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On the Importance of Confident Error Bands for Extrapolations of σ_{pp}^{tot} to High Energies

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Abstract

Elastic proton-proton scattering is the most simple process in high-energy hadronic interactions. One of the main tasks in this field is to detemine the total proton cross section σ_{pp}^{tot} in order to reproduce experimental data. Total cross sections are known long ago from accelerator experiments in the energy range $\sqrt{s} \leq 1.8$ TeV and in the range $\sqrt{s} = 6-40$ TeV from Extensive Air Shower. In order to know the σ_{pp}^{tot} energy behavior within the accelerator data range and beyond, it is generally proceeded to fit the available set data and also to predict data by extrapolation to high energies. However, if we analize the diverse works existing in the literature about the extrapolation problem, we find in some of them that the uncertainty associated to the σ_{pp}^{tot} prediction points is relatively large or even in other cases the corresponding uncertainties associated to their predictions are not reported. Besides, the disagreement existing between the extrapolated data to high energies from accelerator data and cosmic data, widely discussed in the literature, can be better studied, if prediction methods would offer a confident error interval. The main goal of different methods is to minimize the involved errors to obtain highly precise predictions. In this work we present an alternative prediction method that allows to determine a confident statistical error interval around each of the σ_{pp}^{tot} predicted points. Predictions are developed on the basis of the multiple-diffraction model to estimate σ_{pp}^{tot} in the center of mass range $10-40$ TeV ($10^{17}-10^{18}$ eV *in lab*) which covers both LHC and the highest cosmic ray energies. We conclude that at least in this case the proposed method is not only more precise that the conventionnal χ^2 technique but also more economic from the point of view of calculation time, because the process is based in a unique calculation instead of multiple iterations.

INTRODUCTION

It is experimentally very well known that σ_{pp}^{tot} rises with energy up to 62.7 GeV in the centre-of-mass; later in the 80's such a rising for $\sigma_{\bar{p}p}^{tot}$ was also known when the $S\bar{p}pS$ collider became operational; the Tevatron has confirmed this tendency up to 2 TeV , equivalent to E=10^{15} eV in the laboratory [1], [2], [3], [4], [5]. At the same time the difference $\Delta\sigma = \sigma_{\bar{p}p}^{tot}$ - σ_{pp}^{tot} goes to zero as $s^{-0.57}$ with increasing energy $\sqrt{s}$ [6]. On this basis, and from the fact that it does not affect the goal of this paper, we asume for symplicity that both σ_{pp}^{tot} and $\sigma_{\bar{p}p}^{tot}$ are equal asymptotically. Besides, when no danger of confusion arises, we designate in a generic way σ_{tot} for any of them.

To go to higher energies we have to rely on cosmic rays estimations, which cover the range $\sqrt{s} = 6-40$ TeV in the center of mass [7], [8]. On the other hand, we can estimate the σ^{tot} high energy behaviour beyond the accelerator data range by fitting in a model-dependent way the available data set and then to predict data by extrapolation to higher energies. Actually the extrapolation is based in purely theoretical, empirical or semi-empirical methods widely accepted because it is a useful tool to draw inferences about the σ_{pp}^{tot} energy behavior. The pioneer work was given in [9] with very good results and extended in [10]. However, a careful analysis shows the comparison between the extrapolated data from accelerators and the actual estimations made from cosmic rays to be difficult. The origin lies in the indirect way in which total cross sections are estimated from cosmic rays, nowadays widely discussed in the literature [11], [12]. Depending on the particular assumptions, the values may oscillate by large amounts [13]. The problem could be better studied if prediction methods would offer a confident error interval, because the ability of a statistical method to reproduce data of any physical quantity with high precision gives the pattern for the prediction of out of the range data. Prediction procedures of significant physical quantities represent a useful tool in drawing inferences about the behaviour of the out-of- the range data and so, about the generator events. Theoretical predictions out of the range of a data set involve a certain degree of uncertainty. With the aim of evaluating the confidence of such predictions it is convenient to determine the uncertainty associated to the predictions of the data.

In this context, popular methods generally use the χ^2 technique, based on the minimization of the quadratic sum of data deviations with respect to the employed mathematical model of prediction. In this work we present an alternative prediction method that allows to determine a confident statistical error interval around each of the σ^{tot} predicted points. As an application, predictions are developed on the basis of the multiple-diffraction model to estimate σ^{tot} in the centre of mass range 10-40 TeV ($10^{17}-10^{18}$ eV in lab) which covers both the future LHC accelerator (CERN, Geneva) range and σ^{tot} from cosmic ray data at the highest energies available.

