Integrated Bayesian Experimental Design

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Abstract. Any scientist planning experiments wants to optimize the design of a future experiment with respect to best performance within the scheduled experimental scenarios. Bayesian Experimental Design (BED) aims to find the optimal design of an experiment by maximizing an expected utility function that quantifies the goals of the experiment. The expectation marginalizes over the uncertain physical parameters of interest, and the possible values of future data. Here we adopt an information-theoretic utility, appropriate when the goal is simply to aquire information efficiently. The goal of the Integrated Bayesian Experimental Design (IBED) concept is to design different, complementary experiments jointly to obtain optimal benefits from the complementary strengths of the constituent experiments. The Bayesian Integrated Data Analysis (IDA) concept of linking interdependent measurements to provide a validated data base and to exploit synergetic effects will be used to design meta-diagnostics. The applications address the design of experiments to diagnose plasmas in a fusion experiment. An example is given by the Thomson scattering (TS) and the interferometry (IF) diagnostics individually, and a set of both. In finding the optimal experimental design for the meta-diagnostic, TS and IF, the strengths of both experiments can be combined to synergistically increase the reliability of results.

Keywords: Bayesian Experimental Design, Integrated Data Analysis, fusion diagnostics

INTRODUCTION

The design of diagnostic experiments for fusion devices is of major concern to meet the requirements for answering the physical questions necessary to design next generation fusion devices. Wendelstein 7–X, presently under construction, will be a magnetic fusion device providing data from complementary and redundant diagnostic measurements. Two of those diagnostics, the Thomson scattering (TS) and the interferometry (IF) diagnostics, will provide complementary but partially redundant information about the plasma density. TS provides spatially and temporally resolved electron temperature T_e and electron densities n_e whereas IF provides line-integrated density measurements with high precision. The combination of both aims at improved local resolution compared to the results from IF alone and improved density precision compared to the results from TS alone. The Integrated Data Analysis (IDA) concept allows to combine data from different experiments to obtain improved results [1]. The synergetic effects obtained by linking interdependent heterogeneous measurements are expected to be increased by linking the design of sets of diagnostics at a very early stage. The concept of Integrated Bayesian Experimental Design (IBED) aims in finding optimal experimental settings for groups of heterogeneous, complementary diagnostics.

Both methods, IDA and IBED, provide useful tools when data of different experiments are interdependent in the sense that they refer to the same quantity of interest. Since the results of Bayesian data analysis are independent of analyzing data jointly or subsequently, IDA and IBED must not be interpreted as extensions to Bayesian analysis. A virtue of doing experimental design in a Bayesian setting is that Bayesian inference is internally consistent. The joint design of multiple experiments pose the same conceptual problem as when one designs a single experiment because the same principles and theory apply. Besides the conceptual simplicity of the Bayesian method, the integration of the analysis of data from interdependent and complementary experiments as well as the integration of their design provide major steps towards a robust and reliable data analysis not only in fusion science. The present applications in fusion science are challenging because they pose a multi-variate and non-linear design problem.

An overview on classical and Bayesian experimental design can be found for example in [2]. In a recent paper we introduced the framework for quantified experimental design of fusion diagnostics and presented an effective way to calculate the cumbersome integrals [3]. The present paper shows the applications of the IBED concept on the design of TS and IF individually, and, ultimately, sketches the experimental design on the combined *meta-diagnostic* (TS+IF).

BAYESIAN EXPERIMENTAL DESIGN

The quantification of the terminology *best performance* cannot be a derived from first principles. It has to consider the benefit of the experimental results with respect to the information yield which allows to answer the interesting scientific question. We want to have experiments which provide small estimation uncertainties as well as experiments which solve physical problems such as deciding about the validity of different physical models. Experimental design is a decision theoretic problem based on optimizing utility functions, $U(D,\eta)$, with respect to design parameters η. The utility function U depends on the data D of a future experiment. Since we want to have an optimal design not only for a single data set but for different experimental scenarios with a variety of measured data we have to optimize the *expected utility function*

$$EU(\eta) = \int dD\, P(D|\eta)\, U(D,\eta). \tag{1}$$

where all relevant future data were marginalized. The marginalization takes care of data D which are uncertain due to statistical and systematical uncertainties, which vary due to lack of knowledge about the behavior of the physical system, and which are subject to changes in the physical scenarios such as parameter scans.

