(Kernel) Density Estimation

IML WG meeting: Unsupervised learning

Anton Poluektov

University of Warwick, UK
Budker Institute of Nuclear Physics, Novosibirsk, Russia

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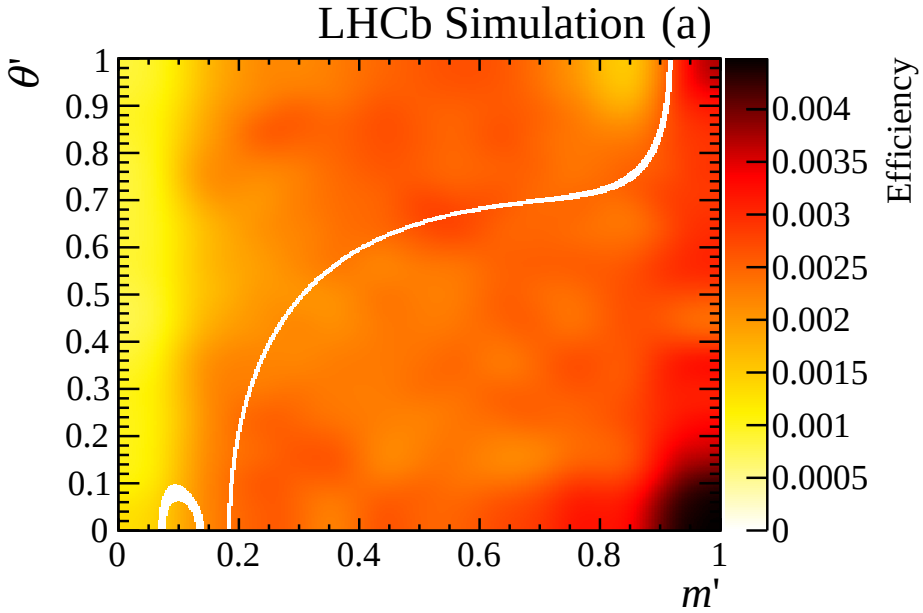
Introduction

- No need to explain that the essential part of every HEP analysis is density estimation.
  - Modelled PDF when we need to measure some parameters from ML fit
  - Empirical PDF (*e.g.* `KeysPDF`, polynomial) when we need some *ad hoc* description of some shape (background, efficiency, ...)
- Speaking in terms of today's meeting, density estimation is an example of unsupervised learning
  - Take a (training) sample
  - Try to predict response (probability density) for a point that is not in the sample.
- Here I will concentrate on model-independent density estimation, mostly kernel density estimation (KDE), based on experience from LHCb analyses.

Simplest case: histogramming

Simplest method of density estimation: histogramming. Certainly, no need to tell you about it.
Frequently used extension of this technique at LHCb: cubic spline smoothing (1D, 2D). See, e.g., [PRD 90, 072003 (2014)]



Efficiency over 2D phase space of $B_s \to DK\pi$ decay.

- Interpolation by cubic spline between bins.
- Continuous PDF (and its 1st and 2nd derivatives).
- Binning effect is still present.

Kernel density estimation (KDE) basics

Let x_i be the data points from which we have to estimate the PDF. Kernel density estimator is

$$P_{\mathrm{KDE}}(x) = \sum_i K(x - x_i)$$

Here $K(x)$ is a kernel. Can use various forms, here I will use the parabolic one:

$$K(x) = 1 - (x/h)^2$$

Optimal in some sense (although the others, such as Gaussian, are almost as good).
Note the resulting $P_{\mathrm{KDE}}(x)$ in $i \to \infty$ limit is rather a convolution of the true PDF with the kernel $K(x)$. Thus, structures with the width $\leq$ kernel width are smeared.
Kernel width h (bandwidth) needs to be optimised to reach balance between bias (wide kernels) and stat. fluctuations (narrow kernels).
For HEP-related discussion, see

[K. Cranmer, Comp. Phys. Comm. 136 (2001) 198-207]

KDE: bandwidth choice and adaptive kernels

There are ways to estimate the optimal bandwidth h for specific densities, *e.g.* for Gaussian PDF

$$h^* = \sigma \left(\frac{4}{3n} \right)^{1/5}$$

For optimal performance, bandwidth h should depend on *local* density in the point x_i:

