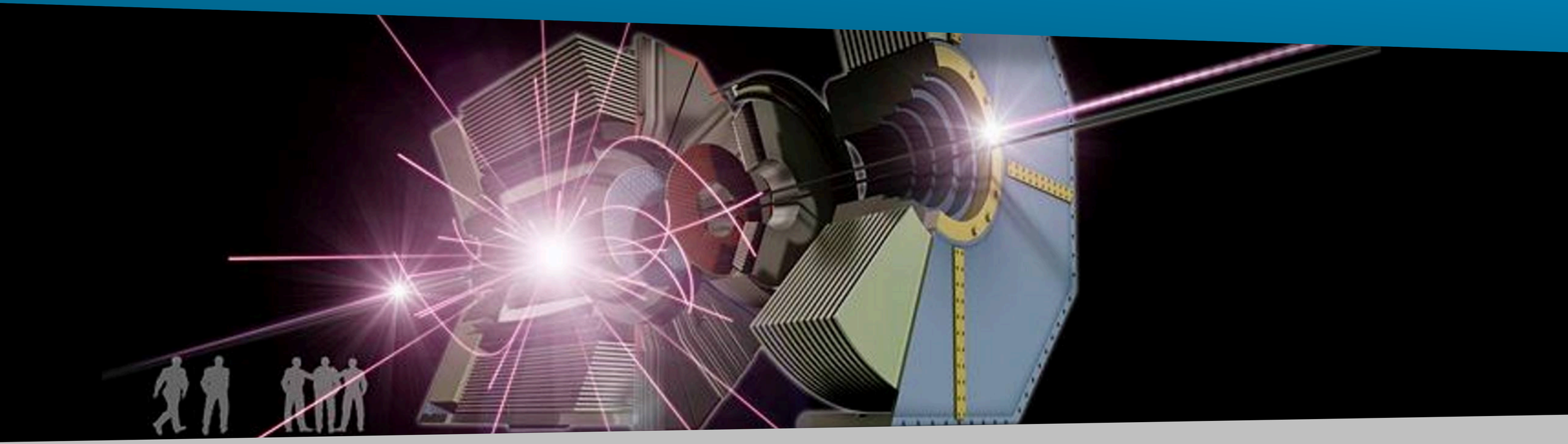
A hands-on introduction of PyRooUnfold



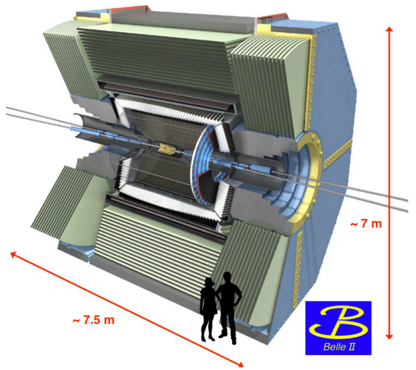
Version: v2.0.0

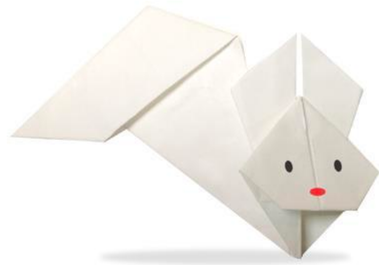
Lu Cao, 8 August 2024

Recap of Unfolding

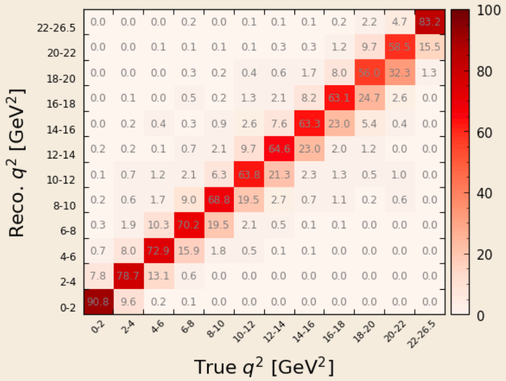
- Measured spectra are usually distorted and transformed by various detector effects (resolution, acceptance, etc.)
- Unfolding procedure is necessary/crucial for “shape” measurement

Unfolding





- Detector effects can be extracted with MC and wrap into migration matrix (also called response matrix)



M(i, j) indicates the probability (%) to observe an event in bin *i* if it had a generator-level value in bin *j*

- Unfolded spectra should recover MC truth in executable bias tests (not only Asimov); and avoid oscillating result while keeping minimal bias
- NO universally “excellent” method! Performance highly depends on data shape, resolution, statistics, etc.
- **Need validation for each specific case**

