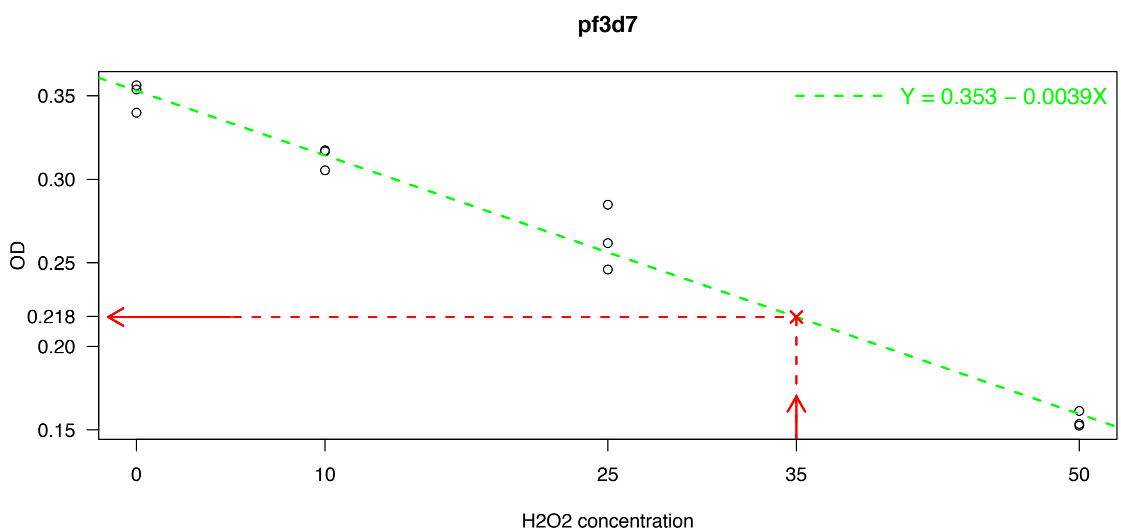
# Prediction and Calibration

# 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

$$\begin{aligned} E(\hat{y}) &= \beta_0 + \beta_1 x \\ \text{var}(\hat{y}) &= \sigma^2 \left( \frac{1}{n} + \frac{(x - \bar{x})^2}{SXX} \right) \end{aligned}$$

where $y = \beta_0 + \beta_1 x$ is the true mean response.

# Why?

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

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

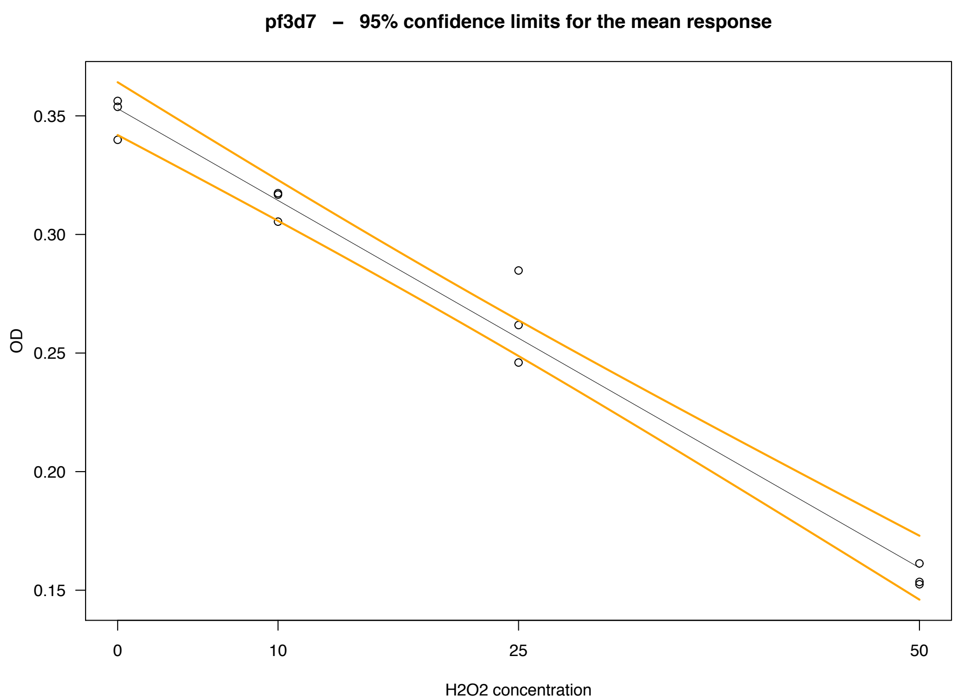
# Confidence intervals

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.

