

# Notes on posterior flavour separation of fragmentation functions using SIDIS data

In this set of notes we discuss a possible strategy to achieve flavour separation of a preexisting set of fragmentation functions (FFs) using data for semi-inclusive deep-inelastic scattering (SIDIS) with performing a fit. The application domain of this method is the inclusion of the COMPASS data for the production of unidentified charged hadrons ( $h^\pm$ ) in the set NNFF1.1h presented in Ref. [1].

## 1 The methodology

The COMPASS experiment released SIDIS data for unidentified charged-hadrons production [2] in the form of multiplicities separately for  $h^+$  and  $h^-$ . Thanks to the partonic structure of the corresponding observable, this data, if included in a determination of FFs, allows one to separate, not only flavour species, but also flavour from ant flavour. This contrasts with single-inclusive  $e^+e^-$  annihilation (SIA) data and hadro-production in  $pp$  collision that are only able to constrain a limited number of flavour combinations. This is the reason why the NNFF1.1h set, that is based on SIA and  $pp$  data only, does not deliver a reliable flavour separation. In these notes we devise a method that allows for the inclusion of the COMPASS data in the NNFF1.1h without the need of a new fit. The method is based on the Bayesian reweighting procedure.

The NNFF sets adopt the following parameterisation basis:

$$\{D_{u^+}^{h^\pm}, D_{d^++s^+}^{h^\pm}, D_{c^+}^{h^\pm}, D_{b^+}^{h^\pm}, D_g^{h^\pm},\} \quad (1.1)$$

at the initial scale  $Q_0 = 5$  GeV, with  $q^+ = q + \bar{q}$ . This choice, particularly the reduced number of combinations, is dictated by the fact that the data set included in the fits is only sensitive to this number of combinations. It is thus apparent that no separation of  $q$  and  $\bar{q}$  and also of  $d^+$  and  $s^+$  is achievable. This led us to parameterise the 5 combinations in Eq. (1.1) in place of the 11 independent combinations at  $Q_0$  for each hadronic charge. To obtain a separation from SIDIS data we first assume charge conjugation symmetry to connect the FFs of hadrons of opposite charge:

$$D_{q(\bar{q})}^{h^+} = D_{\bar{q}(q)}^{h^-}. \quad (1.2)$$

This symmetry is exact in QCD and holds at all scales. This allows us to consider the FFs of a single charge, we choose  $h^+$ . Second, we assume that “sea-type” quark flavours are symmetric with respect to charge conjugation<sup>(1)</sup>. In particular, for strange, charm, and bottom we assume that:

$$D_q^{h^+} = D_{\bar{q}}^{h^+}, \quad q = s, c, b. \quad (1.3)$$

The 5 FF combinations in Eq. (1.1) for each hadronic charge along with the constraints in Eqs. (1.2) and (1.3), brings us to 8 degrees of freedom constrained. To get to 11 we need three more degrees of freedom that we constrain using the COMPASS data. We parameterise these three additional degrees of freedom in terms of three auxiliary functions  $C(x)$ ,  $H(x)$  and  $G(x)$  introduced through the following (trivial) identities:

$$D_{u^+}^{h^+}(x, Q_0) = C(x)D_{u^+}^{h^+}(x, Q_0) + [1 - C(x)]D_{u^+}^{h^+}(x, Q_0), \quad (1.4)$$

and identify:

$$D_u^{h^+}(x, Q_0) = C(x)D_{u^+}^{h^+}(x, Q_0), \quad \text{and} \quad D_{\bar{u}}^{h^+}(x, Q_0) = [1 - C(x)]D_{u^+}^{h^+}(x, Q_0). \quad (1.5)$$

Then:

$$D_{d^++s^+}^{h^+}(x, Q_0) = H(x)D_{d^++s^+}^{h^+}(x, Q_0) + [1 - H(x)]D_{d^++s^+}^{h^+}(x, Q_0), \quad (1.6)$$

