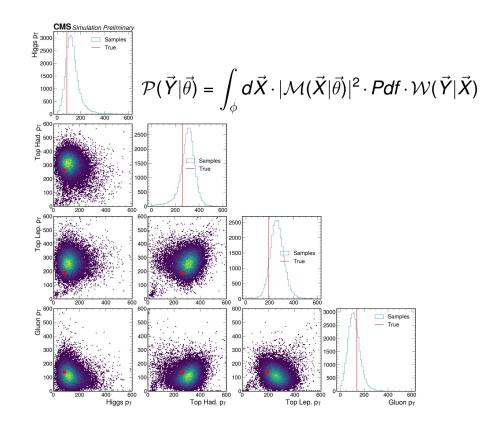
Computing

optimal observables from the matrix element method with conditional normalizing flows

Davide Valsecchi (ETH Zurich) for the CMS Collaboration

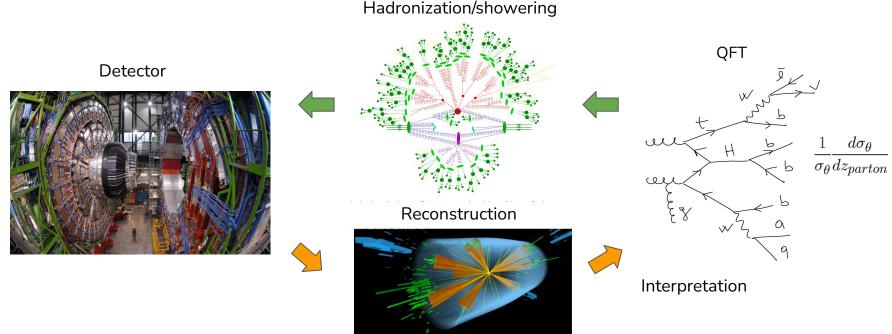
CMS-DP-2023-85





Intro and motivation

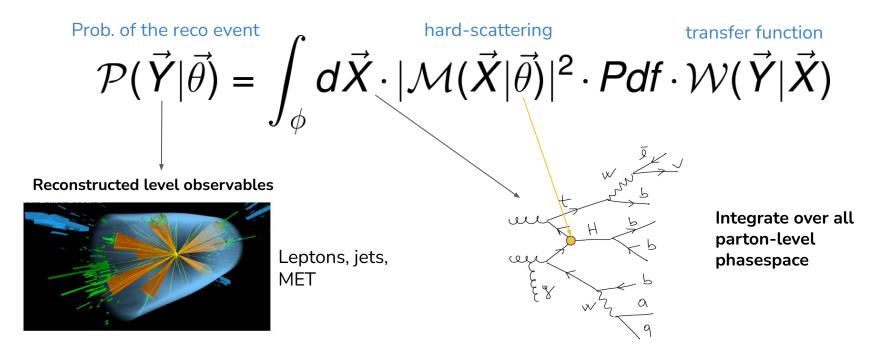




- HEP relies on a complex chain of high fidelity simulators to model the signals in our detectors
 - \rightarrow full likelihood of an event x is **intractable** $p(x|z) = \int dz_{detector} \int dz_{shower} p(x|z_{detector}) p(z_{detector}|z_{shower}) p(z_{shower}|z)$
- The Matrix Element Method is a way to link directly the detector-level info with the theory

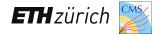
The matrix element method master formula

Estimation of the probability that a reconstructed event \mathbf{y} , is generated by a physical process defined by $\mathbf{\theta}$ parameters.



A transfer function W(Y|Z) models the probability that the reconstructed event parton-level configuration

Example: MEM for EFT

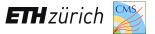


LHC EFT WG Group2 report: arxiv

- Goal: compute each term of the likelihood expansion with the MEM
 - \rightarrow <u>Encapsulate the full event kinematic</u> information in a single likelihood ratio
- Extract limit on Wilson coefficients with optimal observables with a unbinned or standard binned fit to CMS data

LHC EFT WG Group2 report: arxiv

Classical MEM computation

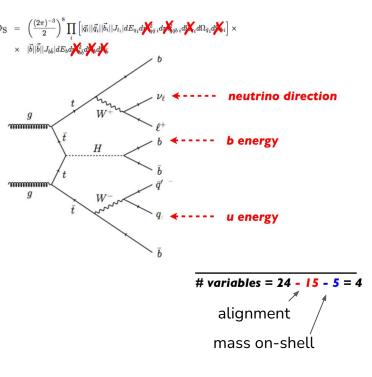


Example of MEM for ttH(bb) process

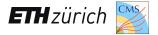
From Bianchini's talk at DataScience@LHC 2015

1. consider **generator-level particles as aligned to jets**

- a. > jets than needed \rightarrow all possible permutations and sum
- b. < objects than needed \rightarrow discard the event or integrate out the missing partons
- 2. Assume full reconstruction, particles mass on-shell
- 3. Compute the numerical integral with VEGAS over the free d.o.f.
- 4. **Permute** the jet-parton assignment \rightarrow **extremely time consuming**



A new approach based on generative ML



Model the conditional probability of parton-level events given a reconstructed event using normalizing flows

General **strategy** based on:

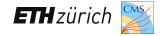
- Precision-Machine Learning for the Matrix Element Method 2310.07752 (see next talk!)
- Two Invertible Networks for the Matrix Element Method 2210.00019
- Invertible Networks or Partons to Detector and Back Again 2006.06685

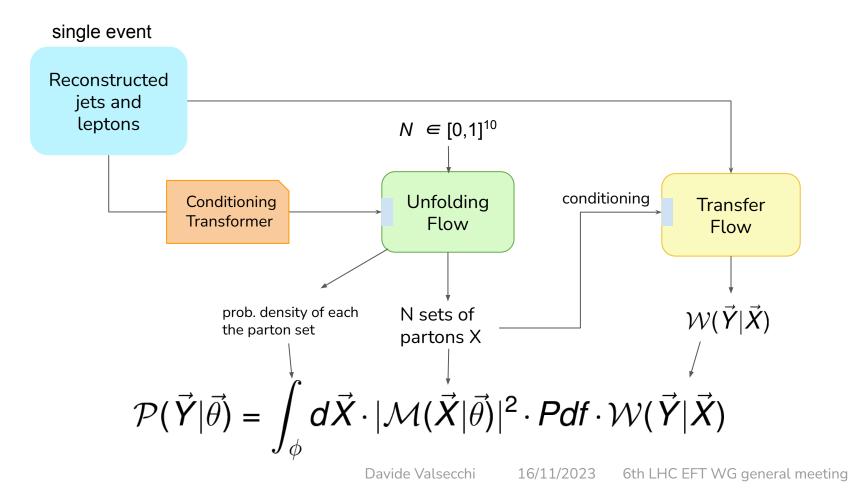
First application of the method on the experiment side:

- **Complex ttH(bb) channel** in the semileptonic final state (1 lepton, >6 jets):
 - MEM used for sig/bkg discrimination in CMS analyses: doi:10.1007/JHEP03(2019)026, CMS-PAS-HIG-19-011
- Full CMS detector simulation including pileup
- All jet multiplicities considered

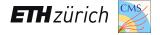
Today talk: generating generator-level events for MEM integration

MEM computation

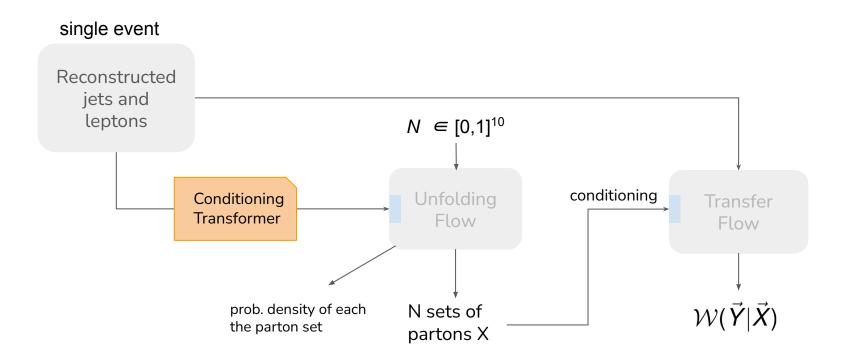




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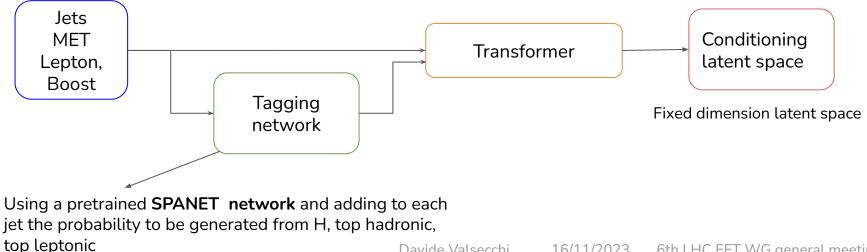


Conditioning transformer



Conditioning on reconstructed events

- **ETH** züri
- Sampled particle sets for the MEM integral computation strongly depends on the reconstructed objects.
- Use a **transformer** to extract a fixed-size conditioning latent space for the unfolding flow
 - can handle additional radiation and missing objects \rightarrow
 - avoids direct jet-parton combination \rightarrow
- The conditioning latent space should be correlated with the most probable partons

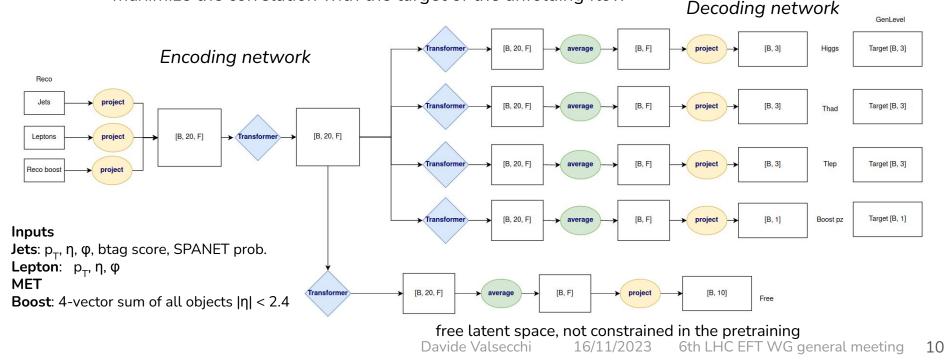


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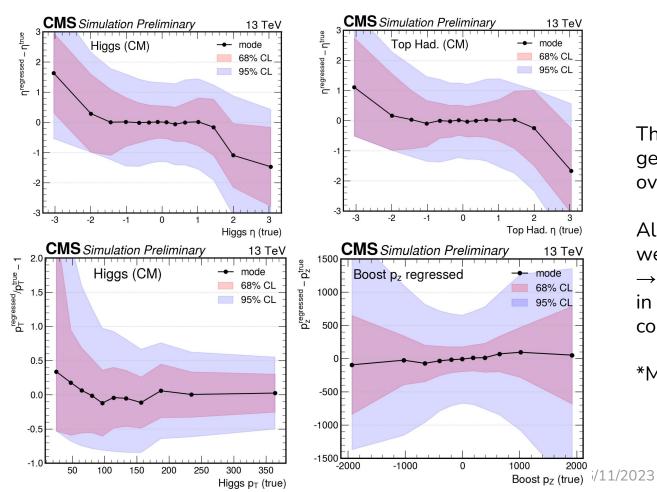
Conditioner pre-training

- Idea: pretrain the conditioning transformer with a **regression** of the **generator-level particles**: higgs, top_{had}, top_{lep} (p_T , η , ϕ) + total event boost p_Z

- \rightarrow additional radiation (gluon) computed from momentum balance
- \rightarrow maximize the correlation with the target of the unfolding flow



Parton regression performance



The regression of the generator-level particles is overall unbiased

ETH zürich

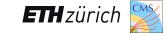
Also the total p_Z of the event is well regressed \rightarrow the particles can be boosted in the centre-of-mass (CM) correctly.