Unfolding Methods

Method	Description	Parameters	Comments	Function in PyRooUnfold
Bin-by-bin correction	unregularised, correct bin content with MC bin-by-bin factors	-	assumes no inter-bin migration; could have biases from the MC model	do_BinByBin
Matrix inversion	unregularised matrix inversion with singular value removal	-	give large bin-bin correlations and magnify statistical fluctuations; not accurate for small matrices	do_Invert
TUnfold	matrix inversion with 0-, 1-, or 2-order polynomial, an adjustable regularisation term of neighbouring bins	reg. strength τ	optimal tau can be chosen by scanning L-curve; better when nbin_mea > bin_true. By default, tau is determined internally by plotting log10(chi2 squared) against log10(tau)	do_TUnfold(τ)
Bayes	use Bayes' theorem to invert response matrix, regularisation by stopping iterations before reaching "true" inverse	iteration n (default 4)	n needs to be tuned with statistics, bins	do_Bayes(*n*)
IDS	iterative, dynamically stabilised method, uses stat. significance of the data-MC differences in each bin for regularisation	iteration n	allows to treat the effects of new structures in data and the large fluctuations from background subtraction	do_Ids(*n*)
SVD	singular value decomposition, regularisation with a smooth cut-off on small singular value contribution	k = 1..nbins	k too small: dominated by MC truth k too large: dominated by stat. fluctuations k needs to be tuned with bins, sample size	do_Svd(*k*)
GP	Gaussian Process (GP) method, uses RooUnfoldInvertT to get an initial solution and uses a marginal likelihood minimization to find the optimal regularization. [arXiv: 1811.01242]	kernel choice (only radial "1" is implemented now)	kernel function needs to describe truth well, and global regularisation strength may be varied locally along the spectrum by using a non-stationary kernel	do_GP

PyRooUnfold

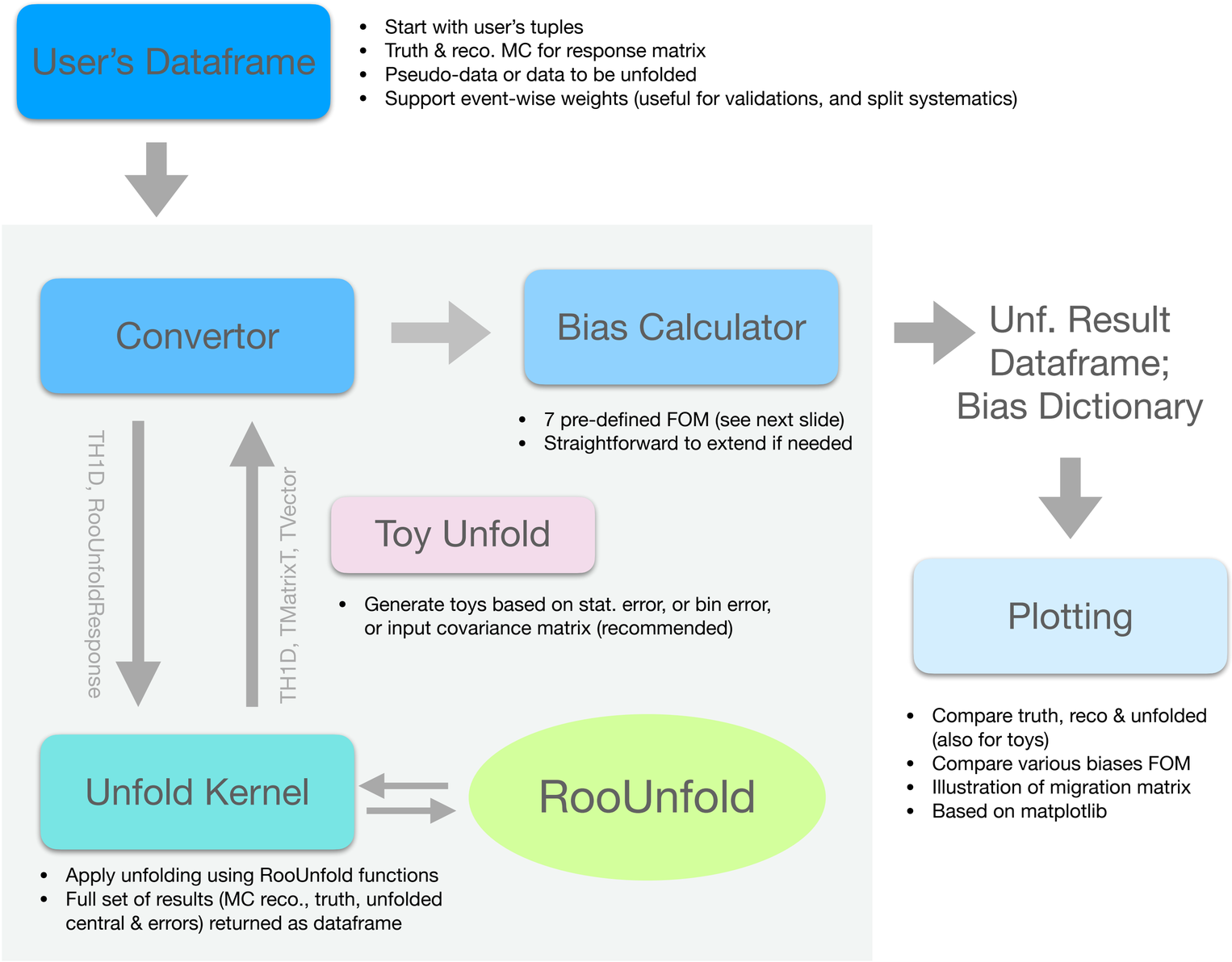
Not only **A Python wrapper of RooUnfold**

Included in the current version:

- Interface of all above methods and major features of RooUnfold
- Toys generation with input error/cov.
- Bias calculator
- Commonly needed plotting functions

Versions/Tags:

- v2.0.0: compatible with RooUnfold 3.0.0(2)
- v1.0.0: compatible with RooUnfold 2.0.1



Bias Study F.O.M.

