MOMENT MORPHING[a]

Interpolation between multi-dimensional histograms

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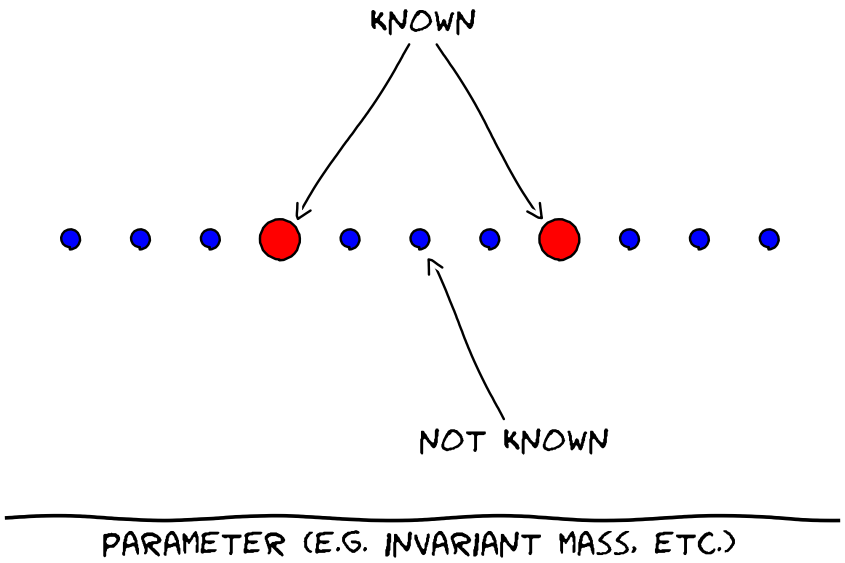
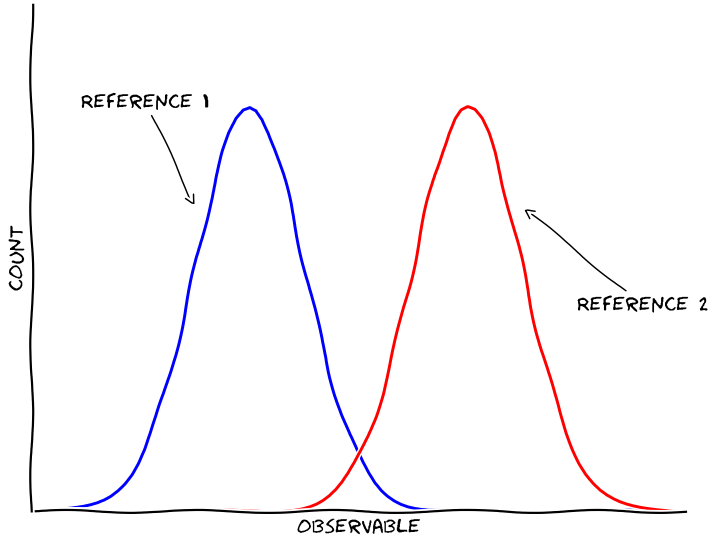
[a]M. Baak, S. Gadatsch, R. Harrington and W. Verkerke 2014.

- Given a set of measurements $\mathbf{x}$, and a hypothesis $\boldsymbol{\alpha}$, what is the probability of the data under this hypothesis?
  - Define a **probability model** $f(\mathbf{x}|\boldsymbol{\alpha})$
- Generally no analytical predictions for $f(\mathbf{x}|\boldsymbol{\alpha})$ available at LHC
  - Monte Carlo simulation (**CPU expensive** and **time consuming**) for "reference" parameter values
- Statistical inference requires maximizing the likelihood
  - Likelihood function must be defined for all values of $\boldsymbol{\alpha}$
- **Interpolate between available samples**
  - **Assumption:** resolution is larger than simulated step size



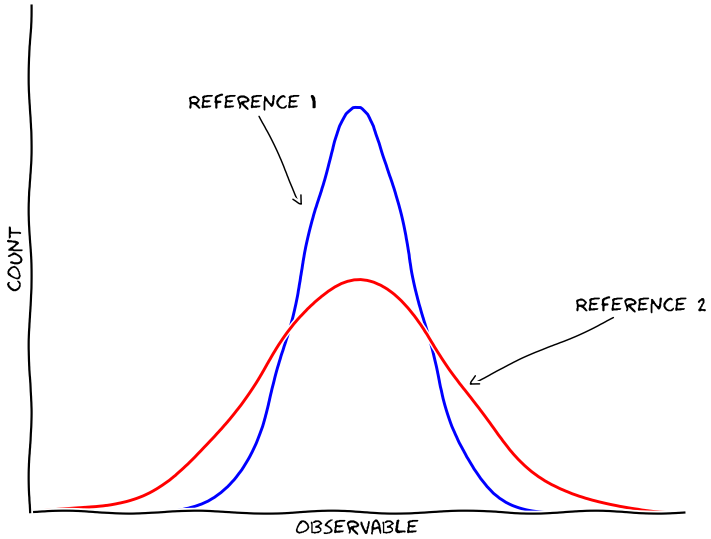
DOMINANT EFFECTS ON (PHYSICS) DISTRIBUTIONS

Changing **mean**



E.g. shifting mass peak, etc.

Changing **variance**



E.g. resonance width, etc.

In the following construct a continuous parametric model for all other parameter values

STEP 1 – VERTICAL MORPHING

- Suppose $f(\mathbf{x}|m)$ is known for n values of m
- Write Taylor series up to order $n-1$ around a reference value m_0