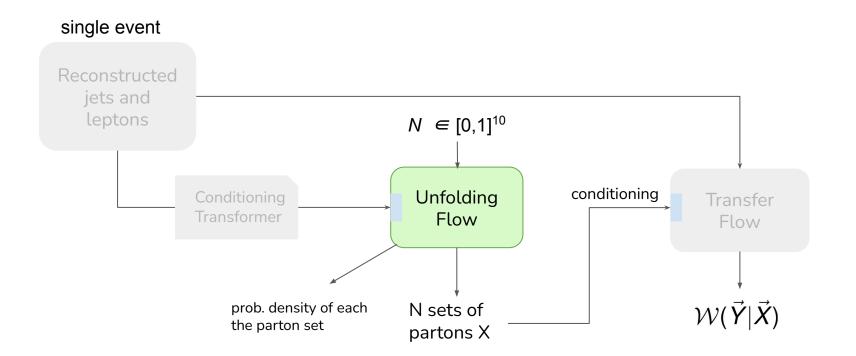
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*More plots in backup

Unfolding flow





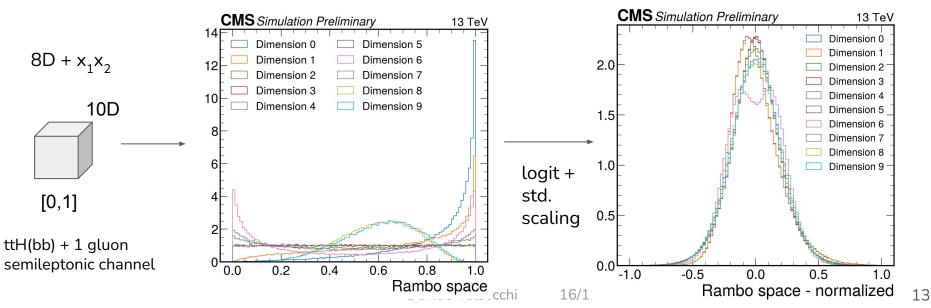
Phase space representation

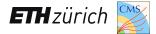
Need to parametrize 4-momenta of particles in an event in a way suitable to be modeled by normalizing flows.

Using the **RamboOnDiet** <u>1308.2922</u> algorithm \rightarrow analytical mapping, compact and fast

- parametrizes events in the CM frame
- D = 3N-4 numbers $\in [0,1]$ to describe N particles final state
- almost flat phase-space density (for massless particles)
- 2 additional numbers for the momentum fractions of the scattering partons $x_1 x_2$

Also look at Enhanced latent spaces for improved collider simulations 2305.07696





Flow architecture

Reconstructed particles

Conditioning

Transformer

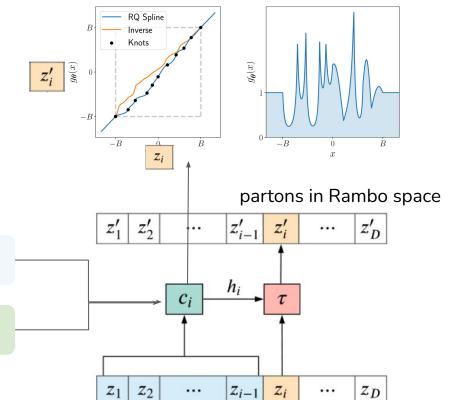
Implemented the flow as Rational Quadratic Spline <u>1906.04032</u> flow with autoregressive blocks.

The conditioning vector is made up from the regressed partons converted to Rambo space and a free latent vector.

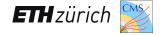
Regressed partons

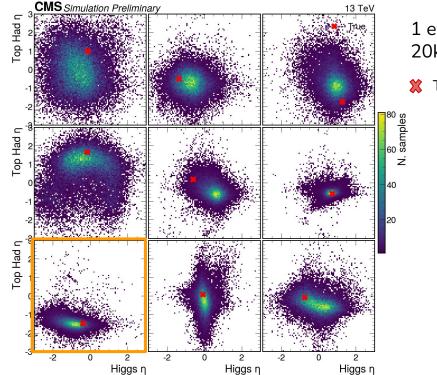
Latent vector

Parton space



Unfolding flow samples





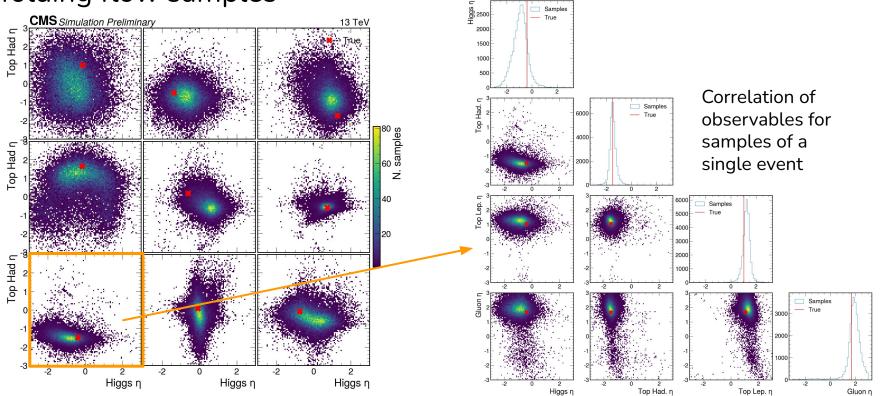
1 event in each box 20k samples

True gen-level particles

The unfolding flow learns the conditional probability *P***(partons/reconstructed event)** and generates partons in the most probable configurations.

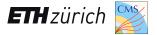
Unfolding flow samples

ETH zürich

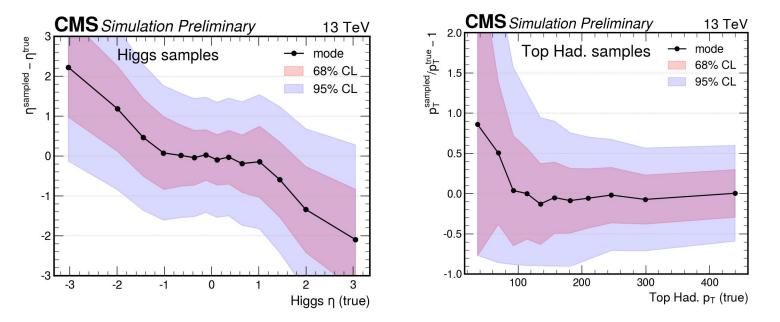


CMS Simulation Preliminary

The unfolding flow learns the conditional probability *P***(partons/reconstructed event)** and generates partons in the most probable configurations.



