Constrained Least Square Techniques in Fits of QCD Parameters

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10th September 2015

Abstract

The method of constrained least squares is brought to use in the object-oriented data to theory comparison framework Alpos, using the FORTRAN based implementation in Apcalc as well as a newly developed C++ implementation of the method. Reformulations of different definitions of χ^2 functions in the framework of constrained least squares are studied, and the validity is verified by fits of the strong coupling constant with data sets taken at the H1 experiment. A fit of the strong coupling constant is also performed with inclusive jet cross sections measured at the ATLAS detector. First studies on the use the method in fits for parton density functions are performed, where problems concerning the numerical stability of the fit are observed and reported.

Contents

1. Introduction

Quantum Chromodynamics (QCD) is the theory of strong interactions between coloured particles, e.g. quarks and gluons in the standard model, for a review see e.g. [1]. In calculations in the framework of perturbative QCD, the strong coupling constant α_S[1] enters as a free parameter, which needs to be determined by experiments. This is the only free parameter of the perturbative part of QCD, if the masses of particles are considered to be known or negligible. However, the perturbative procedure is only applicable in hard scattering processes with sufficient high energy scale, where quarks and gluons can be considered as free particles. Thus, parton density functions (PDFs) are needed to account for non-perturbative effects in the scattering of hadrons, or the scattering of other particles with hadrons. This makes PDFs an essential ingredient for any prediction at hadron colliders like the Large Hadron Collider (LHC). The PDFs as well as the strong coupling constant are currently only determinable by fits to experimental data. Therefore, fit methods are required to provide estimates for these theory parameters from experiments. Additionally to the widely used least square approach, an alternative constraint least square technique can be considered. This will provide an alternative approach and thus enable double checks for biases in fits, but also allows for a more general fitting method. This report is on the implementation of this method and the application to α_S fits, and first studies on the application in PDF fits. In section two, a particular data set is defined as a reference for the following studies. In section three, the method of constrained least squares is introduced in contrast to the standard least square approach. Afterwards, in section 4, different standard χ^2 definitions are considered, reformulated in the framework of constrained least squares and fits of α_S are performed with these definitions in both approaches. The strong coupling constant is fitted with inclusive jet data taken at the ATLAS detector at energies of $\sqrt{s} = 2.76$ TeV and $\sqrt{s} = 7$ TeV in section 5. Fits to parton density functions are attempted in section 6. The results are summarised in the final section 7.

2. Reference Data

The method described in section 3.2 is applied in fits of the strong coupling constant α_S, in order to validate the method and the implementation as described in section 4 and 5. As a reference the inclusive jet cross section measurement in electron/positron[2]-proton collisions at the H1 [2] experiment is chosen. It provides a useful benchmark model, firstly as the α_S fit result is published and discussed, such that simple comparisons with these published results are possible. Secondly it provides an advanced correlation structure

[1] Throughout this report, quoted values for α_S generally refer to $\alpha_s(M_Z)$, the strong coupling constant at the scale of the mass of the Z boson, although the scale will be suppressed in the notation for convenience reasons.

[2] From here on, the term "electron" will be used to refer to electrons as well as positrons, if not explicitly stated otherwise.

between different sources of uncertainties which is well understood and a statistical covariance matrix, such that the fit method can be tested in a challenging environment.

2.1. Experiment

The H1 is a detector which was taking data from electron-proton collisions at the HERA accelerator. The most important detector components are the tracking system consisting of a silicon tracker (CST) and jet chambers (CJC1 and CJC2). The tracking system is surrounded by a liquid argon sampling calorimeter (LAr) consisting of an electromagnetic and a hadronic part. The return yoke for the 2.76 T magnetic field is equipped with streamer tubes for muon measurements. In the forward direction a lead-fibre calorimeter (SpaCal) is assembled.

The used inclusive jet cross section measurement analysed data taken from 2003 to 2007 at a electron energy of $E_e = 27.6$ GeV and a proton energy of $E_p = 920$ GeV corresponding to an integrated luminosity of 351 pb^{-1}.