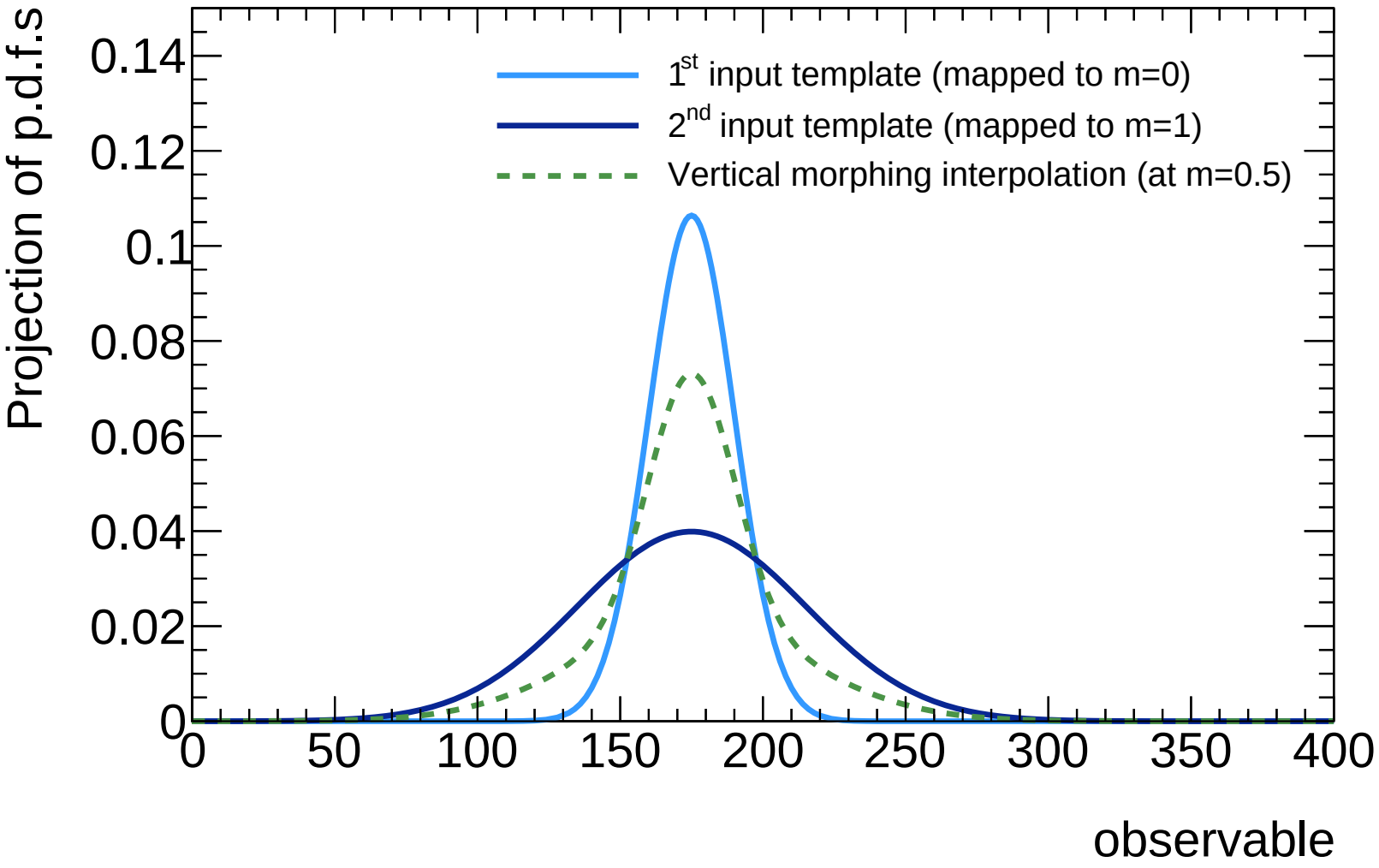
$$f(\mathbf{x}|m_i) \approx \sum_{j=0}^{n-1} \underbrace{(m_i - m_0)^j}_{=M_{ij}} \underbrace{\frac{1}{j!}\frac{\mathrm{d}^{(j)} f(\mathbf{x}|m_0)}{\mathrm{d}m^{(j)}}}_{=f_j'(\mathbf{x}|m_0)} \quad \Leftrightarrow \quad f_j'(\mathbf{x}|m_0) = \sum_{i=0}^{n-1} \left(M^{-1}\right)_{ji} f(\mathbf{x}|m_i)$$

- Predicted template shape at any value m' is a linear combination of the reference templates (**"vertical" morphing**)

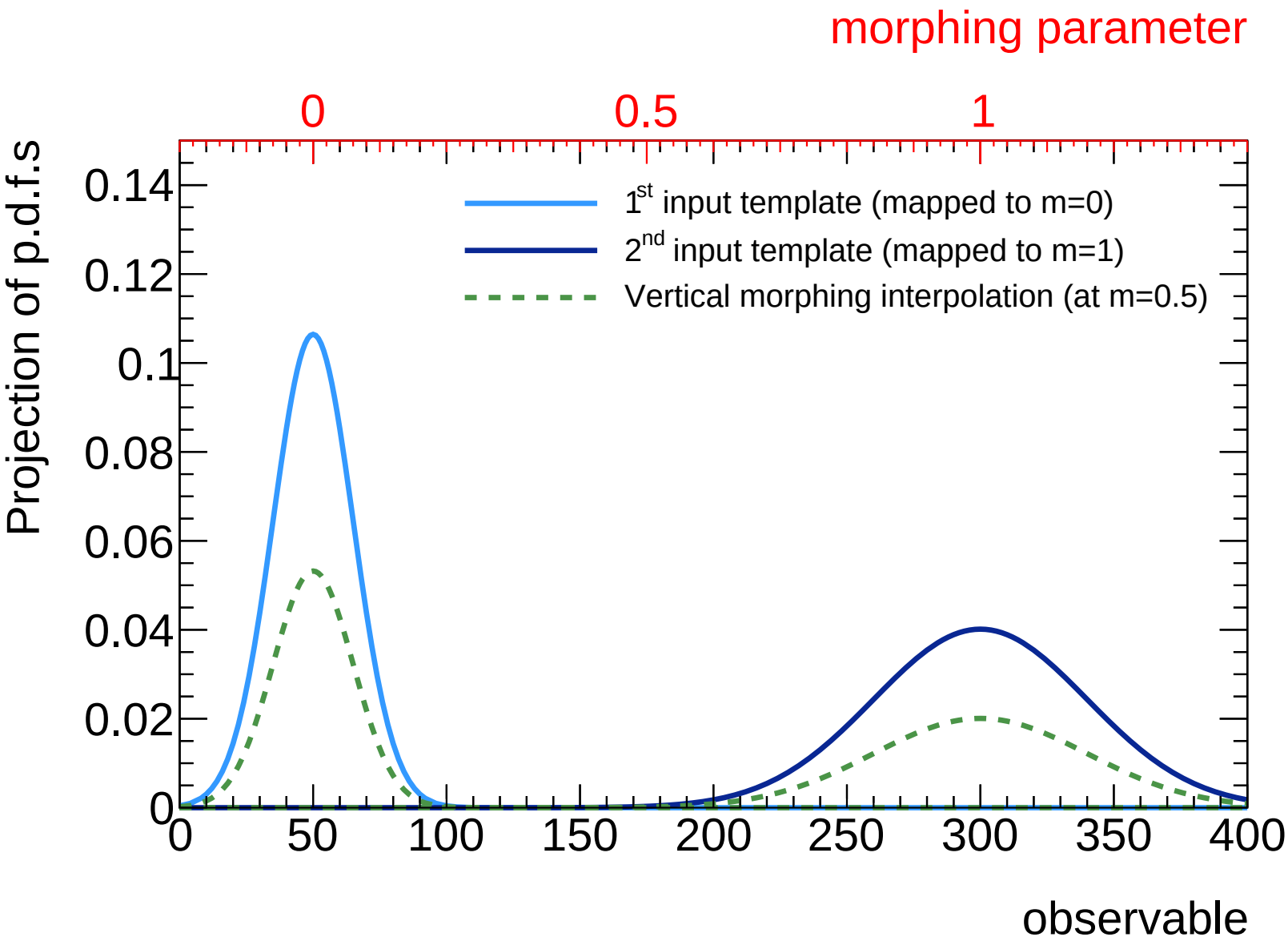
$$f_{\text{pred}}(\mathbf{x}|m') = \sum_{i=0}^{n-1} \underbrace{\sum_{j=0}^{n-1} (m' - m_0)^j \left(M^{-1}\right)_{ji}}_{=c_i(m')} f(\mathbf{x}|m_i)$$

