

# **Integrated Data Analysis of the DIII-D Density Profile**

L. Stagner<sup>1</sup>, W.W. Heidbrink<sup>1</sup>, MA Van Zeeland<sup>2</sup>, and L. Zeng<sup>2</sup>

<sup>1</sup>University of California–Irvine, Irvine, California, USA

<sup>2</sup>General Atomics, P.O. Box 85608, San Diego, California 92186-5608, USA

## **Abstract**

## **1 Introduction**

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## **2 Integrated Data Analysis**

As fusion experiments expand, so does the number of diagnostics used to probe the underlying physics. With the increase in diagnostics the number of interrelations among the diagnostics increases accordingly. While each diagnostic can act independently it is often advantageous to combine the data sets to acquire the most accurate result that is consistent with all the information available. This causes difficulties when trying to combine multiple data sets that cover complementary areas of interest. Bayesian data analysis give a comprehensive, scalable, and automated framework for combining complementary diagnostics.

## 2.1 The Bayesian perspective

Bayesian statistics differs from the prevailing frequentist statistics that is taught in most introductory courses. The difference between the two views is in the definition of probability. In the Bayesian perspective, probability represented a degree of belief or plausibility that an event was true, based on the information available. This school of thought is opposed to frequentist view that probability is a long run relative frequency with which the event occurs, given infinitely many repeated experimental trials.[1]

While the frequentist view is seemingly more objective, it is limited in its straightforward application since some things cannot have long run relative frequencies and, as a result, cannot be analysed by probability theory. For instance a constant, such as the mass of an object, cannot be analysed by a straightforward application of the frequentist definition of probability as a long run relative frequency. To use the frequentist view you first have to relate the mass to the data through some function called the *statistic*. Since statistic is subject to random noise it becomes the random variable to which the rules of probability can then be applied. The issue with this approach is that there is no natural way of choosing the best statistic.[2] The founders of the field have a plethora of ad hoc rules and tests to determine which statistic should be used in any situation. These rules and tests hides much of the mechanics and assumptions inherent in the analysis and the consequences can often turn up at the worst possible moments.

The bayesian definition has no such difficulty since nearly anything can be thought of as a probability and the framework explicitly formulates all assumptions. That is not to say that it is without its issues. The frequentist view is often much easier to use because it hides most of the difficulties from the user. In bayesian statistics you have to be very careful with the assumptions that are made since it can drastically affect the results. Also, the calculation of optimal parameters is also a challenging numerical exercise in Bayesian statistics. It was partially for this reason that the frequentist view arose into prominence. It was only in the mid 20<sup>th</sup> century with the advent of computers and efficient sampling algorithms that Bayesian statistics has begun its resurgence. In recent years Bayesian analysis has become essential to many scientific fields such as cosmology and artificial intelligence.[1]

## 2.2 Mathematical Formulation

In 1946, Richard Cox began to formulate the rules for logical and consistent reasoning by considering how we might quantify our beliefs about the truth of an event or object. He concluded that the real numbers we attached to our beliefs followed the rules of probability:[2]

$$prob(X|I) + prob(\bar{X}|I) = 1 \quad (2.1)$$

and

$$prob(X, Y|I) = prob(X|Y, I) \times prob(Y|X, I) \quad (2.2)$$

Here  $\bar{X}$  denotes that  $X$  is false and the vertical bar ‘|’ means ‘given’. All the probabilities are conditional on  $I$  to denote the relevant background information available, since there is no such thing as an absolute probability.

Equation 2.1 and 2.2 are called the sum and product rules, respectively. The sum and product rule form the basic equations of probability theory. From these two rules we can derive the core equations used in bayesian statistics: Bayes’ theorem

$$prob(X|Y, I) = \frac{prob(Y|X, I) \times prob(X|I)}{prob(Y|I)} \quad (2.3)$$

and marginalization.

$$prob(X|I) = \int_{-\infty}^{\infty} (X, Y|I) dY \quad (2.4)$$

The power behind Bayes theorem can best be recognized with a change of notation.

