Jet Propulsion Laboratory
California Institute of Technology

SEE Data Fitting Techniques: From Eyeball Mark IV to Generalized Linear Models (and Beyond?)

Module 9b: Fitting Data is about more than extracting parameters

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Acronyms and Abbreviations

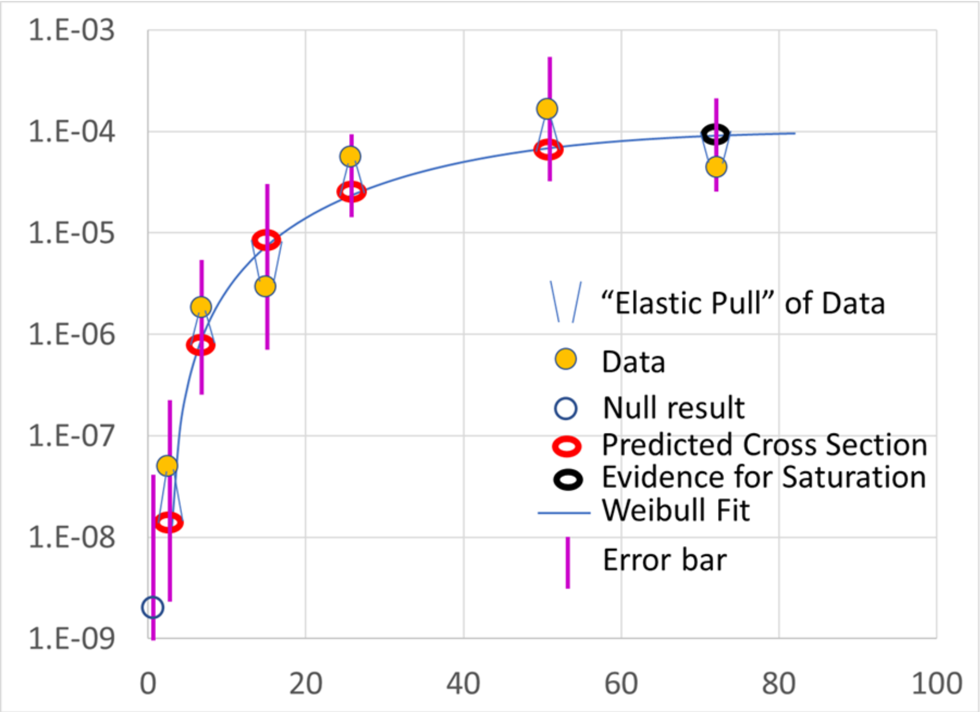
- CL—Confidence Level
- DOF—Degrees of Freedom
- DDR2—Double Data Rate (2nd generation)
- DRAM—Dynamic Random Access Memory
- FOM—Figure of Merit
- GLM—Generalized Linear Model
- GOF—Goodness of Fit
- LET—Linear Energy Transfer
- LLS—Logarithmic Least Squares
- MC—Monte Carlo
- MLE—Maximum Likelihood Estimator
- OLS—Ordinary Least Squares
- SDRAM—Synchronous DRAM
- SEE—Single-Event Effect
- SEU—Single-Event Upset
- WC—Worst-Case

Agenda

I. Motivation for Fitting—A cartoon
II. Challenges of fitting SEE data
   A. Why ordinary least squares doesn't work
   B. Alternatives to OLS
III. Generalized Linear Models
   A. Best Estimates and Confidence Intervals
   B. Selecting the worst-case rates
IV. A few applications

Fitting Data to a distribution

Fitting data to a distribution is not just about simplifying the analysis—it can reveal the physics behind your data



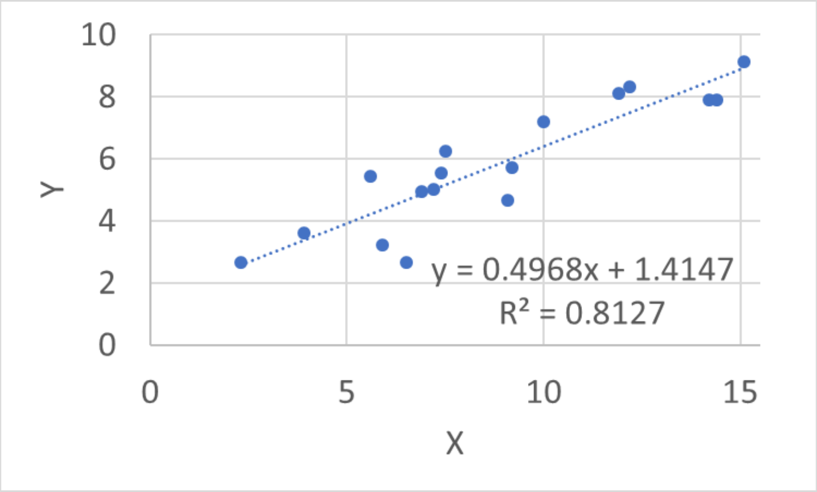
- Fitting data to a curve is a tug of war
  - Assumed form of the curve tugs one way
  - Data tug the other
  - Goodness of Fit (GOF) metric gives strength of pull

- Qualitative factors of fit form also important
  - A form that saturates is inappropriate if data do not
- Different GOF metrics for different fit methods
  - Eyeball Mark IV: "Looks good to me!"
  - Least-squares methods: sum of squared differences between model and data
  - χ^2 fit similar but normalizes differences to model prediction.
  - Generalized Linear model (GLM)—GOF is likelihood, but reflects assumed form of the errors
- Fitting methods assume different error distributions
  - Eyeball fits are subjective
  - Least-squares and χ^2 fit assume data errors~normal
  - GLM can handle Poisson errors as well as others