Quality of the sampled partons



The quality of the sampled partons configuration is evaluated by sampling 30 sets per 1.5M events and analyzing the bias w.r.t of the target true partons.

The bias of the sampled particles is on average small in the bulk of the distributions and increases in the tails.

Overall the performance is very correlated with the one of the **regression** for the conditioning network.

Conclusions



- → First steps for the full-fledged application on **CMS simulation** of the novel strategies (2210.00019,2006.06685) for the Matrix Element Method computation with generative models on a **complex final state**, like ttH(bb)
- → The full reconstructed event information is analyzed by a transformer to regress the
 4-momenta of the generator-level particles. This information is then used to generate set of particles with a normalizing flow.
- \rightarrow The quality of the generative model is promising and it can be further optimized
- \rightarrow The next step is to model the transfer function W(reco|hard)
- \rightarrow All plots and public results on <u>CMS-DP-2023-85</u>



Questions?

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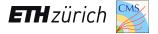
Backup

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References

- 1. Matrix Element Method in HEP: Transfer Functions, Efficiencies, and Likelihood Normalization <u>1101.2259</u>
- 2. Phase Space Sampling and Inference from Weighted Events with Autoregressive Flows 2011.13445
- 3. i-flow: High-dimensional Integration and Sampling with Normalizing Flows 2001.05486
- 4. MadNIS Neural Multi-Channel Importance Sampling 2212.06172
- 5. Normalizing Flows: An Introduction and Review of Current Methods <u>1908.09257</u>
- 6. Normalizing Flows for Probabilistic Modeling and Inference <u>1912.02762</u>
- 7. Masked Autoregressive Flow for Density Estimation <u>1705.07057</u>
- 8. Neural Spline Flows <u>1906.04032</u>
- 9. RAMBO on diet <u>1308.2922</u>
- 10. LHC EFT WG Report: Experimental Measurements and Observables 2211.08353
- 11. Invertible Networks or Partons to Detector and Back Again 2006.06685
- 12. Two Invertible Networks for the Matrix Element Method 2210.00019
- 13. Modified Differential Multiplier Method paper
- 14. Measurement of the ttH and tH production rates in the H \rightarrow bb decay channel with 138fb-1 of proton-proton collision data at $\sqrt{s=13 \text{ TeV} \text{ CMS-PAS-HIG-19-011}}$
- 15. Attention is all you need <u>1706.03762</u>
- 16. SPANet: Generalized Permutationless Set Assignment for Particle Physics using Symmetry Preserving Attention <u>2106.03898</u>
- 17. POWHEG: NLO calculations in shower Monte Carlo P. Nason, JHEP 0411 (2004) 040, hep-ph/0409146 [paper]
- 18. An Introduction to PYTHIA 8.2 1410.3012

Conditioner transformer training



The pretraining regression is performed with multiple components:

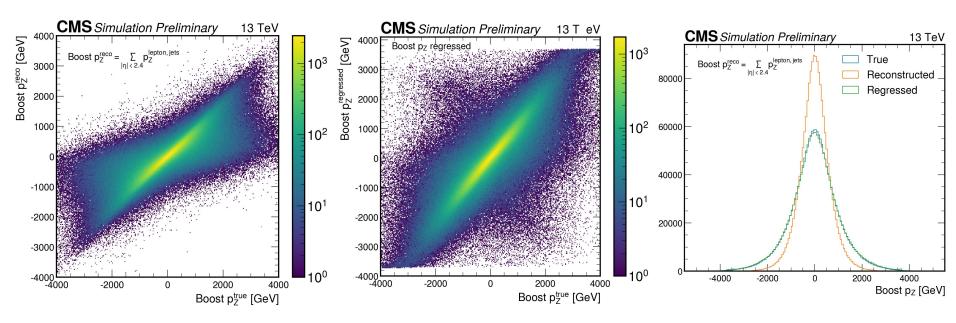
- **Huber** loss for single particles + event boost p₇ + computed gluon
- **MMD** loss for single particles + full 13D space \rightarrow keeps distributions coherent

Trained using the Modified Differential Multiplier Method (MDMM) technique to balance the difference losses (<u>paper</u>)

Conditioner transformer configuration:

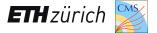
- Encoder: 4 layers, 8 heads, 64D latent vector, 512 hidden layer,
- Decoders: 4 layers, 4 heads, 64D latent vector, 512 hidden layer
- Total weights: 1.8M

Parton regression performance - Boost

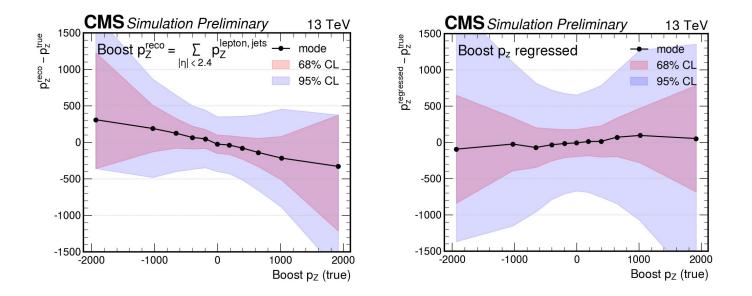


The conditioning transformer regresses the event boost in order to be able to bring the partons to the center-of-mass.

The left figure shows the correlation between true boost p_z and the boost p_z estimated by summing all the reconstructed objects with $|\eta| < 2.4$. The figure in the middle shows the regressed boost p_z which improved a lot the correlation. The plot on the right shows the 1D profile of the boost p_z for the truth level, the reconstructed estimation and the regression.



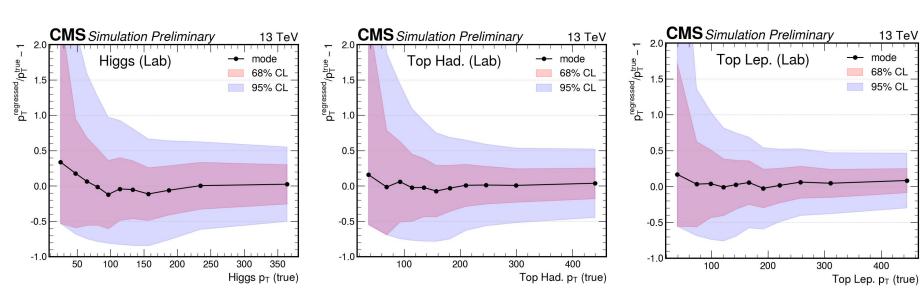
Parton regression performance - Boost



The conditioning transformer regresses the event boost in order to be able to bring the partons to the center-of-mass.

