Adaptive scanning – a proposal how to scan theoretical predictions over a multi-dimensional parameter space efficiently

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Abstract

A method is presented to exploit adaptive integration algorithms using importance sampling, like VEGAS, for the task of scanning theoretical predictions depending on a multi-dimensional parameter space. Usually, a parameter scan is performed with emphasis on certain features of a theoretical prediction. Adaptive integration algorithms are well-suited to perform this task very efficiently. Predictions which depend on parameter spaces with many dimensions call for such an adaptive scanning algorithm.

1 Introduction

Most observations in elementary particle physics so far are well described by the Standard Model of particle physics. However, it is widely believed that the Standard Model is only an effective low-energy limit embedded in a larger theory which is not known at present. Extensions of the Standard Model of particle physics usually are equipped with a lot of additional parameters compared to the Standard Model which describe new physics at energy scales not probed so far by experiment. The predictions of promising extensions of the Standard Model for physical observables should be calculated and studied in detail, either to find hints for new physics or to exclude alternative models or, at least, to constrain their parameters.

A way to study such predictions is performing parameter scans. But what exactly is a parameter scan? A parameter scan may be defined as the process of calculating numerical values for a theoretical prediction for a sufficient amount of points in parameter space, such that, sufficient smoothness of the prediction’s dependence on the parameters assumed, a clear understanding of the range of values for the prediction arises. Usually, in this process all other known restrictions on the parameters are taken into account. Thus, only meaningful, i.e. not otherwise excluded, points in parameter space are sampled. In high energy physics the most common goal of a parameter scan over a prediction of an alternative model is to restrict the parameter space of the model by comparison of the prediction with experimental results. Specifically, one wants to find the regions in parameter space where a theoretical prediction for an observable either matches the measured value within error bars, or, if nothing has been observed, respects exclusion limits on possible observables drawn from experiments. This is a typical situation. In practice, of course, things are sometimes more involved.

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Common techniques for parameter scans are sampling a rigid grid of points in parameter space or choosing points at random with a uniform distribution. For the latter sometimes special non-uniform probability functions are used for plotting reasons, e.g. to have the sample points uniformly distributed on a logarithmic scale. But, in the same way as a rigid grid of samples or the naive Monte Carlo approach are not the best options for evaluating numerically multi-dimensional integrals efficiently these parameter scan techniques are not optimal for multi-dimensional parameter spaces. The amount of calculation time needed for a parameter scan may easily get out of hand for parameter spaces with many dimensions, for instance the minimal supersymmetric standard model (MSSM) with general parameters — especially, if time-consuming calculations are necessary already for each sampled parameter point, as for instance in many predictions for hadron colliders.

The basic observation made in this note is that finding regions of interest for a function in a multi-dimensional parameter space and finding a good approximation to the integral of a multi-dimensional function can be attacked by the same method in a very efficient way. That means, essentially, existing algorithms for adaptive integration by importance sampling (implemented e.g. in VEGAS [1]) can also be used to perform an what will here be called “adaptive parameter scan”.

In section 2 a formulation of our proposal is given, furnished in section 3 with a concrete example from the study of an MSSM cross section prediction, and summarized in section 4.

2 Algorithm

By an adaptive parameter scan we mean the task to scan a function $f$, depending on a set of $N$ parameters $(p_1, \ldots, p_N)$, over a hypercube $\{(p_1, \ldots, p_N) | p_i^{\text{min}} \leq p_i \leq p_i^{\text{max}}, i = 1, \ldots, N\}$ in order to find regions of parameter space where some “importance function” $G(f, p_1, \ldots, p_N)$ becomes large. To that end an approximation to the integral

$$I = \int_{p_1^{\text{min}}}^{p_1^{\text{max}}} dp_1 \cdots \int_{p_N^{\text{min}}}^{p_N^{\text{max}}} dp_N G(f(p_1, \ldots, p_N), p_1, \ldots, p_N) \quad (1)$$

is evaluated by an adaptive integration algorithm using importance sampling (e.g. VEGAS) and each point in parameter space is stored during the process. The idea is to choose $G$ in such a way that the (for some specific reasons) preferred values of $f$ (and possibly $p_i$) lead to large values of $G$ and that therefore the parameter regions where $G(f, p_i)$ is large (i.e. where $f$ and possibly the $p_i$ take on preferred values according to the specific reasons which lead to the choice of $G$) are more thoroughly sampled by an adaptive integration algorithm based on importance sampling. Examples are:

- $G(f) = f$ to emphasize regions with large values of $|f|$,  
- or $G(f) = 1/f$ to emphasize regions with small values of $|f|$,  
- or $G(f) = \Theta(-f)f$ to emphasize regions with large $|f|$ but with $f$ negative.

As is well known from adaptive Monte Carlo integration algorithms, any other, more complicated, parameter region can always be embedded in a hypercube with little loss of efficiency.

