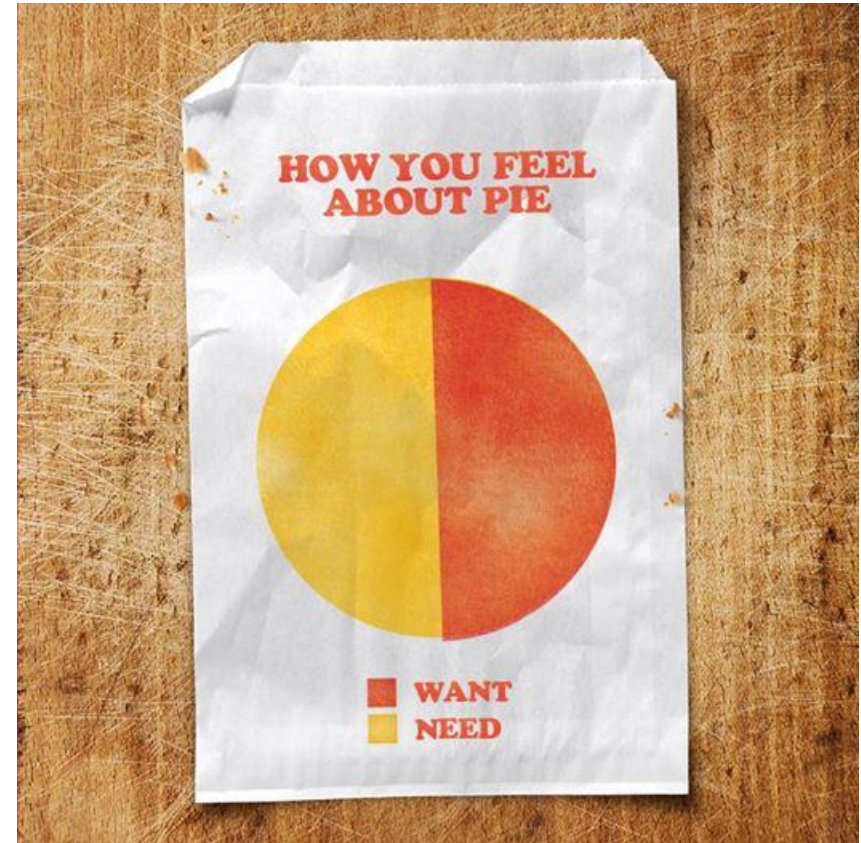


Model Measures: Are they fit for purpose?

Tim Wright

NZMUGS Conference, 2014

- ‘Fit for Purpose’
- Draft MUGS Data Comparison Guidelines (GEH)
- Expanded review of:
 - GEH
 - R^2
 - RMSE
- I am no statistician (but I love statistics !)
- ‘Keeping it real’



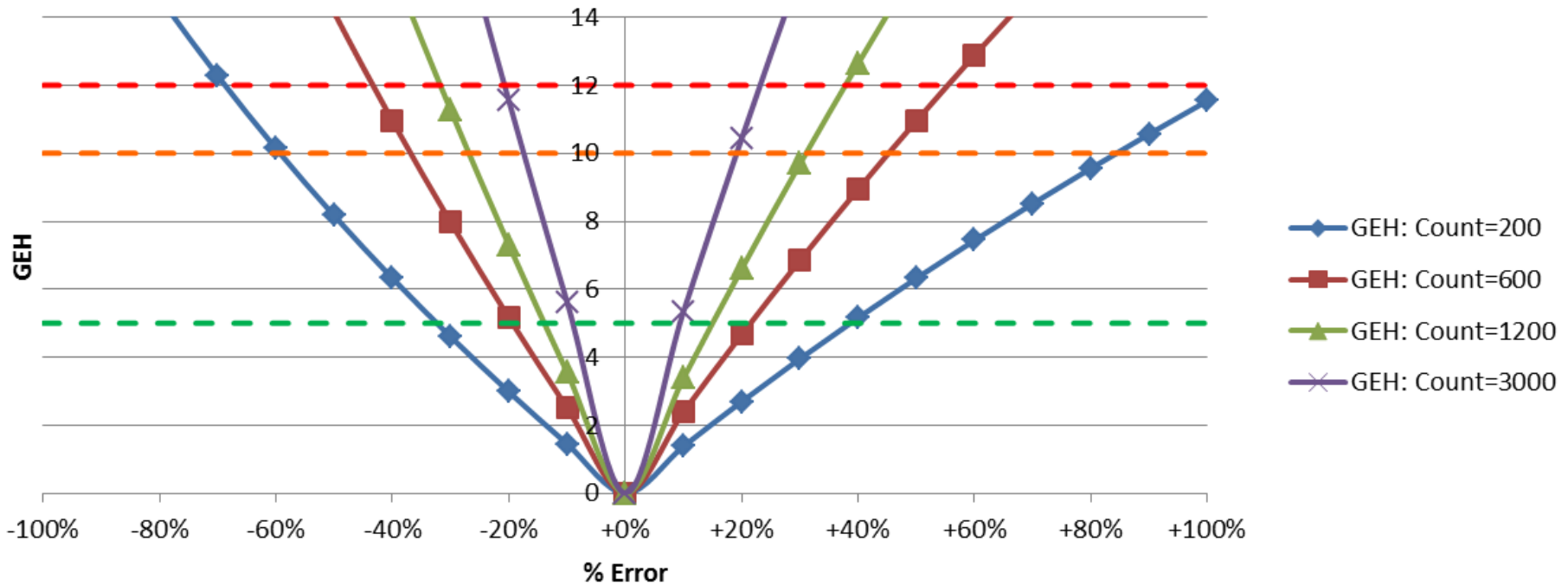
“For every grain of sand on Earth, there are 10,000 stars in the observable universe”

“1 Million seconds is around 12 Days. 1 Billion seconds is around 32 years”

