The optimal model will have enough components to accurately fit data and be predictive, but remain simple enough for interpretation. Additionally, the model is subject to over-fitting constraints.

Three metrics are used to evaluate the utility of adding a new component (a):

R^2X: sum of squares for the variation in the **X** matrix

$$R^2X = 1 - \frac{\Sigma(X_{model,a} - X_{obs})^2}{\Sigma(X_{obs}^2)}$$

R^2Y: sum of squares for the variation in the **Y** matrix

$$R^2Y = 1 - \frac{\Sigma(Y_{model,a} - Y_{obs})^2}{\Sigma(Y_{obs}^2)}$$

Q^2Y: fraction of the total variation in the **Y** matrix that can be predicted

$$Q^2Y = [1.0 - \Pi(PRESS/SS)_a]$$

<u>PRESS = Prediction Error Sum of Squares</u>

1) Remove an individual data element (i,k)
2) Fit model
3) Predict the element i,k that was withheld

   $(observed_{i,k} - predicted_{i,k})^2$
4) Repeat until each element has been withheld once and only once