$$\hat{y} = g(x) = \underbrace{\bar{y}_{red}}_{b_0} + \underbrace{(\bar{y}_{green} - \bar{y}_{red})}_{b_1} x \quad , \quad \text{let } n_g = \sum x_i , \; p_g = \bar{x} = \frac{n_g}{n}, \; n_r = n - n_g$$

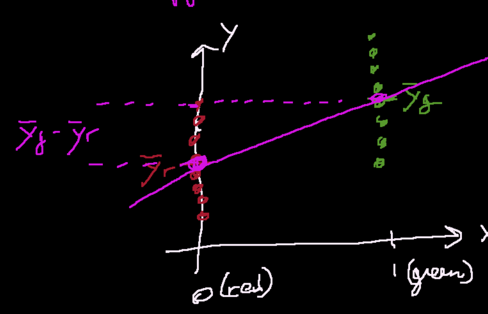
$$\bar{y} = \frac{1}{n}\left(\sum y_i\right) = \frac{1}{n}\left(\sum_{i:green} y_i + \sum_{i:red} y_i\right) = \frac{\sum_G y_i}{n} \cdot \frac{n_g}{n_g} + \frac{\sum_R y_i}{n} \frac{n_r}{n_r}$$

$$= p_g \frac{\sum_G y_i}{n_g} + (1-p_g) \frac{\sum_R y_i}{n_r} = \underbrace{p_g \bar{y}_g + (1-p_g)\bar{y}_r}$$

$$b_1 = \frac{\overbrace{\sum x_i y_i}^{n_g \bar{y}_g = \sum_G y_i} - n \overbrace{\bar{x}}^{p_g} \bar{y}}{\underbrace{\sum x_i^2}_{n_g} - n \underbrace{\bar{x}^2}_{p_g}} = \frac{n_g \bar{y}_g - n p_g \bar{y}}{n_g - n p_g^2} \cdot \frac{\frac{1}{n}}{\frac{1}{n}} = \frac{\cancel{p_g} \bar{y}_g - \cancel{p_g} \bar{y}}{\cancel{p_g} - p_g^{\cancel{2}}} = \frac{\bar{y}_g - \bar{y}}{1-p}$$

$$= \frac{\bar{y}_g - (p_g \bar{y}_g + (1-p_g)\bar{y}_r)}{1-p_g} = \frac{\cancel{(1-p_g)} \bar{y}_g - \cancel{(1-p_g)} \bar{y}_r}{\cancel{1-p_g}} = \bar{y}_g - \bar{y}_r$$

$$b_0 = \bar{y} - b_1 \underbrace{\bar{x}}_{p_g} = \cancel{p_g \bar{y}_g} + (1-\cancel{p_g})\bar{y}_r - \cancel{(\bar{y}_g - \bar{y}_r) p_g} = \bar{y}_r$$



What if x \in {red, green, blue}? This is then p=2 and we need an OLS solution for p > 1. But intuitively...

$$g(x) = \begin{cases} \bar{y}_{red} & \text{if } x = red \\ \bar{y}_{green} & \text{if } x = green \\ \bar{y}_{blue} & \text{if } x = blue \end{cases} = \underbrace{\bar{y}_{red}}_{b_0} + \underbrace{(\bar{y}_{green} - \bar{y}_{red})}_{b_1} \overset{\mathbb{1}_{x=green}}{\overset{\|}{x_1}} + \underbrace{(\bar{y}_{blue} - \bar{y}_{red})}_{b_2} \overset{\mathbb{1}_{x=blue}}{\overset{\|}{x_2}}$$