It should be mentioned that a completely different form of a parameter scan appears in [2] which also makes use of an integration over parameter space.
The end result is a set of points in parameter space which may allow to give meaningful answers to questions like

- "What are the regions of large cross section ?",
- "Where are the regions in parameter space where the observable is small enough to be consistent with present data ?",
- "In what regions of parameter space are the radiative corrections to some observable negative ?".

If there are complicated parameter restrictions to be taken into account the method proves to be very powerful. By setting the importance function zero in disallowed regions and non-zero otherwise, the algorithm can adapt to the allowed region of parameter space. Thus, even if no other feature of the theoretical prediction is emphasized (i.e. $G(f) = 1$ in the allowed region), the algorithm focuses iteratively on the allowed region, which is not the case in the naive Monte Carlo approach.

For the integration of a function by an adaptive Monte Carlo algorithm the approximate value and error of the integral estimate is most important, while the sampled points are essentially of no interest. For adaptive scanning it’s just the opposite. Most interesting are the sampled points, while the approximate value of the estimate and its error are quantities to control the thoroughness of the scan.

3 Example

In order to demonstrate the usefulness of the proposed method we apply it to a concrete physics example based on a previous calculation [3]. Parts of these results have been already presented elsewhere [4]. We want to study the MSSM prediction for the cross section $\sigma$ of the process $e^+e^- \rightarrow H^\pm W^\mp$, where $H^\pm$ denotes a charged Higgs boson and $W^\mp$ a charged electroweak vector boson. For our example we choose a center–of–mass energy $\sqrt{s} = 500$ GeV for the colliding $e^+e^-$ pair, which is typical for a future high energy linear collider, and for the mass of the charged Higgs boson $m_{H^\pm} = 250$ GeV. In this situation the production of charged Higgs pairs would just be kinematically forbidden and the process under study would be one of the relevant production channels for the charged Higgs search at a linear collider of this energy. The cross section of this loop-induced process is rather small. Therefore, it is interesting to scan the MSSM parameter space with an emphasis on regions with comparatively large cross section.

In the following we compare the results of a parameter scan performed in three different ways. For simplicity we scan over a 6-dimensional subset of the MSSM parameter space in the ranges

$$1 \leq \tan \beta \leq 50, \ -2000 \text{GeV} \leq \mu, A_t, A_b \leq 2000 \text{GeV}, \ 50 \text{GeV} \leq M_{Sf.}, M_2 \leq 2000 \text{GeV},$$

where $\tan \beta$ is the ratio of the two Higgs vacuum expectation values in the MSSM, $\mu$ is the supersymmetric Higgs mass term, $A_t$ and $A_b$ are soft-breaking trilinear couplings, $M_{Sf.}$ is a common sfermion mass scale and $M_2$ a common gaugino mass scale. The other two gaugino mass parameters $M_1$ and $M_3$ are fixed by GUT relations. A more detailed description of the parameters and relations can be found in [5], which has been used for the calculation.
Figure 1: Cross section values in picobarn obtained by the three ways of scanning the parameter space plotted on a logarithmic scale versus one scan parameter, (a) \( \tan \beta \), (b) \( M_{Sf.} \), and (c) \( X_t = A_t - \mu / \tan \beta \).

of the cross section together with the computer programs FeynArts and FormCalc [6]. In order to restrict our scan to meaningful combinations of parameters we discard all points in parameter space where experimental bounds on masses of so far undiscovered particles, like Higgs bosons, sfermions and gauginos, are violated, and where corrections to the electroweak rho-parameter by superpartner loop-contributions strongly disagree with the measured value. We choose the bounds listed in [5], which might seem too conservative for a real physics analysis but are sufficient for our demonstration purpose. For all adaptive scans discussed in the following the importance function \( G \) was set to zero for discarded points, thus influencing the adaptive scan.

We perform the parameter scan using

(A) the naive Monte Carlo approach, i.e. just randomly sampling points in the given hypercube,

(B) the adaptive Monte Carlo approach using VEGAS with 11 iterations and 2000 sample points per iteration with the “regular” importance function \( G(\sigma) = \sigma \), i.e. integrating \( \sigma \) over
the hypercube and recording the sampled points,

(C) the adaptive Monte Carlo approach using VEGAS with 12 iterations and 2000 sample points per iteration with the importance function $G(\sigma) = \theta(\sigma - \sigma_0) \cdot \sigma$, where $\sigma_0 = 5 \cdot 10^{-4}$pb and $\theta(x) = 0$ for $x < 0$ and $\theta(x) = 1$ for $x > 0$.