Figure of Merit	Description	Nickname
$\sum_i b_i$	Sum of absolution biases in each bin, $b_i = N_i^{\text{unfolded}} - N_i^{\text{true}}$	a
$\sum_i b_i / N_i^{\text{true}}$	Sum of normalized absolute biases $(N_i^{\text{true}} \neq 0)$	b
$\sum_i b_i$	Sum of biases, which can be zero when significant biases are present in individual bins but cancel in the sum (balanced oscillation)	c
$\sqrt{\sum_{i,j} Cov_{i,j}}$	The square root of the sum of all elements of the post-unfold covariance matrix.	d
$\sum_i \frac{b_i}{\sqrt{\sum_{i,j} Cov_{i,j}}}$	Ratio of the sum of absolute biases and the error taking into account bin-to-bin correlations.	e
$\sqrt{\left(\sum_i b_i\right)^2 + \sum_{i,j} Cov_{i,j}}$	The total biases absorbing the total error with bin-to-bin correlations, which is used to check the general oscillation.	f
$\sum_i \frac{b_i}{\sqrt{Cov_{ii}}}$	The summed ratio of the absolute bias and unfolding error in each bin.	g
$\Phi(\frac{b_i}{\sigma_i} + 1) - \Phi(\frac{b_i}{\sigma_i} - 1)$	Coverage probability of intervals $[N_i^{\text{unfolded}} - \sigma_i, N_i^{\text{unfolded}} + \sigma_i]$, assuming N_i^{unfolded} is Gaussian distributed and Φ is the normal cumulative distribution function.	h

Every type has a good reason but also has limitations. Checking a combination of several is needed.

How-to

Single-run unfolding

```
from pyroounfold.unfold import unfold

example_q2 = unfold(

    df_train = df_mc,
    weight_train = df_mc['weight_train'],

    df_test = df_mc,
    weight_test = df_mc['weight_test'],

    name_var_true = 'true_q2',
    name_var_reco = 'reco_q2',

    show_var = r'$q^{2}$',# for plotting

    bins = q2_bins

    #optional input:

    reco_bin_error

    reco_cov

    kcovtoy

    mc_stat_err

)
```

← df for defining migration matrix Asimov unfolding, if train = test

← df of unfolding target, can be re-set by example_q2.**set_hist_measure**(bin_centre, bin_error)

← column names of variables

← binning of variables

← reco. bin-wise uncertainties need to propagated in unfolding

← reco. covariance matrix, alternative of bin-wise uncertainties

← Error propagation method (RooUnfold):

False - default, errors from the covariance matrix given by the unfolding (propagate reco_bin_error & reco_cov)

True - based on the variation of internal toys tests

see next slide

MC Stat. Error from Migration Matrix

`mc_stat_err` <- Interfaced argument from RooUnfolding::SystematicsTreatment dosys

Include systematic errors from response matrix due to limited MC statistics?

```
0 [kNoSystematics]:leave out the effect of MC statistical uncertainties on the migration matrix.
1 [kGammas]: include the effect by running internal toys
2 [kAlphas]: to exclude measurement errors.
3 [kAll IncludeSystematics()default]: all included
4 [kNoStatistics]
```

How-to

Single-run unfolding

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Bayes	use Bayes' theorem to invert response matrix, regularisation by stopping iterations before reaching "true" inverse	iteration n (default 4)	n needs to be tuned with statistics, bins	do_Bayes(*n*)
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GP	Gaussian Process (GP) method, uses RooUnfoldInvertT to get an initial solution and uses a marginal likelihood minimization to find the optimal regularization. [arXiv: 1811.01242]	kernel choice (only radial "1" is implemented now)	kernel function needs to describe truth well, and global regularisation strength may be varied locally along the spectrum by using a non-stationary kernel	do_GP

Regularisation parameter can be indicated as input:

```
example_q2.do_Svd(5)
```

```
example_q2.do_Bayes(30)
```

```
example_q2.do_Invert()
```
← apply unfolding using matrix-inversion method

```
example_q2.result_df
```
← result of unfolding

```
example_q2.result_cov
```
← post-unfolding covariance matrix

	bin_index	truth_central	measured_central	unfolded_central	unfolded_error	coverage_perbin
0	0	0.578678	0.578678	0.598678	0.119736	0.598678
1	1	0.296794	0.296794	0.290794	0.058159	0.290794
2	2	0.652948	0.652948	0.658948	0.131790	0.658948
3	3	0.606196	0.606196	0.616196	0.123239	0.616196
4	4	0.643521	0.643521	0.623521	0.124704	0.623521
5	5	0.624760	0.624760	0.604760	0.120952	0.604760
6	6	0.682689	0.682689	0.782689	0.156538	0.782689
7	7	0.682324	0.682324	0.682324	0.136465	0.682324
8	8	0.681740	0.681740	0.681740	0.136348	0.681740
9	9	0.635936	0.635936	0.635936	0.127187	0.635936