2.2. Theory

On parton level, the cross section for inclusive jet production in electron proton scattering can be calculated perturbatively. In the so called Breit frame of reference, where the boson radiated from the electron collides heads on with a parton of the proton, the cross section on parton level can be expressed as

$$\sigma^{\text{parton}} = \sum_{a,n} \alpha_S^n(\mu_r) c_{a,n}(x, \mu_r, \mu_f) \otimes f_a(x, \mu_f) \ , \tag{1}$$

where $c_{a,n}$ are perturbative coefficients to be calculated from Feynman diagrams, f_a is the parton density function for parton a. The parameters μ_r and μ_f denote the renormalisation and factorisation scale. They are chosen to be $\mu_r^2 = (Q^2 + (p_T^{\text{jet}})^2)/2$ and $\mu_f^2 = Q^2$ with Q^2 denoting the negative square of the exchanged four momentum and p_T the transverse jet momentum. Corrections have to be applied to take into account non perturbative hadronisation effects and electroweak corrections. Both are parametrised by bin-wise factors c_i^{had}, c_i^{ew} and used to calculate the cross section in each bin i as

$$\sigma_i^{\text{hadron}} = \sigma_i^{\text{parton}} c_i^{\text{had}} c_i^{\text{ew}} \tag{2}$$

The perturbative coefficients are determined at NLO using predictions from NLOJet++ [3] interfaced to fastNLO [4] [5]. The PDF set MSTW2008nlo [6] [7], which was determined at a value of the strong coupling of $\alpha_S = 0.118$, is used.

3. The Method of Constrained Least Squares

It is a common problem to find the set of parameters of a theory which best fits some measured data. Two methods designed to solve this problem, referred to as "standard least square" and "constrained least square", are described here. Both are based on the minimisation of some expression χ^2, but differ in the construction of this expression, and in the implementation of the connection of data and theory.

3.1. Standard Least Squares

The "standard least squares" shall name the widely used approach to construct residuals of every measured data point y_i as

$$r_i = y_i - f_i(a_j) \tag{3}$$

where f_i denotes the theory prediction fir y_i in terms of a set of parameters a_i. The χ^2 expression is defined as the weighted sum over the residuals squared:

$$\chi^2 = \sum_{ij} r_i W_{ij} r_j \tag{4}$$

with some weight matrix W_{ij} which can be chosen to be the inverse of the co-variance matrix of the data points $W_{ij} = V_{ij}^{-1}$. With this weight, the case of uncorrelated data reduces to

$$\chi^2 = \sum_i \frac{r_i^2}{\sigma_i^2} \tag{5}$$

with the uncertainty σ_i of the data point y_i. More advanced definitions of χ^2 expressions are described in chapter 5.

3.2. Constrained Least Squares

The method of "constrained least squares" is an alternative approach to the one discussed above [8]. For every measured data point $y_{i,0}$ a correction is calculated by

$$\Delta y_i = y_i - y_{0,i} \tag{6}$$

where y_i is the "true" value according to the fitted model. The weighted sum over these corrections,

$$\chi^2 = \sum_{ij} \Delta y_i W_{ij} \Delta y_j \tag{7}$$

is minimised with respect to the corrections Δy_i, but this time subject to some constraints F_i, which are functions of the corrected data points and the current values of parameters,

$$F_i = F_i(y_j + \Delta y_j, a_j + \Delta a_j) \tag{8}$$

where a_j in this case denotes the initial value of the parameters. Of course again a natural choice for the weights is $W_{ij} = V_{ij}^{-1}$. The actual form of the constraints can vary, as they may also impose some physical constraint like conservation laws, normalisation rules or known geometric properties of the measured data. However, in the case where they are only used to realise the connection of a data point to its respective theory prediction, they can be formulated as

$$F_i = y_i - f_i(\hat{a}_j) = y_{i,0} + \Delta y_i - f_i(a_j + \Delta a_j) \tag{9}$$

Other formulations and the translation of more advanced standard χ^2 definitions are as well discussed in chapter 5

4. Implementation

The method of constrained least squares is implemented in the `FORTRAN` based program `Apcalc` [9]. The essential functionality is re-implemented in `C++`. Both methods are used in the `Alpos` [10] data to theory comparison framework.

4.1. Alpos

The `C++` based `Alpos` framework is used to interface theory predictions with measured data and uncertainties. User code may implement additional

- Datasets, providing data and uncertainties for a new measurement.
- Functions, providing necessary tools for theory predictions.
- Tasks, providing tools to access and modify theory parameters.

Two `tasks` were implemented

- `AApcFitter` featuring the `FORTRAN` code from `Apcalc`.
- `AConstLQFitter` featuring the new `C++` implementation of the constrained least square method.

