HS³ - Overview of supported types and components

06. April 2023

1 Introduction

With the introduction of pyhf [1], a JSON format for likelihood serialization has been put forward. However, an interoperable format that encompasses likelihoods with a scope beyond stacks of binned histograms was sorely lacking. With the release of ROOT 6.26/00 [2] and the experimental RooJSONFactoryWSTool therein, this gap has now been filled.

This document sets out to document the syntax and features of the HEP Statistics Serialization Standard (HS³) for likelihoods and statistical models in general, as to be adopted by any HS³-compatible statistics framework.

Please note that this document as well as the HS³ standard are still in development and can still undergo minor and major changes in the future. This document describes the syntax of version 0.2 of the HS³ standard.

1.1 How to read

In the context of this document, any JSON object is referred to as a component. A key-value-pair inside such a component is referred to as a component. If not explicitly stated otherwise, all components mentioned are mandatory.

The components located inside the top-level object are referred to as top-level components.

1.2 Terms and Types

This is a list of used types and terms in this document.

struct	$key:value$ mapping, keys are of type $\mathbf{string}.$ Represented with { }
array	array of items (either ${\bf strings}$ or ${\bf numbers})$ without keys. Represented with []
string	references to objects, names and arbitrary information. Represented with " $"$
number	either floating or integer type values

Boolean values; they can be encoded as true and false or 1 and 0 respectively

All structs inside an array should always have a component name.

Within most top-level components, any one string given as a value to any component should always refer to the name of another, fully qualified component, unless explicitly stated otherwise. Top-level components in which this is not the case are explicitly marked as such.

2 Top-level components

In the following the top-level components of HS^3 and their parameters/arguments are described. Each component is completely *optional*, but certain components might depend on other components, which need to be provided in that case. The only exception is the component metadata containing the version of HS^3 , which is always required. In short the supported top-level components are

distributions (optional) array of distributions

functions (optional) array of mathematical functions

data (optional) array of data (or simulated data)

likelihoods (optional) array of combinations of distributions and data

domains (optional) array of domains, describing ranges of parameters;

parameter_points

(optional) array of parameter points, to be used as starting points for minimizations or to document best-fit-values or nominal truth values of datasets

analyses (optional) array of suggested analyses to be run on the models in this file

metadata required struct containing meta information; required HS³ version number,

(optional), e.g., authors, paper references, package versions, data/analysis

descriptions

misc (optional) struct containing miscellaneous information, e.g. optimizer settings,

plotting colors, etc.

In the following each of these are described in more detail with respect to their own structure.

2.1 Distributions

The top-level component distributions contains an array of distributions in struct format. Each distribution has to have the components type denoting the kind of distribution described and a component name. Distributions in general have the following keys:

name custom string

type string that determines the kind of distribution, e.g. gaussian_dist

each distribution has individual parameter components for the various individual parameters. For example, distributions of type gaussian_dist have the specific components mean, sigma and x. In general, these components can contain strings as references to other objects, numbers or boolean values. Depending on the parameter and the type of distribution, they appear either

in single item or array format.

Example: Distributions

In the following all implemented distributions are listed in detail.

2.1.1 Exponential distribution

The PDF of the exponential distribution is defined as

ExponentialPdf
$$(x, c) = \mathcal{N} \cdot \exp(c \cdot x),$$
 (1)

where \mathcal{N} is a normalisation constant that depends on the range and values of the arguments.

2.1.2 Gaussian/Normal distribution

The PDF of a Gaussian/Normal distribution is defined as

GaussianPdf
$$(x, \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(\frac{(x-\mu)^2}{\sigma^2}\right).$$
 (2)

name custom string

 ${\tt type} \hspace{1.5cm} {\tt gaussian_dist} \hspace{1.5cm} or \hspace{1.5cm} {\tt normal_dist}$

 \mathbf{x} number or name of the variable x

mean number or name of the parameter used as mean value μ

sigma number or name of the parameter encoding the root-mean-square width σ .

