Lack-of-fit Tests to Indicate Material Model Improvement or Experimental Data Noise Reduction

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Finding parameters for material models

- there are many choices of material models
- commercial finite element codes have implemented dozens
- selecting the best model isn't simple
- selecting the best set of parameters
- FEA results compare to experimental results
- lack-of-fit may be a useful tool for these responses

What is lack-of-fit

A lack-of-fit test is a statistical test that answers whether:

- Does the variation between my model and data come from the inadequacy of my model?
- Or is the variation a result of the inherent noise in the test data?

This is what lack-of-fit looks like

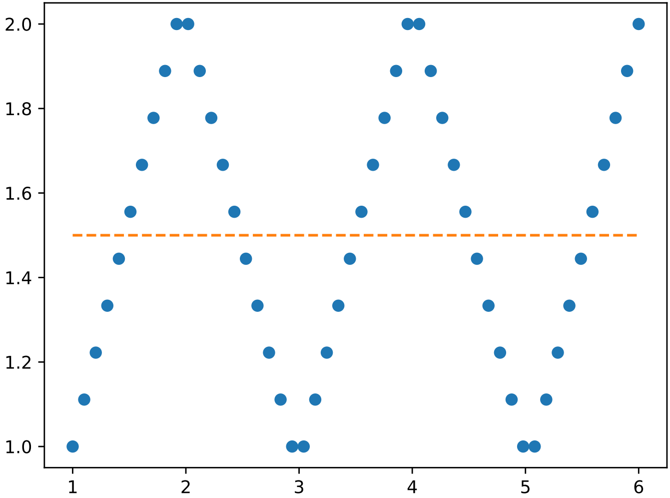


Figure 1: A constant model is fit to a collection of data points where lack-of-fit is apparent.

However this model is adequate with the provided data

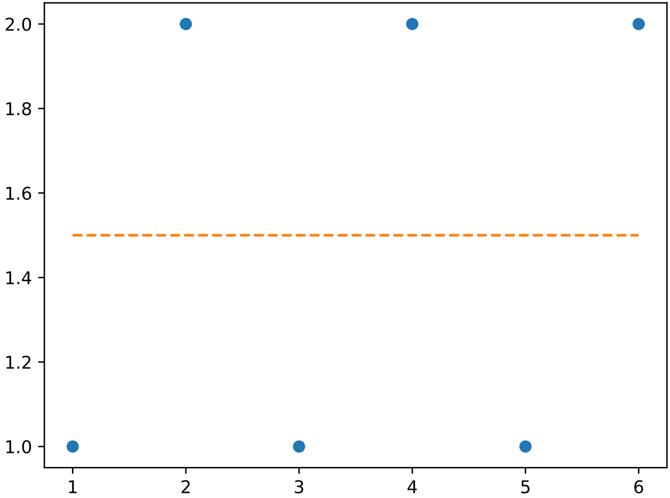


Figure 2: A constant model is fit to a collection of data points where the model adequately describes the data.

Traditional lack-of-fit test

There is a statistical test to check for lack-of-fit in cases when it may be difficult to see.

- partitioning sum of squares
- pure-error and lack-of-fit
- F-test
- analysis of variance (ANOVA)
- requires true replicates

$$F = \frac{\text{lack-of-fit}}{\text{pure-error}} \tag{1}$$

True replicates and noise

It just so happens that it's easy to calculate the pure-error with true replicates.

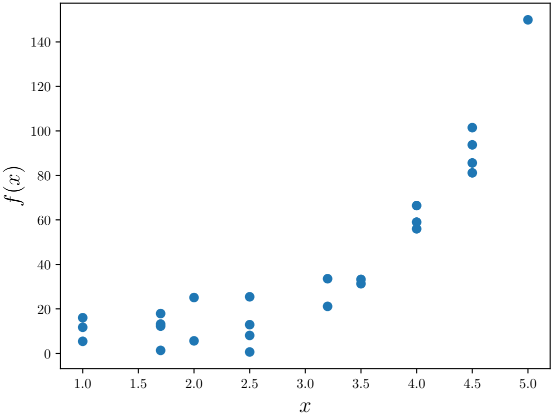


Figure 3: An example demonstrating true replicates. There are multiple $f(x)$ for a unique x.

