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The impact of statistical models on scalings derived from multi-machine H-mode threshold experiments

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Abstract
The predicted H-mode power threshold, P_{L-H}, for ITER is generally estimated from the international global H-mode threshold database (IGDBTH) by ordinary least squares log–linear (OLS) regressions. Such fits assume that errors are uncorrelated and (i) errors in P_{L-H} are much greater than those in the other parameters, (ii) errors are normally distributed and (iii) relative errors are equal for all experiments. In this paper, the validity of this statistical model for the IGDBTH is examined, by use of the more generalized maximum-likelihood method. Results indicate that all three assumptions bias the resulting scaling and so need to be relaxed. A fit relaxing all three constraints lies outside the error bars of the OLS, indicating that the choice of the statistical model makes a significant contribution to the resulting scaling. A chi-squared analysis shows that none of the studied models are entirely consistent with the data, indicating that further refinement of the physical and statistical model is required. For ITER-like parameters, a maximum-likelihood analysis shows a predicted threshold of 38.4 MW, compared with 31.1 MW for the OLS, indicating that OLS tends to under predict and that quoted confidence intervals tend to be too small. However, further studies of the sources of errors in the IGDBTH would be required before estimates based on more detailed statistical models can be given with confidence.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

As ITER, along with several other next step fusion devices, takes the H-mode for its baseline scenario [1], the power required to access the H-mode on these devices is a key parameter. The international global H-mode threshold database (IGDBTH) [2] provides data describing H-mode threshold experiments on 13 machines and predictions of the H-mode power threshold for next step machines, such as ITER, are made using empirical fits to this database. Such analyses have been performed using ordinary least squares log–linear regression (OLS) [3] and, more recently, with errors-in-variables log–linear orthogonal regression (EVOR) [4]. These fits use different statistical models, which result in different predictions from the same dataset. This paper uses a more general fitting method, based on the maximum-likelihood (M-L) method [5], to study the impact of statistical models on fits to the IGDBTH. The paper is structured as follows: section 2 discusses the mathematical formalism used in the paper. This is then used to produce scaling laws based on differing statistical models in section 3. Section 4 considers the consistency of the different methods with the data. In section 5, the results are brought together and conclusions drawn.

2. Mathematical formalism

Several forms of scaling laws and data selection criteria have been applied to the IGDBTH but, as this paper only considers the impact of statistical models on scalings, only one example need be considered here. The chosen physics model is a power law fit of the threshold power in megawatts, P, to the plasma surface area in metres square, S, magnetic field in T, B, and electron density in $10^{20}\cdot\mathrm{m}^{-3}$, n,

$$P = c_1 \cdot S^{c_2} \cdot B^{c_3} \cdot n^{c_4}, \tag{1}$$

where c_j, $j = 1, \ldots, J = 4$, are the free parameters to be fit. The dataset used will be IAEA04R of [3] and [4], which contains $I = 1298$ observations. The observations of the dependent variable, power, will be denoted P_i and those of the independent variables by $\boldsymbol{x}_{i,j}$, where $j = 1, \ldots, J - 1 = 3$, $\boldsymbol{x}_{i,1} = S_i$, $\boldsymbol{x}_{i,2} = B_i$ and $\boldsymbol{x}_{i,3} = n_i$.

The M-L method seeks the solution to a fitting problem by finding the combination of free parameters that result in the maximum probability density for the measured data. Formally, an expression for the probability density of the data is constructed, using the assumed physics and statistics models, and then this is maximized. The most general statistical model considered here is one in which all the measured parameters have a normal distribution with known standard deviations. The standard deviation for the power is denoted $\sigma_{\mathrm{p},i}$ and those for S, B and n by $\sigma_{i,j}$. The likelihood for a given set of measurements can then be expressed as

$$p\left(\boldsymbol{P}|\boldsymbol{x},\boldsymbol{c}\right) \propto \left(\prod_{i=1}^{I} \sigma_{\mathrm{eff},i}^{-1}\right) \cdot \exp\left(-\frac{1}{2}\chi^2\right) \tag{2}$$

where,

$$\chi^2 = \sum_{i=1}^{I} \frac{(P_i - f(\boldsymbol{x}_i;\boldsymbol{c}))^2}{\sigma_{\mathrm{eff},i}^2} \quad , \qquad \sigma_{\mathrm{eff},i}^2 = \sigma_{p,i}^2 + \sum_{j=1}^{J} \left(\frac{\partial f(\boldsymbol{x}_i;\boldsymbol{c})}{\partial \mathrm{x}_{i,j}}\right)^2 \sigma_{i,j}^2,$$

and $f(\mathbf{x};\mathbf{c})$ describes the function being fitted to P. $\sigma_{\mathrm{eff},i}$ represents the error in P together with the propagated errors from S, B and n. The best fit is derived by minimizing (2) for the $J = 4$ free parameters. Equation (2) will be solved numerically in the following sections using the MINUIT [6] package.