- Coefficients c_i add up to 1

A TOY EXAMPLE



A TOY EXAMPLE



- Linear transformation of the input observables $f(\mathbf{x}|m_i) \to f(\mathbf{x}'|m_i)$
  - Translating referred to as **"horizontal" morphing**

$$x'_{ij} = (x_j - \mu'_j) \underbrace{\frac{\sigma_{ij}}{\sigma'_j}}_{=a_{ij}} + \mu_{ij} \quad \text{with} \quad \begin{aligned} \mu'_j(m) &= \sum_i c_i(m) \cdot \mu_{ij} \\ \sigma'_j(m) &= \sum_i c_i(m) \cdot \sigma_{ij} \end{aligned}$$

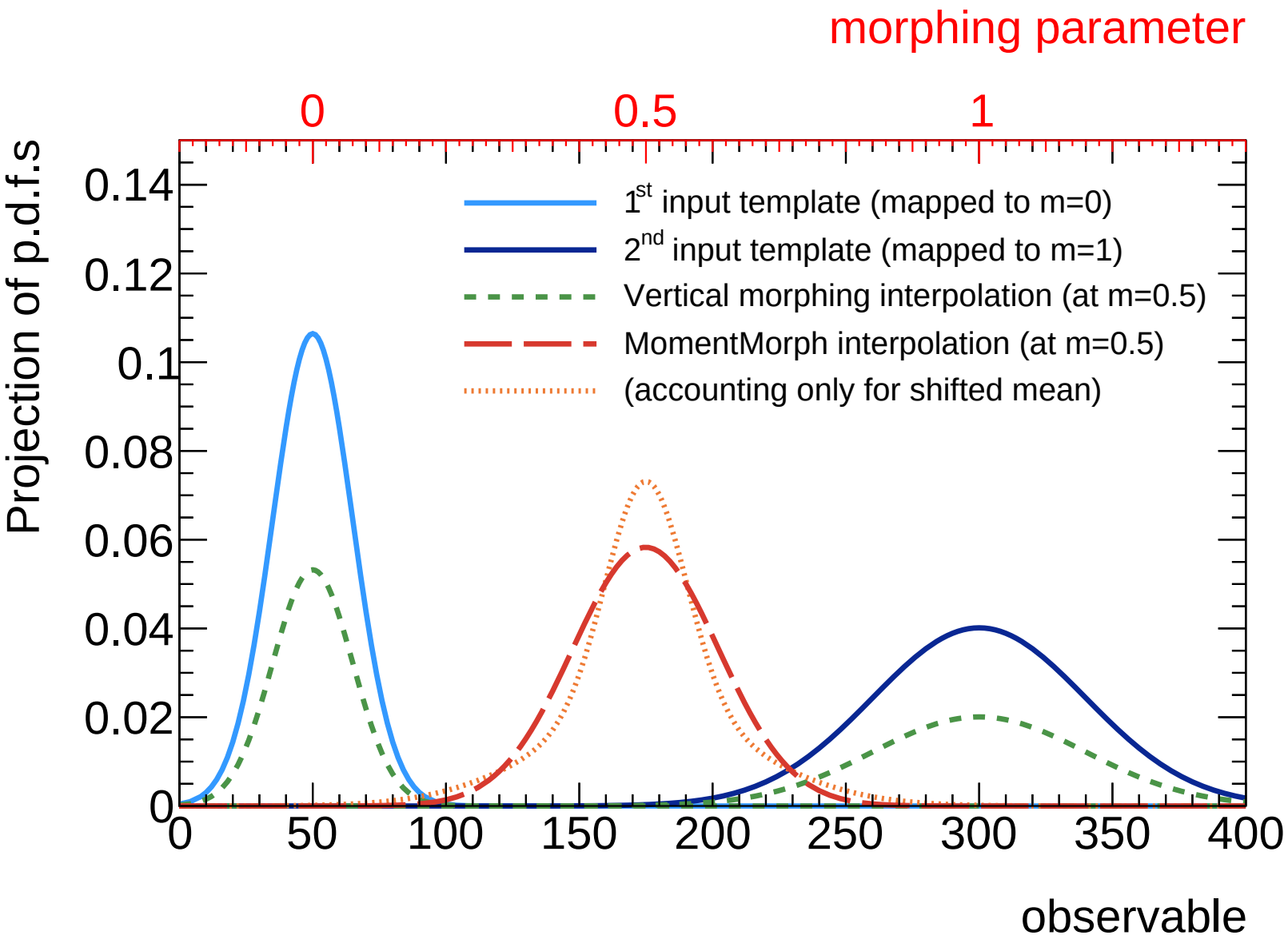
- Normalization only changed by the Jacobian

$$\int_{-\infty}^{+\infty} f(\mathbf{x}'|m_i)\mathrm{d}\mathbf{x} = \frac{1}{\prod_j a_j(m)} \int_{-\infty}^{+\infty} f_i(\mathbf{x}|m_i)\mathrm{d}\mathbf{x}$$