2.1.3 Log-normal Distribution

The PDF of the Log-normal distribution is defined as

$$LogNormalPDF(x, m_0, k) = \frac{1}{\sqrt{2\pi \cdot \ln(k) \cdot x}} \cdot \exp\left(\frac{-\ln^2(\frac{x}{m_0})}{2\ln^2(k)}\right).$$
(3)

name custom string

type lognormal_dist

 \mathbf{x} number or name of the variable x

mean number or name of the parameter used as mean value m_0

 \mathbf{k} number or name of the parameter k describing the shape

2.1.4 Multivariate Normal distribution

The PDF of the multivariate normal distribution is defined as

MvNormalPDF(
$$\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\Sigma}$$
) = $(2\pi)^{-k/2} \det(\boldsymbol{\Sigma})^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\mathsf{T} \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right)$, (4)

with Σ being positive-definite.

name custom string

type multinormal_dist

 \mathbf{x} array of numbers or names of the variables \mathbf{x}

mean array of length k of the parameters used as locations μ

covariances array of arrays of dimension $k \times k$ containing numbers or names for the

covariance matrix Σ . In general, the covariance matrix Σ needs to be positive

semi-definite.

2.1.5 Poisson distribution

The PDF of a Poisson distribution is defined as

$$P_{\lambda}(k) = \frac{\lambda^k}{k!} e^{-\lambda}.$$
 (5)

type poisson_dist

 \mathbf{x} number or name of the variable x serving as observable k.

2.1.6 Argus Background distribution

The PDF of the Argus background distribution is defined as

$$\operatorname{Argus}(m, m_0, c, p) = \mathcal{N} \cdot m \cdot \left[1 - \left(\frac{m}{m_0} \right)^2 \right]^p \cdot \exp \left[c \cdot \left(1 - \left(\frac{m}{m_0} \right)^2 \right) \right]$$
 (6)

and describes the ARGUS background shape.

type argus_dist

number or name of the variable m used as mass mass

resonance number or name of the parameter used as resonance m_0

slope number or name of the parameter used as slope c

power number or name of the parameter used as exponent p.

Addition of distributions 2.1.7

The PDF of this so-called Mixture Distribution is a sum of PDFs f_i :

$$MixturePdf(x) = \sum_{i=1}^{n-1} c_i * f_i(\vec{x})$$
 (7)

where the c_i are coefficients and \vec{x} is the vector of variables. If the number of coefficients is one less than the number of distributions, c_n is computed from the other coefficients as

$$c_n = 1 - \sum_{i=1}^{n-1} c_i \tag{8}$$

namecustom string

 $mixture_dist$ type

summands array of names referencing distributions

coefficients array of names of coefficients c_i or numbers to be added

2.1.8 Product Distribution

The PDF of the product of PDFs of independent distributions f_i is defined as

$$\operatorname{ProductPdf}(x) = \prod_{i}^{n} f(x). \tag{9}$$

custom string name product dist

type

factors array of names referencing distributions

2.1.9 Continuous Uniform Distribution

The PDF of a continuous uniform distribution is defined as:

UniformPdf
$$(x, a, b) = \frac{1}{b - a}$$
 $a \le x \le b.$ (10)

 $\verb"max" number or name of the parameter used as upper bound of range $b$$

min number or name of the parameter used as lower bound of range a

2.1.10 Polynomial Distribution

The PDF of a polynomial distribution is defined as

PolynomialPdf
$$(x, a_0, a_1, a_2, ...) = \sum_{i=0}^{n} a_i x^i = a_0 + a_1 x + a_2 x^2 + ...$$
 (11)

name custom string

type polynomial_dist

 \mathbf{x} number or name of the variable x

coefficients array of coefficients a_i . The length of this array implies the degree of the

polynomial.