The concept of information theoretic measures using the Shannon information entropy is employed to construct a utility function which measures the information gain provided by an experiment. A measure of information gain is given by the Kullback-Leibler (KL) distance (mutual information, negative information entropy) between the posterior pdf $P(\phi|D,\eta)$ and the prior pdf $P(\phi)$

$$U_{\mathrm{KL}}(D,\eta) = \int d\phi\; P(\phi|D,\eta)\; \log \frac{P(\phi|D,\eta)}{P(\phi)}. \tag{2}$$

Integrating over the parameter space ϕ, the KL distance is a measure of what we can learn from the experimental data D. The KL distance provides an interpretable measure of information gain. The information gain is measured in bits if we use the base-2 logarithm. A simple example showing the dependence of information gain on the precision of measured data can be found in [3].

Using $U_{\mathrm{KL}}(D,\eta)$ and employing Bayes theorem the expected utility (EU) function is

$$EU_{\mathrm{KL}}(\eta) \quad = \quad \iint dD\, d\phi\; P(\phi)\, P(D|\phi,\eta)\, \log \frac{P(D|\phi,\eta)}{P(D|\eta)} \tag{3}$$

where

$$P(D|\eta) = \int d\phi\; P(D|\phi,\eta)\, P(\phi) \tag{4}$$

is the prior predictive value (ppv) (prior predictive probability for the data, marginal likelihood, evidence of the data).

In the theory of BED, the prior distribution $P(\phi)$ encodes all the information available before consideration of the new data. Compared to an inferential problem the prior in BED has to be modified to address the parameter space of interest. Since the prior may extend beyond the useful region of parameter space a restriction of the parameter space allows to select experimental scenarios of interest. To prevent the design process from "wasting effort" on uninteresting parts of parameter space, we truncate the prior to the region of interest, and renormalize it. If, for some parameter values, the distribution is set to zero this does not mean that these parameter values are never expected to be observed but that for these parameter values it is not necessary to have an optimal experimental design. In fusion science, an optimal experiment has to be robust against changes of the experimental scenarios of interest. On the one hand, experimental scenarios often change due to different physical goals and, on the other hand, due to an unexpected behavior of the plasma (this is why we are doing experiments at all). Therefor, a prior in BED should reflect not only the knowledge we have about a parameter in a certain physical situation but, in addition, the prior has to comprise the wide variety of the possible situations. Henceforth, $P(\phi)$ should be interpreted as a renormalized prior which summarizes all parameter values *relevant* for future experimental scenarios of interest. $P(\phi)$ does not depend on the design parameters η.

The likelihood pdf $P(D|\phi,\eta)$ describes the statistics of the data and depends on the design parameters η either via the measurement uncertainty or via the data descriptive model.

An efficient way to calculate the EU is shown in [3]. For given design parameters η we draw a pair of values (D^*,ϕ^*) from the joint distribution $P(D,\phi|\eta)$ by drawing subsequently a set of parameter values from $P(\phi)$ and a data vector from $P(D|\phi^*,\eta)$. $P(D^*|\eta)$ (4) can be calculated by quadrature (for low-dimensional parameter spaces) or by Monte Carlo integration. The author made good experience with the VEGAS algorithm which could be modified for a reasonable first guess for the initial grid ([3] and references therein). Repeating this process and averaging the logarithm of the ratio of the likelihood and the ppv, $\log[P(D|\phi,\eta)/P(D|\eta)]$, provides a Monte Carlo estimate of equation (3).

