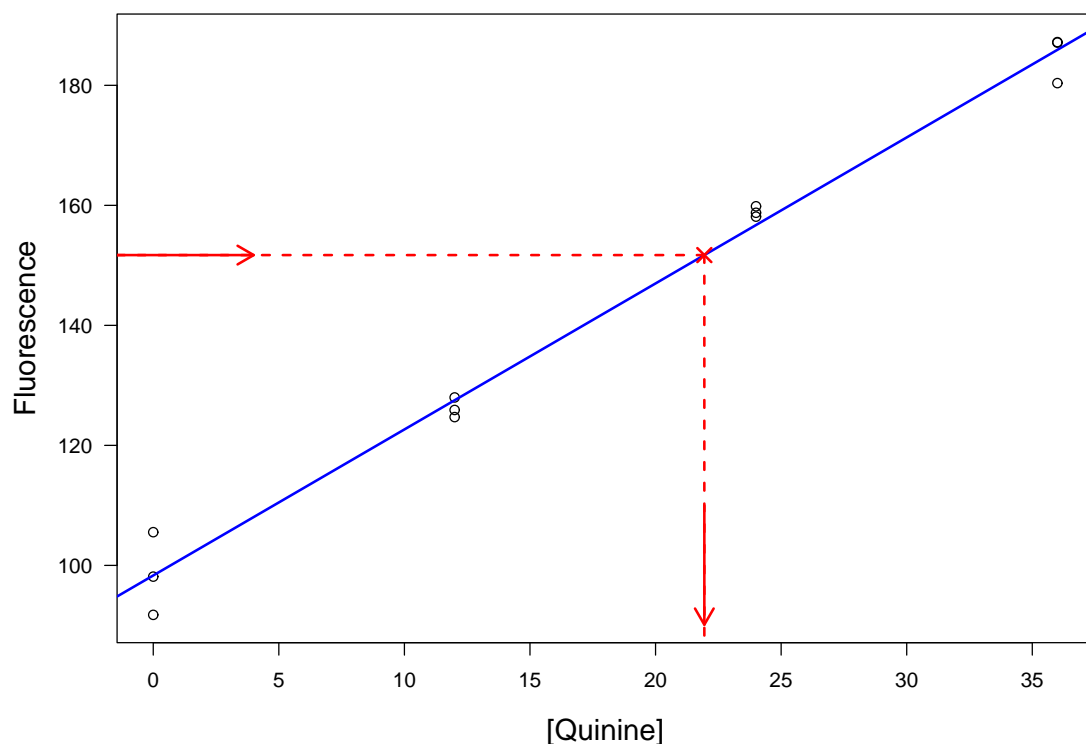
We have a number of pairs  $(x,y)$  to get a calibration line/curve.  
 $x$ 's basically without error;  $y$ 's have measurement error

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

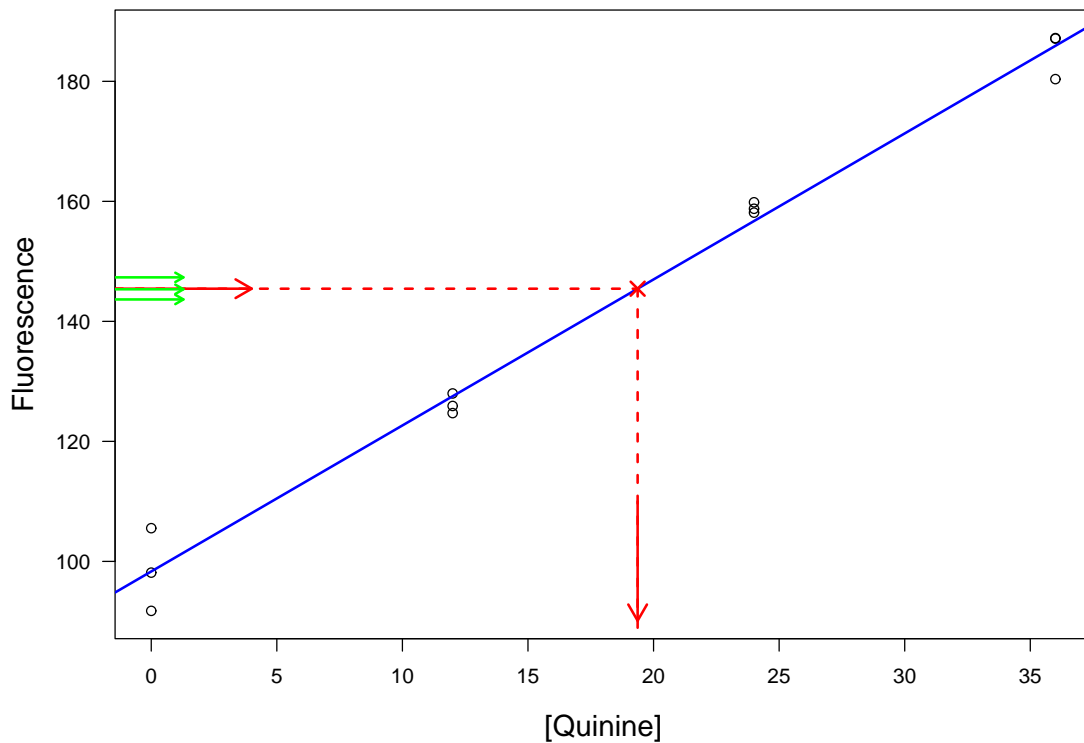
$$y^* = \beta_0 + \beta_1 x^* + \epsilon$$