THE STATISTICAL PREDICTION TECHNIQUE

The validity of any statistical method to predict a given physical quantity out of the range values (extrapolation) depends on its precision to reproduce the employed data (interpolation, namely fitting). A fundamental task of any prediction method is to minimize the error band of the predicted set of values. In the specific case of σ^{tot} what is searched is to obtain a prediction beyond the energy range of the employed data with the minimum of dispersion. Instead of the usual χ^2 technique to determine a confident interval around each predicted value, we propose here the use of the *Forecasting technique* [18] as a valid alternative. This method is based on the *multiple linear regresion* theory and consists in determining a prediction equation for a quantity y (dependent variable), that in turns depends on k independent variables (x_i), that is

$$E(y) = \sum_{i=0}^{k} \gamma_i f_i(x_i) \tag{1}$$

(with $f_o(x_o) = 1$) , where f_i are arbitrary functions of x_i, and γ_i are the fitting constants. In the generalized version the variable x_i may depend on other parameters, i.e., $x_i = x_i(s, t, ..)$.

To solve the prediction problem involved in equation (1), the matrix formalism is used. Denoting with Y the matrix of $(n \times 1)$-dimension of the dependent variables and with X the matrix of $[n \times (k + 1)]$-dimension of the k independent variables, the row $x_{11}x_{12}.....x_{1k}$ determines the value y_1 of the dependent variable, the row $x_{21}, x_{22}, ...x_{2k}$ determines the value y_2 and so on. The variables contained in the matrixes X, Y can be related by the matrix equation Y = XB, which is the matrix expression of the prediction equation (1). The $[(k + 1) \times 1]$-dimension matrix B contains the values of the constants γ_i needed to write in explicit form the prediction equation (1) [18] . We then have

$$B = (X^t X)^{-1} X^t Y \tag{2}$$

where X^t denotes the transposed matrix of X and $(X^t X)^{-1}$ denotes the inverse matrix of $X^t X$. As we can see essentially this equation minimizes the quadratic sum of the deviations of points (x_{ij}, y_j) with respect to the prediction equation proposed through equation (1). With those matrixes several statistical estimators are easily determined, such as the Sum of Square Errors (SSE)

$$SSE = Y^t Y - B^t (X^t Y) \tag{3}$$

and the Mean Square Error (S_d^2) given as

$$S_d^2 = \frac{SSE}{[n - (k + 1)]} \tag{4}$$

where the denominator defines the number of degrees of freedom for errors, given by the number of γ_i - parameters. Once these estimators are calculated, we then evaluate the uncertainty band with a $100(1-\delta)\%$ of precision degree considering two cases. First, for fitting (prediction within the range of data) by means of

$$INTB = y \pm t_{\delta/2}^{n-p} \left\{ S_d^2 A^t (X^t X)^{-1} A \right\}^{1/2} \tag{5}$$

Secondly, for extrapolation (prediction out of the data range) with

$$EXTB = y \pm t_{\delta/2}^{n-p} \left\{ S_d^2 \left[1 + A^t \left(X^t X \right)^{-1} A \right] \right\}^{1/2} \tag{6}$$

Here y denotes the central prediction corresponding to the set data included in $X - matrix$, $t_{\{\delta/2\}}^{\{n-p\}}$ denotes Student's {t} -distribution for the n values of the independent variables with p degrees of freedom, and $\delta/2$ denotes the degree of precision. $INTB(+)$, $EXTB(+)$ and $INTB(-)$, $EXTB(-)$ denote the corresponding Upper and Lower bounds respectively. The matrix A denotes the column-matrix of $(k + 1) \times 1$ dimension, which elements $\{1, x_1, x_2, \ldots, x_k\}$ correspond to the numerical values of the γ_i appearing in equation (1). A^t is the transposed matrix of A. In the estimations which follow we have set $\delta/2 = 0.125$ which corresponds to 95% precision.