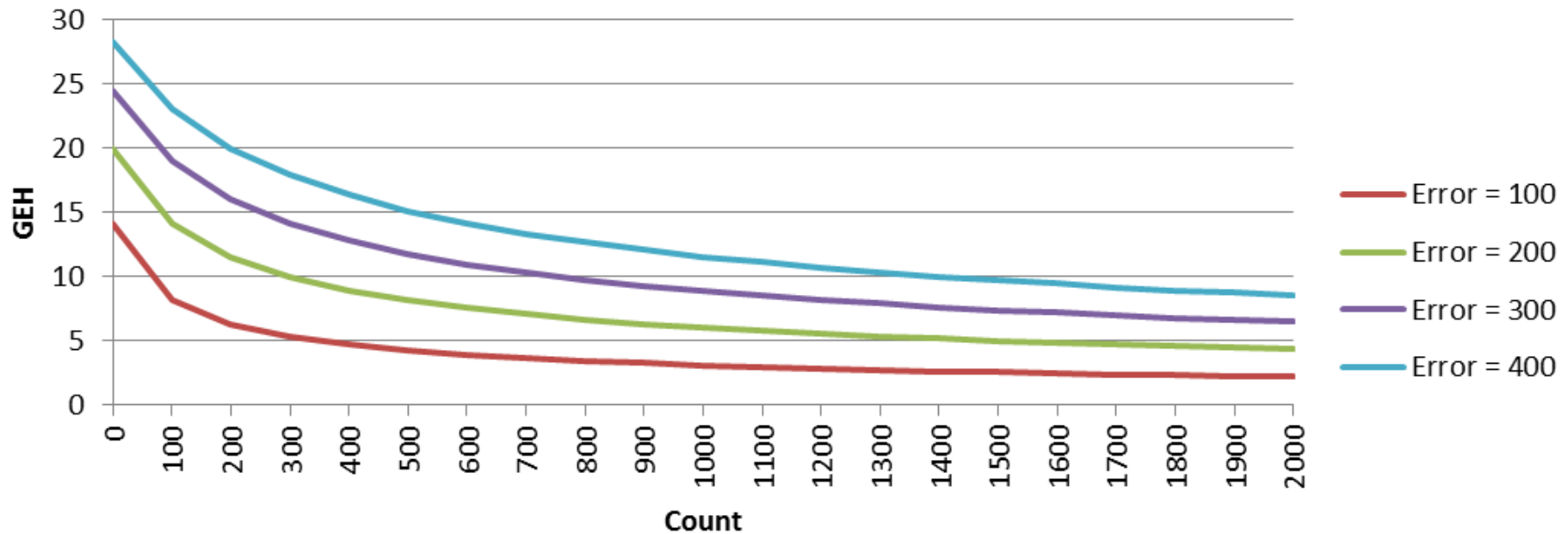
- $\sqrt{\frac{(M-O)^2}{(M+O)/2}}$
- $\frac{\sqrt{(M-O)^2}}{\sqrt{(M+O)/2}}$
- $\frac{(M-O)}{\sqrt{(M+O)/2}}$
- $\frac{\textit{Difference}}{\sqrt{\textit{Average}}}$

- Single measure of overall fit

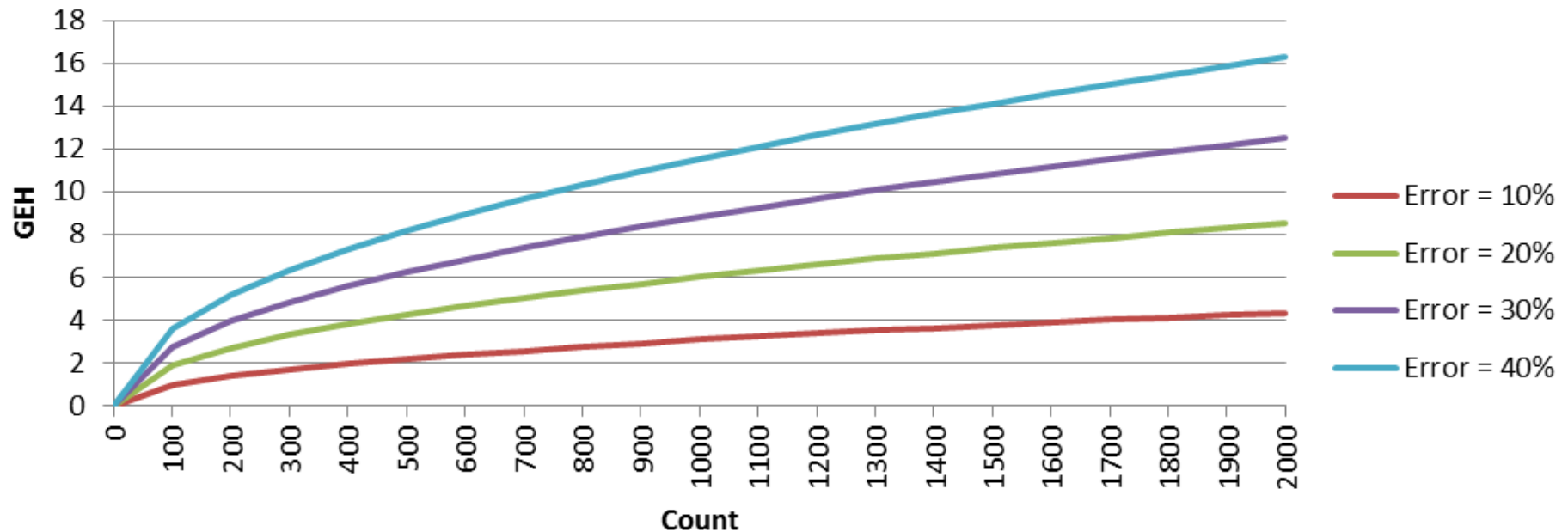
Variation of GEH with %Error for Example Counts