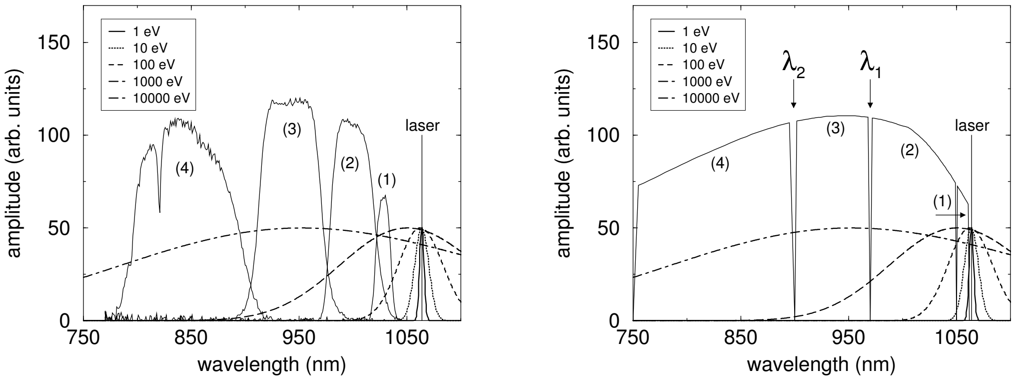

FIGURE 1. 4 spectral filters as a function of the wavelength and 5 different Thomson scattering functions for temperatures $T_{\mathrm{e}} = 1\mathrm{eV} - 10\mathrm{keV}$ (scaled). The left panel shows a typical set of filters used in a previous experiment and the right panel shows the modeled filters for a future experiment. Typical experimental design parameters are given by the two transition wavelengths λ_1 and λ_2.

APPLICATIONS

Our work on experimental design is motivated by the Wendelstein 7-X fusion device which is in its construction phase. The fusion device was designed to study advanced stellarator concepts for a future fusion power plant. The physical scenarios to be studied require elaborate experimental diagnostics capabilities to be designed for best performance under a set of wide plasma parameters. Two of the most important ("level 0") plasma diagnostics are the TS and the IF diagnostics.

Example 1: Thomson Scattering

TS provides spatially and temporally resolved electron temperature T_{e} and electron densities n_{e} profiles by means of laser scattering on electrons in a hot plasma [4]. A simplified version of the future TS experiment has a two-dimensional parameter vector $\phi = (T_{\mathrm{e}}, n_{\mathrm{e}})$. The data, $D = \{D_j\}$, from TS light measurements may be modeled by $D_j = I_j + \varepsilon_j$, where ε_j is a noise term and I_j is the light intensity given by

$$I_j \propto n_{\mathrm{e}} \int \tau_j(\lambda)\, S(\lambda, T_{\mathrm{e}})\, d\lambda. \tag{5}$$

Spectral filters $\tau_j(\lambda), j = 1 \ldots 4$, cut out bands of the scattering function $S(\lambda, T_{\mathrm{e}})$ of the spectral shape of the scattered light of the laser beam. The left panel of Figure 1 shows typical spectral responses of four different filters as a function of the wavelength λ and 5 different scattering functions for temperatures $T_{\mathrm{e}} = 1\mathrm{eV} - 10\mathrm{keV}$. At low temperatures the scattering function is centered at the laser wavelength (1064 nm). For increasing temperatures the scattering function broadens and the center shifts to smaller wavelengths due to relativistic effects. The relative weights of the 4 measured intensities allow to determine T_{e} and their absolute intensities allow to infer n_{e}. The