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<sup>1</sup> In fact, since we are considering all possible charged hadrons in the final state, it is not strictly true that strange, charm, and bottom are sea-distributions. However, the hadronic yield is dominated by pions for which this assumption is more justified.

and we identify:

$$D_{d+}^{h+}(x, Q_0) = H(x)D_{d++s+}^{h+}(x, Q_0), \quad \text{and} \quad D_{s+}^{h+}(x, Q_0) = [1 - H(x)]D_{d++s+}^{h+}(x, Q_0). \quad (1.7)$$

But since we assume  $D_s^{h+} = D_s^{h+}$ , we have that:

$$D_s^{h+}(x, Q_0) = D_s^{h+}(x, Q_0) = \frac{1}{2}[1 - H(x)]D_{d++s+}^{h+}(x, Q_0). \quad (1.8)$$

Finally, we introduce the third function as follows:

$$D_{d+}^{h+}(x, Q_0) = G(x)D_{d+}^{h+}(x, Q_0) + [1 - G(x)]D_{d+}^{h+}(x, Q_0), \quad (1.9)$$

and identify:

$$D_d^{h+}(x, Q_0) = G(x)D_{d+}^{h+} = G(x)H(x)D_{d++s+}^{h+}(x, Q_0), \quad (1.10)$$

and:

$$D_d^{h+}(x, Q_0) = [1 - G(x)]D_{d+}^{h+} = [1 - G(x)]H(x)D_{d++s+}^{h+}(x, Q_0). \quad (1.11)$$

At the end of the day, we can parameterise the flavour separation in terms of  $C(x)$ ,  $H(x)$ , and  $G(x)$  using Eqs. (1.5), (1.8), (1.10), and (1.11). The final goal is the determination of these functions. Despite, in principle, they are totally unknown, we can in practice impose some phenomenologically-motivated constraints on them. First we require that the auxiliary functions in the range  $x \in [0, 1]$  are between 0 and 1:

$$0 \leq C(x), H(x), G(x) \leq 1, \quad x \in [0, 1]. \quad (1.12)$$

The reason is that we want that the flavour-separated distributions contribute constructively to their original combinations. We then assume that for  $x$  very close to one all flavour-separated distributions contribute with the same amount to their original combinations. This translates into:

$$C(1) = H(1) = G(1) = \frac{1}{2}. \quad (1.13)$$

To fulfill the requirements above it is convenient to define:

$$\begin{aligned} C(x) &= \frac{1}{2}c(x) + \frac{1}{2}, \\ H(x) &= \frac{1}{2}h(x) + \frac{1}{2}, \\ G(x) &= \frac{1}{2}g(x) + \frac{1}{2}, \end{aligned} \quad (1.14)$$

with:

$$-1 \leq c(x), h(x), g(x) \leq 1, \quad x \in [0, 1], \quad (1.15)$$

and:

$$c(1) = h(1) = g(1) = 0. \quad (1.16)$$

The simplest possible parameterisation for the functions  $f = \{c, h, g\}$  is:

$$f(x) = Ax^\alpha(1-x)^\beta. \quad (1.17)$$

The constraint in Eq. (1.16) is implemented by requiring:

$$\beta > 0. \quad (1.18)$$

In addition, for  $f$  not to diverge at small values of  $x$ , we also require:

$$\alpha \geq 0. \quad (1.19)$$

The constraint in Eq. (1.15) is implemented by requiring that the function  $f$  computed in its (unique) stationary point  $x_0$  in the interval  $[0, 1]$  is bound to be in the interval  $[-1, 1]$ . This will finally result in a constraint on the normalisation factor  $A$ . To do so, we first find the stationary point of  $f$  by requiring its derivative to be zero:

$$\left. \frac{df}{dx} \right|_{x=x_0} = Ax_0^{\alpha-1}(1-x_0)^{\beta-1}[\alpha - (\alpha + \beta)x_0] = 0 \quad \Rightarrow \quad x_0 = \frac{\alpha}{\alpha + \beta}, \quad (1.20)$$

so that:

$$f(x_0) = A \left( \frac{\alpha}{\alpha + \beta} \right)^\alpha \left( \frac{\beta}{\alpha + \beta} \right)^\beta = A \frac{\alpha^\alpha \beta^\beta}{(\alpha + \beta)^{\alpha + \beta}}. \quad (1.21)$$