4.2. Using Apcalc in Alpos

The `Apcalc` program is used in the `AApcFitter` task in `Alpos`. Different calculations for constraints are implemented as discussed in section 5. The functions `apc`, `apcres`, `apcpul` and `apccova` from `Apcalc` are used to provide the basic derivative calculation and solving of the linear equation, print out of results, calculation of pulls and co-variance matrix, respectively.

4.3. Implementation of the method and use in Alpos

The basic functionality of the `Apcalc` program was re-implemented in `C++` using the `Eigen` library [11]. The provided class `Apccpp` has to be initialised with a vector containing all measured values and starting values as parameters. By convention, slightly different to `Apcalc`, the unmeasured parameters have to be given as the last entries in the vector, and the later provided co-variance matrix of size $m \times m$ will be considered as the co-variance matrix for the first m entries of X. The main function to be used by the user is `bApcpp`, which is used in a similar way as `APC` in `apcalc`:

```
Apccpp Example(evX);
do {
   VectorXd evNewX =  Example.evGetX();  // get corrected X
   VectorXd evF = Constraint(evNewX);    // user defined code for constraint
} while(Example.bApcpp(evF, emV));
```

where the above code corresponds to one iteration. The function `bApcpp` will return `true` as long as more evaluations of F are needed to calculate the derivative. The derivative with respect to the i-th entry of X is calculated by varying the value of this entry to positive and negative direction and calculating the difference of the constraints at these two values. Thus, two evaluations of F are needed per entry in X. When all derivatives are calculated, the function `bSolveEquation` is used, which determines the matrix

$$M = \begin{pmatrix} -V & 0 & V^T A_m^T \\ 0 & 0 & A_{um}^T \\ A_m V & A_{um} & -A_m V A_m^T \end{pmatrix} \tag{10}$$

where A_m denotes the derivative matrix of the constraints with respect to measured values, and A_{um} the derivative matrix with respect to unmeasured values, e.g. parameters. This matrix is used to calculate the inverse of the matrix

$$L = \begin{pmatrix} V^{-1} & 0 & A_m^T \\ 0 & 0 & A_{um}^T \\ A_m & A_{um} & 0 \end{pmatrix} \tag{11}$$

and thus solving the system of linear equations

$$\begin{pmatrix} V^{-1} & 0 & A_m^T \\ 0 & 0 & A_{um}^T \\ A_m & A_{um} & 0 \end{pmatrix} \begin{pmatrix} \Delta\vec{y}_m \\ \Delta\vec{y}_{um} \\ \vec{\lambda} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -\vec{C}(\vec{y_0}) \end{pmatrix} \tag{12}$$

making use of the fact that V is usually known rather than V^{-1}. The inverse is found by the exchange algorithm, for example described in [12]. It is implemented in the function `emInvertMatrix(MatrixXd emV, int iN)` which inverts the matrix, assuming that the necessary steps have already been applied to the top left $iN \times iN$ matrix. Solving this system of equations corresponds to finding the constrained minimum as described in section 3 for a linear constraint. If n measured values and parameters were provided, the top left $n \times n$ part of the inverse of the matrix L corresponds to the co-variance matrix of the fitted values, such that this is available right after the inversion. In the case of a nonlinear constraint this procedure should be repeated iteratively. There function `bIsFinished` can be used to check for convergence, it will be `true` if the change in χ^2 and the average absolute value of the constraints were sufficient small after the last iteration, or if the maximum number of iterations is reached. The latter should be interpreted as non-convergence of the fit, `bIsConverged` can be used to check for convergence without considering the number of iterations. This implementation is used in the `AConstLQFitter` task in `Alpos`.

5. Definitions of χ^2 and Constraints

Various definitions of χ^2 expressions are possible, realising different assumptions on statistical properties of the measured uncertainties. First the concept of nuisance parameters is introduced for the treatment of correlated systematic uncertainties, and its realisation in the used framework is sketched. Afterwards, different χ^2 definitions are considered together with their equivalent in terms of constrained least squares. Numerical values for standard least square fits using `Minuit`[3] [14] are compared to the result of the constrained least square fit.

