Consistent multi-differential histogramming and summary statistics with YODA2

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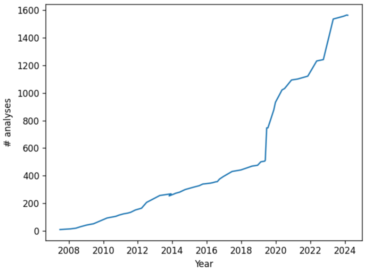
Introduction

- Yet more Objects for Data Analysis!
  [yoda.hepforge.org]
- lightweight and general purpose library for binned statistical data analysis
- first released in 2013
- written in C++ and programmatically usable from C++ and Python, complemented by a set of command-line tools for dataset inspection, manipulation and combination



- emerged from the sub-field of Monte Carlo event generator analysis and tuning in HEP, but library is deliberately agnostic of any particular application
- tools wrapping around YODA include [Rivet] and [Contur]
  - as such, widely used for event generator analysis, tuning, analysis preservation and reinterpretation efforts

Summary statistics

Analytic first- and second-order statistical moments for probably density function $f(x) \equiv \mathrm{d}P/\mathrm{d}x$

$$\langle x \rangle \equiv \int_{x \in X} x f(x)\,\mathrm{d}x$$

$$\langle x^2 \rangle \equiv \int_{x \in X} x^2 f(x)\,\mathrm{d}x$$

$$\sigma^2(x) \equiv \langle x^2 \rangle - \langle x \rangle^2$$

Weighted moments

Weighted mean and variance:

$$\langle x \rangle = \frac{\sum_n w_n x_n}{\sum_n w_n}$$

$$\sigma^2(x) = \mathcal{B} \cdot \frac{\sum_n w_n \left(x_n - \sum_m w_m x_m\right)^2}{\left(\sum_n w_n\right)} = \frac{\left(\sum_n w_n x_n^2\right) \cdot \left(\sum_n w_n\right) - \left(\sum_n w_n x_n\right)^2}{\left(\sum_n w_n\right)^2 - \sum_n w_n^2}$$

with weighted Bessel factor:

$$\mathcal{B} = \frac{N_\text{eff}}{N_\text{eff} - 1} = \frac{(\sum_n w_n)^2}{(\sum_n w_n)^2 - \sum_n w_n^2}$$

for effective fill count:

$$N_\text{eff} = \frac{(\sum_n w_n)^2}{\sum_n w_n^2}$$

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- generalise measured variable x to vector variable-space Ω
  - composed of vectors ω with differential volume elements $\mathrm{d}\Omega$
- partition Ω into disjoint (sub)set of bins $\{\Omega_b\} \subset \Omega$

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$$\langle \omega^{(i)} \rangle_b \equiv \int_{\omega \in \Omega_b} \omega^{(i)} f(\omega)\, \mathrm{d}\Omega$$

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- need to recover unbinned values when expanding the partition to whole space
- need to recover differential properties of the pdf itself as $\Omega_b \to \mathrm{d}\Omega(\omega)$
- merging bins must converge to the same result as having originally constructed a lower-dimensional or less finely binned partition of space

Design principles I

- Differential consistency
  - unlike list of (weighted) fill counts, histogram is a binned best-estimate of a continuous distribution
  - crucial to take $f(\boldsymbol{x}) \equiv \mathrm{d}P/\mathrm{d}\boldsymbol{x}$ notation literally since optimal estimation requires non-uniform binning

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- Integral consistency
  - ability to project higher- into lower-dimensional binnings without biasing integral quantities
  - including integrally consistent constructions of binned profiles from higher-dimensional histograms