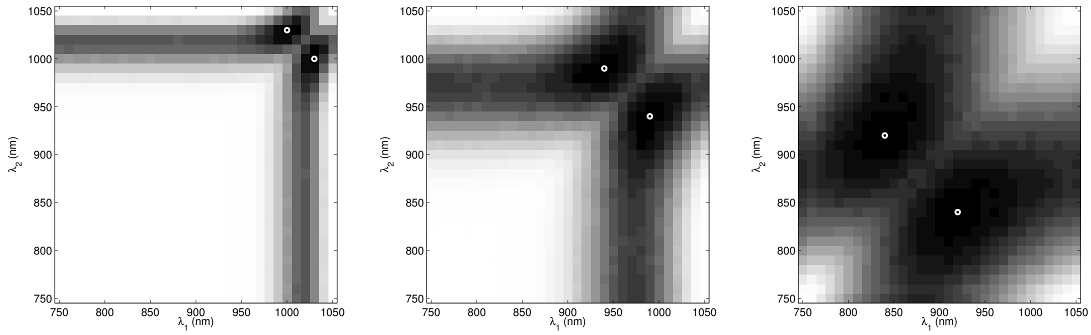

FIGURE 2. Expected utility as a function of filter cutoffs λ_1 and λ_2, and of the parameter range of interest: $T_\mathrm{e} = 0.01 - 0.25$ keV [10.7-11.6 bits] (left); $T_\mathrm{e} = 0.25 - 1$ keV [9.3-11.1 bits] (middle); $T_\mathrm{e} = 1 - 10$ keV [9.0-11.3 bits] (right).

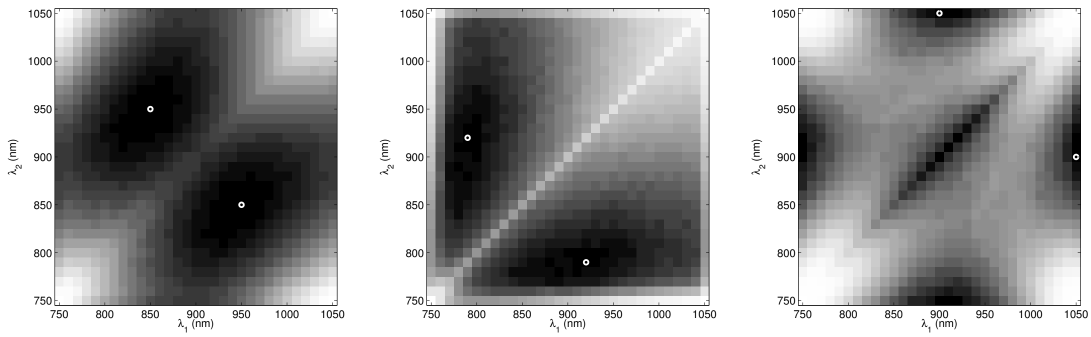

FIGURE 3. Expected utility as a function of filter cutoffs λ_1 and λ_2, and of the statistics of the data ($T_\mathrm{e} = 0.25 - 10$ keV): $\sigma \propto \sqrt{D}$ [10.7-11.6 bits] (left); $\sigma \propto D$ [6.6-9.0 bits] (middle); $\sigma = \mathrm{const}$ [10.8-12.7 bits] (right).

spectral channels close to the laser line provide information about the small temperatures whereas those far from the laser line are necessary for the large temperatures. The right panel of Figure 1 shows the spectral bands of a planned future TS experiment where the spectral bands are modeled with boxes multiplied with a sensitivity curve experimentally calibrated. The filter cutoffs λ_1 and λ_2 are part of the design parameters η and will be discussed in this work. Other design parameters and design criteria were discussed in a previous work [3].

The likelihood is assumed to be Gaussian with variance $\sigma^2 \propto D$, similar to that used for the TS experiments at the fusion device ASDEX Upgrade. Figure 2 shows the EU as a function of the filter cutoffs, $EU(\lambda_1, \lambda_2)$. The left panel depicts the results with a prior pdf $P(T_\mathrm{e} \in [0.01 - 0.25]\ \mathrm{keV}) = \mathrm{const}$ and 0 elsewhere which is close to the situation at the plasma edge where small temperatures are observed. The middle panel shows the result for scenarios $T_\mathrm{e} = 0.25 - 1$ keV and the right panel for $T_\mathrm{e} = 1 - 10$ keV which comprises the interesting parameter values in the plasma center. As expected, the optimal design values depend on the relevant range of the plasma parameter T_e.