How-to

Single-run unfolding

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Regularisation parameter can be indicated as input:

```
example_q2.do_Svd(5)
```

```
example_q2.do_Bayes(30)
```

```
example_q2.do_Invert()   ← apply unfolding using matrix-inversion method
example_q2.result_df     ← result of unfolding
example_q2.result_cov    ← post-unfolding covariance matrix
```

	bin_index	truth_central	measured_central	unfolded_central	unfolded_error	coverage_perbin
0	0	0.578678	0.578678	0.598678	0.119736	0.598678
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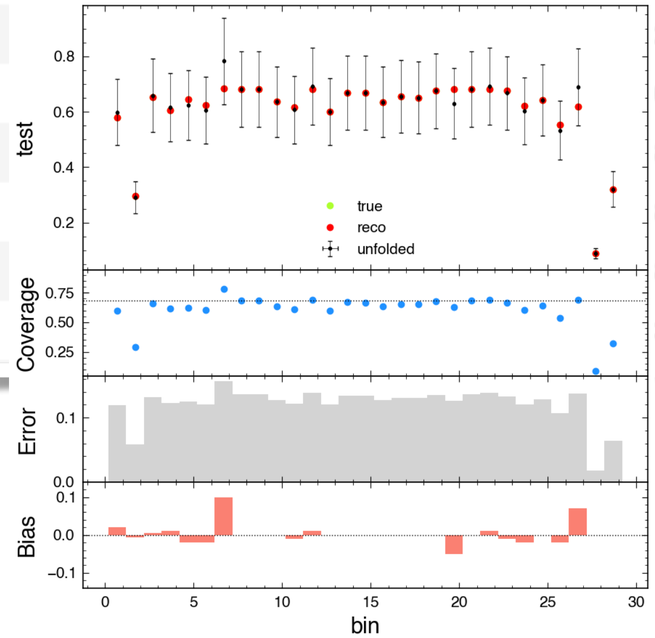
3	3	0.606196	0.606196	0.616196	0.123239	0.616196
4				23521	0.124704	0.623521
5				04760	0.120952	0.604760
6				82689	0.156538	0.782689
7				82324	0.136465	0.682324
8				81740	0.136348	0.681740
9				35936	0.127187	0.635936




```
fig = plot_compare_single_run_check(example_q2.result_df, bins, x_title='bin', y_title='test')
```

How-to

Toys unfolding

```
from pyroounfold.toy_unfold import toy_unfold

example_toy = toy_unfold(

    df_train = df_train,
    weight_train = df_train['weight'],
    df_test = df_test,
    weight_test = df_test['weight'],
    name_var_true = 'truth',
    name_var_reco = 'measured',
    show_var = 'variable',
    bins = my_bins,

    toy_size =1000

## optional input
    kcovtoy
    mc_stat_err

    reco_cov

    reco_bin_error

    )
```

← same as defined in single-run unfolding

← number of toys

← if reco_cov is given, toys will be generated based on it with multivariate Gaussian

← if no reco_cov, toys generation is based on reco_bin_error using Gaussian;
if none of above two are given, Poisson distribution based on stat. error of bin count will be used.
Generated toys are stored as dataframe example_toy.toys_df.

```
example_toy.do_toyUnfold( method='Invert',
                          get_fom=True)

example_toy.do_toyUnfold( method='Svd', para=5,
                          get_fom=True)
```

← apply unfolding with chosen method/parameters

← flag to calculate and save bias F.O.M.

```
example_toy.result_cen_mean
```

← median of central values from unfolded toys

```
example_toy.result_cen_err
```

← standard deviation of errors from unfolded toys

```
example_toy.result_coverage_perbin
```

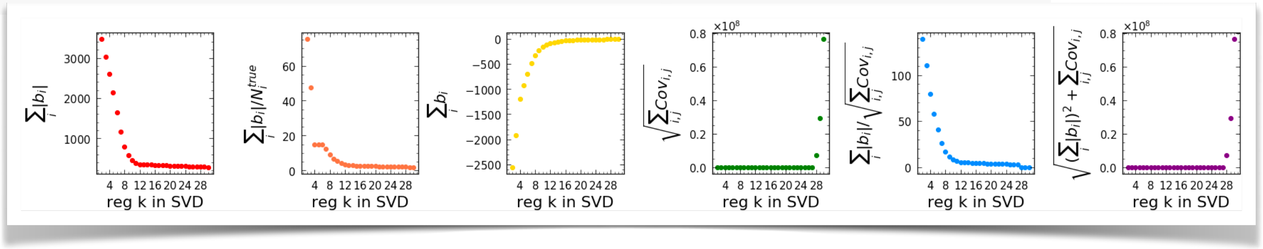
← averaged coverages from unfolded toys for each bin

For toys:

```
example_toy.dict_fom
```
← result of bias FOM if get_fom=True; returned as *dictionary* {‘fom_a’, ‘fom_b’, … nicknames listed previously }

For toys & various regulation parameters:

```
svd_cen, svd_err, svd_fom = example_toy.do_toyUnfold_scan( method='Svd', para_arr=np.arange(2,30), get_fom=True)
```



For single-run unfolding:

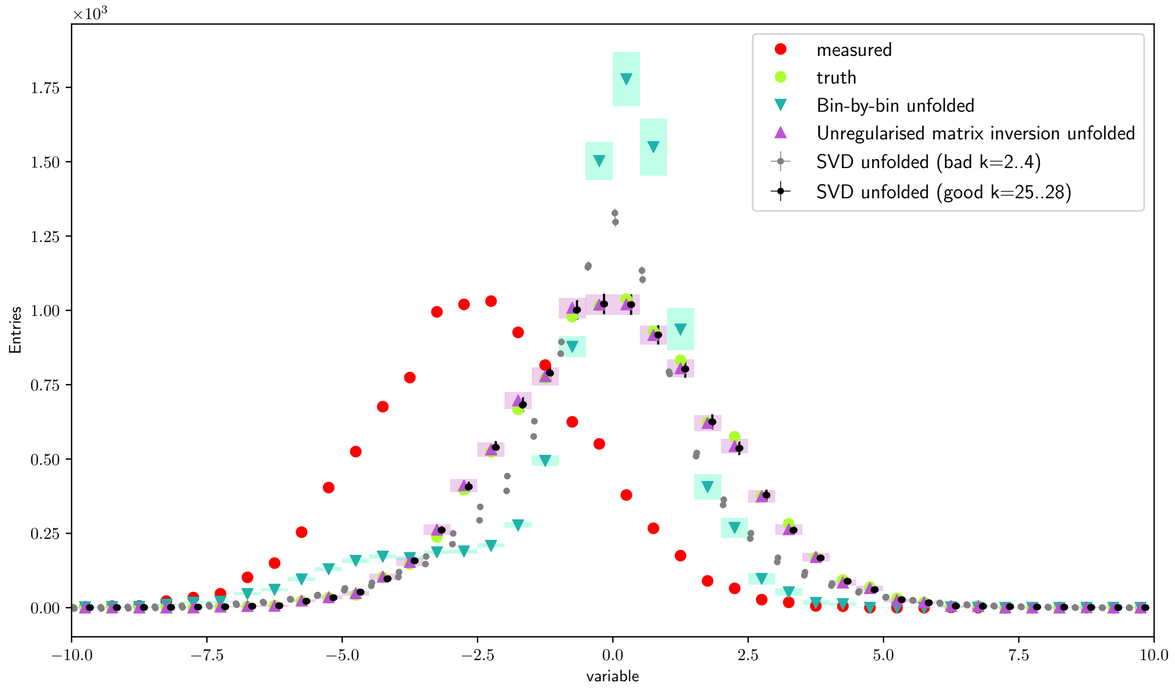
```
example_q2.do_Svd(5)

example_q2.check_bias()
```
← calculate and save bias F.O.M.

```
example_q2.bias_a
example_q2.bias_b
```
← results of bias F.O.M, bias_a, …, bias_h

Figure of Merit	Description	Nickname
$\sum_i \lvert b_i \rvert$	Sum of absolution biases in each bin, $b_i = N_i^{\text{unfolded}} - N_i^{\text{true}}$	a
$\sum_i \lvert b_i \rvert / N_i^{\text{true}}$	Sum of normalized absolute biases ($N_i^{\text{true}} \neq 0$)	b
$\sum_i b_i$	Sum of biases, which can be zero when significant biases are present in individual bins but cancel in the sum (balanced oscillation)	c
$\sqrt{\sum_{i,j} Cov_{i,j}}$	The square root of the sum of all elements of the post-unfold covariance matrix.	d
$\sum_i \frac{\lvert b_i \rvert}{\sqrt{\sum_{i,j} Cov_{i,j}}}$	Ratio of the sum of absolute biases and the error taking into account bin-to-bin correlations.	e
$\sqrt{\left(\sum_i \lvert b_i \rvert\right)^2 + \sum_{i,j} Cov_{i,j}}$	The total biases absorbing the total error with bin-to-bin correlations, which is used to check the general oscillation.	f
$\sum_i \frac{\lvert b_i \rvert}{\sqrt{Cov_{ii}}}$	The summed ratio of the absolute bias and unfolding error in each bin.	g
$\Phi(\frac{b_i}{\sigma_i} + 1) - \Phi(\frac{b_i}{\sigma_i} - 1)$	Coverage probability of intervals $[N_i^{\text{unfolded}} - \sigma_i, N_i^{\text{unfolded}} + \sigma_i]$, assuming N_i^{unfolded} is Gaussian distributed and Φ is the normal cumulative distribution function.	h

Validation Method And Parameters



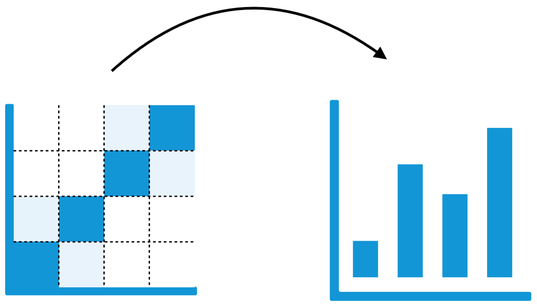
- In this test, matrix-inv and SVD (good k) recover the truth centres well.
- Regulation parameter *k* in SVD:

