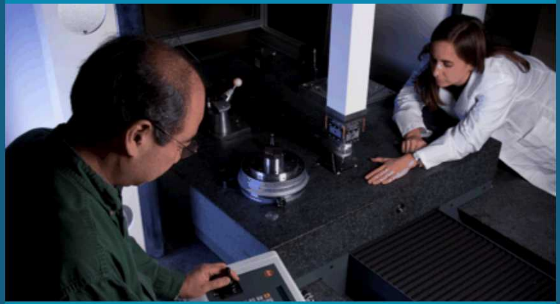
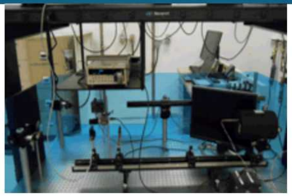
SAND2018-9321C

Calculating Interval Uncertainties for Calibration Standards That Drift with Time





PRESENTED BY

Collin J. Delker

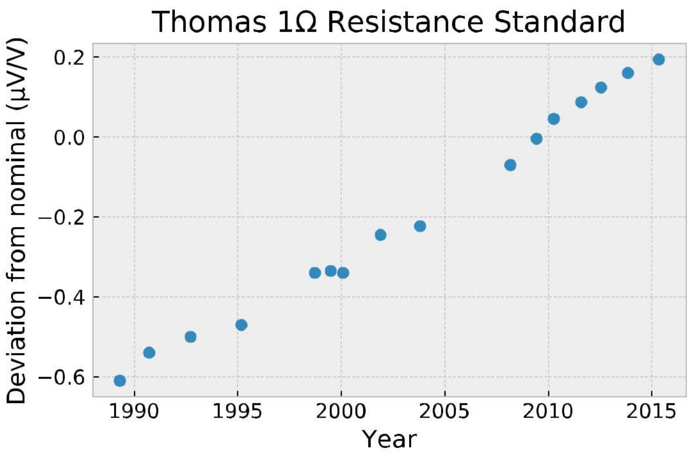
E. Auden, M. Benner, E. Forrest, R. Johnson, T. Kypta, T. Moss, J. Novak, E. O'Brien, K. Sanchez, R. Sandoval, O. Solomon, G. Smith

SAND: XXXXXXXXX

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

MOTIVATION

Many calibration standards drift over time due to physical aging mechanisms. How should this drift be accounted for in an uncertainty budget?



- **ISO 17025**: Report time-of-test uncertainty only
- **DOE/NNSA**: Must certify an interval uncertainty accounting for **drift**, shipping, usage, etc.


Thomas-Type Resistor


Current shunt

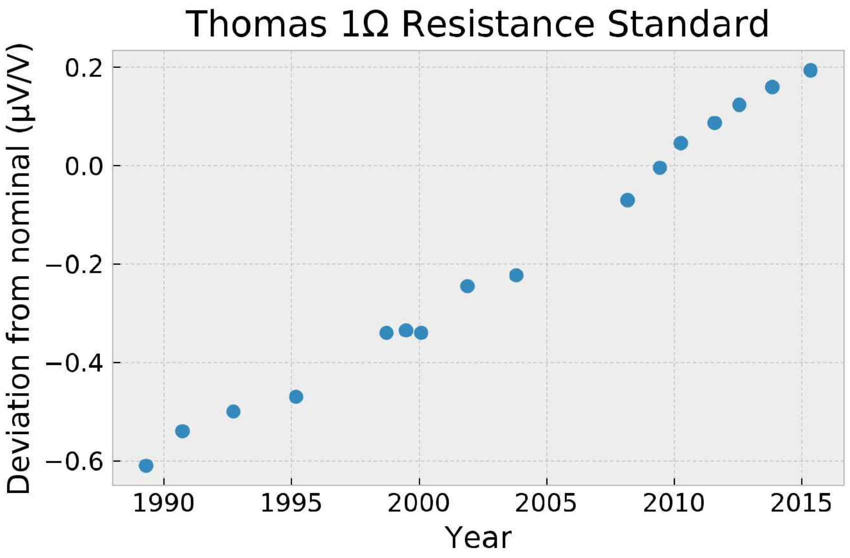

Zener DCV standard


Voltage Divider

UNCERTAINTY COMPONENTS

- Type A Measurement Uncertainty
- Type B System Uncertainty
- Expected drift and drift uncertainty

- Goal: Provide an uncertainty statement that is valid until the next calibration due date



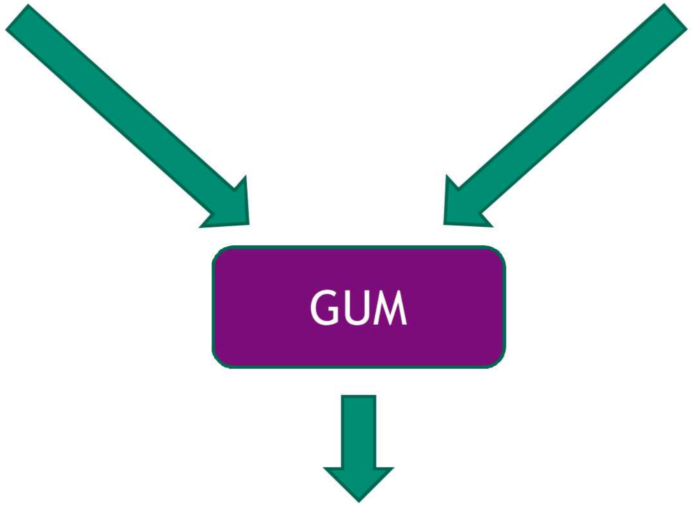
TIME-OF-TEST UNCERTAINTY

System Uncertainty

- Measurement Model
- Calibration Standards
- Environmental Conditions
- Stimulus Settings, etc.