## Example

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# Another example



## Regression for calibration

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

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

$y_j^*$  for  $j = 1, \dots, m$

with  $y_j^* = \beta_0 + \beta_1 x^* + \epsilon_j^*$ ,  $\epsilon_j^* \sim \text{iid Normal}(0, \sigma)$

for some  $x^*$

Goal: Estimate  $x^*$  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  $\hat{x}^* = (\bar{y}^* - \hat{\beta}_0) / \hat{\beta}_1$  where  $\bar{y}^* = \sum_j y_j^* / m$

## 95% CI for $\hat{x}^*$

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

$$\text{Let } g = T / [|\hat{\beta}_1| / (\hat{\sigma} / \sqrt{SXX})] = (T \hat{\sigma}) / (|\hat{\beta}_1| \sqrt{SXX})$$

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

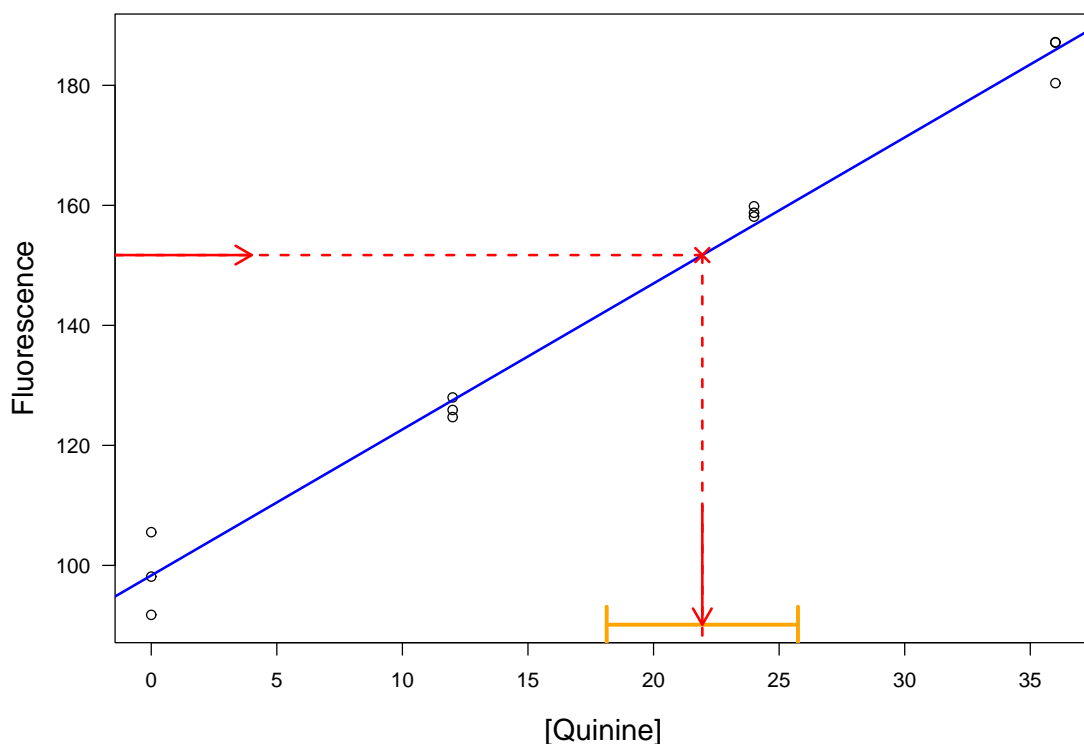
In this case, the 95% CI for  $\hat{x}^*$  is  $(-\infty, \infty)$ .

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

$$\hat{x}^* \pm \frac{(\hat{x}^* - \bar{x}) g^2 + (T \hat{\sigma} / |\hat{\beta}_1|) \sqrt{(\hat{x}^* - \bar{x})^2 / SXX + (1 - g^2) (\frac{1}{m} + \frac{1}{n})}}{1 - g^2}$$