Typically don't have true-replicates

Often we're determining material parameters for a model to match a collection of experimental responses. For this type of response we'll need a different formulation of F.

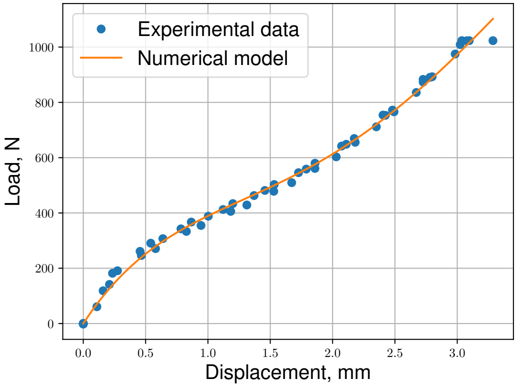


Figure 4: A collection of uniaxial tests and a FE model using a strain dependent Young's modulus.

Calculating the unbiased variance of fit - error

For the previous example, we can easily calculate the unbiased variance of our numerical model compared to the test data. This is analogous to the sum of square of residuals.

$$\mathbf{e} = f(\mathbf{x}) - \hat{f}(\mathbf{x}) \tag{2}$$

$$\hat{\sigma}^2 = \frac{\mathbf{e} \cdot \mathbf{e}^\mathsf{T}}{n - n_\beta} \tag{3}$$

If the model is a perfect fit to the data, $\hat{\sigma}^2 = 0$.

$\hat{\sigma}^2$ is the **error** of fit.

Estimating the noise in test data

There are multiple methods to estimate the variance (or noise) within test data. The methods that stand out in literature are the GSJ[1] and Hart[2] variance estimators.

GSJ:

- lines every three consecutive data points
- intended for non-linear regression
- widely used

Hart:

- uses regression model fit to data
- similar to spline interpolation

The GSJ variance estimator constructs a pseudo-residual vector between the line of every three consecutive points.

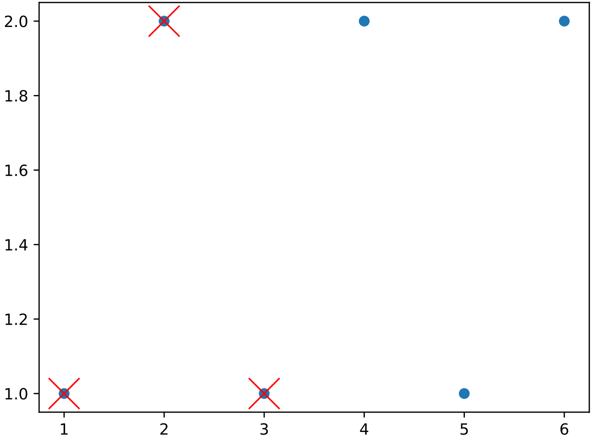


Figure 5: Select three consecutive points.

GSJ variance estimator 2 of 3

We can fit a line in between the first and third data point. This line is assumed to represent the data.

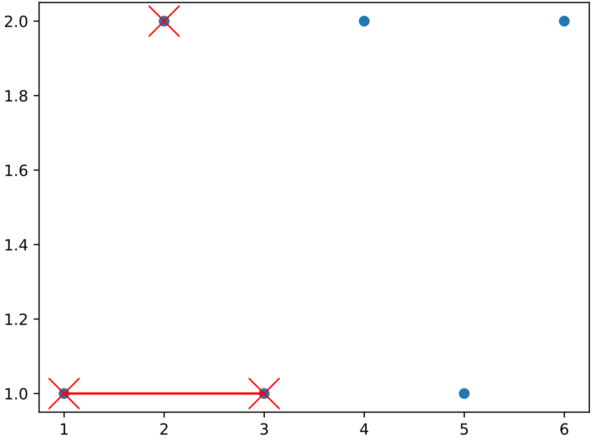


Figure 6: Line created between the first and third point.