THE MULTIPLE DIFFRACTION MODEL

Let us now illustrate the use of our statistical prediction method within the context of the problem mentioned in the introduction, i.e., the determination of σ^{tot} at very high energies. Among the different alternatives we choose Glauber's multiple diffraction theory [14] applied to hadron-hadron scattering [15] under the particular approach given in [16]. It has the advantage of using only five parameters: two of them, α and β, associated with the form factor G_N of the nucleon, and three ($C(s)$, a and $\lambda(s)$) associated with the elementary parton-parton amplitude $f(q, s)$. Within this approach σ^{tot} in the Multiple Diffraction Method is determined through the following expression:

$$\sigma_{tot} = 4\pi \int_0^\infty bdb \left\{ 1 - e^{-\Omega(b,s)} cos\left[\lambda\Omega(b, s)\right] \right\} J_0(qb) \tag{7}$$

where b is the impact parameter, $q^2 = -t$ the four-momentum transfer squared among the protons and J_o is the zero-order Bessel function. The critical ingredient is the so-called opacity function $\Omega(b, s)$ given by the equation

$$\Omega(b, s) = \int_0^\infty qdq \; G^2 Imf(q, s).J_0(q, b) \tag{8}$$

An explicit expression is

$$\Omega(b, s) = C\{E_1 k_0(\alpha b) + E_2 k_0(\beta b) + E_3 k_{ei}(ab) + E_4 k_{er}(ab) + b\left[E_5 k_1(\alpha b) + E_6 k_1(\beta b)\right]\} \tag{9}$$

where k_0, k_1, k_{ei}, and k_{er} are the modified Bessel functions, and E_1 to E_6 are functions of the free parameters. This equation was numerically evaluated for nine energies, seven for pp (13.8, 19.4, 23.5, 30.7, 44.7, 52.8, 63.5 GeV) and two for $\bar{p}p$ (546 and 1800 GeV) [17].

THE STATISTICAL ERROR BANDS

The confidence intervals for σ_{tot} are estimated through a two-step process:

In the first place the values of the free parameters of the model were obtained through a detailed analysis of the values of both the differential elastic cross section ($\frac{d\sigma}{dq^2}$) and the ratio of the Real to the Imaginary part of the forward elastic scattering amplitude, $\rho = Ref(q,s)/Imf(q,s)$ and their behaviour with energy, from the ISR to the Tevatron. Two of them, a y β are constant with energy, $a^2 = 8.20$ GeV^2 and $\beta^2 = 1.80$ GeV^2. The whole procedure to obtain the three energy dependent free parameters is described in detail in [21]. A parametric fitting of those free parameters $C(s)$, $\alpha^{-2}(s)$ and $\lambda(s)$ can be expressed with the help of the following analytic expressions

$$C(s) = 19.24521 - 2.86114\ ln(s) + 0.22616\ ln^2(s) \quad (10)$$

$$\alpha^{-2}(s) = 1.8956 - 0.03937\ ln(s) + 0.01301\ ln^2(s) \quad (11)$$

$$\lambda(s) = 0.01686 + 0.00125\left(1 - e^{-ln(s/400)/0.18549}\right) + 0.19775\left(1 - e^{-ln(s/400)/3.74642}\right) \quad (12)$$

$\sqrt{s}$ (GeV)	$C(s)$ (GeV^{-2})	$\alpha^{-2}(s)$ (GeV^{-2})	$\lambda(s)$
13.8	9.9039	2.0945	-0.12816
19.4	10.082	2.1469	-0.02848
23.5	10.225	2.1798	0.00975
30.7	10.474	2.2296	0.04942
44.7	10.923	2.3075	0.08786
52.8	11.159	2.3451	0.10064
62.5	11.421	2.3849	0.11172
546	16.872	3.0634	0.18035
1800	21.518	3.5685	0.19501
14000	32.239	4.6555	0.20703
16000	33.056	4.7359	0.20749
30000	37.102	5.1298	0.20927
40000	39.062	5.3188	0.20993
100000	45.757	5.9568	0.21153

Table 1. Values of $C(s)$, $\alpha^{-2}(s)$ and $\lambda(s)$ from equations (10) - (12) considering experimental values up to 1800 GeV and extrapolating up to 100 TeV.

Table 1 summarizes the results, quoting the values obtained for the model parameters $C(s)$, $\alpha^{-2}(s)$ and $\lambda(s)$ as a function of the energy $\sqrt{s}$. For the following discussion on extrapolation, we have included five supplementary energy points, in addition to the energies at which experimental values are available, which represent the central values at five chosen extrapolation energies: 14, 16, 30, 40 and 100 TeV. In the second step, applying the procedure described through equations (1) - (6), the upper and lower bounds for $C(s)$, $\alpha^{-2}(s)$ and $\beta(s)$ are determined at each one of the energy values. We obtain in this way the upper and lower confidence intervals for each of the three parameters. The results are shown in figures 1, 2 and 3 for $C(s)$, α^{-2} and $\lambda(s)$ respectively. Next, from those previous calculated upper and lower confidence intervals values for $C(s)$, $\alpha^{-2}(s)$ and $\beta(s)$ we determine the corresponding upper and lower confidence intervals for σ_{tot}. Tables 2 and 3 summarize the central, upper and lower σ_{tot} values, to be compared with the experimental values. The final results of the overall procedure are shown in figures 5 and 6.