5.1. Nuisance Parameters

Correlated systematic uncertainties can be treated by the inclusion of an additional parameter b_j for every systematic uncertainty j, which is taken to be measured to be 0 with uncertainty 1. Let the effect of this systematic on the data point i be given by Γ_j^i as absolute value, or by $\gamma_j^i = \Gamma_j^i / y_{0,i}$, where $y_{0,i}$ denotes the measured value of the data point i. Note that, given a concrete model of the uncertainty, one or both of these values might not ultimately characterise the distribution of the uncertainty and are only meant to represent a numerical value. There are different ways to parametrise the effect of these systematic uncertainties in the fit. In any case, a shift is applied to the theory prediction t_i corresponding to the data point i. This shift can be parametrised in the following ways

- A Additive, $t_i \to t_i + b_j \Gamma_j^i$
- M Multiplicative, $t_i \to t_i \exp b_j \gamma_j^i$
- Approximately multiplicative, $t_i \to t_i(1 + b_j \gamma_j^i)$

When combining several systematic uncertainties with different treatments, one needs to decide in which order to add and multiply different shifts. For the constrained least square fits, there are two ways implemented to add systematic uncertainties:

A adding <u>after</u> multiplying with all multiplicative systematic uncertainties

[3]The `TMinuit` implementation in `ROOT` [13] is used.

MA adding before multiplying with all multiplicative systematic uncertainties

If all systematic uncertainties are additive, both ways are equivalent. Alternative, all systematic uncertainties can be treated approximately multiplicative.

5.2. Simple χ^2

The simplest approach is to define

$$\chi^2 = \sum_{ij} (d_i - t_i) V_{ij}^{-1} (d_i - t_i) \tag{13}$$

with measured data values d_i and theory predictions in terms of the free parameters t_i. This notation will be kept throughout the report. The matrix V_{ij} in this case is the absolute co-variance matrix of the measured values, which implicitly assumes a normal distribution of the uncertainties. This corresponds to take constraints

$$F_i = d_i - t_i \tag{14}$$

for the constrained least square approach and using the full co-variance matrix as weight matrix.

5.3. Log Normal based χ^2

A modified version of the simplest χ^2 expression introduced above is introduced in reference [2] and reads

$$\chi^2 = \sum_{ij} (\log(d_i) - \log(t_i)) V_{ij}^{-1} (\log(d_i) - \log(t_i)) \ , \tag{15}$$

treating the uncertainties as log-normal distributed instead of normal as in the previous section. The matrix V in this case contains the relative uncertainties rather than absolute ones. The corresponding constraint can be formulated by taking $d_i \to \hat{d}_i = \log(d_i)$ and set the constraint to

$$F_i = \hat{d}_i - \log(t_i) \tag{16}$$

The weight matrix again is taken to be the matrix containing relative co-variances. Nuisance parameters can be included, in the case where all systematic uncertainties are treated as multiplicative, the full χ^2 definition used in [2] is recovered. For this case, a fit to inclusive jet data at the H1 experiment was performed using `Minuit` for the standard least square fit, and compared to the result of the constrained leas square fit which are presented in table 2. Both methods agree well on the value of α_S as well as of the nuisance parameters and uncertainties, and reproduce the result of [2].

5.4. χ^2 with variable variance

A χ^2 definition motivated by the ones used in references [15] and [16] reads

$$\chi^2 = \sum_i \frac{[t_i(1 - \sum_j \gamma^i_j b_j) - d_i]^2}{\delta^2_{\text{stat},i} d_i t_i + \delta^2_{\text{uncorr},i} t_i^2} + \sum_j b_j^2 \tag{17}$$

which already includes nuisance parameters according to the approximate multiplicative parametrisation. As previously, γ^i_j denotes the relative systematic uncertainty. The $\delta_{\text{stat},i}$ and $\delta_{\text{uncorr},i}$ denote statistical (Poisson like) and uncorrelated relative uncertainties. Their different behaviour is accounted for by the different calculation of their contribution to the absolute co-variance matrix from the respective relative uncertainties. Note that the shift due to systematic uncertainties is not included in the denominator, which is considered the default behaviour.

It is not possible to dynamically change the definition of V in the constrained least square framework, however a similar setup can be considered. First, the constraints are taken to be

$$F_i = t_i(1 - \sum_j \gamma^i_j b_j) - d_i \tag{18}$$

which also already includes the parametrisation of the systematic uncertainties according to the approximate multiplicative prescription. The behaviour of the denominator is accounted for by taking V to be a diagonal matrix with diagonal elements

$$V_{ii} = \delta^2_{\text{stat},i} d_i t_i + \delta^2_{\text{uncorr},i} t_i^2 \tag{19}$$

and updating this after every iteration with the fitted theory parameters, but with the initial provided data.