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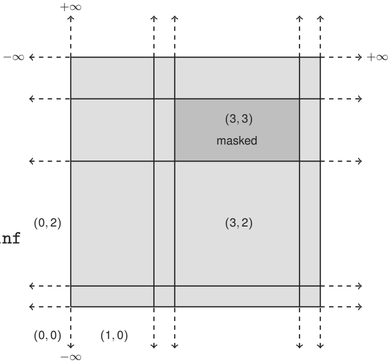
- User friendliness
  - aim to provide a “clean” programmatic interface expressed in terms of statistical and data-analytic concepts and hence well-matched to the goals and skill-sets of data scientists
  - hide the complexity of advanced language features used internally to make high levels of abstraction possible while enforcing statistical consistency and type-safety
  - intentionally limited to binned statistical analysis only, with zero library dependencies for core C++ operation, to assist embedding into applications

Experience from YODA1

- design goals partially established already at the time of YODA1 release in 2013, but structural issues motivated a ground-up rewrite
- limited data-object dimensionality and only continuous-valued axes supported
- inability to store arbitrary data-types in binnings
- correct but limited treatment of overflow bins
- no unified scheme for local and global bin indexing in multiple dimensions
- internal code duplication to support C++ and Python APIs for several different dimensionalities and binned-content types
- mismatching of the “inert" scatter datatype from e.g. HepData to the binned “live” objects from MC runs
- limited and inconvenient implementation of uncertainty breakdowns and correlations on scatter types

Bin partitioning

- new `Axis` class templated on edge type
- (classic) continuous axis triggered by `std::is_floating_point` trait
  - N bins defined by $N+1$ edges, plus under- and overflow bin
  - active uses of IEEE 754 FP standard; infinity binning:
    bin edges: `-inf -1.0 -0.5 0.0 0.5 1.0 +inf`
    bin widths: `+inf 0.5 0.5 0.5 0.5 +inf`



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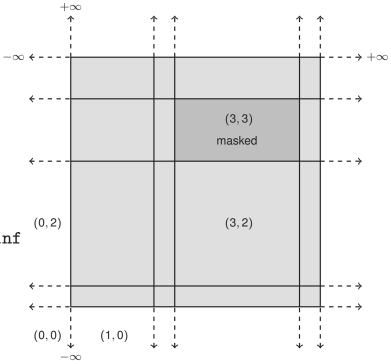

- (new) discrete axis for all other types
  - bins along discrete axis only have their edge label
  - N bins defined by N edges, plus otherflow bin
  - useful for multiplicities, cutflows, . . .
- `Binning` class permits slicing and marginalisaing across global fill-space and translates local indices into a global index and vice versa

Bin content

- `Bin` wrapper class that links bin content with the local and global binning properties
  - every bin has a `dVol()` method (also `dLen()`, `dArea()` aliases in 1D and 2D)
  - access to axis-specific quantities via templated accessor methods
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- Live content: `Dbn`
  - distribution class from YODA1, now generalised to arbitrary dimensions
  - keeps track of *exact* first and second order moments (and mixed moments $\sum_n w_n x_n y_n$)
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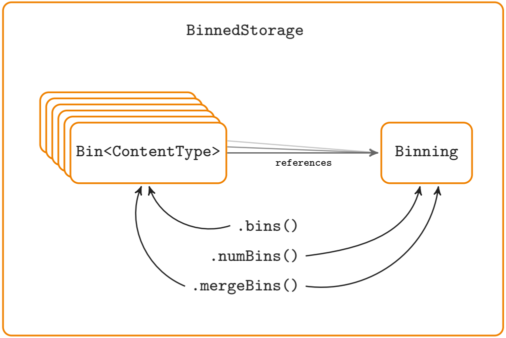
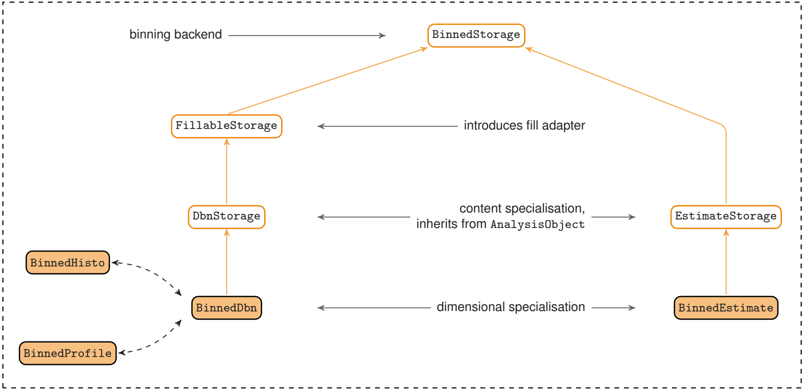
  - fill provides `fill` method accepting next coordinate set, optional weight and optional fill fraction
- Inert content: `Estimate`
  - a central value with an associated error breakdown
  - errors encoded as labelled uncertainty pairs corresponding to {down,up} variations of a nuisance parameter
  - support for correlated/uncorrelated treatment of different NPs
  - arithmetic operations respect (un-)correlated error treatment