Type A Uncertainty

- Repeated Measurements
- N Measurements Repeated on M days, etc.



$$\sigma_{test} = \sqrt{\sigma_{sys}^2 + \sigma_{typeA}^2}$$

DETERMINING DRIFT RATE – LINEAR REGRESSION

Standard line fit function minimizes residual distances between measured y_i and fit line y(x):

$$y = A + Bx$$

Fit parameters:

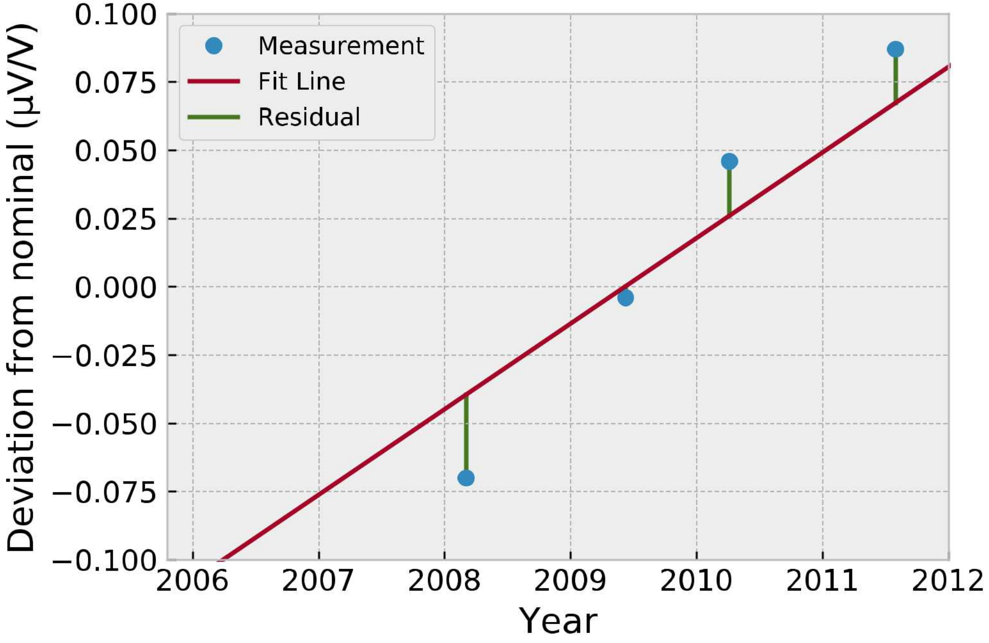
$$A = \frac{\Sigma x_i^2 \Sigma y_i - \Sigma x_i \Sigma x_i y_i}{\Delta}$$

$$B = \frac{N \Sigma x_i y_i - \Sigma x_i \Sigma y_i}{\Delta}$$

$$\Delta = N \Sigma x_i^2 + (\Sigma x_i)^2$$

Parameter Uncertainties:

$$\sigma_A = \sigma_y \sqrt{\frac{\Sigma x_i^2}{\Delta}} \qquad \sigma_B = \sigma_y \sqrt{\frac{N}{\Delta}}$$



Excel's LINEST function makes the **assumption** that uncertainty in every data point is equal to average residual:

$$\sigma_y^2 = \frac{\Sigma (y_i - A - Bx_i)^2}{N - 2}$$

DETERMINING DRIFT RATE – LINEAR REGRESSION

The residual scatter already includes known uncertainties, so if you assume σ_y and also include known uncertainty, you have double counted. You did all that work to determine time-of-test uncertainty: use it!

$$\sigma_y^2 = \frac{\Sigma(y_i - A - Bx_i)^2}{N-2}$$

$$\sigma_y = \sigma_{test} = \sqrt{\sigma_{sys}^2 + \sigma_{typeA}^2}$$

Line fit calculation is the same, but use the known σ_y. Calculate fit by hand or use a function like Python's numpy.polyfit() with *w* parameter, or R's lm() with *weights* parameter.

$$\sigma_A = \sigma_y\sqrt{\frac{\Sigma x_i^2}{\Delta}} \qquad \sigma_B = \sigma_y\sqrt{\frac{N}{\Delta}}$$

Note that σ_y can also vary with time, such as by varying Type A uncertainty each year or changing equipment during the device's history. Expressions for σ_A and σ_B can be weighted appropriately.

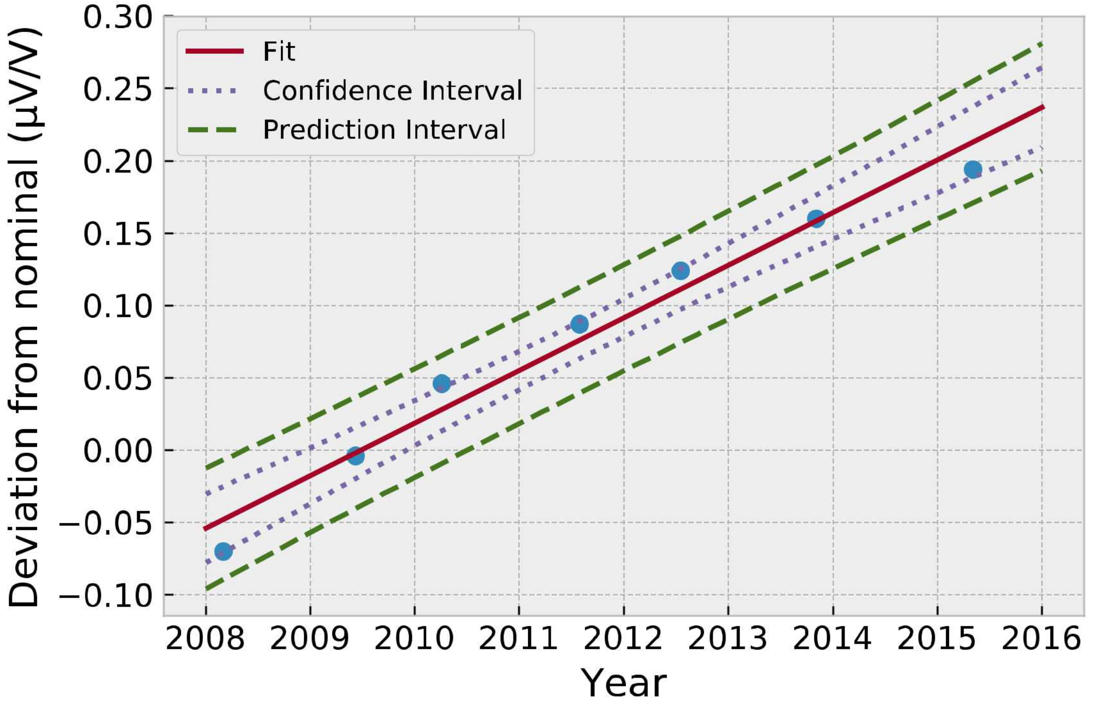
CONFIDENCE AND PREDICTION INTERVAL

The calculated σ_B gives uncertainty in the slope of the line. To identify the uncertainty of the line itself and a point predicted by the line at the next calibration due date, use confidence and prediction intervals.