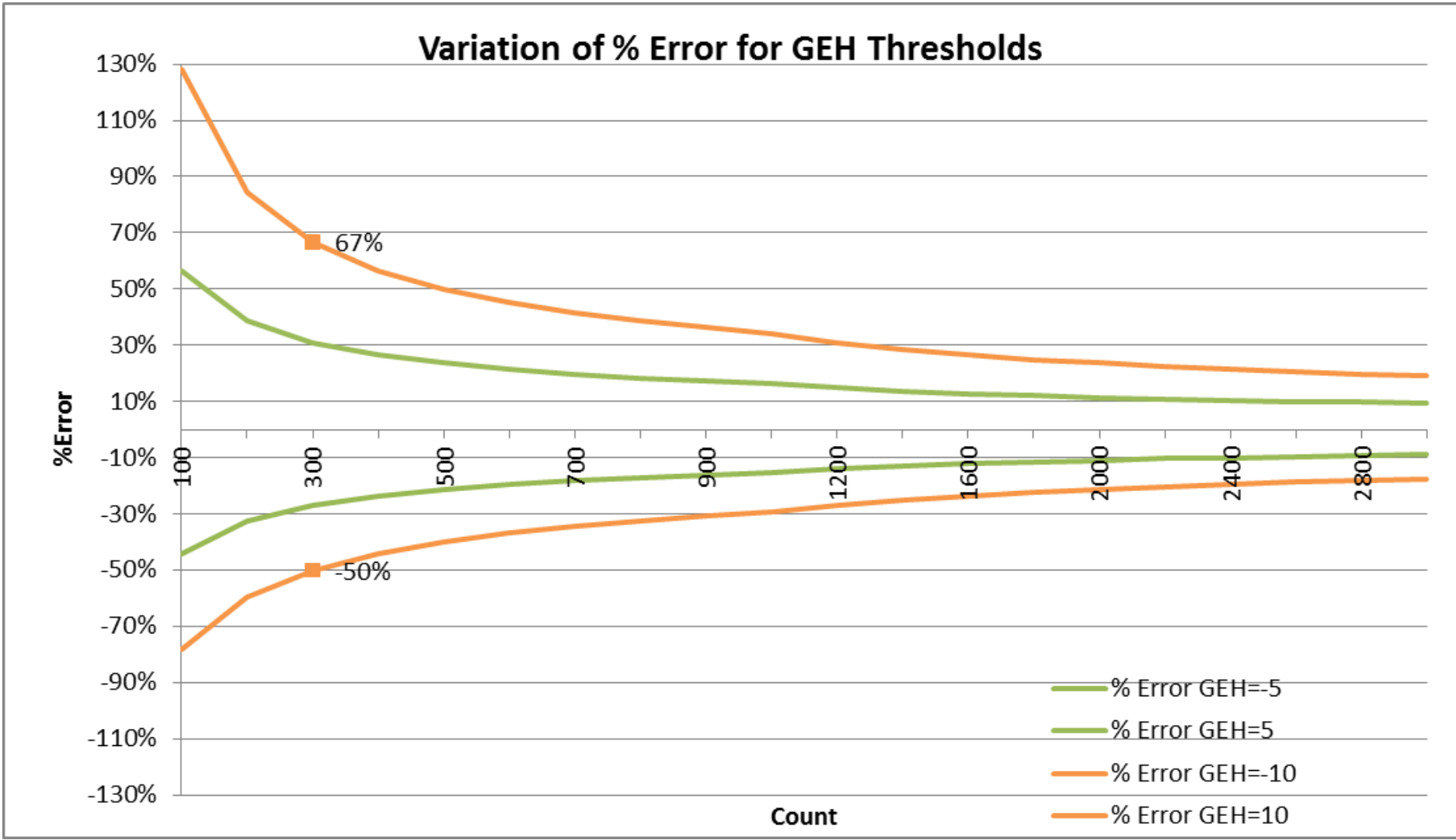


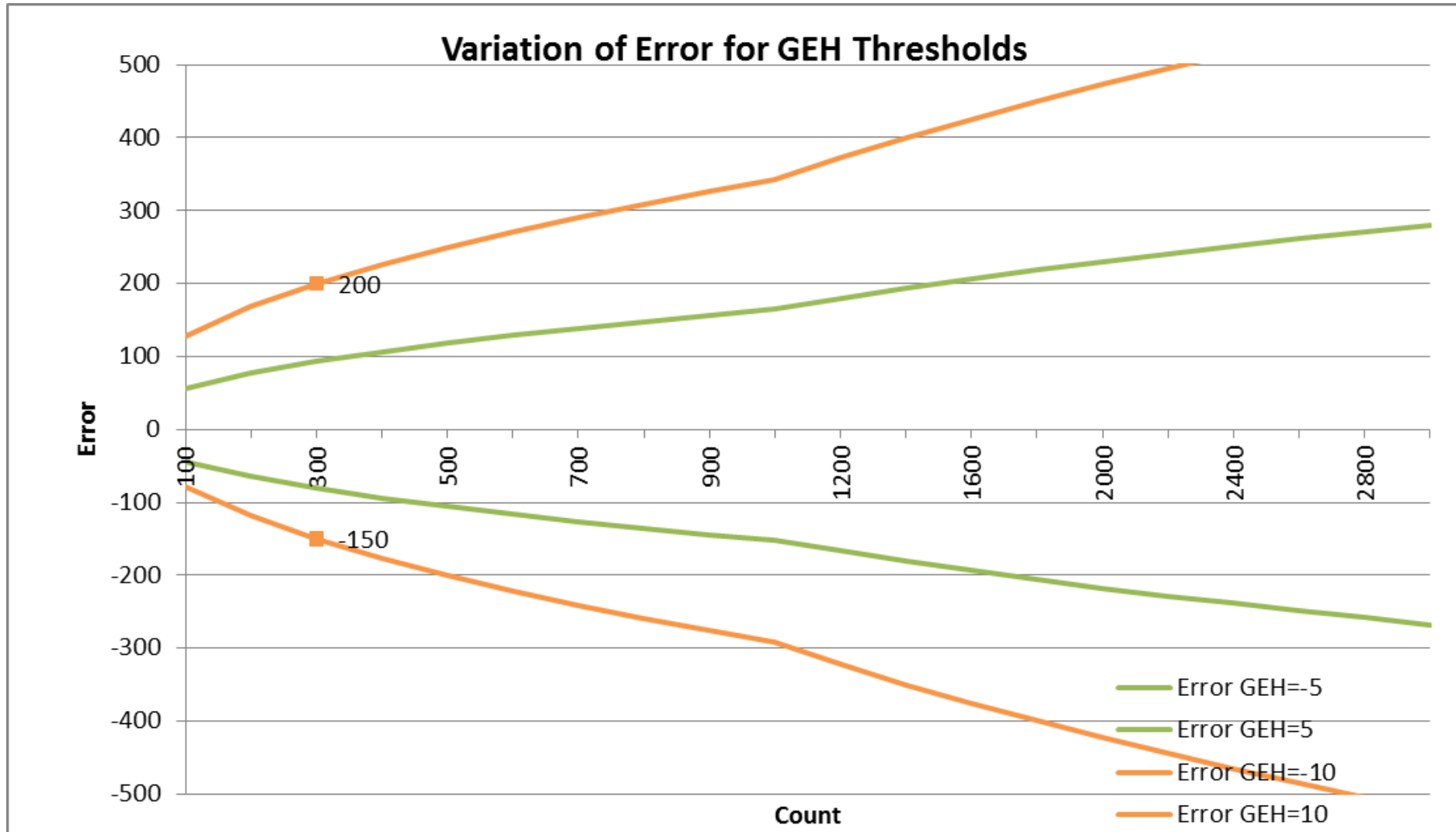
Variation of GEH with Count for Constant Error