Combined bin partitioning and content

- new `BinnedStorage` class can hold arbitrary types
  - supports index-based `bin(i)` and coordinate-based `binAt(x)` lookups
  - supports bin masking (`mask(i)`, `maskAt(x)`) to emulate "gaps" (in place of bin erasure)



A generic storage for binned quantities



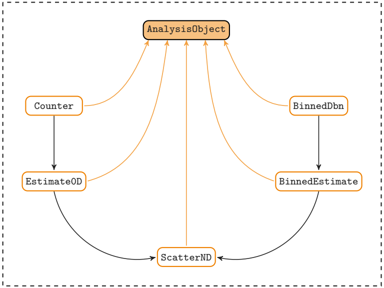
- new `FillableStorage` class inherits from `BinnedStorage`
  - introduces a fill adapter that handles the bin-content manipulation for each `fill` call
  - `fill` function returns bin position (global index) or `-1` if a coordinate was `nan`

Standard histograms and profiles

- intermediate DbnStorage layer introduces Dbn-specific methods (e.g. global integral, variance etc.)
- BinnedDbn is the user-facing type with various aliases for familiar classes
  - mixes in axis-specific method names (xMean(), yEdges(), etc.)
  - BinnedHisto<double,int> = BinnedDbn<2,double,int>
  - BinnedProfile<string> = BinnedDbn<2,string>
  - Histo2D = HistoND<2> = BinnedHisto<double,double> = BinnedDbn<2,double,double>
  - Profile1D = ProfileND<1> = BinnedProfile<double> = BinnedDbn<2,double>

Type and dimensionality reductions

- live `BinnedDbn` objects reduce to inert `BinnedEstimate` objects
  - with `Estimate1D = EstimateND<1> = BinnedEstimate<double>`
  - slice along axis `n` using `EstimateND<N>().mkEstimates<n>();` to yield vector of `EstimateND<N-1>`
- 0-dimensional variants with live `Counter` reducing to `Estimate0D`



- both live and inert types reduce to `Scatter` objects for plotting
- all user-facing types inherit from the `AnalysisObject` base class, which provides the attribute system to store metadata
- all types support global scaling operations; arbitrary transformations (e.g. lambda functions) can also be applied to all *inert* data types (estimates, points)

Example: construction and filling

```
// declaration examples
Histo1D h1; // histogram with 1 continuous axis
Profile2D p1; // profile with 2 continuously binned axes + 1 unbinned axis
HistoND<5> h2; // histogram with 5 continuous axes


// constructor examples
Histo1D h3(10, 0, 100); // 10 bins between 0 and 100
const std::vector<double> edges = {0, 10, 20, 30, 40, 50};
Histo1D h4(edges);
BinnedHisto<int, std::string> h5({ 1, 2, 3 }, { "A", "B", "C" });


// fill examples
Histo1D h6(5, 0.0, 1.0);
h6.fill(0.2);
Profile1D p2(5, 0.0, 1.0);
p2.fill(0.2, 3.5);


// marginalisation examples
Histo2D h7 = p1.mkHisto(); //< marginalise over unbinned axis
Histo1D h8 = h7.mkMarginalHisto<1>(); //< marginalise over secomd binned axis
Histo1D h9 = p1.mkMarginalProfile<0>(); //< marginalise over first binned axis
```