The deviation between second point and line is calculated for every three consecutive points. These deviations are used to approximate the noise.

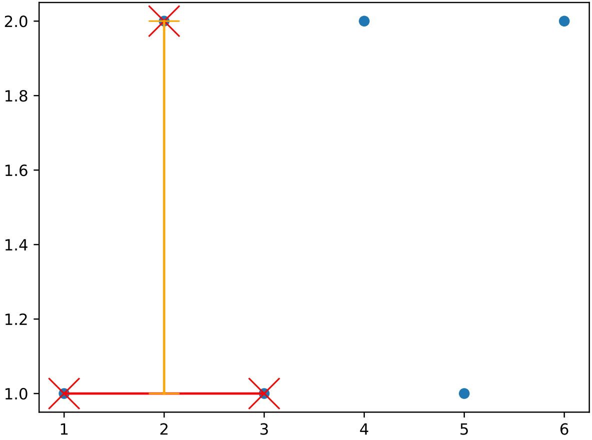


Figure 7: Deviation between the second point and pseudo-line.

Lack-of-fit test as comparison of variance

$$F = \frac{\hat{\sigma}^2}{\hat{\sigma_e}^2} = \frac{\textbf{Error}}{\textbf{Noise}} \tag{4}$$

When the variance of fit is equal to the variance within test data, $F = 1.0$, then there is no lack-of-fit.

When the variance of fit is much larger than the variance within test data, F is larger than one, then there is lack-of-fit.

F follows the F-distribution

A P-value can be calculated for a particular F and then used to accept/reject the following null hypothesis.

$$H_0 : \text{Model adequately represents data} \tag{5}$$

If we reject the null hypothesis, then there is lack-of-fit.

A load-dependent Poisson's ratio

There is no lack-of-fit in this example. The deviation between the trend and data can be entirety explained by the variation in the data from noise.

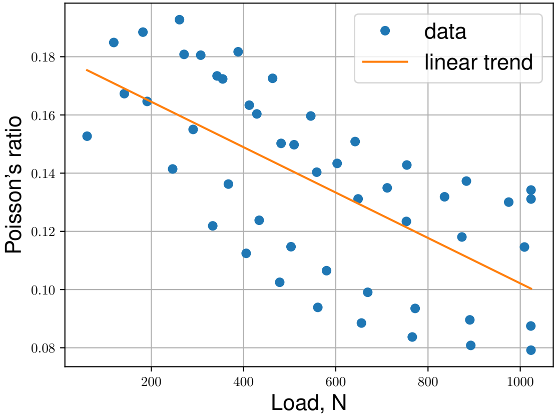


Figure 8: A collection of observed Poisson's ratios as a function of Load.

Improved load-dependent Poisson's ratio

With better process control in our tests we can reduce the noise in the test data improving the overall model.

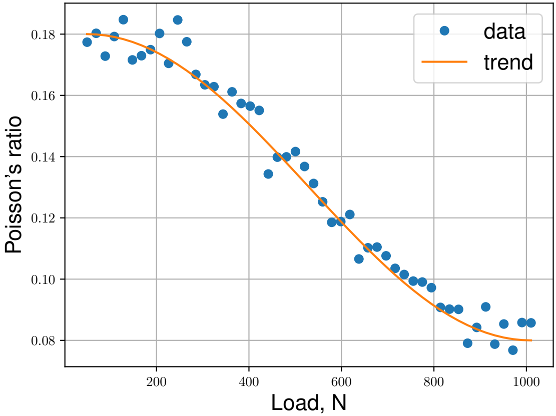


Figure 9: Improved observed Poisson's ratios as a function of Load.

Non-linear orthotropic model for PVC-coated polyester

I simultaneously determine all of the $\boldsymbol{\beta}$ parameters in a single optimization of a warp, fill, and 45° bias uniaxial test. Each uniaxial test has a FE model which is matched to an experimental response [3].