6. Fit for α_S using ATLAS inclusive jet data

Another α_S fit is performed using cross sections of inclusive jet production in proton-proton collisions at the LHC. It is again performed in the standard least square and the constrained least square framework and the results are compared with each other and with the world average.

6.1. Data

Inclusive jet cross sections measurements at the ATLAS detector at two different values of the centre of mass energy $\sqrt{s}$ of the protons are used. The measurement at $\sqrt{s} = 2.76$ TeV [17] was performed in 2011 with an integrated luminosity of 0.2 pb^{-1}. The second used measurement used data taken in 2011, corresponding to 37 pb^{-1}, at $\sqrt{s} = 7$ TeV [18]. Both measurements used the same detector calibration, such that the corresponding systematic uncertainties are correlated between them.

6.2. Theory

Cross sections for inclusive jet production in proton-proton collisions can be determined in a similar way as described in section 2.2. Equation (1) for the cross section at parton level is replaced by

$$\sigma = \sum_{n,i,j} \alpha_S^n(\mu_r) f_{1,i}(x,\mu_f) \otimes f_{2,j}(x,\mu_f) \otimes c_{i,j,n}(x,\mu_r,\mu_f) \ , \tag{20}$$

where $c_{i,j,n}$ perturbative factors and f_1 and f_2 denote the PDFs for the respective protons. The coefficients are again determined at NLO in the fastNLO framework, and the MSTW2008nlo PDF set determined at $\alpha_S = 0.118$ is used. The renormalisation and factorisation scales are set to be equal to the transverse jet momentum, $\mu_r = \mu_f = p_T^{\text{jet}}$.

6.3. Fit

The fit is performed with the standard least square approach using `Minuit`, and in the constrained least square framework. The log normal based χ^2 described in section 5.3 is used including nuisance parameters. Results for α_S are presented in table 1. They agree well with each other, and are compatible with the world average of $\alpha_S = 0.1185 \pm 0.0006$ published in [1] The distributions of the nuisance parameters for the two separate measurements and for the combined fit are shown in figures 1, 2 and 3. They are expected be symmetrically distributed with mean value 0, which is roughly the observed behaviour.

Table 1: Results of the α_S fits to inclusive cross section measurements at the ATLAS experiment [17] [18], for the constrained least square approach and the standard least square approach using `Minuit`, both with the log normal based prescription with nuisance parameters. Shown are fitted values of α_S with uncertainties, and the final χ^2/n_{df} value.

Data	Constr. Lq.	χ^2/n_{df}	Minuit	χ^2/n_{df}
2.76 TeV	0.12211 ± 0.00323	1.0510	0.12211 ± 0.00324	1.0507
7 TeV	0.11670 ± 0.00228	0.5563	0.11670 ± 0.00229	0.5563
combined	0.12086 ± 0.00181	1.0501	0.12086 ± 0.00181	1.0501

7. Fits to Parameters of Parton Density Functions

After the method is implemented and the equivalence of χ^2 definitions and constraints is validated, it is attempted to apply the method of constrained least squares to fits of parameters of parton density functions (PDF). This would enable to make use of the possibility to naturally include physical requirements into the fit by means of additional constraints implementing the sum rules. A review on sum rules can be found at [19]

7.1. Parametrisation

The PDF is parametrised at the starting scale $Q_0^2 = 1.9$ GeV^2. The values at higher scales are calculated using the `QCDNUM` program [20]. The parametrisation of the PDF used is introduced in reference [21], and is therefore referred to as "HERAPDF parametrisation". The functions are defined as

$$xg(x) = A_g x^{B_g}(1-x)^{C_g} \tag{21}$$

$$xu_v(x) = A_{u_v} x^{B_{u_v}}(1-x)^{C_{u_v}}(1+E_{u_v}x^2) \tag{22}$$

$$xd_v(x) = A_{d_v} x^{B_{d_v}}(1-x)^{C_{d_v}} \tag{23}$$

$$x\bar{U}(x) = A_{\bar{U}} x^{B_{\bar{U}}}(1-x)^{C_{\bar{U}}} \tag{24}$$

$$x\bar{D}(x) = A_{\bar{D}} x^{B_{\bar{D}}}(1-x)^{C_{\bar{D}}} \tag{25}$$

which respectively parametrise the gluon distribution, the u and d valence quark distribution and the u-type and d-type anti quark distribution. The parameter $B_{\bar{U}}$ is set equal to $B_{\bar{D}}$ and B_{u_v} equal to B_{d_v}. Further, A_g, A_{u_v}, $A_{\bar{u}}$ and A_{d_v} are determined by sum rules and physical considerations, leaving in total 10 parameters for the fit.