2.1.11 HistFactory Distribution

HistFactory [3] is a language to describe statistical models consisting only of "histograms" (which is used interchangeably with "step-functions" in this context). Each HistFactory distribution describes one "channel" or "region" of a binned measurement, containing a stack of "samples", i. e. binned distributions sharing the same binning (step-functions describing the signal or background of a measurement). Such a model is shown in Figure 1. Each of the contributions may be subject to modifiers.

$$HistFactoryPdf(x, \vec{\theta}) = \prod_{b \in bins} Poisson(n|\lambda)$$
 (12)

where λ is the prediction in the given bin. This prediction is computed as

$$\lambda = \sum_{s \in \text{samples}} \left[\left(d_s(x) + \sum_{\delta \in M_{\delta}} \delta(x, \theta_{\delta}) \right) \prod_{\kappa \in M_{\kappa}} \kappa(x, \theta_{\kappa}) \right]$$
(13)

Here $d_s(x)$ is the distribution associated with the sample s, a step function

$$d_s(x) = \chi_b^{y_s}(x) \tag{14}$$

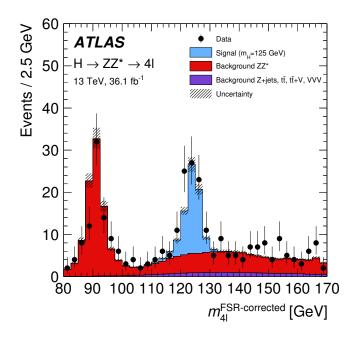


Figure 1: A binned statistical model describing a High Energy Physics measurement, in this case of the $H \to 4\ell$ process by the ATLAS collaboration.

In this section, $\chi_b^{y_s}(x)$ denotes a generic step function in the binning b such that $\chi_b(x) = y_{s,i}$, some constant, if $x \in [b_i, b_{i+1})$. The $y_{s,i}$ in this case are the bin contents (yields) of the histograms. The M_{κ} are the multiplicative modifiers, the M_{δ} are the additive modifiers. Each of the modifiers is either multiplicative (κ) or additive (δ) . All samples and modifiers share the same binning b. The modifiers depend on a set of nuisance parameters θ , where each modifier can only depend on one θ_i , but the θ_i can take the form of vectors and the same θ_i can be shared by several modifiers. By convention, these are denoted α if they affect all bins in a correlated way, and γ if they affect only one bin at a time. The types of modifiers are

- A uncorrelated shape systematic or shapesys modifier is a multiplicative modifier that scales each single bin by the value of some independent parameter γ . Here, $\theta_i = \vec{\gamma}$, where the length of $\vec{\gamma}$ is equal to the number of bins in this region.
- A correlated shape systematic or histosys modifier is an additive modifier that adds or subtracts a constant step function χ^f , scaled with a single factor α . The modifier contains a data section, which contains the subsections hi and lo that help to define the step function χ^f . They contain contents, which define the bin-wise additions or subtractions for $\alpha = 1$. Here, $\theta_i = \alpha$.
- A normalization systematic or normsys modifier is a multiplicative modifier that scales the entire sample in this region with the same constant factor f that is a function of α . The modifier contains a data section, which contains the values hi and 10 that help to define f. There are different functional forms that can be chosen for f. However, by convention $f(\alpha = 0) = 1$, $f(\alpha = +1) =$ "hi" and $f(\alpha = -1) =$ "10". In this case, $\theta_i = \alpha$.

- A normalization factor or normfactor modifier is a multiplicative modifier that scales the entire sample in this region with the value of the parameter μ itself. In this case, $\theta_i = \mu$.
- The staterror modifier is a shorthand for encoding uncorrelated statistical uncertainties on the values of the step-functions, using a variant of the Barlow-Beeston Method [4]. Here, the relative uncertainty on the sum of all samples in this region containing the staterror modifier is computed bin-by-bin. Then, a constrained uncorrelated shape systematic (shapesys) is created, encoding these relative uncertainties in the corresponding Poisson (or Gaussian) constraint term.

type of modifier	description	definition	free parameters
shapesys	Uncorrelated Shape systematic	$\kappa(x, \vec{\gamma}) = \chi_b^{\gamma} \cdot \chi_b^f$	$\gamma_0,, \gamma_n$
histosys	Correlated Shape systematic	$\delta(x,\alpha) = \alpha * \chi_b^f$	α
normsys	Normalization systematic	$\kappa(x,\alpha) = f(\alpha)$	α
normfactor	Normalization factor	$\kappa(x,\mu) = \mu$	μ
${\tt shapefactor}, {\tt stat_error}$	Shape factor	$\kappa(x, \vec{\gamma}) = \chi_b^{\gamma}$	$\gamma_0,, \gamma_n$