- Final p.d.f. is **self-normalized**

$$p(\mathbf{x}|m') = \sum_i c_i(m') f(\mathbf{x}', m_i) \prod_j a_j(m')$$

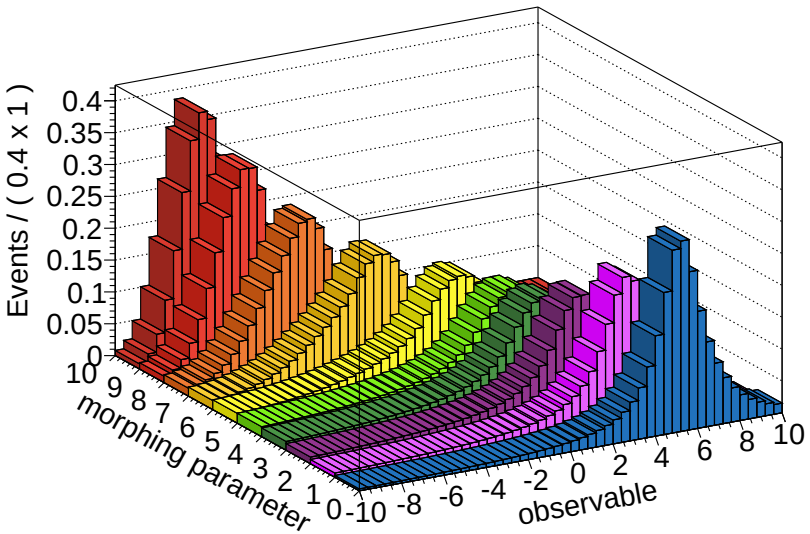
BACK TO THE TOY EXAMPLE



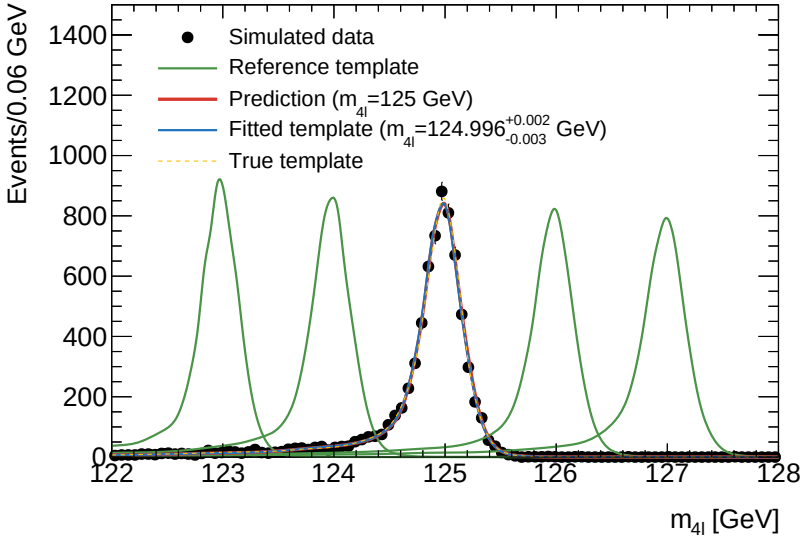
EXAMPLE CODE

```
// This example builds two normal distributions and uses moment morphing to
// interpolate between the templates using RooFit.
using namespace RooFit;

// Create a persistable container for RooFit projects, allowing to use a simplified
// scripting language to build the p.d.f.s needed in this example
RooWorkspace w("w", 1);

// Build two normal distributions, corresponding to different values in the morph
// parameter space. They share the same observable, but have otherwise different
// moments, i.e. mean and width.
w.factory("RooGaussian::gaussian1(obs[0,400],50,15)");
w.factory("RooGaussian::gaussian2(obs,300,40)");

// Build a RooMomentMorph p.d.f. which interpolates between the normal distributions
// created before. The interpolation is parametrized by the parameter alpha and the
// reference templates map to alpha=0 and alpha=1 respectively.
w.factory("RooMomentMorph::morphpdf(alpha[0,1],obs,{gaussian1,gaussian2},{0,1})");

// Set the morphing parameter alpha explicitly to 0.5.
w::alpha->setVal(0.5);

// Create a frame to draw the p.d.f. from before and show the input templates as
// solid blue curves and the moment morph p.d.f. at alpha=0.5 in dashed red.
RooPlot* frame = w::obs->frame();
w::gaussian1->plotOn(frame, LineColor(kBlue), LineStyle(kSolid));
w::gaussian2->plotOn(frame, LineColor(kBlue), LineStyle(kSolid));
w::morphpdf->plotOn(frame, LineColor(kRed), LineStyle(kDashed));
frame->Draw();
```