Therefore, for  $-1 \leq f(x_0) < 1$ , one needs that:

$$-\frac{(\alpha + \beta)^{\alpha + \beta}}{\alpha^\alpha \beta^\beta} \leq A \leq \frac{(\alpha + \beta)^{\alpha + \beta}}{\alpha^\alpha \beta^\beta}. \quad (1.22)$$

Finally, by extracting randomly the parameters  $A$ ,  $\alpha$ , and  $\beta$  of the function  $f$  defined in Eq. (1.17) in the ranges allowed by the inequalities in Eqs. (1.18), (1.19), and (1.22) for each of the functions  $c(x)$ ,  $h(x)$ , and  $g(x)$ , we can generate a random flavour separation<sup>(2)</sup>. We can then test the obtained flavour separation against the experimental data by computing the corresponding  $\chi^2$ . Having a broad set of random flavour separations would subsequently allow to apply Bayesian reweighting (possibly followed by unweighting) to select the flavour separations that best describe the data. Fig. 1.1 shows the behaviour of 100 random flavour-separation functions:

$$F(x) = \frac{1}{2}f(x) + \frac{1}{2}, \quad (1.23)$$

generated according to the recipe discussed above.

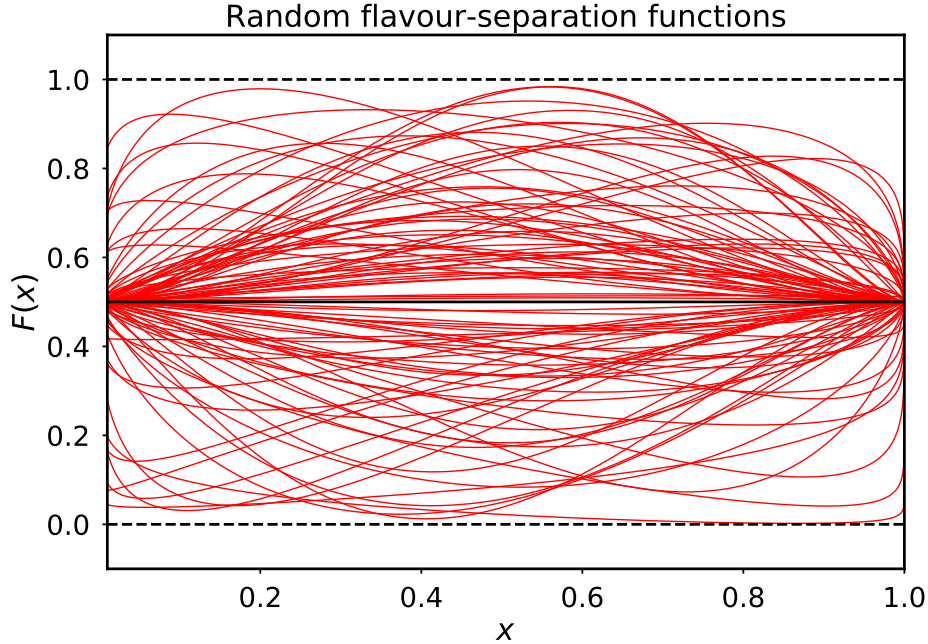


Fig. 1.1: Set of 100 random flavour-separation functions.