Modifiers can be constrained. In essence, the likelihood picks up a penalty term for changing the corresponding parameter too far away from its nominal value. If a modifier has a constraint, which can be of the type Gauss for a unit gaussian, Poisson for a Poissonian, or LogNormal, a corresponding constraint term will be considered in addition to the aux_likelihood section of the likelihood, constraining the parameter to its nominal value. The nominal values are $\alpha=0$, $\gamma=1$, $\mu=1$.

array of structs representing the axes. If given each struct needs to have the component name. Further, (optional) components are max, min and nbins.

samples array of structs containing the samples of this channel. For details see below.

Struct of one sample:

name custom string

data struct containing the components contents and errors, depicting the data

contents and their errors. Both components are arrays of the same length.

modifiers array of structs with each struct containing a component name and a type of modifier. Further (optional) components are data and constraints both

depending on the type of modifier. For details on these components, see the

description above.

```
HistFactory

{
    "name": "myAnalysisChannel",
    "type": "histfactory_dist",
```

¹The variation consists of summarizing all contributions in the stack to a single contribution as far as treatment of the statistical uncertainties is concerned.

```
"axes": [
      {
            "max": 1.0,
            "min": 0.0,
            "name": "myRegion",
"nbins": 2
      }
],
 "samples": [
      {
            "name": "mySignal",
"data": {
                  "contents": [ 0.5, 0.7 ],
                  "errors": [ 0.1, 0.1 ]
             "modifiers": [
                  {
                        "name": "Lumi",
"type": "normfactor"
                  },
                        "name": "mu_signal_strength",
"type": "normfactor"
                  },
                       "constraint": "Gauss",
"data": { "hi": 1.1, "lo": 0.9 },
"name": "my_normalization_systematic_1",
"type": "normsys"
                  },
                        "constraint": "Poisson",
                        "name": "staterror",
"type": "staterror"
                  },
                        "constraint": "Gauss",
"data": { "hi": { "contents": [ -2.5, -3.1 ] }, "lo": { "
                            contents": [ 2.2, 3.7 ] } },
                        "name": "my_correlated_shape_systeamtic_1",
"type": "histosys"
                   },
                   {
                        "constraint": "Poisson",
                       "data": { "vals": [ 0.0, 1.2 ] },
"name": "my_uncorrelated_shape_systematic_2",
"type": "shapesys"
            ]
      },
            "name": "myBackground"
            . . .
     }
]
```

2.2 Functions

The top-level component functions describes an array of mathematical functions in struct format to be used as helper objects. Similar to distributions each entry is required to have the components type and name. Other components are dependent on the kind of functions. Functions in general have the following components:

name custom string

type string that determines the kind of function, e.g. sum

each function has individual parameter keys for the various individual parameters. For example, functions of type sum have the parameter key summands. In general, these keys can describe strings as references to other objects or numbers. Depending on the parameter and the type of function, they appear either in single item or array format.

Example: Functions

In the following the implemented functions are described in detail.

2.2.1 Product

A product of values or functions a_i .

$$\operatorname{Prod} = \prod_{i}^{n} a_{i} \tag{15}$$

name custom string

type product

factors array of names of the elements of the product or numbers.

2.2.2 Sum

A sum of values or functions a_i .

$$Sum = \sum_{i}^{n} a_{i} \tag{16}$$

name custom string

type sum

summands array of names of the elements of the sum or numbers.

2.2.3 Generic Function

Note: Use of this function type is discouraged in favour of more specific function types.

A generic mathematical function, encoded by a string.

This function type is intended to encapsulate elementary mathematical operations such as addition("+"), subtraction("-"), multiplication("*") and division("/"). For any function-calls, such as exp, pow, min, max or similar, the behavior is undefined. Frameworks developers are encouraged to use their frameworks built-in just-in-time-compiler or interpreter to parse this expression without pre-processing and raise an exception when this fails.

expression a string with a generic mathematical expression. Simple mathematical syntax

common to programming languages should be used here, such as x-2*y+z. For

any non-elementary operations, the behavior is undefined.