Take-home message:

choose method / tune para. with cautions for each specific case

Validation Scenario

Asimov



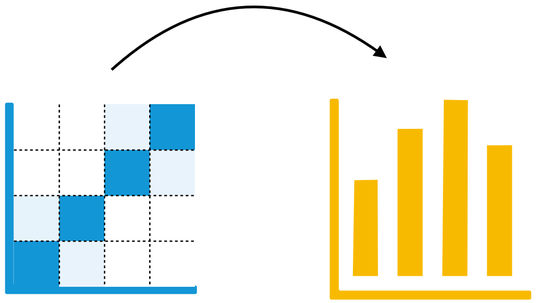
Nominal migration matrix

Nominal MC

train

test

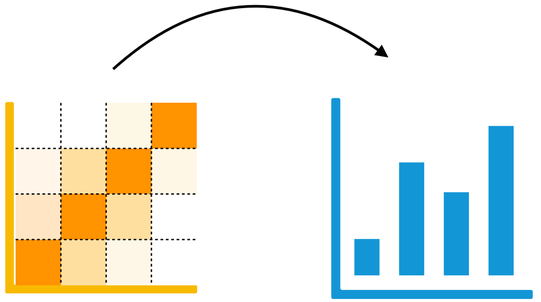
Varied type A



Nominal migration matrix

Varied MC

Varied type B



Varied migration matrix

Nominal MC

- Asimov test is mandatory validation but might be not sufficient
- Varied MC / migration matrix provide test scenario for potential mis-modelled shape and resolution in MC
- Such variations can be used to evaluate systematic uncertainty

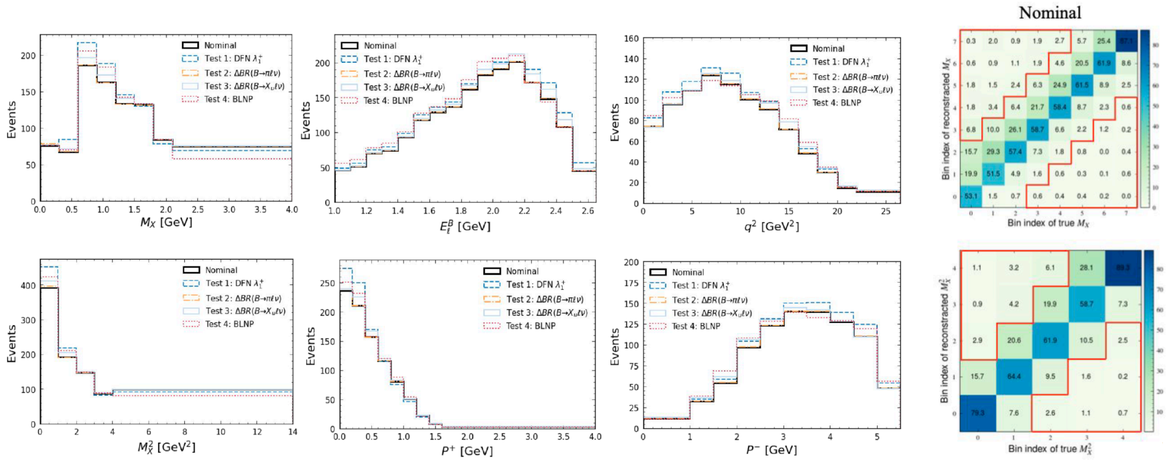
Benchmark Tests of Unfolding Differential $B \to X_u \ell \nu$ Spectra

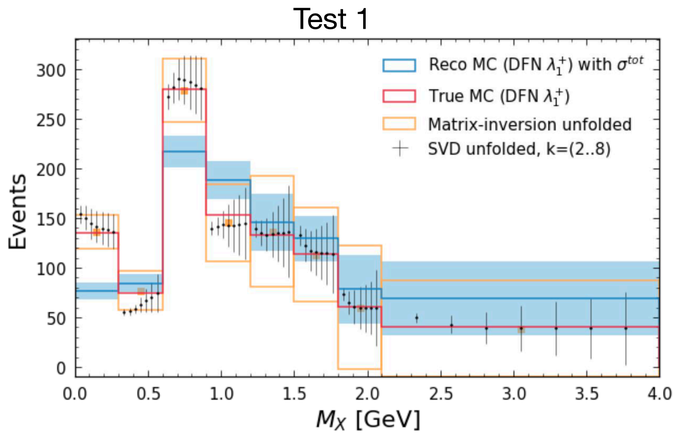
Type A:

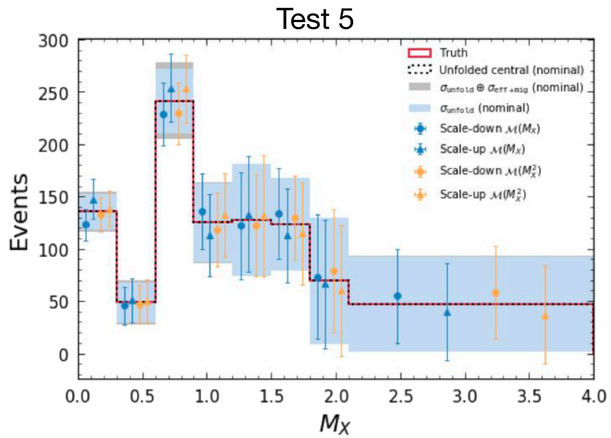
- Use nominal migration matrix to **unfold shifted MC:**
  - **Test 1**: shifted on one eigen-direction of inclusive modelling para. **DFN λ_1^+**
    - Enlarge +50% unc. in used DFN model for testing at an extreme point (max. 60 MeV for m_b and 0.6 for a)
  - **Test 2**: shifted 1σ on excl. component **BR(B→ πlν)**
  - **Test 3**: shifted 1σ on incl. **BR(B→ X_ulν)**
  - **Test 4**: replace DFN to **BLNP**