$$u_{conf}(t) = \sigma_y \sqrt{\frac{1}{N} + (t - \bar{t})^2 \left(\frac{\sigma_B}{\sigma_y}\right)^2}$$

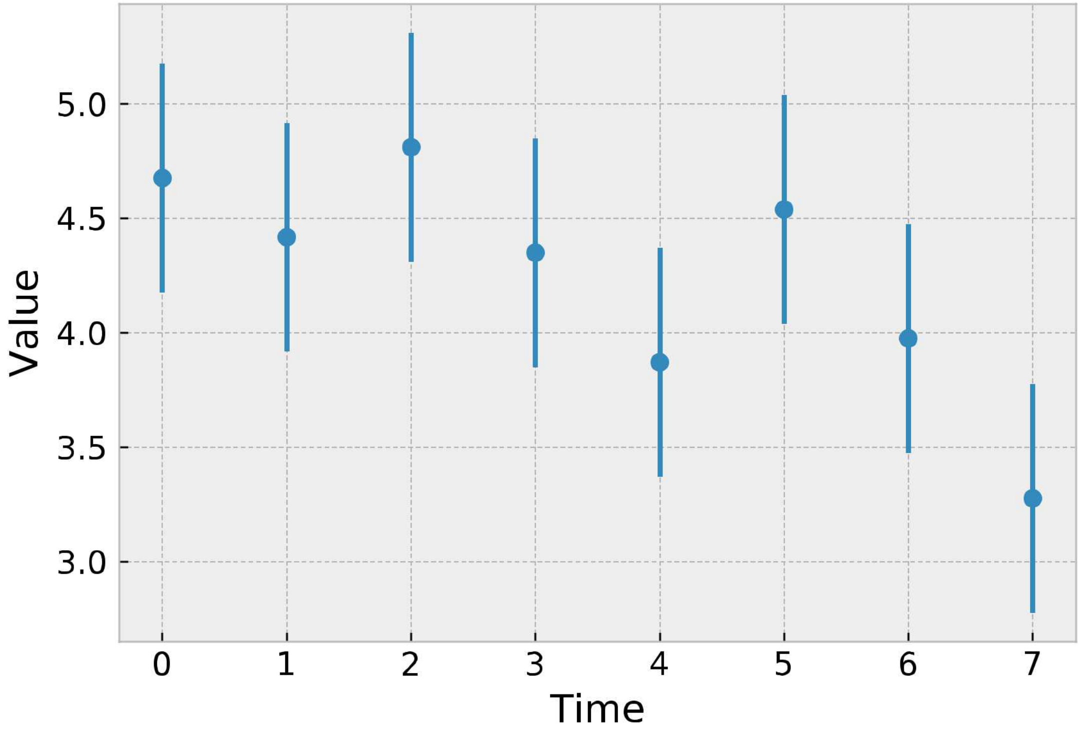
$$u_{pred}(t) = \sqrt{\sigma_y^2 + u_{conf}^2(t)}$$

$$= \sigma_y \sqrt{1 + \frac{1}{N} + (t - \bar{t})^2 \left(\frac{\sigma_B}{\sigma_y}\right)^2}$$

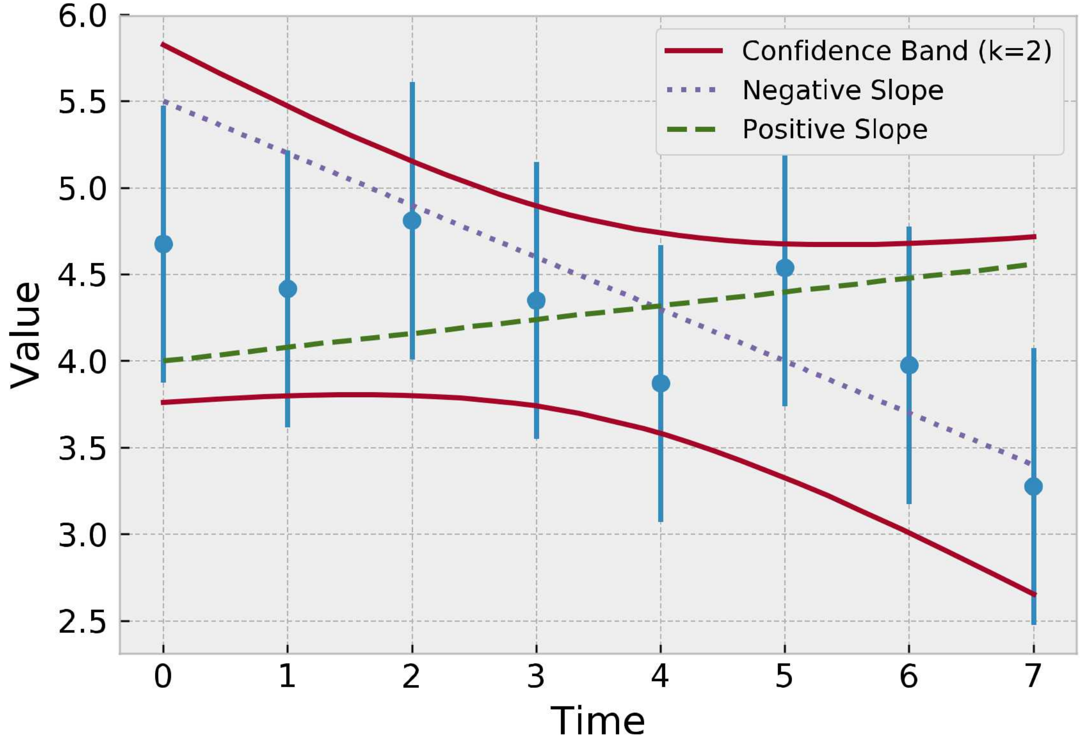


SLOPE TEST

Data appears to have negative drift slope…



yet fit-line to 95% confidence can be positive or negative!



