NNLOPS accurate Drell-Yan production

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ABSTRACT: This document contains instructions for the promotion of VJ-Minlo Les Houches event files from NLO to NNLO accuracy in the description of inclusive Drell-Yan production observables, by a reweighting procedure making use of the DYNNLO program [1].

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1 Introduction

This manual explains how to run the code (that makes use of the Minlo procedure) in the Zj/DYNNLOPS and Wj/DYNNLOPS directories, in conjunction with the DYNNLO program, to get NNLOPS accuracy for inclusive Drell-Yan production.

In order to obtain the needed source code, the user has to download the DYNNLOPS directory from the Zj or Wj main directory, using the following command

```
svn co [--revision n] --username anonymous --password anonymous \ svn://powhegbox.mib.infn.it/trunk/User-Processes-V2/DYNNLOPS. The DYNNLOPS directory contains five folders
```

- aux: a directory containing auxiliary files (e.g. to combine histograms, make plots, etc.);
- Docs: a directory containing the manual;
- COMMON: a directory containing all files common to W and Z production;
- WNNLOPS and ZNNLOPS: directories containing files specific of W or Z production.

As there is no fundamental difference between obtaining NNLOPS accurate results for Z and W production using this code, in the following we will give instructions for the case of Z production. For the W case, the commands listed in the rest of this document need to be changed straightforwardly.

2 NNLO input

A fundamental ingredient required to obtain NNLO accurate event samples is a triple differential distribution for the Z boson Born kinematics. We here give instructions on how to obtain such distributions, in a format suitable for upgrading the ZJ-Minlo events via the Zj/DYNNLOPS reweighting code.

1. Make sure the LHAPDF package is installed:

```
https://lhapdf.hepforge.org
```

In particular, for the installation of DYNNLO, the command lhapdf-config --libdir should return the location of the installed LHAPDF libraries.

2. Download DYNNLO from the following URL:²

```
http://theory.fi.infn.it/grazzini/codes/dynnlo-v1.5.tgz
```

- 3. Unpack the tarball in a convenient location
 - \$ cp /Downloads/dynnlo-v1.5.tgz ./
 - \$ tar -xzvf dynnlo-v1.5.tgz
 - \$ ls dynnlo-v1.5

Under the parent directory dynnlo-v1.5 one should find subdirectories bin, doc, obj, src, and a makefile.

- 4. Enter the DYNNLO parent directory
 - \$ cd dynnlo-v1.5
- 5. Replace (or link) the ${\tt DYNNLO}$ default ${\tt makefile}$ with the one from the
 - Zj/DYNNLOPS/ZNNLOPS/dynnlo-patches directory
 - \$ cp /path/to/Zj/DYNNLOPS/ZNNLOPS/dynnlo-patches/dynnlo.makefile ./makefile
- 6. Link (or copy using the -L option) the DYNNLO patches directory into the parent directory
 - \$ cp -r -L /path/to/Zj/DYNNLOPS/ZNNLOPS/dynnlo-patches ./
- 7. Build the code
 - \$ make

A message --> DYNNLO compiled with LHAPDF routines <-- indicates success. You might need to set the environmental variable LD_LIBRARY_PATH to the output of lhapdf-config --libdir, although the patched dynnlo.makefile contains commands that should take care of this automatically.

- 8. Copy over the template input file
 - \$ cd bin

¹In this case the Born kinematics is fully specified in terms of the rapidity of the boson, an (arbitrary) angle describing the final state leptons and the invariant mass of the lepton pair.

²Make sure that version 1.5 is used, since a problem with the dependence of the genuine NNLO results upon varying the factorisation scale was fixed by the DYNNLO authors in version 1.5.

- 9. Edit the input file as desired. The input file is nothing but a standard DYNNLO input file and may be run simply by typing
 - \$./dynnlo < dynnlo.infile >> my.log
 yielding a nnlo.top and nnlo3D.top histogram file.