## 2 Efficient computation of the SIDIS cross section

In this section, we will manipulate the formulas for the SIDIS cross section so to make them optimal from the point of view of the implementation. The goal is to make their numerical computation as efficient as possible. The SIDIS differential cross section for the exchange of a virtual photon can be written as:

$$\frac{d^3\sigma}{dx dQ dz} = \frac{4\pi\alpha^2}{Q^3} \left[ \frac{Y_+}{x} F_2(x, z, Q^2) - \frac{y^2}{x} F_L(x, z, Q^2) \right], \quad (2.1)$$

where we have defined:

$$Y_+ = 1 + (1 - y)^2. \quad (2.2)$$

<sup>2</sup> For obvious reason, we need to limit the values of  $\alpha$  and  $\beta$  also from above. We choose  $\alpha, \beta < 2$  because this value seems to give a uniform distribution.

The structure functions  $F_2$  and  $F_L$  are given at NLO by the following convolution:

$$F(x, z, Q) = x \sum_{q\bar{q}} e_q^2 \left[ (C_{qq}(x, z|Q) \otimes f_q(x|Q) + C_{qg}(x, z|Q) \otimes f_g(x|Q)) \otimes d_q(z|Q) \right. \\ \left. + (C_{gq}(x, z|Q) \otimes f_q(x|Q)) \otimes d_g(z|Q) \right], \quad (2.3)$$

where  $\{f_q, f_g\}$  are the quark and gluon PDFs and  $\{d_q, d_g\}$  are the quark and gluon FFs,  $e_q$  is the electric charge of the quark  $q$  and  $\{C_{qq}^{2,L}, C_{qg}^{2,L}, C_{gq}^{2,L}\}$  are the relevant partonic cross sections. Importantly, the perturbative coefficients of the coefficient functions  $C$  factorise as follows:

$$C(x, z) = \sum_t c_t O_t^{(1)}(x) O_t^{(2)}(z), \quad (2.4)$$

where  $c_t$  are numerical coefficients, and  $O_t^{(1)}$  and  $O_t^{(2)}$  are one-dimensional functions of  $x$  and  $z$ , respectively. Since we are interested in isolating the FFs at some initial scale  $Q_0$ , we also write:

$$d_{q(g)}(z|Q) = T_{q(g)i} d_i(z|Q) = T_{q(g)i} \Gamma_{ij}(z|Q, Q_0) \otimes d_j(z|Q_0), \quad (2.5)$$

where  $\Gamma_{ij}$  is the appropriate evolution operator and  $T_{q(g)i}$  is the rotation matrix from the evolution to the physical basis. Now, for the generic structure function, let us define:

$$\mathbb{C}_j(z|x, Q, Q_0) = \left[ C_{qq}(x, z|Q) \otimes \left( \sum_{q\bar{q}} e_q^2 f_q(x|Q) T_{qi} \right) + \left( \sum_{q\bar{q}} e_q^2 T_{qi} \right) C_{qg}(x, z|Q) \otimes f_g(x|Q) \right. \\ \left. + C_{gq}(x, z|Q) \otimes \left( \sum_{q\bar{q}} e_q^2 f_q(x|Q) \right) T_{gi} \right] \otimes \Gamma_{ij}(z|Q, Q_0) \\ = \mathbb{K}_i^{\text{SIDIS}}(z|x, Q) \otimes \Gamma_{ij}(z|Q, Q_0), \quad (2.6)$$

where we have used the fact that, in the zero-mass scheme, the quark hard cross sections do not depend on the specific quark flavour, such that:

$$F(x, z, Q) = \sum_j \mathbb{C}_j(z|x, Q, Q_0) \otimes d_j(z|Q_0). \quad (2.7)$$