Cauchy distribution ➟ Crystal Ball line shape ➟ normal distribution



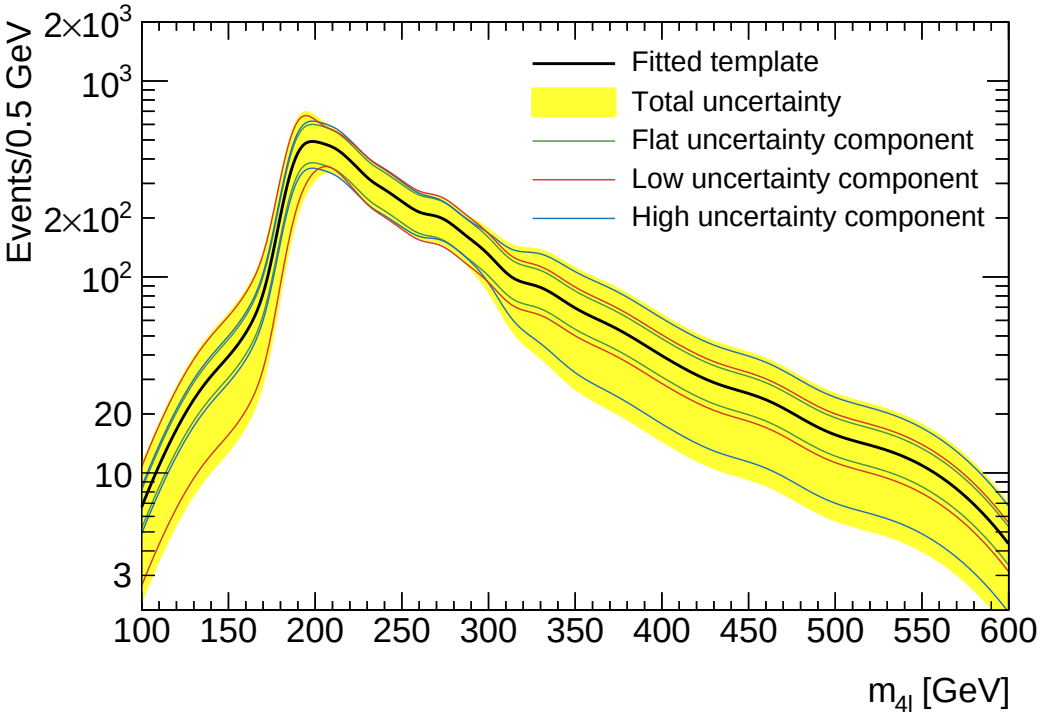
Standard Model Higgs boson decaying to four leptons

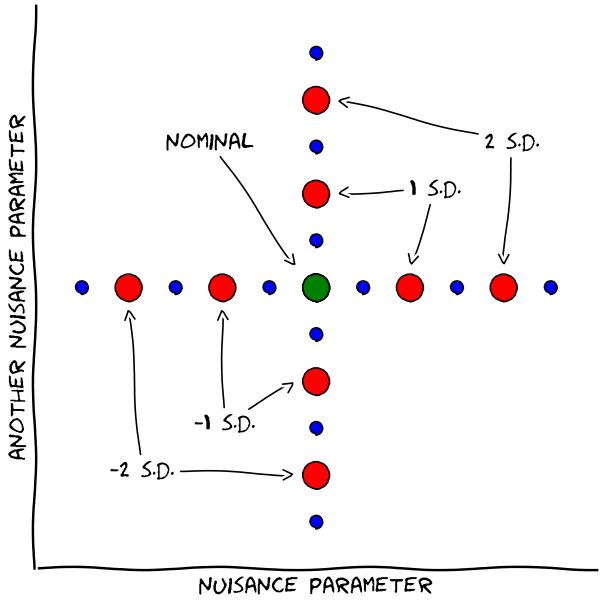


- Variations around a nominal distribution
  - Typically just the nominal distribution and $\pm 1\sigma$ variations simulated

$$f(x|\theta)\big|_{\theta=0,\pm 1} \rightarrow f(x|\theta) \text{ for all } \theta$$

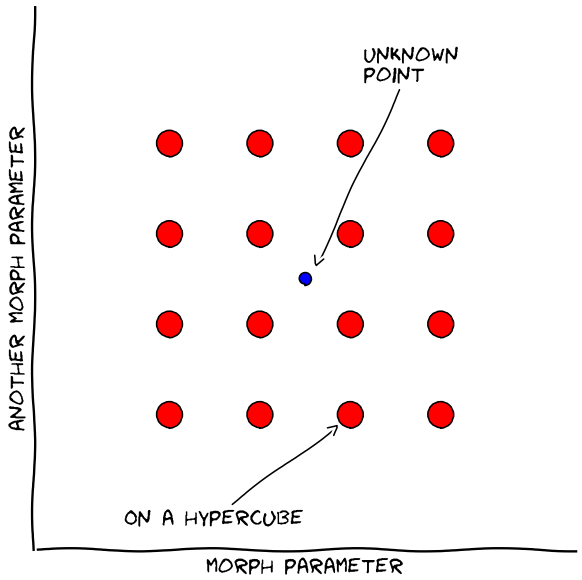
- Assume that systematic effects in physics measurement **factorize**: $L(\alpha_i, \alpha_j) = L(\alpha_i)L(\alpha_j)$





- Used for background description in ATLAS $H \rightarrow ZZ^* \rightarrow 4\ell$ analysis
- Illustration for three uncertainties
  - Flat, low $m_{4\ell}$, high $m_{4\ell}$