$$h_i = h_0 P(x_i)^{1/N}$$

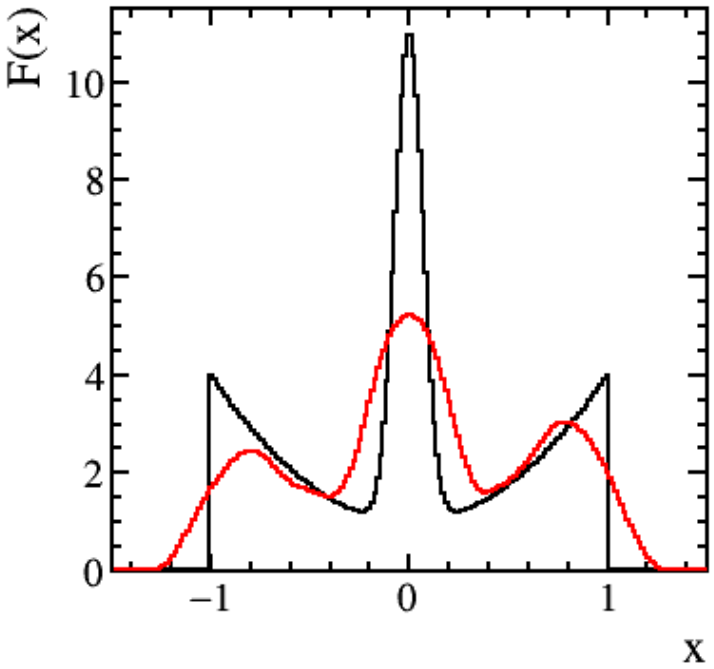
True density $P(x)$ unknown $\Rightarrow$ iterative procedure (adaptive KDE):

- First iteration: fixed kernel
- Second iteration: BW given by the PDF at the 1st iteration.
- ...

KDE implementations

- `RooFit`: `RooKeysPDF` (1-dim), `RooNDKeysPDF` (N-dim).
  - Gaussian kernel
  - Both fixed and adaptive kernels
  - Boundary correction using data reflection
- `scikit-learn`: `sklearn.neighbors.KernelDensity`.
  - Choice of various kernels
  - Only fixed kernel
  - Different metrics
  - Optimisation using KD-tree $\Rightarrow$ faster lookup
- My own implementation (`Meerkat`): see below
  - Attempt to solve problems related to boundary effects and curse of dimensionality.

KDE: boundary effects



$P_{\text{true}}(x) = 1+3x^2+10e^{-x^2/0.1^2}$

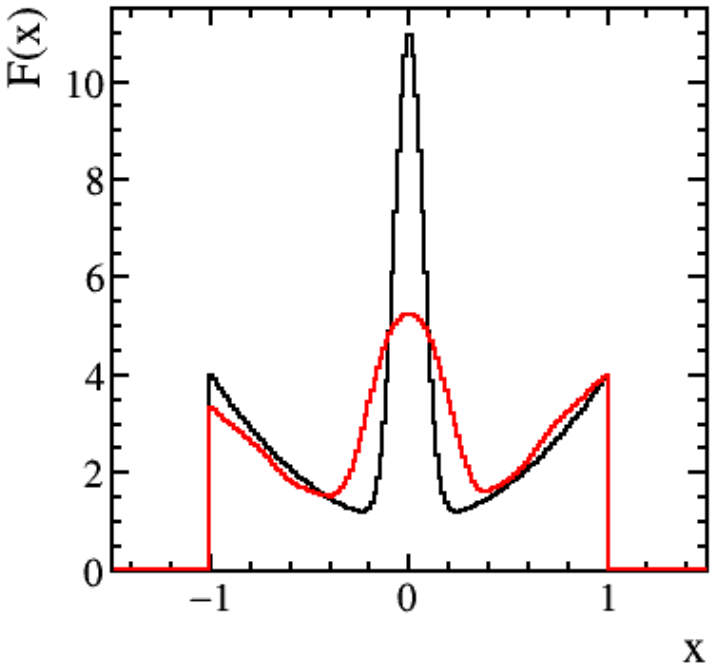
The usual problem with KDE is boundary effects.

Methods to correct for this:

- Data reflection.
- Kernel modification near boundary.

Normally work with simple boundaries (1D, linear). Not easy to apply to *e.g.* conventional Dalitz plots.

KDE: correcting for boundary effect



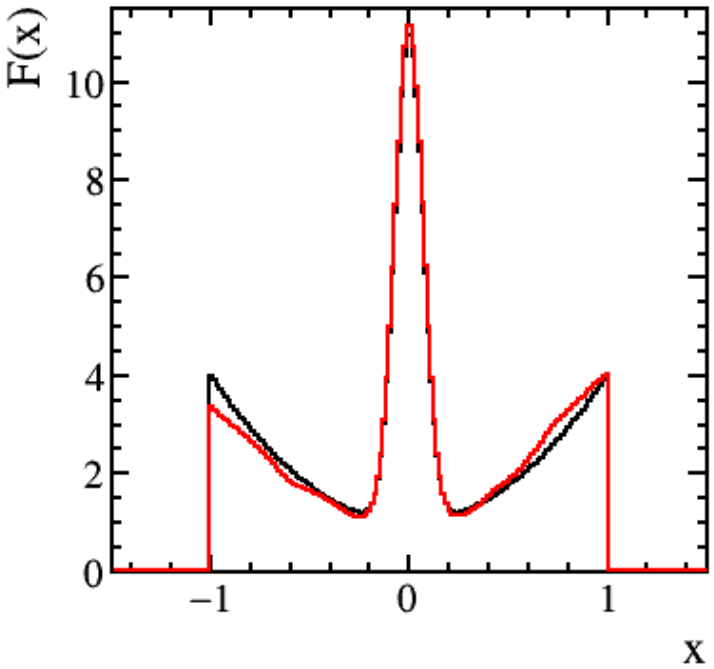
$$P_{\text{true}}(x) = 1+3x^2+10e^{-x^2/0.1^2}$$