# Confidence limits



# 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 $\sigma^2$

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

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

# Prediction intervals

Hence

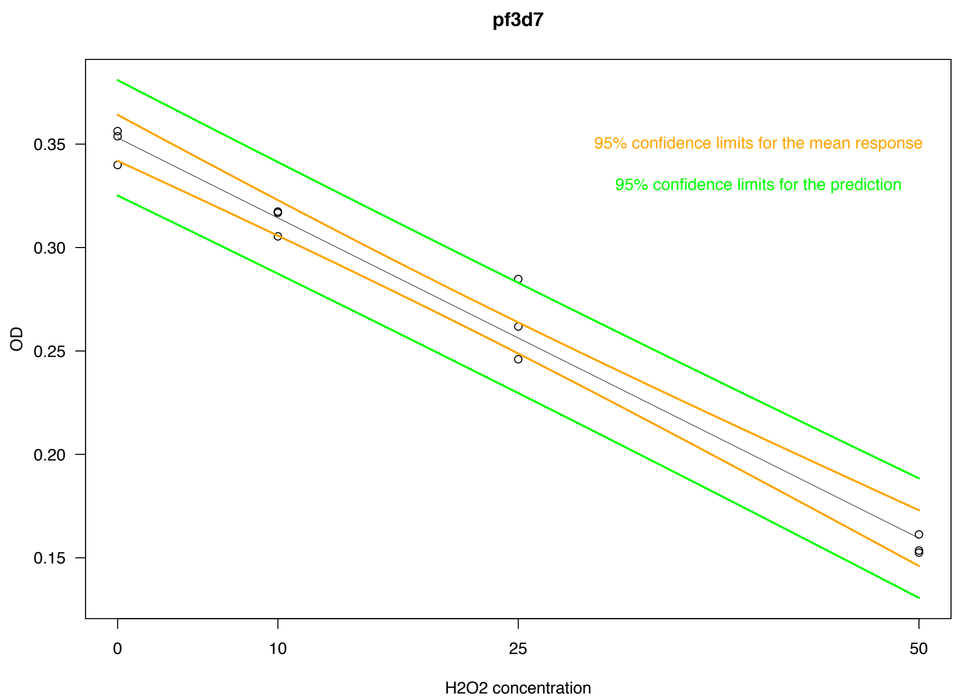
$$\hat{y}^\star \pm t_{(1 - \frac{\alpha}{2}), n-2} \times \hat{\sigma} \times \sqrt{1 + \frac{1}{n} + \frac{(x - \bar{x})^2}{SXX}}$$