Using the perturbative expansion of the hard cross sections and Eq. (2.4), the factor  $\mathbb{K}^{\text{SIDIS}}$  in Eq. (2.6) can be written more explicitly as:

$$\mathbb{K}_i^{\text{SIDIS}}(z|x, Q) = \left( \sum_{q\bar{q}} e_q^2 f_q(x|Q) T_{qi} \right) \delta(1-z) \\ + a_s(Q) \sum_t c_{qq,t} \left[ O_{qq,t}^{(1)} \otimes \left( \sum_{q\bar{q}} e_q^2 f_q(Q) T_{qi} \right) \right] (x) O_{qq,t}^{(2)}(z) \\ + a_s(Q) \left( \sum_{q\bar{q}} e_q^2 T_{qi} \right) \sum_t c_{qg,t} \left[ O_{qg,t}^{(1)} \otimes f_g(Q) \right] (x) O_{qg,t}^{(2)}(z) \\ + a_s(Q) T_{gi} \sum_t c_{gq,t} \left[ O_{gq,t}^{(1)} \otimes \left( \sum_{q\bar{q}} e_q^2 f_q(Q) \right) \right] (x) O_{gq,t}^{(2)}(z), \quad (2.8)$$

with:

$$a_s(Q) = \frac{\alpha_s(Q)}{4\pi}. \quad (2.9)$$

Note that, given the evolution and physical basis, one has that  $T_{gi} = \delta_{gi}$  and  $T_{qg} = 0$ . Finally, defining:

$$\mathbb{K}_i^{\text{SIDIS}}(z|x, Q) = \frac{4\pi\alpha^2}{Q^3} \left[ \frac{Y_+}{x} \mathbb{K}_{2,i}^{\text{SIDIS}}(z|x, Q) - \frac{y^2}{x} \mathbb{K}_{L,i}^{\text{SIDIS}}(z|x, Q) \right], \quad (2.10)$$

one has:

$$\frac{d^3\sigma}{dx dQ dz} = \sum_j \mathbb{K}_i^{\text{SIDIS}}(z|x, Q) \otimes \Gamma_{ij}(z|Q, Q_0) \otimes d_j(z|Q_0). \quad (2.11)$$

## 2.1 Integrating over the phase space

For implementation reasons, we take as a reference for our calculations the cross section differential in  $x$ ,  $Q$  and  $z$  integrated over the final-state phase space (bins):

$$\sigma = \int_{Q_{\min}}^{Q_{\max}} dQ \int_{x_{\min}}^{x_{\max}} dx \int_{z_{\min}}^{z_{\max}} dz \frac{d^3\sigma}{dx dQ dz}, \quad (2.12)$$

However, sometimes the photon invariant mass  $Q$  is replaced by the inelasticity  $y$  of the process defined as in terms of the center-of-mass energy  $\sqrt{s}$  as:

$$Q^2 = xys. \quad (2.13)$$

In this case the integral over the phase space takes the form:

$$\sigma = \int_{y_{\min}}^{y_{\max}} dy \int_{x_{\min}}^{x_{\max}} dx \int_{z_{\min}}^{z_{\max}} dz \frac{d^3\sigma}{dx dy dz} = \int_{\sqrt{x_{\min} y_{\min} s}}^{\sqrt{x_{\max} y_{\max} s}} dQ \int_{\bar{x}_{\min}}^{\bar{x}_{\max}} dx \int_{z_{\min}}^{z_{\max}} dz \frac{d^3\sigma}{dx dQ dz}, \quad (2.14)$$

with:

$$\bar{x}_{\min} = \max \left[ x_{\min}, \frac{Q^2}{sy_{\max}} \right] \quad \text{and} \quad \bar{x}_{\max} = \min \left[ x_{\max}, \frac{Q^2}{sy_{\min}} \right]. \quad (2.15)$$

Often, cross sections are measured within a fiducial region defined as:

$$W = \sqrt{\frac{(1-x)Q^2}{x}} \geq W_{\min}, \quad y_{\min} \leq y \leq y_{\max}, \quad Q \geq Q_{\min}. \quad (2.16)$$

