Preprint: arXiv:2510.21041

HadStruct Collab: K. Orginos, J. Karpie, H. Dutrieux, S. Zafeiropoulos

Gaussian processes for Inferring Parton Distributions

WONPAQCD December 4, 2025

Yamil Cahuana Medrano

CENTER for NUCLEAR FEMTOGRAPHY
WILLIAM & MARY CHARTERED 1693
FULBRIGHT
Jefferson Lab

Outline

Particularities of doing a fit and solving the inverse problem

- ✓ Motivation: LQCD and PDFs
- ✓ Pseudo-PDFs
- ✓ Gaussian processes
  - ➢ Bayesian approach
  - ➢ Levels of inference (3 ways to write Bayes)
- ✓ Conclusion

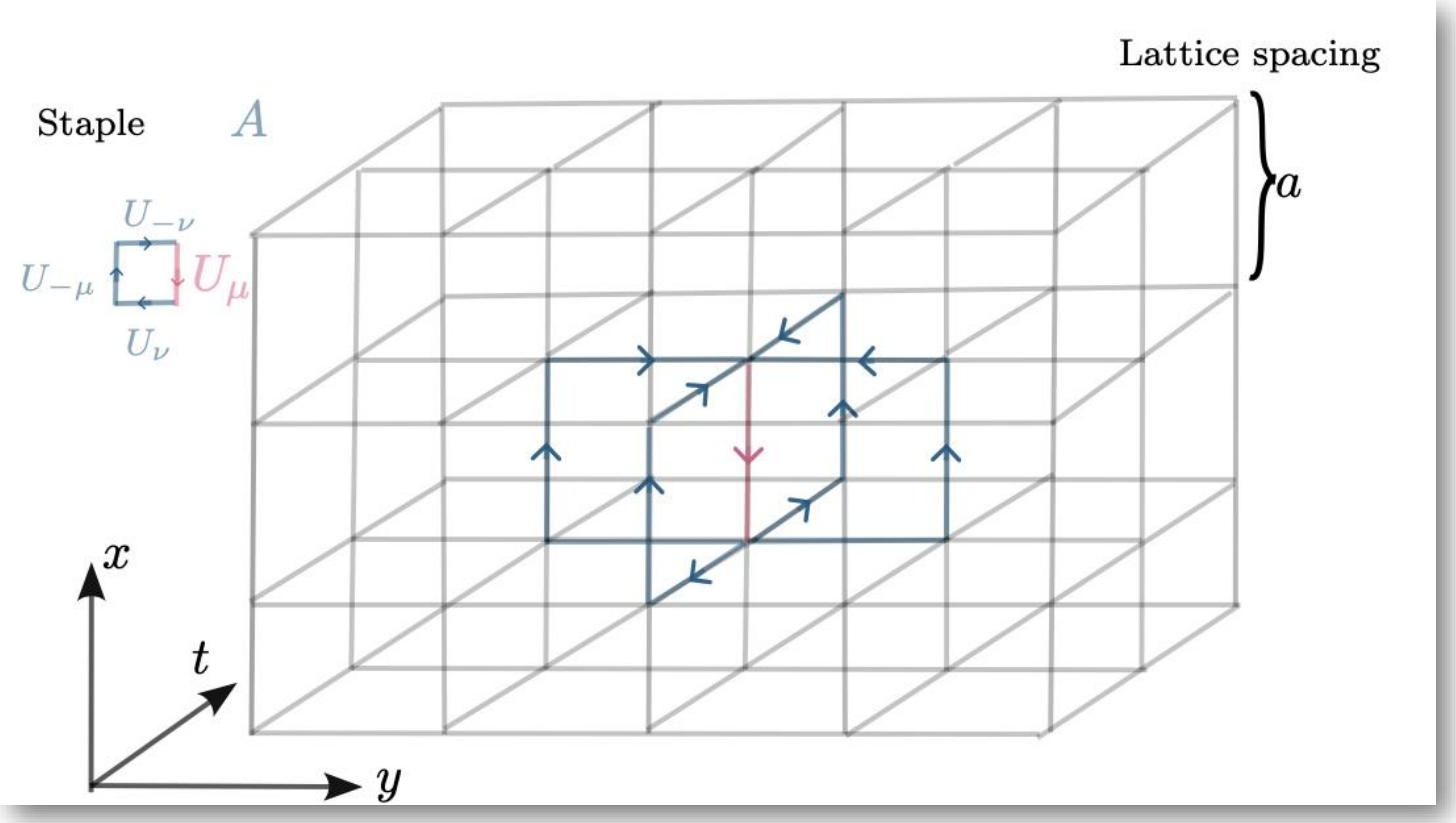
Motivation

PDF ⟷ LQCD

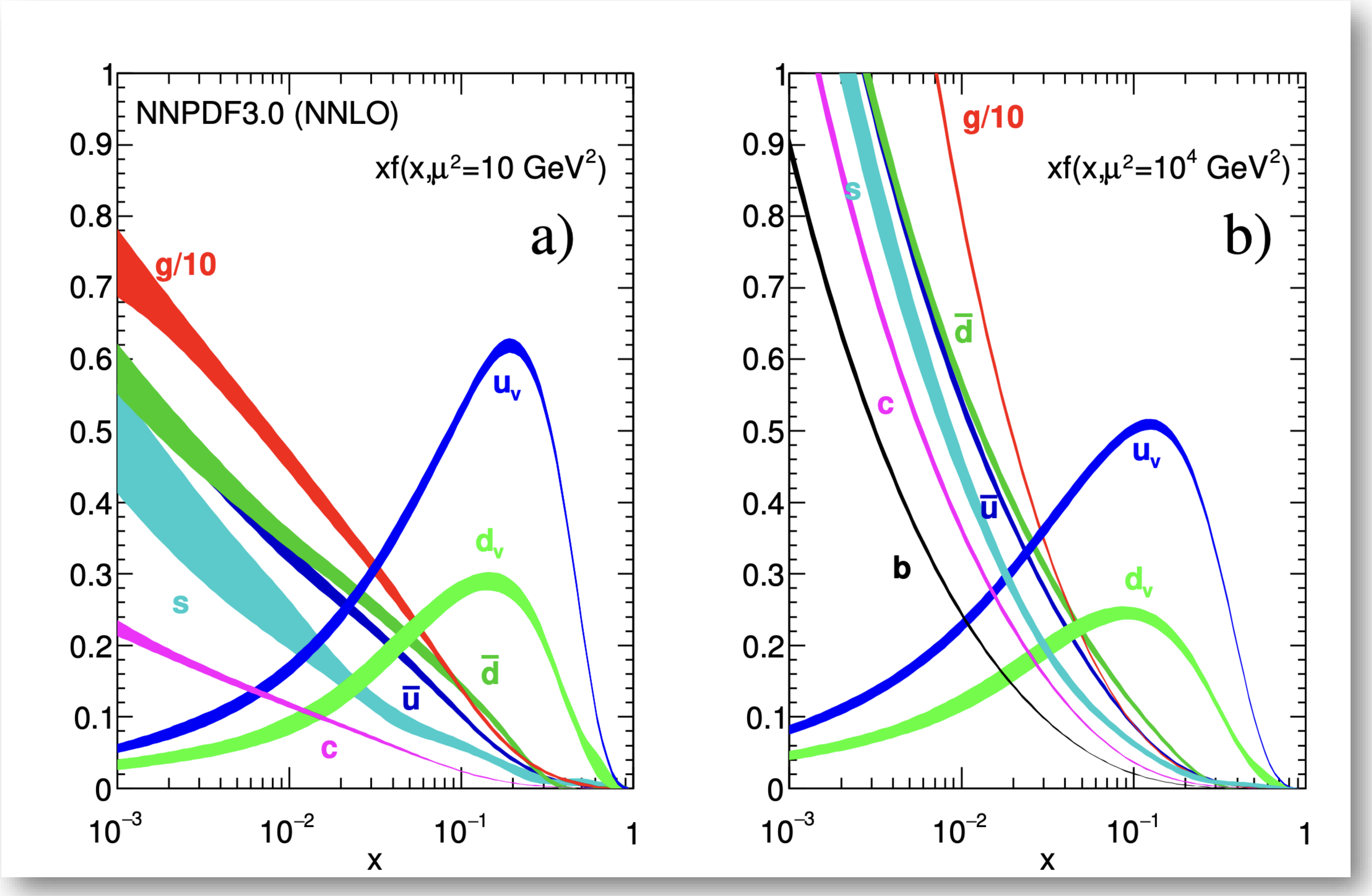
My Introduction to LQCD… and PDFs

$$\mathcal{L}_{QCD} = -\frac{1}{4}F^{\alpha}_{\mu\nu}F^{\mu\nu}_{\alpha} + \overline{\psi}(i\not{D} - m_i)\psi_i$$

$$\langle \mathcal{O}(fields)\rangle = \frac{1}{Z}\int D[fields]\mathcal{O}(fields)e^{-S_{QCD}(fields)}$$