How well does g predict? We need a "model performance metric". In the SVM this was accuracy or misclassification error. Here, it will can also be what we use internally in the algorithm:

$$SSE := \sum_{i=1}^{n} e_i^2 = \sum (y_i - g(x_i))^2$$

Is SSE interpretable? No, let's take the mean at least, call that mean squared error (MSE):

$$MSE = \frac{1}{n-2} SSE$$

But this is still in the squared unit of the phenomenon so it's still uninterpretable. We can take the square root of MSE called root mean squared error (RMSE):

$$s_e = RMSE = \sqrt{\frac{1}{n-2} \sum e_i^2} = \sqrt{MSE}$$

RMSE is in the same unit as y (it is akin to the standard deviation of the residuals s_e). Also, from the CLT,

$$[g(x) \pm 1.96 \cdot RMSE]$$

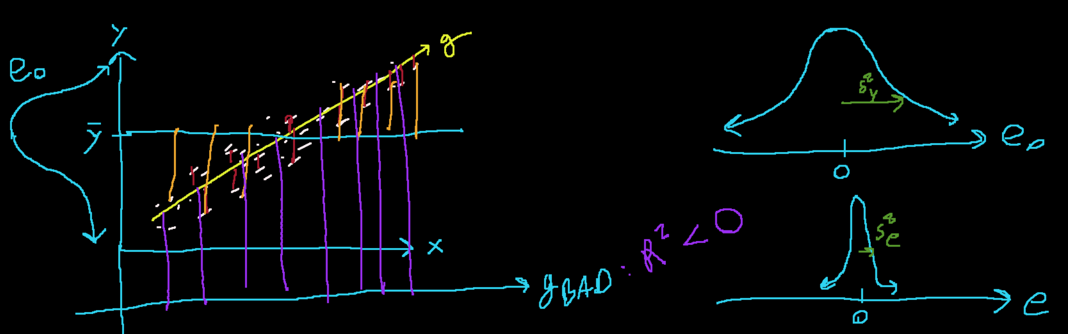
is approx a 95% confidence interval for the true y at that x. RMSE is a very important metric in regression models.

Another important error / performance metric is "R-squared" which is the "proportion of variance explained". We will now explain this definition.

Consider the null model, $g_0 = \bar{y}$. What is the SSE of this model? Let's call it SSE_0.

$$SSE_0 = \sum_{i=1}^{n} e_{0,i}^2 = \sum_{i=1}^{n} (y_i - \bar{y})^2 = \underbrace{SST} = (n-1) s_y^2$$

sum of squares total

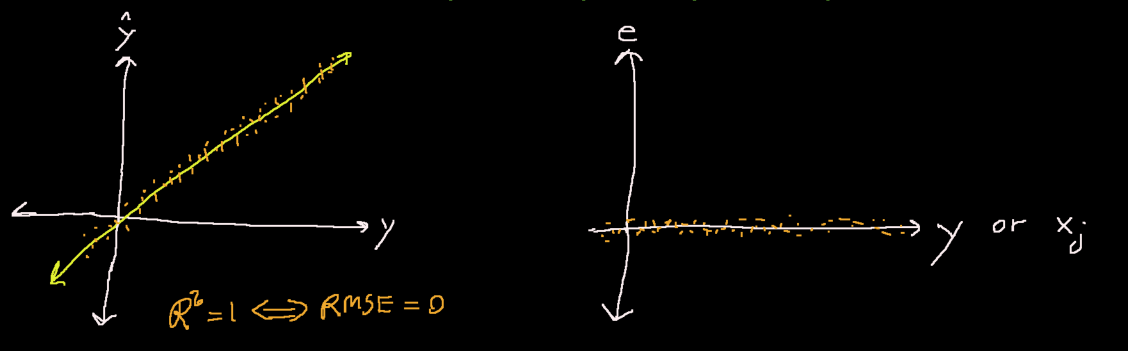


$$\frac{SSE}{SST} = \frac{(n-1) s_e^2}{(n-1) s_y^2} = \frac{s_e^2}{s_y^2}$$

$$R^2 = \frac{SST - SSE}{SST} = \frac{(n-1) s_y^2 - (n-1) s_e^2}{(n-1) s_y^2} = \frac{\overbrace{s_y^2 - s_e^2}^{\Delta s^2}}{s_y^2} = \frac{\Delta s^2}{s_y^2}$$

R-squared can never be more than 100%. But R-squared can be negative. This occurs when s^2_e > s^2_y meaning the model is predicting worse than g_0 = ybar.