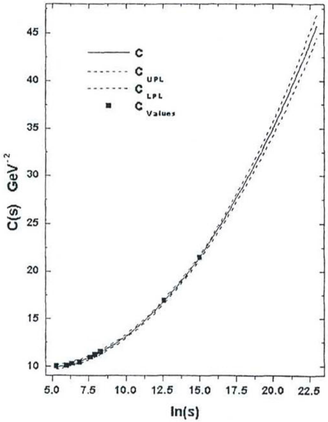

Fig. 1. The parameter $C(s)$ and its confidence interval.

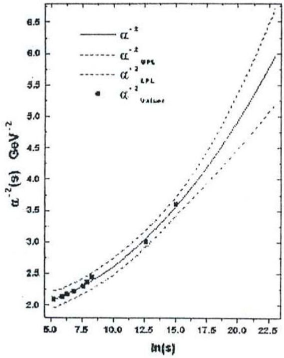

Fig. 2. The parameter $\alpha^{-2}(s)$ and its confidence interval.

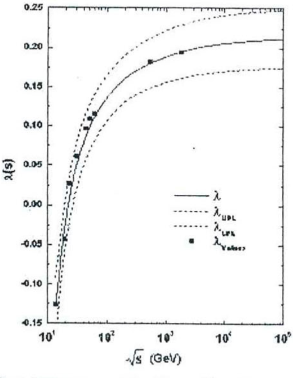

Fig. 3. The parameter $\lambda(s)$ and its confidence interval.

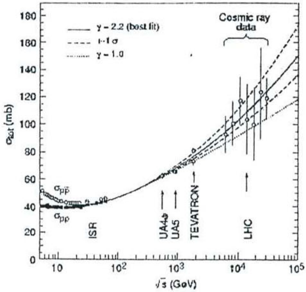

Fig. 4. σ_{exp}^{tot} from accelerator and from cosmic rays. Solid line indicates the best $\chi 546, \rho^2$. The two dashed lines delimitate the region of uncertainty. After [20].

$\sqrt{s}$ (GeV)	σ_{tot} (mb)	σ_{tot}^{upper} (mb)	σ_{tot}^{lower} (mb)	σ_{exp}^{tot} (mb)
13.8	38.30	39.24	37.38	38.36 ± .04
19.4	38.92	39.80	38.05	38.97 ± .04
23.5	39.44	40.32	38.58	38.94 ± .17
30.7	40.37	41.25	39.49	40.14 ± .17
44.7	42.00	42.93	41.08	41.79 ±.16
52.8	42.84	43.79	41.90	42.67 ± .19
62.5	43.77	44.75	42.80	43.32 ± .23
546	61.78	63.11	60.49	61.5 ± 1.5
1800	76.02	78.43	73.68	76. ±1.6
14000	106.51	113.07	99.96	- - -
16000	108.73	115.67	101.79	- - -
30000	119.60	128.43	110.64	- - -
40000	124.74	134.57	114.77	- - -
100000	142.01	155.34	128.28	- - -

Table. 2. Central, upper and lower values for σ_{tot} obtained with the forecasting technique. Experimental values (σ_{exp}^{tot}) are quoted for comparison. Data has been use up to 546 GeV, corresponding to Fig. 5.

$\sqrt{s}$ (GeV)	σ_{tot} (mb)	σ_{tot}^{upper} (mb)	σ_{tot}^{lower} (mb)	σ_{exp}^{tot} (mb)
13.8	38.29	39.35	37.31	38.36 ± .04
19.4	38.92	39.90	37.95	38.97 ± .04
23.5	39.44	40.41	38.48	38.94 ± .17
30.7	40.34	41.33	39.39	40.14 ± .17
44.7	41.93	42.99	40.97	41.79 ±.16
52.8	42.76	43.85	41.78	42.67 ± .19
62.5	43.67	44.80	42.68	43.32 ± .23
546	61.62	63.20	60.68	61.5 ± 1.5
1800	76.17	78.19	75.10	76. ±1.6
14000	108.27	112.99	105.10	- - -
16000	110.67	115.65	107.27	- - -
30000	122.41	128.78	117.79	- - -
40000	128.05	135.13	122.78	- - -
100000	147.14	156.77	139.46	- - -

Table. 3. Central, upper and lower values for σ_{tot} obtained with the forecasting technique. Experimental values (σ_{exp}^{tot}) are quoted for comparison. Data has been use up to 1800 GeV, corresponding to Fig. 6.