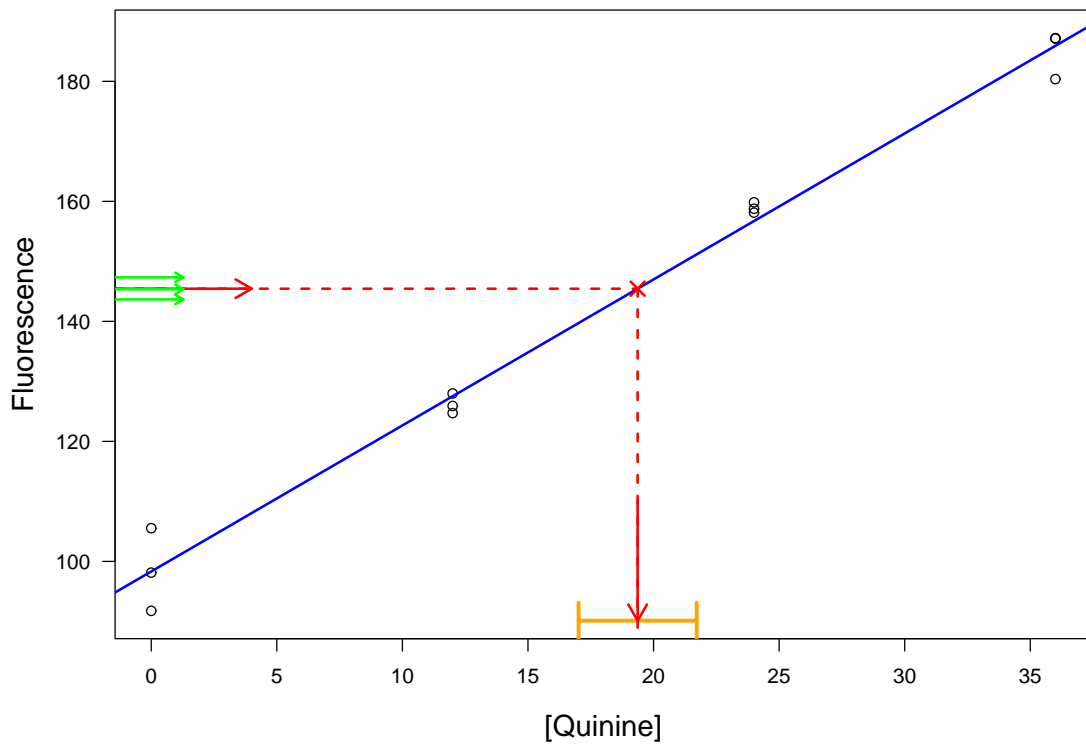
For very large  $n$ , this reduces to  $\hat{x}^* \pm (T \hat{\sigma}) / (|\hat{\beta}_1| \sqrt{m})$

## Example



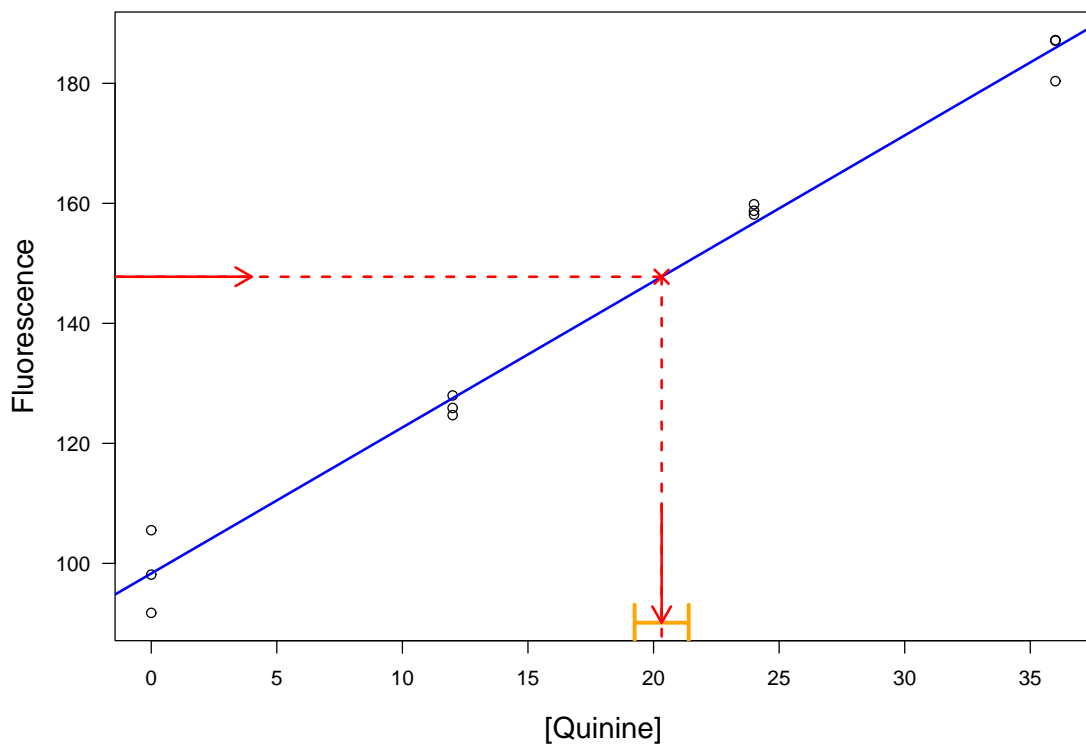
# Another example

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# Infinite m

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# Infinite n