The first file contains one-dimensional distributions which can be used for phenomenological studies. The second file is the one of interest here, as it contains a set of three-dimensional distributions which can be used for reweighting ZJ-Minlo events. As each histogram consists of $25^3 = 15625$ bins, very high statistics are required to properly populate the tails of the distributions. For the analysis presented in [2] we ran 100 instances of DYNNLO with the following parameters:

```
15 10000000 ! itmx1, ncall1 30 10000000 ! itmx2, ncall2
```

Changing the random seed rseed for each run. To combine the runs we provide a fortran program, merge3ddata.f, in the aux folder. As it can use big amounts of memory, we recommend compiling with the following flags

\$ gfortran -mcmodel=medium -o merge3ddata merge3ddata.f

To then merge the nnlo3D.top files into a file called dynnlo.top do the following

```
$ ./merge3ddata 1 file_1.top ... file_N.top
$ mv fort.12 dynnlo.top
```

We would like to note here that, due to the way DYNNLO computes the real contribution of the cross-section, the errors of the nnlo3D.top files (and nnlo.top) are not reliable. In order to asses the precision on the three dimensional distributions, we provide a small program, 3dto1d.f, which will integrate the three-dimensional distributions into three one-dimensional distributions. After compilation it is run by

\$./3dto1d dynnlo.top

which will produce a file fort.12 with one-dimensional distributions.

In the case where a user might not be interested in high rapidity events, it is presumably reasonable to run with fewer points than suggested here.

10. Finally, make sure that all input parameters (width, mass, couplings, pdfs) should be the same in DYNNLO and ZJ-Minlo. (The patched DYNNLO program outputs all relevant physical parameters).

3 Zj-MiNLO events

The other fundamental ingredient needed for the NNLO reweighting procedure are ZJ-Minlo Les Houches events. A few modifications of the standard code are needed to obtain three-dimensional distributions and to maintain consistency of the physical parameters in DYNNLO

and ZJ-MiNLO. In order to include them, it is sufficient to replace the default POWHEG makefile with the patched one:

\$ cp DYNNLOPS/ZNNLOPS/powheg-patches/powheg.makefile ./makefile

In DYNNLOPS/ZNNLOPS/powheg-patches/powheg.input a template input file can also be found. If the code is run with the patches out of the box and the above input file, consistency between DYNNLO and ZJ-MiNLO should be achieved. However, we stress again that it is up to the user to make sure this is the case.

Few comments are helpful:

- 1. A large number of physical parameters used by the ZJ-Minlo code, such as the Fermi constant, are assigned by the subroutine init_couplings defined in the file Zj/init_couplings.f. As in the case of the DYNNLO mdata.f file, some of the parameters in this file are irrelevant. Nevertheless, in Zj/DYNNLOPS/ZNNLOPS/powheg.input all these parameters can be changed. The version we provide is consistent with our patched version of mdata.f
- 2. For detailed instructions on setting up the ZJ-MiNLO program to perform numerous runs in parallel see section 4.1 in /path/to/W2jet/Docs/manual-BOX-WZ2jet.pdf
- 3. We add that although it is not strictly necessary to generate the ZJ-MiNLO events using a NNLO PDF, in the limited studies that we have carried out to date we used the same (NNLO) PDF set in ZJ-MiNLO and DYNNLO.
- 4. As was the case when obtaining NNLO distributions, a large number of events is needed to populate the tails of the three-dimensional distributions. For the study carried out in [2] we used 20 million events to compute denominators.