2.3 Data

The component data contains an array of data sets in struct format. Each data set needs to contain the components type and name. Other components are dependent on the type of data set as depicted in the following

name custom string

type string that determines the format of the observations

each type of observations has different parameter keys. Some of these are

optional and marked accordingly in the more detailed description below

A detailed description of the different types with examples can be found below.

2.3.1 Point Data

Point data describes a measurement of a single number, with a possible uncertainty (error).

name custom string

type point

value of this data point

error (optional) error of this data point

Example: Point Data

2.3.2 Unbinned Data

Unbinned data describes a measurement of multiple data points in a possibly multi-dimensional space of variables. These data points can be weighted.

custom string name unbinned type entries array of arrays containing the coordinates/entries of the data axes array of structs representing the axes. If given each struct needs to have the component name. Further, (optional) components are max, min and nbins. (optional) array of values containing the weights of the individual data points, weights to be used for χ^2 comparisons and fits. If this component is not given, weight 1 is assumed for all data points. If given, the array needs to be of the same length as entries.

(optional) array of arrays containing the errors/uncertainties of each entry. If entries_error given, the array needs to be of the same shape as entries.

```
"data":[
 {
   "name":"data1",
```

```
"type": "unbinned",
"weights":[
  9.0,
  18.4
"entries":[
  [1],
  [2]
],
"entries_errors":[
  [0.3],
  [0.6]
"axes":[
  {
    "name": "variable1",
    "min":1,
    "max":3
  },
  ]
},
```

2.3.3 Binned Data

Binned data describes a histogram of data points with bin contents in a possibly multi-dimensional space of variables.

name custom string

type binned

contents array of values representing the contents of the binned data set

axes array of structs representing the axes. If given each struct needs to have the

component name. Further, (optional) components are max, min and nbins.

uncertainty (optional) struct representing the uncertainty of the contents. It consists of up

to three components:

type denoting the kind of uncertainty, for now only Gaussian

distributed uncertainties denoted as gaussian_uncertainty

are supported

sigma array of the standard deviation of the entries in contents.

Needs to be of the same length as contents

correlation (optional) array of arrays denoting the correlation between

the contents in matrix format. Must be of dimension length of contents × length of contents. It can also be set to 0

to indicate no correlation.

Example: Binned Data

```
"data":[
 {
   "name":"data2",
    "type":"binned",
   "contents":[
     9.0,
      18.4
   ],
    "axes":[
      {
        "name": "variable1",
        "nbins":2,
        "min":1,
        "max":3
   ]
 },
```

This type can also be used to store pre-processed data utilizing the uncertainty component

Example: Pre-processed binned Data

```
"uncertainty" : {
    "type": "gaussian_uncertainty",
    "correlation" : 0,
    "sigma" : [ 3, 4 ]
},
    "axes":[
    {
        "name":"variable1",
        "nbins":2,
        "min":1,
        "max":3
      },
      ...
]
```

2.4 Likelihoods

The component likelihoods contains an array of likelihoods in struct format which are defined as combinations of distributions and observations. Distributions and observations can only be integrated as keys in string format as references to distributions and observations implemented in their respective components. Thus, the components of a likelihood struct are:

name custom string

distributions array of strings referencing the used distributions

data array of strings referencing the used data, must be of the same length as the array of distributions

2.5 Domains

The component domains contains an array of domains. These contain information on ranges of parameters and variables in struct format. Each domain must contain a name and a type

although right now only the product_domain type is supported. A domain consists of the following components:

The component axes itself is an array of ranges each containing the components min, max and name.

min lower bound of range

2.6 Parameter points

The component parameter_points contains an array of parameter configurations. These can be starting values for minimizations, parameter settings used to generate toy data, best-fit-values obtained, or points in parameter space used for different purposes.

```
Example: Parameter points

"parameter_points":[
{
```

The component parameters is an array of components each containing

name custom string

value number, value of variable

const (optional) boolean, whether variable is constant or not. Default is false.

