N-Tuples and compact matrix element representations

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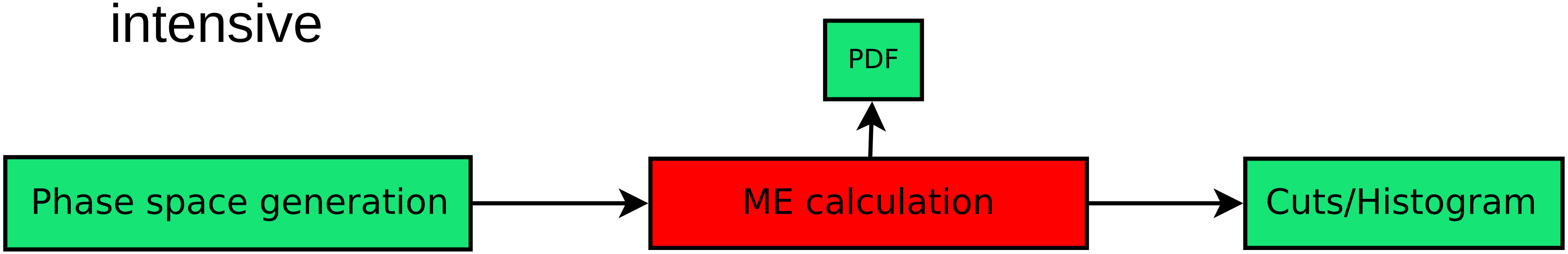
Plan

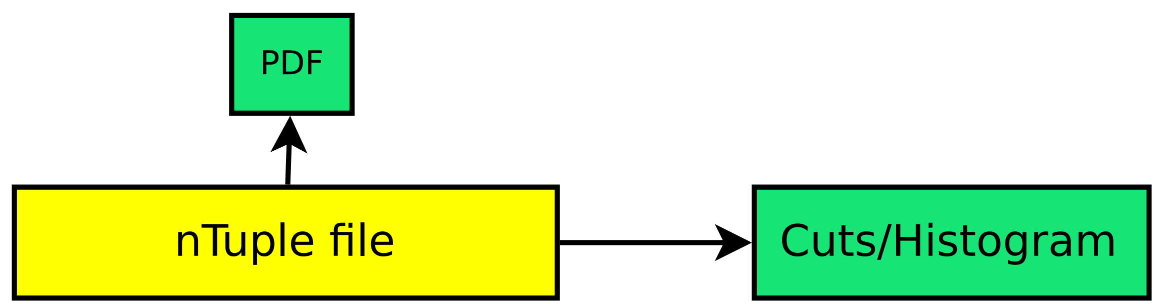
- nTuples
- NNLO ntuples
- Orthogonal functions for phasespace

n-Tuple files [arXiv:1310.7439]

- High multiplicity NLO calculations are computationally intensive



- Matrix elements are expensive
- Jet clustering, observables, PDF evaluation are relatively cheap
- Store matrix element, PS point and the information necessary to change scales

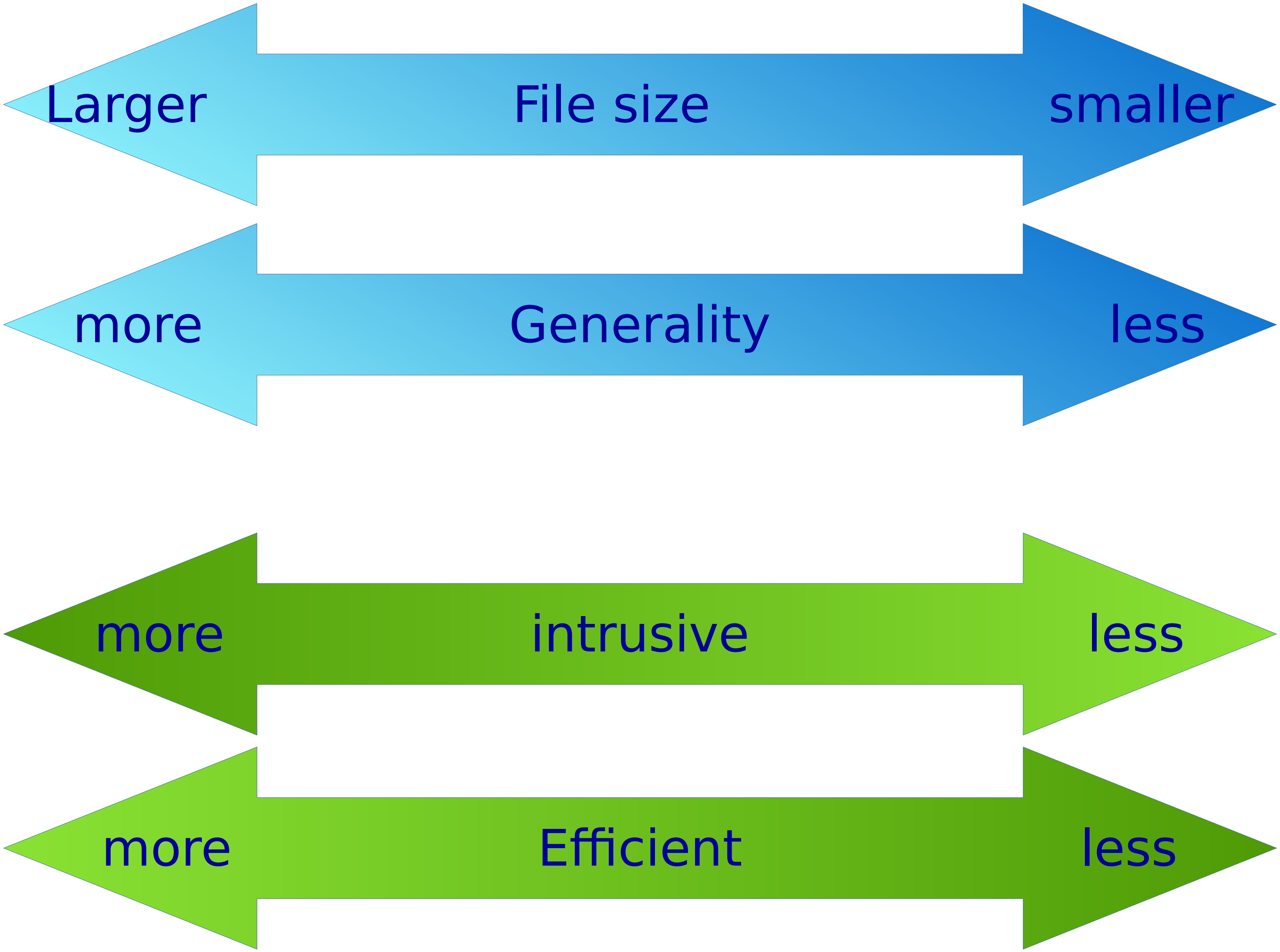


NLO nTuple files [arXiv:1310.7439]

- Advantages
  - One can change the analysis cuts, add observables
  - Cheap scale variation and PDF errors (otherwise extremely expensive)
  - Easy communication between theorists and experimenters
  - No need for specific know-how of the tool which produced the NLO calculation
  - Easier to “endorse” an event file than a program
- Disadvantage
  - Large files
  - Generation cuts need to be loose enough to accommodate many analysis $\rightarrow$ efficiency cost

NNLO nTuple files

- Trade offs



Compact Matrix element representations

nTuple file

- A nTuple file is a weighted sample to represent the integral

$$\sigma = \int d\phi_n \frac{d\sigma}{d\phi} C(\phi)$$

- Where *C* is a set of cuts designed to be as inclusive as possible
- ϕ is the phasespace, and also include the integration over the PDFs for hadronic initial states
- For hadronic initial states we need to create new nTuples
  - For new collider energies
  - For different jet pt cuts

Compact representation

- Question: if calculating the differential cross section is the difficult part, how can I store as much information as possible about it in a way that I can reuse it more?
- I can try to represent the underlying probability density
  - Is it a probability density?
    - Yes at LO
    - Not at NLO
    - It should be for an infrared-safe observable
- Goal is to build a basis of phasespace functions that can build any infrared safe observable
- Consider 1 $\rightarrow$ n process (e+e-, Higgs decay)

Orthogonal PS function

- Let's introduce as set of orthonormal functions of phasespace
- The exact form of the parametrisation is not very relevant
  - Map coordinates to either [0,1] or [-1,1]
  - Arrange for flat Jackobian:

$$\int d\phi f(\phi) = \int dx_1 \cdots dx_k f(\phi(x_1, ..., x_k))$$

  - Use polynomial orthogonal basis

$$\int_{x_{min}}^{x_{max}} \Phi_i(x)\Phi_j(x)\, dx = \delta_{ij}$$

- The basis function for the phasespace

$$\Phi_{i_1,...,i_k}(x_1, ..., x_k) = \Phi_{i_1}^{(1)}(x_1)...\Phi_{i_k}^{(k)}(x_k)$$

Orthogonal PS function

- So we can now write any (reasonable) function of phase-space as

$$f(\phi) \approx \sum_{i_1,\ldots,i_k} c_{i_1,\ldots,i_k} \Phi_{i_1,\ldots,i_k}(\phi)$$

- The number of indices corresponds to the number of free parameters (including azimuthal symmetry)
  - For 2 particle PS: 1
  - For 3 particle PS: 4
  - $3n$-5 for n particle PS
- Becomes quickly too many dimensions (curse of dimensionality)