Type B:

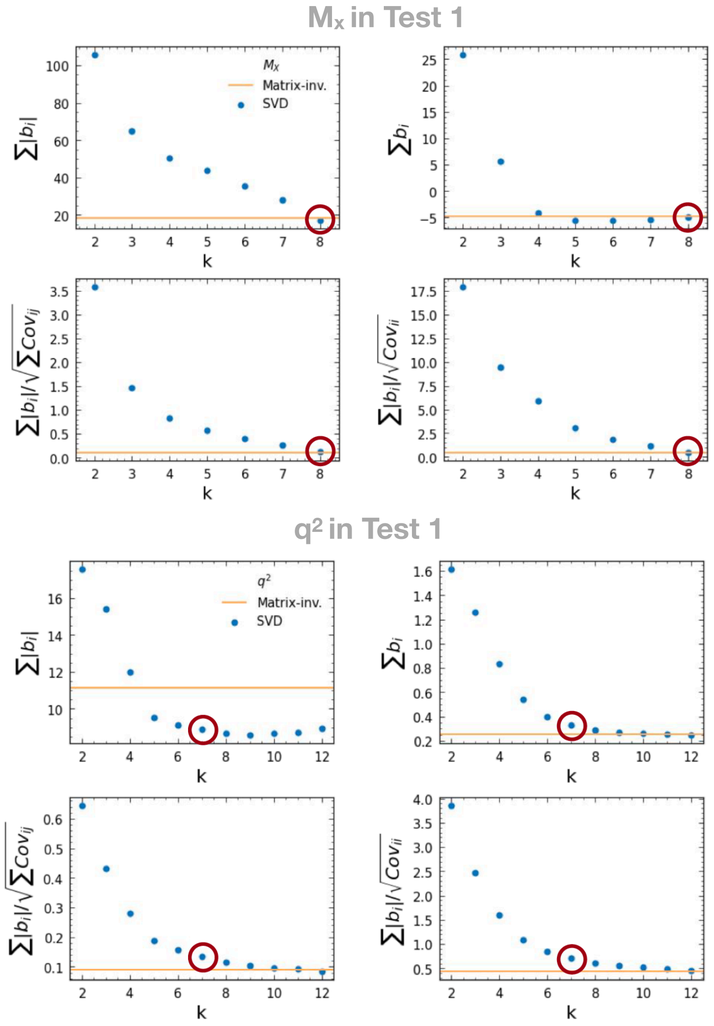
- **Test 5**: varied resolution effects in M_X and M_X^2 migration matrix by ±100% in tail region







- Bias FOM evaluated for tuning *k* in SVD method for each kin. variable
- Matrix-inv result shown as comparison
- Good *k* should be satisfied in all tests



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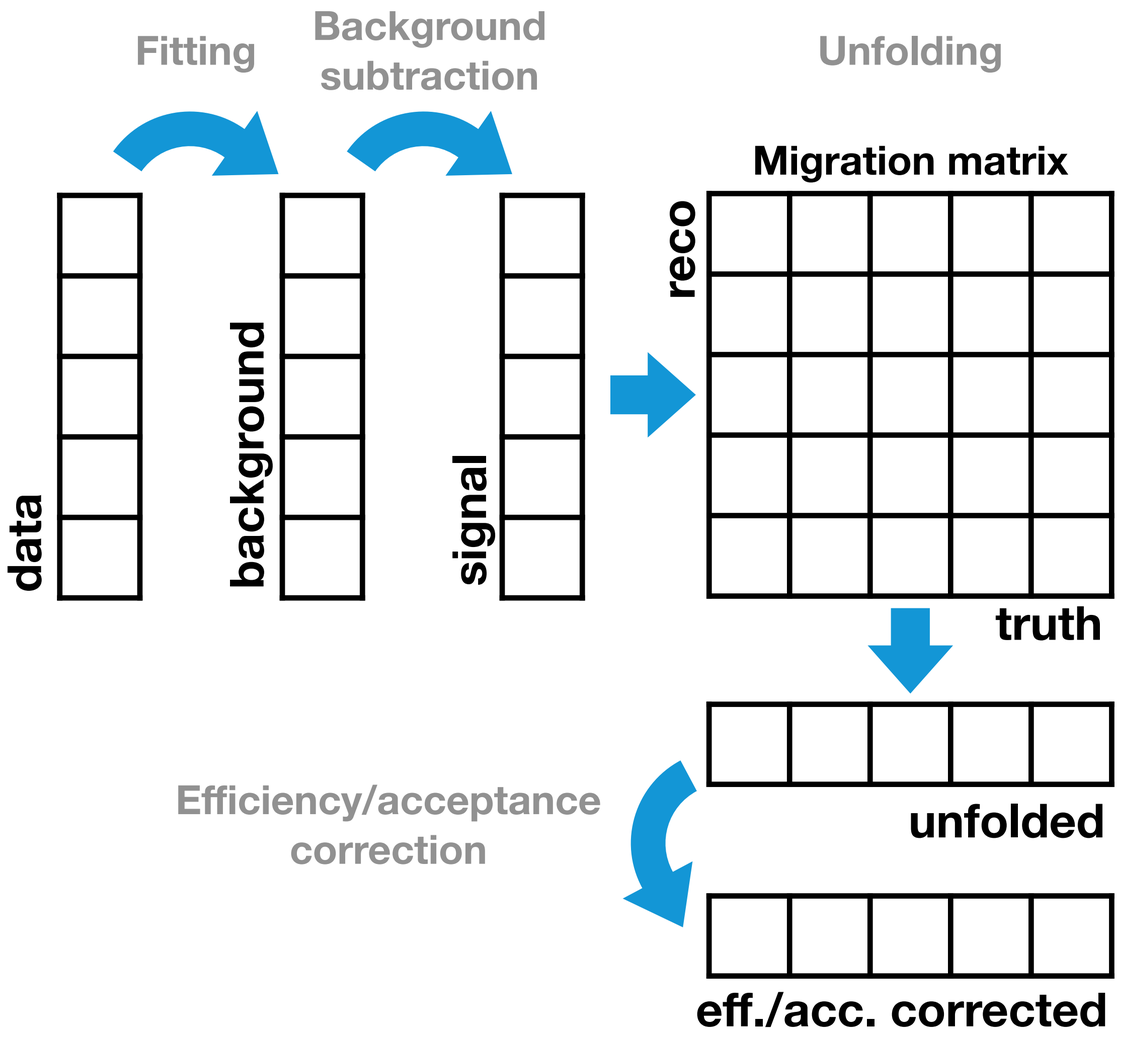
About Error Propagation