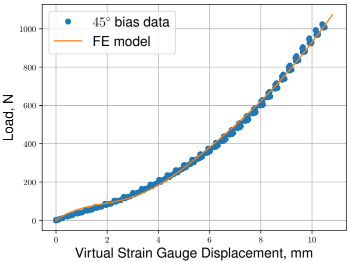
$$E_1(\varepsilon_1) = \beta_0 + \beta_1\varepsilon_1 + \beta_2\varepsilon_1^2 + \beta_3\varepsilon_1^3 \tag{6}$$

$$E_2(\varepsilon_2) = \beta_4 + \beta_5\varepsilon_2 + \beta_6\varepsilon_2^2 \tag{7}$$

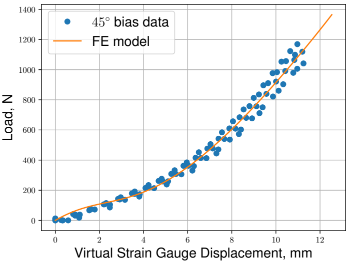
$$G_{12}(\gamma_{12}) = \beta_7 + \beta_8\gamma_{12} + \beta_9\gamma_{12}^2 \tag{8}$$

45° bias test - consider these two different results

It's difficult to spot lack-of-fit.



(a) Lack-of-fit is present. $F = 1.6$ P=0.001

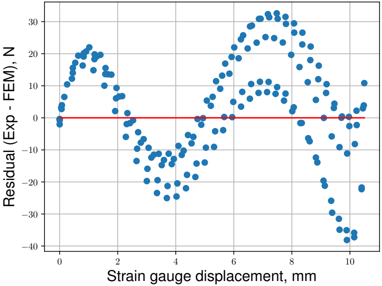


(b) No lack-of-fit. $F = 0.8$ P=0.79

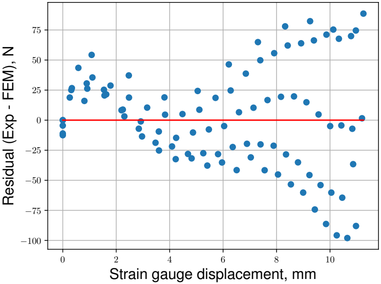
Figure 10: Results of a uniaxial 45° bias test for two different PVC-coated polyesters.

Lack-of-fit can be thought of as a pattern

Clearly see the lack-of-fit in the residual plots.



(a) Lack-of-fit is present. $F = 1.6$ P-value=0.001



(b) No lack-of-fit. $F = 0.8$ P-value=0.79

Figure 11: Lack-of-fit is apparent in the results on the left, but not in the results on the right. The red line at 0 marks where a perfect model would match every data point exactly.

Hysteresis loops for modeling metal forming process

- kinematic hardening material model
- five experimental load-unload-load cycles
- used for modeling metal forming process

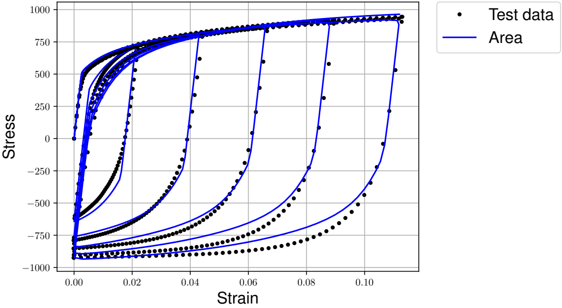


Figure 12: Comparison of numerical model and test data for five hysteresis loops.

Lack-of-fit in sections of Hysteresis loops

Without doing any calculations we can see regions in the residual plot where lack-of-fit is present. The figures shows the first hysteresis cycle.