The left figure shows the bias in the estimation of the true boost p_z computed by summing all the reconstructed objects with $|\eta| < 2.4$. The figure on the right shows the bias in the estimation of the true boost p_z using the boost regressed by the conditioning transformer. The bias at high p_z is reduced by the regression.

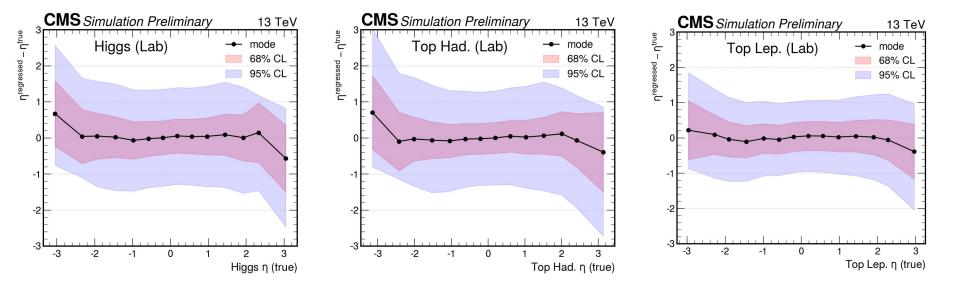
Parton regression performance - Lab Frame



The plots show the performance of the regression performed by the conditioning transformer. The bias in the regression of the p_T of the higgs, hadronically decaying top quark (Top Had), and leptonically decaying top quark (Top Lep), is shown in bins of the true p_T of the particles in the lab frame.

The regression is overall unbiased: at high p_T the 68% confidence level interval reaches an uncertainty in the regressed p_T of ~30%, whereas at low p_T (< 50 GeV) the uncertainty is larger.

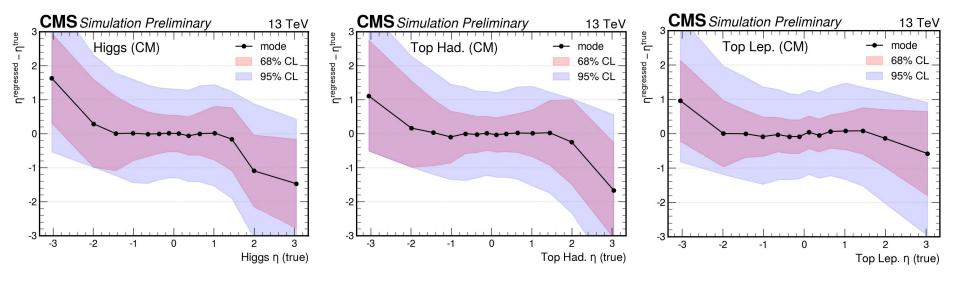
Parton regression performance - Lab Frame



The plots show the performance of the regression performed by the conditioning transformer. The bias in the regression of the η of the higgs, hadronically decaying top quark (Top Had), and leptonically decaying top quark (Top Lep), is shown in bins of the true η of the particles in the lab frame.

The regression is overall unbiased, apart from the region $|\eta| > 2.5$ which covers the very tail < 3% of the particle distribution.

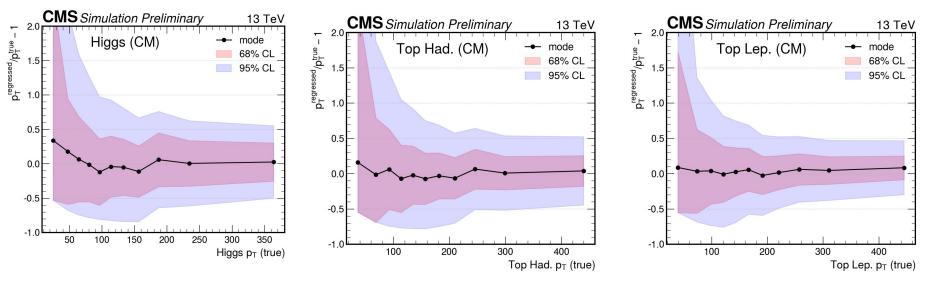
Parton regression performance - CM Frame



The plots show the performance of the regression performed by the conditioning transformer, after bringing the regressed partons in the center-of-mass (CM) using the regressed event boost. The bias in the regression of the η of the higgs, hadronically decaying top quark (Top Had), and leptonically decaying top quark (Top Lep), is shown in bins of the true η of the particles in the CM frame.

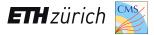
The regression is overall unbiased, apart from the region $|\eta| > 1.5$ which covers the tail $<\sim 10\%$ of the particle distribution. The performance is slightly worse than in the lab frame due to the imperfect regression of the total boost p_z , used for the transformation.

Parton regression performance - CM Frame

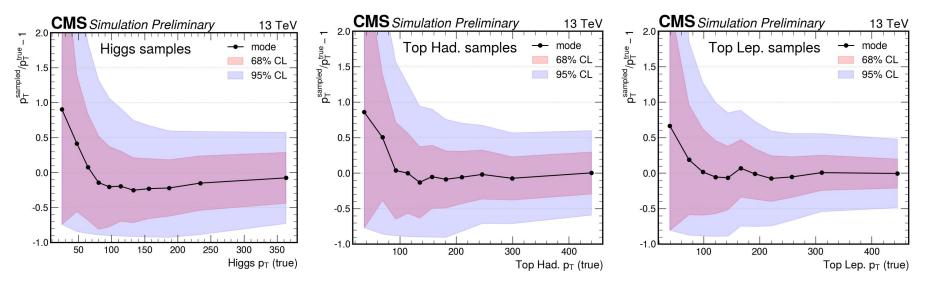


The plots show the performance of the regression performed by the conditioning transformer, after bringing the regressed partons in the center-of-mass (CM) using the regressed event boost. The bias in the regression of the p_{T} of the higgs, hadronically decaying top quark (Top Had), and leptonically decaying top quark (Top Lep), is shown in bins of the true p_{T} of the particles in the CM frame.