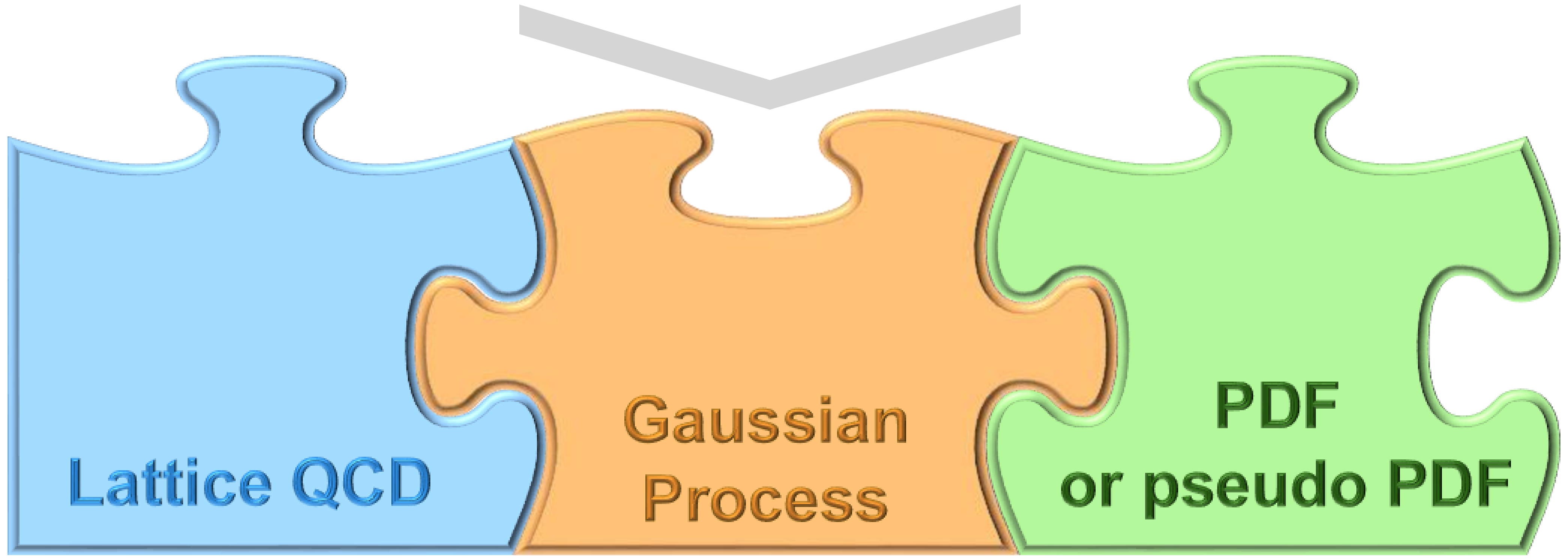


`Parton distributions and lattice QCD calculations
arXiv:1711.07916v3



Parton distributions for the LHC run II
10.1007/jhep04(2015)040

$$f_q(x,\mu) = \int_{\infty}^{\infty}\frac{dz^-}{2\pi}e^{-xP^+z^-}\langle P|\,\bar{\psi}(z^-)U(0;z^-)\psi(0)\,|P\rangle$$



PDFs on Euclidean Lattice

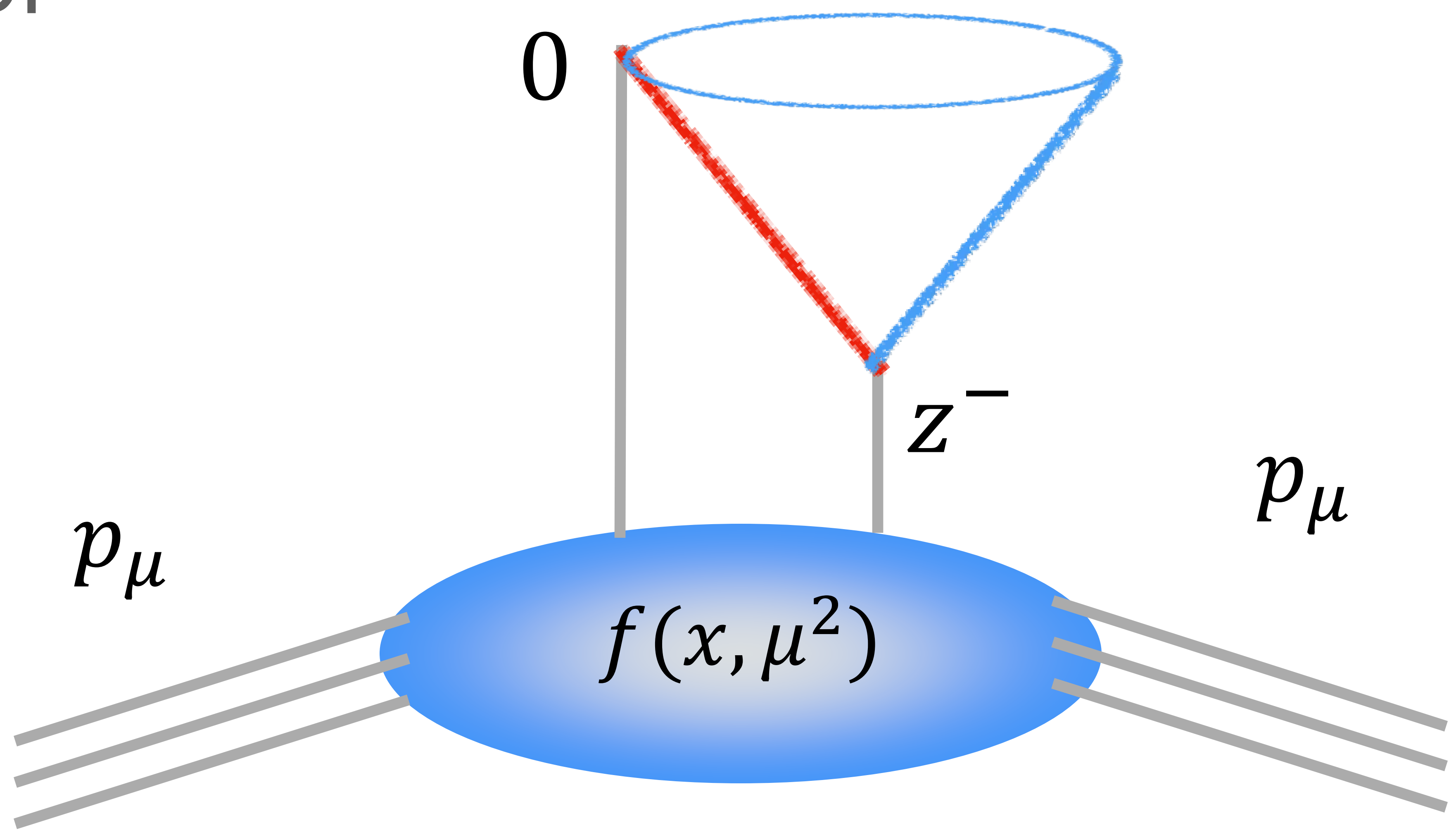
J. Collins, Foundations of Perturbative QCD
A.Radyushkin, Phys. Rev. D 96, 034025 (2017)
X. Ji, Phys. Rev. Lett. 110, 262002 (2013).

Pseudo-PDFs

$$M^\alpha(p,z) =< p|\bar\psi(z)\gamma^\alpha U(z;0)\psi(0)|p >= p^\alpha \mathcal{M}(\nu, z^2) + z^\alpha \mathcal{N}(\nu, z^2)$$

PDF

$\alpha = +$ $z_\alpha = (0, z^-, 0_T)$ $p_\alpha = (p^+, \frac{m_p^2}{2p^+}, 0_T)$

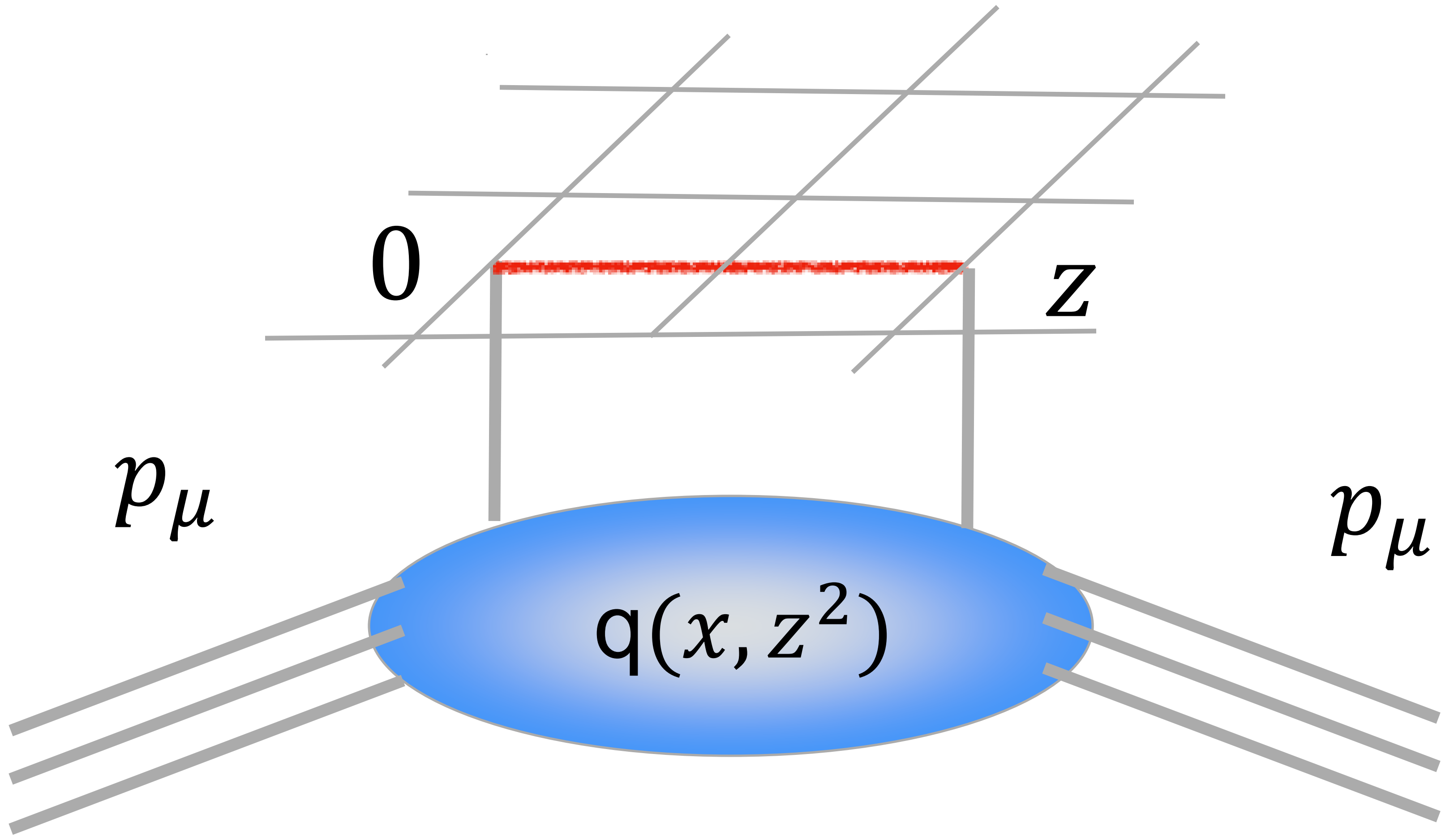


$$\mathcal{M}(-p_+z_-, 0) = \int_{-1}^1 dx f(x) e^{-ixp_+z_-}$$

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\nu \mathcal{M}(-\nu, 0) e^{-ix\nu}$$

Pseudo-PDF

$\alpha = 0$ $z_\alpha = (0,0,0,z_3)$ $p_\alpha = (p_0, 0, 0, p_3)$



$$\mathfrak{M}(\nu, z^2) = \frac{\mathcal{M}(\nu,z^2)}{\mathcal{M}(0,z^2)} = \int_{-1}^1 dx q(x,z^2) e^{-ix\nu}$$

$$q(x,z^2) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\nu \mathfrak{M}(\nu, z^2) e^{ix\nu}$$

Inverse problem

Which equation should I use?