Table 1. Summary of fits of equation (1) to IAEA04R assuming errors on logged parameters are normally distributed.

Statistical model	$c_1 \cdot 10^2$	c_S	c_B	c_n
(1) OLS	7.7	0.80	0.65	0.44
(2) M-L with (i), (ii) and (iii)	7.7	0.80	0.65	0.44
(3) EVOR	7.5	0.85	0.58	0.56
(4) EVOR with mean errors	7.5	0.85	0.58	0.56
(5) M-L with (ii) and (iii) only	7.5	0.85	0.58	0.56
(6) M-L with (iii) only	7.7	0.97	0.32	0.88
(7) OLS adjusted for log bias	7.6	0.80	0.65	0.44

3. Fits to the threshold database

For the fits, the measured parameters are taken from IGDBTH and their standard deviations as those calculated in [4]. For comparison, the OLS and EVOR fits are also calculated directly using the SAS package [7]. The errors given in [4], are fractional errors estimated for each machine: they can be thought of as rough estimates of the true errors. The errors are all assumed to be uncorrelated and normally distributed and so they are appropriate to the formalism of section 2.

3.1. Simple OLS fit

OLS fits are based on the statistical model described in section 2 with three further assumptions:

(i) that errors in P are much greater than in the other parameters
(ii) that the relative errors may be taken as equal for all experiments
(iii) that the logs of P, S, B and n are essentially normally distributed

With these further assumptions, P, S, B and n can be replaced in (2) by their log values and $f(\boldsymbol{x};\boldsymbol{c})$ takes on a linear form. The standard deviations are replaced by the relative errors, $s_{p,i} = s_p$ and $s_{i,j} = 0$, and the exponent in equation (2) reduces to a quadratic in $\boldsymbol{c}$ and equation (2) can be minimized by linear algebra.

The resulting fit of this statistical model to IAEA04R is shown in table 1, where the global value of the relative error in P is calculated as the square root mean square of the individual terms, $s_p^2 = (1/I)\sum_{i=1}^{I} s_{p,i}^2$. Fit 1 represents the SAS OLS fit and Fit 2 a M-L fit with the assumptions outlined above. As can be seen, the fits are equal demonstrating that OLS fits do indeed use this model. The validity of each of the assumptions made will now be studied in turn.

3.2. Inclusion of errors on independent variables

Assumption (i), that errors in P are much greater than in the other parameters ($\sigma_{p,i} \gg \sigma_{i,j}$), has already been shown to be in need of relaxation [4]. The mean relative error of $s_n \approx 0.065$ is over 40% of that of $s_P \approx 0.156$, for example. If assumption (i) is relaxed, equation (2) has a more complicated form, but it can be shown [8] that it can still be solved analytically. This is the statistical model used in EVOR.

In table 1, Fits 3 and 4 represent SAS EVOR fits and Fit 5 a M-L fit with the assumptions outlined above. Fit 3 shows the case where s_p and s_j are calculated as indicated in section 3.1., and Fit 4 where they are calculated as $s_p = (1/I)\sum_{i=1}^{I} s_{p,i}$, an alternative method also used in the literature [9]. Fit 3 and Fit 4 are identical to 2 decimal places, indicating that the method is not sensitive to which of these methods is chosen. Comparing the M-L fit to either of the

Table 2. Summary of fits of equation (1) to IAEA04R assuming errors on parameters are normally distributed.

Statistical model	$c_1 \cdot 10^2$	c_S	c_B	c_n
8. M-L, Errors on P only	5.6	0.86	0.72	0.58
9. M-L	6.0	0.96	0.45	0.80

EVOR fits, it can be seen that the resulting scalings agree, demonstrating that EVOR fits do indeed use this model. Comparing the EVOR fit with the OLS fit, it can be seen that the resulting scalings are indeed different. This indicates that assumption (1) does indeed need to be relaxed as not doing so results in biasing of the scaling.