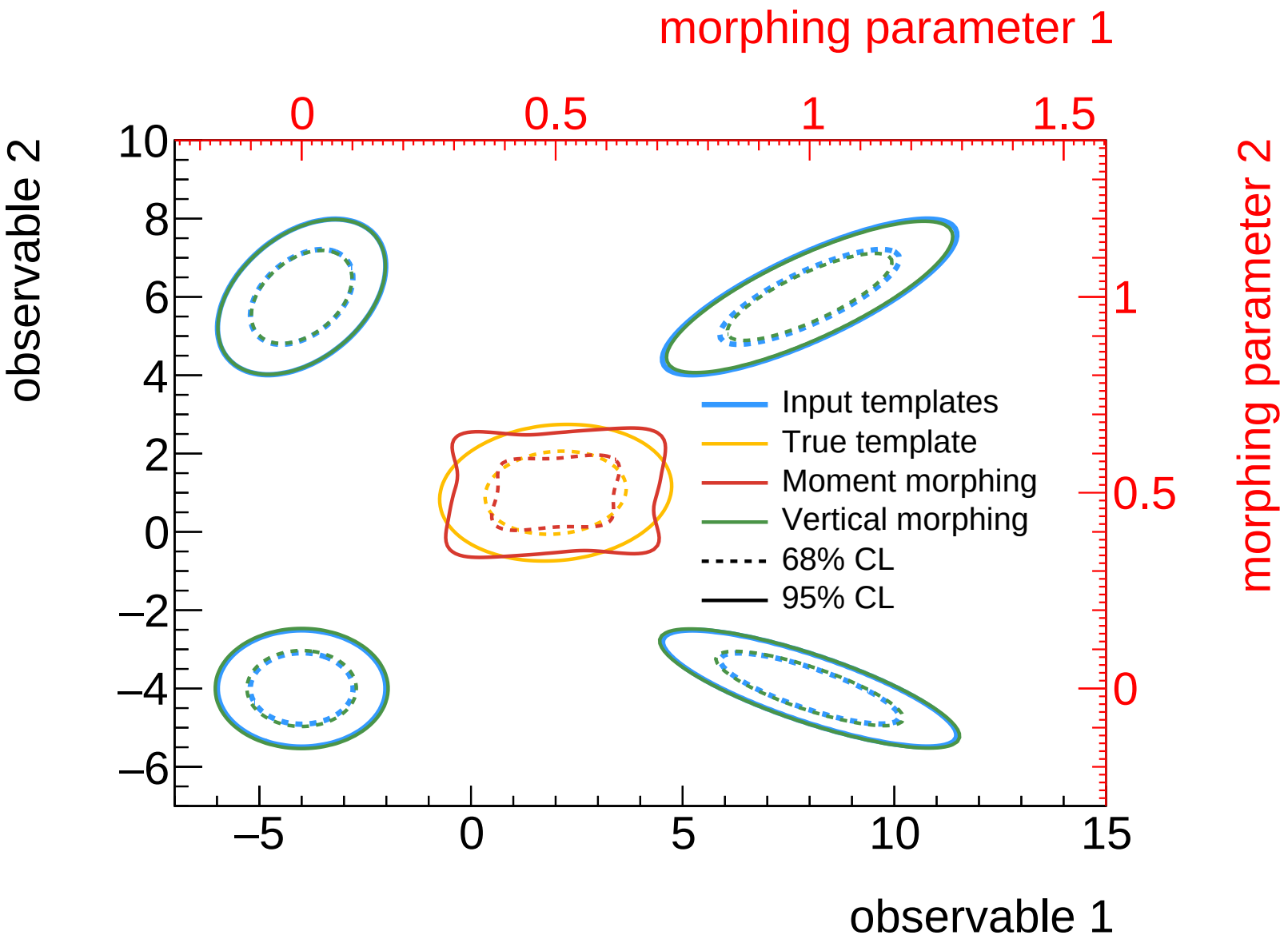
- Extendable to $M \geq 1$ observables and $N \geq 1$ model parameters
  - Reference points on a N-dimensional hypercube
- new! Model the impact of a non-factorizable response: $L(\alpha_i, \alpha_j) \neq L(\alpha_i)L(\alpha_j)$
  - E.g. b-tagging calibration depends (somewhat) on jet calibration



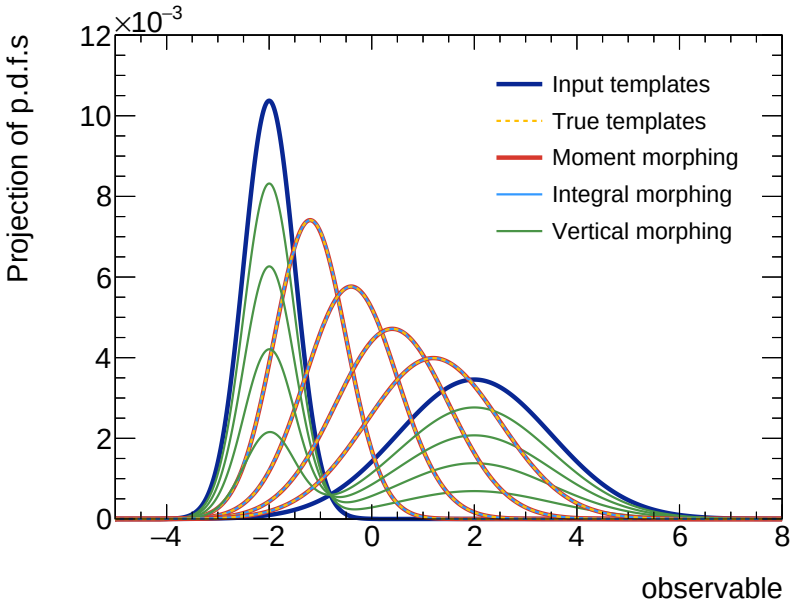

```
// Define axes that span a hypercube
RooBinning dim1(1, 0.0, 1.0);
RooBinning dim2(1, 0.0, 1.0);

// Attach reference distributions to bin boundaries
RooMomentMorphND::Grid referenceGrid(dim1, dim2);
referenceGrid.addPdf(*gauss1, 0, 0);
referenceGrid.addPdf(*gauss3, 1, 0);
referenceGrid.addPdf(*gauss2, 0, 1);
referenceGrid.addPdf(*gauss4, 1, 1);
```

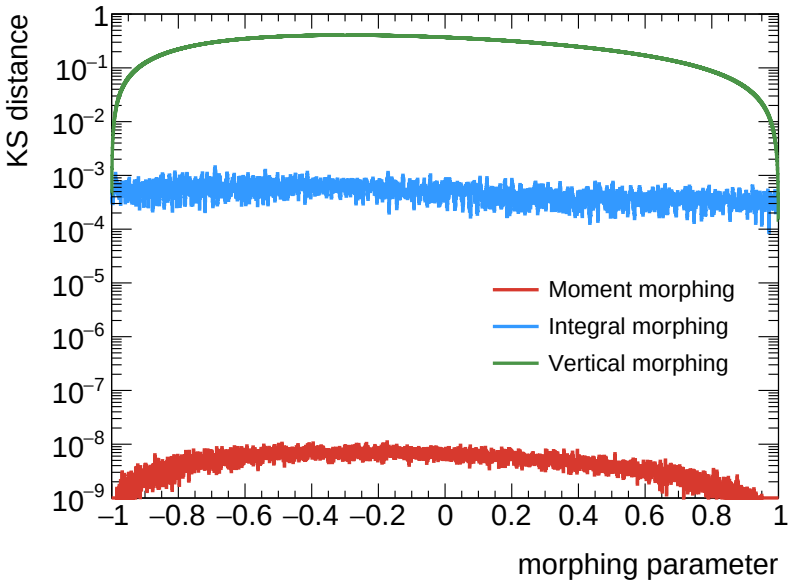
- Subject to changes in the covariance moments

AN EXAMPLE IN TWO DIMENSIONS



Exact for any distribution with linearly changing first and second moments and fixed higher-order moments