A.Radyushkin, Phys. Rev. D 96, 034025 (2017)

$$q(x,z^2) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\nu e^{-ix\nu}\mathfrak{M}(\nu,z^2)$$

or

$$\mathfrak{M}(\nu,z^2) = \int_{-1}^{1} dx e^{ix\nu} q(x,z^2)$$

We might need to make assumptions about the behavior of ITD

$$\mathcal{L} \equiv \int_{-1}^{1} dx e^{ix\nu}$$

because…

- ✓ We have some additional information on q(x). This can be implemented in our prior.
- ✓ Compact support in the integral (Finite elements helps to achieve machine precision).
- ✓ Avoid modeling the bilocal operator(or M(z,p)) which may bias the result.

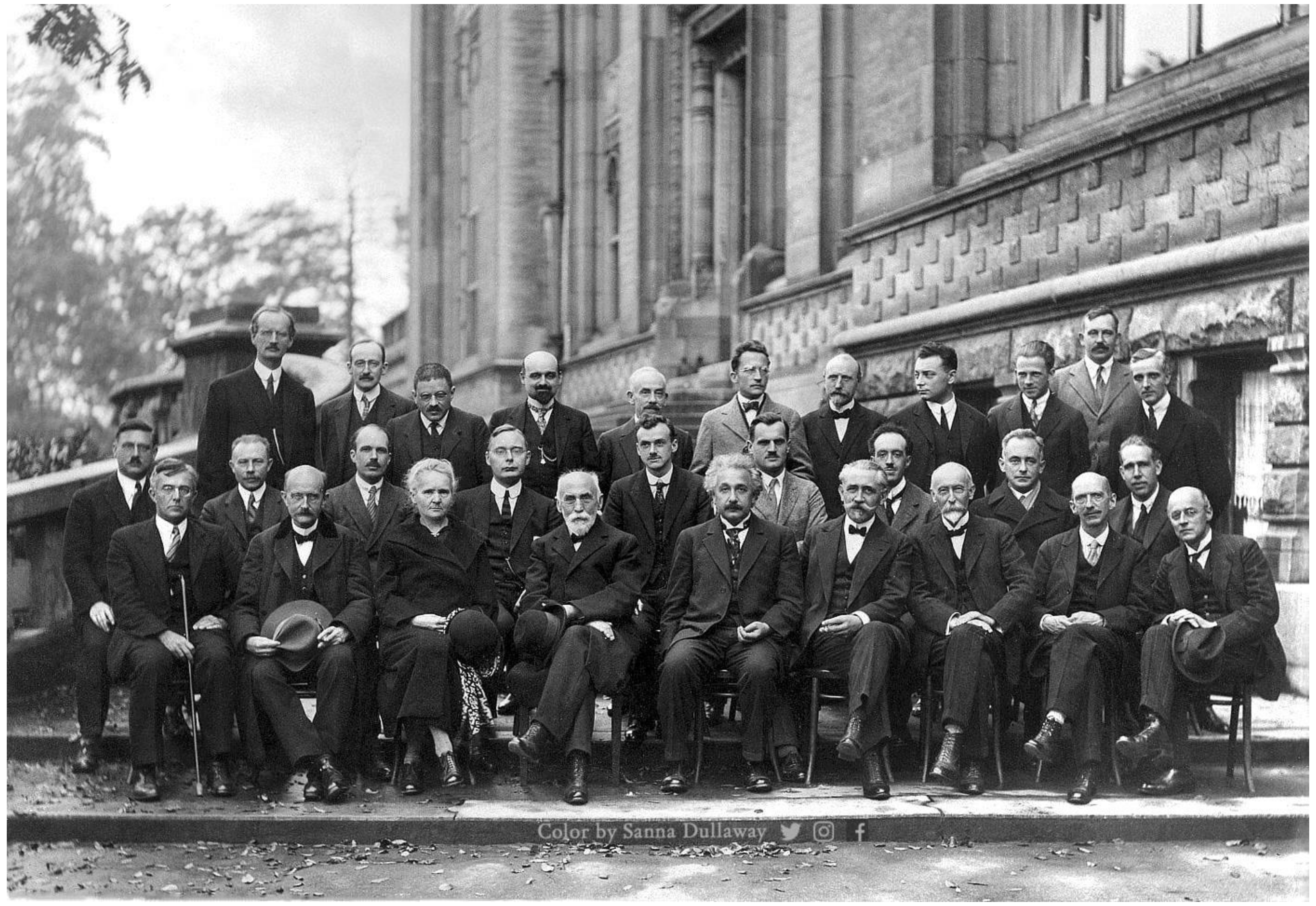
Inverse problem

Probabilistic approach

- Colorize Black and White Photos

Forward map = Easy

$\mathcal{L}$

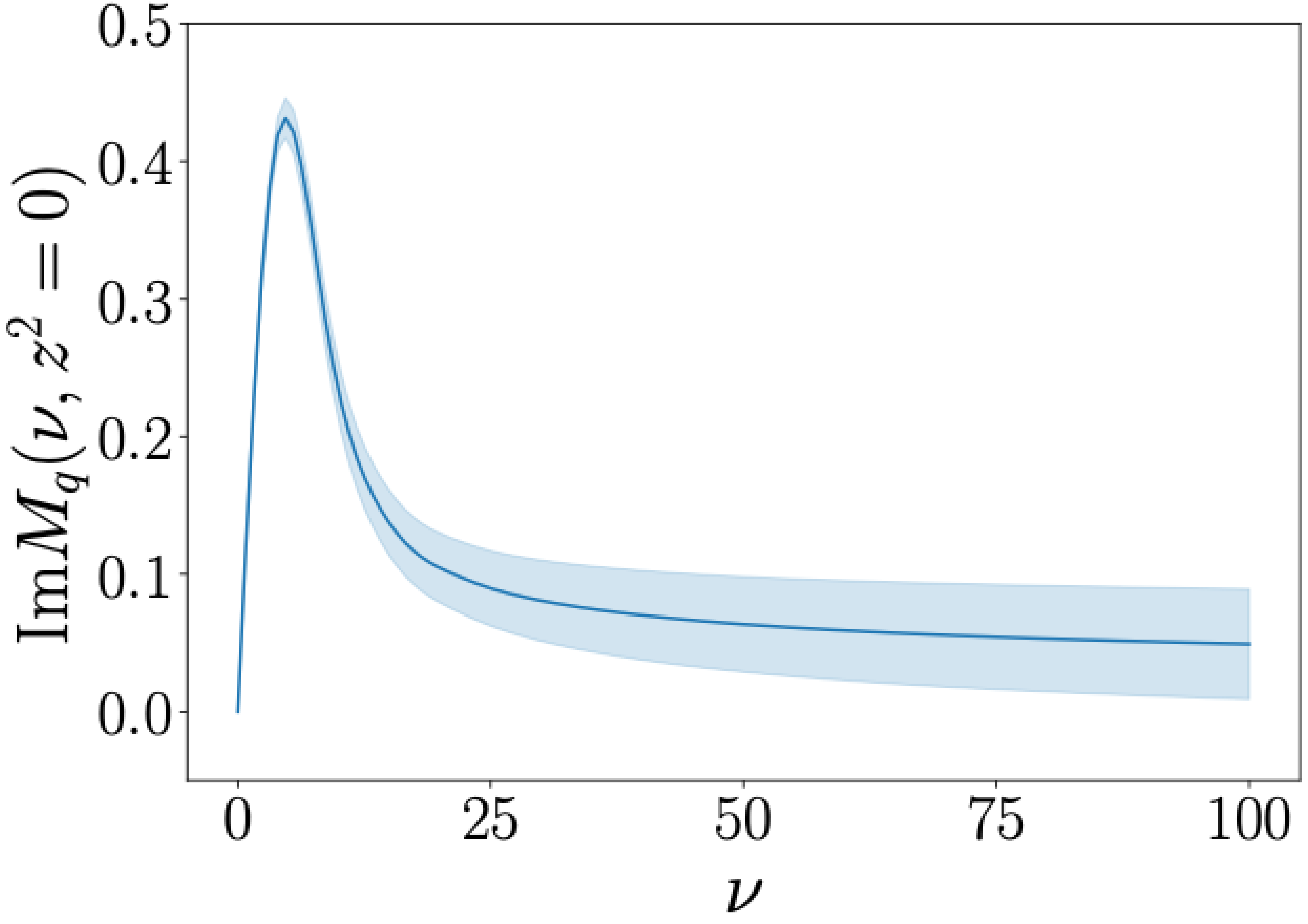


$\mathcal{L}^{-1}$

Inverse problem (Closure test)