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

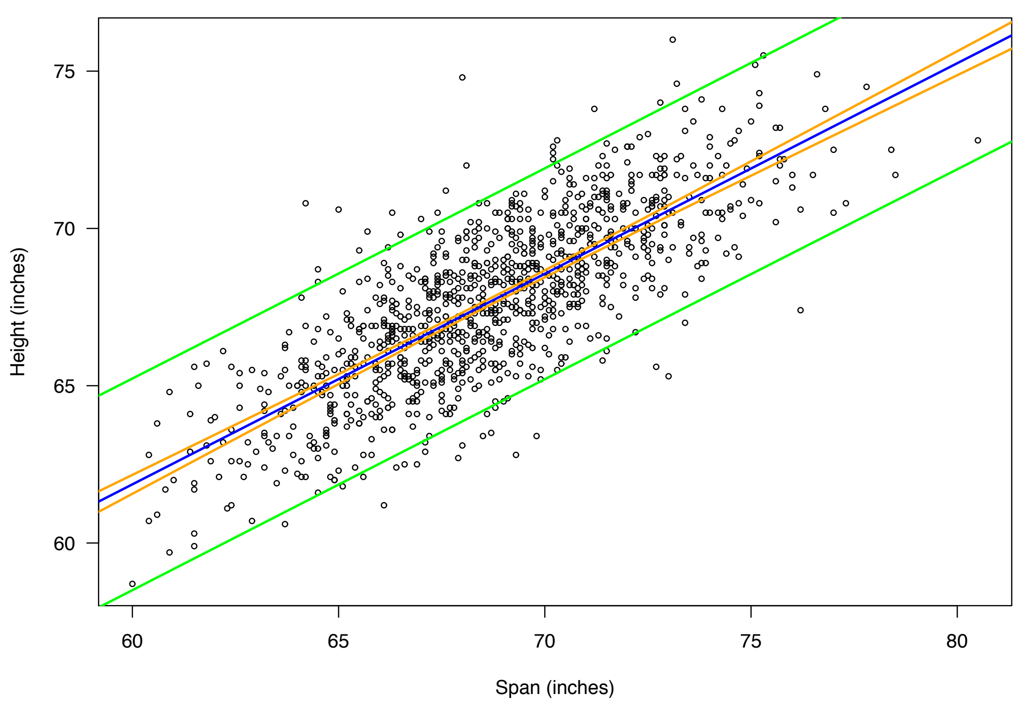
$\longrightarrow$ When n is very large, we get roughly