The regression is overall unbiased: at high p_T the 68% confidence level interval reaches an uncertainty in the regressed p_T of ~30%, whereas at low p_T (< 50 GeV) the uncertainty is larger. The performance is overall unchanged w.r.t of the regression result in the lab frame.

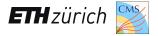


Quality of the sampled partons

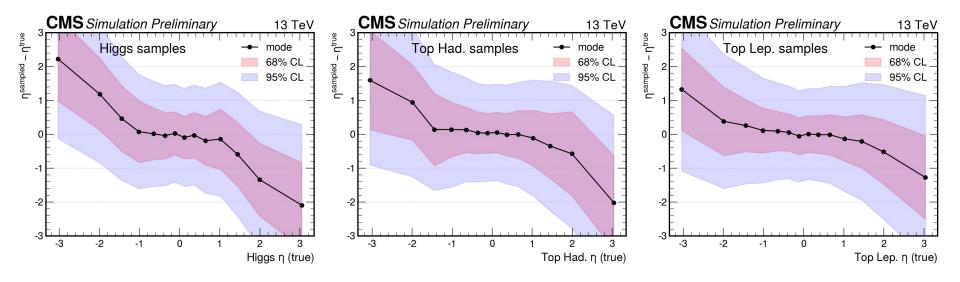


The quality of the sampled partons configuration is evaluated by sampling 30 sets per 1.5M events and analyzing the bias w.r.t of the target true partons. The plots show the bias of the sampled partons in bins of the true p_T of the particles in the CM frame.

The average bias of the samples reaches 20% in the bulk of the distribution (100 GeV) for the higgs parton, while it is very close to 0% for the top quarks. The bias is very small at high pT, while at very low pt (<50GeV), it increases up to 100%.



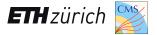
Quality of the sampled partons



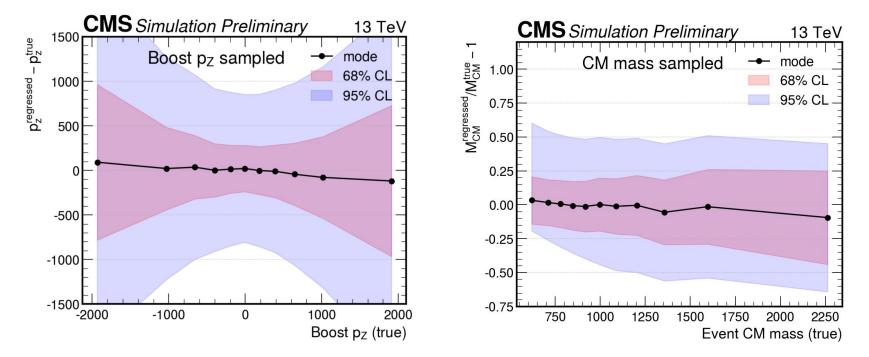
The quality of the sampled partons configuration is evaluated by sampling 30 sets per 1.5M events and analyzing the bias w.r.t of the target true partons. The plots show the bias of the sampled partons in bins of the true η of the particles in the CM frame.

The average bias of the samples is close to 0 in the bulk of the distribution, while it reached $\Delta \eta \sim 1$ in the tails (only 10% of the events have $|\eta_{CM}| > 1.5$). In general, the performance of the sampling is highly correlated with the one of the regression, as expected, since the unfolding flow is conditioned with the regressed partons.

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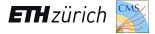
Quality of the sampled boost



The unfolding flow models also the incoming parton energy fractions alongside the final state partons in the CM frame.

The bias of the sampled incoming parton energies is shown by plotting the event total CM mass and the event total boost p_7 . Both the distributions are very well modelled by the flow.

Unfolding flow architecture and training



Unfolding flow configuration:

- Conditioning vector dimension: 16
- Number of transforms: 6
- Flow type: RQS autoregressive
- Number of spline bins: 40
- Spline network: 64 hidden features, 2x512 feedforward networks
- Number of trainable parameters:
 5.3M (flow)+ 1.8M (conditioner) = 7.1M

The flow is trained **simultaneously my maximum likelihood** and by **sampling** parton configurations and comparing them with the target.

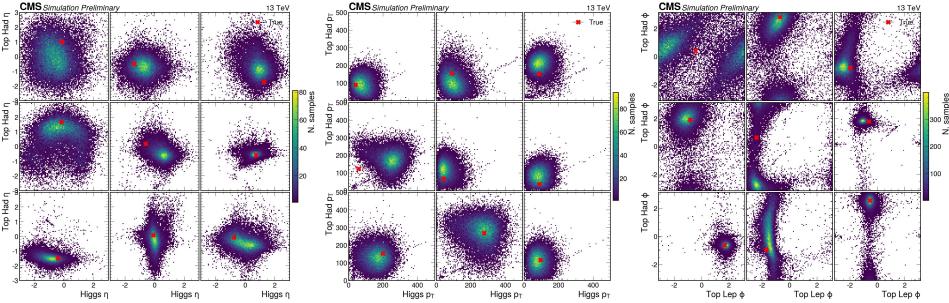
The training took 20 hours on a A100 Nvidia GPU over a 1.5M events training dataset.

2 approaches to evaluate the quality of the flow:

- sample 20k parton sets for a few random events and inspect their distributions
- samples 20 partons sets for 1.5M of testing events and analyze the bias w.r.t of the true partons

Goal for **importance sampling:** minimize **bias**, sample points with the same probability of the integrand function.





- The unfolding flow learns the conditional probability *P(partons/reconstructed event)* and generates partons in the most probable configurations.
- Each box in the figures shows 20k sampled partons for a given event.
- The red cross shows the true value of the partons position/energy in each event.