Why Fitting σ vs. LET Data Is Challenging

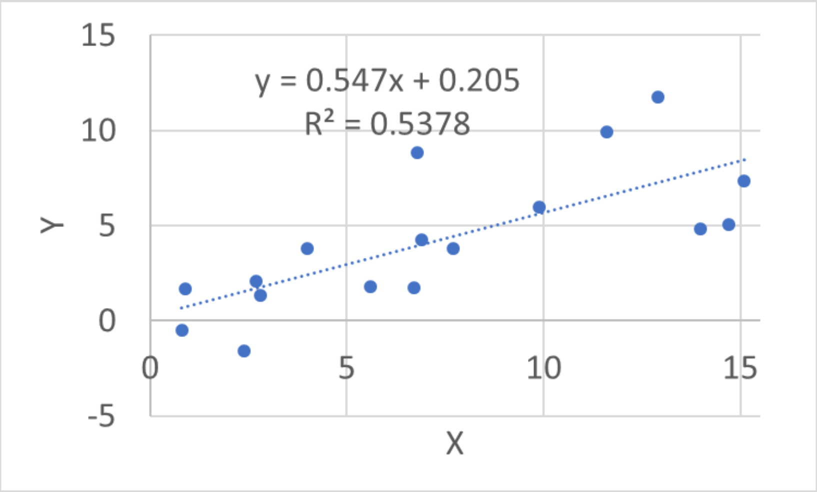
- SEE cross section data pose several challenges
  - Cross section points are distributed according to Poisson statistics—may be broad
  - Errors on different cross section points may have very different magnitudes
  - Cross section may vary across many orders of magnitude
    - This means errors on saturation are likely to be much larger even if percentage error is smaller
    - Makes Least-Squares methods problematic—errors near saturation tend to dominate.
    - Higher low-LET ion fluxes magnify importance of errors near onset, but saturated cross section also important
  - Goal of hardness assurance is to bound SEE rates, but this is subjective unless confidence levels can be established
- These challenges are partially why many experts still use eyeball fits, despite
  - Making rate estimations difficult to compare between experts/agencies
  - Complicating comparison of predictions with on-orbit data

Why Not Ordinary Least Squares (OLS)



Both curves generated with a linear model y=0.5x+1, but data on right is noisier

Errors on data are uncorrelated, random and unbiased and normally distributed.



- Ordinary Least Squares fails for SEE data because SEE data meet only 3 of 7 OLS assumptions
    - SEE cross section is NOT linear in the fitting variables.
    - **Average error IS zero.**
    - Poisson errors on cross sections depend on observed counts—so they are not independent of the cross sections
    - Error observations are independent
    - Errors do not have constant variance (~square root of event count)
    - Independent variables are independent
    - Error term is not Normal

Alternatives to OLS

- χ^2 minimization still presumes errors on measurements are normal: $\chi^2 = \sum {(\sigma_i^o - \sigma_i^E)^2}/{\sigma_i^E}$
- Not true for SEE data
  - May perform adequately if all cross sections based on large event counts
- How does OLS typically fail for SEE cross section vs. LET?
  - Error magnitudes near saturation much larger than those near onset→poor constraint on onset LET
- Replacing absolute differences with difference of logarithms result in better overall fit
  - Assuming n cross section measurements with observed cross sections $\{\sigma_i^o\}$ and predicted cross sections $\{\sigma_i^p\}$ the following quantity has been observed empirically to produce a good fit if error on $\{\sigma_i^o\}$ are negligible
  - $LLS = \sum_{i=1}^{n} \left({(\ln(\sigma_i^o) - \ln(\sigma_i^p))^2}/{\sigma_i^p} \right)$
  - Disadvantages
    - Approach assumes errors are negligible and yields only a single best fit—no bounding fits/rates
- If Poisson or other errors are not negligible, need a more flexible fitting approach

How About Likelihood Techniques?

- Maximum Likelihood techniques provide many of the characteristics needed for SEE data fitting
  - Intuitive—likelihood is just the joint probability of our data given our assumed distribution
  - Finds both best-fit and confidence contours in parameter space (follow χ^2 because likelihood Λ~normal near its maximum)
  - Unfortunately, only works with probability distributions and Weibull cross section is a “form” or “shape,” not a distribution

	Failure Doses
$D1$	95.91037
$D2$	93.58756
$D3$	117.8288
$D4$	129.0717
$D5$	105.9007

Likelihood

$$\Lambda(\{\vec{D}\}, m, s)) = N(D_1, m, s) * N(D_2, m, s) * N(D_3, m, s) * N(D_4, m, s) * N(D_5, m, s)$$

$\mathcal{L}$(CL)~Max LIK*EXP(-0.5*INVχ^2(1-CL,DOF));(DOF=# parameters=2 for Normal)