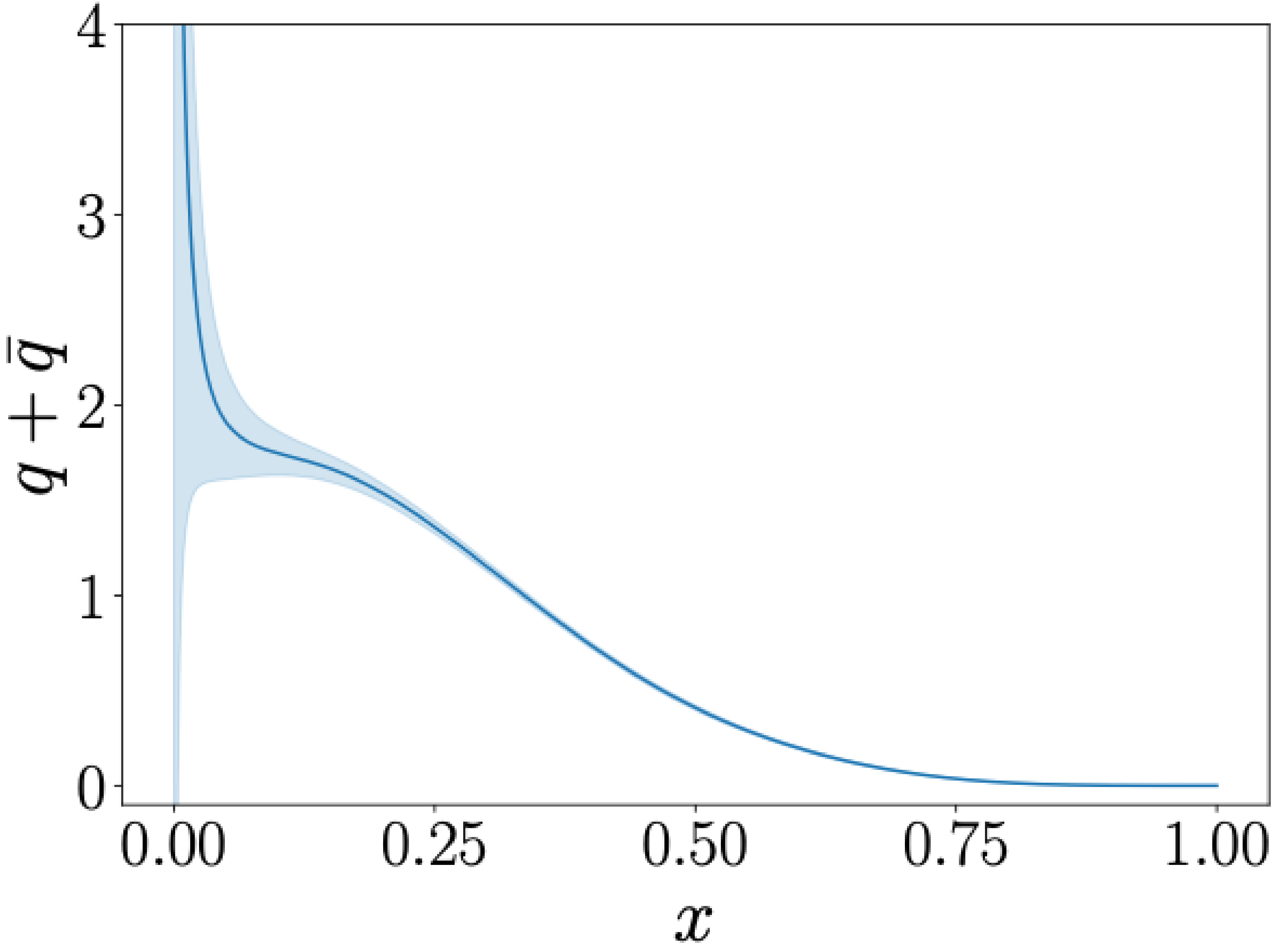
NNPDF 4.0 (imaginary component)

NNPDF Collaboration, The Path to Proton Structure at One-Percent Accuracy



Forward map = Easy $\mathcal{L}$

$\mathcal{L}^{-1}$

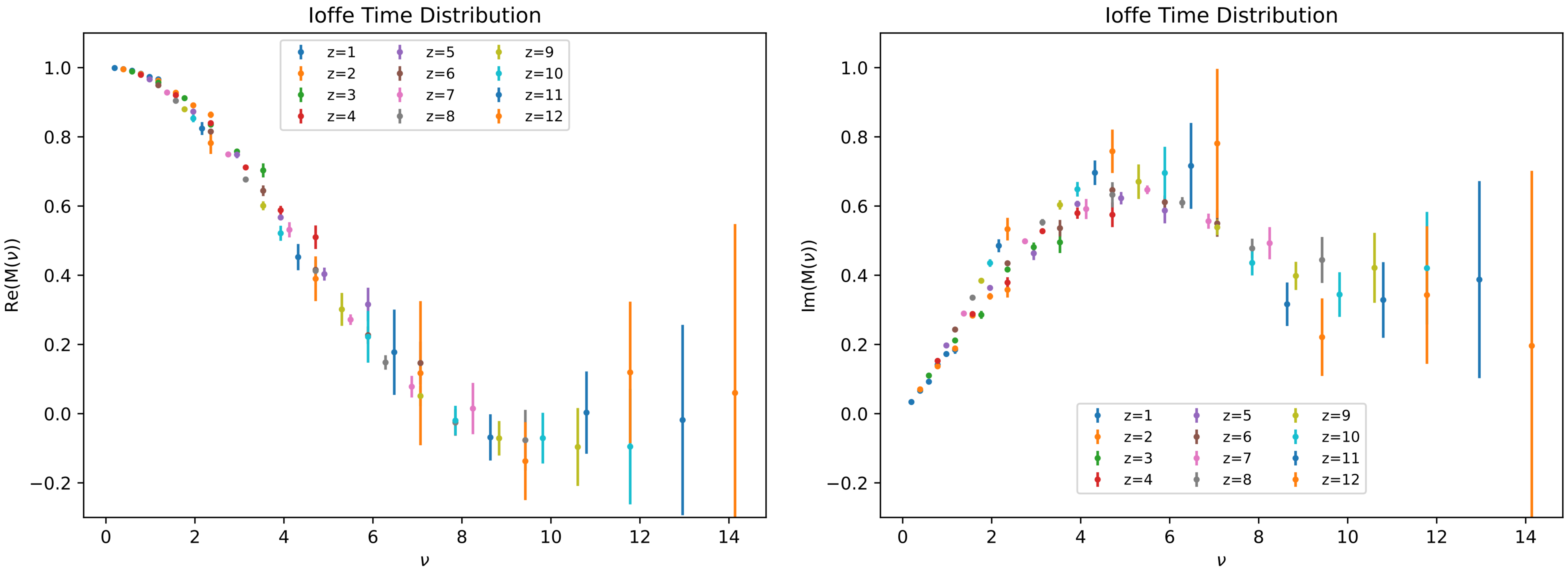


$$\mathfrak{M}(\nu) = \int_{-1}^{1} dx e^{ix\nu} q(x)$$

Available lattice data

Unpolarized iso-vector PDF of the nucleon

Lattice details: 2+1 flavors of clover improved Wilson quarks with a lattice spacing a = 0.094(1) fm and a pion mass of 358(3) MeV