Here's some other useful plots especially when p > 1:



$$R^2 = 1 \iff RMSE = 0$$

$$R^2 \uparrow \iff RMSE \downarrow$$

If R^2 = 99%, does this mean the model is for sure "good"? No. Because if the initial variance was so very large, even a 99% reduction wouldn't result in a small residual variance i.e. RMSE still could be high after 99% variance reduction.

We now would like to generalize the least squares estimation algorithm to cases where p > 1. Let's begin with p = 2.

$$\mathcal{H} = \left\{ w_0 \overset{\vec{x}\vec{w}}{+} w_1 x_1 + w_2 x_2 : \underbrace{w_0, w_1, w_2 \in \mathbb{R}}_{\vec{w} \in \mathbb{R}^3} \right\}$$

$$SSE = \sum_{i=1}^{n} e_i^2 = \sum (y_i - \hat{y}_i)^2 = \sum (y_i - w_0 - w_1 x_{1,i} - w_2 x_{2,i})^2$$

$$b_0 = \underset{w_0 \in \mathbb{R}}{\text{argmin}} \{SSE\}, \quad b_1 = \underset{w_1 \in \mathbb{R}}{\text{argmin}} \{SSE\}, \quad b_2 = \underset{w_2 \in \mathbb{R}}{\text{argmin}} \{SSE\}$$

This problem can be solved more simply with matrix algebra and a matrix equation:

$$\mathbb{D} = \langle X, \vec{y} \rangle, \quad \text{let } X = [\vec{1}_n \; \vec{x}_{\cdot 1} \; \vec{x}_{\cdot 2}] = \begin{bmatrix} 1 & x_{11} & x_{12} \\ 1 & x_{21} & x_{22} \\ 1 & x_{31} & x_{32} \\ \vdots & \vdots & \\ 1 & x_{n1} & x_{n2} \end{bmatrix}$$

$$\text{e.g. } \hat{y}_1 = \vec{x}_1 \vec{w}, \; \hat{y}_2 = \vec{x}_2 \vec{w} \; \ldots$$

$$\underbrace{\hat{\vec{y}} = X\vec{w}} = \begin{bmatrix} w_0 + w_1 x_{11} + w_2 x_{12} \\ w_0 + w_1 x_{21} + w_2 x_{22} \\ \vdots \\ w_0 + w_1 x_{n1} + w_2 x_{n2} \end{bmatrix}$$

$$\text{define } \vec{e} := \vec{y} - \hat{\vec{y}}$$

$$SSE = \sum_{i=1}^{n} e_i^2 = \vec{e}^\top \vec{e} = (\vec{y} - \hat{\vec{y}})^\top (\vec{y} - \hat{\vec{y}}) = (\vec{y}^\top - \hat{\vec{y}}^\top)(\vec{y} - \hat{\vec{y}})$$

$$= \vec{y}^\top \vec{y} - \hat{\vec{y}}^\top \vec{y} - \overbrace{\vec{y}^\top \hat{\vec{y}}}^{\hat{\vec{y}}^\top \vec{y}} + \hat{\vec{y}}^\top \hat{\vec{y}} = \vec{y}^\top \vec{y} - 2 \hat{\vec{y}}^\top \vec{y} + \hat{\vec{y}}^\top \hat{\vec{y}}$$

$$= \vec{y}^\top \vec{y} - 2 (X\vec{w})^\top \vec{y} + (X\vec{w})^\top X\vec{w} = \vec{y}^\top \vec{y} - 2 \vec{w}^\top X^\top \vec{y} + \vec{w}^\top X^\top X \vec{w}$$