MaxLik | 90% CL=.1*MaxLik | 95% CL=.05*MaxLik | 99% CL=.01*MaxLik

mean \ sigma	7.4	10.4	13.4	16.4	19.4	22.4	25.4	28.4	31.4	34.4	37.4	40.4	43.4	46.4	49.4	52.4
76.45	6.1E-31	6.8E-20	1.2E-15	1.2E-13	1.2E-12	4.4E-12	9.0E-12	1.3E-11	1.6E-11	1.6E-11	1.6E-11	1.5E-11	1.3E-11	1.2E-11	1.0E-11	8.5E-12
80.45	3.5E-26	1.7E-17	3.5E-14	1.1E-12	6.1E-12	1.5E-11	2.3E-11	2.8E-11	2.9E-11	2.7E-11	2.5E-11	2.1E-11	1.8E-11	1.5E-11	1.3E-11	1.1E-11
84.45	4.7E-22	2.1E-15	6.3E-13	7.6E-12	2.4E-11	4.1E-11	5.1E-11	5.3E-11	4.9E-11	4.2E-11	3.6E-11	2.9E-11	2.4E-11	2.0E-11	1.6E-11	1.3E-11
88.45	1.4E-18	1.3E-13	7.3E-12	3.9E-11	7.8E-11	1.0E-10	1.0E-10	9.1E-11	7.6E-11	6.2E-11	4.9E-11	3.9E-11	3.0E-11	2.4E-11	1.9E-11	1.5E-11
92.45	1.0E-15	3.5E-12	5.4E-11	1.5E-10	2.0E-10	2.0E-10	1.8E-10	1.4E-10	1.1E-10	8.4E-11	6.3E-11	4.8E-11	3.7E-11	2.8E-11	2.2E-11	1.7E-11
96.45	1.7E-13	4.7E-11	2.6E-10	4.2E-10	4.3E-10	3.6E-10	2.7E-10	2.0E-10	1.5E-10	1.1E-10	7.7E-11	5.7E-11	4.3E-11	3.2E-11	2.5E-11	1.9E-11
100.45	6.7E-12	3.0E-10	7.9E-10	8.8E-10	7.3E-10	5.3E-10	3.7E-10	2.6E-10	1.8E-10	1.3E-10	8.9E-11	6.5E-11	4.7E-11	3.5E-11	2.7E-11	2.0E-11
104.45	6.0E-11	9.0E-10	1.5E-09	1.4E-09	1.0E-09	6.8E-10	4.5E-10	3.0E-10	2.0E-10	1.4E-10	9.7E-11	7.0E-11	5.1E-11	3.7E-11	2.8E-11	2.1E-11
108.45	1.3E-10	1.3E-09	1.9E-09	1.6E-09	1.1E-09	7.3E-10	4.8E-10	3.1E-10	2.1E-10	1.4E-10	1.0E-10	7.1E-11	5.2E-11	3.8E-11	2.9E-11	2.2E-11
112.45	6.1E-11	9.1E-10	1.5E-09	1.4E-09	1.0E-09	6.8E-10	4.5E-10	3.0E-10	2.0E-10	1.4E-10	9.7E-11	7.0E-11	5.1E-11	3.7E-11	2.8E-11	2.1E-11
116.45	6.8E-12	3.0E-10	7.9E-10	8.9E-10	7.3E-10	5.3E-10	3.7E-10	2.6E-10	1.8E-10	1.3E-10	8.9E-11	6.5E-11	4.8E-11	3.5E-11	2.7E-11	2.0E-11
120.45	1.8E-13	4.7E-11	2.6E-10	4.2E-10	4.3E-10	3.6E-10	2.7E-10	2.0E-10	1.5E-10	1.1E-10	7.7E-11	5.7E-11	4.3E-11	3.2E-11	2.5E-11	1.9E-11
124.45	1.1E-15	3.5E-12	5.5E-11	1.5E-10	2.0E-10	2.0E-10	1.8E-10	1.4E-10	1.1E-10	8.4E-11	6.3E-11	4.8E-11	3.7E-11	2.8E-11	2.2E-11	1.7E-11
128.45	1.5E-18	1.3E-13	7.4E-12	3.9E-11	7.8E-11	1.0E-10	1.0E-10	9.1E-11	7.6E-11	6.2E-11	4.9E-11	3.9E-11	3.0E-11	2.4E-11	1.9E-11	1.5E-11
132.45	4.9E-22	2.2E-15	6.4E-13	7.6E-12	2.4E-11	4.2E-11	5.1E-11	5.3E-11	4.9E-11	4.3E-11	3.6E-11	3.0E-11	2.4E-11	2.0E-11	1.6E-11	1.3E-11
136.45	3.7E-26	1.8E-17	3.5E-14	1.1E-12	6.1E-12	1.5E-11	2.3E-11	2.8E-11	2.9E-11	2.7E-11	2.5E-11	2.1E-11	1.8E-11	1.5E-11	1.3E-11	1.1E-11