Variation of GEH with Count for Constant Error







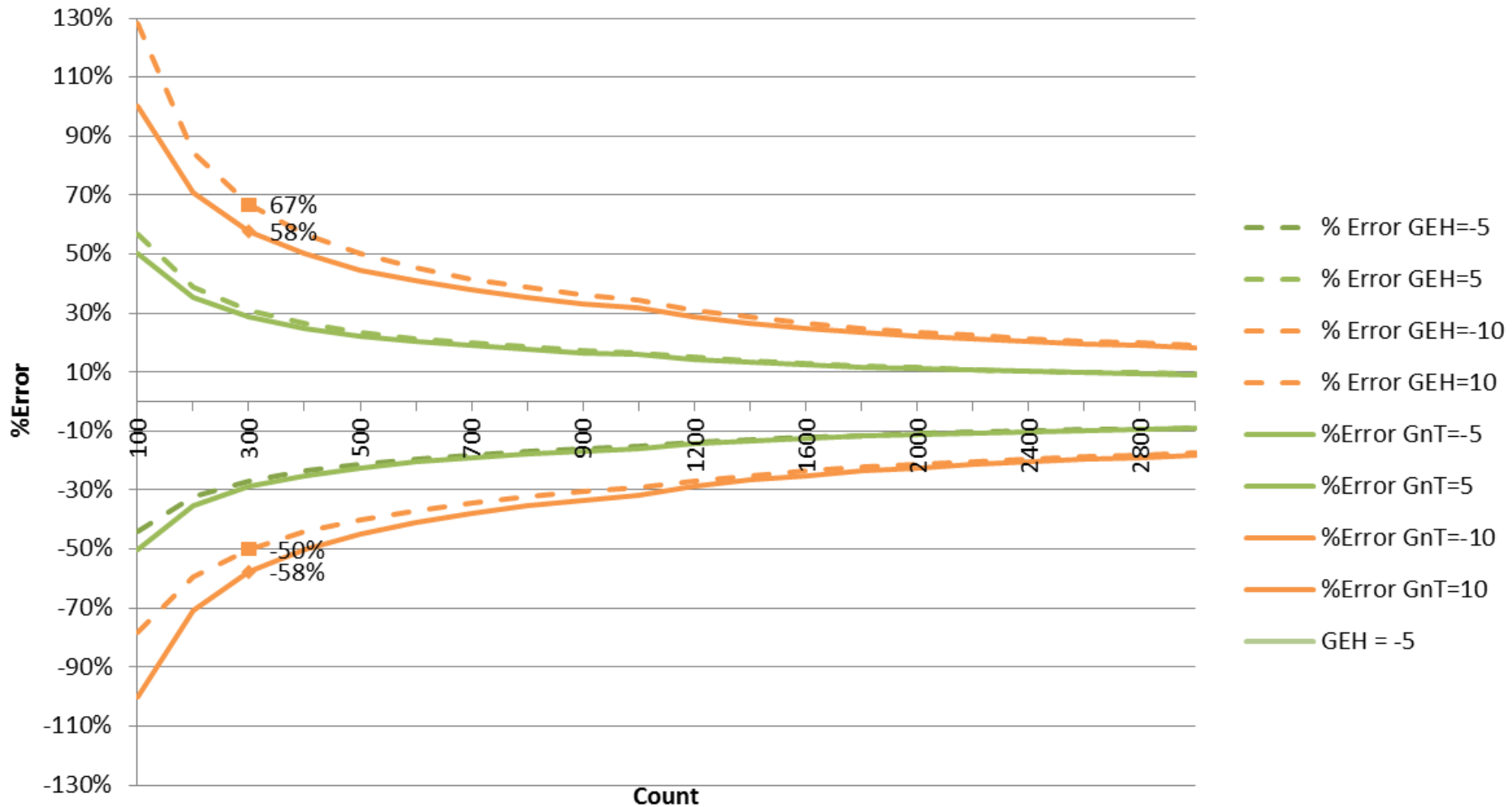
	Model 1	Model 2
Count	400	400
Modelled	500	300
Error	100	-100
% Error	25%	-25%

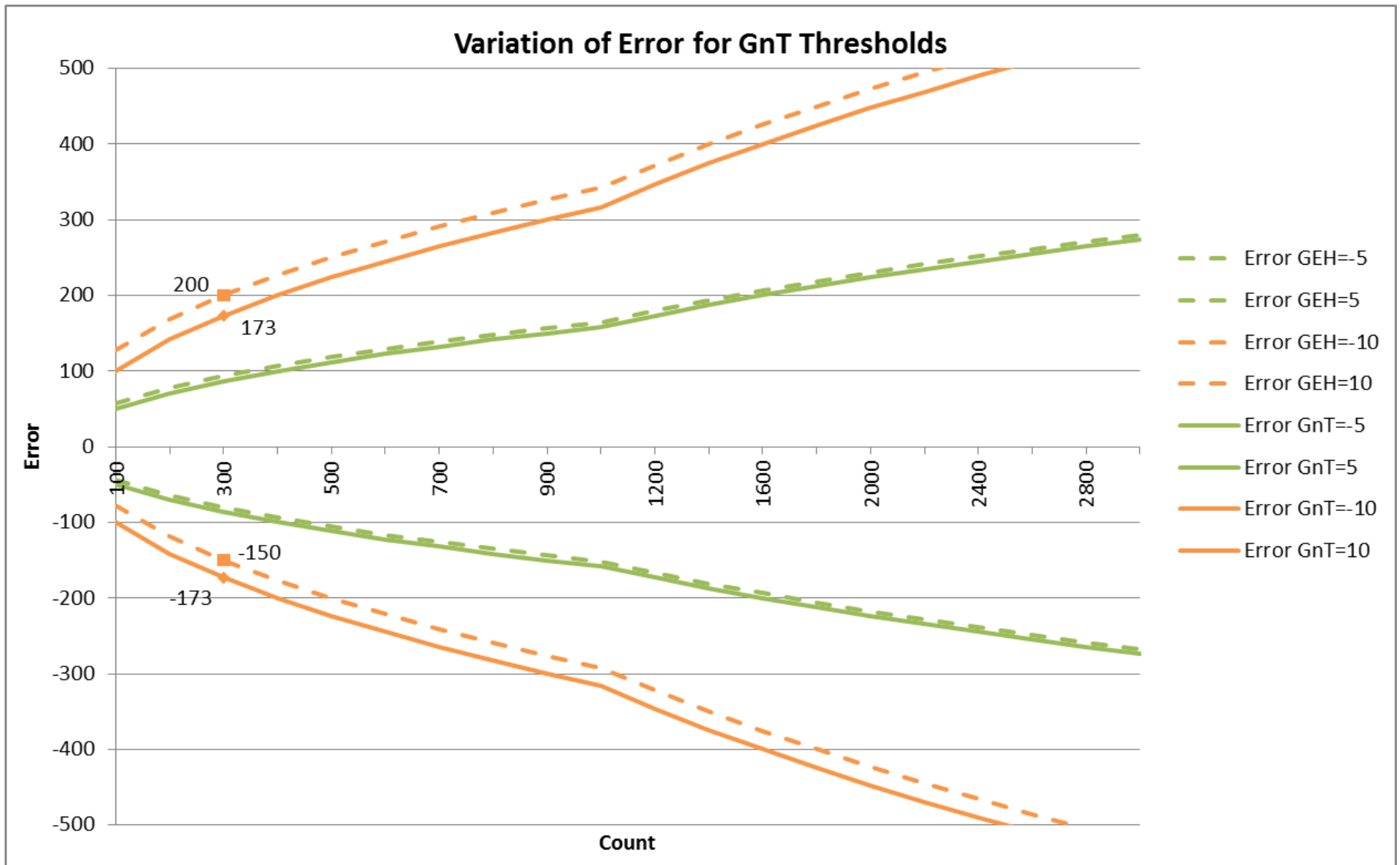
	Model 1	Model 2
Count	900	900
Modelled	600	1200
Error	-300	300
% Error	-33%	33%