$$prob(hypothesis|\{data\}, I) = \frac{prob(\{data\}|hypothesis, I) \times prob(hypothesis|I)}{prob(\{data\}|I)} \quad (2.5)$$

or as denoted in most parameter estimation problems:

$$\mathcal{P}(\vec{\alpha}|\vec{d}, I) = \frac{\mathcal{L}(\vec{d}|\vec{\alpha}, I)\pi(\vec{\alpha}|I)}{\mathcal{Z}(\vec{d}|I)} \quad (2.6)$$

where  $\vec{\alpha}$  are the parameters to be inferred. The terms in the above equation have formal names.  $prob(hypothesis|I)$  is called the *prior*. The prior encodes

the current state of knowledge about the parameters before we have analyzed any new data. When we have acquired new information the prior is modified by the first term,  $\text{prob}(\{\text{data}\}|\text{hypothesis}, I)$  called the *likelihood*. The product of the likelihood and the prior give  $\text{prob}(\text{hypothesis}|\{\text{data}\}, I)$ , which is called the *posterior*. The posterior encodes our final state of knowledge after all the data has been incorporated. The maximum value of the posterior gives us the best estimate of the parameters we trying to infer. The last term,  $\text{prob}(\{\text{data}\}|I)$ , is called the *evidence* or *marginal likelihood*. In parameter estimation problems the evidence can be ignored since it is essentially a normalization constant. However, in model comparison problems it is of vital importance.

### 2.3 Choosing the Best Prior

It was noted earlier that one has to be extra careful with the assumptions that are made prior to incorporating data. Quite fittingly, these assumptions are encoded in the choice of prior. This process can be difficult and if often done incorrectly. In order to choose the best prior three main schools of thought for choosing priors have been developed.

The first school of thought is to choose a prior that expresses specific, definite information about a parameter. If, for instance, a parameter is known, through past experience or expert testimony, to have a value around  $1 \pm 0.2$  with upper bound of 2. It would not be uncommon for someone to assign a prior that is a Gaussian with a mean of 1 and standard deviation of 0.2 that is zero for values greater than 2. Informative priors are both a major advantage and can also be a major pitfall. If our prior knowledge was incorrect and the upper bound is around 5, depending on the amount of data, we may have biased the posterior such that it doesn't reflect the truth. We must then be careful not to bias our results without proper justification. Informative priors also suffer from the fact that there is not a well defined procedure for choosing them.

The second school of thought is to be as non-informative as possible. This method should be used when we have no prior information about the parameter in question. The most common type of non-informative prior is called the Jeffreys' Prior. The key property of the Jeffreys' Prior is that it is invariant under re-parameterization. The Jeffreys' prior is defined as

$$\pi(\vec{\alpha}) \propto \sqrt{\det \mathcal{I}(\vec{\alpha})} \quad (2.7)$$

where  $\mathcal{I}$  is the Fisher information. One of the main problems with the Jeffreys' Prior is that it can be improper in the sense that it cannot be normalized to one (although there are ways around this). Improper priors should not be used since it can lead to paradoxes.[1] The Jeffreys' Prior is also sometimes impossible to calculate and is therefore of limited use.

The third school of thought is to choose the prior that has the largest Shannon information entropy that is still consistent with the given testable information. The idea is that entropy is a measure of “uninformativeness” so picking the most ‘uninformative’ prior that is still consistent with testable information would be the best choice. Mathematically, this is the constrained optimization problem:

$$Q = - \int \pi(x) \log\left(\frac{\pi(x)}{m(x)}\right) dx - \lambda C(x) \quad (2.8)$$

where  $p(x)$  is the prior,  $m(x)$  is the Lebesgue measure which ensures invariance under transformation,  $\lambda$  is the Lagrange multiplier, and  $C(x)$  is the constraint function. For example, if we knew the mean of a parameter, using the principle of maximum entropy the best prior would be a Poisson distribution. Likewise, if we knew both the mean and the variance of the parameter the principle would yield a gaussian. The principle of maximum entropy provides a balanced and systematic approach to problem of picking the right prior. It is for these reasons that we will endeavor to apply the principle of maximum entropy whenever possible.

## 2.4 Model Comparison

In a bayesian framework it is possible to compare two competing models to see which one best describes the observed measurements. Let  $\vec{d}$  be some observed data. A model  $M$  has parameters  $\vec{\alpha}$ , with prior  $\pi(\vec{\alpha}|M)$  and likelihood  $\mathcal{L}(\vec{d}|\vec{\alpha}, M)$ . Applying marginalization, the model evidence is defined as:

$$\mathcal{Z}(\vec{d}|M) = \int \mathcal{L}(\vec{d}|\vec{\alpha}, M) \pi(\vec{\alpha}|M) d\vec{\alpha} \quad (2.9)$$

You will notice the above equation is of the same form as Eq. 2.6 with  $M \rightarrow I$ . To compare two models  $M_1$  and  $M_2$  one may compute the ratio of the models evidences, called the Bayes Factor[1]:

$$B(M_1, M_2) = \frac{\mathcal{Z}(\vec{d}|M_1)}{\mathcal{Z}(\vec{d}|M_2)} \quad (2.10)$$