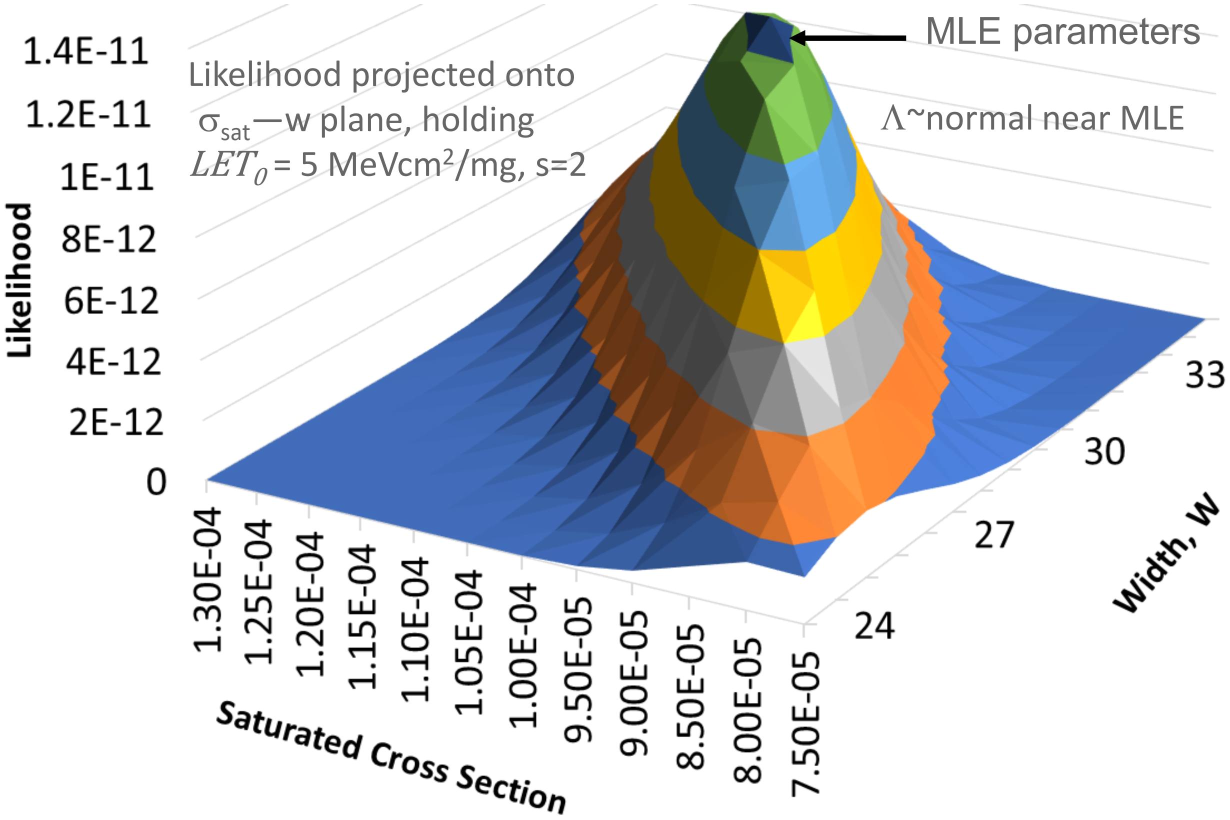
Generalized Linear Models (GLM)

- GLM extend MLE to more complicated models
  - Start with exponential-family probability distribution
  - Instead of numerical parameters, insert the model
  - Example: Weibull form of $\sigma(LET, LET_0, \sigma_{sat}, w, s)$
  - Select LET_0, σ_{sat}, w and s to maximize likelihood

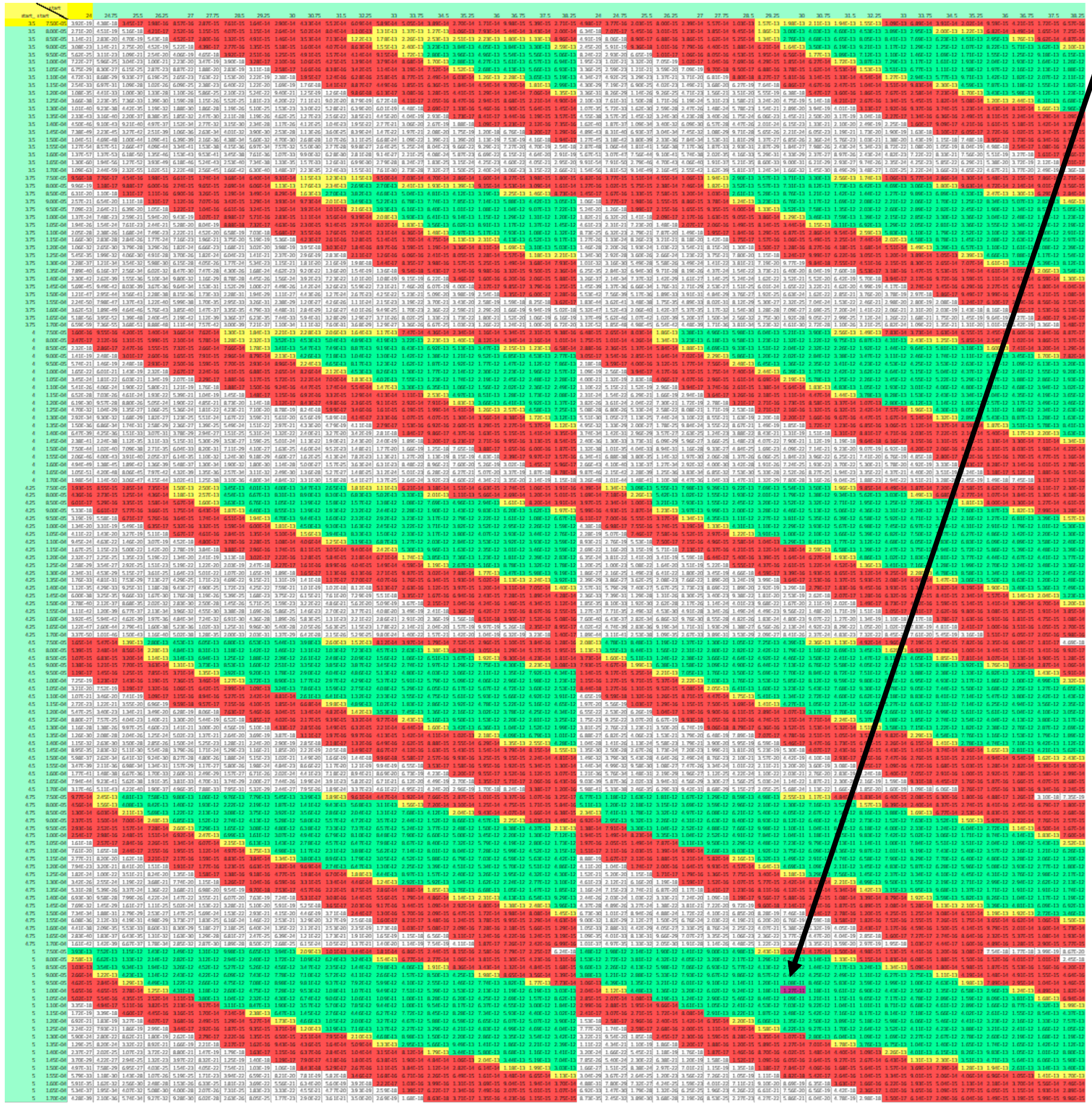
- A GLM for SEE?
  - Inputs=observables (LETs, fluences $\{F_i\}$, event counts $\{N_i^o\}$)
    - Modeled counts $N_i^p = F_i \times \sigma(LET_i)$ (Weibull form)
    - Likelihood $\Lambda = \prod_{i=1}^{n} Poisson(N_i^o, N_i^p)$
    - Maximize Λ with respect to, LET_0, σ_{sat} , w and s
    - Can be implemented as a 4D grid search in Excel
    - Determine confidence contours based on usual χ^2 relation
    - Can also select parameters that maximize SEE rate from among all combinations in a given CL (WC rate @ CL)