Coefficients

- The coefficients are determined through integration over phasespace

$$c_{i_1,\ldots,i_k} = \int d\phi\, \Phi_{i_1,\ldots,i_k} f(\phi)$$

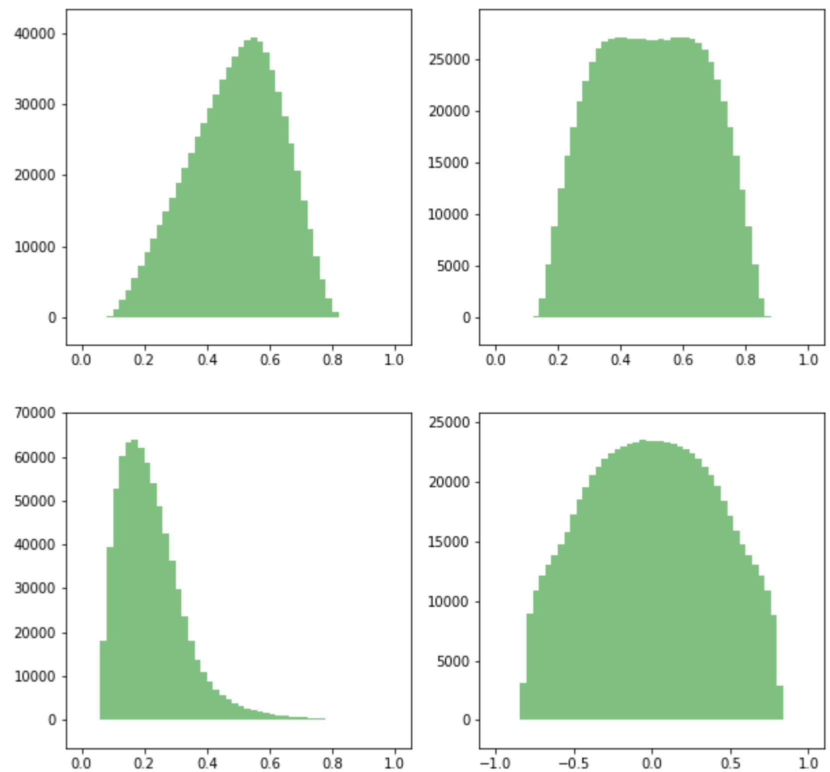
- Using this representation we have

$$\begin{aligned} \sigma &= \int d\phi_n \frac{d\sigma}{d\phi} C(\phi) \\ &= \sum_{i_1,\ldots,i_k} c_{i_1,\ldots,i_k} \int d\phi_n \Phi_{i_1,\ldots,i_k}(\phi) C(\phi) \\ &= \sum_{i_1,\ldots,i_k} c_{i_1,\ldots,i_k} d_{i_1,\ldots,i_k} \end{aligned}$$

- Phase-space integration for matrix elements and cuts can be separated

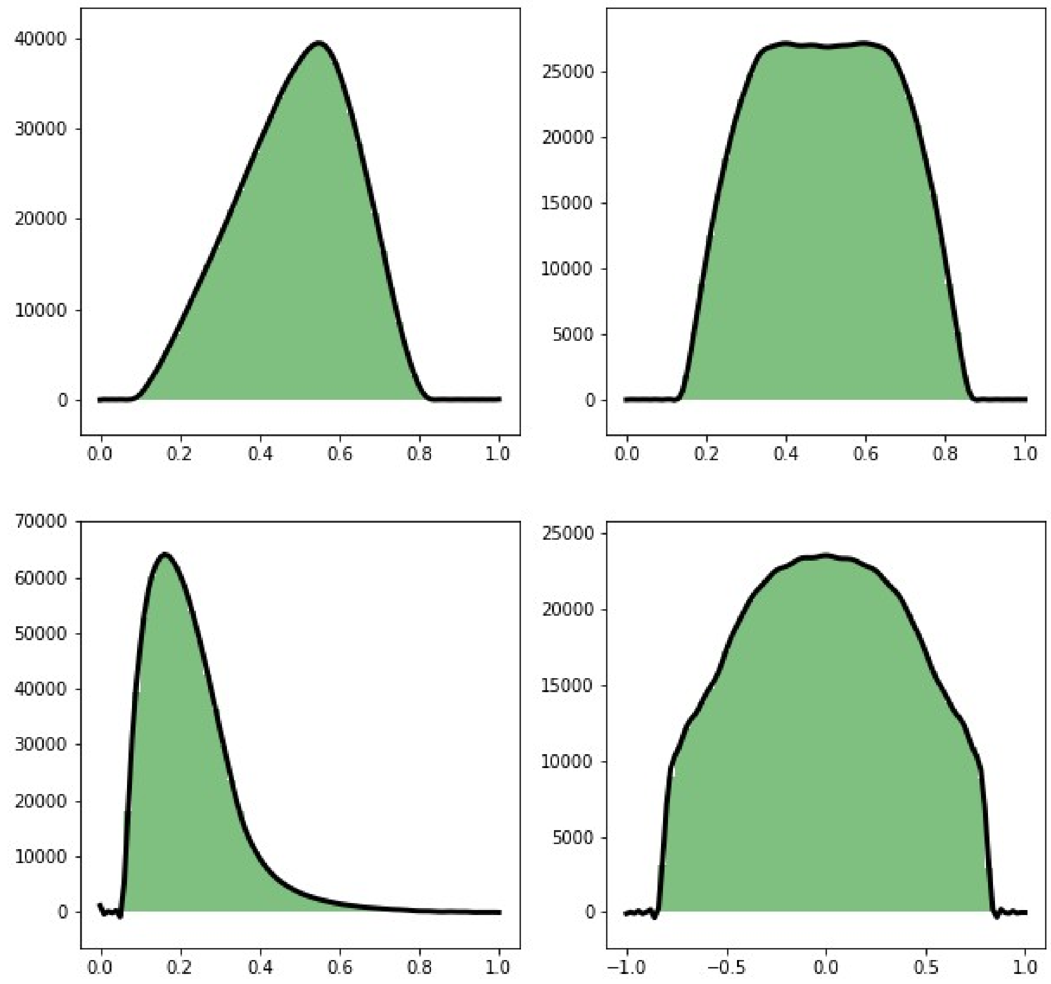
Example

- e+e- → 3j LO
  - Fix centre of mass energy to 1
  - Require 3 jets using R=0.1 and transverse momentum 0.25
- The densities $\frac{d\sigma}{dx_i}$ in phase space look like this:



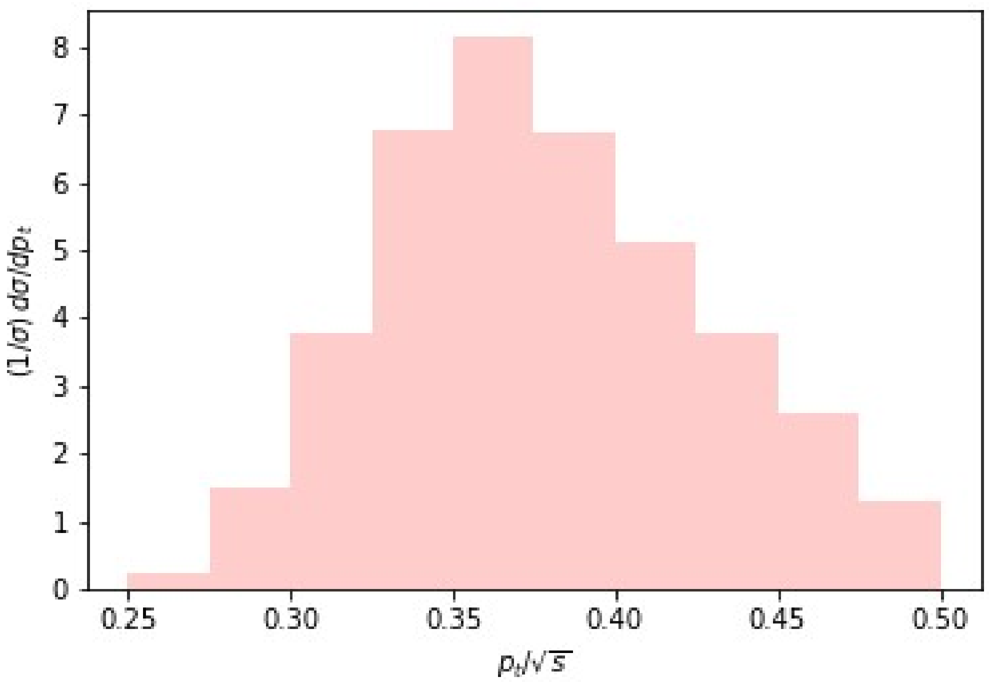
Estimate of the densities

- Calculate the coefficients for the density with 50 coefficients per dimension
- Reconstruct the density and compare with the histograms:



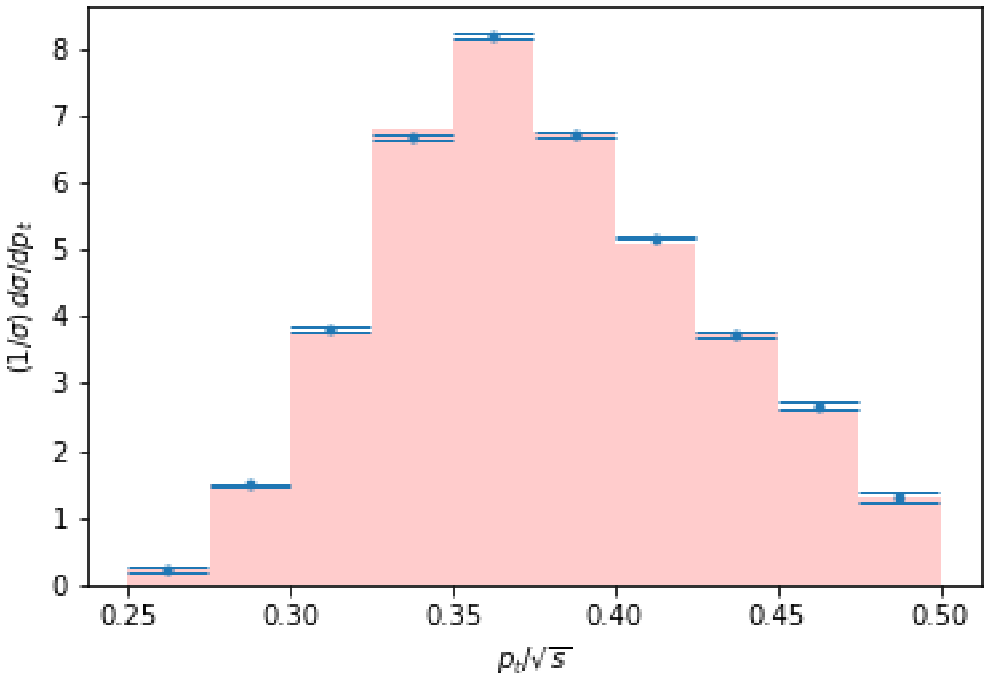
Observable

- Observables: bins in first jet transverse momentum



Reconstructed distribution

- Here are the reconstructed histograms

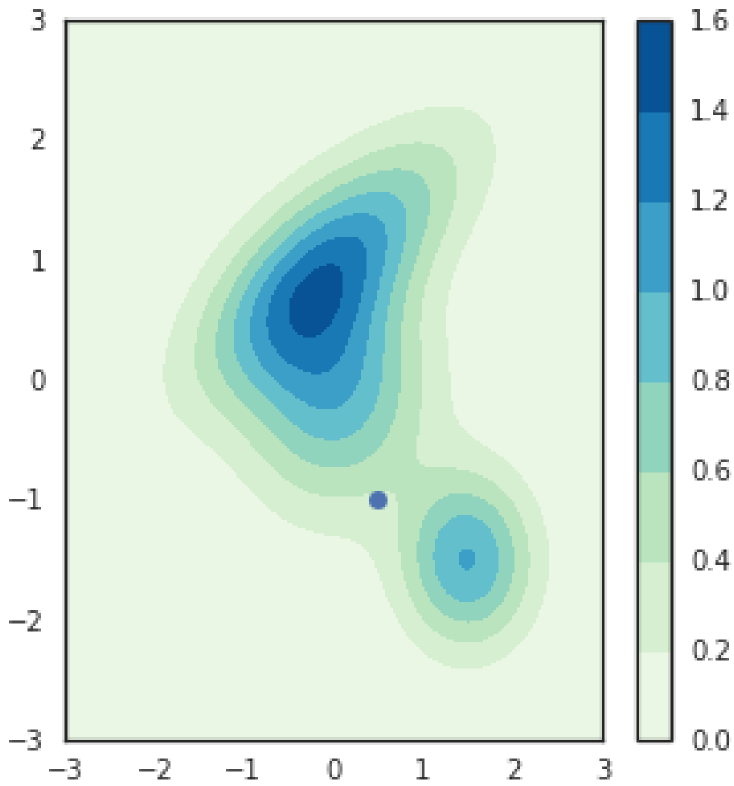


Generating samples

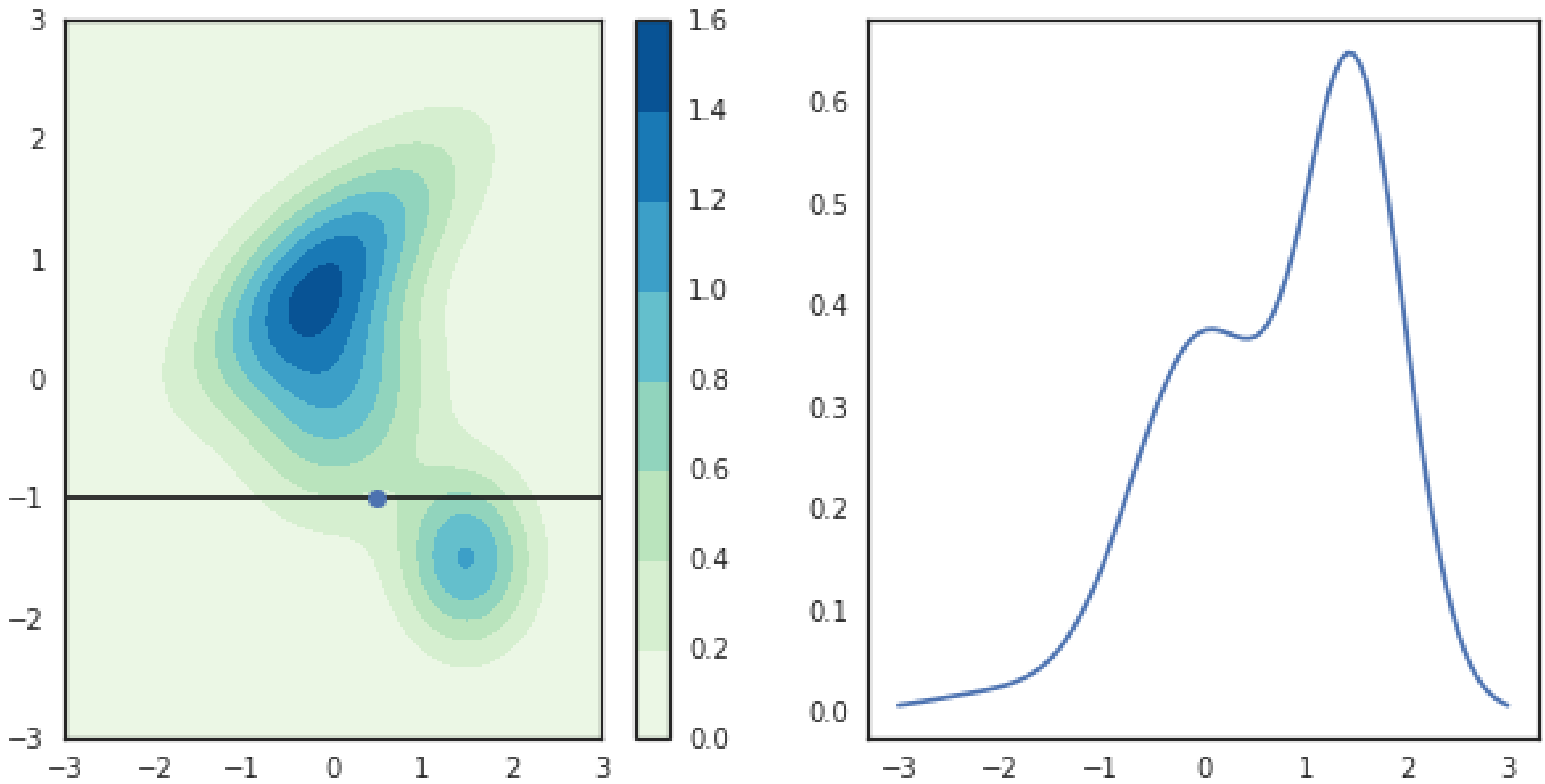
- One advantage of having an approximation for the density is that we can draw samples from it
- We can use Gibbs sampling
  - Start somewhere and repeat the following algorithm
    - Given a point $$X^i = (x_1^{(i)}, ...x_k^{(i)})$$
    - Generate the next values for each coordinate x_j successively according to the conditional probability

$$x_j^{(i+1)} \simeq P(x_j | x_1^{(i+1)}, .., x_{j-1}^{(i+1)}, x_{j+1}^{(i)}, ..., x_k^{(i)})$$

Gibbs sampling



Gibbs sampling



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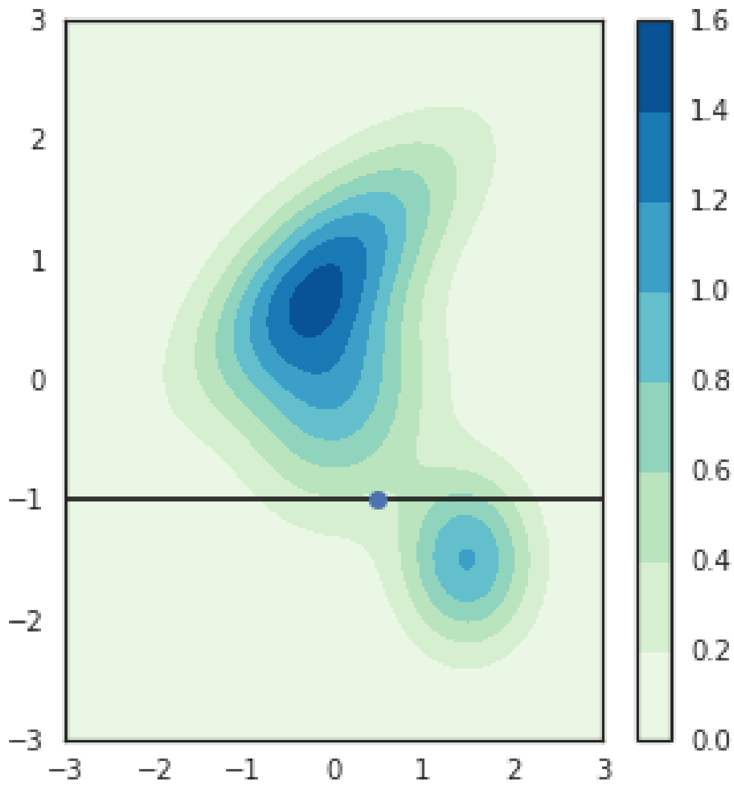

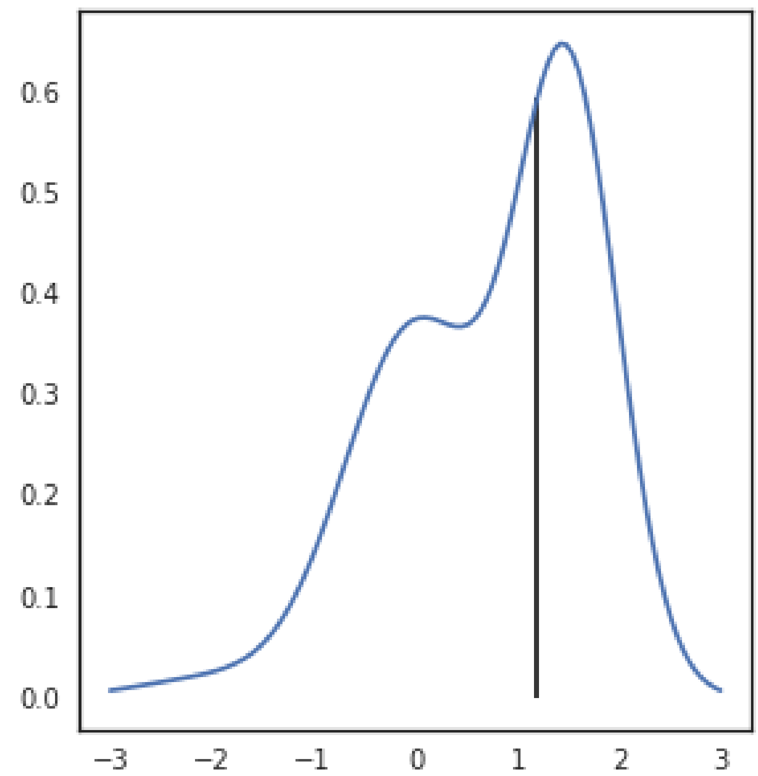

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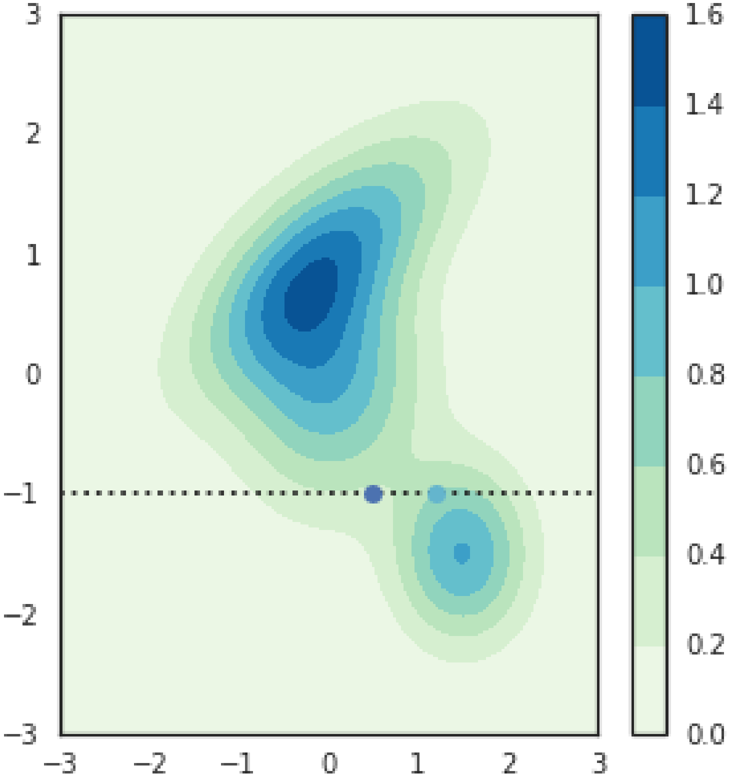