Example: looping and indexing

```
size_t nbinsX = 4, nbinsY = 6;
double lowerX = 0, lowerY = 0;
double upperX = 4, upperY = 6;
Histo2D h2(nbinsX, lowerX, upperX,
           nbinsY, lowerY, upperY);

// loop over bins and fill with increasing weight
double w = 0;
for (auto& b : h2.bins()) { //< iterators passes through using templated bin wrappers
  h2.fill(b.xMid(), b.yMid(), ++w);
}

for (size_t idxY = 0; idxY < h2.numBinsY(true); ++idxY) { //< true includes overflows
  for (size_t idxX = 0; idxX < h2.numBinsX(true); ++idxX) { //< true includes overflows
    std::cout << "\t(" << idxX << "," << idxY << ")\t=\t";
    std::cout << h2.bin(idxX, idxY).sumW();
  }
  std::cout << std::endl;
}
std::cout << std::endl;

# H2 bins using local indices + under/overflows:
#   (0,0) = 0 (1,0) =  0 (2,0) =  0 (3,0) =  0 (4,0) =  0 (5,0) = 0
#   (0,1) = 0 (1,1) =  1 (2,1) =  2 (3,1) =  3 (4,1) =  4 (5,1) = 0
#   (0,2) = 0 (1,2) =  5 (2,2) =  6 (3,2) =  7 (4,2) =  8 (5,2) = 0
#   (0,3) = 0 (1,3) =  9 (2,3) = 10 (3,3) = 11 (4,3) = 12 (5,3) = 0
#   (0,4) = 0 (1,4) = 13 (2,4) = 14 (3,4) = 15 (4,4) = 16 (5,4) = 0
#   (0,5) = 0 (1,5) = 17 (2,5) = 18 (3,5) = 19 (4,5) = 20 (5,5) = 0
#   (0,6) = 0 (1,6) = 21 (2,6) = 22 (3,6) = 23 (4,6) = 24 (5,6) = 0
#   (0,7) = 0 (1,7) =  0 (2,7) =  0 (3,7) =  0 (4,7) =  0 (5,7) = 0
```

YODA I/O

- generalising the existing V2 ASCII format to arbitrary dimensions and supporting `std::string`-based edges required a little restructuring:

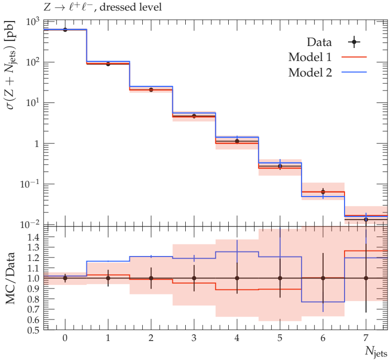
```
BEGIN YODA_HISTO1D_V3 /H1D_d
Path: /H1D_d
Title:
Type: Histo1D
---
# Mean: 3.470588e-01
# Integral: 1.700000e+01
Edges(A1): [0.000000e+00, 5.000000e-01, 1.000000e+00]
# sumW          sumW2           sumW(A1)        sumW2(A1)       numEntries
0.000000e+00    0.000000e+00    0.000000e+00    0.000000e+00    0.000000e+00
1.000000e+01    1.000000e+02    1.000000e+00    1.000000e-01    1.000000e+00
7.000000e+00    4.900000e+01    4.900000e+00    3.430000e+00    1.000000e+00
0.000000e+00    0.000000e+00    0.000000e+00    0.000000e+00    0.000000e+00
END YODA_HISTO1D_V3

BEGIN YODA_BINNEDHISTO<S>_V3 /H1D_s
Path: /H1D_s
Title:
Type: BinnedHisto<s>
---
# Mean: 3.750000e-01
# Integral: 8.000000e+00
Edges(A1): ["A"]
# sumW          sumW2           sumW(A1)        sumW2(A1)       numEntries
5.000000e+00    2.500000e+01    0.000000e+00    0.000000e+00    1.000000e+00
3.000000e+00    9.000000e+00    3.000000e+00    3.000000e+00    1.000000e+00
END YODA_BINNEDHISTO<S>_V3
```