4 Reweighting

The NLO-to-NNLO weight factor assigned to the VJ-MiNLO events is differential in the vector boson phase space (Φ_B) and the transverse momentum of the leading jet (p_T) , at the NNLO level in the DYNNLO case, and at the level of the hardest emission cross section (Les Houches events) in VJ-MiNLO. It is given by

$$\mathcal{W}\left(\Phi_{B}, p_{\mathrm{T}}\right) = h\left(p_{\mathrm{T}}\right) \frac{\int d\sigma^{\mathrm{NNLO}} \, \delta\left(\Phi_{B} - \Phi_{B}\left(\Phi\right)\right) - \int d\sigma_{B}^{\mathrm{MINLO}} \, \delta\left(\Phi_{B} - \Phi_{B}\left(\Phi\right)\right)}{\int d\sigma_{A}^{\mathrm{MINLO}} \, \delta\left(\Phi_{B} - \Phi_{B}\left(\Phi\right)\right)} + \left(1 - h\left(p_{\mathrm{T}}\right)\right), \tag{4.1}$$

where

$$d\sigma_A = d\sigma h \left(p_{\rm T} \right) \,, \tag{4.2}$$

$$d\sigma_B = d\sigma \left(1 - h\left(p_{\rm T}\right)\right)\,,\tag{4.3}$$

with h a monotonic profile function

$$h(p_{\rm T}) = \frac{(\beta m_{\rm V})^2}{(\beta m_{\rm V})^2 + p_{\rm T}^2},$$
 (4.4)

and β a constant parameter. On convoluting $W(\Phi_B, p_T)$ with the VJ-MiNLO differential cross section and integrating over p_T one finds, exactly,

$$\left(\frac{d\sigma}{d\Phi_B}\right)^{\text{NNLOPS}} = \left(\frac{d\sigma}{d\Phi_B}\right)^{\text{NNLO}}.$$
(4.5)

For a proof of why such a reweighting procedure leads to NNLO accuracy in general, we refer the reader to [2, 3].

The role of the profile function h and, in particular, the β parameter within it, is, roughly speaking, to determine how to spread out the NLO-to-NNLO corrections along the $p_{\rm T}$ axis. For $\beta=\infty$ the corrections are spread uniformly in $p_{\rm T}$ (see e.g. fig. 3 of ref. [3]), while for $\beta=1$ they are concentrated in the region $p_{\rm T}<\beta\,m_V$. In the latter respect the β parameter plays a similar role to the resummation scale in dedicated resummation calculations, and as such we favour that β be set consistently with the preferred values in those. Thus we recommend $\beta=1$ in carrying out the reweighting. Indeed for $\beta=1$ we find good agreement with dedicated NNLL+NNLO calculations of the Z boson transverse momentum and the 0-jet veto efficiency where the resummation scale was set to m_Z .

We should emphasise that, while our NNLOPS simulation is formally NNLO accurate for inclusive quantities, the accuracy of its resummation of all-orders large logarithms is, formally, categorically not at the NNLL+NNLO level. We recommend that the predictions of such calculations be used to 'tune' the NNLOPS simulation (in particular the β parameter) to approximate the yet higher order, large logarithmic, terms which it does not take into account. Setting $\beta=1$ appears to do a very good job in this respect, thus it is the default, recommended, value in the following. If the reweighting is performed using eq. (4.1), the value of β can be changed by just modifying in a straightforward way the file get_zdamp.f (get_wdamp.f for W production).

4.1 A simple run

The code to be used in order to produce an NNLO-reweighted event file can be found in the DYNNLOPS/ZNNLOPS/Reweighter directory. After compiling it (FastJet needs to be linked), the program has to be run with the following command line:

```
$ ./minnlo <ZjMinLO-eventfile> <nr-DYNNLOfiles> <DYNNLO-file1>
[ <DYNNLO-file2>...] [<ZjMinLO-file1> <ZjMinLO-file2> ....]
```

where ZjMiNLO-eventfile is a LH file (suffix .1he) containing events produced with ZJ-MiNLO, obtained as described in sec. 3, nr-DYNNLOfiles denotes the number of DYNNLO files containing the 3D distributions (more then one is needed for instance when computing uncertainty bands using scale variation), DYNNLO-file* are output files of DYNNLO, computed as described in sec 2. The number of files given in the input line must correspond to nr-DYNNLOfiles. Finally, ZjMiNLO-file* contain three-dimensional histograms computed using ZJ-MiNLO events. These last arguments are optional. If these files are not present in the command line, the reweighing program computes them and stops. We call this stage one. When the ZjMiNLO-file* are computed by the reweighing program using

the ZjMiNLO-eventfile, the first weight present in the LHE file will produce a file called MINLO-W1-denom.top, the second weight a file called MINLO-W2-denom.top and so on.