3.3. *Inclusion of machine-to-machine variation in errors*

Assumption (ii), that the relative errors may be taken as equal for all experiments ($s_{p,i} = s_p$ and $s_{i,j} = s_j$), is an approximation as the relative errors in all parameters have been shown to vary from tokamak to tokamak [4] with $s_{p,i} = 0.06$–0.23, $s_{S,i} = 0.01$–0.10, $s_{B,i} = 0.01$–0.03 and $s_{n,i} = 0.02$–0.10. This assumption can be easily relaxed in the M-L analysis and the resulting fit, taking the relative errors for each tokamak given in [4], is given as Fit 6 in table 1. As with assumption (i), the relaxation of this assumption has had a clear effect on the resulting scaling indicating that assumption (ii) does need to be relaxed as not doing so biases the result of the scaling. It should be noted at this point that (ii) alone can be relaxed within the OLS method, but not within the EVOR method. Neither OLS or EVOR can thus relax both (i) and (ii) together.

3.4. *Relaxation of normally distributed logs constraint*

Assumption (iii) is that the logs of P, S, B and n are essentially normally distributed. This is the case for very small relative errors on all parameters ($s_{i,j}, s_{p,i} \ll 1$) but as these errors become larger the log distribution becomes strongly asymmetric. The assumption can be easily relaxed in the M-L analysis, by simply using the P, S, B and n themselves in equation (2) rather than their logs.

The effect of relaxing this one assumption can be seen by comparing the OLS fit of table 1 (Fit 1) with Fit 8 of table 2. Fit 8 contains the same assumptions, (i) and (ii), as the OLS but with minimisation performed with P, S, B and n directly. It can be seen that relaxing this assumption alone has had a marked effect on the scaling.

An example of the effect of log-skewing is indicated in figure 1 which shows the distribution of the logarithm of a normally distributed variable $x = N(x_0, \sigma_x)$, with $x_0 = 1$ and $\sigma_x = 0.5$, where $N(\boldsymbol{x}_0, \sigma)$ denotes the normal distribution with mean value $\boldsymbol{x}_0$ and standard deviation, (SD) σ. The distribution of $\ln x$ is very different from that derived by simple error propagation, $N\left(\ln x_0, \sigma_x \big/ x_0\right)$, which is that assumed by OLS. Firstly, the $\ln x$ distribution has a different mean (E $(\ln x) \approx \ln x_0 - \sigma^2 \big/ 2.x_0^2$, where ***E(X)*** denotes the expectation value of the variable ***(X)*** and standard deviation, and, secondly, its distribution is skewed. The former can be corrected for in OLS, simply by replacing the logged variables by their expected values, and this has been done in the log-shifted fit, Fit 7 of table 1. It can be seen that the resulting scaling differs little from the standard OLS. This method is akin to taking the logs as being distributed like $N(E[\ln x], SD[\ln x])$ which can be seen from figure 1 to be a poor representation of their true distribution, due to the large skewing. This demonstrates that it is the skewing of the log distribution that is the dominant contribution to the biasing of OLS.

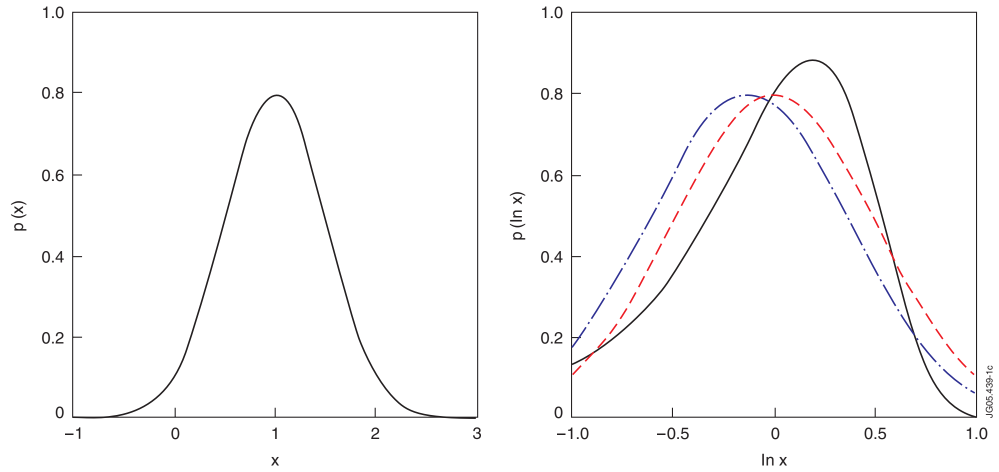

Figure 1. The probability density distribution of (*a*) a normally distributed variable, $x = N(1,0.5)$ and (*b*) its log, both shown as solid black lines. Also shown in (*b*), the distributions $N(0,0.5)$ as dotted (red) and an adjusted normal distribution $N(E[\ln x]SD[\ln x])$ as dot-dashed (blue).