- **GEH:** $\frac{\text{Difference}}{\sqrt{\text{Average}}}$
- $\sqrt{\text{Average}}$ Reflects uncertainty in the count
- What is the Purpose ?
 - To identify possible issues for further investigation
- **GnT:** $\frac{\text{Difference}}{\sqrt{\text{Observed}}}$



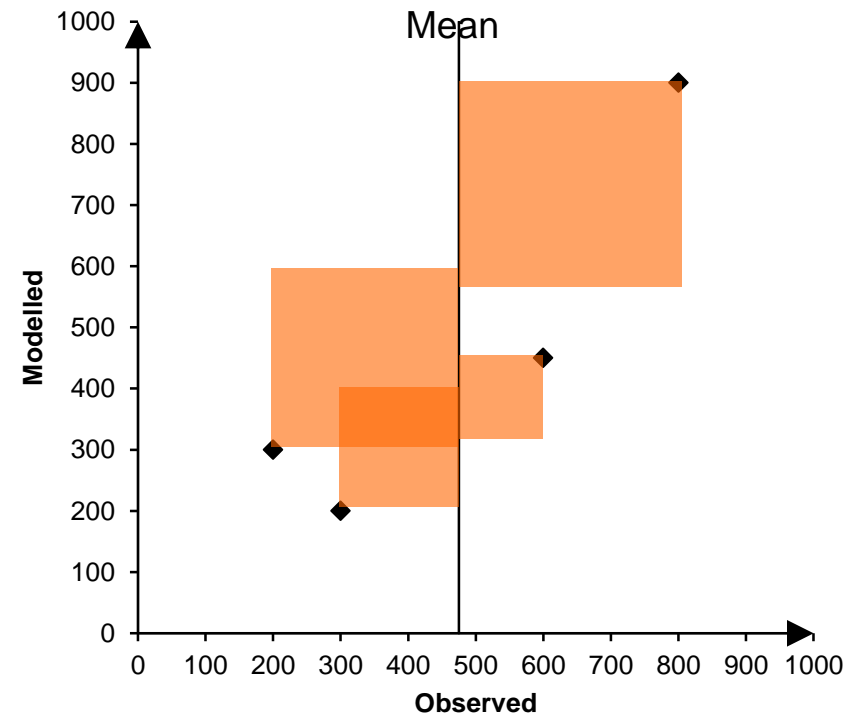
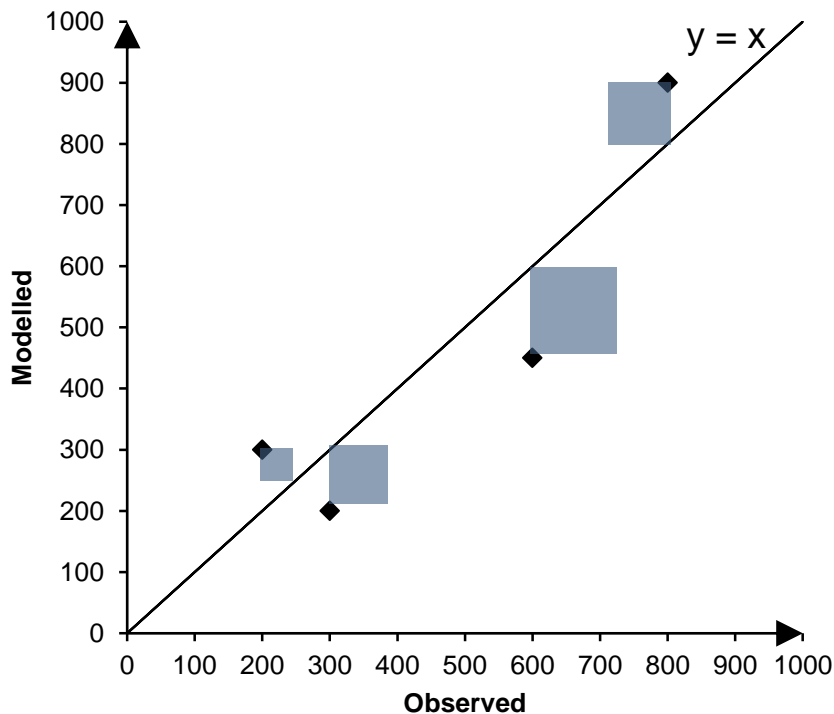
Variation of % Error for GnT Thresholds





- $R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$

- $R^2 = 1 - \frac{\text{Errors}^2 \text{ Summed}}{\text{Difference between a count and the mean count}^2 \text{ Summed}}$



R²: A Comparison



Observed	Modelled	GEH	% Error (M-O)/O	Error ² (M-O) ²	Diff ² (O-Av) ²
400	380	1.0	-5%		
450	473	1.0	+5%		
500	475	1.1	-5%		
505	530	1.1	+5%		
510	485	1.1	-5%		
515	541	1.1	+5%		
520	494	1.2	-5%		
525	551	1.1	+5%		
530	504	1.2	-5%		
600	630	1.2	+5%		