Simple correction: divide result of KDE by the convolution of kernel with flat density:

$$P_{\text{corr}}(x) = \begin{cases} \frac{\sum_{i=1}^{N} K(x-x_i)}{(U \otimes K)(x)} & \text{for } x \in X, \\ 0 & \text{otherwise.} \end{cases}$$

$$U(x) = \begin{cases} 1 & \text{for } x \in X, \\ 0 & \text{otherwise.} \end{cases}$$

KDE: correcting for boundary effect



$$P_{\text{true}}(x) = 1 + 3x^2 + 10e^{-x^2/0.1^2}$$

$$P_{\text{appr}} = 1 + 10e^{-x^2/0.1^2}$$

Suppose we approximately know how the PDF behaves at the boundaries. A more sophisticated correction:

$$P_{\text{corr}}(x) = \frac{\sum_{i=1}^{N} K(x - x_i)}{(P_{\text{appr}} \otimes K)(x)} \times P_{\text{appr}}(x).$$

replaces KDE by an approximation PDF at boundaries and in regions with narrow structures.

Relative KDE

$$P_{\mathrm{corr}}(x) = \frac{\sum_{i=1}^{N} K(x - x_i)}{(P_{\mathrm{appr}} \otimes K)(x)} \times P_{\mathrm{appr}}(x).$$

In other words, we represent the PDF as a product:

$$P_{\mathrm{corr}}(x) = f(x) P_{\mathrm{appr}}(x)$$

where $P_{\mathrm{appr}}(x)$ is known and describes narrow structures and boundaries, and $f(x)$ is slowly-varying and is represented by the kernel density.

An intermediate solution between the model-based and model-independent density estimators.

Can be generalised to any complex boundaries, weighted distributions (including negative weights, sWeights), variable (adaptive) kernels.

[A.P., JINST 10 P02011 (2015)]

Relative KDE: multidimensional case

So, we have an approach that performs KDE over some approximation PDF. How does this help in the case of multiple dimensions?
Multiple dimensions typically need wide kernel (or very large samples). A couple of examples how approximation PDF can help:

- If your multidimensional PDF is approximately factorisable:
  - Approximation PDF is the product of PDFs in lower dimensions.
  - Relative KDE with wide kernel describes residual correlations.
- Efficiency shape in multiple dimensions:
  - Approximation PDF from high-statistics fast MC sample (e.g. generator-level MC with simple kinematic cuts) and narrow kernel.
  - Relative KDE based on full Geant simulation and wider kernel.

Meerkat library

[http://meerkat.hepforge.org]

The procedure described above is implemented in the Meerkat library (Multidimensional Efficiency Estimation using Relative Kernel Approximation Technique). Obviously not limited to efficiency estimation. Direct usage of relative KDE formulas is *slow* because convolution should be done in every point x. For practical applications, use binned approach with multilinear interpolation:

$$P_{\text{interp}}(x) = \frac{Bin\left[\sum_{i=1}^{N} K(x - x_i)\right]}{Bin\left[(P_{\text{appr}} \otimes K)(x)\right]} \times P_{\text{appr}}(x).$$

Time to estimate the PDF is linear with the size of the sample, and memory is constant (no need to store the whole data sample in memory). Very large data sample can practically be used (I've used 10^8 sample for 5D distribution).

Usage of Meerkat

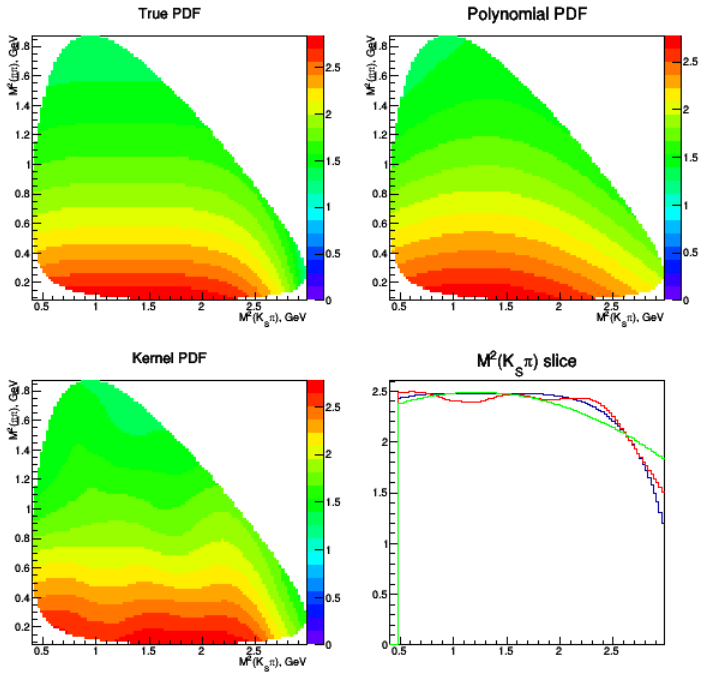
[http://meerkat.hepforge.org]