2.7 Analyses

The component analyses contains an array of possible (automated) analyses. To that extent, likelihoods, parameters of interest and the affiliated domains are listed. Description of the components:

name	custom string
likelihood	name as reference to a likelihood defined in the top-level component ${\tt likelihoods}$
aux_likelihood_terms	(optional) array of names of some distributions defined under ${\tt distributions}$ to be used as auxiliary likelihood terms (see below)
parameters_of_interest	(optional) array of names as reference to parameters that are interesting for the analysis at hand
parameter_domain	name of a domain to be used for the parameters, defined in the top-level component ${\tt domains}$
data_domain	name of a domain to be used for the variables in data, defined in the top-level component ${\tt domains}$
aux_likelihood	(optional) name of a constraint term to be used, defined in the top-level component ${\tt distributions}$
init_value	(optional) name of an initial value to be used, defined in the top-level component parameter_points

prior

(optional) name of a prior distribution, defined in the top-level component distributions. This could, for example, be a product distribution of all the individual priors.

All parameters of all distributions in the likelihood must either be listed under the domain referenced, or set to const in the parameter point referenced. Interpretation in Bayesian context of the components parameter_domain, aux_likelihood, init_value and aux_likelihood_terms imply a prior distribution. Alternatively, a prior distribution may also be directly defined through the component prior.

Auxiliary likelihood terms are additional terms to be added to the likelihood. They are intended to reflect subsidiary measurements, typically employing some simple distributions types like Gaussian, Poisson or log-normal. While these subsidiary measurements could easily be stored as full likelihood terms in the corresponding likelihood, this is often inconvenient, since these subsidiary measurements often follow a conventional form of being centered around some default value, mostly 0 or 1, which would then need to be stored as a separate dataset under data. Thus, by convention, distributions listed under aux_likelihood_terms use the following default-values as data:

```
gaussian_dist 0
poisson_dist 1
lognormal_dist 1
```

Example: Analyses

2.8 Metadata

The top-level component $\mathtt{metadata}$ contains meta-information related to the creation of the file. The component $\mathtt{hs3_version}$ stores the HS^3 version and is required for now. Overview of the components:

hs3_version (required) HS³ version number for reference

packages (optional) array of structs defining packages and their version number used in the creation of this file, depicted with the components name and version respectively

authors (optional) array of authors, either individual persons, or collaborations

publications (optional) array of document identifiers of publications associated with this filedescription (optional) short abstract/description for this file

```
Example: Metadata

"metadata" :
{
    "hs3_version" : "0.2.0",
    "packages" : [
        {
            "name": "ROOT",
            "version": "6.28.02"
        }
    ],
    "authors": ["The ATLAS Collaboration", "The CMS Collaboration"],
    "publications": ["doiABCDEFG"]
}
```

2.9 Miscellaneous

The top-level component misc contains arbitrary, user-created information in struct format.

```
Example: Miscellaneous

"misc" :
{
    "custom key 1" : "custom information 1"
}
```

This top-level component is intended to store any and all additional information, including useror backend-specific meta-information. Examples include, but are not limited to:

- colors and styles for drawing distributions in this file
- suggested settings for samplers or minimizers when working with the distributions in this file
- comments explaining design choices made when building the model in this file
- suggested names and paths for output files to be used by backends working with this file

References

- 1. Heinrich, L., Feickert, M. & Stark, G. pyhf version 0.6.3. https://github.com/scikit-hep/pyhf/releases/tag/v0.6.3.
- 2. An, S. et al. root-project/root version 6.26. Mar. 2022.
- 3. Cranmer, K., Lewis, G., Moneta, L., Shibata, A. & Verkerke, W. *HistFactory: A tool for creating statistical models for use with RooFit and RooStats* tech. rep. (New York U., New York, Jan. 2012). https://cds.cern.ch/record/1456844.
- 4. Barlow, R. & Beeston, C. Fitting using finite Monte Carlo samples. *Computer Physics Communications* 77, 219–228. ISSN: 0010-4655. https://www.sciencedirect.com/science/article/pii/001046559390005W (1993).