As a final step, all three assumptions of section 3.1 can be relaxed and a full fit made to equation (2). The result is given as Fit 9 of table 2. This is the fit for the statistical model where P, S, B and n are all assumed to have normally distributed uncorrelated errors, which vary from tokamak to tokamak. When compared with OLS, the M-L fit to equation (2) differs strongly indicating that the combined effect of the assumptions of section 3.1 is to produce a biasing in the original fit.

3.5. Further statistical models

In all the above analyses errors were assumed to be uncorrelated and normally distributed. The M-L method can be easily extended to alternate error distributions, by replacing the probability distribution in equation (2) with the one appropriate to the chosen statistical model. Correlations between errors in P, S, B and n, for a given experiment, would be expected to be weak, but other choices of variables may require such correlations to be addressed. Correlations between measurements from different experiments on the same machine, due perhaps to calibration errors, are more likely and could be similarly included. Examples of non-normal error distributions might derive from power stepped L–H threshold experiments where the threshold is known only to lie somewhere between two measurements. In such cases, the M-L would tend towards discriminant analyses [10].

Another area for consideration is the distribution of the independent data. All methods used in this paper assume that the underlying independent data are drawn randomly. This is clearly not the case as technical and physical constraints on individual machines, coupled with the varying amounts of data from each machine, result in correlations of the independent parameters. An example of this, showing the n–S correlation, can be seen in figure 3. These effects can be included in M-L analyses by either extended M-L and/or by including availability in the analysis [5]. Weighting methods have been applied to other plasma physics databases [11, 12] in an attempt to redress such problems and could equally be applied to the IGDBTH. Bayesian methods [13], which have been applied to other plasma physics databases [14, 15], could also be used to include such effects as they naturally include such

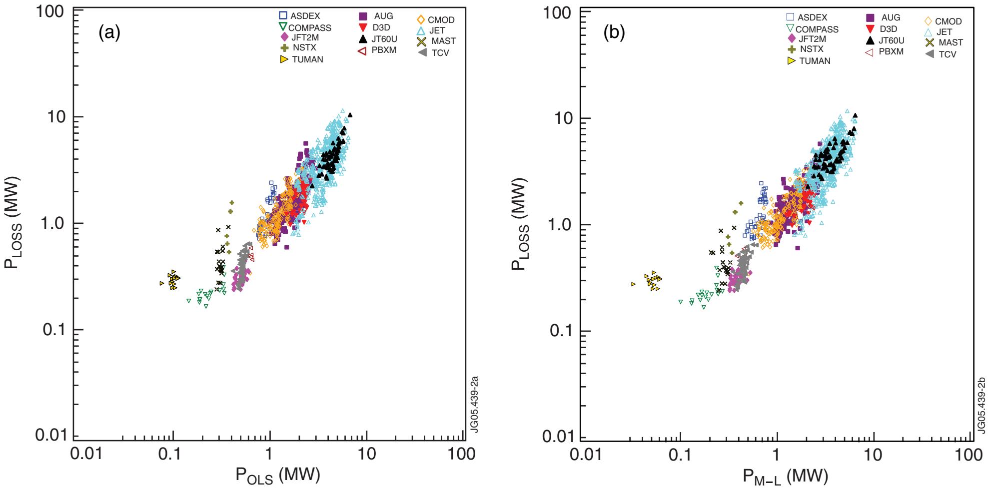

Figure 2. (*a*) The observed loss power at the L–H threshold, P_{LOSS}, against that predicted from an OLS fit, P_{OLS}, for the IAEA2004R dataset drawn from the IGDBTH. (*b*) The observed loss power at the L–H threshold, P_{LOSS}, against that predicted from the full M-L fit, $P_{\text{M-L}}$, for the IAEA2004R dataset drawn from the IGDBTH.

Table 3. Summary of fits for a selected set of statistical models.