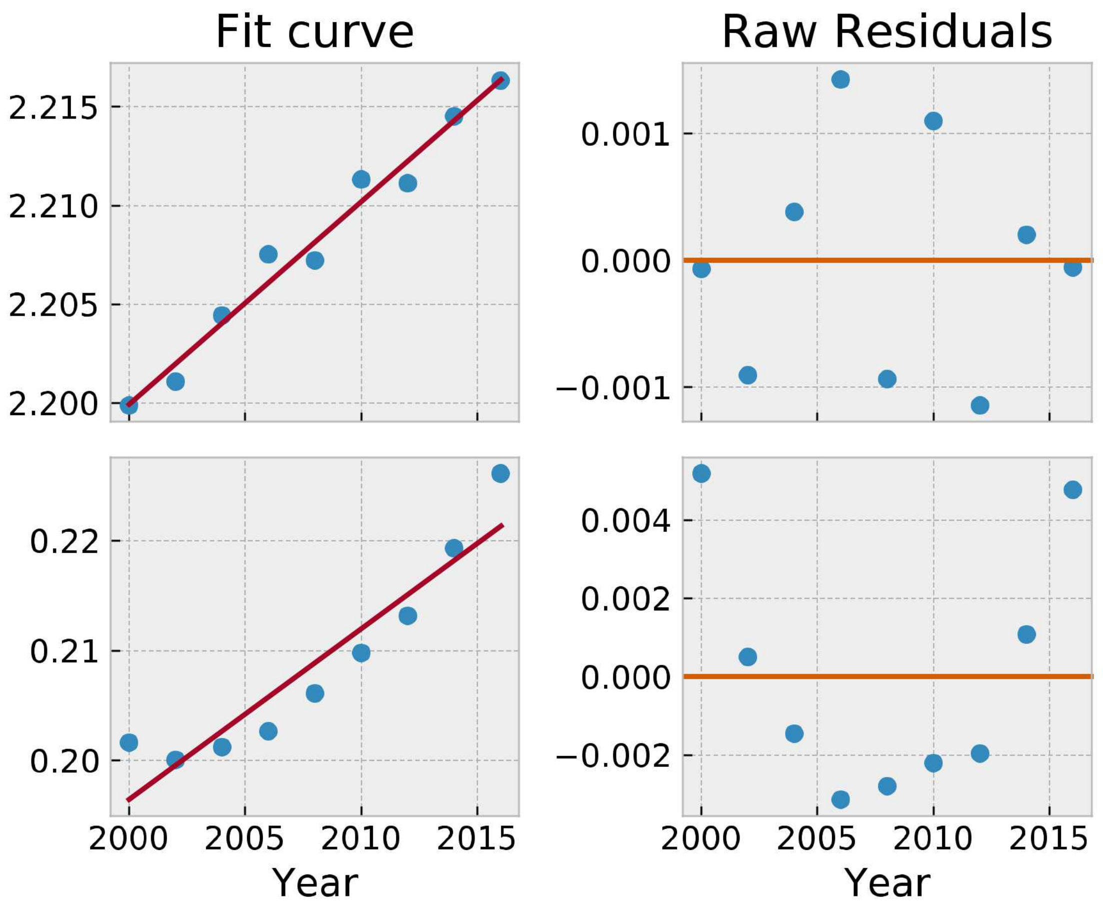
If slope B $\pm$ k σ_B contains 0, the slope has no statistical significance.
Make sure your device passes the slope test before adjusting for drift.

IS THE DRIFT LINEAR?

Raw residuals normally distributed about 0 indicate the model (line) is a good model to use for the data.

Straight line describes data well

Polynomial would probably work better



IDEAL WAY TO REPORT UNCERTAINTY OF DRIFTING DEVICE

The ideal way: report predicted value and uncertainty as function of time over the interval.

$$y(t) = (A + B \cdot t) \pm \left[k \cdot \sigma_y \sqrt{1 + \frac{1}{N} + (t - \bar{t})^2 \left(\frac{\sigma_B}{\sigma_y} \right)^2} \right]$$

$$y(t) = (9.9445 \times 10^{-5} \cdot t - .002795) \pm \left[0.02815 \sqrt{0.31443(t - 4235.1)^2 + 26} \right]$$

Who wants to evaluate this formula every time the asset is used?

Be careful of units. Is t in days? Years? Is t the time since last calibration, since the beginning of the device's history, or seconds since January 1, 1970?

Quick, how many days has it been since the thing was calibrated on May 15?

HOW TO COMBINE UNCERTAINTIES INTO SINGLE VALUE?

Method 1: Add in the expected drift

$$u_c = k\sqrt{\sigma_{test}^2 + u_{conf}^2(t = t_{next})} + \text{abs}(rate \cdot interval)$$

Method 2: RSS in the expected drift

$$u_c = k\sqrt{\sigma_{test}^2 + u_{conf}^2(t = t_{next}) + (rate \cdot interval)^2}$$

HOW TO COMBINE UNCERTAINTIES INTO SINGLE VALUE?

Method 3: Apply GUM guidance on known correction factors (GUM F.2.4.5)

Correction Factor

$$b(t) = r \cdot t \qquad \bar{b} = \frac{r(t_2 - t_1)}{2}$$

Uncertainty in Average Correction

$$u^2(\bar{b}) = \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} (b - \bar{b})^2 \mathrm{d}t = \frac{r^2}{12}(t_1^2 - 2t_1 t_2 + t_2^2)$$

Uncertainty in Determining Correction

$$\overline{u^2[b(t)]} = \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} u_{conf}^2(t) \mathrm{d}t$$