These constraints have the effect of reducing the phase space of some bins placed at the edge of the fiducial region. The net effect is that of replacing the  $x$  integration bounds in both Eqs. (2.12) and (2.14) with:

$$x_{\min} \rightarrow \bar{x}_{\min} = \max \left[ x_{\min}, \frac{Q^2}{sy_{\max}} \right] \quad \text{and} \quad x_{\max} \rightarrow \bar{x}_{\max} = \min \left[ x_{\max}, \frac{Q^2}{sy_{\min}}, \frac{Q^2}{Q^2 + W_{\min}^2} \right]. \quad (2.17)$$

Therefore, also the integral in Eq. (2.14) can be recasted in the form of Eq. (2.12). Using Eq. (2.11), we finally have that:

$$\sigma = \sum_j \left[ \int_{z_{\min}}^{z_{\max}} dz \left[ \int_{Q_{\min}}^{Q_{\max}} dQ \left[ \int_{x_{\min}}^{x_{\max}} dx \mathbb{K}_i^{\text{SIDIS}}(z|x, Q) \right] \otimes \Gamma_{ij}(z|Q, Q_0) \right] \otimes d_j(z|Q_0) \right]. \quad (2.18)$$

This expression provides the optimal structure for the implementation in APFEL++ in terms of integrations and convolutions. Indeed, upon integration in  $x$ , one finds:

$$\int_{x_{\min}}^{x_{\max}} dx \mathbb{K}_i^{\text{SIDIS}}(z|x, Q) = c_i(Q; x_{\min}, x_{\max}) \mathbb{L}_i(z), \quad (2.19)$$

so that:

$$\begin{aligned} \int_{Q_{\min}}^{Q_{\max}} dQ \left[ \int_{x_{\min}}^{x_{\max}} dx \mathbb{K}_i^{\text{SIDIS}}(z|x, Q) \right] \otimes \Gamma_{ij}(z|Q, Q_0) &= \int_{Q_{\min}}^{Q_{\max}} dQ c_i(Q; x_{\min}, x_{\max}) \mathbb{L}_i(z) \otimes \Gamma_{ij}(z|Q, Q_0) \\ &= \int_{Q_{\min}}^{Q_{\max}} dQ \mathbb{M}_j(z|x_{\min}, x_{\max}, Q, Q_0) \\ &= \mathbb{N}_j(z|x_{\min}, x_{\max}, Q_{\min}, Q_{\max}, Q_0) \end{aligned} \quad (2.20)$$

and finally:

$$\sigma = \sum_j \int_{z_{\min}}^{z_{\max}} dz \mathbb{N}_j(z|x_{\min}, x_{\max}, Q_{\min}, Q_{\max}, Q_0) \otimes d_j(z|Q_0) = \sum_j \mathbb{O}_j(z_{\min}, z_{\max}, x_{\min}, x_{\max}, Q_{\min}, Q_{\max}, Q_0). \quad (2.21)$$

### 3 Computation of the single-inclusive $e^+e^-$ annihilation cross section

From the point of view of the numerical computation, the single-inclusive  $e^+e^-$  annihilation (SIA) cross section can be regarded as a simplified version of the SIDIS one. Specifically, for SIA the variable  $x$  is just absent and there is no integration over the scale  $Q$  because  $Q = \sqrt{s}$  with  $\sqrt{s}$  fixed and determined by the collision energy of the lepton pair. In addition, in all cases considered in our analysis, data are delivered for specific values of the variable  $z$  such that no integration over  $z$  is required. Finally, the observable is computed as:

$$\frac{1}{\sigma} \frac{d\sigma}{dz} = \sum_j \mathbb{K}_i^{\text{SIA}}(z|Q) \otimes \Gamma_{ij}(z|Q, Q_0) \otimes d_j(z|Q_0). \quad (3.1)$$

This equation closely resembles Eq. (2.11) but the  $\mathbb{K}_i^{\text{SIA}}$  functions have a simpler structure and, up to a factor  $\sigma_0/\sigma$ , where  $\sigma_0$  is the leading-order total cross section, are already computed by APFEL up to  $\mathcal{O}(\alpha_s^2)$ .

## References

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