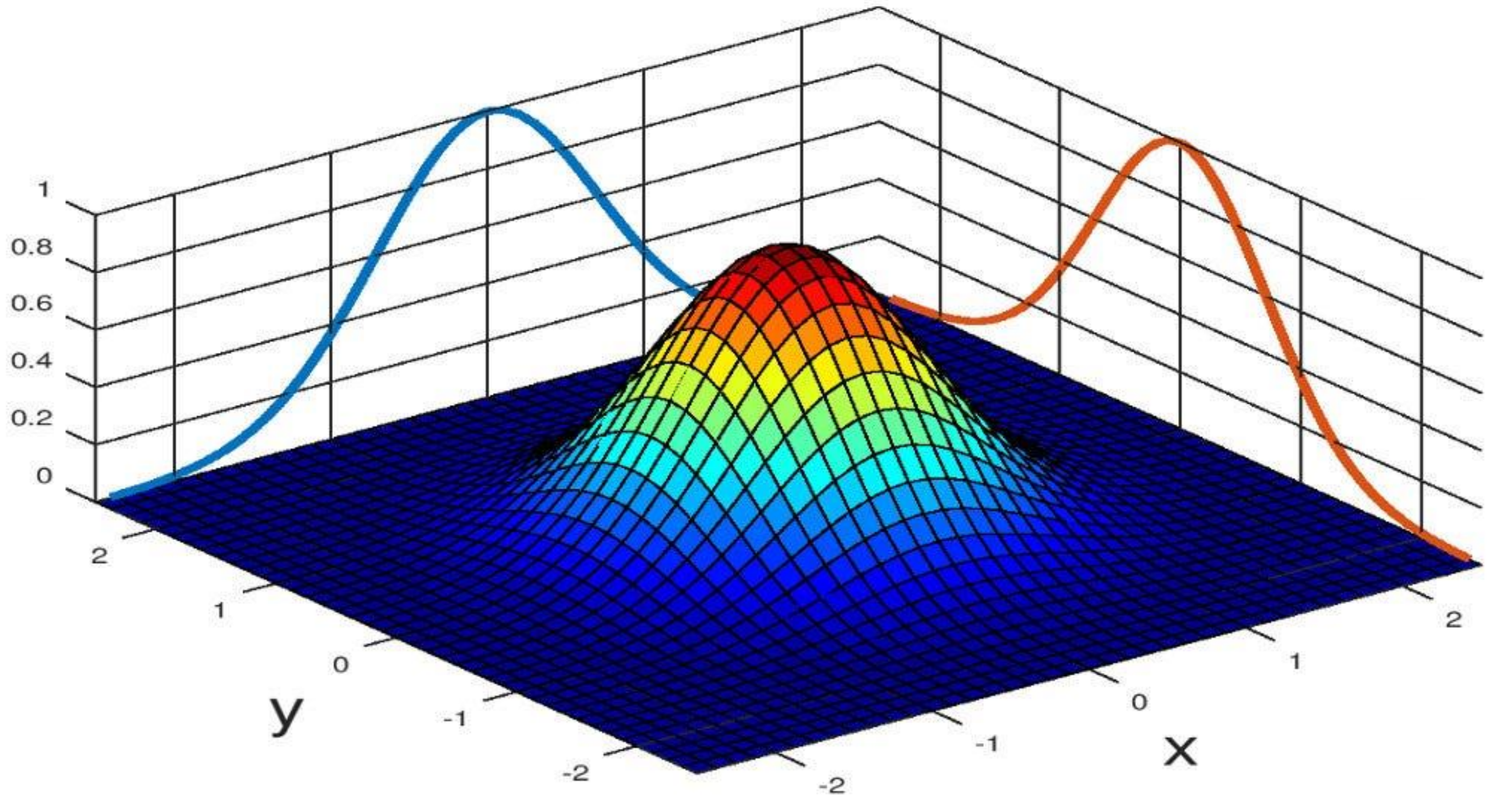


Colin Egerer, Forward and Off-Forward Parton Distributions from Lattice QCD

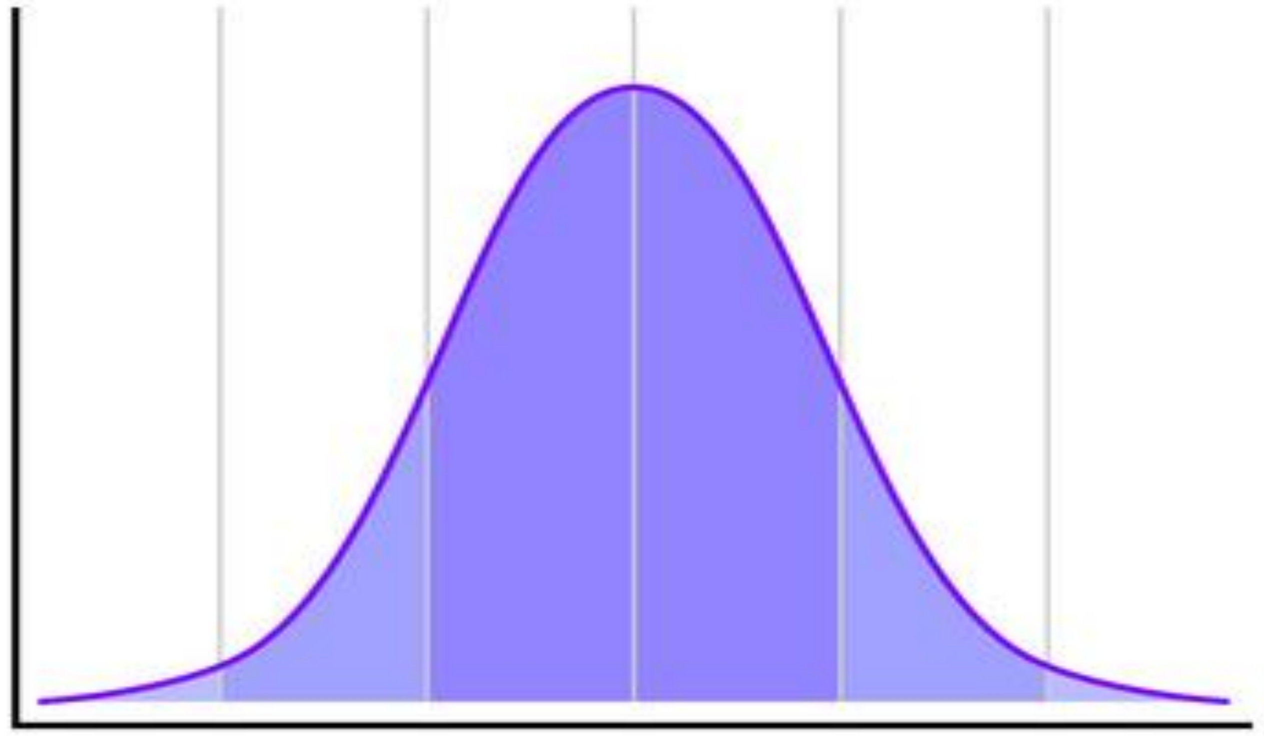
Gaussian process!!!

= Stochastic Process…

$\vec{\mu}_i, \sigma_{ij}$

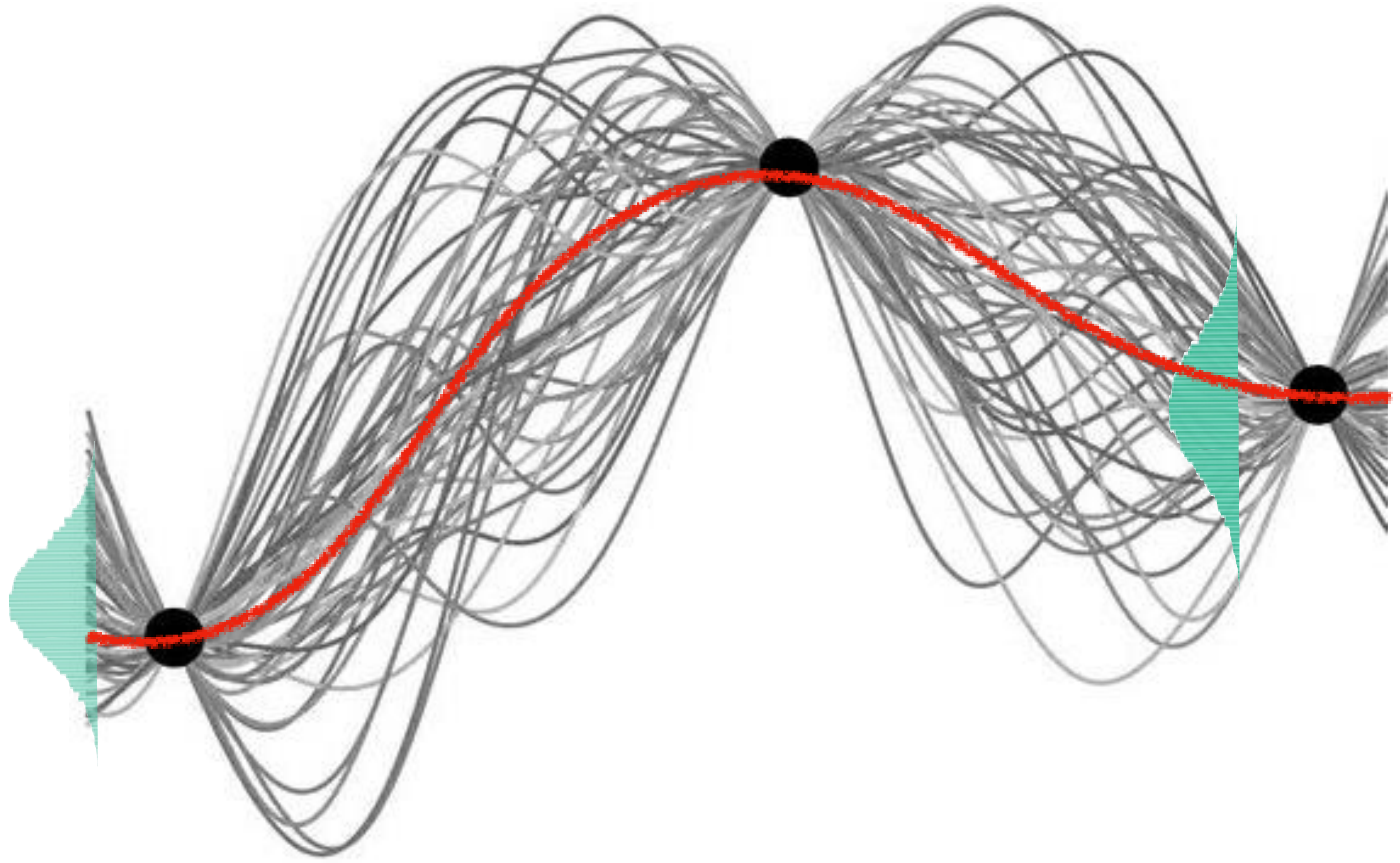


μ, σ



Normal Distribution

$\mu(x), \sigma(x, x')$ or $K(x, x')$



Try to imagine an infinite dimensional normal distribution

Machine Learning of Nonlinear Partial Differential Equations. arXiv: 1708.00588
Gaussian Processes for Machine Learning, E. Rasmussen and C. K. I. Williams

Gaussian process

Parametric vs/and/or Non-parametric

Gaussian Processes for Machine Learning, E. Rasmussen and C. K. I. Williams

Parametric

$$\chi^2(q(x;\theta)) = \frac{1}{2}(M_i - \mathcal{L}_{\nu_i} q(x;\theta)) C_{ij}^{-1} (M_j - \mathcal{L}_{\nu_j} q(x;\theta))$$

$$q(x;\theta)_{PDF} = N x^{\alpha}(1-x)^{\beta}$$

$$\hat{q}(x) = \min_{\theta}\left(\chi^2(q(x;\theta))\right)$$

$$P(\theta|M^i) = \frac{e^{-\chi^2(q(x;\theta))} P(\theta)}{P(M^i)}$$

Bayesian, but still parametric

If we do not parametrize, what we do in this case?