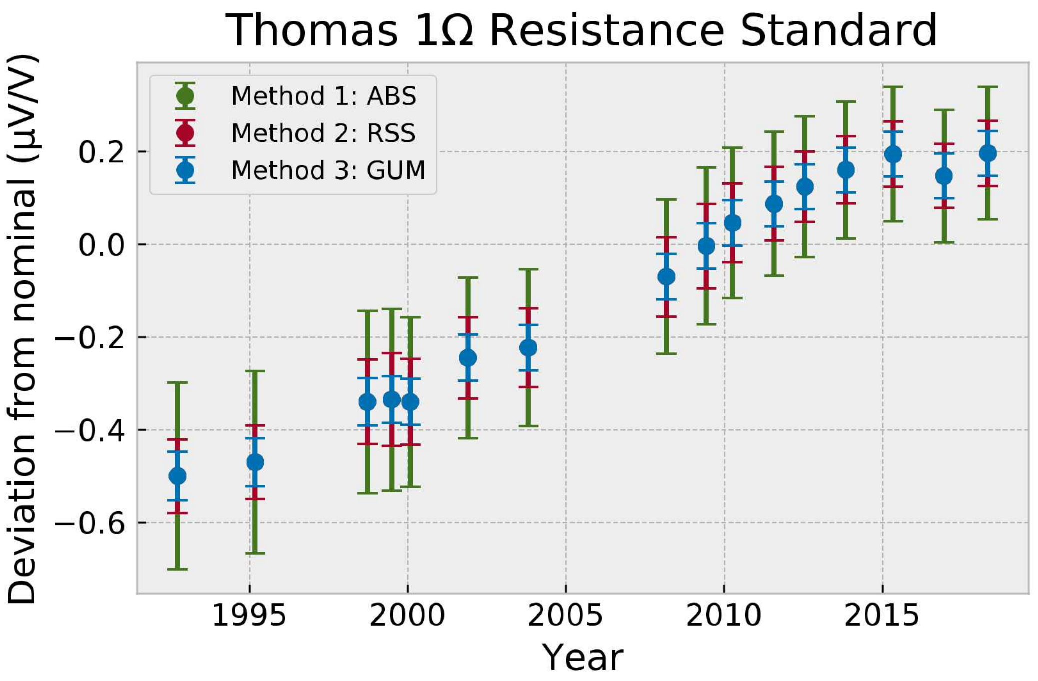
Other Uncertainty in Measurement

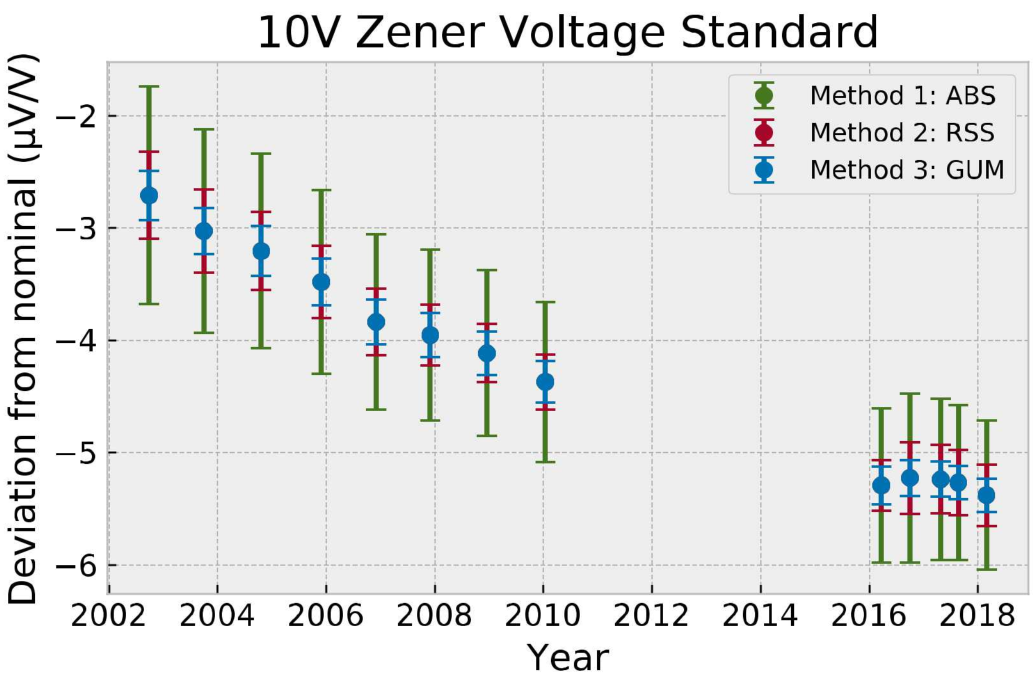
$$\overline{u^2[y(t)]} = \sigma_{test}^2$$

$$u_c = k\sqrt{u^2(\bar{b}) + \overline{u^2[b(t)]} + \overline{u^2[y(t)]}}$$

$$y = y' + \bar{b} \pm u_c$$

CASE STUDIES





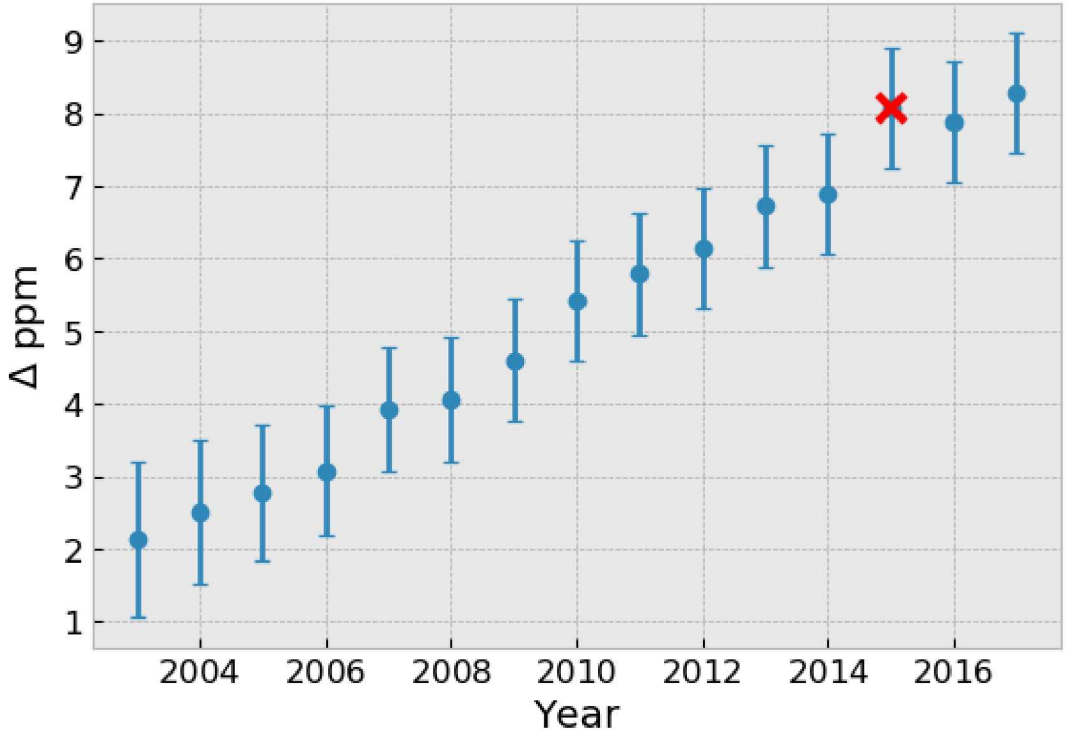
2018 Uncertainty Components (μV/V)	Thomas 1Ω	Zener 10V
Time-of-Test Uncertainty (k=1)	0.022	0.11
Confidence Interval (k=1)	0.0079	0.065
Drift Rate (μV/V/year)	0.036	-0.20
Expanded Uncertainty Method 1 (ABS)	0.14	0.66
Expanded Uncertainty Method 2 (RSS)	0.070	0.27
Expanded Uncertainty Method 3 (GUM)	0.048	0.15