- Create a *phase space* from the building blocks provided.
- Optionally create an *approximation density*.
- Fill the relative KDE PDF.
- Store the binned version of it into a file (or export to ROOT histograms for 1D or 2D).
- Use it in e.g. your ML fits (as a ROOT histogram, as RooFit PDF, or as interpolated binned density using the class provided).

Both `C++` interface (for compiled programs or `CINT`, `CLang`) and `Python` interface are provided.
Currently used in several LHCb analyses for efficiency, background description (especially for non-trivial phase spaces, such as Dalitz plots), for parametrisation of PID response. Up to 5 dimensions.
Most of the analyses are ongoing, so no public plots with real data. Can only show some toy MC results.

Example of Meerkat usage: Dalitz plot efficiency

```
md = 1.8646   # D0 mass
ma = 0.497    # KS0 mass
mb = 0.139    # Pi mass
mc = 0.139    # Pi mass
# Define Dalitz phase space for D0->KsPiPi
# Variables are x=m^2(ab), y=m^2(ac)
phsp = DalitzPhaseSpace("PhspDalitz",
       md, ma, mb, mc)
# Create polynomial approximation PDF
poly = PolynomialDensity("PolyPDF",
       phsp,     # Phase space
       2,        # Power of polynomial
       ntuple,   # Input ntuple
       "x","y", # Ntuple variables
       50000)    # Sample for MC normalisation
# Create kernel PDF from the generated sample
kde = BinnedKernelDensity("KernelPDF",
       phsp,     # Phase space
       ntuple,   # Input ntuple
       "x","y", # Variables to use
       200,200, # Numbers of bins
       0.4, 0.4,# Kernel widths
       poly,     # Approximation PDF
       50000)    # Sample for MC convolution
```



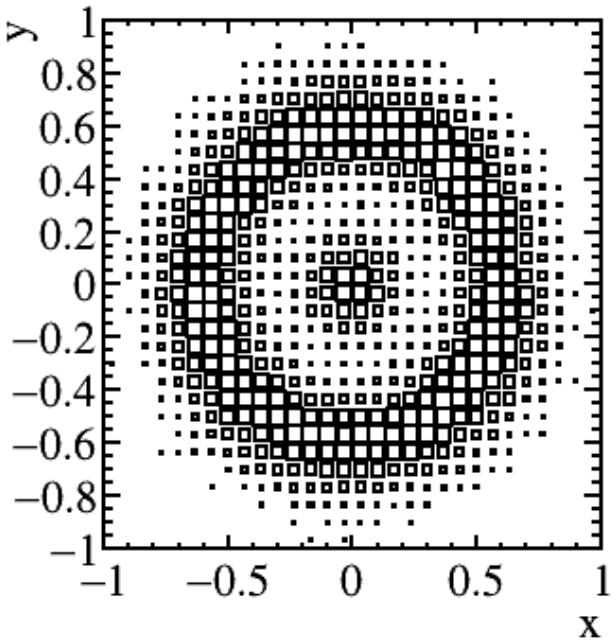
Gaussian Mixture Model

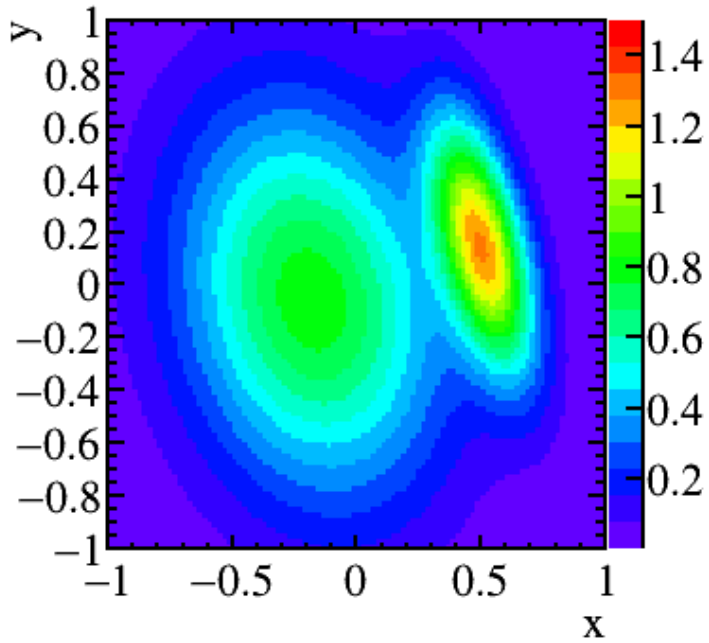
- Sum of multivariate Gaussian components with different normalisations, widths and correlations.
- Classical estimation algorithm: expectation-maximization method (EM).
  - Iterative procedure for a given number of Gaussians.
  - Expectation step: assign each data point to its Gaussian component (e.g. using weights)
  - Maximization step: calculate the new parameters of the Gaussian component from the assigned points (mean, covariance).
- EM works well without boundaries, or at least when the Gaussians are significantly away from boundaries (such that mean and covariance gives a good approximation). Difficult to describe distributions close to uniform.