Statistical model	$c_1 \cdot 10^2$	c_S	c_B	c_n	χ^2_N	P_{ITER}
OLS	7.7 ± 0.3	0.80 ± 0.01	0.65 ± 0.03	0.44 ± 0.03	7.43	31.1 ± 7.1 %
EVOR	7.5 ± 0.3	0.85 ± 0.02	0.58 ± 0.03	0.56 ± 0.03	7.09	34.3 ± 7.2 %
M-L	6.0 ± 0.3	0.96 ± 0.02	0.45 ± 0.04	0.80 ± 0.05	6.26	38.4 ± 9.8 %

information as a prior distribution. In this context, it should be noted that the M-L method used here corresponds exactly to a Bayesian method with the model described in section 2, a uniform prior distribution for the free parameters and independent variables and the power law linearised about its value for the measured parameters.

4. Errors and confidence

The observed threshold power is plotted against that calculated by the OLS fit (Fit 1) and the M-L fit (Fit 9) in figures 2(*a*) and (*b*), respectively. By eye, the agreement between the data and both fits is similar. The spread of the data is fairly wide, with the scalings describing some of the trend in the data from machines such as ASDEX-Upgrade, C-Mod, COMPASS, DIII-D, JET and JT60-U. Other machines, such as ASDEX and TCV, seem to be less well described. The observed H-mode power threshold for TUMAN-3M lies systematically above both scalings. This is believed to be because the TUMAN-3M data are all taken from limiter discharges, rather than the single null discharges which make up the majority of the dataset. For a fuller understanding of how well the scalings describe the data, the errors in the scalings themselves must first be quantified.

The covariance matrix for the free parameters, $\boldsymbol{c}$, describes the variance of all $J = 4$ free parameters along with their covariances. The resulting errors are given for the OLS, EVOR and M-L in table 3. It should be noted that, as a consistency check, the errors for the OLS fit were found to agree with those calculated by the standard OLS regression method [5]. All the

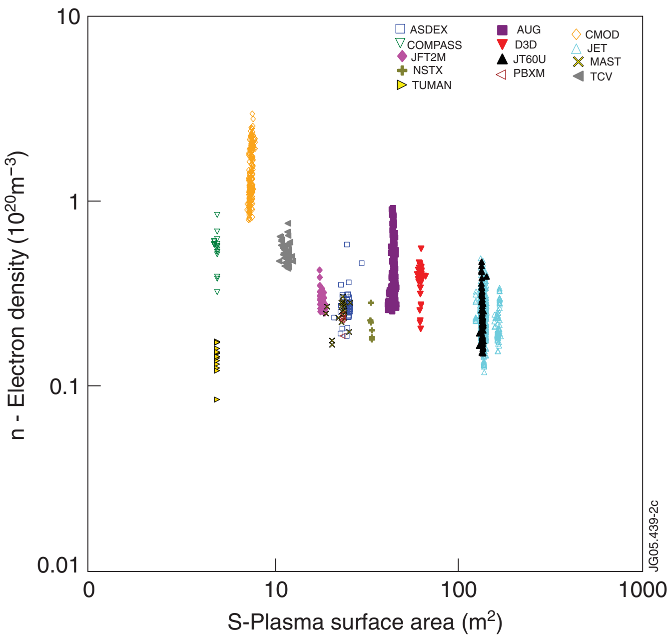

Figure 3. The electron density, n, against the plasma surface area, S, for IAEA2004R dataset drawn from the IGDBTH. The negative n–s correlation can be clearly seen.

methods differ from the others, in at least one coefficient, by more than the predicted errors. This is because the errors are calculated assuming that the statistical model used for a particular fit is correct. The fact that the three fits differ by more than their errors means that the choice of model has a significant effect on the outcome of the fit. Partly the IGDBTH is sensitive to the choice of the statistical model because of correlations that exist between the parameters. S and n have the strongest correlation, $\rho_{nS} = -0.73$, as can be seen in figure 3. This correlation means that if the exponents of these two parameters are raised or lowered together, then the predicted power, for points in the database, does not change greatly.