The last approach already uses some knowledge about the range of values $\sigma$ can take on and is a rather radical way to focus on large values of $\sigma$ by disfavoring all regions with $\sigma < 5 \cdot 10^{-4}$pb by setting the importance function to zero there. The VEGAS settings of approaches (B) and (C) are such that the number of valid points is approximately equal (14874 and 15466) and (A) has the same number of points as (C). Thus, the performance of the three methods can be judged easily by comparing Figures 1 and 2. Note that we don’t consider a rigid grid of points. While this might give good results for parameter spaces of low dimensionality, calculation time will blow up like $n^N$, where $n$ is the desired number of sample points per scan parameter and $N$ the number of scan parameters. Already for 10 points per parameter this would require in our example $10^6$ points to calculate.
In the following the results for the three ways of scanning the parameter space are discussed. Figures 1 and 2 show the cross section plotted versus one of the scan parameters on a logarithmic and linear scale, respectively. For brevity we don’t show plots for all scan parameters. As interesting examples we plot the cross section versus \(\tan \beta\) (Figures 1(a) and 2(a)), \(M_{Sf}\) (Figures 1(b) and 1(b)) and versus \(X_t = A_t - \mu / \tan \beta\) (Figures 1(c) and 1(c)). The latter combination of parameters controls the mixing between interaction- and mass-eigenstates in the scalar top sector of the MSSM and is well known to control the size of many quantum effects in the MSSM. Figures 1(a) and 2(a) show that there is a strong dependence on \(\tan \beta\), such that even in the scan results a slope can be guessed, which most of the cross section values follow closely. Comparing the different ways of scanning there is clearly a depletion of points with lower values of \(\sigma\) for the adaptive approaches compared to the naive approach, whereas the enhancement of sampled points with larger \(\sigma\)-values are better seen in Figures 1(b) and 2(b) and (c).

In Figures 1(b) and 2(b) the adaptive scan using the \(\theta\)-function to disfavor lower values of \(\sigma\) (approach (C)) already defines a clear upper boundary of possible \(\sigma\)-values over a wide range in \(M_{Sf}\). Only for \(M_{Sf}\) below \(\approx 300\) GeV more statistics is needed to get a clear boundary.

Figures 1(c) and 2(c) show that the adaptive scans, (B) and (C), resolve the areas of large \(X_t\) that lead to large cross section, which is not the case for the naive approach. The adaptive scans also reveal two areas of large cross section around \(X_t \approx \pm 1000\) GeV which would need more statistics to be clearly resolved. The naive scan, having the same number of points as the other two results, fails to see such detail. These areas of large cross section actually correspond to the large cross section area for low \(M_{Sf}\) in Figures 1(b) and 2(b).

Figure 3 shows the cross section versus the two important parameters \(M_{Sf}\) and \(X_t\). As all three scans have roughly the same number of sampled points, the improvement in finding

\[\text{(3)}\]

There is only one point of large cross section in this area which gives a faint hint of what might be going on in that region of parameter space. One would need a tremendous amount of additional sampled points in order to resolve it with the naive approach.
parameter regions of large cross section for the adaptive scans is obvious. But, it should be mentioned that the results presented here are meant to demonstrate the performance of the different methods. For a physics study the amount of sampled points would be much higher and also a combination of scans with different importance functions is conceivable.

A quantitative view on the performance of the different approaches is given in Figure 4 which shows for each of the three approaches the relative density $D(n, m)$ of sampled points in cross section bins $[m \cdot 10^{-n}, (m + 1) \cdot 10^{-n}]$ picobarn, with $n \in \{3, \ldots, 8\}, m \in \{1, \ldots, 9\}$. $D(n, m)$ is defined as the number of points per bin, $N(n, m)$, normalized to the total number of sampled points,

$$D(n, m) = \frac{N(n, m)}{\sum_{n, m} N(n, m)}.$$  

In the naive approach the density of sampled points is just the distribution of cross section values which emerges for a random choice of parameter values in the given hypercube of scan parameters. The adaptive approaches gain relative densities of sampled points in the large cross section area which are one to two orders of magnitude higher than for the naive approach.

The method of adaptive scanning has been successfully applied in two other analyses [7, 8]. The authors of [8] performed a parameter scan over a 16–dimensional subset of the MSSM parameter space. Encouraged by the results, they even performed a more general, 66–dimensional scan including many more parameters that only indirectly influence their observables, obtaining results consistent with the smaller scan.

4 Summary

We present a new method to perform parameter scans for theoretical predictions: “adaptive scanning”. The method is designed to handle parameter spaces of large dimensionality and is very efficient if there is an emphasis on certain features of the prediction. Furthermore,
in cases where parts of the parameter space are excluded or forbidden by further restrictions our method of scanning can focus adaptively on the allowed region. The scan of a prediction \( f(p_i) \) over (a portion of) a parameter space \( \{p_i\} \) with emphasis on certain features is realized by defining an importance function \( G(f, p_i) \) and sampling adaptively more points in regions where \( G \) is large. This is done by numerically estimating the integral of \( G \) over (a portion of) parameter space with an adaptive Monte Carlo integration algorithm which is based on importance sampling and by recording the sampled points. The method can be straightforwardly implemented as a computer program using VEGAS with a suitable random number generator and a function to be called by VEGAS which calculates the desired function \( G \) and stores the sampled parameter points. The method is modular and flexible: One is free to choose the function \( G \) and it is simple to use different integration algorithms. Any sophistication present in implementations of adaptive integration algorithms, for instance parallelization, may be exploited for our method of parameter scanning. An exemplary FORTRAN code using VEGAS is available from the author upon request.

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