Variance of Cross-Validated χ^2

To understand the uncertainty associated with the empirical χ^2 values for both the training and test datasets, we compute the **empirical variance** across repeated trials, and compare it to the **theoretical variance** predicted by chi-squared statistics.

Empirical Variance Calculation

For each model complexity (polynomial degree) m, and each of the T random trials, we compute:

$$\chi^{2(t)}_{A}(m) = \frac{1}{\sigma^2} \sum_{i=1}^{N} \left(y_{A,i}^{(t)} - \hat{y}_{A,i}^{(t)} \right)^2, \quad t = 1, 2, \ldots, T$$

Then the sample mean and variance are:

$$\overline{\chi^2{}_A}(m) = \frac{1}{T} \sum_{t=1}^{T} \chi^{2(t)}_{A}(m)$$

$$\mathrm{Var}[\chi^2{}_A](m) = \frac{1}{T} \sum_{t=1}^{T} \left(\chi^{2(t)}_{A}(m) - \overline{\chi^2{}_A}(m) \right)^2$$

The same formulas hold for the test dataset $\chi^{2(t)}_{B}(m)$.

Theoretical Variance of Chi-Squared Distribution

If the model is correct and the residuals are Gaussian, then the quantity χ^2 follows a chi-squared distribution with ν degrees of freedom. The mean and variance of a chi-squared random variable with ν degrees of freedom are:

$$\mathbb{E}[\chi^2] = \nu, \quad \mathrm{Var}[\chi^2] = 2\nu$$

We apply this to estimate the theoretical variance for both datasets:

$$\mathrm{Var}_{\mathrm{theory}}(\chi^2{}_A) = 2(N - m)$$
$$\mathrm{Var}_{\mathrm{theory}}(\chi^2{}_B) = 2(N + 3m)$$

Here, N is the number of data points in each dataset, and m is the number of fit parameters (i.e., polynomial degree + 1).

Comparison and Visualization

In the plot:

- The empirical standard deviations $\sqrt{\mathrm{Var}({\chi^2}_A)}$ and $\sqrt{\mathrm{Var}({\chi^2}_B)}$ are shown as vertical error bars.
- The theoretical standard deviations $\sqrt{2(N-m)}$ and $\sqrt{2(N+3m)}$ are shown as shaded bands centered on the average χ^2 values.

This comparison helps evaluate whether the observed variability in χ^2 aligns with expectations under the assumption of Gaussian noise and a well-calibrated model.