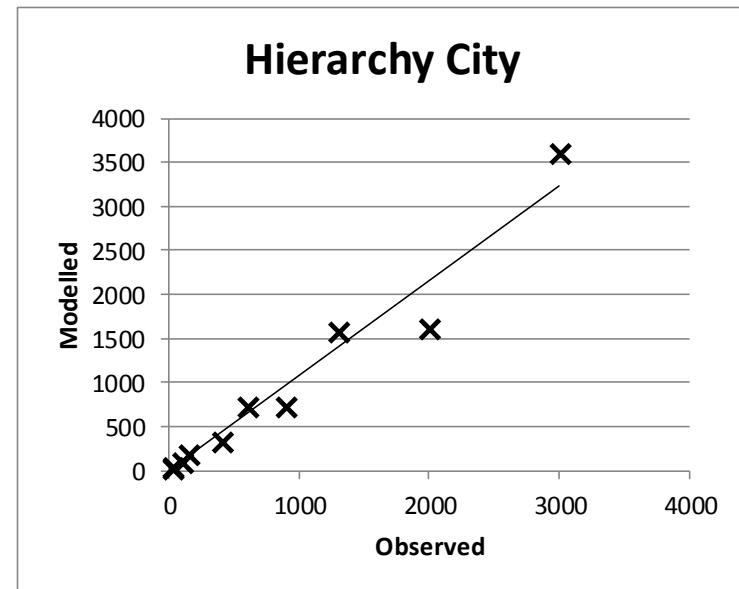
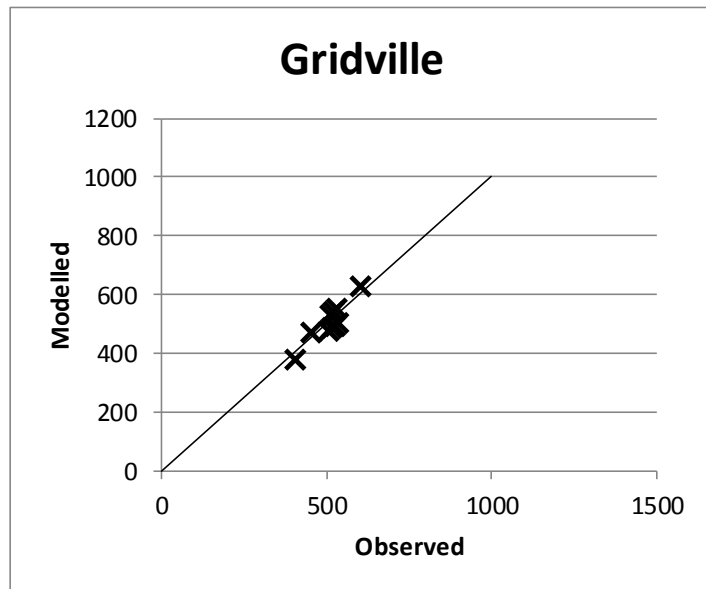
506 Ave

Totals:
R²:

Observed	Modelled	GEH	% Error (M-O)/O	Error ² (M-O) ²	Diff ² (O-Av) ²
20	16	0.9	-20%		
25	30	1.0	+20%		
100	80	2.1	-20%		
150	180	2.3	+20%		
400	320	4.2	-20%		
600	720	4.7	+20%		
900	720	6.3	-20%		
1300	1560	6.9	+20%		
2000	1600	9.4	-20%		
3000	3600	10.4	+20%		

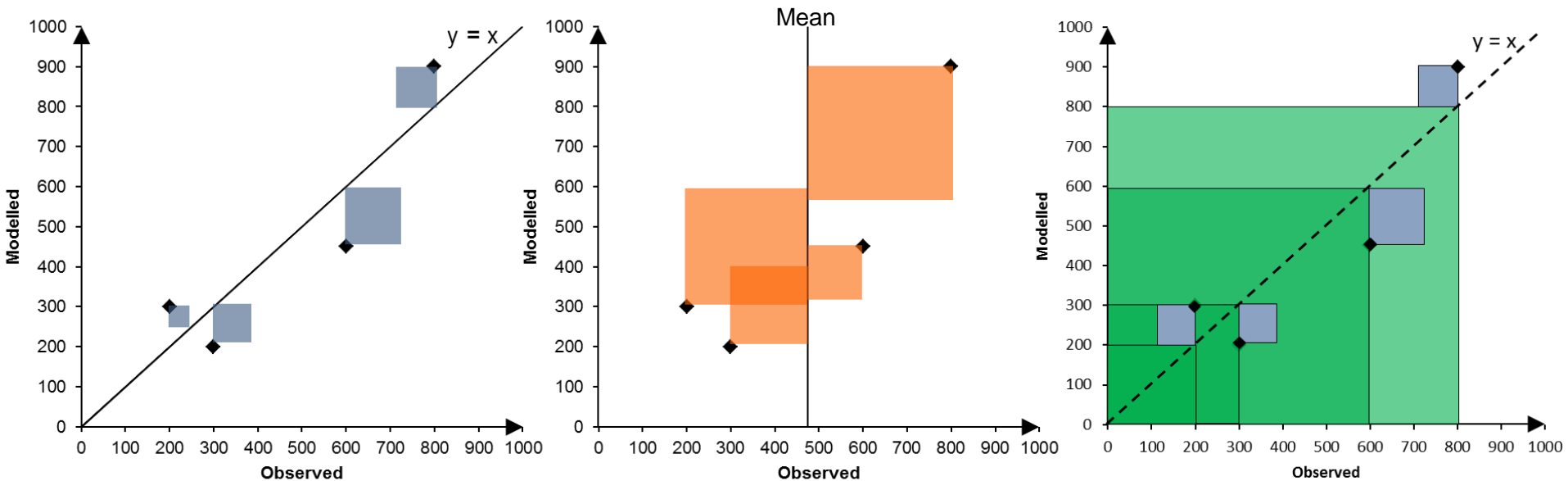
850 Ave

Totals:
R²:



R²: An Alternative ?

- $R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$
- $R^2 = 1 - \frac{\text{Error}^2, \text{Summed}}{\text{Difference between a Count and the Mean Count}^2, \text{Summed}}$
- Alternative: $R^2 = 1 - \frac{\text{Error}^2, \text{Summed}}{\text{Count}^2, \text{Summed}}$



R²: A Modification ?



Observed	Modelled	GEH	% Error (M-O)/O	Error ² (M-O) ²	Obs ² (O) ²
400	380	1.0	-5%	400	160,000
450	473	1.0	+5%	506	202,500
500	475	1.1	-5%	625	250,000
505	530	1.1	+5%	638	255,025
510	485	1.1	-5%	650	260,100
515	541	1.1	+5%	663	265,225
520	494	1.2	-5%	676	270,400
525	551	1.1	+5%	689	275,625
530	504	1.2	-5%	702	280,900
600	630	1.2	+5%	900	360,000