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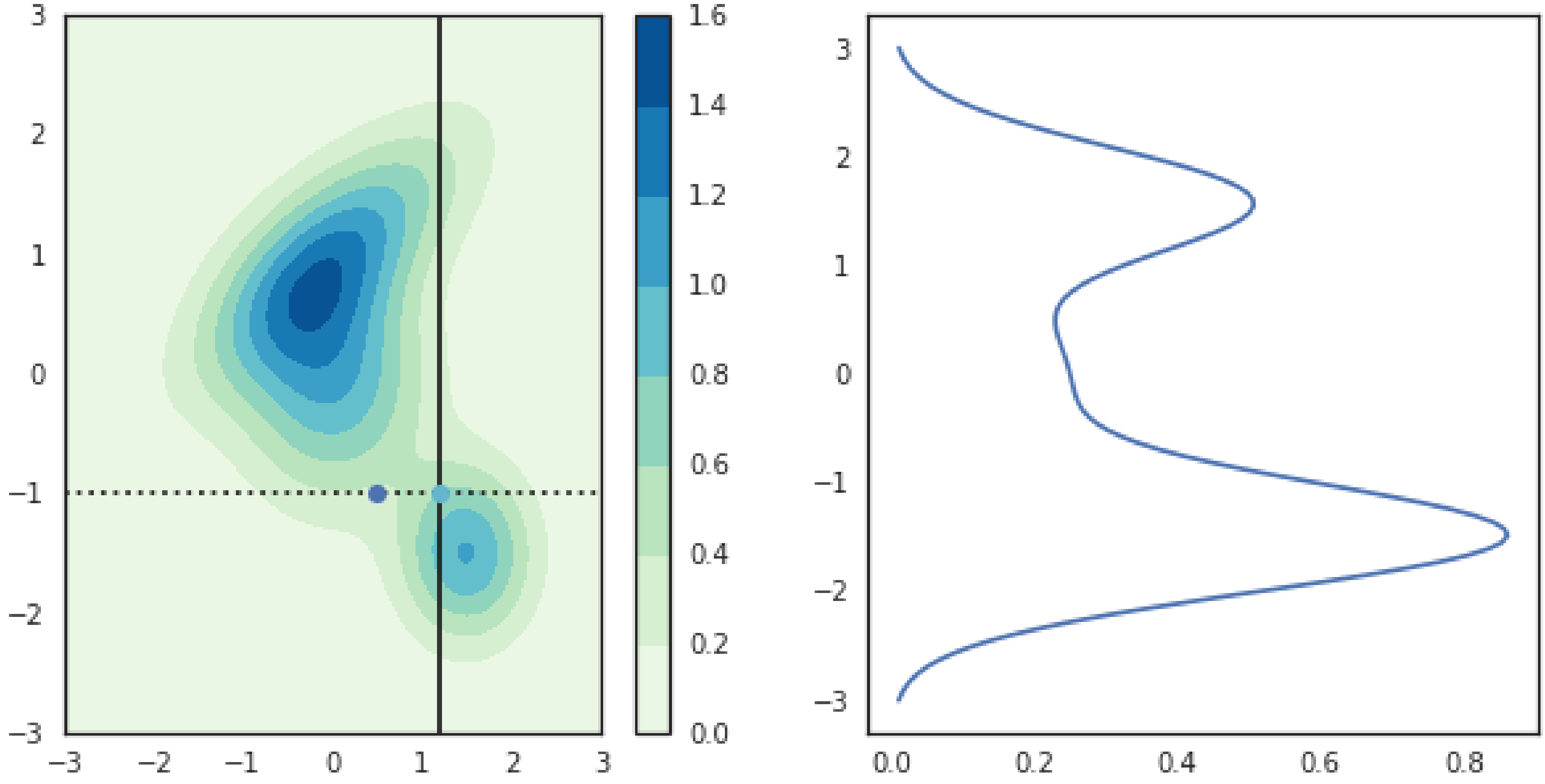

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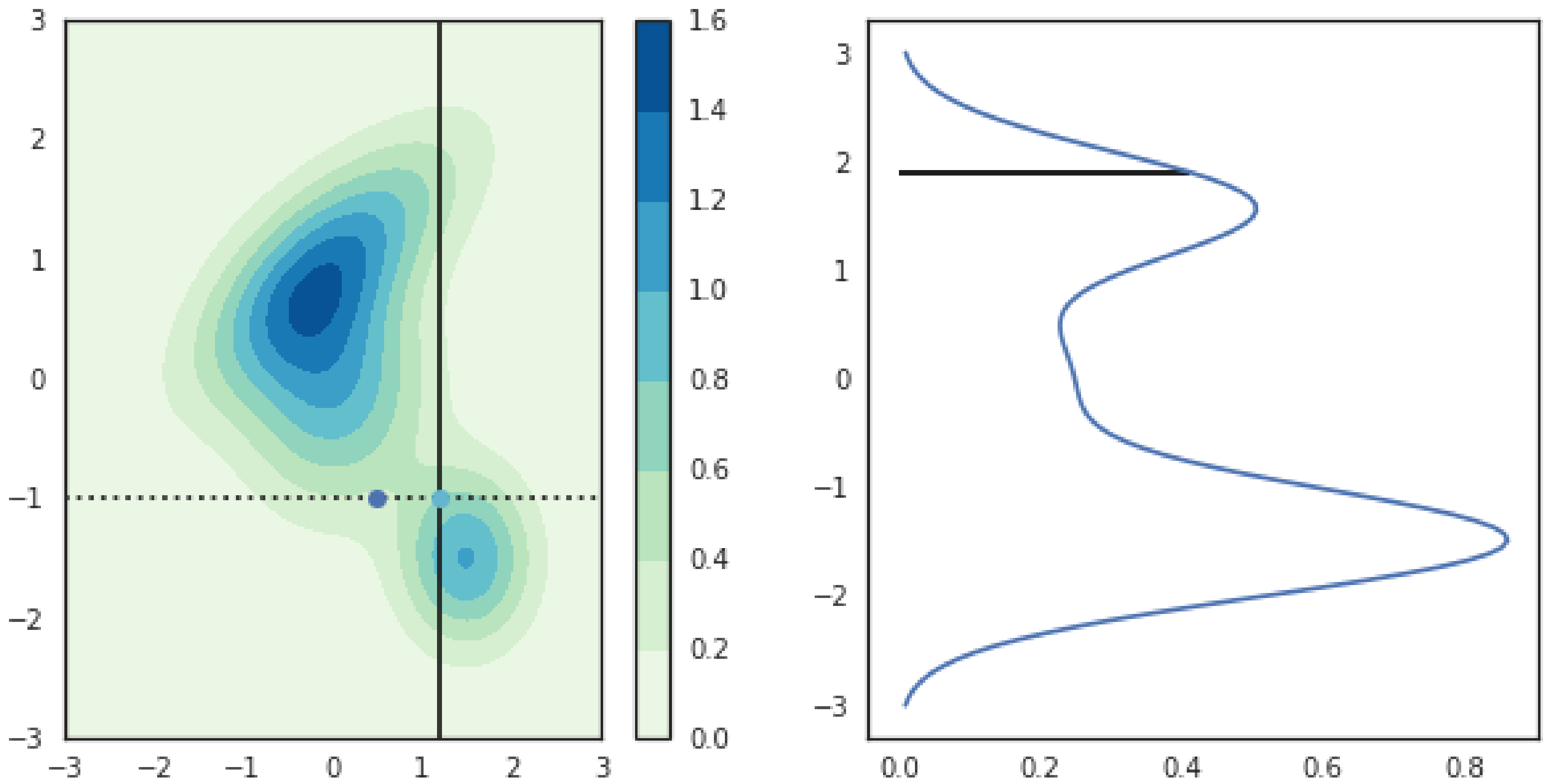

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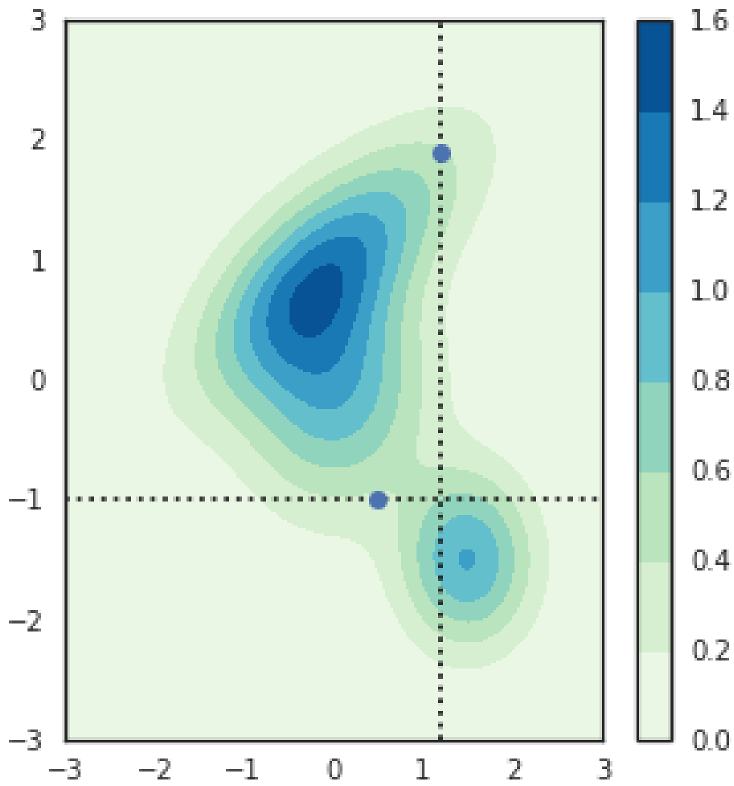