Gaussian Mixture Model

Can use bruteforce fitting at the maximisation step of EM:

- Choose one Gaussian component and do ML fit of its parameters.
- Repeat for each component.
- Increase number of components one by one.





Generally better results than KDE for small samples and PDFs with irregularities (*e.g.* background samples with limited statistics).
$\sim$ 20 Gaussian components usable with modern h/w, esp. GPU.

Using Bayesian classifier (ANN, etc.)

Use supervised learning technique to perform unsupervised learning task.

[B. Viaud, EPJ. Plus 131 (2016), 6, 191]

- Take two samples:
  1. Sample to estimate density ("efficiency")
  2. Uniform distribution in the phase space
- Train classifier to distinguish the two samples based on distribution variables x_i.
- If the classifier gives Bayesian probability $P(x)$ for the point to belong to sample 1 ("probability to pass selection"), it can be interpreted as the local PDF density.
- Classifiers that can be used: NeuroBayes, TMVA with Bayesian regularization ([Comp. Phys. Comm. 182 (2011) 2655-2660]).

Another possible approach: train ANN with backpropagation algorithm specifically designed to reproduce probability density. See, e.g. [Comp. Phys. Comm. 135 (2001) 167175].

Summary

- Model-independent density estimation is a crucial point in many HEP analyses.
- A few techniques are on market, with their advantages and drawbacks. Just a few examples:
  - Histogramming
  - Kernel density estimation
  - Gaussian mixture model
  - Multivariate Bayesian classifiers
- including some which I haven't covered here
  - Orthogonal polynomials
  - k-nearest neighbours
- A few possibilities are either not tried, or not widely known, and in many cases the convenient implementation is lacking. Any volunteers?

Backup

Classes of Meerkat library

Derived from `AbsPhaseSpace`:

- `OneDimPhaseSpace` — 1D range
- `DalitzPhaseSpace` — 2D Dalitz plot phase space
- `ParametricPhaseSpace` — range $[z_{\min}(\vec{x}), z_{\max}(\vec{x})]$ as `TFormula`'s
- `CombinedPhaseSpace` — direct product of other phase spaces

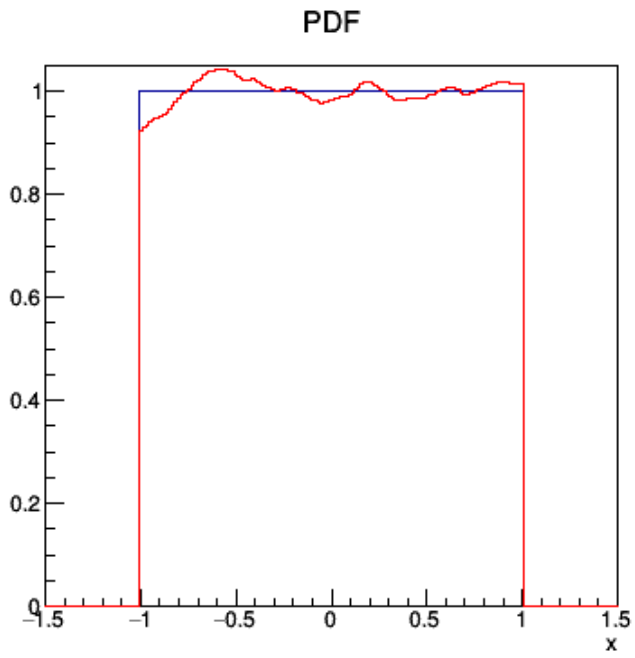
Derived from `AbsDensity`:

- `UniformDensity` — Constant PDF over any phase space
- `FormulaDensity` — PDF given by `TFormula` (up to 4D)
- `KernelDensity` — Unbinned KDE (*slow*! use binned instead)
- `BinnedDensity` — Binned PDF from any `AbsDensity` or file
- `BinnedKernelDensity` — Binned KDE, fixed kernel
- `AdaptiveKernelDensity` — Binned KDE, adaptive kernel
- `FactorisedDensity` — Product of any AbsDensities

OneDimPdf: Estimate 1D PDF with fixed kernel

This is the simples example: 1D PDF in range $(-1, 1)$ with flat approximation PDF.