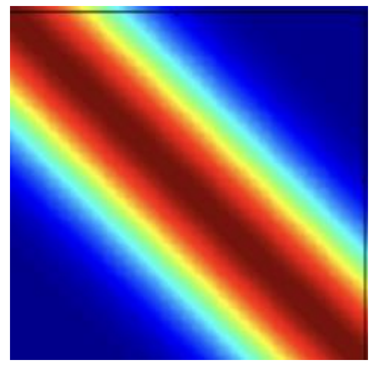
Non-Parametric

$$\hat{q}(x) = \min_{q \in H}\left(\chi^2(q(x)) + \|\mathcal{P}q\|_H^2\right)$$

Imposes additionally conditions on the Hilbert space

$$H = \{q(x) \,|\, \text{continuous? smooth? square-integrable} \}$$

$$\|\mathcal{P}q\|_H^2 \to q(x) K^{-1}(x,x') q(x')$$



$$K(x,x') = \sigma e^{\frac{|x-x'|^2}{2l^2}}$$

We can recover a parametric feature

$$q(x) \to q(x) - q_{PDF}(x)$$

$$P(q(x)|M^i) = \frac{e^{-\chi^2(q(x))} e^{-\|\mathcal{P}q\|_H^2}}{P(M^i)}$$

Bayesian approach

Levels of inference

$$\text{Posterior} = \frac{\text{Likelihood} \quad \text{Prior}}{\text{Evidence}}$$

Parametric Models

3rd

$$P(\mathcal{H}_i|M^l) = \frac{P(M^l|\mathcal{H}_i)P(\mathcal{H}_i)}{P(M^l)}$$

Model Average/Selection of Models, depending on the approximation

$\mathfrak{q}(x) \quad \mathfrak{q}(x)\mathfrak{q}(x)$

2nd

$$P(\theta|M^l,\mathcal{H}) = \frac{P(M^l|\theta,\mathcal{H})P(\theta|\mathcal{H})}{P(M^l|\mathcal{H})}$$

The hyper parameters can be conditioned to the data and the model.

$< q(x) > \quad < q(x)q(x) >$

1st

$$P(q(x)|M^l,\theta,\mathcal{H}) = \frac{P(M^l|q(x),\theta,\mathcal{H})P(q(x)|\theta,\mathcal{H})}{P(M^l|\theta,\mathcal{H})}$$

Solved analytically (path integral techniques)

$\bar{q}(x) \quad \overline{q(x)q(x)}$

Marginal Likelihood or Evidence = Likelihood of the next level of inference

$$\{functions, Parameters, Hypothesis, Data\} \equiv \{q(x), \theta, \mathcal{H}, M^l\}$$

1st level of inference

Gaussian processes à la Feynman

Posterior = $\dfrac{\text{Likelihood}\ \text{Prior}}{\text{Evidence}}$

$$\bar{q}(x;\theta) = \int q(x) P(q(x)|M^l,\theta,\mathcal{H}) D[q(x)]$$

$$\overline{q(x)q(x)} = \int q(x)q(x) P(q(x)|M^l,\theta,\mathcal{H}) D[q(x)]$$

Everything is "gaussian" in this level of inference(It's like solving a free field theory).

$$P(q(x)|M^l,\theta,\mathcal{H}) = \frac{P(M^l|q(x),\theta,\mathcal{H})P(q(x)|\theta,\mathcal{H})}{P(M^l|\theta,\mathcal{H})}$$

My prior and likelihood have an analytic expression:

Likelihood
$$P(M^l|q(x),\theta,\mathcal{H}) = N_{likelihood} e^{-\frac{1}{2}(M_i - \mathcal{L}_{\nu_i} q(x)) C^{-1}_{ij} (M_j - \mathcal{L}_{\nu_j} q(x))}$$

Prior
$$P(q(x)|\theta,\mathcal{H}) = N_{prior} P_{const} e^{-\frac{1}{2}(\int dx dx' (q(x) - q_{PDF}(x)) K^{-1}(x,x')(q(x') - q_{PDF}(x'))}$$

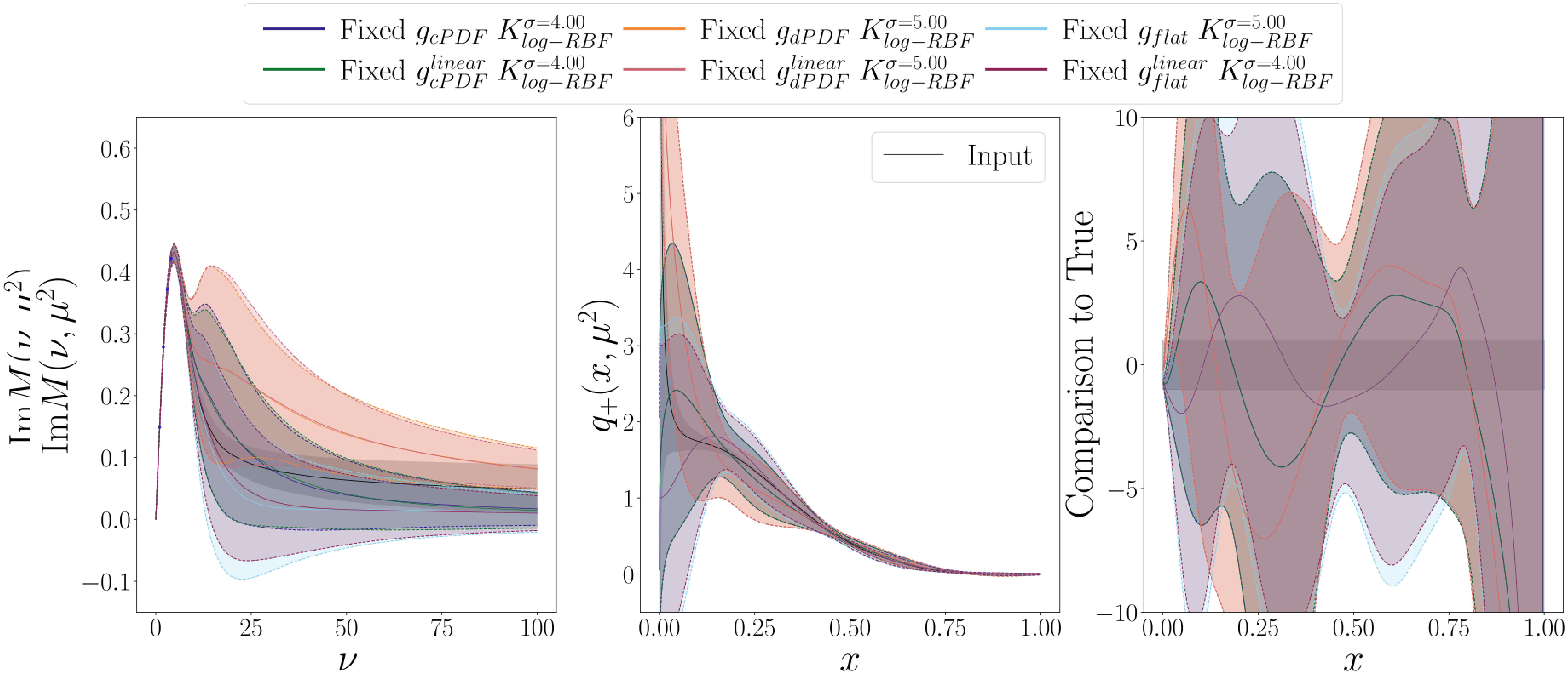
$$P_{const} = e^{-\frac{1}{2\lambda}(\int_0^1 dx q(x) - 1)^2 - \frac{1}{2\lambda_c}(\int_0^1 dx q(x)\delta(1-x))^2}$$

Normalization and q(x=1)=0

Evidence
$$P(M^l|\theta,\mathcal{H}) = \int D[q(x)] P(M^l|q(x),\theta,\mathcal{H}) P(q(x)|\theta,\mathcal{H})$$

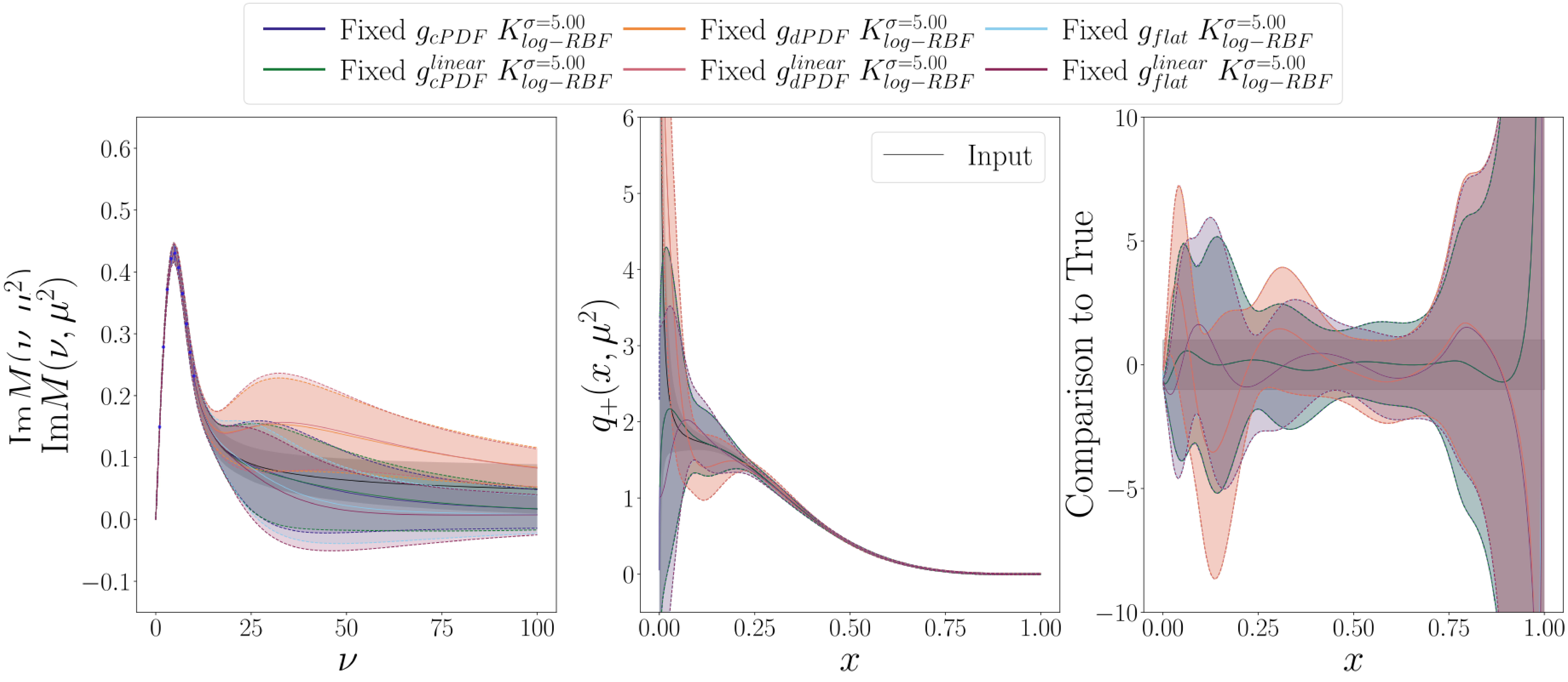
1st Level of inference

Fix parameters (4 data points)