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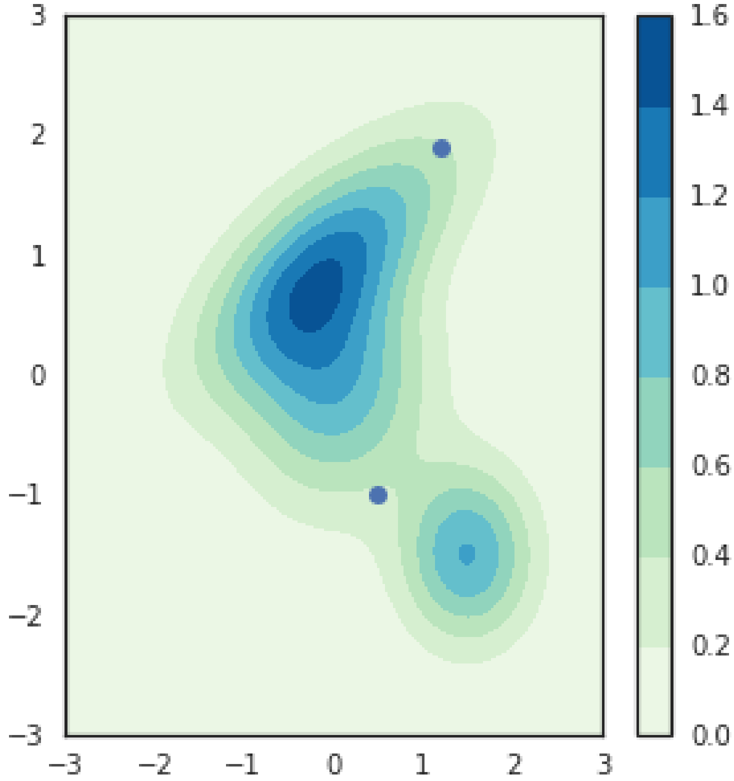

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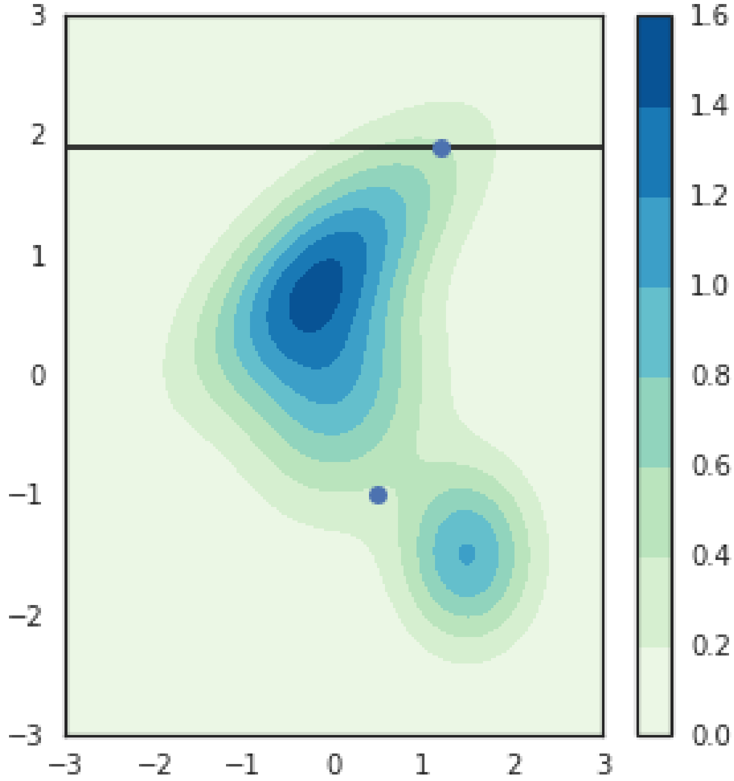

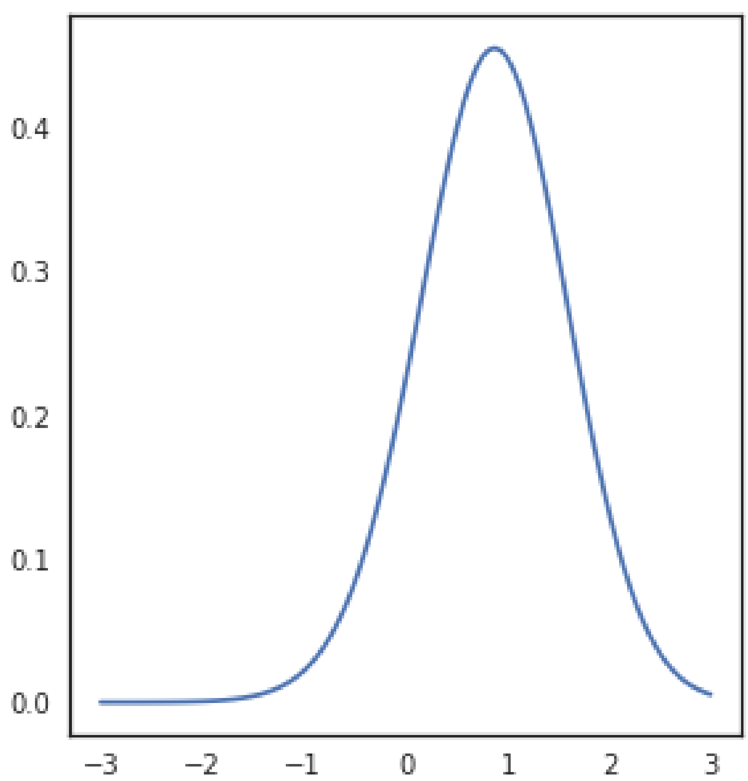

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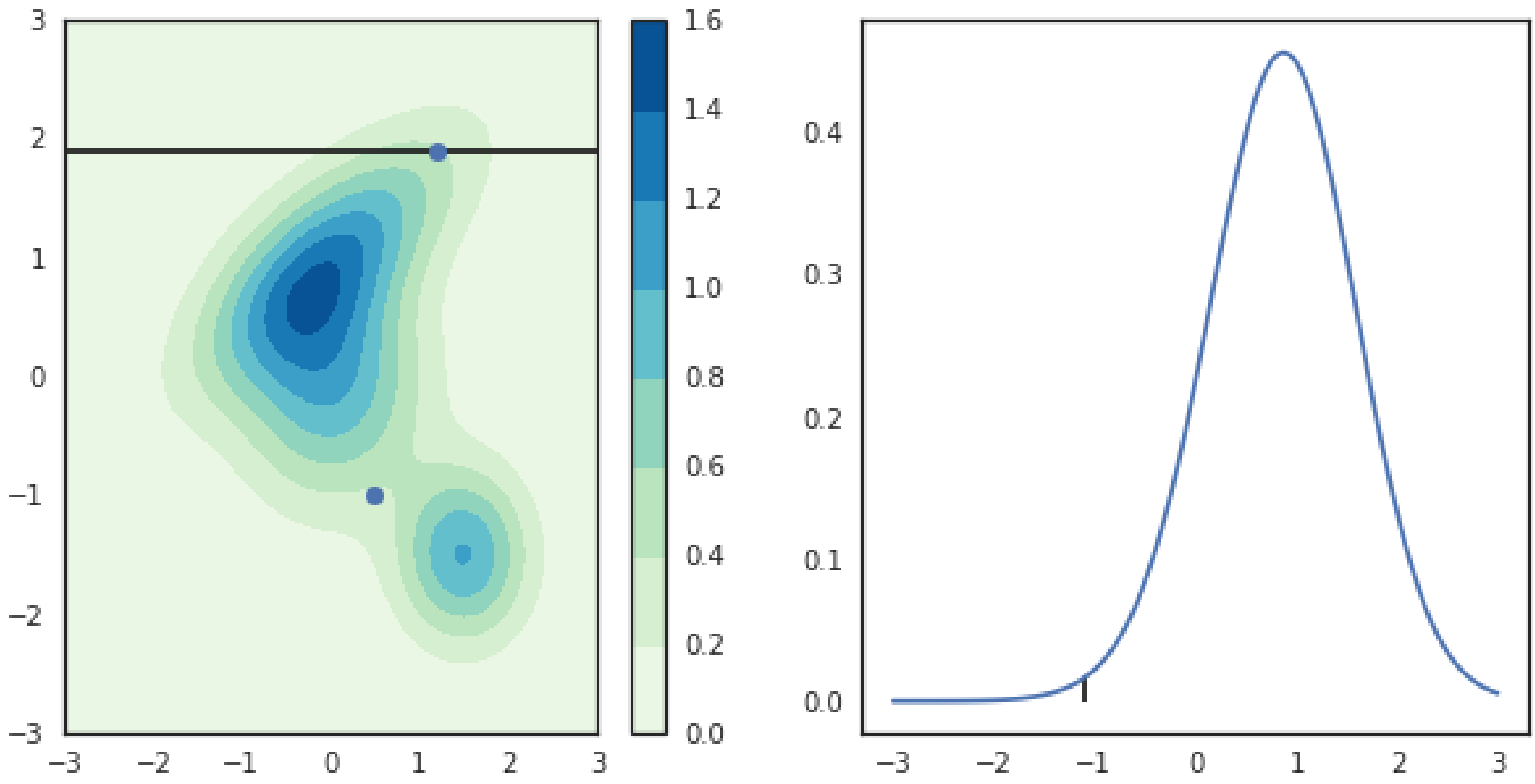