- Confidence Contours for Likelihood
  - ~ Λ normality near MLE means CL~χ^2 distributed (DOF=4)

$$\Lambda(\{\vec{x}\}, CL) \Big/ \Lambda(\{\vec{x}\}, MAX) \sim \exp(-0.5 * INV\chi^2(1 - CL, DOF))$$



What the Grid Search Looks Like



- Best Fit (Max Likelihood)
- 90% Confidence Contour
- 95% Confidence Contour
- 99.99% Confidence Contour)

- Grid search for MLE Weibull parameters
  - Each rectangular tile holds 2 variables (LET_0, s) constant
  - W and σ_{sat} are varied over an adjustable, credible range
  - Increment LET_0 and/or s, repeat (20 × 20=400 tiles)
    - » 160000 parametric combinations
- Establishing confidence contours: Example for 90% CL
  - Any fit w/ likelihood $>\Lambda_{Max}\times\exp(-0.5*\mathrm{Inv}\chi^2(1\text{-}90\%,4))$ $=\sim 0.02\Lambda_{Max}$ lies within the 90% CL
    - » The better the data, the fewer the fits lie within the CL
    - » Of the many fits for each CL, which has the highest rate?
  - Procedure is similar for any CL

Picking the WC Rate for Confidence Level CL

- CREME96 calculations for 160000 fits (or even 1000 fits) likely prohibitively time consuming.
- Instead, us Figure of Merit to identify promising fits in a particular CL likely to yield high rate: $FOM = C_{Env} \times {}^{\sigma_{sat}}/_{(LET_0 + w\times 0..288^{1/s})^2}$.
- Select 10-20 fits yielding highest FOM rate to input to CREME96
- FOM and CREME96 rate agree well for σ_{sat}>100μm^2 and LET_0<50 MeVcm^2/mg; even when they disagree FOM a good indicator of high rates
- Resulting WC rate for confidence CL tends to conservatively bound rate more than CL% of the time—less conservative as data improves

		2.58	2.58	2.58	2.58	2.58	2.58	2.58	2.58	2.58	2.58	2.58	2.58	2.58	2.58	2.58	2.58	2.58	2.58	2.58	2.58
		50	55	60	65	70	75	80	85	90	95	100	105	110	115	120	125	130	135	140	145
0.13	0.0025	0	0	0.00036	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.13	0.003	0	0	0.00043	0.00037	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.13	0.0035	0	0	0	0.00043	0.00037	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.13	0.004	0	0	0	0	0.00043	0.00037	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.13	0.0045	0	0	0	0	0.00048	0.00042	0.00037	0	0	0	0	0	0	0	0	0	0	0	0	0
0.13	0.005	0	0	0	0	0	0.00046	0.00041	0	0	0	0	0	0	0	0	0	0	0	0	0
0.13	0.0055	0	0	0	0	0	0	0.00045	0.0004	0	0	0	0	0	0	0	0	0	0	0	0
0.13	0.006	0	0	0	0	0	0	0.00049	0.00043	0	0	0	0	0	0	0	0	0	0	0	0
0.13	0.0065	0	0	0	0	0	0	0	0.00047	0.00042	0	0	0	0	0	0	0	0	0	0	0
0.13	0.007	0	0	0	0	0	0	0	0.00051	0.00045	0	0	0	0	0	0	0	0	0	0	0
0.13	0.0075	0	0	0	0	0	0	0	0.00054	0.00048	0.00043	0	0	0	0	0	0	0	0	0	0
0.13	0.008	0	0	0	0	0	0	0	0	0.00052	0.00046	0.00042	0	0	0	0	0	0	0	0	0
0.13	0.0085	0	0	0	0	0	0	0	0	0.00055	0.00049	0.00044	0	0	0	0	0	0	0	0	0
0.13	0.009	0	0	0	0	0	0	0	0	0	0.00052	0.00047	0	0	0	0	0	0	0	0	0
0.13	0.0095	0	0	0	0	0	0	0	0	0	0.00055	0.0005	0.00045	0	0	0	0	0	0	0	0
0.13	0.01	0	0	0	0	0	0	0	0	0	0.00058	0.00052	0.00047	0	0	0	0	0	0	0	0
0.13	0.0105	0	0	0	0	0	0	0	0	0	0	0.00055	0.0005	0.00045	0	0	0	0	0	0	0
0.13	0.011	0	0	0	0	0	0	0	0	0	0	0.00058	0.00052	0.00048	0	0	0	0	0	0	0
0.13	0.0115	0	0	0	0	0	0	0	0	0	0	0.0006	0.00055	0.0005	0.00045	0	0	0	0	0	0
0.13	0.012	0	0	0	0	0	0	0	0	0	0	0	0.00057	0.00052	0.00047	0	0	0	0	0	0