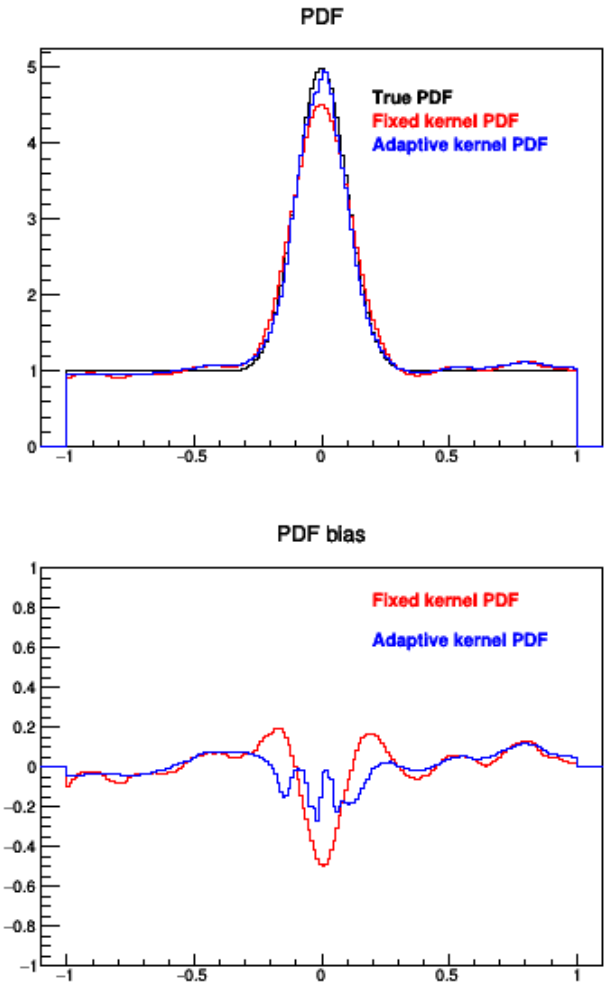
```
# Create phase space
phsp = OneDimPhaseSpace("Phsp1D", -1, 1)
# Create kernel PDF from the ntuple
kde = BinnedKernelDensity("KernelPDF",
        phsp,    # Phase space
        ntuple, # Input ntuple
        "x",     # Variable to use
        1000,    # Number of bins
        0.2,     # Kernel width
        0,       # Approx. PDF (0 for flat)
        100000   # Sample for MC convolution
      )
# Write the result
kde.writeToFile("OneDimPdfBins.root")
# Project result to 1D histogram
hist = TH1F("hist","Kernel PDF",200,-1.5,1.5)
kde.project(hist)
```



OneDimAdaptiveKernel: Varying kernel width

If your PDF contains sharp peaks, you may want adaptive PDF with kernel width depending on density: $\sigma \propto P^{-1/N_{\mathrm{dim}}}$

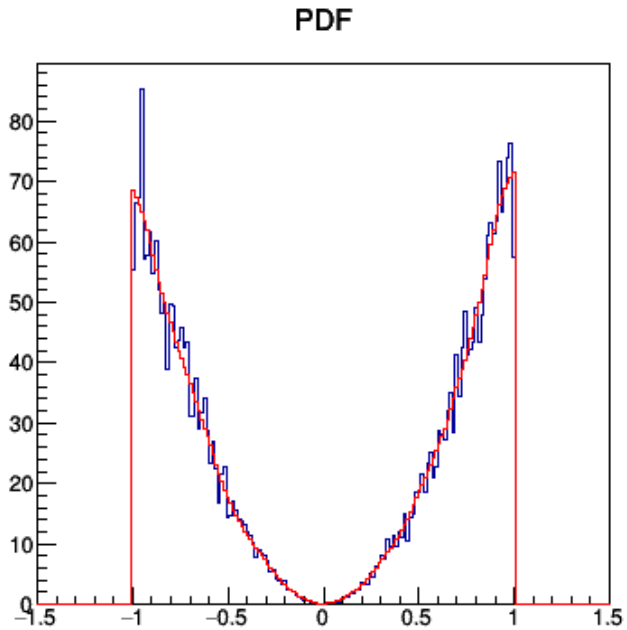
```
# Create phase space
phsp = OneDimPhaseSpace("Phsp", -1, 1)
# Create kernel PDF from the ntuple
kde = BinnedKernelDensity("KernelPDF",
        phsp, ntuple,
        "x", 1000, 0.1,
        0, 0, 100000)
# Create adaptive kernel PDF with the kernel
# width depending on the binned PDF
# from the last step
ada = AdaptiveKernelDensity("AdaPDF",
        phsp, ntuple,
        "x", 1000,
        0.1,  # width corresponding to pdf=1
        kde,  # density for width scaling
        0, 100000)
```



WeightedTuple: Estimate PDF from weighted distribution

Can work with weighted distributions. Example: uniform distribution in $x \in (-1, 1)$, but weight $w \propto x^2$.

