Root-Mean-Square-Deviation/Error (RMSD/RMSE)

The **root-mean-square-deviation** (RMSD) or **root-mean-square-error** (RMSE) is a frequently used measure of the differences between values (sample or population) predicted by a model or an **estimator** and the values observed. It represents the square root of the second **sample moment** of the differences between predicted values and observed values or the **quadratic mean** of these differences. These **deviations** are called **residuals** when the calculations are preformed over the data sample that was used for estimation and are called **errors** (or prediction errors) when computed out-of-sample.

Data:

actual: (x, y)	predicted: (x, y)	$\bar{\mathbf{x}} = 2$	$\bar{\mathbf{y}} = 3$
(1, 1)	(1, 0.5)	$\mathbf{s_x} = 0.816$	$\mathbf{s_y} = 2.160$
(2, 2)	(2, 3)		
(2, 3)	(2, 3)		
(3, 6)	(3, 5.5)	(Prediction Formula: $\hat{y} = 2.50x - 2$)	

Insight: The i^{th} residual will be equal to the i^{th} y-value for a given x, minus the predicted y-value for a given x:

$$r_i = y_i - \hat{y} \tag{1}$$

Calculate Residuals:

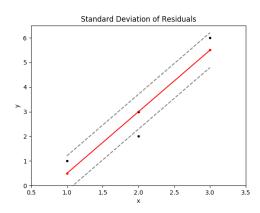
$$r_1 = 1 - 0.5$$
 \Rightarrow $r_1 = 0.5$ $r_2 = 2 - 3$ \Rightarrow $r_2 = -1$ $r_3 = 3 - 3$ \Rightarrow $r_3 = 0$ $r_4 = 6 - 5.5$ \Rightarrow $r_4 = 0.5$

Insight: Similar to typical standard deviation, but take the distance between a point and the model's **prediction**, sum the result, and like a sample standard deviation, divide by n-1, then take the square-root of the result.

$$\sqrt{\frac{\sum r_i}{n-1}} \tag{2}$$

Calculate Standard Deviation of Residuals:

$$\sqrt{\frac{(0.5)^2 + (-1)^2 + (0)^2 + (0.5)^2}{3}} \qquad = \qquad \sqrt{\frac{1.5}{3}} \qquad = \qquad \sqrt{\frac{1}{2}} \qquad \approx \qquad \boxed{0.707}$$



Summary: This is used to find out how much a model disagrees with the actual data. A **lower number** means a **better** fit to the model.