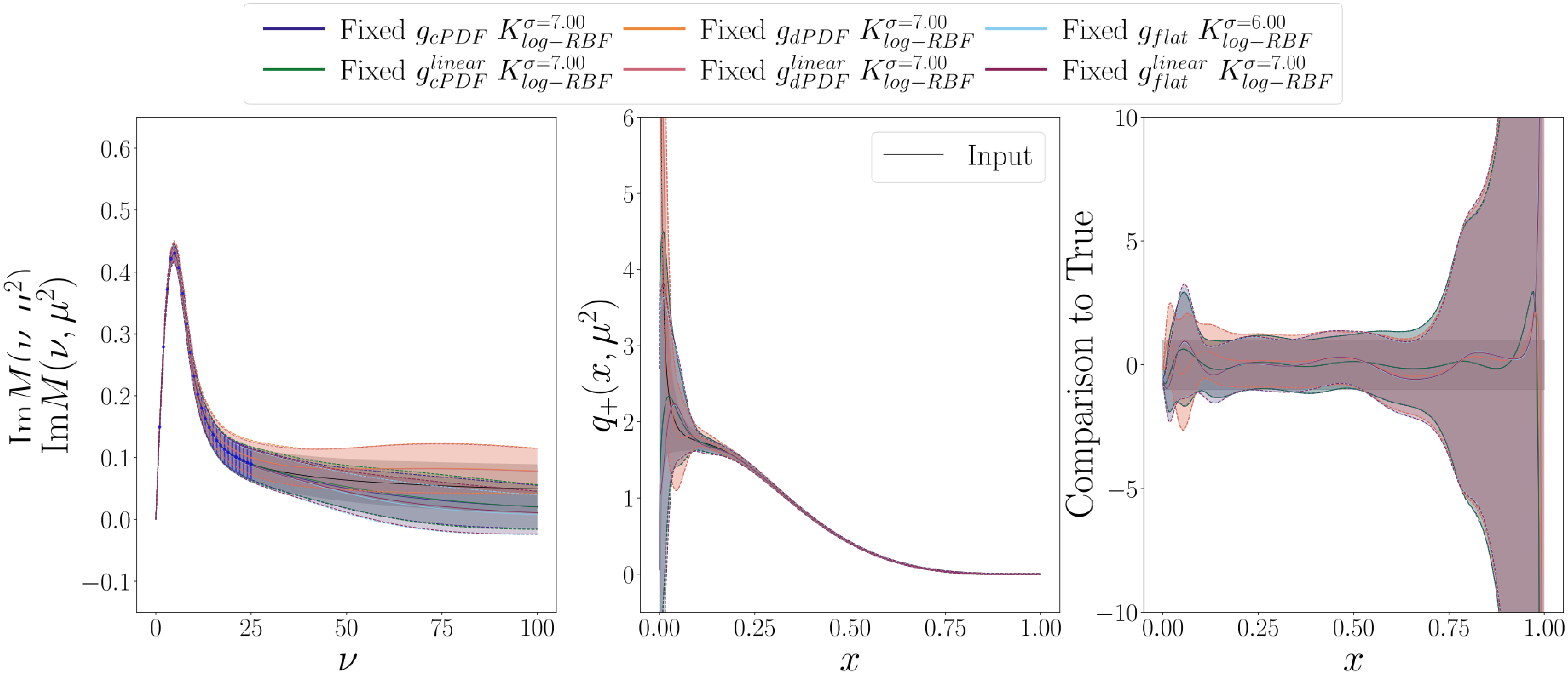
1st Level of inference

Fix parameters (10 data points)



1st Level of inference

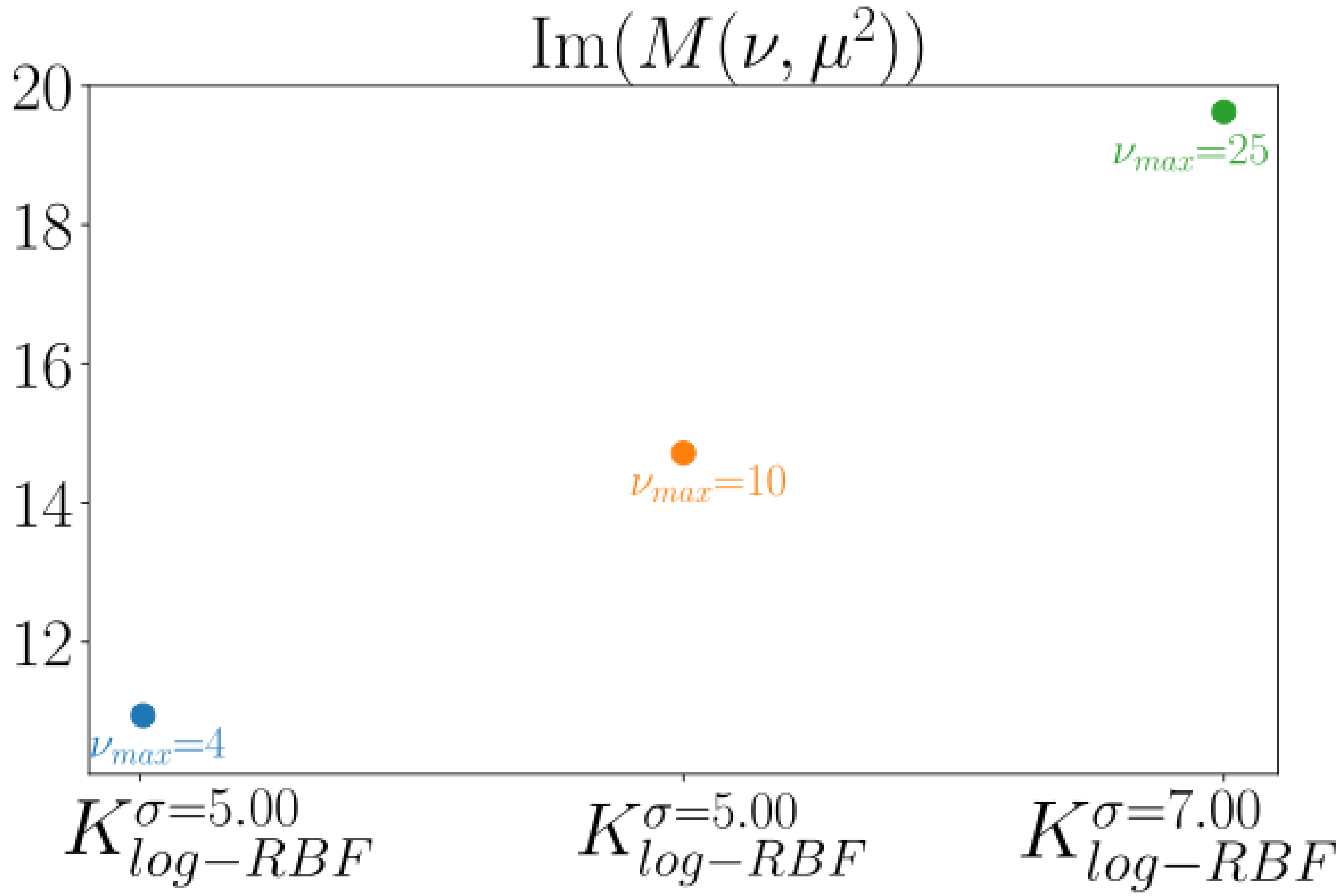
Fix parameters (25 data points)