COMPARE THE METHODS USING MONTE CARLO

Approach:

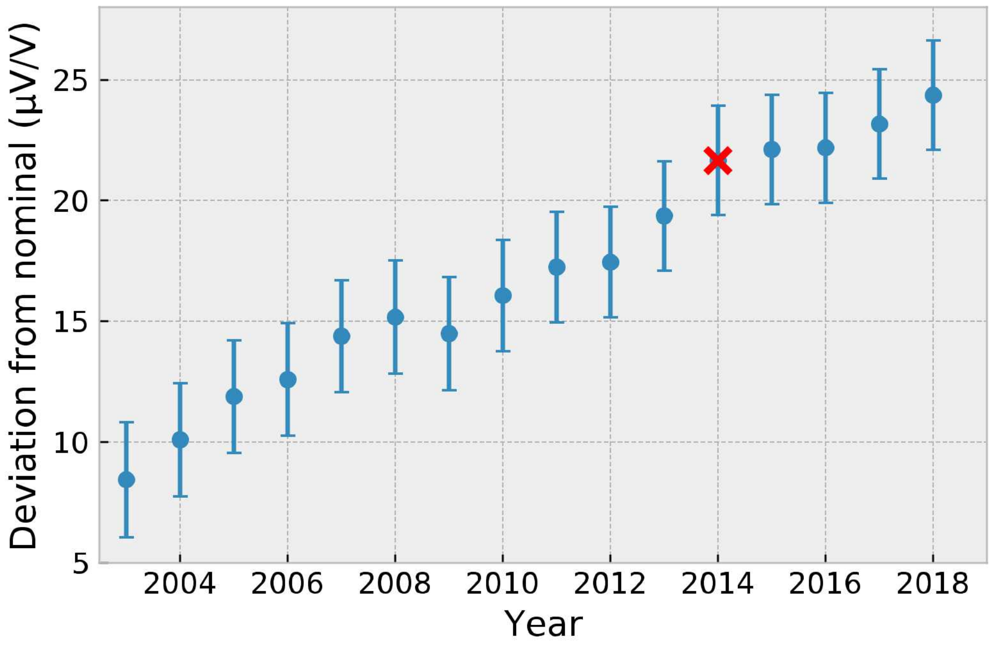
- Simulate many possible drift lines. Try different drift rate and time-of-test uncertainty.
- Start with 5 data points (1997-2002, not shown) to get enough data to start regression
- Error bars at each point are based on calculated drift uncertainty using data from all previous years expanded to 95% coverage
- Compare this uncertainty with next year's data point. Count out-of-tolerance rate.

One of N Monte Carlo data sets
Red X point is OOT

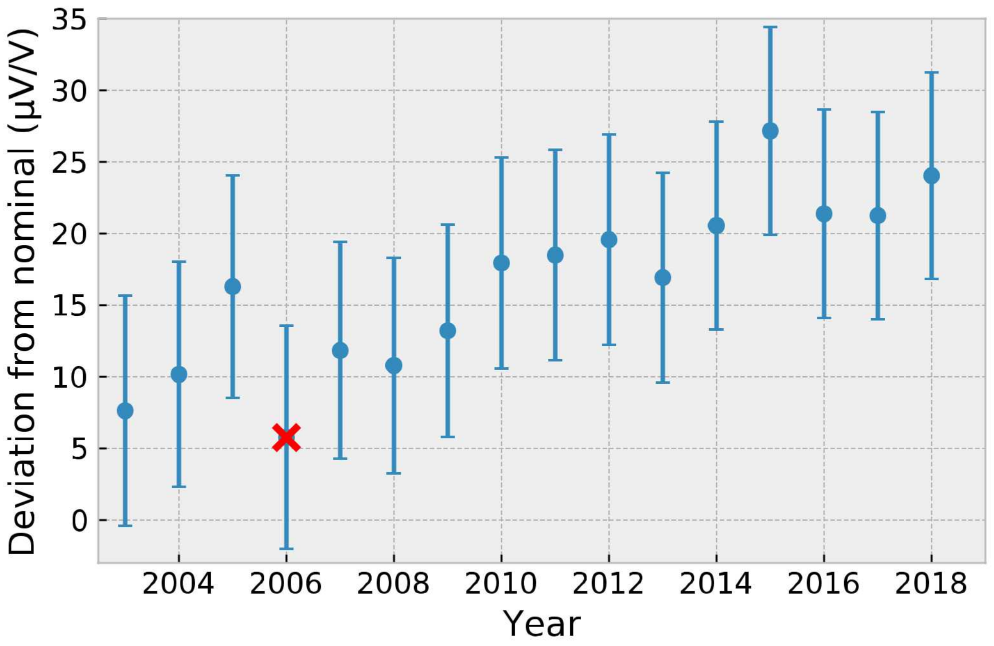


MONTE CARLO RESULTS

Low time-of-test uncertainty (Method 3 shown)



High time-of-test uncertainty (Method 3 shown)