If fit is within CL, cell=FOM rate, otherwise, 0

LET_0=.13,σ_{sat}=0.01, w=95,s=2.58

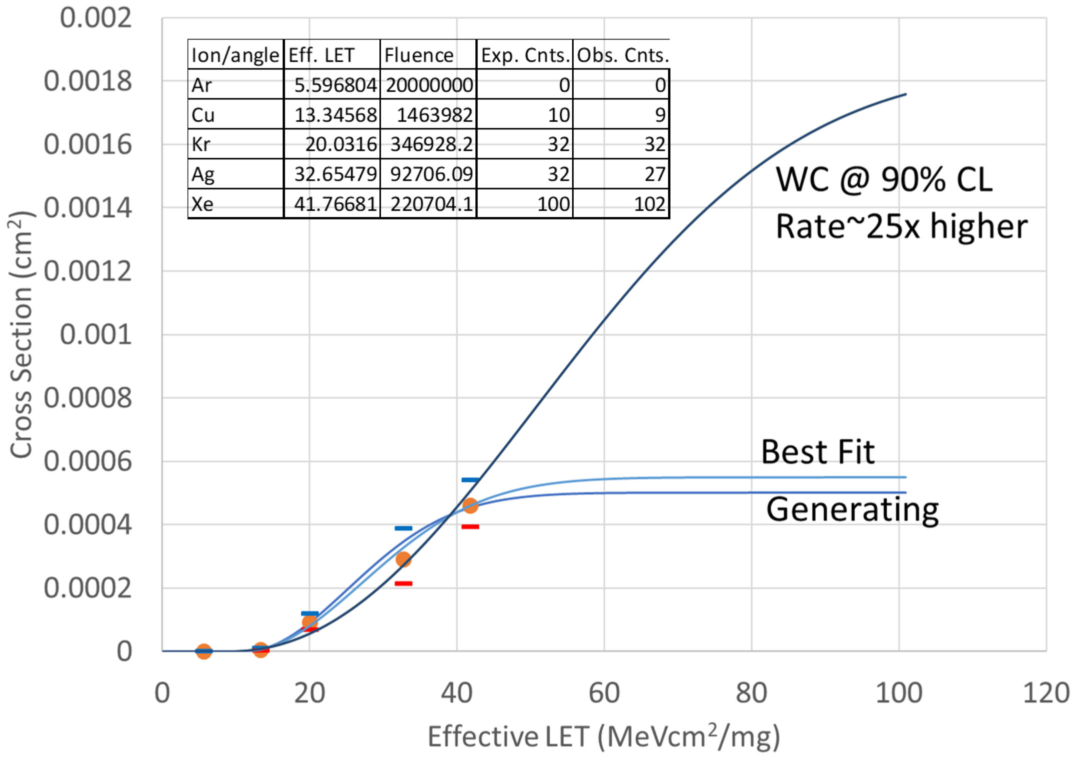
LET_0=.13,σ_{sat}=0.011, w=100,s=2.58

LET_0=.13,σ_{sat}=0.0115, w=100,s=2.58

OK, We Have A Method—What Is It Good For?

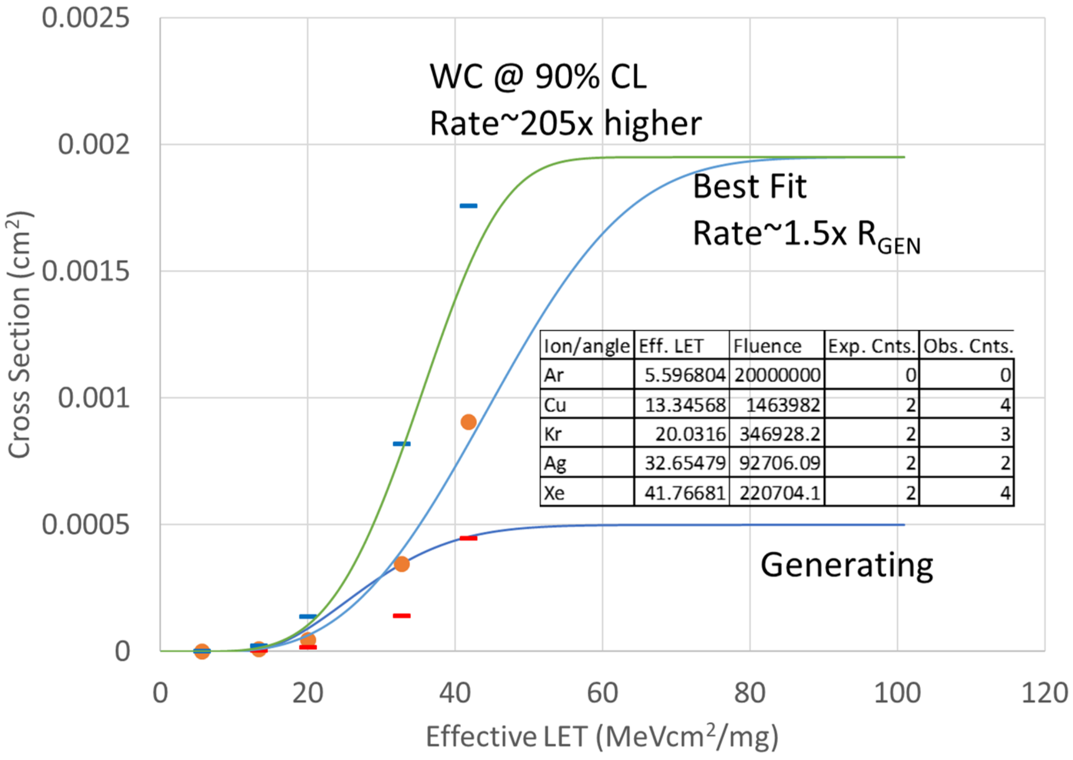
- Useful data-quality metric: Ratio of WC rate @ 90% CL to Best-Fit (MLE) rate
  - For good data, this ratio tends to be 2-3x
  - Can carry out simulations to optimize ratio for purposes of test planning or on-the-fly decisions during test
    - What combination of ions, event counts, etc. provides best constraints on possible fits to the data?