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

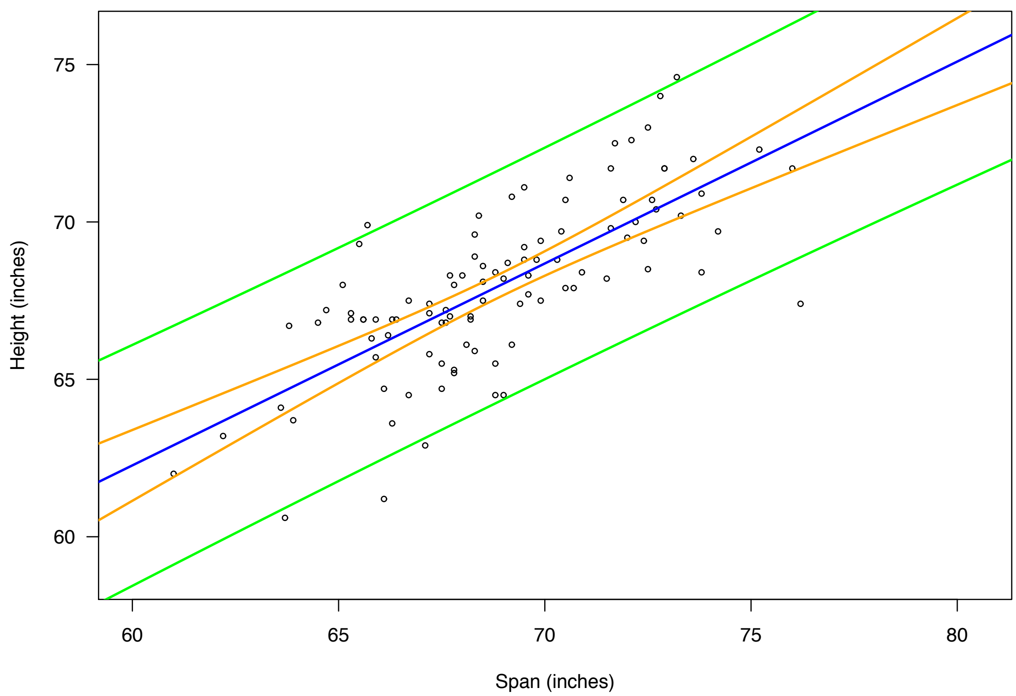
# Prediction intervals




# 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

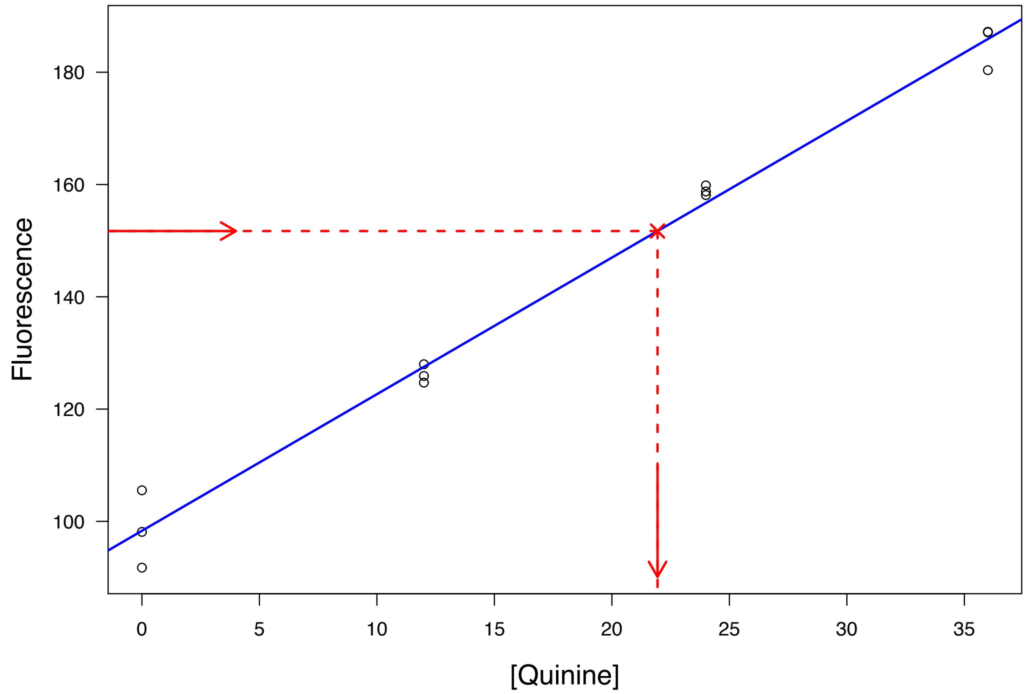
$$y = \beta_0 + \beta_1 x + \epsilon \qquad \text{where } \epsilon = \text{error}$$

$\longrightarrow$ Another common situation:

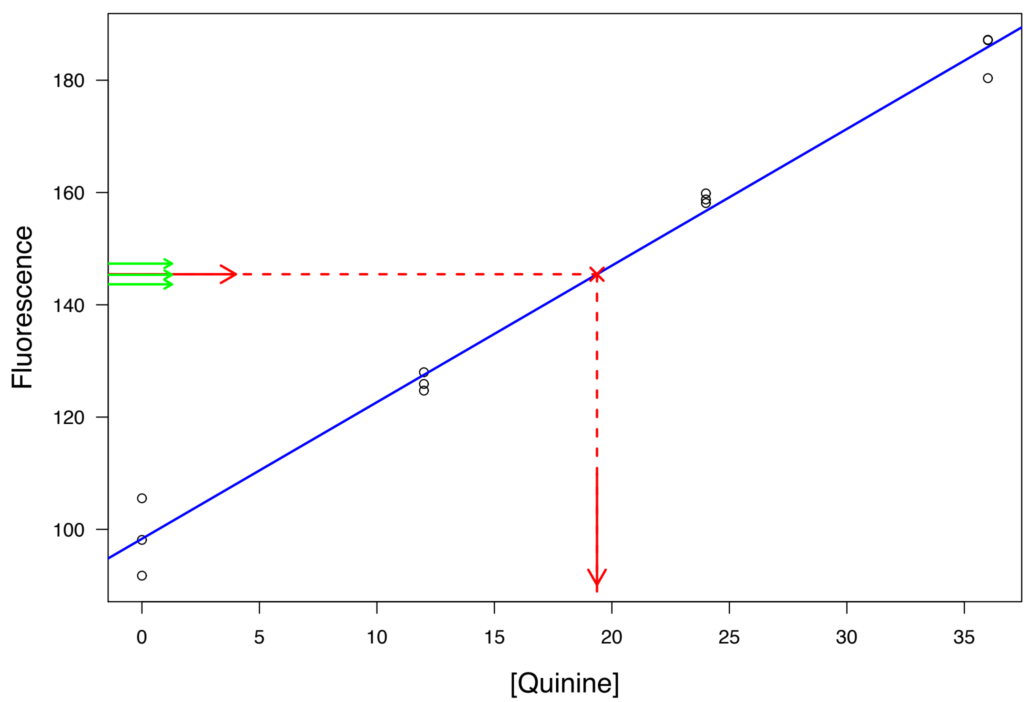
- ○ We have a number of pairs (x,y) to get a calibration line/curve.
- ○ x's basically without error; y's have measurement error.
- ○ We obtain a new value, $y^\star$, and want to estimate the corresponding $x^\star$:

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

# 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$(0, \sigma)$

$y^\star_j$ for $j = 1, \ldots, m$

with $y^\star_j = \beta_0 + \beta_1 x^\star + \epsilon^\star_j$, $\epsilon^\star_j \sim$ 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 $\bar{y}^\star = \sum_j y^\star_j / m$

# 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 $H_0 : \beta_1 = 0$!

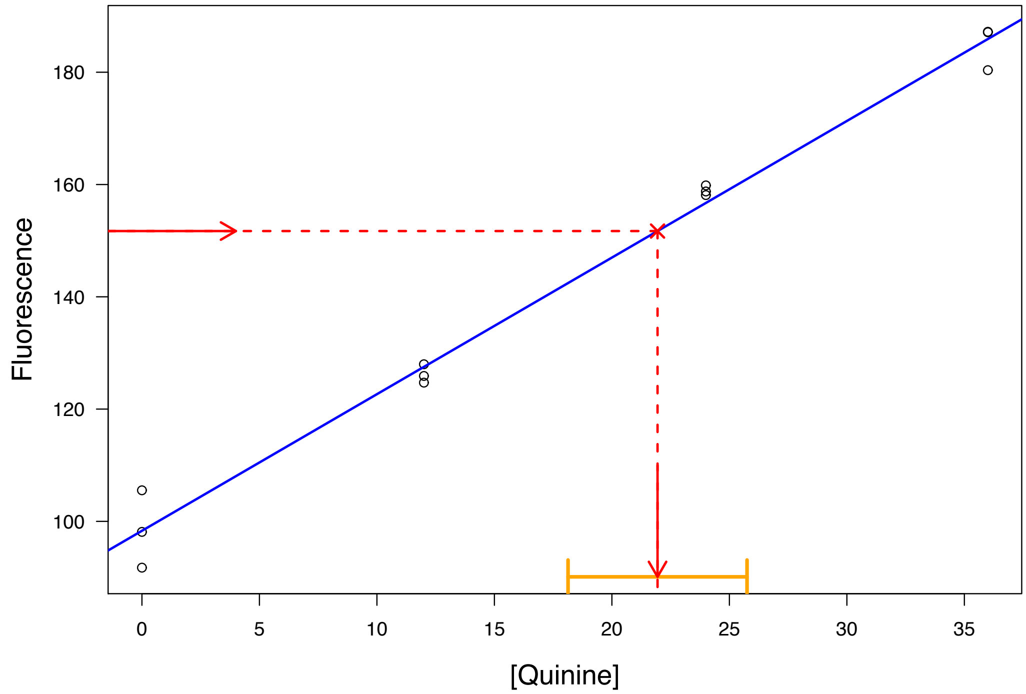
In this case, the 95% CI for $\hat{x}^\star$ is $(-\infty, \infty)$.