Rather than producing just one huge event file, it is also possible to compute the MINLO-W*-denom.top files on each event sample and then combine the resulting distributions using the program merge3ddata.f (in aux). With the generated MINLO-W*-denom.top files one can then go on and perform the actual NNLO reweighing including in the command line these files. We call this stage two. The files have to be given in the same order as the corresponding weights in the LH file. Otherwise the reweighting will be incorrect.

Here follows an example on how to go through both stages, assuming that the user has a ZJ-MiNLO event file called pwgevents.lhe containing 7 weights and 3 DYNNLO files called dynnlo-mur0.5-muf0.5.top, dynnlo-mur1.0-muf1.0.top and dynnlo-mur2.0-muf2.0.top. The program should be called as

This will result in an output of MINLO-W1-denom.top, MINLO-W2-denom.top, MINLO-W3-denom.top, MINLO-W4-denom.top, MINLO-W5-denom.top, MINLO-W6-denom.top, MINLO-W7-denom.top.

To perform stage two the user would run

which will produce a file called pwgevents.lhe-nnlo.⁴ This LH file is the final output of the minnlo NLO-to-NNLO reweighter program, and can now be read and showered by Pythia or Herwig, as it is usually done with LH event files generated by the POWHEG BOX. It is important to notice that the new NNLO weight attached to each event is written after the event record, in the line comprised between the partonic momenta and the end-of-event tag (</event>). Similarly to the format of a POWHEG BOX output when the reweighting machinery is used, this line starts with the text

```
#new weight,renfact,facfact,pdf1,pdf2
```

followed by a weight and other information. In a LH file obtained with the minnlo reweighter, the names of the DYNNLO-output files are appended at the end of this line, and the NNLO weight to be used is the first number appearing, which will obviously be different from the original weight contained in ZJMiNLO-eventfile. This different weight, together with the appended identifier at the end of each line starting with #new weight, should be the only differences between the input and output LH files. Notice that the NNLO-reweighted output file will always contain the #new weight line(s), even if the original LH file ZJMiNLO-eventfile didn't.

³In this case, care has to be take to produce files in different directories.

⁴As usual, the shell will match and expand MINLO-W*-denom.top to the list of files MINLO-W1-denom.top, MINLO-W2-denom.top,..., MINLO-W7-denom.top, which is the actual input read by the minnlo program.

The program takes few hours to reweight a LH file produced by ZJ-MiNLO containing 20 million events. The output printed on the terminal at run time is self explanatory. We have also included a template script (runminnlo_template.sh) to help the user.

4.2 Estimating uncertainties

The conservative ansatz we recommend in estimating errors (the one employed in ref. [2, 3]) is that the $\mu_{\rm R}$ and $\mu_{\rm F}$ scales in the NNLO and NLO inputs should be varied in a fully independent way. In doing so we regard the uncertainties in the normalisations of distributions as being independent of the respective uncertainties in the shapes, at least in the region covered by the profile function $h(p_{\rm T})$, i.e. in the low $p_{\rm T}$ domain. Normalisation uncertainties are determined by the DYNNLO program, while shape uncertainties are due to ZJ-MiNLO. Outside of the low $p_{\rm T}$ region, the uncertainty is given by the standard ZJ-MiNLO computation (which uses in that region $\mu_{\rm R} = \mu_{\rm F} = p_{\rm T}$ as central scale choice).