7.2. Data

For the PDF fit, data from deep inelastic scattering in electron/positron-proton collisions taken at the H1 and the ZEUS experiments [21] is used. Both detectors were taking data at the HERA accelerator between 1994-2000.

7.3. Fit with `Minuit`

The fit is first done in the framework of standard least squares in `Minuit`, using the HERAFitter style χ^2 prescription. It yields the result presented in table 3.

7.4. Constrained Least Square Fit

The constrained least square fit for the same parametrisation was attempted, but no numerical stable result was found. Possible reasons are discussed in the following:

- Correlations between different parameters. Table 4 shows the correlations between parameters and global correlations as obtained by the standard least square fit with `Minuit`. It can be seen that some parameters are highly correlated, which may cause problems for the used method and the applied iterative procedure for non-linear constraints.

- Insufficient accuracy in underlying calculations. Another possibility is that the calculation of the PDF at higher scales than Q_0 is not sufficient accurate to allow for a precise derivative calculation by the method used in `Apcalc`.

8. Conclusion

The constrained least square method was implemented in the `Alpos` framework, and was used to successfully reproduce published fits of the strong coupling constant α_S and agrees with results of standard least square. Different χ^2 definitions can be reformulated as fitting procedures in the constrained least square framework. Fits of α_S are also performed for inclusive jet cross section measurements at the ATLAS detector. Again agreement between the two methods is found, and values of α_S are obtained which are compatible with the current world average. The attempted fit of the PDF parameters failed to find a stable solution. Possible reasons might be insufficient accuracy in underlying calculations spoiling the derivative calculation or high correlations between parameters.

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A. Tables

Table 2: Results of the α_S fits to inclusive cross section measurements at the H1 experiment [2], for the constrained least square approach and the standard least square approach using `Minuit`, both with the log normal based prescription. Shown are fitted values for nuisance parameters and α_S with uncertainties, and the final χ^2 value, where the number of degrees of freedom is $N_{df} = 23$.

Parameter	Constr. Lq	uncert.	Minuit (Lq)	uncert.
Ee1	−0.118574	0.989151	−0.118398	0.989156
Ee2	0.164451	0.973625	0.163633	0.973634
Ee3	0.130504	0.96193	0.130967	0.961934
Ee4	−0.548446	0.942674	−0.548347	0.942675
Ee5	0.15678	0.986295	0.156297	0.986295
Ee6	0.033113	0.998928	0.0333391	0.998928
IDe1	0.156884	0.986565	0.156834	0.986572
IDe2	−0.0945082	0.987231	−0.0934895	0.987236
IDe3	−0.109699	0.988528	−0.110129	0.988529
IDe4	0.170533	0.991857	0.170156	0.991857
IDe5	−0.379062	0.930441	−0.379606	0.930441
IDe6	−0.00120012	0.976528	-5.08426×10^{-05}	0.976528
JES	−0.839874	0.835335	−0.837921	0.835432
LArN	−0.0387863	0.998956	−0.038135	0.99899
Lumi	−0.193932	0.97356	−0.195303	0.974438
Mod1	0.577884	0.907091	0.57753	0.907105
Mod2	0.264247	0.920891	0.264944	0.920892
Mod3	−0.0514873	0.933844	−0.0521898	0.93385
Mod4	0.721486	0.924786	0.72196	0.924787
Mod5	−0.46755	0.939925	−0.467944	0.939926
Mod6	0.201529	0.900293	0.201099	0.900293
RCES	0.013186	0.986554	0.0128818	0.986617
ThE1	−0.0461547	0.994451	−0.0460038	0.994454
ThE2	0.0777942	0.992977	0.0768791	0.992979
ThE3	0.0284282	0.996139	0.0286272	0.996139
ThE4	−0.108905	0.998369	−0.108811	0.998369
ThE5	0.0828137	0.985539	0.0821319	0.98554
ThE6	0.0110961	0.998206	0.0107733	0.998206
TrCl	−0.0775727	0.995817	−0.0722268	0.995954
Trig	−0.0930872	0.993971	−0.0968922	0.994169
α_S	0.117389	0.00222235	0.117388	0.00222624
χ^2	24.7464		24.7465	

Table 3: Fitted values of pdf parameters for fit with `Minuit` to data published in [21].