DISCUSSION AND CONCLUSIONS

In order to evaluate the quality of the forecasting technique let us compare it with well-known versions of the standard χ^2 method. In Table 4 we quote results of the χ^2 method for two cases: in the first one, a fit to σ^{tot} including data up to 546 GeV [19], which we call χ^2_{546}; in the second one, a more strong version of the same fit, this time fitting simultaneously σ^{tot} and the ρ parameter [20], which we call $\chi^2_{546,\rho}$, again including data up to 546 GeV. We compare their predictions for σ^{tot} at several energies with our predictions which we call F_{546}. The empty spaces in Table 4 are due to the fact that the authors of the fits do not quote values at those energies. As it can be seen, when the extrapolated energy point is the same (data at 14, 16 and 40 TeV), the forecasting errors F_{546} are only half of the χ^2_{546} ones. They are even smaller that the errors obtained with the improved fit $\chi^2_{546,\rho}$. This shows that the forecasting method is, at least in this case, more precise that the classical χ^2. Graphically, the results are represented in Figure 4 for the predictions of the $\chi^2_{546,\rho}$ fit and in Figure 5 for the predictions of the forecasting F_{546}. The inclusion of more experimental points improves obviously the predictions. This is clearly illustrated in Fig. 6, where we have applied the forecasting technique taking into account energies up to 1800 GeV. The error bands are smaller, and the corresponding values are put in Table 4 in the F_{1800} column.

On the other hand, as we emphasized in the description of the method, for its use in a computer the forecasting is much faster than the χ^2 because there is only one iteration to be done. We conclude that the use of the *Forecasting method* in the specific case of σ_{pp}^{tot}, constrains the possible high energy values of σ_{tot} to a narrow band; it may then be employed as a valuable tool in the comparison between the values for σ_{tot} estimated from Cosmic Ray experiments and the extrapolations from accelerator data.

$\sqrt{s}$ (TeV)	χ^2_{546} (mb)	F_{546} (mb)	χ^2_{ρ} (mb)	F_{1800} (mb)
1.8	76.7 ± 4.0	$76.0^{+2.4}_{-2.3}$	76.5 ± 2.3	$76.2^{+2.0}_{-1.0}$
14	112 ± 13	106.5 ± 6.5		$108.3^{+4.7}_{-3.2}$
16		108.7 ± 7.0	111 ± 8.0	$110.7^{+5.0}_{-3.4}$
30		$119.6^{+8.8}_{-9.0}$		$122.4^{+6.4}_{-4.6}$
40		$124.7^{+9.8}_{-10.0}$	130 ± 13	$128.0^{+7.1}_{-5.2}$
100		$142.0^{+13.3}_{-13.7}$		$147.1^{+9.6}_{-7.6}$

Table 4. Comparison of σ_{tot} with the forecasting (F) and the χ^2 techniques. F_{546} and F_{1800} correspond to σ_{tot} evaluated up to 546 and 1800 GeV respectively.

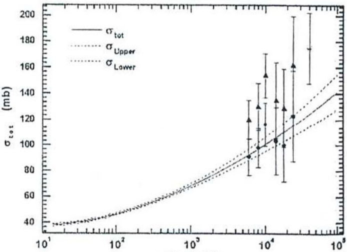

Fig. 5. σ_{tot} from the forecasting technique (solid line) together with the region of uncertainty (dotted lines) using data up to 546 GeV.

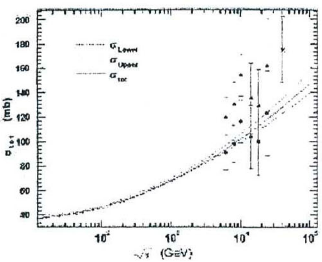

Fig. 6. σ_{tot} from the forecasting techniques (solid line) together with the region of uncertainty (dotted lines) using data up to 1800 GeV.

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