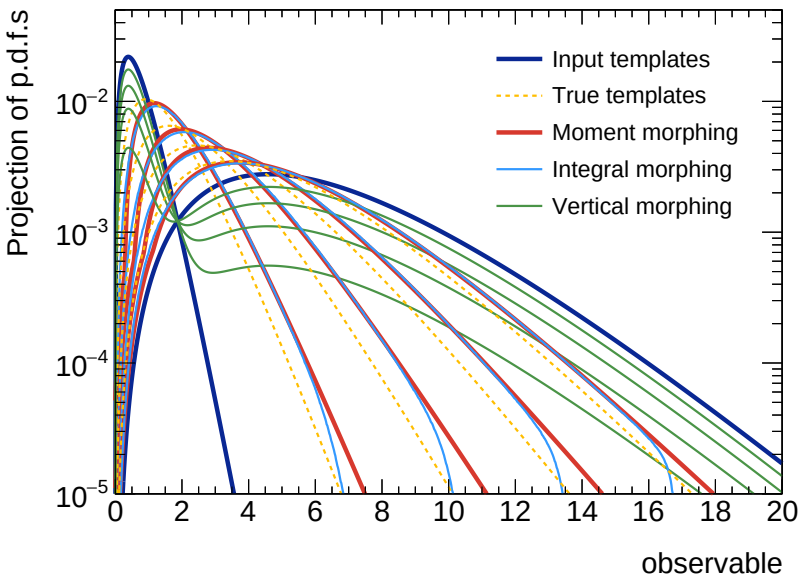


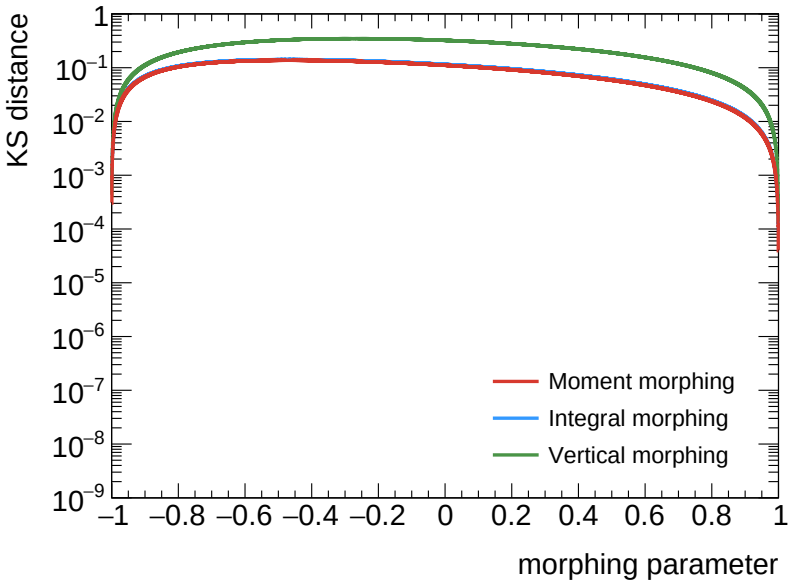
Comparison of ***moment morphing***[a] *with* ***vertical morphing***[b] *and* ***integral morphing***[c] *using the Kolmogorov-Smirnov distance between interpolated and true shape as metric*

[a] M. Baak, S. Gadatsch, R. Harrington and W. Verkerke 2014.
[b] E.g. K. Cranmer, G. Lewis, L. Moneta, A. Shibata, and W. Verkerke 2012, and Ref. [a].
[c] A.L. Read 1999.

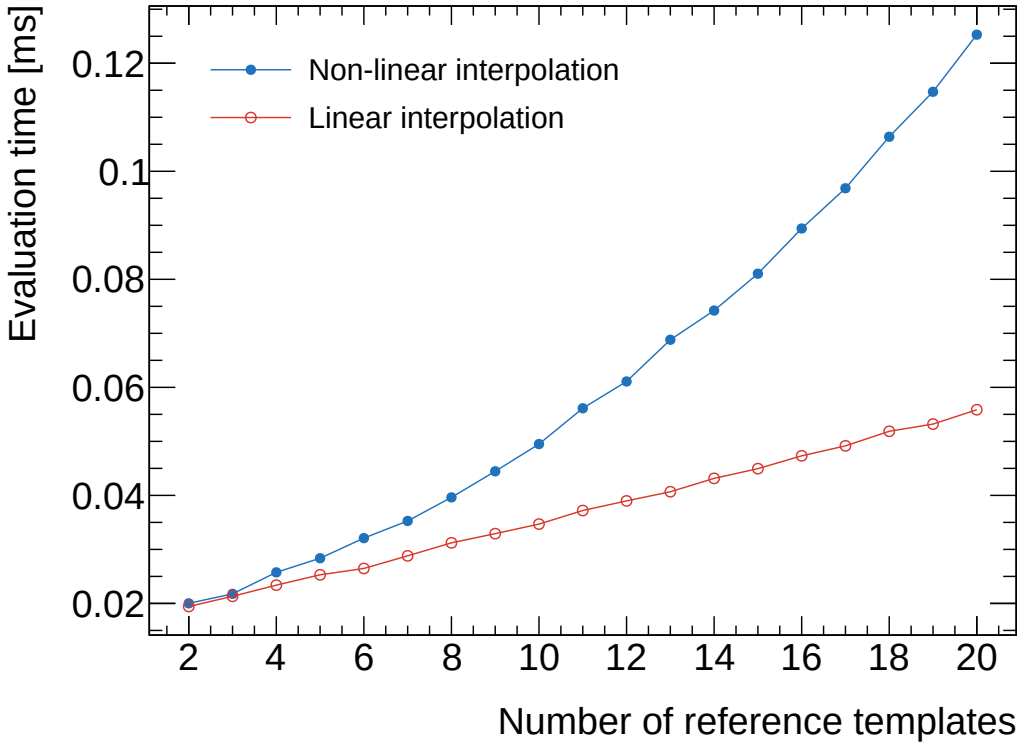
Deviations from exact prediction due to

- ⚠ (Local) non-linearity of the first and second moment
  - ☞ Approximate by piece-wise linear interpolation or higher order polynomial
- ⚠ Any dependence on higher moments
  - ☞ Empirically accounted for, but accuracy depends on distributions