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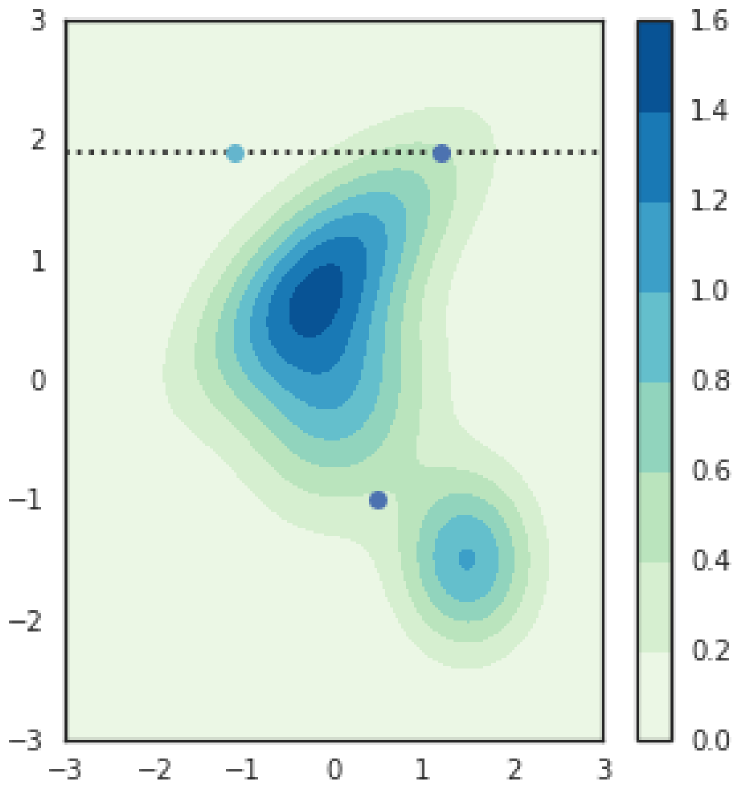

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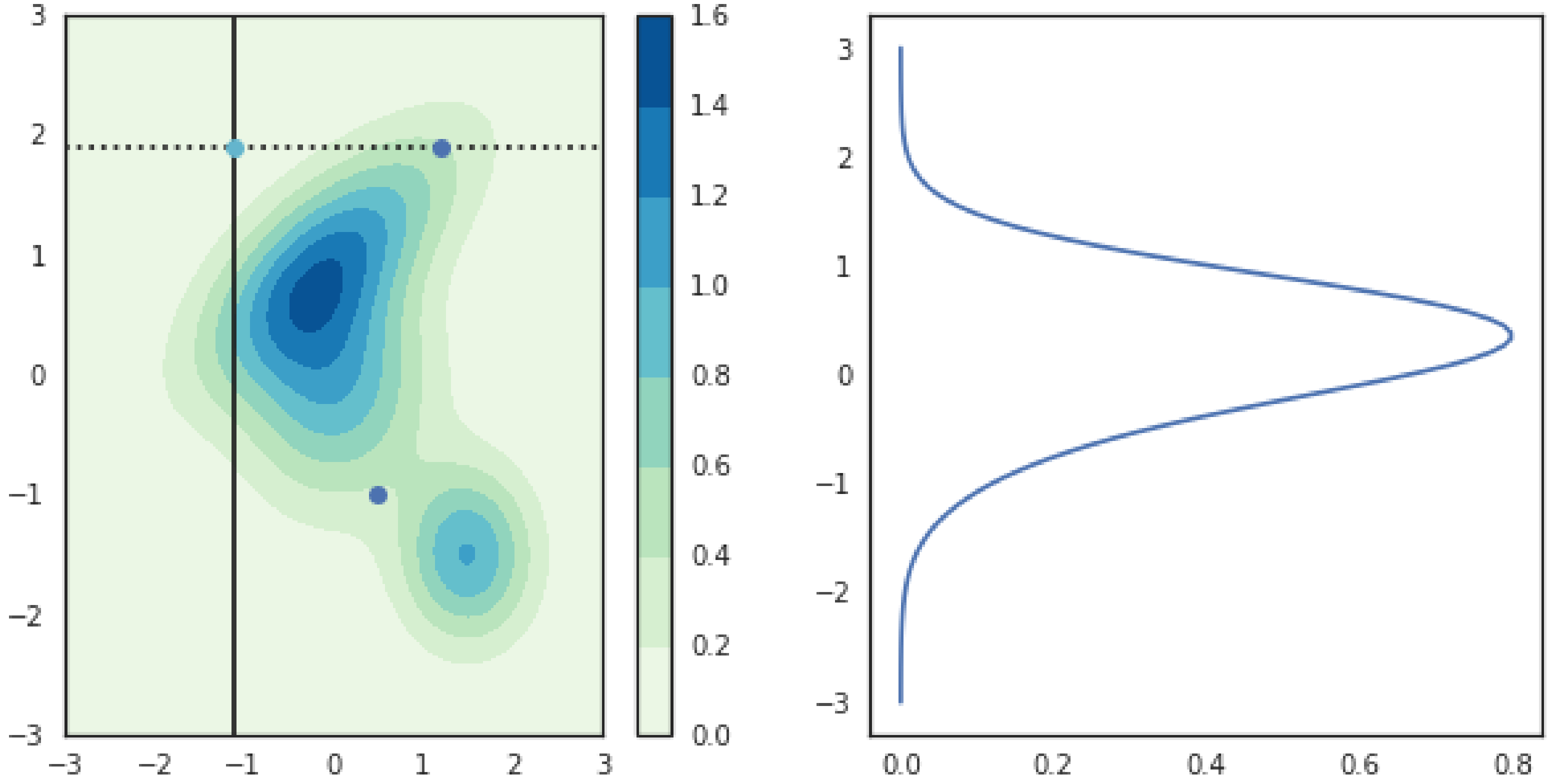

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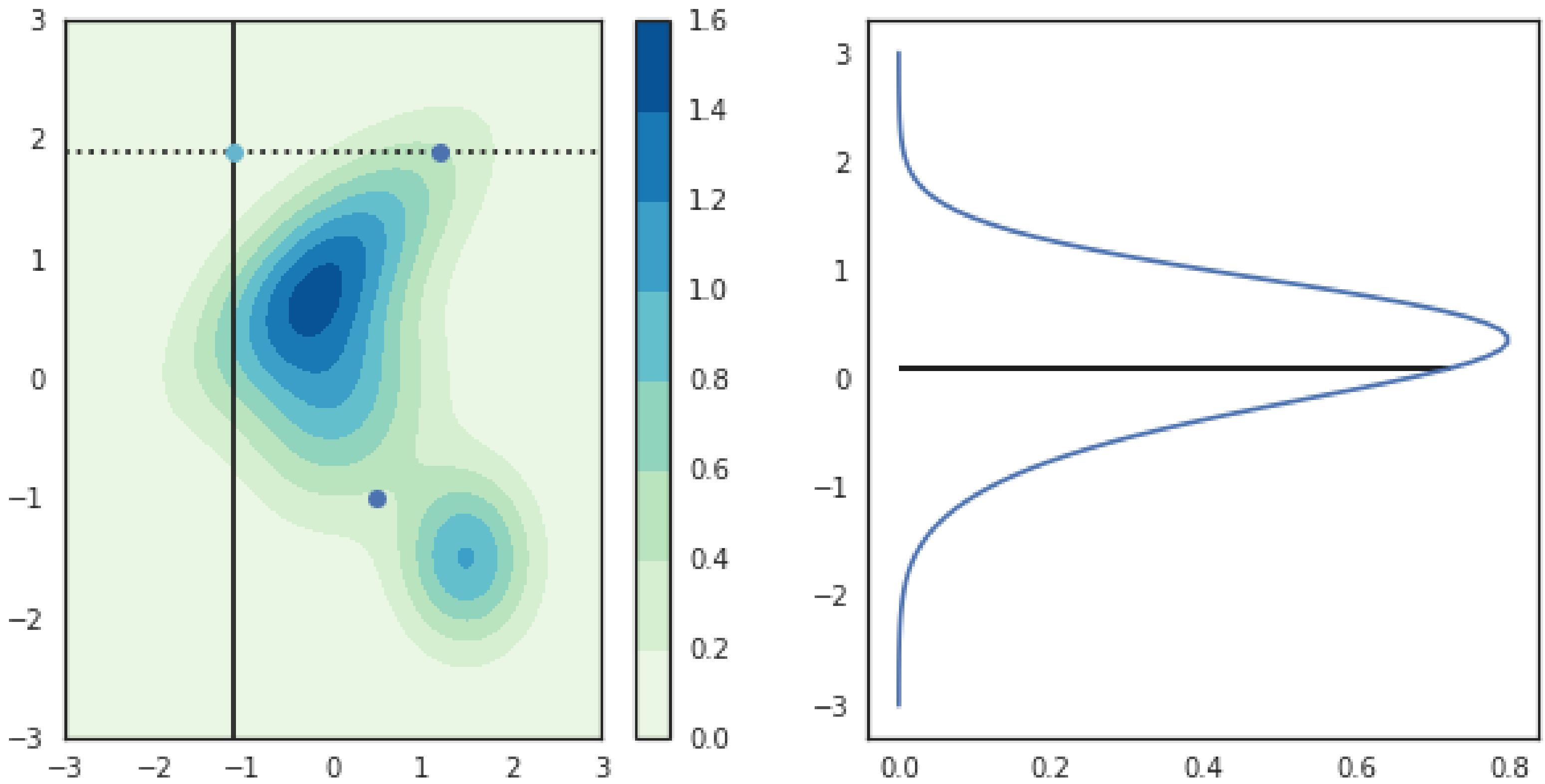

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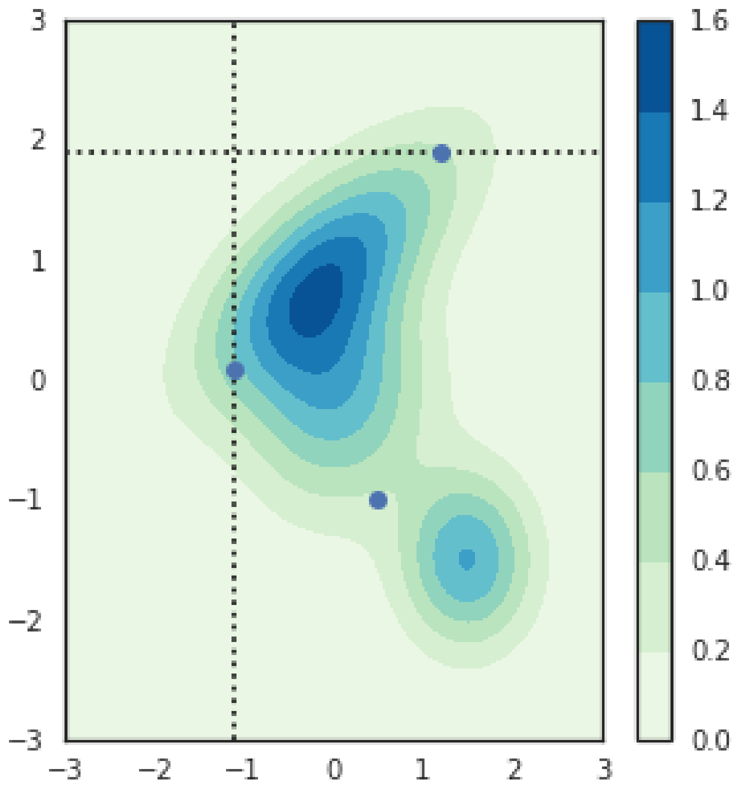