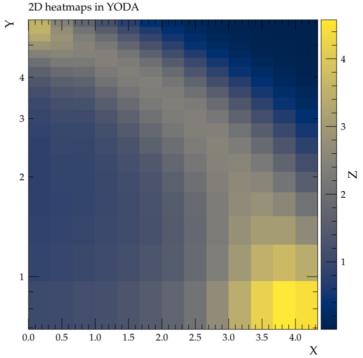
- already the default on HepData! (old format still available via `YODA1` option)

- YODA2 reader can still read old ASCII format from YODA1

Plotting

- `matplotlib`-based plotting machinery produces **self-consistent Python scripts** allowing for better customisation of plots (no YODA installation required)





- plots drawn from `Scatter` objects
  - final abstraction layer to seperate style choices for rendering data from statistical analysis

Summary

- histograms are a powerful tool and often taken for granted
- summary statistics grouped into binned ranges of e.g. an independent variable
- fixed data size regardless of how many “fill" events are aggregated into them
- directly linked to core concepts in differential and integral calculus
- a decade after its first release, YODA backend underwent a ground-up redesign
- statistical analysis objects generalised to arbitrary dimensions and edge types along different axes – with the help of modern C++ design patterns
- YODA 2.0.0 has been out for a couple of months now – check it out: [yoda.hepforge.org]

Backup

Unweighted moments

Unweighted mean and variance for finite-size sample with $1 \leq n \leq N$:

$$\langle \hat{x} \rangle_\mathrm{U} \equiv \frac{\sum_{n=1}^{N} x_n}{N}$$

$$\sigma^2_\mathrm{U}(\hat{x}) \equiv \frac{\sum_{n=1}^{N} (x_n - \langle x \rangle)^2}{N-1}$$

$$= \langle x^2 \rangle_\mathrm{U} - \langle x \rangle^2_\mathrm{U}$$

$$= \frac{\sum_{n=1}^{N} x_n^2}{N-1} - \frac{\left(\sum_{n=1}^{N} x_n\right)^2}{(N-1)^2}$$

Counts and efficiencies

Closely related quantities are Poisson mean and variance:

$$\langle \hat{x} \rangle_{\mathrm{P}} \equiv N$$

$$\sigma^2_{\mathrm{P}}(\hat{x}) \equiv N$$

Classic Monte Carlo scaling then given by

$$\frac{\sigma_{\mathrm{P}}(\hat{x})}{\langle \hat{x} \rangle_{\mathrm{P}}} = \frac{\sqrt{N}}{N} = \frac{1}{\sqrt{N}}$$

Sample efficiency for selected events N_{sel} from a known number of total events N is

$$\hat{\epsilon} \equiv \frac{N_{\mathrm{sel}}}{N}$$

Binomial statistics gives an estimator for the uncertainty on the efficiency

$$\hat{\sigma}^2(\hat{\epsilon})_{\mathrm{B}} = \frac{\hat{\epsilon}(1 - \hat{\epsilon})}{N}$$

Connection to differential calculus

- statistical histogram: a **discrete approximation to entire probability density function** $f(\Omega) = \mathrm{d}P/\mathrm{d}\Omega$ or population density $\mathrm{d}N/\mathrm{d}\Omega$, not just a collection of fill counts

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  - generally not desirable for finite bins to have the same width
  - using non-uniform bin sizes ensures statistical relative uncertainty on bin populations is equally distributed across histogram
  - failing to divide by the bin measure distorts the distribution away from its physical shape