Unfolded flow samples: single event correlations

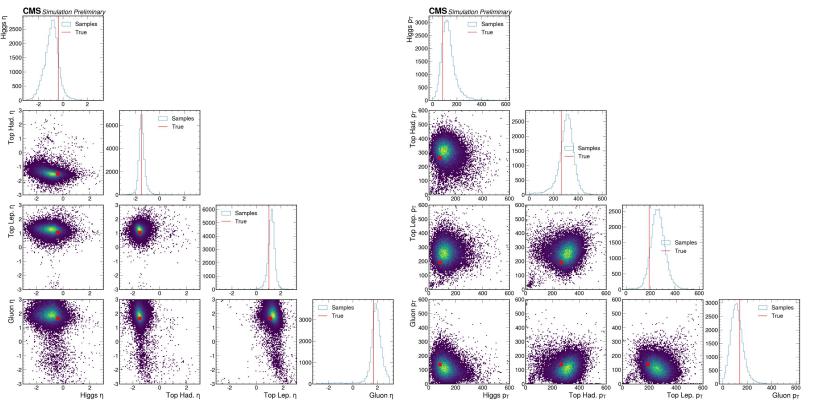
Top Had.

Fop Lep

Gluo

Higgs n

Top Had. n



Correlation between η (left) and p_{τ} (right) of the sampled generator-level particle for a single event.

Gluon η

Top Had. pT

Top Lep. pT

The red cross/line shows the true value of the partons position/energy in each event. Davide Valsecchi 16/11/2023 6th LHC EFT WG general meeting

Top Lep. n

Gluon pt

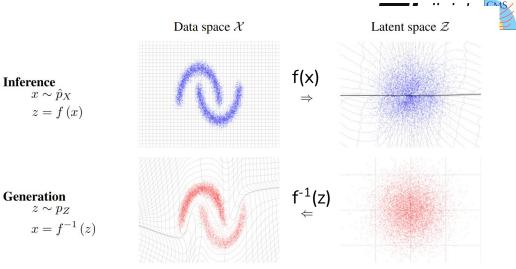


Normalizing flows : More formally

From the rules of change of integration variables

 $p_X(x) = p_Z(f(x)) \left| \det\left(\frac{\partial f(x)}{\partial x^T}\right) \right|$ $\log\left(p_X(x)\right) = \log\left(p_Z(f(x))\right) + \log\left(\left|\det\left(\frac{\partial f(x)}{\partial x^T}\right)\right|\right),$

where f(x) goes in the "normalizing" direction to the z latent space.



We can both **sample** and evaluate the **density**

- If the p.d.f in the l**atent space is tractable** (multidim gaussian, uniform)
- if the transformation is invertible

Requirement: the jacobian of the transformation must be computed in an efficient way \rightarrow this defines the possible implementation of the flows

 $\mathbf{z}_{0} \xrightarrow{f_{1}(\mathbf{z}_{0})} \mathbf{z}_{1} \cdots \mathbf{z}_{i-1} \xrightarrow{f_{i}(\mathbf{z}_{i-1})} \mathbf{z}_{i} \xrightarrow{f_{i+1}(\mathbf{z}_{i})} \cdots \mathbf{z}_{K} = \mathbf{x}$ $(\mathbf{z}_{0} \xrightarrow{f_{1}(\mathbf{z}_{0})} \underbrace{\mathbf{z}_{1} \cdots \mathbf{z}_{i-1}}_{\mathbf{z}_{0} \sim p_{0}(\mathbf{z}_{0})} \xrightarrow{\mathbf{z}_{K} \sim p_{K}(\mathbf{z}_{K})} \xrightarrow{\mathbf{z}_{K} \sim p_{K}(\mathbf{z}_{K})}$

Expressiveness: transformations are composable!

$$(T_2 \circ T_1)^{-1} = T_1^{-1} \circ T_2^{-1}$$

det $J_{T_2 \circ T_1}(\mathbf{u}) = \det J_{T_2}(T_1(\mathbf{u})) \cdot \det J_{T_1}(\mathbf{u})$

ccni 💷 🗸 🗸

Prob. of the reco event hard-scattering transfer function

$$\mathcal{P}(\vec{Y}|\vec{\theta}) = \int_{\phi} d\vec{X} \cdot |\mathcal{M}(\vec{X}|\vec{\theta})|^2 \cdot Pdf \cdot \mathcal{M}(\vec{Y}|\vec{X})$$

- From first principles: MadGraph, OpenLoop -
- Only component depending on the **parameters** $\boldsymbol{\theta}$ -
- It can become the **slowest** part in the evaluation of the MEM -
- It can be "multi-channel": non trivial dependency on the different Feynman diagrams -
- Parton distribution functions need to be convoluted as: _

$$\int_{\phi} d\vec{X} \sum_{a,b} \int_{x_1,x_2} dx_1 dx_2 f_a(x_1, Q^2) \cdot f_b(x_2, Q^2) \cdot |\mathcal{M}(x_1, x_2, \vec{X}|Q^2, \vec{\theta})| \cdot \mathcal{W}(\vec{Y}|\vec{X})$$

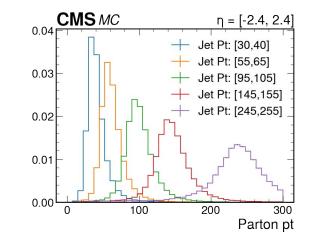
MEM: the transfer function

arxiv:1101.2259





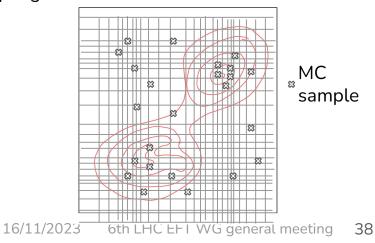
- "Core" of the MEM method: models the probability to get a reconstructed event given a parton configuration
- It is the main factor driving the power and precision of the method
- δ for leptons, more complex for jets
- Usually it is **factorized by object** taking many assumptions:
 - objects matching and geometrical alignment
 - ignore out-of-acceptance objects
 - additional term for MET and initial state radiation.