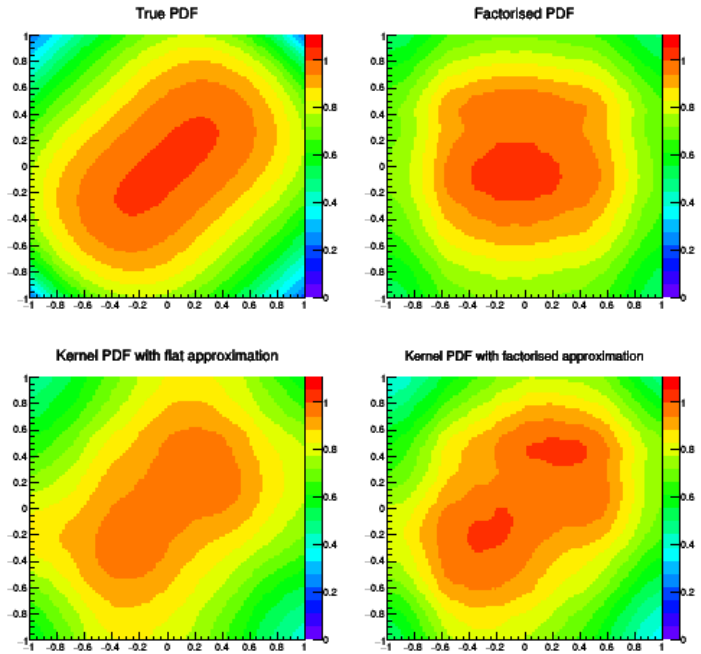
```
# Create phase space
phsp = OneDimPhaseSpace("Phsp", -1, 1)

# If number of variables passed to constructor
# is larger by 1 than the phase space
# dimensionality, the last variable is
# considered as weight
kde = BinnedKernelDensity("KernelPDF",
        phsp,
        ntuple, # Input ntuple
        "x",    # Variable to use
        "w",    # Weight variable
        1000,   # Number of bins
        0.2,    # Kernel width
        0,      # Approx. PDF (0 for flat)
        100000  # Sample for MC convolution
      )
```



CombinedPdf: 2D phase space

Rectangular phase space, factorised density used as approximation for KDE

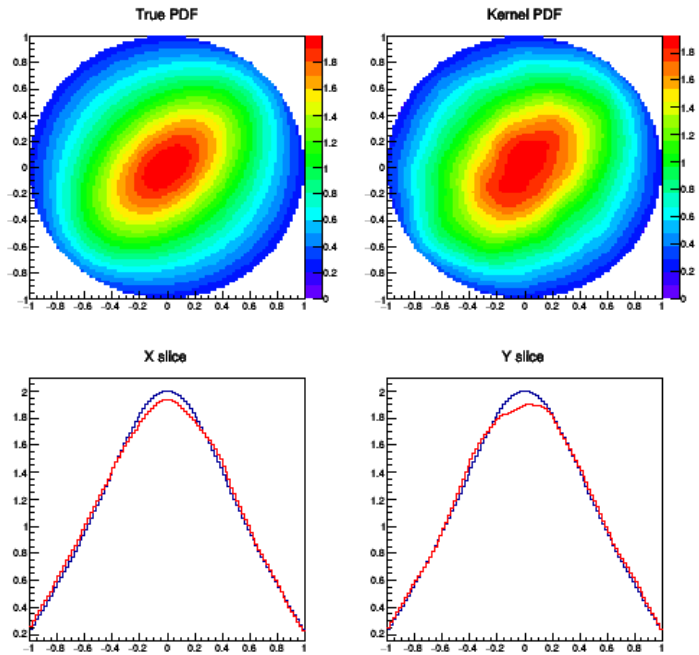
```
# Define 1D phase spaces
phsp_x = OneDimPhaseSpace("PhspX", -1, 1)
phsp_y = OneDimPhaseSpace("PhspY", -1, 1)
# Define combined phase space for the two vars
phsp = CombinedPhaseSpace("PhspCombined",
           phsp_x, phsp_y)
# Densities for projections
kde_x = BinnedKernelDensity("KernelPDF_X",
           phsp_x, ntuple, "x", ... )
kde_y = BinnedKernelDensity("KernelPDF_Y",
           phsp_y, ntuple, "y", ... )
# Factorised density
fact = FactorisedDensity("FactPDF",
        phsp,kde_x,kde_y)
# Create kernel PDF with factorised approximatio
kde_factappr = BinnedKernelDensity(
        "KernelPDFWithFactApprox",phsp, ntuple,
        "x","y",   # Variables
        100,100,   # Numbers of bins
        0.4, 0.4, # Kernel widths
        fact,      # Approximation PDF
        100000)    # Sample size for MC convolution
```