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  - using non-uniform bin sizes ensures statistical relative uncertainty on bin populations is equally distributed across histogram
  - failing to divide by the bin measure distorts the distribution away from its physical shape
- actual bin populations are better computed using a discrete binning expressed in terms of finite probabilities rather than densities
  - awkward workaround: multiply each density by the fill volume
  - prefer to refer to this not as a histogram but a bar chart, reflecting its typical use

Profiles

- useful class of histogram mixing binned and unbinned variable subspaces
- allow characterisation of the unbinned dimensions Υ via their moments as projected into each partition of the bin-space Θ
  - allow statistical aggregation of finite samples into "independent variable" bins $\theta \in \Theta_b$, while characterising the mean dependence of the unbinned dependent variables y on θ
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  - linearity of statistical moments again ensures consistency when merging bins
- unbinned space Υ can in general be multidimensional but canonical bin value then ambiguous
- definiteness retained for single-dimensional unbinned space with moments $\langle y \rangle$ and $\langle y^2 \rangle$
  - profile canonical bin value is the mean $\langle y(\Theta) \rangle$ as a function of binned coordinates
  - nominal uncertainty given by standard error $\hat{\sigma}_{\bar{y}}(\theta) = \hat{\sigma}_b / \sqrt{N_b}$ for effective sample count N_b in bin $b \subset \theta$

Variadic templates and parameter packs

- Metaprogramming using C++17 takes care of generalisation to arbitrary dimensions:

```
#include <iostream>
#include <string>
#include <tuple>
#include <vector>

template <typename... Args>
class MyHisto {
public:
  MyHisto(const std::vector<Args>& ... edges)
    : _axes(edges ...) { }

  size_t dim() const { return sizeof...(Args); }

  template<size_t I>
  void printBinning() const {
    if constexpr (I < sizeof...(Args)) {
      std::cout << "Axis" << (I+1) << "has";
      std::cout << std::get<I>(_axes).size();
      std::cout << "bins." << std::endl;
      printBinning<I+1>();
    }
  }

  void print() const {
    std::cout << dim() << "D:" << std::endl;
    printBinning<0>();
  }

private:
  std::tuple<std::vector<Args>...> _axes;
};
```

Support of YODA2 in Rivet4

- Rivet adopted YODA2 starting with its 4.0 series
  - all reference data shipped with Rivet has been converted to the new types
  - HepData already supports YODA2 by default: writes out `BinnedEstimate` objects
- `TypeRegister`: edge combination of `double`, `int` and `string` pre-registered for 1D and 2D objects, others can be registered on the fly:
  - `RIVET_REGISTER_TYPE(YODA::BinnedHisto<double,int,string,double>)`
  - `RIVET_REGISTER_BINNED_SET(double, double, string, int)`
- routines adjusted to use discrete binning where appropriate
- Rivet's custom `BinnedHistogram` class got replaced with a `HistoGroup` class (a `FillableStorage` with a “group axis" and a `BinnedHisto` as bin content)

```
Histo1DGroupPtr _hist; //< Histo1DGroup = HistoGroup<double,double>
...
book(_hist, { 1.0, 2.0, 3.0, 4.0 });
for (auto& bin : hist->bins()) {
  book(bin, 1, 1, bin.index());
}
...
_hist->fill(val1, val2);
...
normalize(_hist); // or: scale(_hist, crossSection()/sumOfWeights());
divByGroupWidth(_hist); // divide by bin width along group axis
```

Better support for massive MPI applications

- YODA2 inheritance structure makes it straightforward to `serialize` the data
  - numerical content of `AnalysisHandler` can be translated into `std::vector<double>`
  - arrays of primative types lend themselves better to MPI communication
- corresponding `deserialize` method to load the data block back into an `AnalysisHandler` for merging
- reduced I/O load from parsing info files in the initialisation phase
- more profiling and optmisations envisaged for the Rivet4 series