To determine goodness of fit then, a statistical model must be chosen and a measure of the consistency of the data and fit to it must be determined. This is done here by taking the value of χ^2 in equation (2), which can be shown to have an expected value of $I - J = 1294$. The normalized χ^2, $\chi^2_N = \chi^2/(I - J)$, thus has an expectation value of 1 and can be shown to have a standard deviation approximated by $2/\sqrt{I} \approx 0.06$ [5]. In this paper, the assumed statistical model is one with all three assumptions of section 3.1 relaxed. The resulting values of χ^2_N are given in the final column of table 3. It can be seen that the M-L has the lowest χ^2_N, followed by EVOR, with the OLS being the weakest representation of the data, given the assumption that the chosen statistical model is correct. In each case, the differences between these methods are significantly larger than the standard deviation of χ^2_N.

However, it can also be seen from table 3 that for the M-L fit $\chi^2_N = 6.26$, which is significantly much greater than one. This implies that the combined physical and statistical model used in this paper does not sufficiently describe the data. This may be because the wrong form of the physical model has been chosen, important physics variables have been ignored, the size of the errors in the statistical model have been underestimated and/or a more detailed statistical model is required. The physical model is clearly very crude, and the statistical model is still relatively simple, so it is perhaps not surprising that the resulting χ_N^2 is so far from unity. Alternative physical models, including ones with further restrictions on the dataset or physics-based constraints on the scalings, could be studied within the M-L framework. The statistical model could be refined as discussed in section 3.5 or by improving the estimates of the calculated errors for each observation in the dataset. This would involve an analysis of the sources of errors in each machine to provide a reliable estimate of the error on each observation of each parameter used in the fits. The facility to store the individual errors on each parameter would also have to be added to the IGDBTH database.

In the final column of table 3, the power required for a H-mode transition on ITER is given, assuming $S = 683$, $B = 5.3$ and $n = 0.5$. The results would be for a pure deuterium ITER plasma, and it should be noted that with the observed $P \propto M^{-1}$ scaling [16], where M is the mean hydrogenic atomic mass, the predict threshold for deuterium–tritium plasmas would be somewhat lower and that for pure hydrogen plasmas somewhat higher. The error bars are derived by propagating the errors on the fitted parameters and, again, represent one standard deviation. 95% confidence intervals, representing two standard deviations, can be calculated from them. For example, the 95% confidence interval for the M-L fit is $\boldsymbol{P} = 30.9$–45.9. There is a clear difference in the predicted power, largely coming from the variation in size scaling through the parameter S. Thus, the choice of the statistical model has a similarly large impact on the final scaling. This would suggest that OLS and EVOR scalings do, in general, underestimate the predicted power threshold for ITER. Perhaps more importantly, these results suggest that the error bars on the predicted power for the existing scalings are too small. As uncertainty exists in the choice of the statistical model itself, a conservative procedure would be to base confidence intervals on results from a set of statistical models rather than on just one.

Comparing the three fits of table 3 with other recent fits to the IGDBTH [3, 17–19], which are all OLS fits to subsets of the full database, the OLS and EVOR are seen to lie within the range of the previous fits. In contrast, the M-L fit corresponds to the strongest density scalings and weakest field scalings previously observed. This could be interpreted as evidence against the M-L or equally as a demonstration that the previous OLS fits introduced a bias. A more concerning consistency check for the M-L is that its density and field scalings lie outside previous fits obtained when taking data from only one machine, with the one exception of the $P \propto n^{0.79} \cdot B^{0.56}$ observed for ASDEX-Upgrade [17]. For the ITER predictions, the M-L fit lies towards the high end of the scalings but is not the highest.

5. Conclusion

By using the more general M-L method, the statistical model used in both OLS and EVOR fits has been assessed. The assumptions that (i) the errors in P are much greater than in the other parameters, (ii) the relative errors do not vary from experiment to experiment and (iii) the logs of P, S, B and n are normally distributed have all been shown to be in need of relaxation and to introduce a significant level of biasing in the resulting fits. For the third assumption, this has been shown to be due to the skewing effect of taking the logarithm of a normal distribution.

The sensitivity of the fit to the statistical model illustrates the importance of taking care in its selection. The most sophisticated model used in this paper has a goodness of fit measure of $\chi_N^2 = 6.26$, which indicates that there are still important missing details in the physical and/or statistical model. For ITER this model predicts a threshold power of 38.4 MW, significantly higher than either OLS, 31.1 MW, or EVOR, 34.3 MW. This indicates that OLS and EVOR fits tend to underestimate the ITER predicted power threshold. The sensitivity of the M-L fits to the calculated errors, which are only roughly estimated at present, means that these errors must be better understood before a single statistical model, and hence a single fitting method, can be chosen. For the present, confidence intervals based on a set of statistical models are the most appropriate.

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