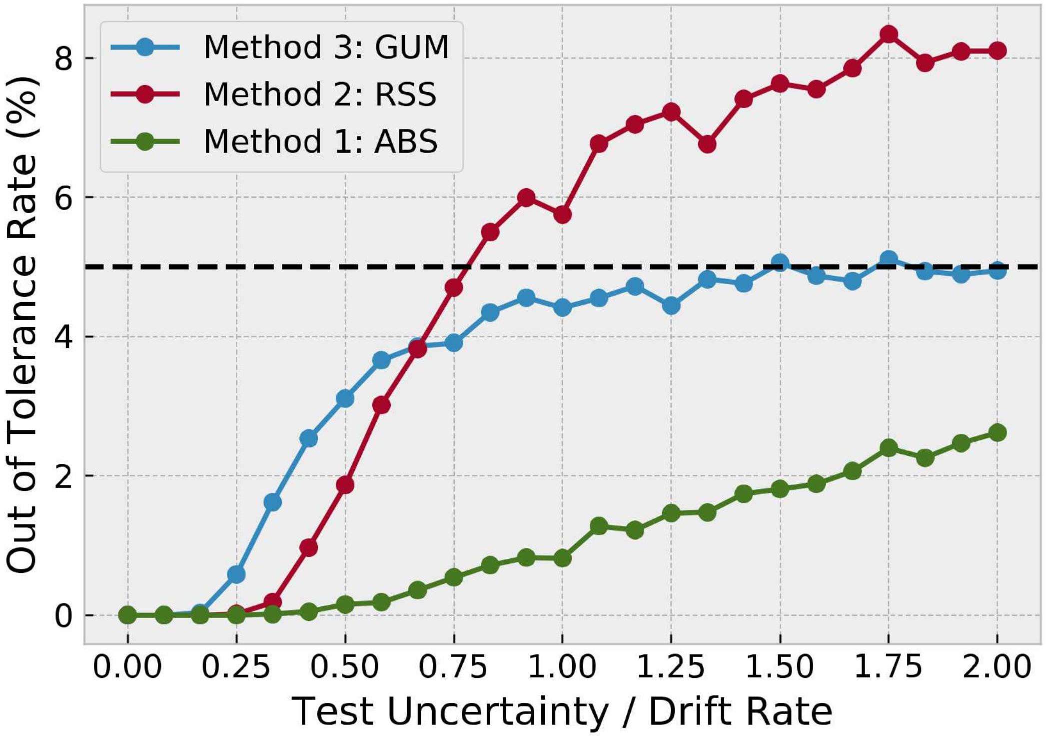
	OOT Rate
Method 1 (ABS)	0.51 %
Method 2 (RSS)	4.85 %
Method 3 (GUM)	4.37 %

	OOT Rate
Method 1 (ABS)	3.63 %
Method 2 (RSS)	8.11 %
Method 3 (GUM)	4.84 %

MONTE CARLO RESULTS

Sweep the ratio of uncertainty to drift rate. As test uncertainty approaches 0, the drift line can be predicted exactly and OOTs go to zero, regardless of method.

The GUM Method stays near a 5% OOT rate for typical uncertainty ranges.

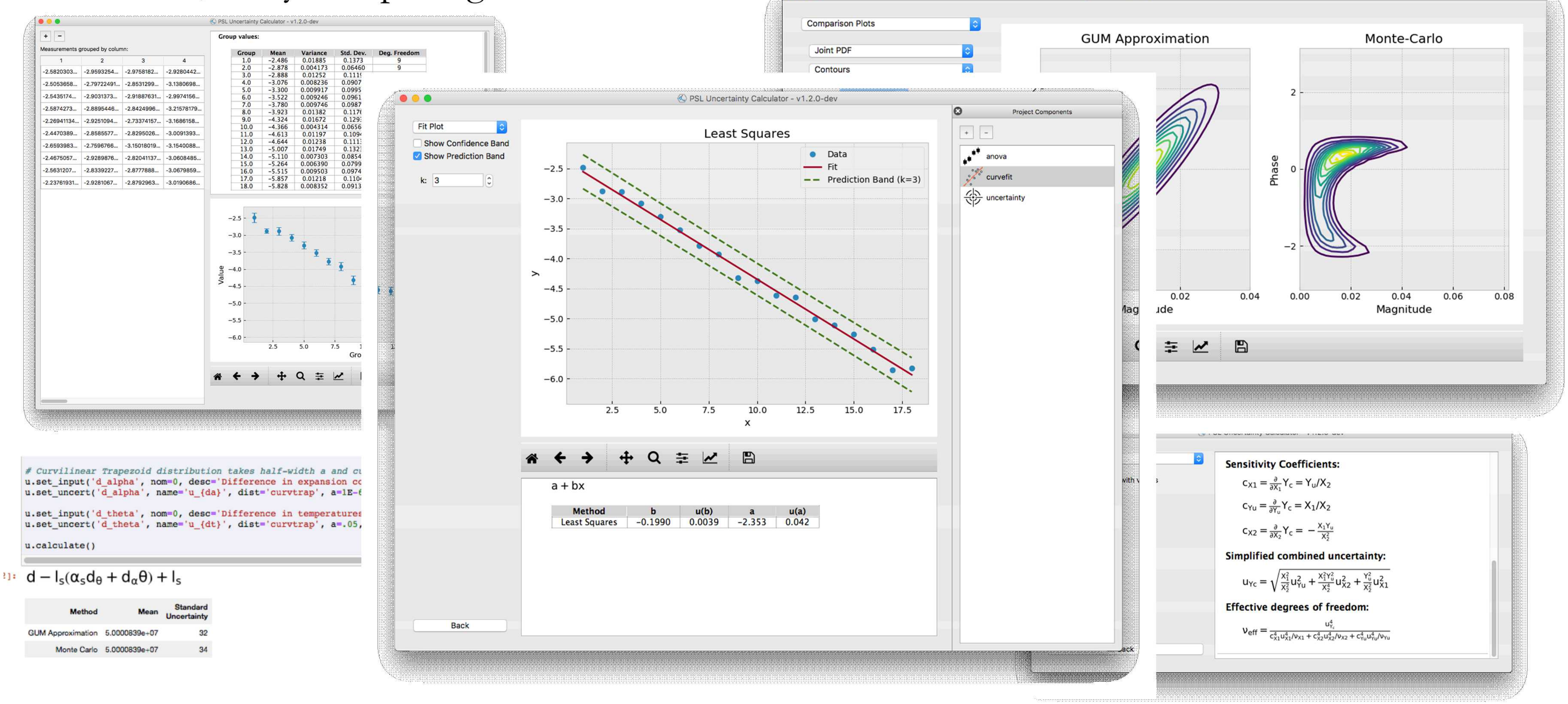


CONCLUSIONS

- The GUM Method is consistent with GUM, generates approximately 95% in tolerance rate for k=2 uncertainty. It can also be adapted for nonlinear drift.
- Absolute value method is more conservative and easier to implement.
- Recommendations:
  - Always be clear which method is being used to account for drift.
  - Report value and uncertainty as functions of time for reference, then use the GUM method for reporting a single value applicable to entire interval.
  - Evaluate model using slope test, residual analysis, etc., every year. Watch for step changes in drift rate.
  - Compare residual average with calculated uncertainty. If wildly different, there may be something off in the uncertainty calculation!