Parameter	Fitted Value	Uncertainty
B_g	0.315859	0.0323106
C_g	9.41796	0.687771
B_{u_v}	0.706674	0.0183122
C_{u_v}	5.12833	0.240229
E_{u_v}	10.5675	2.22162
C_{d_v}	4.58529	0.372283
$C_{\bar{U}}$	1.33633	0.190079
$A_{\bar{D}}$	0.113807	0.00385015
$B_{\bar{D}}$	-0.213225	0.00462787
$C_{\bar{D}}$	2.83034	0.748938

Table 4: Correlations between PDF parameters from fit with `Minuit` to data published in [21].

	Global	B_g	C_g	B_{u_v}	C_{u_v}	E_{u_v}	C_{d_v}	$C_{\bar{U}}$	$A_{\bar{D}}$	$B_{\bar{D}}$	$C_{\bar{D}}$
B_g	0.99620	1.000	0.920	0.708	−0.187	−0.400	0.183	0.098	−0.610	−0.711	−0.332
C_g	0.99818	0.920	1.000	0.694	−0.198	−0.445	0.329	0.103	−0.522	−0.576	−0.589
B_{u_v}	0.99548	0.708	0.694	1.000	−0.473	−0.709	0.025	0.401	−0.325	−0.393	−0.075
C_{u_v}	0.99808	−0.187	−0.198	−0.473	1.000	0.923	0.132	−0.743	−0.350	−0.258	−0.084
E_{u_v}	0.99817	−0.400	−0.445	−0.709	0.923	1.000	0.061	−0.617	−0.093	−0.016	0.059
C_{d_v}	0.98893	0.183	0.329	0.025	0.132	0.061	1.000	−0.170	−0.333	−0.279	−0.792
$C_{\bar{U}}$	0.98701	0.098	0.103	0.401	−0.743	−0.617	−0.170	1.000	0.554	0.439	0.056
$A_{\bar{D}}$	0.99191	−0.610	−0.522	−0.325	−0.350	−0.093	−0.333	0.554	1.000	0.968	0.256
$B_{\bar{D}}$	0.99443	−0.711	−0.576	−0.393	−0.258	−0.016	−0.279	0.439	0.968	1.000	0.228
$C_{\bar{D}}$	0.99688	−0.332	−0.589	−0.075	−0.084	0.059	−0.792	0.056	0.256	0.228	1.000

B. Figures

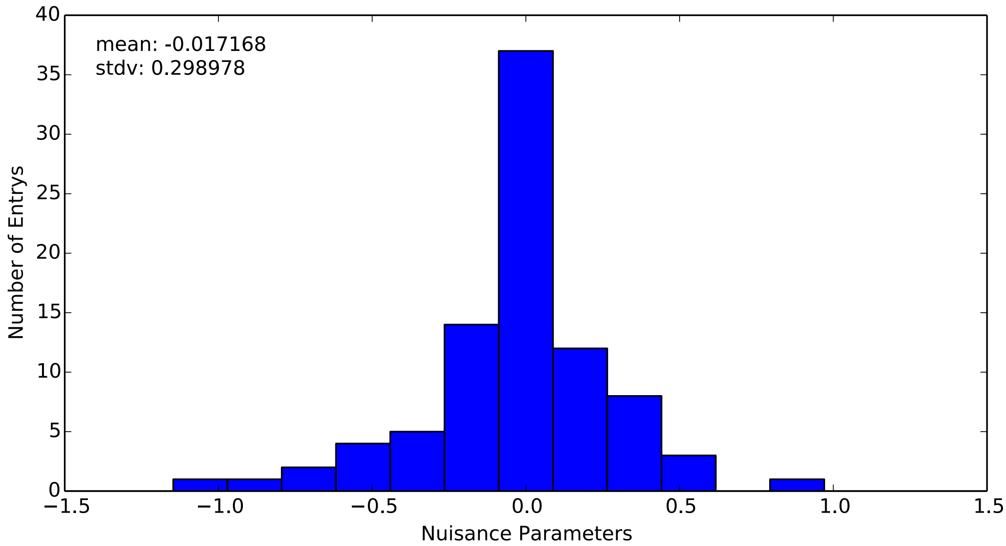

Figure 1: Distribution of nuisance parameters for inclusive jet data measured with the ATLAS detector at a centre of mass energy of the proton-proton system of $\sqrt{s} = 2.76$ TeV [17], obtained with the constrained least square fit described in section 6.