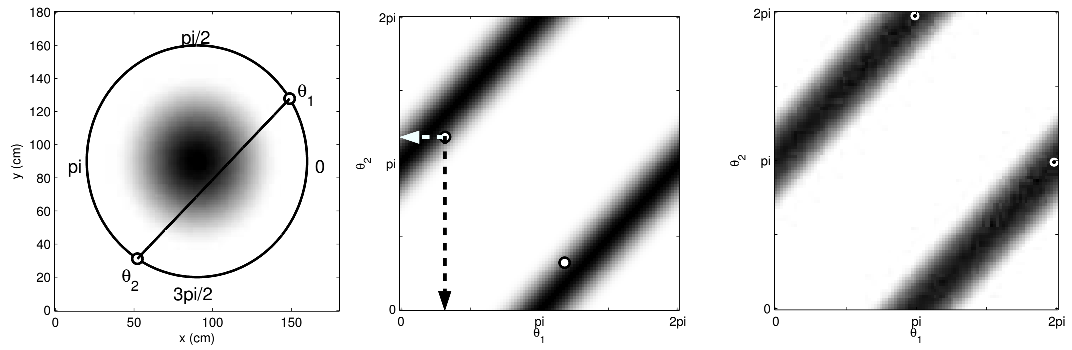

FIGURE 4. Left: 2-dim density distribution with line-of-sight parameterized with the angles θ_1 and θ_2; middle and right: measured phase shift [0-8.4 fringes] and expected utility as a function of θ_1 and θ_2 [0-2.7 bits]; The maximum EU is obtained for every LOS going through the center of the plasma.

The change of the EU as a function of the density interval is of minor importance (not shown here) because the cutoff wavelengths λ_1 and λ_2 are most crucial only for the relative information determining the temperature values. These results help to quantify the usually applied intuitive procedure for TS design. Choosing prior pdfs according to the parameter regimes of most interest we have a sensitive tool to study the performance of the experiment as well as to study the robustness of the design against unexpected scenarios. Extensions to non-uniform prior pdfs are straightforward.

In addition to the dependence of the design on the prior pdfs of the physical parameters, the optimal design depends critically on the statistics of the data. Figure 3 shows EUs for 3 different statistics: $\sigma \propto \sqrt{D}$ (left), $\sigma \propto D$ (middle), and $\sigma = \text{const}$ (right). Since $\sigma \propto \sqrt{D}$ is the most realistic statistic it was chosen as the reference for the previously shown results. The results show clearly that all types of uncertainties deteriorating the measured data have to be critically assessed. A thorough assignment of the likelihood is crucial for finding best performance of the future experiment. At the moment, we are assessing in the very detail the uncertainties involved in the TS experiment at ASDEX Upgrade to obtain a most reliable likelihood for the design of the future TS experiment planned at Wendelstein 7-X. Deviances from the previously shown statistics are expected due to various types of uncertainty sources.

Example 2: Interferometry

IF provides line-integrated density measurements with high precision. The phase shift of a laser beam traversing through a plasma is measured relative to vacuum. The measured phase shift is $D = \Phi + \varepsilon$, where the phase shift Φ is proportional to the wavelength of the laser λ_L and the line integrated plasma density $n_e(r)$,