If the Bayes factor is greater than one favor model  $M_1$  and values less than one favor model  $M_2$ . Jefferys[3] gave the following qualitative interpretation of a Bayes factor:

$\mathbf{B}(M_1, M_2)$	Interpretation
$B(M_1, M_2) < .10$	Strong Evidence for $M_2$
$.10 < B(M_1, M_2) < .33$	Moderate Evidence for $M_2$
$.33 < B(M_1, M_2) < 1.0$	Weak Evidence for $M_2$
$1.0 < B(M_1, M_2) < 3.0$	Weak Evidence for $M_1$
$3.0 < B(M_1, M_2) < 10.$	Moderate Evidence for $M_1$
$B(M_1, M_2) > 10.$	Strong Evidence for $M_1$

## 2.5 Combining multiple diagnostics

One of the advantages of bayesian statistics is that it provides a systematic framework for combining data sets from multiple sources. This can be seen from Eq. 2.6. Consider just two data points  $D_1$  and  $D_2$ . Bayes theorem would yield:

$$prob(H|D_1, D_2, I) \propto prob(D_1, D_2|H, I) \times prob(H|I) \quad (2.11)$$

We can use Bayes theorem to express the posterior to be conditional on  $D_1$ .

$$prob(H|D_1, D_2, I) \propto prob(D_2|H, D_1, I) \times prob(H|D_1, I) \quad (2.12)$$

This shows that the prior in Eq. 2.11 can be replaced by the posterior based on  $D_1$ .

If  $D_1$  and  $D_2$  are independent then

$$prob(D_1|H, D_2, I) = prob(D_1|H, I) \quad (2.13)$$

and

$$prob(D_2|H, D_1, I) = prob(D_2|H, I) \quad (2.14)$$

Substituting Eq. 2.14 into Eq. 2.12 and applying Bayes theorem to the prior yields:

$$prob(H|D_1, D_2, I) \propto prob(D_2|H, I) \times prob(D_1|H, I) \times prob(H|I) \quad (2.15)$$

This result can be generalized for  $K$  data points as

$$prob(H|D, I) \propto \left( \prod_{k=0}^K prob(D_k|H, I) \right) \times prob(H|I) \quad (2.16)$$

This result forms the basis for integrated data analysis. So long as all the data is independent from each other, we can assign different likelihoods for each data point. This allows for the data to have different types of errors. For instance, we could combine a diagnostic that is subject to systematic error with a diagnostic whose error is distributed according to a Poisson or Gaussian distribution. Using orthodox methods this could not be done easily, but within a bayesian framework it flows naturally from the basic equations.

Looking more closely at Eq. 2.16 you will notice that each likelihood is dependent on  $H$ . If we put Eq. 2.16 into the notation of Eq. 2.6:

$$\mathcal{P}(\vec{\alpha}|D, I) \propto \left( \prod_{k=0}^K \mathcal{L}(D_k|\vec{\alpha}, I) \right) \times \pi(\vec{\alpha}|I) \quad (2.17)$$

We can easily see that integrated data analysis requires that we have a forward model for each diagnostic that depends on a set of common parameters  $\vec{\alpha}$ . The requirement of a forward model for each diagnostic forces one to formulate a model linking the physics underlying a measurement to the resulting measurement. Mathematically, for  $J$  number of diagnostics:

$$d_j = f_j(\vec{\beta}, \vec{\gamma}_j) \quad (2.18)$$

where  $d_k$  and  $f_j$  is the theoretical measurement and forward model for diagnostic  $j$ , respectively. The vector  $\vec{\beta}$  are the common parameters that are shared between diagnostics. The vector  $\vec{\gamma}_j$  are parameters that are unique to each diagnostic. These are also called *nuisance* parameters since they are of no particular interest but are needed for the forward model. These nuisance parameters mean that we need to modify the definition of the prior in Eq. 2.18 to

$$\pi(\vec{\alpha}|I) = \pi(\vec{\beta}|I) \times \left( \prod_{j=0}^J \pi(\vec{\gamma}_j|I) \right) \quad (2.19)$$

If there are no nuisance parameters for the diagnostics the above equation reduces to the prior of Eq. 2.17.