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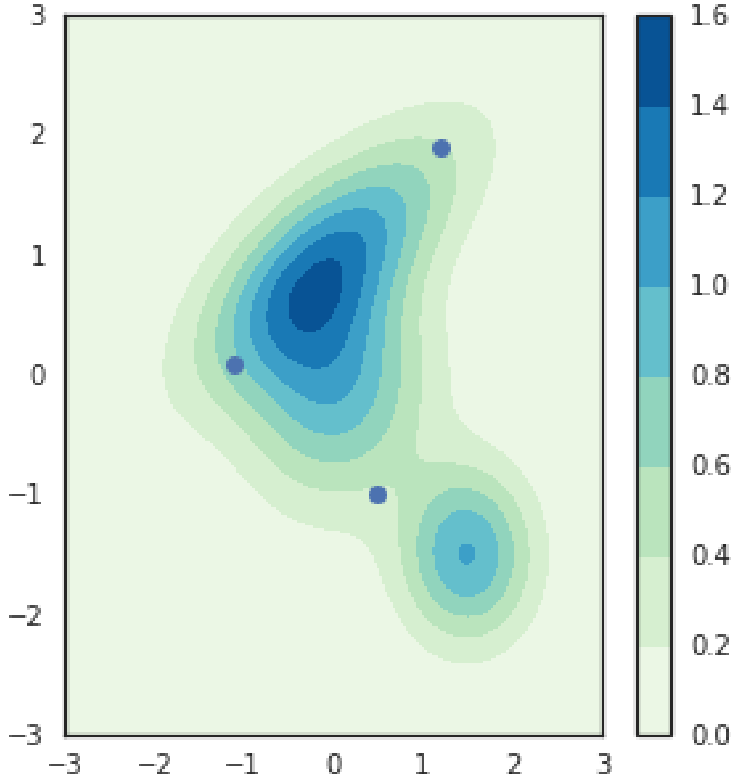


Conditional probability

- With our expression for the probability density

$$f(x_1, ..., x_k) = \sum_{i_1,...,i_k} c_{i_1,...,i_k} \Phi_{i_1}(x_1) \cdots \Phi_{i_k}(x_k)$$

  it is easy to calculate the conditional probabilities

- They are naturally expressed in terms of the basis functions

$$P(x_j | x_1, ..., x_{j-1}, x_{j+1}, ..., x_k) = \sum_j d_j \Phi_j(x_j)$$

  with

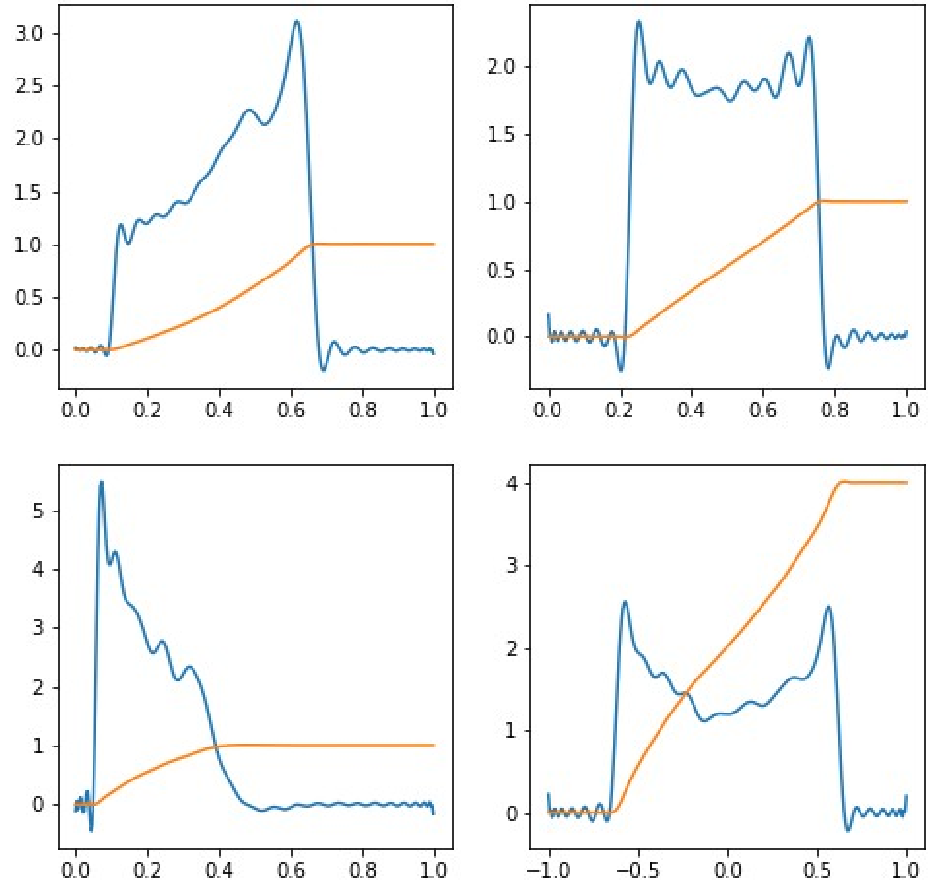
$$\begin{aligned} d_j &= \sum c_{i_1,...,i_{j-1},j,i_{j+1},...,i_k} \Phi_{i_1}(x_1) \cdots \Phi_{i_{j-1}}(x_{j-1}) \\ &\quad \times \Phi_{i_{j+1}}(x_{j+1}) \cdots \Phi_{i_k}(x_k) \end{aligned}$$

Conditional probability

- In order to draw a new value for x_j we need the cumulative distribution of the conditional probability
- The good news is that it is very easy to perform integration in the orthonormal basis:
  - The primitive of the basis functions can be written in terms of the basis functions
  - Integration is simply a multiplication with a matrix than only needs to be calculated once.
  - For the polynomial basis used here the matrix is very sparse

Example

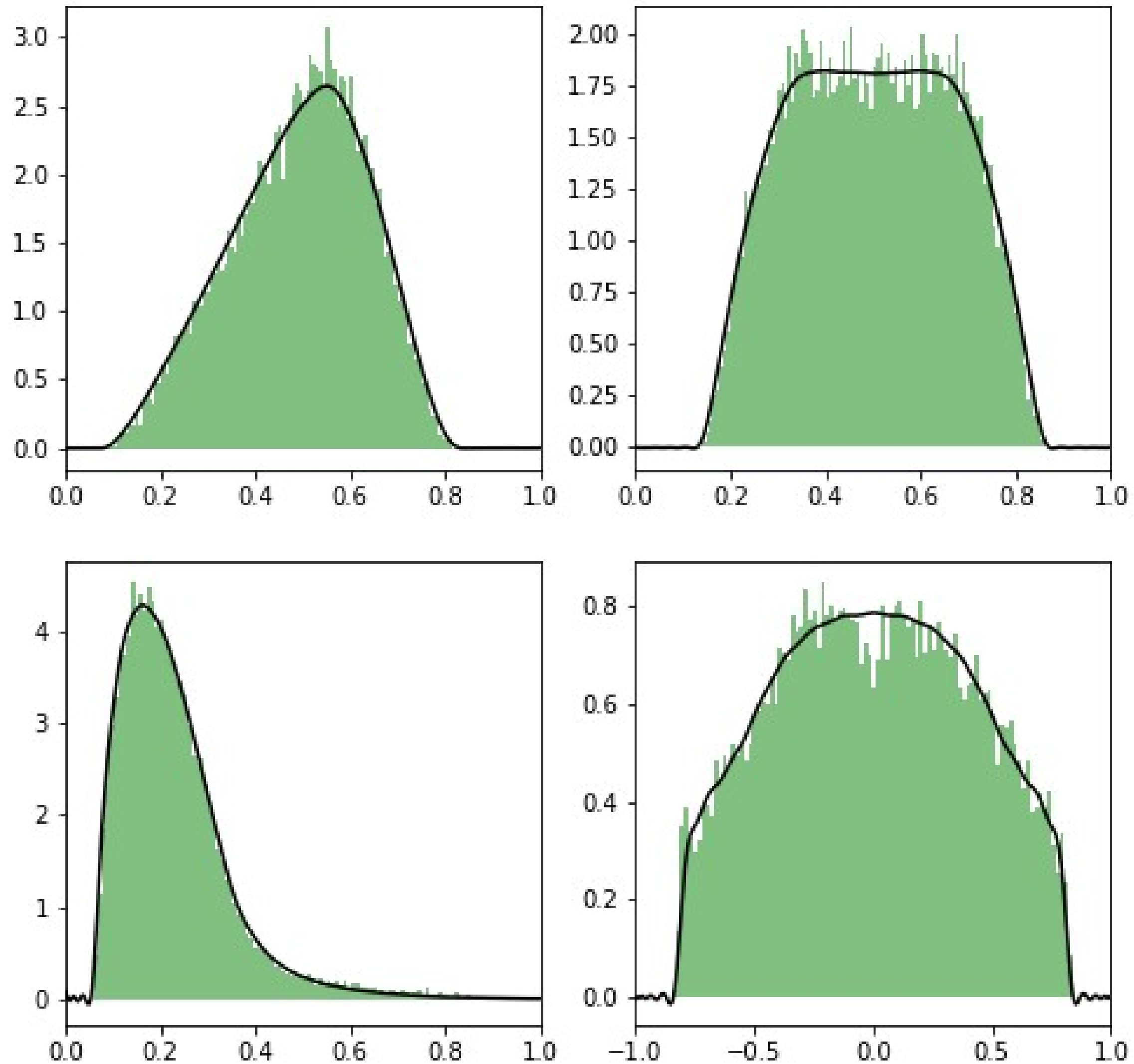
- Conditional distribution



- Fluctuations come from:
  - Truncation of the basis function
  - Limited statistics in the matrix element integration