In order to compute an uncertainty band, one first needs to have obtained multiple outputs from DYNNLO and ZJ-MiNLO with different $\mu_{\rm R}$ and $\mu_{\rm F}$. For the sake of simplicity, we will now describe a case where $\mu_{\rm R}$ and $\mu_{\rm F}$ are kept equal both when running DYNNLO and ZJ-MiNLO. We call this situation a "3x3 pts" scale variation study: for each event we will obtain 9 NNLOPS weights, associated to each of the 9 possible combinations among 3 results from DYNNLO and 3 from ZJ-MiNLO. This procedure is general enough to be straightforwardly adapted to the more general case of a "7x7 pts" scale variation, or variation thereof.

In the "3x3 pts" case, the needed inputs are 3 histogram files from DYNNLO, which we will call DYNNLO-outputfile-HH.top, DYNNLO-outputfile-11.top and DYNNLO-outputfile-22.top, for values of $\mu_{\rm R}=\mu_{\rm F}=\{m_Z/2,m_Z,2m_Z\}$ respectively. Similarly, the user needs to have obtained a LH file from ZJ-MiNLO where 3 weights are associated to each event. This file has to be obtained with the POWHEG BOX reweighting machinery: the 3 lines in between the last line of each event record and the </event> tag should have the format

The NLO-to-NNLO reweighter program should now be invoked in a first steep as:

```
$ ./minnlo ZJMiNLO-events.lhe 3 DYNNLO-outputfile-HH.top \
DYNNLO-outputfile-11.top DYNNLO-outputfile-22.top
```

This will produce the three MiNLO files with three-dimensional distributions. In a second step, one calls

```
$ ./minnlo ZJMiNLO-events.lhe 3 DYNNLO-outputfile-HH.top \
DYNNLO-outputfile-11.top DYNNLO-outputfile-22.top \
MINLO-W1-denom.top MINLO-W2-denom.top MINLO-W3-denom.top
```

At the end of the run, 9 lines will be present after each event record, each one containing the NNLO weight associated to the ZJ-MiNLO result labelled by the values of the pair (<ren.scale factor>, <fact.scale fact>) and the DYNNLO result identified by the name of the file appended to each line.

5 Example analysis

The analysis used for the phenomenological study in ref. [2] can be found in pwhg_analysis-minlo.f. The analysis is compiled in the Zj directory in the usual way by

```
make lhef_analysis
```

It can also be used to analyse events after the showering stage. We provide drivers for both Pythia6 (version 6.4.28) and Pythia8 (version 8.185) which can be compiled by

```
make main-PYTHIA-lhef
make main-PYTHIA8-lhef
```

Note that POWHEG BOX ships with Pythia6.4.25 as standard. It is straightforward to use any other version, by downloading it, and putting it in the main POWHEG BOX directory. For Pythia8 the user has to compile it himself and then set the PYTHIA8LOCATION appropriately.

6 Suggested citations

If you use this code please cite the inclusive Drell-Yan production NNLOPS paper [2] and the VJ-MiNLO paper which precedes and lays much of the foundations for it [4]. The NNLOPS simulation fundamentally relies on the NNLO Drell-Yan boson production calculation of refs. [1], and so these works should also be cited.

A Code description

In this section we briefly record the various additions and modifications to existing DYNNLO and POWHEG BOX code used to produce NNLOPS events.

A.1 DYNNLO

- makefile (DYNNLO-makefile)
 - The DYNNLO makefile is modified by prepending \$(DYNNLOHOME)/dynnlo-patches to the \$DIRS variable, introducing a variable \$PATCHES equal to the concatenation of the following object files in this list, plus the removal of those elements from the other Makefile variables (avoiding duplication). In this way the modified DYNNLO files below are compiled and linked from dynnlo-patches instead of the default versions in the default locations.

• mbook.f

The mtop subroutine, which outputs the DYNNLO histograms to a text file, has undergone a minor modification so as to have the same format as the VJ-MiNLO histogram output, to ease comparisons and for use in the reweighting program.