Statistics good, but poor saturation constraint



Ion/angle	Eff. LET	Fluence	Exp. Cnts.	Obs. Cnts.
Ar	5.596804	20000000	0	0
Cu	13.34568	1463982	10	9
Kr	20.0316	346928.2	32	32
Ag	32.65479	92706.09	32	27
Xe	41.76681	220704.1	100	102

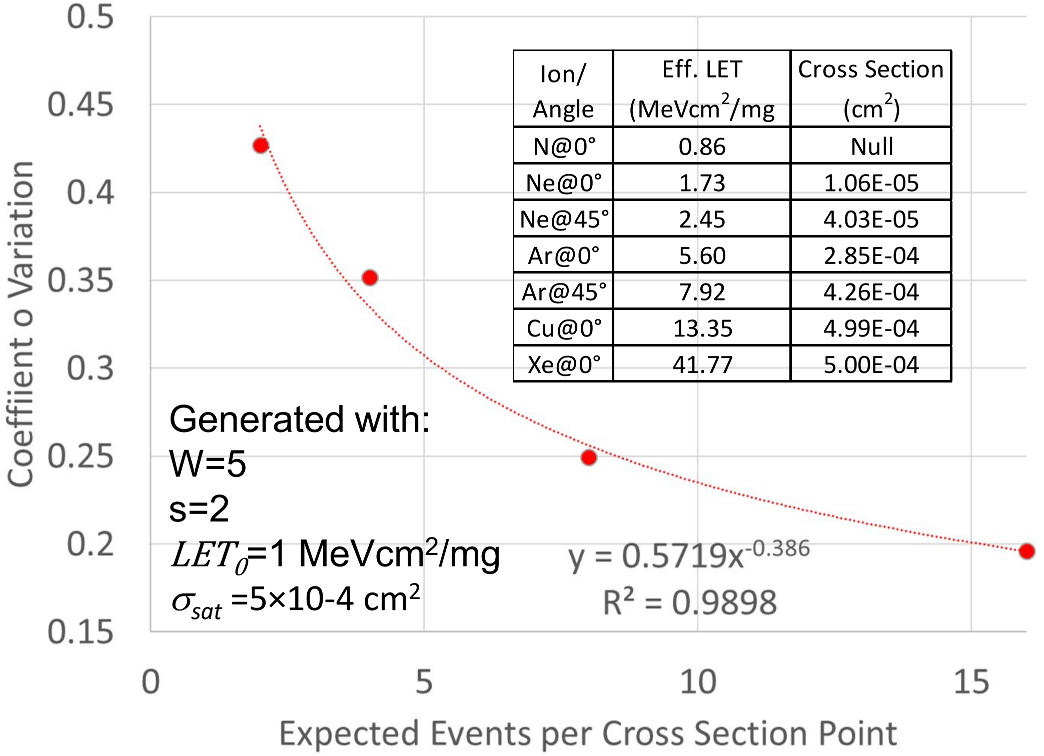
Poor statistics and poor saturation constraint



Ion/angle	Eff. LET	Fluence	Exp. Cnts.	Obs. Cnts.
Ar	5.596804	20000000	0	0
Cu	13.34568	1463982	2	4
Kr	20.0316	346928.2	2	3
Ag	32.65479	92706.09	2	2
Xe	41.76681	220704.1	2	4

Monte Carlo in an Excel File

- More complete picture how variability affects fitting can be obtained using Monte Carlo
- 160000 fit possibilities, iterated >1000 times unmanageable, especially for real time
  - But rate is not equally sensitive to all fit parameters at the same time.
    - Often LET_0 is moderately well constrained by data—trying ~5-7 possibilities is sufficient
    - Most Weibull fits to SEE cross sections have $0.5 \leq s \leq 4$ and rate is not extremely sensitive—5-6 possibilities is sufficient
    - Reduce to 10 possibilities each for σ_{sat} and w and each MC run examines $\leq$ 4200 possibilities
    - Can run ~1000 MC runs in $\leq$ 1 minute
- Resulting Excel file can generate histograms, rank plots and summary statistics for fit parameters, best-fit and WC@CL rates
  - Real-time runs @ accelerator are possible



Ion/ Angle	Eff. LET ($MeVcm^2/mg$	Cross Section (cm^2)
N@0°	0.86	Null
Ne@0°	1.73	1.06E-05
Ne@45°	2.45	4.03E-05
Ar@0°	5.60	2.85E-04
Ar@45°	7.92	4.26E-04
Cu@0°	13.35	4.99E-04
Xe@0°	41.77	5.00E-04