- The final uncertainty of unfolded result is a combination of
  - Propagated pre-unfolding uncertainty (resulted from background subtraction)
  - Variations of unfolded results considering modelling impacts of migration matrix
  - Bias due to choice of method and regularisation parameters

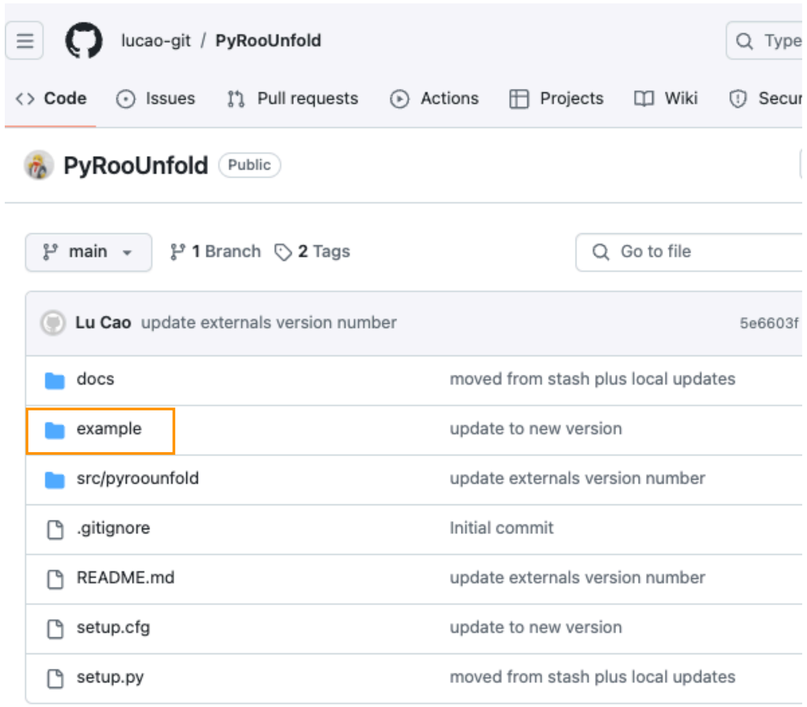
- Experimental systematic sources need to be varied simultaneously for unfolding migration matrix and efficiency correction, preferably also in the procedure of background subtraction (e.g. RooFitUnfold)

- Except bin-by-bin unfolding, most methods handle bin correlation according to regularisation or iteration parameter. Post-unfold correlation (covariance) should be checked



Repository

- Source code provided on https://github.com/lucao-git/PyRooUnfold
- Demo Jupyter notebook can be found in ./example



Install

- Please make sure RooUnfold has been installed before using PyRooUnfold.

If not, please first follow the steps to install RooUnfold
https://gitlab.cern.ch/RooUnfold/RooUnfold/-/blob/master/README.md

or, use a pre-installed RooUnfold (e.g. from CVMFS).

- After installing RooUnfold, please set the environment variable for your RooUnfold libary as

```
export ROOUNFOLD_PATH="/path/for/your/libRooUnfold.so"
```

e.g. in my case

```
export ROOUNFOLD_PATH="/Users/caolu/Workspace/RooUnfold/libRooUnfold.so"
```

or using CVMFS version provided as externals of Belle-II software

```
export ROOUNFOLD_PATH="/cvmfs/belle.cern.ch/el9/externals/v02-02-01/Linux_x86_64/common/lib/li
```

- To install PyRooUnfold, you can first check out the needed version, e.g.

```
git checkout -b v2.0.0
```

and then install the package via

```
pip install .
```

If install via setup.py, you need to include the package into your python library

```
export PYTHONPATH=$PYTHONPATH:<path-of-PyrooUnfold>
```

Versions/Tags

- v1.0.0: compatible with RooUnfold 2.0.1
- v2.0.0: compatible with RooUnfold 3.0.0