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

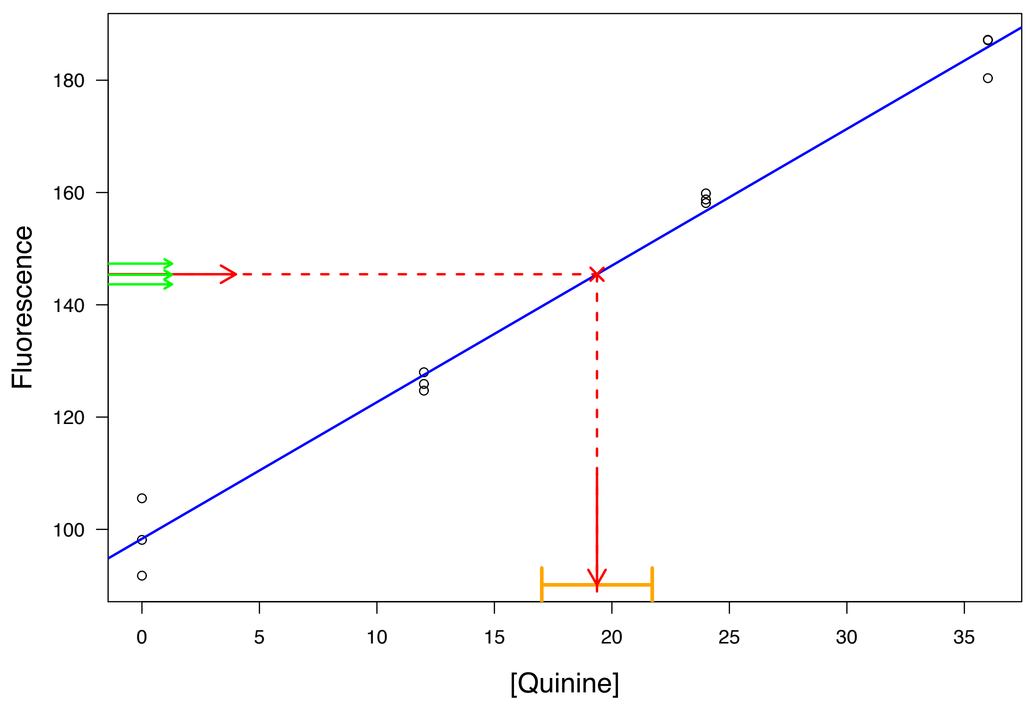
$$\hat{x}^\star \pm \frac{(\hat{x}^\star - \bar{x})\,g^2 + (T\,\hat{\sigma} \,/\, |\hat{\beta}_1|)\sqrt{(\hat{x}^\star - \bar{x})^2/SXX + (1 - g^2)\,(\frac{1}{m} + \frac{1}{n})}}{1 - g^2}$$

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

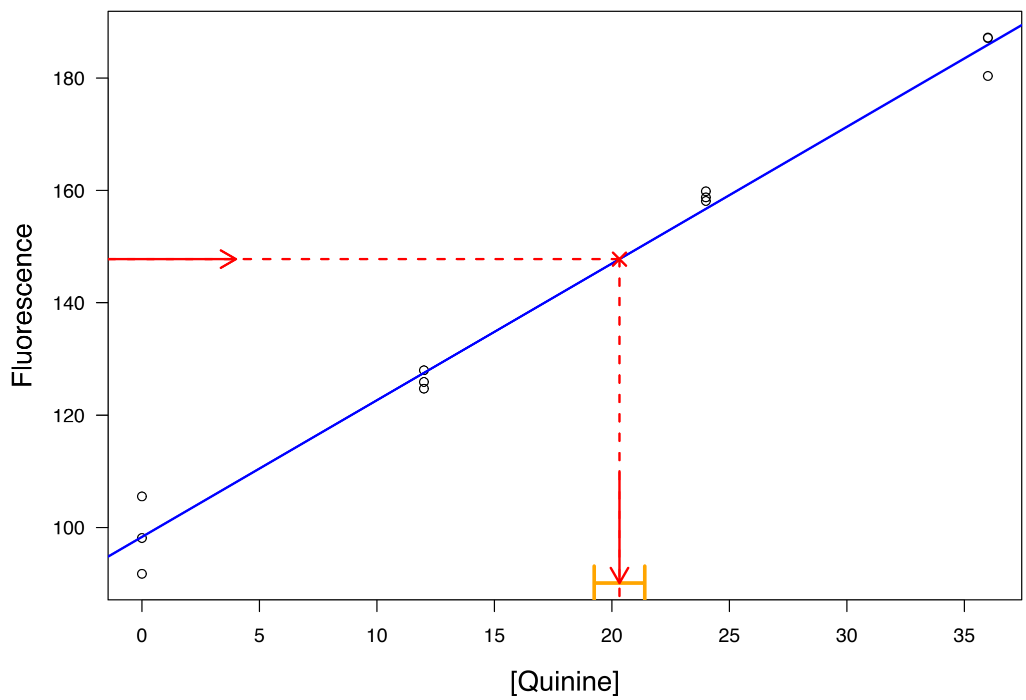
# Example




# Another example



# Infinite m




# Infinite n