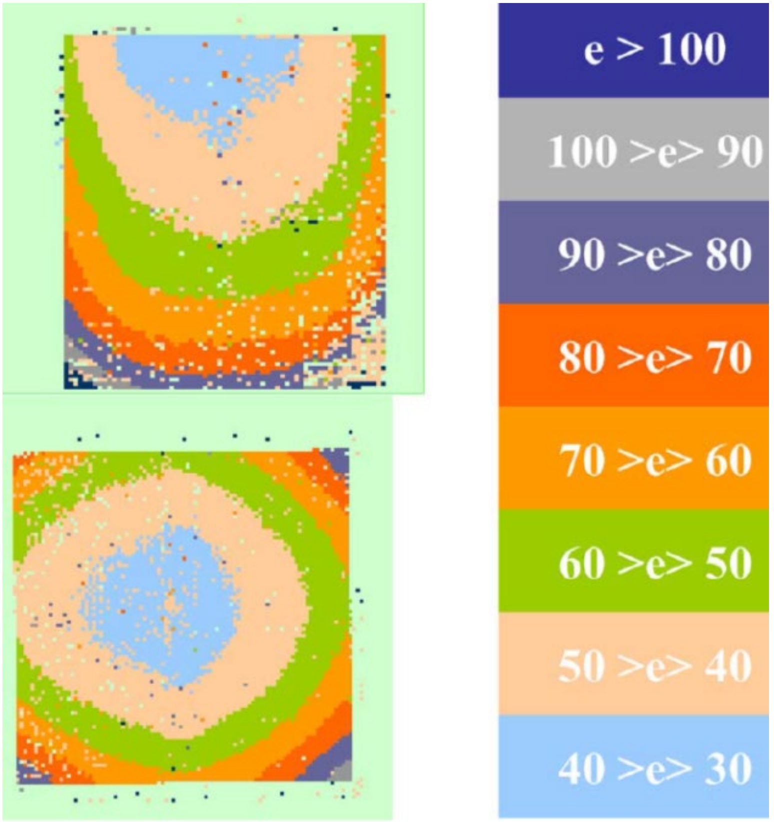
- Coefficient of Variation=standard deviation/mean
- COV decreases ~as power law in expected event count
  - As data quality improves, fit/rate converge to correct values

Generalizing the GLM

Thickness Profile for 2 Thinned DDR2 SDRAMs

Adapted from R. Harboe-Sorenson et al.
IEEE TNS, vol.54, no. 6, pp2125-2130.

Thickness, μm



Non-uniform die thickness, coupled unknown
Sensitive volume location cause LET of ion
Causing SEE mode to be uncertain

- If LET of ion causing an SEE is uncertain, use of a point estimate for LET introduces a systematic error
  - Can model be generalized to account for the uncertainty
  - Only quantities that depend on LET are the predicted counts N_i^p
- Instead of a single LET, we have a distribution, Φ(LET), so
  - $N_i^p = F_i \times \int_{li}^{ui} \Phi_i(LET) \times \sigma(LET) dLET$
  - For i^{th} ion, Φi(LET) ranges from Ll to Lu
  - Rest of model stays the same
- This extension of the SEE GLM submitted for 2021 NSREC
  - Preliminary results indicate systematic errors on rate can exceed 40%
  - Systematic errors do not improve with statistics
- This extension illustrates—if you can quantify the errors, you can treat them with a GLM

But Wait, Don't Answer Yet!

- Big advantage of GLM fitting: can quantify conservatism of rate estimation by confidence level
  - Consistent and repeatable
  - Can compare conservatism across analysts—even if fit was derived using method other than GLM
    - If Λ_{Max} and fit parameters are known, can calculate Λ_{Fit} and then $\Lambda_{Max}/\Lambda_{Fit}$ yields CL based on χ^2 relationship
    - Can be used to calibrate results for other fitting techniques—including Eyeball Mark IV
- Technique also allows exploration between fit parameters and likelihood
  - Correlations between fit parameters as likelihood held near constant reveal interesting features of data
  - Example: if likelihood near constant as w and σ_{sat} increase in lockstep, may indicate saturation not constrained
  - Correlations generally indicate that σ vs. LET may not carry enough information to justify a 4-parameter fit
    - Overfitting can result in systematic errors in rate
- Many other studies possible—Design-of-Experiments, looking for evidence of multiple modes
  - And that's even before you factor in the offer of Ginzu knives!

Conclusions

- Fitting SEE σ vs. LET data poses significant challenges
  - Errors are Poisson—this means not only are errors not normal, they depend on event count n (Standard Deviation~$n^{1/2}$)
  - Cross section (and so event count) is nonlinear in LET
  - Ordinary Least Squares inappropriate
    - Logarithmic Least Squares seems to yield better results, but does not yield bounding fits/rates
- Generalized Linear Model for SEE data yields best (Max. Likelihood) fit but also bounding fit/rate for given CL
  - Results are consistent and reproducible, allowing comparison with other analysts regardless of how their fit was derived
  - Useful tool for a variety of studies—pre-test planning to Design of Experiments
  - Fitting routine can be generalized to include other sources of error (e.g., uncertainty in LET causing a SEE)
  - Can be sufficiently simplified to be used in conjunction with Monte Carlo studies
- GLM are especially useful when event counts underlying cross sections are small
  - However, even for large event counts, approach guarantees a self-consistent, repeatable rate estimate
  - Ratio of WC rate @ 90% CL to best fit rate provides a reliable metric for data quality