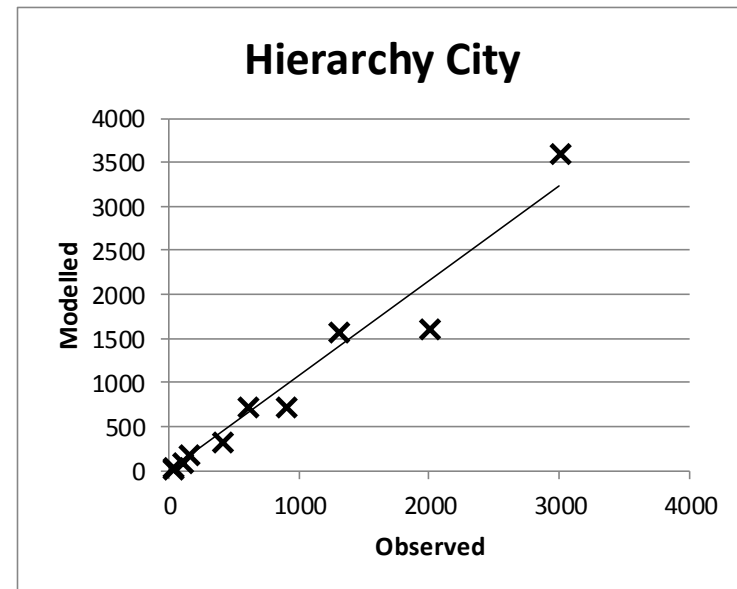
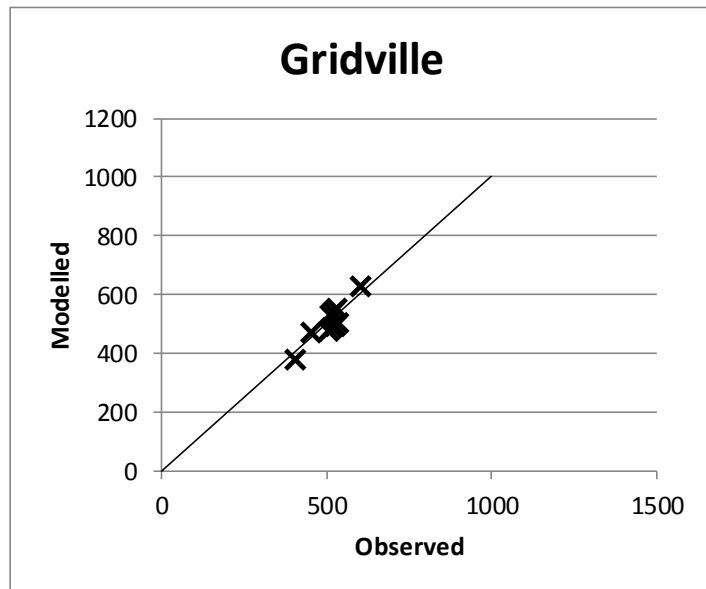
506 Ave

Totals: 6,449 2,579,775
R²: 0.736 0.998

Observed	Modelled	GEH	% Error (M-O)/O	Error ² (M-O) ²	Obs ² (O) ²
20	16	0.9	-20%	16	400
25	30	1.0	+20%	25	625
100	80	2.1	-20%	400	10,000
150	180	2.3	+20%	900	22,500
400	320	4.2	-20%	6,400	160,000
600	720	4.7	+20%	14,400	360,000
900	720	6.3	-20%	32,400	810,000
1300	1560	6.9	+20%	67,600	1,690,000
2000	1600	9.4	-20%	160,000	4,000,000
3000	3600	10.4	+20%	360,000	9,000,000

850 Ave

Totals: 642,141 16,053,525
R²: 0.927 0.960



RMSE Definition (or %RMSE)



- $$\% \text{ RMSE} = \frac{\sqrt{\frac{\sum(M-O)^2}{N-1}}}{\left[\frac{\sum O}{N}\right]} \times 100$$

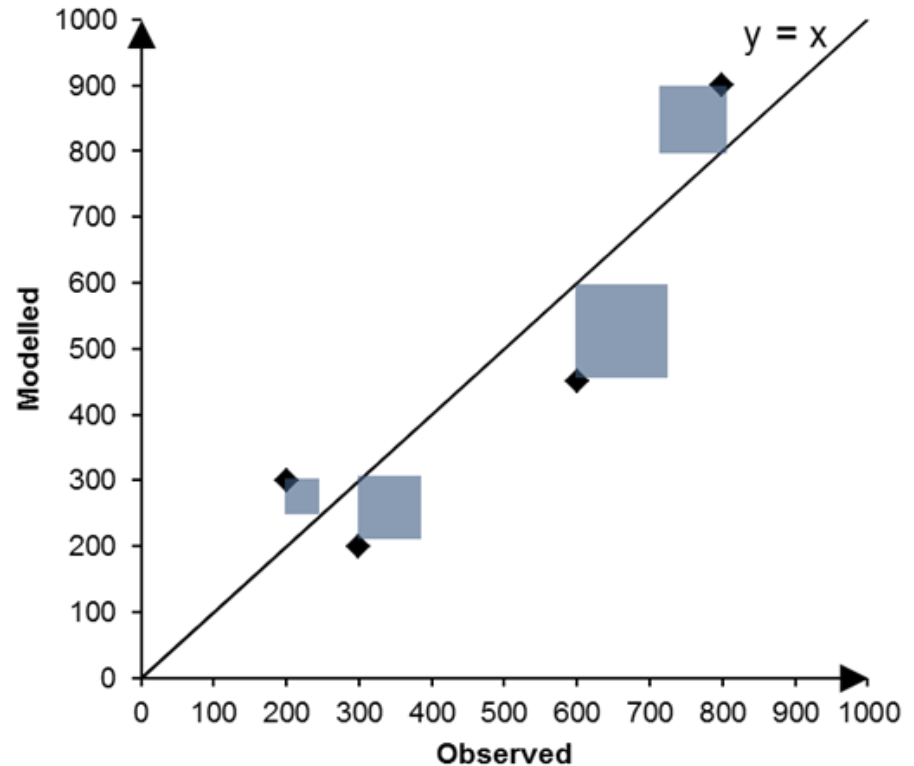
- $$\frac{\sqrt{\frac{\sum \text{Error}^2}{N-1}}}{\text{Ave Count}}$$