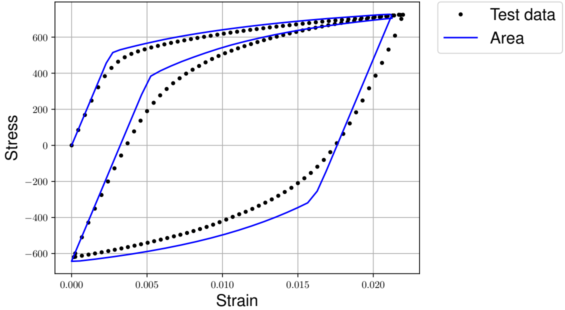
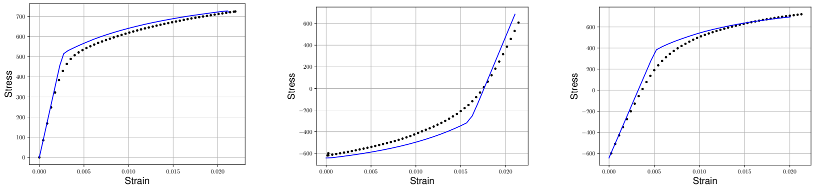


Figure 13: Lack-of-fit is apparent in some sections of the residual plot of the fit to the five hysteresis loops. (P-value load-unload-load: 0.0-0.0-0.0)

As it turns out, these material parameters don't adequately describe this load-unload-load cycle. This is the result of poor optimization.

Partitioning load-unload-load cycle to calculate lack-of-fit

Lack of fit exists when P-value<0.05.



(a) $F=2.8$, P=0.0 (b) $F=25$, P=0.0 (c) $F=7.1$, P=0.0

Figure 14: Showing lack-of-fit in sections of the load-unload-load cycle.

Noise in sections of Hysteresis loops

Applying lack-of-fit to the specific load-unload-load regions we see: 1) no lack-of-fit in the load regions. 2) lack-of-fit in the first unload region.

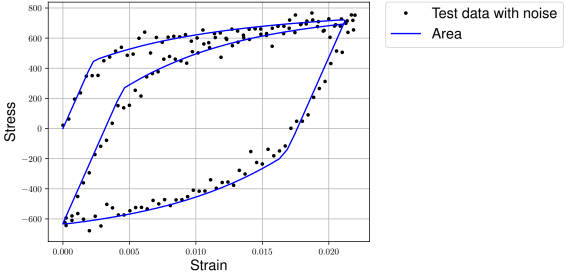
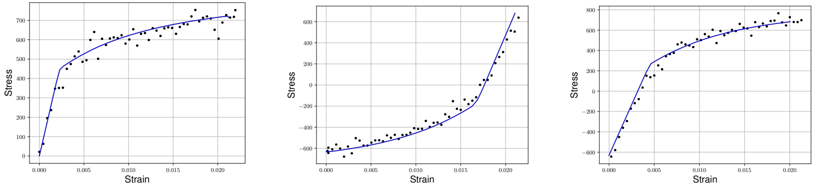


Figure 15: Lack-of-fit is less apparent in some sections of the residual plot of the fit to the five hysteresis loops. (P-value load-unload-load: 0.5-0.0-0.05)

Hybrid outcome: Need to reduce the noise in the load sections, and improve the model in the unload section.

Partitioning load-unload-load cycle to calculate lack-of-fit

Lack of fit exists when P-value<0.05.



(a) $F=0.98$, P=0.52 (b) $F=3.5$, P=0.00 (c) $F=1.83$, P=0.05

Figure 16: Showing lack-of-fit in sections of the load-unload-load cycle with artificial noise.

What could cause lack-of-fit?

So what may cause a systemic departure in your results?

- model is too simple
- modeling parameter are inadequate
- a physical phenomenon not accounted for
- an error in the experiment

Conclusion

$$F = \frac{\textbf{Error}}{\textbf{Noise}} \tag{9}$$

- lack-of-fit as a comparison of variances
- residual plots are useful in visualizing lack-of-fit
- lack-of-fit can be thought of as systematic departure from an expected trend
- another tool to evaluate results

References (are in numerical order) I

T. Gasser, L. Sroka, and C. Jennen-Steinmetz.
Residual Variance and Residual Pattern in Nonlinear Regression.
Biometrika, 73(3):625–633, 1986.

J. D. Hart.
Classical Lack-of-Fit Tests, pages 117–143.
Springer New York, New York, NY, 1997.

C. F. Jekel, G. Venter, and M. P. Venter.
Modeling PVC-coated polyester as a hypoelastic non-linear orthotropic material.
Composite Structures, 161:51–64, feb 2017.