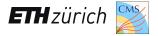


Prob. of the reco event hard-scattering transfer function $\mathcal{P}(\vec{Y}|\vec{\theta}) = \int_{\phi} d\vec{X} \cdot |\mathcal{M}(\vec{X}|\vec{\theta})|^2 \cdot Pdf \cdot \mathcal{W}(\vec{Y}|\vec{X})$

- \rightarrow The integration is over the **partons (+pdfs) complete phase-space**
- \rightarrow The integral is computed numerically with MC sampling
- \rightarrow Very high dimensional \rightarrow needs approximations
- \rightarrow Strong dependence on the coordinate choices
 - needs to be "aligned" with propagators
 - invariant mass constraints
 - Jet-parton alignments
 - additional radiation complex to handle

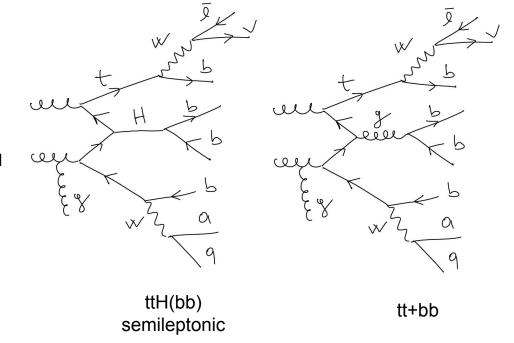


ttH(bb) channel



The MEM has been applied to the problem of signal discrimination for the ttH(bb) CMS analysis.

- \rightarrow Complex process with 2 \rightarrow 8 topology
- \rightarrow 3 channels:
 - single lepton
 - 2 leptons
 - fully hadronic
- → Large irreducible background from tt+bb SM process.
- \rightarrow CMS Analyses:
 - 2016: doi:10.1007/JHEP03(2019)026
 - under review: HIG-19-001 (full Run2)

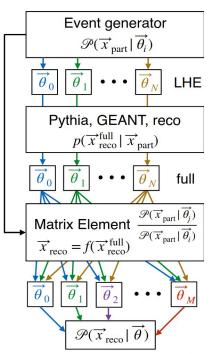


EFT interpretation



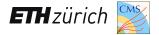
$$\mathscr{P}(\vec{x}_{\text{reco}} \mid \vec{\theta}) \propto \mathscr{P}_0(\vec{x}_{\text{reco}}) + \sum_k \left(\frac{2\theta_k}{\theta_0}\right) \mathscr{P}_{0k}(\vec{x}_{\text{reco}}) + \sum_k \left(\frac{\theta_k}{\theta_0}\right)^2 \mathscr{P}_k(\vec{x}_{\text{reco}}) + \sum_{i < j} \left(\frac{2\theta_i \theta_j}{\theta_0^2}\right) \mathscr{P}_{ij}(\vec{x}_{\text{reco}}) + \sum_{i < j} \left(\frac{2\theta_i \theta_j}{\theta_0^2}\right) + \sum_{i < j} \left(\frac{2\theta_i \theta_j}{\theta_0^$$

- **Goal**: full Run2 measurement of dim6 EFT operators parameters (Wilson coeff.) relevant for ttHbb channel.
- There are 2 possible ways to perform EFT studies in general
 - **one-step**, "direct" measurement: model EFT effects at reco level, build a template analysis, use likelihood profiling to get limits on θ
 - Useful to restrict the number of parameters
 - More complex bookkeeping of MC samples
 - it can reach optimal sensitivity
 - CMS internal, difficult for reinterpretation
 - **two-step**, "unfolding", STXS:
 - fiducial measurements usable for re-interpretation outside of CMS collaboration
 - less optimal, more general



EFT optimal observables

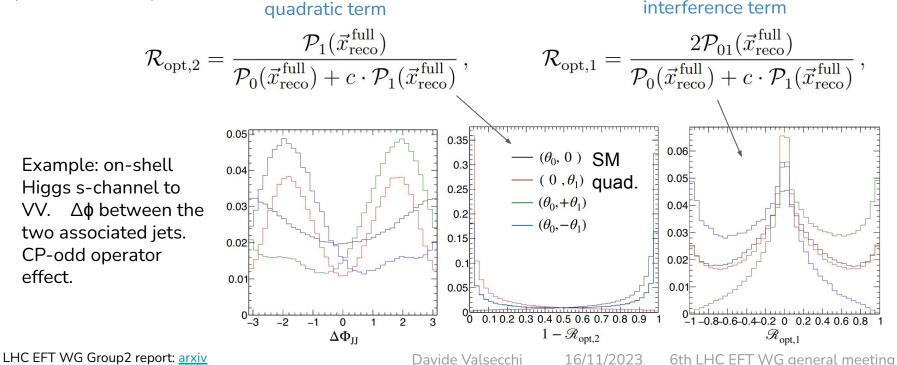
SMEFT quadratic parametrization with dim-6



$$\mathcal{P}(\vec{x}_{\text{reco}} \mid \vec{\theta}) \propto \mathcal{P}_0(\vec{x}_{\text{reco}}) + \sum_k \left(\frac{2\theta_k}{\theta_0}\right) \mathcal{P}_{0k}(\vec{x}_{\text{reco}}) + \sum_k \left(\frac{\theta_k}{\theta_0}\right)^2 \mathcal{P}_k(\vec{x}_{\text{reco}}) + \sum_{i < j} \left(\frac{2\theta_i \theta_j}{\theta_0^2}\right) \mathcal{P}_{ij}(\vec{x}_{\text{reco}})$$

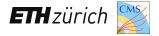
Wilson coefficients

Using Neyman-Pearson lemma one can extract the maximum information from two optimal observables (likelihood ratios).



ng **41**

Importance sampling



An multi-dim integral can be estimated via MC sampling

$$I \approx \frac{V}{N} \sum_{i=1}^{N} f(x_i) \equiv V \langle f \rangle_x, \qquad \sigma_I = \sqrt{\operatorname{Var}} \approx V \sqrt{\frac{\langle f^2 \rangle_x - \langle f \rangle_x^2}{N - 1}} ,$$

If we can find a function g(x) which has a similar shape as f(x) we can improve the variance -> importance sampling

$$I = \int_{\Omega} \frac{f(x)}{g(x)} dG(x) = V \langle f/g \rangle_G, \qquad \sigma_I = V \sqrt{\frac{\langle (f/g)^2 \rangle_G - \langle f/g \rangle_G^2}{N-1}}.$$

$$\int_{\text{bad choice}} \frac{f(x)}{pdf(x)} \int_{\text{initial uniform prior}} \frac{f(x)}{f(x)} \int_{\text{bad choice}} \frac{f(x)}{pdf(x)} \int_{\text{initial uniform prior}} \frac{f(x)}{f(x)} \int_{\text{initial uniform prior}} \frac$$