• mdata.f

- This file contains the values of numerous physical constants in DYNNLO e.g. Fermi's constant G_F , etc. We have edited all parameters in this file to have agreement with the corresponding VJ-MiNLO default settings.

• plotter.f

- This file contains an example analysis for DYNNLO by default. We have modified this analysis to produce three-dimensional histograms. Also a number of distributions relevant for phenomenology is being filled. The three-dimensional histogram range has been set to -5 < y < 5, $-\pi/2 < a_{mll} < \pi/2$ and $0 < \theta_l < \pi$. The distributions have 25 bins in each direction. These values may be altered by the user as desired, by editing the relevant booking subroutine call. However, in this case one must take care to modify the relevant POWHEG BOX analysis file (pwhg_analysis-release.f) used by the reweighting code, under the Vi/DYNNLOPS/VNNLOPS/Reweighter directory.

• setup.f

- This file was modified to use the k_T -algorithm instead of the anti- k_T .

• writeinfo.f

Originally the writeinfo subroutine in this file copied the contents of the input file used in running the program, plus the cross section, as a series of comments to the top of the histogram output file. In order to have a simple uniform format for the VJ-MiNLO and DYNNLO we removed these comments (the bulk of which was simply a copy of the input file used to run the program).

• histofinLH.f

This file takes care of finalising the histograms. As we are using the POWHEG BOX routines to fill our histograms (and a modified version to fill three-dimensional histograms) this file had to be modified to fill the correct histograms and finalise them.

• coupling.f

 We added a printout to the screen of various parameters, to make it easier to compare with the output of VJ-MiNLO.

• boost.f

- Added a routine to go from the lab frame to the CM frame.
- auxiliary.f,pwhg_bookhist-multi.f,pwhg_bookhist-new.f,pwhg_book-multi.h, pwhg_bookhist-new.h,pwhg_math.h

 These files contains the routines to fill histograms, to have a consistent output between DYNNLO and VJ-MiNLO.

A.2 ZJ-MiNLO

• lhapdfif.f

- When using NNLO PDFs Λ_5 is now computed at NLL and not NNLL.

• setlocalscales2.f

– This file is used by the Makefile instead of the default setlocalscales.f. We have changed the routine which computes α_S to be the default POWHEG BOX one, instead of a locally defined prescription. The two prescriptions agree far away from Λ_5 but significant differences show up close to the Landau pole.

• powheg.input / powheg.input-save

Here all values should be set consistently with the values used by DYNNLO.

The rest of the files found in this folder are either a driver for Pythia (as used in [2] or files already described in the section above)

A.3 NNLO reweighting

• Makefile

- The default value for the ANALYSIS variable should be release. FastJet must be linked properly too, and as usual it is recommended to let the Makefile call the fastjet-config command.

• minnlo.f

- This file contains the main program to perform the NLO-to-NNLO reweighting. Some parameters useful for debugging purposes can be found here, as described in the commented section at the beginning of the file. However, the user is recommended not to change them.
- opencount.f, auxilliary.f, lhef_readwrite.f, get_zdamp.f, genclust_kt.f, swapjet.f, miscclust.f, ptyrap.f, r.f
 - These files contain several functions and routines needed by minnlo.f and/or by the analysis subroutine used to process the ZJ-MiNLO LH file and compute $d\sigma_{A/B}^{\text{MINLO}} \delta\left(\Phi_B \Phi_B\left(\Phi\right)\right)$.

[jetlabel.f, jetcuts.f, mxpart.f and npart.f contain common blocks used in the source files.]

• pwhg_analysis-release.f, jet_finder-release.f

- These files contain the minimal analysis needed to extract $d\sigma_{A/B}^{\text{MINLO}} \delta \left(\Phi_B - \Phi_B \left(\Phi \right) \right)$ from the LH input file. They are compiled if ANALYSIS=release is set, which is the default option.

References

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