### 3 Forward modeling of density diagnostics

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### **3.1 Functional form of the density profile**

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### **3.2 Interferometry**

stuff

### **3.3 Reflectometry**

stuff

### **3.4 Thomson scattering**

stuff

### **3.5 Beam emission spectroscopy**

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## **4 Likelihood and prior probabilities**

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### **4.1 Priors**

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#### **4.1.1 Parameter space priors**

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#### **4.1.2 Data space priors**

stuff

### **4.2 Likelihoods**

stuff

#### **4.2.1 Interferometry**

stuff

#### **4.2.2 Reflectometry**

stuff

#### **4.2.3 Thomson scattering**

stuff

#### **4.2.4 Beam emission spectroscopy**

stuff

#### **4.2.5 Combined likelihood probability**

stuff

### **5 Total posterior probability**

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### **5.1 Exploring the posterior**

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### **6 Density profile reconstructions**

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#### **6.1 H-mode reconstruction**

stuff otherstuff

#### **6.2 L-mode reconstruction**

stuff

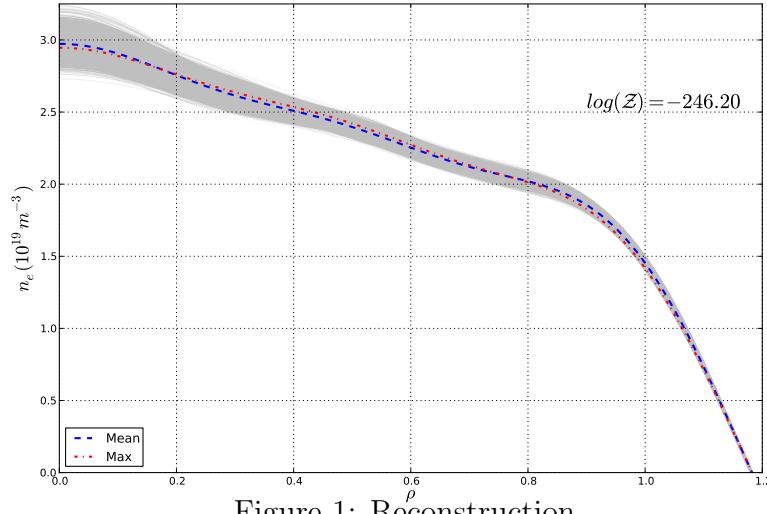


Figure 1: Reconstruction

## 7 Representation of Error

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## 8 Determining discrepant diagnostics

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## 9 Conclusions and future work

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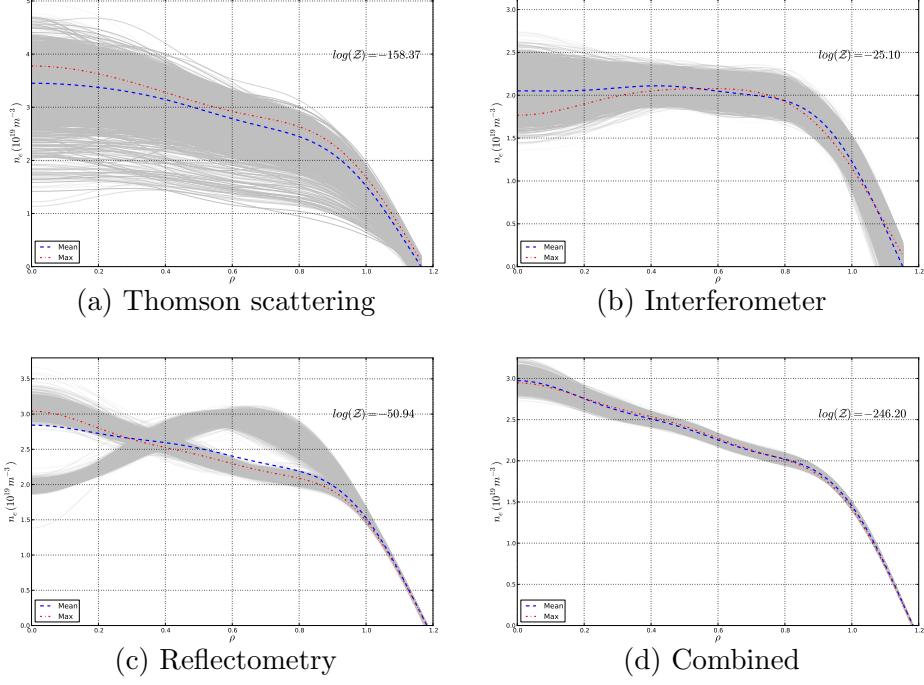


Figure 2: The l-o-n-g caption for all the subfigures (FirstFigure through FourthFigure) goes here.

## References

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- [3] Harold Jeffreys. *Theory of probability*. Oxford University Press, 1998.