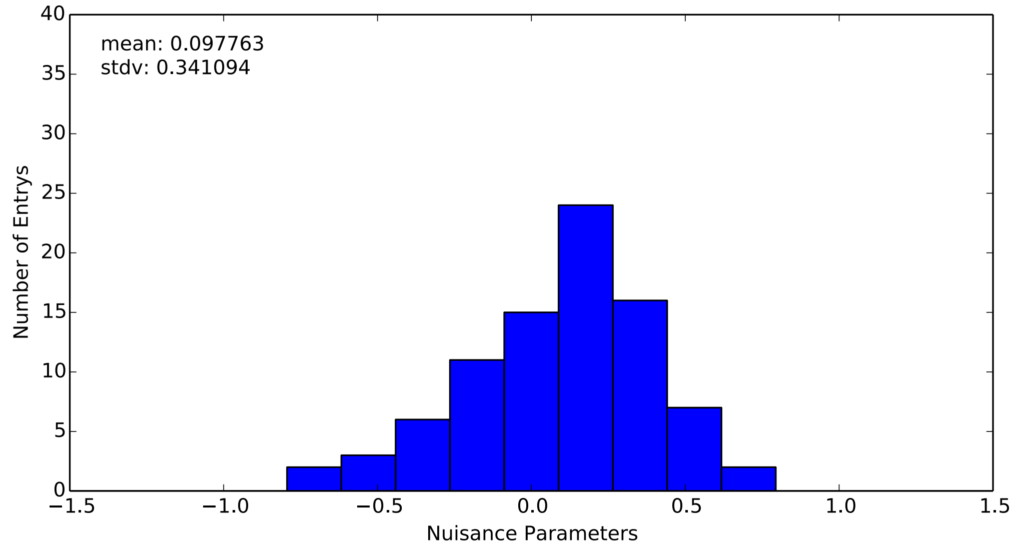

Figure 2: Distribution of nuisance parameters for inclusive jet data measured with the ATLAS detector at a centre of mass energy of the proton-proton system of $\sqrt{s} = 7$ TeV [18], obtained with the constrained least square fit described in section 6.

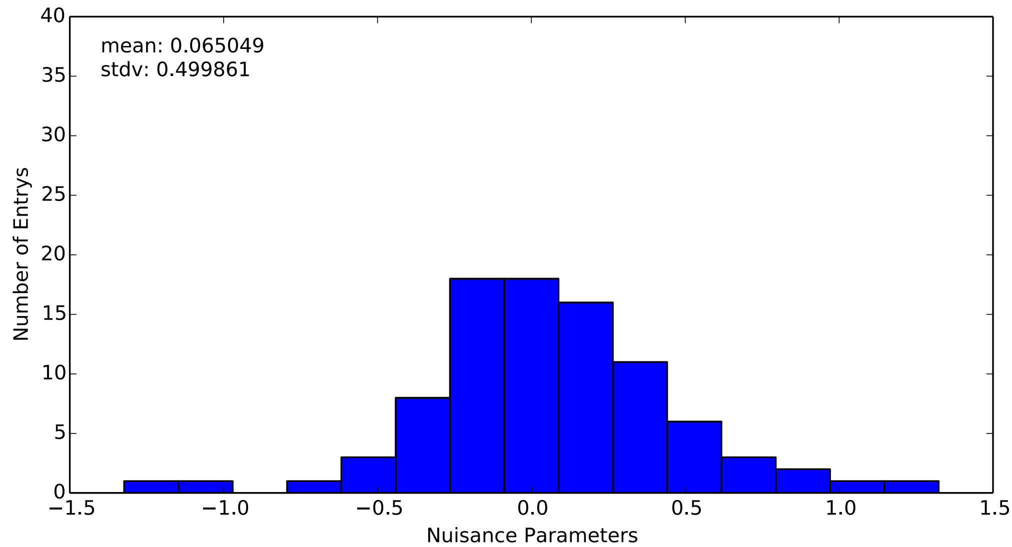

Figure 3: Distribution of nuisance parameters for inclusive jet data measured with the ATLAS detector at a centre of mass energy of the proton-proton system of $\sqrt{s} = 2.76$ TeV [17] and $\sqrt{s} = 7$ TeV [18], obtained with the constrained least square fit described in section 6.