Unweighted events

- Using the Gibbs sampling method we generate an unweighted sample:



Further work

- Lots to do:
  - Use more GPU
  - NLO/NNLO working example
  - Fix numerical issues
    - Polynomial basis chosen is not good with phase-space theta functions
    - Conditional probabilities not well constrained on phasespace boundaries
  - Hadronic example

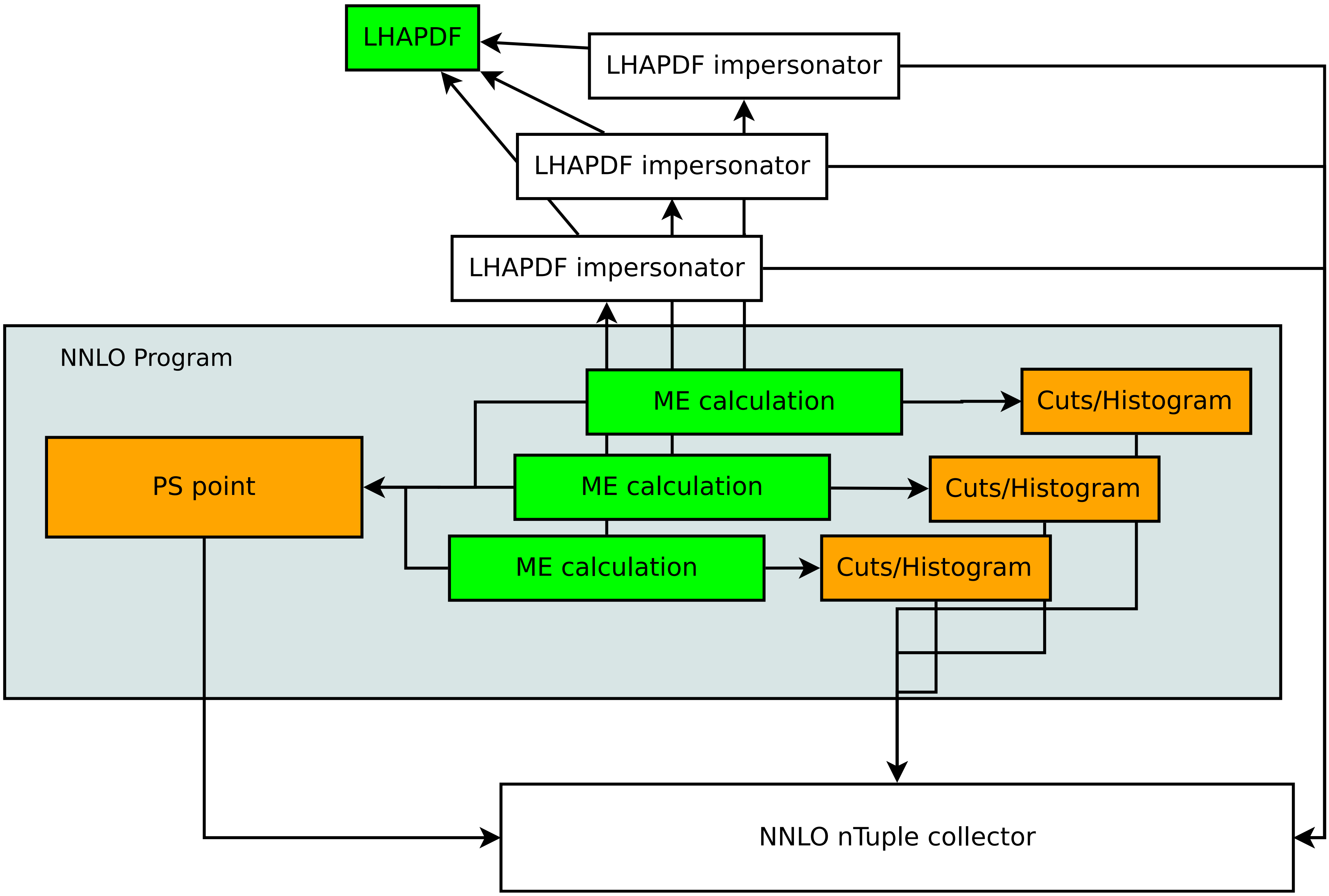
Backup

nTuples for NNLO

nTuples for NNLO

- nTuples have proven useful for NLO
- Can they be as useful for NNLO?
- Same advantages and same disadvantages but amplified:
  - Programs are more complex
  - Larger files:
    - Many more pieces in the calculation
    - More logarithm coefficients
- Main question: is the size reasonable?

Implementation



LHAPDF impersonator

- Allows to alternate vanishing and real pdf to disentangle different pdf terms
- Allows to filter specific initial state
- Reports pdf arguments to the nTuple collector
- Allows to set coupling constant values to one
- Is implemented using a hacking technique so there is no need to modify either
  - the NNLO program
  - the LHAPDF code

Additional difficulties

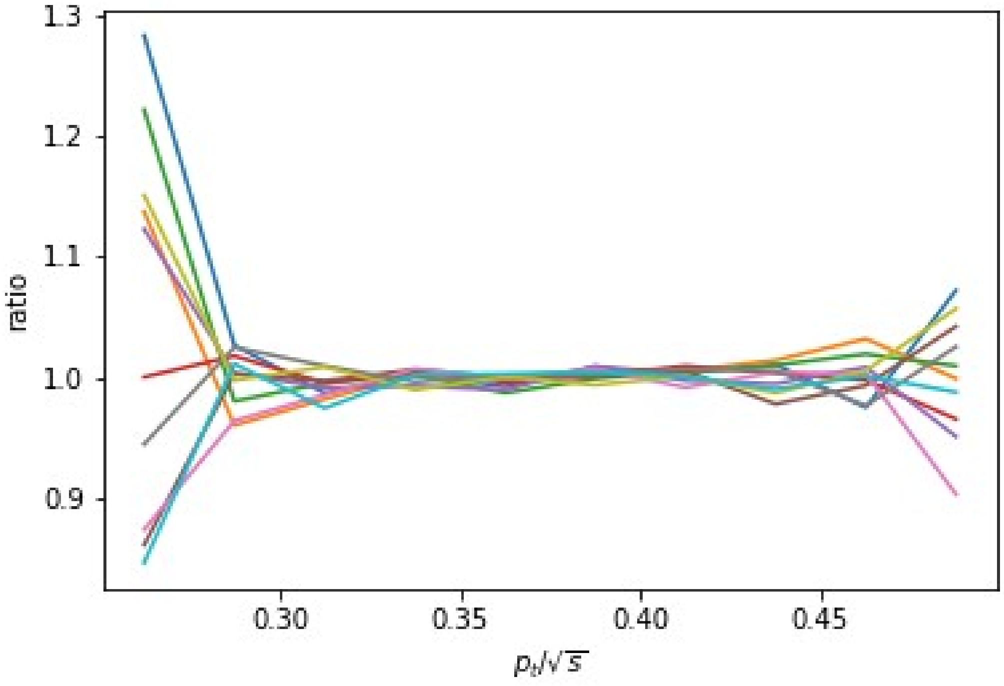
- Caching can cause confusion when the order of pdf, alphas, cuts and histograms are perturbed.
- Need to avoid grid adaptation to ensure synchronisation of the threads

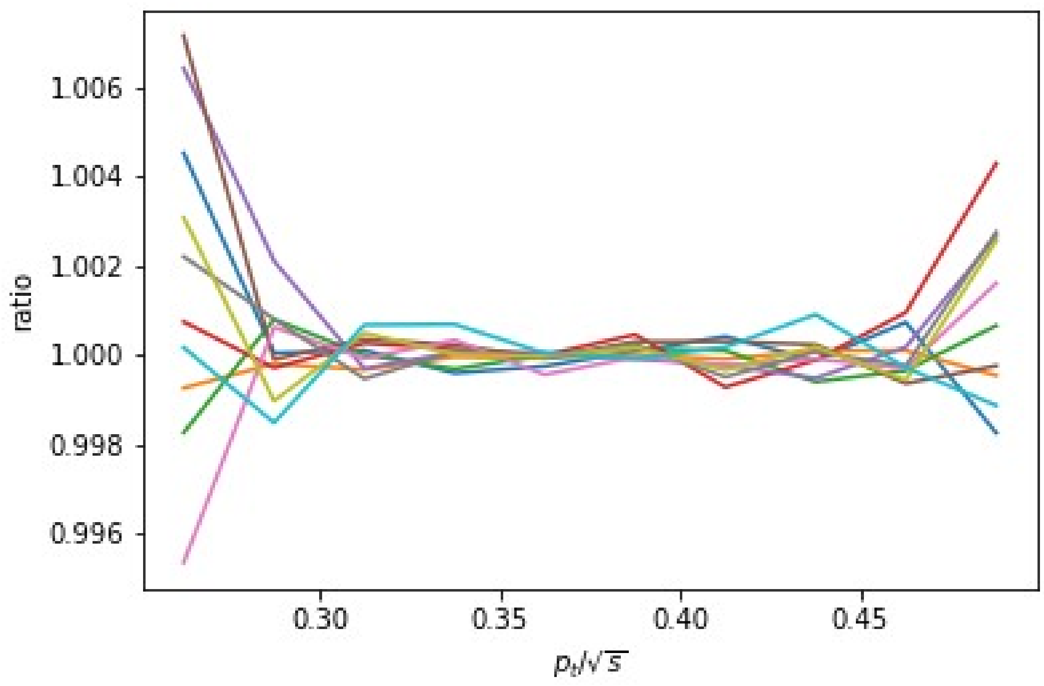
Error estimate

- Two sources of error:
  - Statistical uncertainty on the true value of the coefficients
    - Uncertainty in the matrix element and in the observable
    - This uncertainty can be estimated either
      - during the coefficient determination as a Monte-Carlo error
      - using sub-sampling techniques, with the advantage that correlations between errors are taken into account
  - Truncation error
    - Can be estimated by studying the stability of the prediction as a function of the depth of the expansion.

Coefficient uncertainties

- Observable coefficients
- Matrix elements coefficients





Truncation error

- We can estimate the truncation uncertainty by looking at the convergence as a function of the number of basis function