$$\Phi \propto \lambda_L \int n_e(r)\, dl. \qquad (6)$$

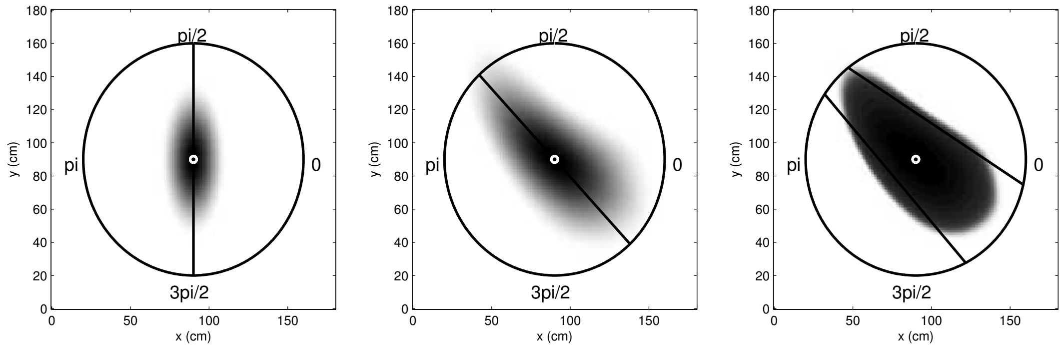

FIGURE 5. 2-dim elliptical (left) and irregular (middle) shape of a parabolic density distribution and a irregular shape with a flat-top and steep gradient at the edge (right). The line-of-sights corresponding to the largest expected utilities are shown.

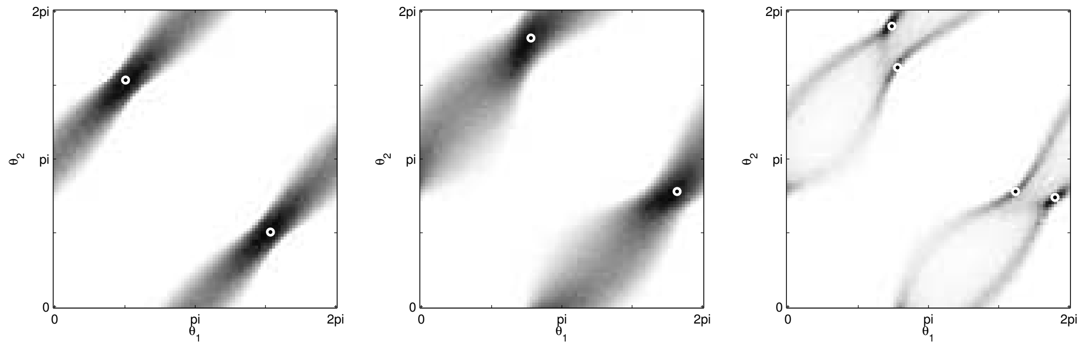

FIGURE 6. Expected utilities as a function of angles θ_1 and θ_2 corresponding to the density profile shapes depicted in Figure 5: [0-2.6 bits] (left), [0-3.2 bits] (middle), [0-1.4 bits] (right).

Design parameters are given by λ_L and the geometrical position of the line-of-sight (LOS) through the plasma. Since the signal-to-noise ratio increases with increasing λ_L, lasers with large wavelengths are preferred as long as deteriorating effects due to beam deflection or vibrations are not annoying. The geometrical positions of the LOSs through the plasma should allow one to invert the line-integrated signal for providing useful information about the density profile. Typically 4-8 LOSs are used to invert the density profile. The left panel of Figure 4 depicts a 2-dimensional parabolic density distribution with a LOS defined by the design parameters θ_1 and θ_2. The parameter of interest ϕ is assumed to be the parabola amplitude. The middle panel shows the measured phase shift as a function of the angles θ_1 and θ_2. LOSs going through the plasma center show the most intense signals. The right panel shows the corresponding EU which increases with the signal-to-noise ratio. There are two symmetries involved: Due to the rotational symmetry of the density profile all designs with $\theta_1 = \theta_2 + \pi(\text{modulo} 2\pi)$ have the same expected utility. The EU is symmetric with respect to swapping θ_1 with θ_2. The likelihood is chosen Gaussian with constant variance.

The plasma of the fusion device W7-X will have various shapes going from triangular over irregular to elliptical shapes. To study the effects of such 2-dim structures Figure 5