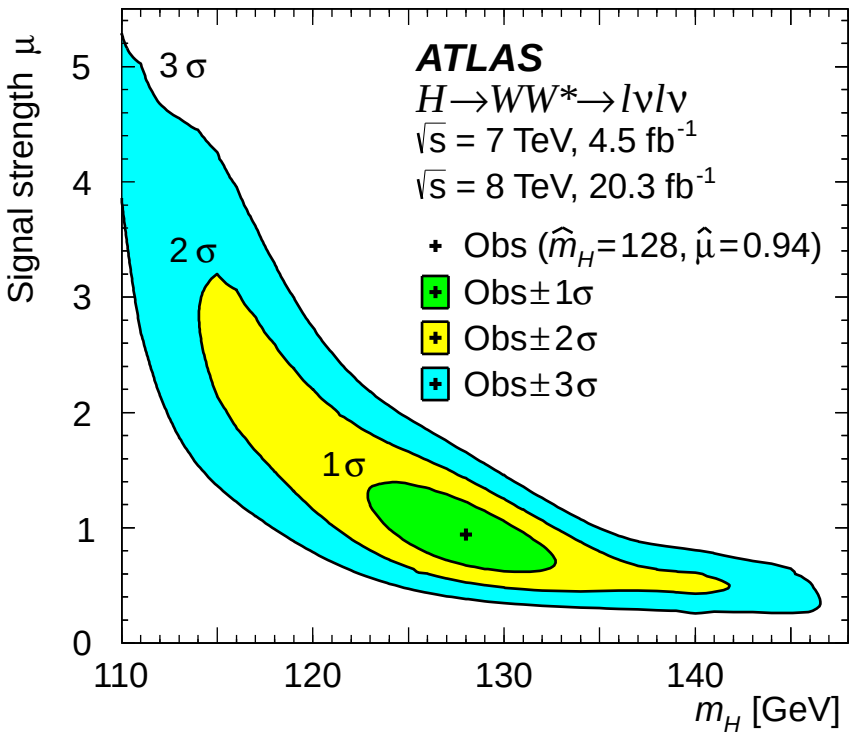
- Numerically stable and fast
  - Caching of expensive components (numerically computed moments, ...)
  - No need to compute normalization of p.d.f.



- Implementation available in the **RooFit** models library in **ROOT**

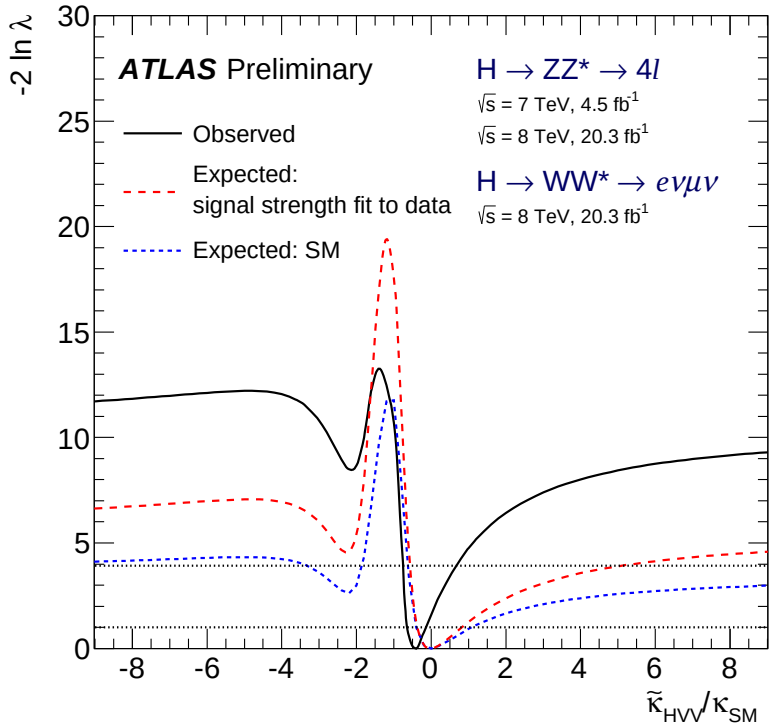
Higgs boson rate in $H \to WW^*$

- Simulated samples available in 5 GeV in m_H



Higgs boson *CP* measurement

- Combination of 1d ($H \to WW^*$) and 2d ($H \to ZZ^*$) moment morphing



[1]The ATLAS Collaboration 2014; The ATLAS Collaboration 2015.

New algorithm to interpolate between Monte Carlo sample distributions

- Generic, simple, fast, stable, accurate
  - Binned histogram and continuous templates in arbitrary dimensions
  - Horizontal and vertical morphing
  - Self-normalized, caching of expensive objects
  - Exact or nearly exact for many typical applications

Backup

- M. Baak, S. Gadatsch, R. Harrington and W. Verkerke, *Interpolation between multi-dimensional histograms using a new non-linear moment morphing method*, arXiv: 1410.7388 [physics.data-an].
- K. Cranmer, G. Lewis, L. Moneta, A. Shibata, and W. Verkerke, *HistFactory: A tool for creating statistical models for use with RooFit and RooStats*,
- A.L. Read, *Linear interpolation of histograms*, Nucl.Instrum.Meth. **A425** pp. 357–360.
- The ATLAS Collaboration, *Observation and measurement of Higgs boson decays to WW* with the ATLAS detector*, arXiv: 1412.2641 [hep-ex].
- The ATLAS Collaboration, *Study of the spin and parity of the Higgs boson in HVV decays with the ATLAS detector*, ATLAS-CONF-2015-008.

- Two input distributions $f_1(x)$ and $f_2(x)$ with cumulative distribution functions

$$F_1(x) = \int_{-\infty}^{x} f_1(x')\mathrm{d}x' \quad \text{and} \quad F_2(x) = \int_{-\infty}^{x} f_2(x')\mathrm{d}x'$$

- Find x_1 and x_2 for which

$$F_1(x_1) = F_2(x_2) = y \equiv \bar{F}(x) \quad \text{with} \quad x = ax_1 + bx_2$$

- Interpolated distribution is

$$\bar{F}^{-1}(y) = a\bar{F}_1^{-1}(y) + b\bar{F}_2^{-1}(y) \quad \Leftrightarrow \quad \bar{f}(x) = \frac{f_1(x_1)f_2(x_2)}{af_2(x_2) + bf_1(x_1)}$$