ParamPhsp: Parametric phase space

More complex phase spaces can be defined with ParametricPhaseSpace

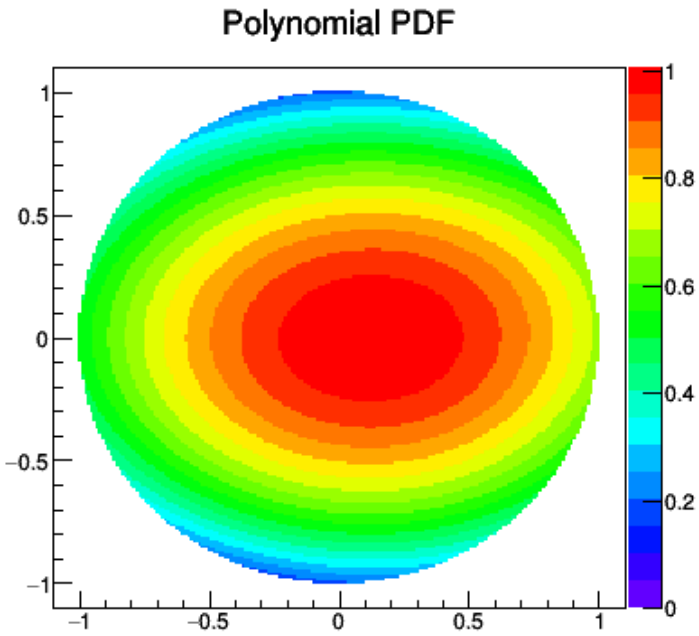
```
# First create 1D phase space for variable x
xphsp = OneDimPhaseSpace("PhspX", -1., 1.)
# Now create parametric phase space for (x,y)
# where limits on variable y are functions of x
phsp = ParametricPhaseSpace("PhspParam", xphsp,
          "-sqrt(1-x^2)", # Lower limit
          "sqrt(1-x^2)",  # Upper limit
          -1., 1.         # Global limits of y
       )
# Create approximation PDF
approxpdf = FormulaDensity("TruePDF", phsp,
          "1.-0.8*x^2-0.8*y^2")
# Create kernel PDF from the generated sample.
# Use polynomial shape as an approximation PDF
kde = BinnedKernelDensity("KernelPDF",
           phsp,       # Phase space
           ntuple,     # Input ntuple
           "x","y",    # Variables to use
           200,200,    # Numbers of bins
           0.2, 0.2,   # Kernel widths
           approxpdf,  # Approximation PDF
           100000      # Sample size for MC convolution
         )
```



TwoDimPolyPdf: Fitted 2D polynomial

You probably don't need Meerkat if your PDF fits well by a polynomial, but polynomial PDF can also be a good approximation PDF. Meerkat can do unbinned 1D and 2D polynomial fits.

```
# First create 1D phase space for variable x
xphsp = OneDimPhaseSpace("PhspX", -1., 1.)
# Now create parametric phase space for (x,y)
# where limits on variable y are functions of x
phsp = ParametricPhaseSpace("PhspParam", xphsp,
          "-sqrt(1-x^2)", # Lower limit
          "sqrt(1-x^2)",  # Upper limit
          -1., 1.         # Global limits of y
       )
poly = PolynomialDensity("PolyPDF",
          phsp,     # Phase space
          4,        # Power of the polynomial
          ntuple,   # input ntuple
          "x", "y",# Variables
          200000    # Sample for MC normalisation
       )
```



DalitzPdf: Dalitz plot

```
md = 1.8646   # D0 mass
ma = 0.497    # KS0 mass
mb = 0.139    # Pi mass
mc = 0.139    # Pi mass
# Define Dalitz phase space for D0->KsPiPi
# Variables are x=m^2(ab), y=m^2(ac)
phsp = DalitzPhaseSpace("PhspDalitz",
       md, ma, mb, mc)
# Create polynomial approximation PDF
poly = PolynomialDensity("PolyPDF",
       phsp,     # Phase space
       2,        # Power of polynomial
       ntuple,   # Input ntuple
       "x","y", # Ntuple variables
       50000)    # Sample for MC normalisation
# Create kernel PDF from the generated sample
kde = BinnedKernelDensity("KernelPDF",
       phsp,     # Phase space
       ntuple,   # Input ntuple
       "x","y", # Variables to use
       200,200, # Numbers of bins
       0.4, 0.4,# Kernel widths
       poly,     # Approximation PDF
       50000)    # Sample for MC convolution
```