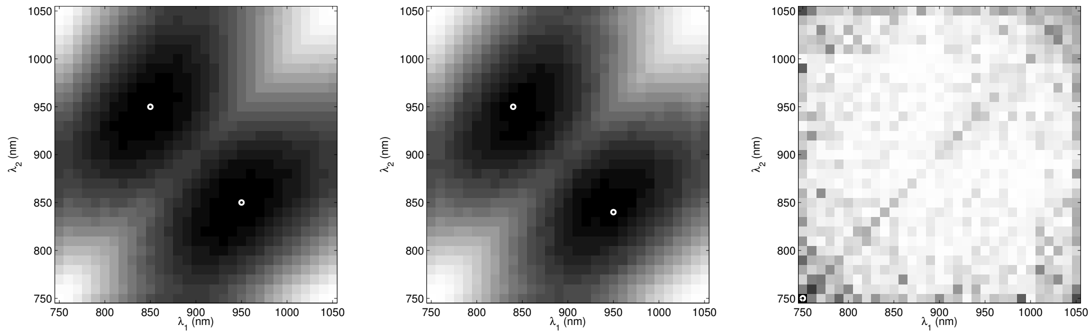

FIGURE 7. Expected utility as a function of filter cutoffs λ_1 and λ_2: TS diagnostic only [9.5-11.7 bits] (left); TS combined with IF diagnostic [19.6-21.5 bits] (middle); TS combined with virtual exact T_e measurement [22.86-22.96 bits] (right);

depicts a 2-dimensional elliptical shape (left) and an irregular shape (middle) both with transformed parabolic density distribution, and an irregular shape with a steep density gradient at the plasma edge (right). For the left and middle profile the parameter of interest ϕ is given by the parabola amplitude and for the right profile it is given by the position of the gradient region.

The corresponding EUs are shown in Figure 6. For the elliptical plasma the largest EU is obtained for a LOS along the long axis (left) similar to the irregular shape with the parabolic profile (middle). The result changes as the density profile becomes flat at the center and steep at the edge. Two local maxima are observed in the EU which belong to the two LOSs tangent to the edges of the plasma. The optimal LOS is no longer going through the center of the plasma. The reason is that the most information about the shape of the profile is obtained at the edges since the profile has its highest variablity here.

As for the TS diagnostic the results depend critically on the statistics of the data. At the moment a test setup is being built to fully assess all uncertainties involved in the IF diagnostic. In the future the positions of a set of 4-8 LOSs will be optimized for reliable reconstruction of density profiles.

INTEGRATED BAYESIAN EXPERIMENTAL DESIGN

Often multiple experiments provide different, complementary information about the phenomenon studied. IBED treats the design of all of the experiments *jointly*, so the complete study optimally benefits from the complementary strengths of the constituent experiments. The combination of the spatially resolving TS diagnostic with the line-integrating very precise IF diagnostic aims at improved local resolution compared to the results from IF alone and improved density precision compared to the results from TS alone. An extensive design of the meta-experiment encompasses 16 (or more) spatial channels of the TS and 4-8 LOSs of the IF diagnostics. First results are shown in Figure 7 where the EU as a function of the TS design parameters λ_1 and λ_2 were shown for three different scenarios: Data of a single spatial channel of the TS diagnostic alone (left), TS data complemented with a very precise measurement of the density n_e (middle) and, alternatively, TS data complemented with a very precise virtual measurement of the temperature T_e (right).

A comparison of the left with the middle panel shows that the design of the TS experiment is robust with respect to additional information provided by the IF experiment since the density information is of minor importance for the cutoff values λ_1 and λ_2. Nevertheless, the EU, and hence the information provided, increases significantly when combining IF data with TS data. In contrast, the right panel shows that a virtual experiment, allowing to determine T_e with high precision, changes the design problem completely. The values of the design parameters can be chosen nearly arbitrarily because the EU is nearly independent on the design variables. T_e is given by the virtual experiment and the density is provided by the overall TS data intensity. In a next step we want to study how the density information from TS influences the design of the IF experiment.

CONCLUSION AND OUTLOOK

The concept of Integrated Bayesian Experimental Design allows one to quantitatively design future experiment or sets of experiments. The design of (meta-)diagnostics depends on the physical scenario of interest and on the statistics of the data. The former one can be varied to study the sensitivity of the design on different or unexpected physical scenarios. The latter one makes it necessary to study in great detail all sources of uncertainties involved in the diagnostics prior to the design of the future experiment.

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