- $$\frac{\sqrt{\frac{\sum \text{Error}^2}{N}}}{\text{Ave Count}}$$

- $$\frac{\sqrt{\text{Average Squared Error}}}{\text{Ave Count}}$$

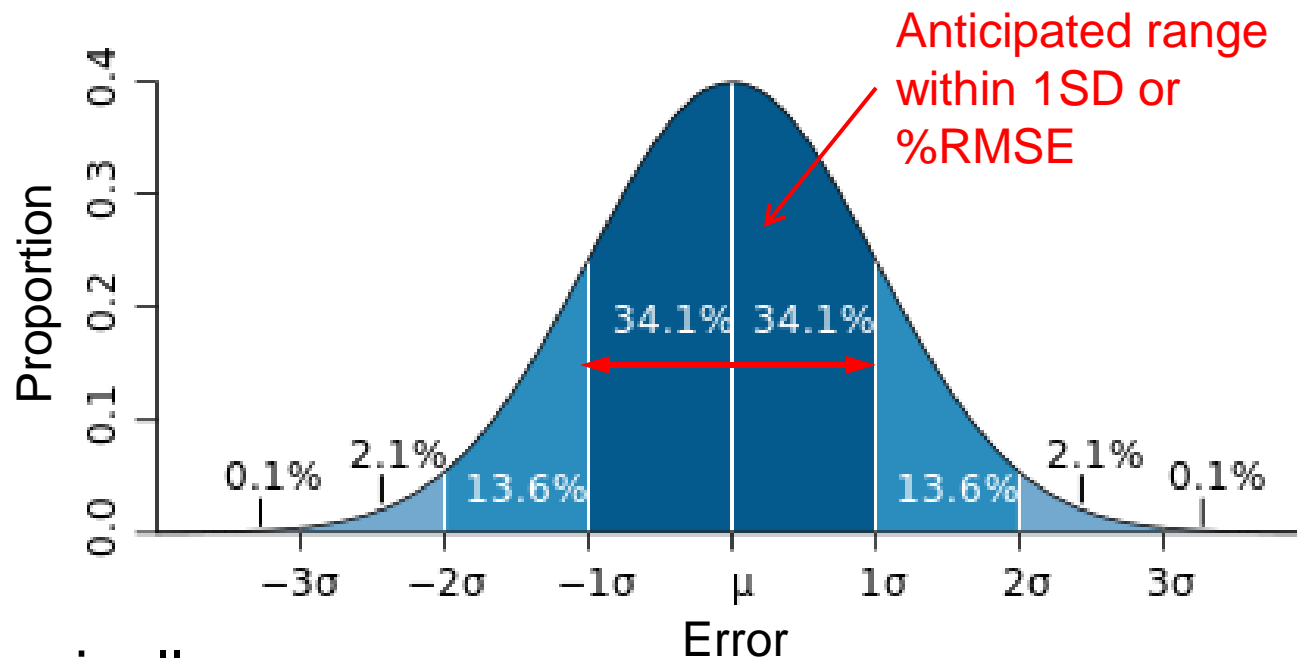
- What does an RMSE of 30% mean ?
- How is this a better measure than the 'weighted average % error', i.e:

- $$\frac{\text{Average Absolute Difference}}{\text{Average Count}} ?$$



%RMSE As a Measure of Confidence

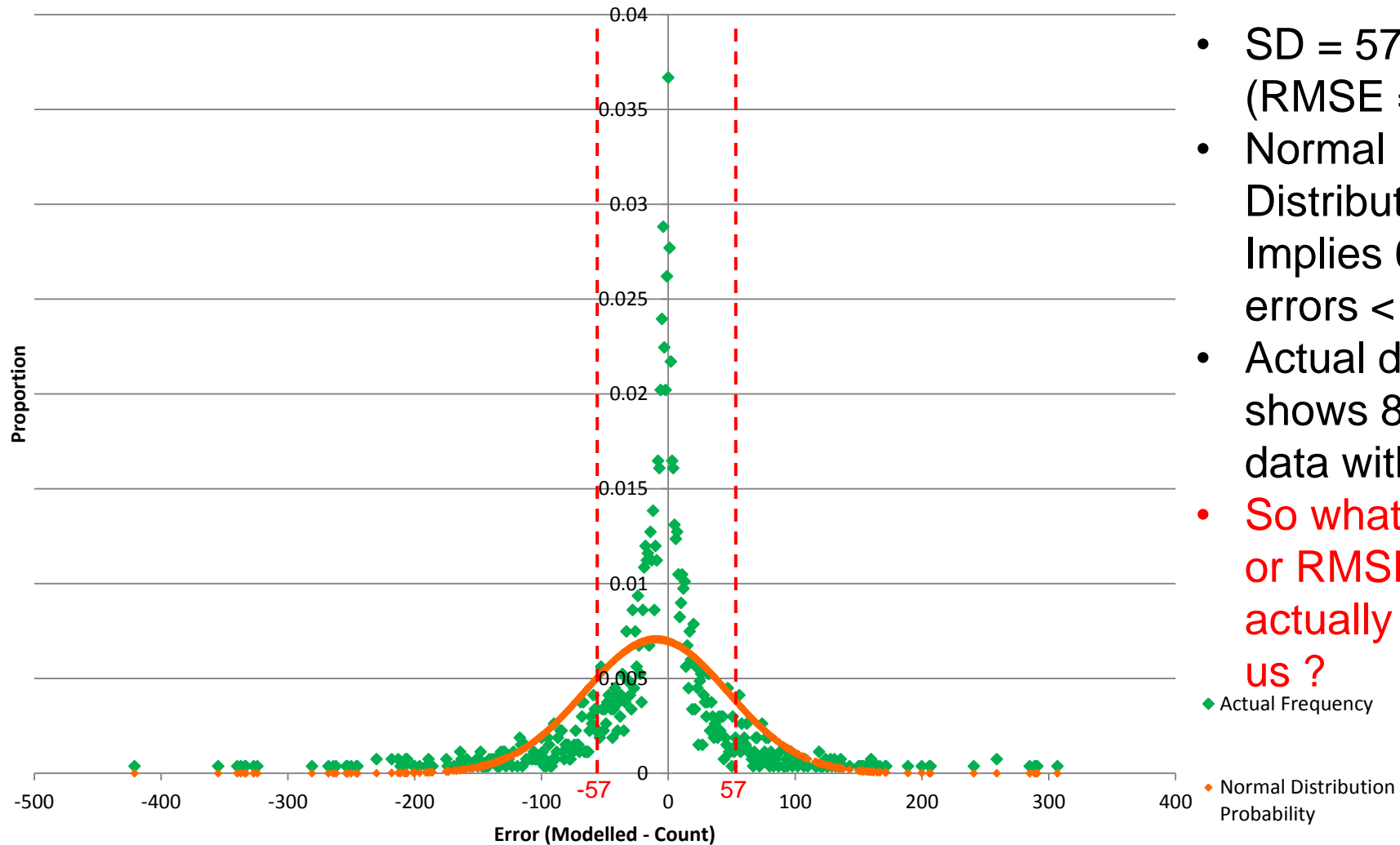
- RMSE closely related to Standard Deviation
- **Theory** is that SD (or RMSE) tells us something about the confidence in the model:



- i.e. typically:
 - 68% of errors < RMSE
 - 95% of errors < 2 x RMSE
- **But** this assumes a normal distribution of errors

%RMSE As a Measure of Confidence

Frequency Distribution of Model Flow Errors vs Normal Distribution



- SD = 57 (RMSE = 24%)
- Normal Distribution Implies 68% of errors < SD
- Actual data shows 81% of data within SD
- **So what is SD or RMSE actually telling us ?**

- Scatter plots are a better indication of overall model fit
- Is the %'Mean Absolute Deviation' i.e. $\frac{\textit{Average Absolute Difference}}{\textit{Average Count}}$ a more direct, simpler, intuitive single measure ?
- E.g. %MAD = 14% vs RMSE = 24%

- Is GnT a better indicator of potential issues with models than GEH ?
- Is R^2 appropriate to our purpose or should this be modified ?
- %RMSE not intuitive and of dubious value. Suggest replacing with %MAD
- Preference is to investigate & document reasons for all significant model vs. data discrepancies prior to and after any ME, rather than focussing on achieving a raft of arbitrary criteria.