COMING SOON: SANDIA'S UNCERTAINTY CALCULATOR

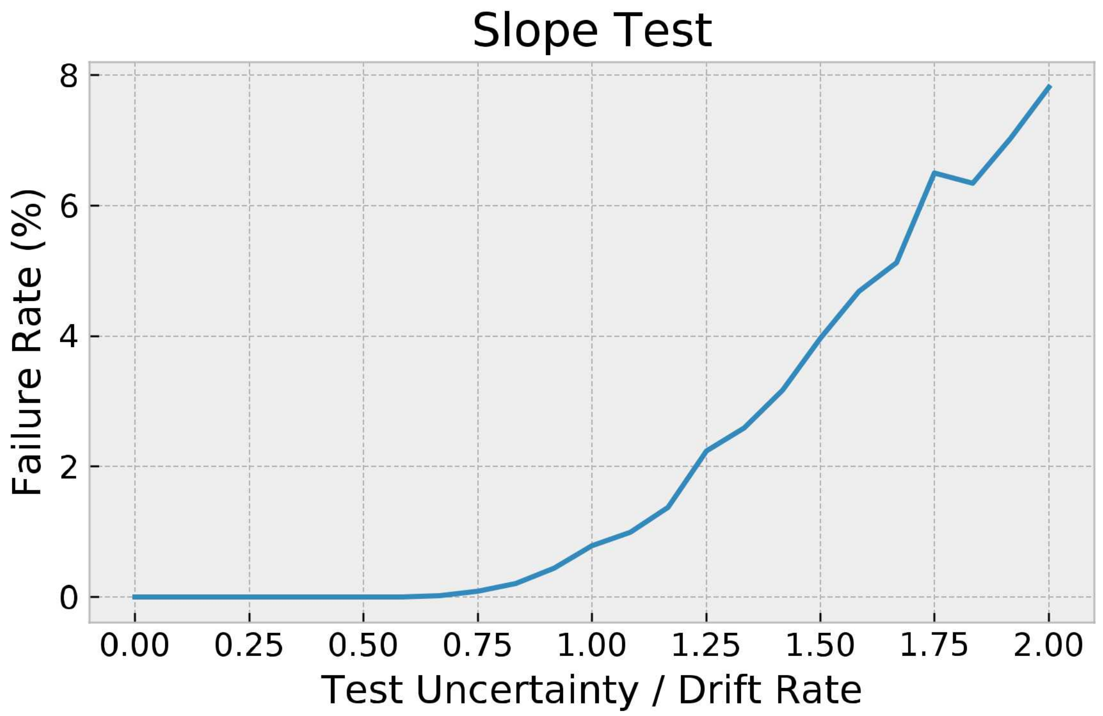
Integrated features include GUM and Monte Carlo uncertainty propagation, curve fit uncertainties, ANOVA, risk analysis, etc. Public open-source. Windows, Mac, Linux user interface, or Python package.



QUESTIONS?

SLOPE TEST FAILURE RATE

Higher uncertainty compared to rate → more slope test failures.



WEIGHTED LINEAR REGRESSION

Each data point has its own weight: $$w_i = \frac{1}{\sigma_{y_i}}$$

$$A = \frac{\Sigma w_i x_i^2 \Sigma w_i y_i - \Sigma w_i x_i \Sigma w_i x_i y_i}{\Delta}$$

$$\sigma_A = \sqrt{\frac{\Sigma w_i x_i^2}{\Delta}}$$

$$B = \frac{\Sigma w_i \Sigma w_i x_i y_i - \Sigma w_i x_i \Sigma w_i y_i}{\Delta}$$

$$\sigma_B = \sqrt{\frac{\Sigma w_i}{\Delta}}$$

$$\Delta = \Sigma w_i \Sigma w_i x_i^2 - (\Sigma w_i x_i)^2$$

METHOD 3 CALCULUS – FOR LINEAR DRIFT

If $t_1 = 0$ and $t_2 = 1$:

Correction Factor

$$b(t) = r \cdot t$$

Average Correction over Interval

$$\bar{b} = \frac{1}{t_2 - t_1}\int_{t_1}^{t_2} b(t)\mathrm{d}t = \frac{r(t_2 - t_1)}{2} \qquad = \frac{r}{2}$$

Uncertainty in Average Correction

$$u^2(\bar{b}) = \frac{1}{t_2 - t_1}\int_{t_1}^{t_2} (b - \bar{b})^2\mathrm{d}t = \frac{r^2}{12}(t_1^2 - 2t_1t_2 + t_2^2) \qquad = \frac{r^2}{12}$$

Uncertainty in Determining Correction

$$\overline{u^2[b(t)]} = \frac{1}{t_2 - t_1}\int_{t_1}^{t_2} u_{conf}^2(t)\mathrm{d}t$$

$$= \frac{1}{N(t_1 - t_2)}\left(\frac{N\sigma_B^2}{3}(t_1^3 - 3t_1^2\bar{t} - t_2^3 + 3t_2^2\bar{t}) + t_1(N\sigma_B^2\bar{t}^2 + \sigma_y^2) - t_2(N\sigma_B^2\bar{t}^2 + \sigma_y^2)\right) \qquad = -\frac{1}{N}\left(\frac{N\sigma_B^2}{12} - \sigma_y^2\right)$$

Other Uncertainty in Measurement

$$\overline{u^2[y(t)]} = \sigma_{test}^2$$

Combined Uncertainty

$$u_c = k\sqrt{u^2(\bar{b}) + \overline{u^2[b(t)]} + \overline{u^2[y(t)]}}$$