KL Divergence

Information gained globally

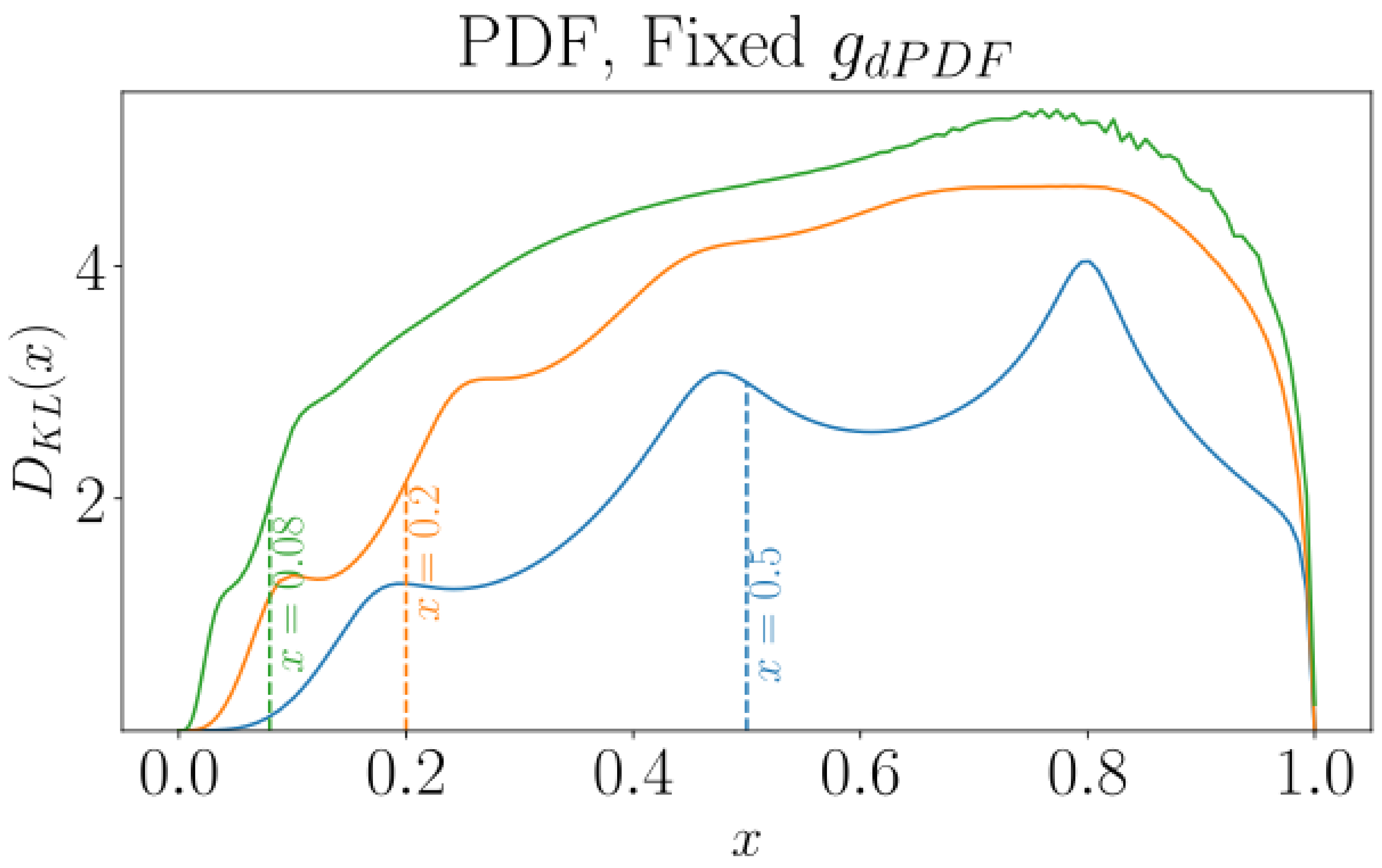
$$D_{KL}(P[q(x)|M,\theta,\mathcal{H}]||P[q(x)|\theta,\mathcal{H}]) = \int D[q(x)]\ P[q(x)|M,\theta,\mathcal{H}] \log\left(\frac{P[q(x)|M,\theta,\mathcal{H}]}{P[q(x)|\theta,\mathcal{H}]}\right)$$

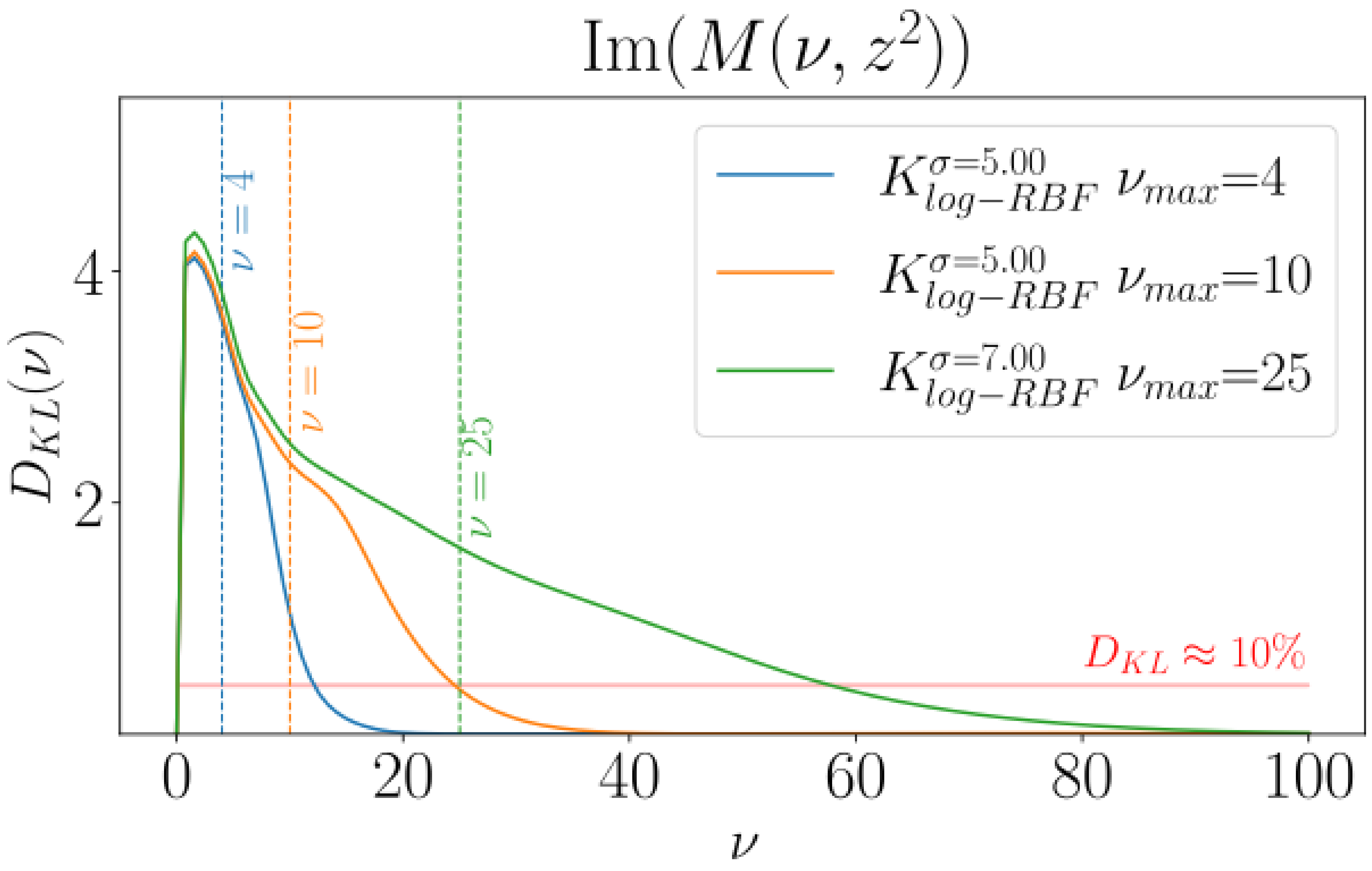


KL Divergence

Information gained locally

$$D_{KL}(x_i) \equiv D_{KL}(P[q_i|M,\theta,I]||P[q_i|\theta,I]) = \int D[q(x_i)]\, P[q_i|M,\theta,I] \log\left(\frac{P[q_i|M,\theta,I]}{P[q_i|\theta,I]}\right)$$





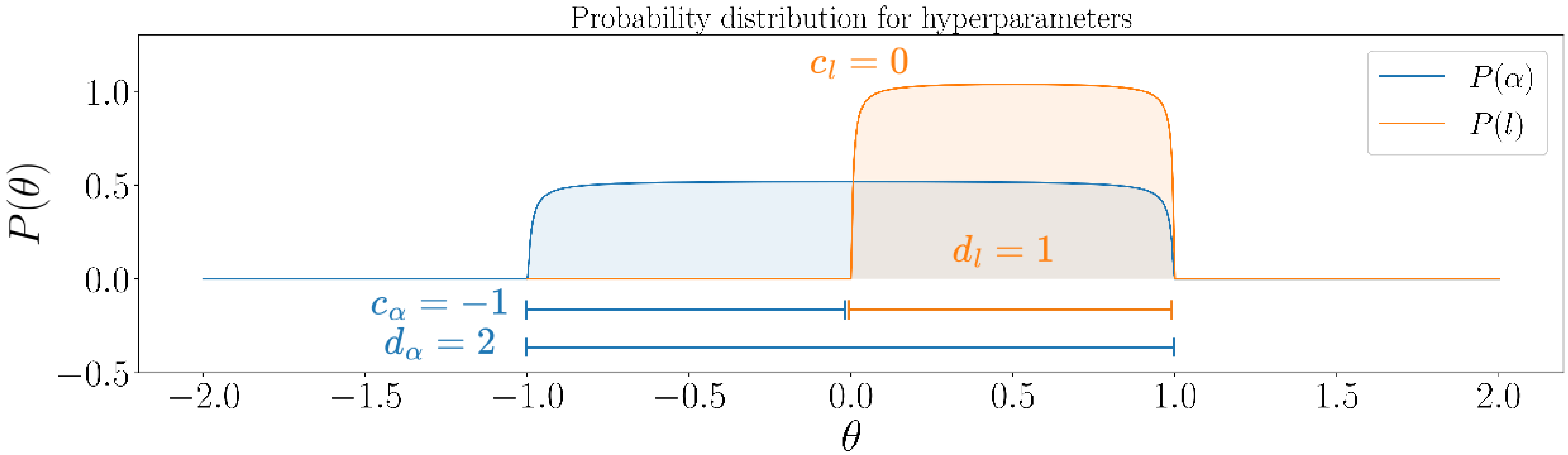
2nd Level of inference

$$P(\theta|M^l, \mathcal{H}) = \frac{P(M^l|\theta, \mathcal{H})P(\theta|\mathcal{H})}{P(M^l|\mathcal{H})}$$

Prior = exponential beta

$$P(\theta|\mathcal{H}) = ne^{-\frac{\hat{\theta}^a(1-\hat{\theta})^b}{2\cdot B(a+1,b+1)}}$$

$$\hat{\theta} = \frac{\theta - c}{d}$$

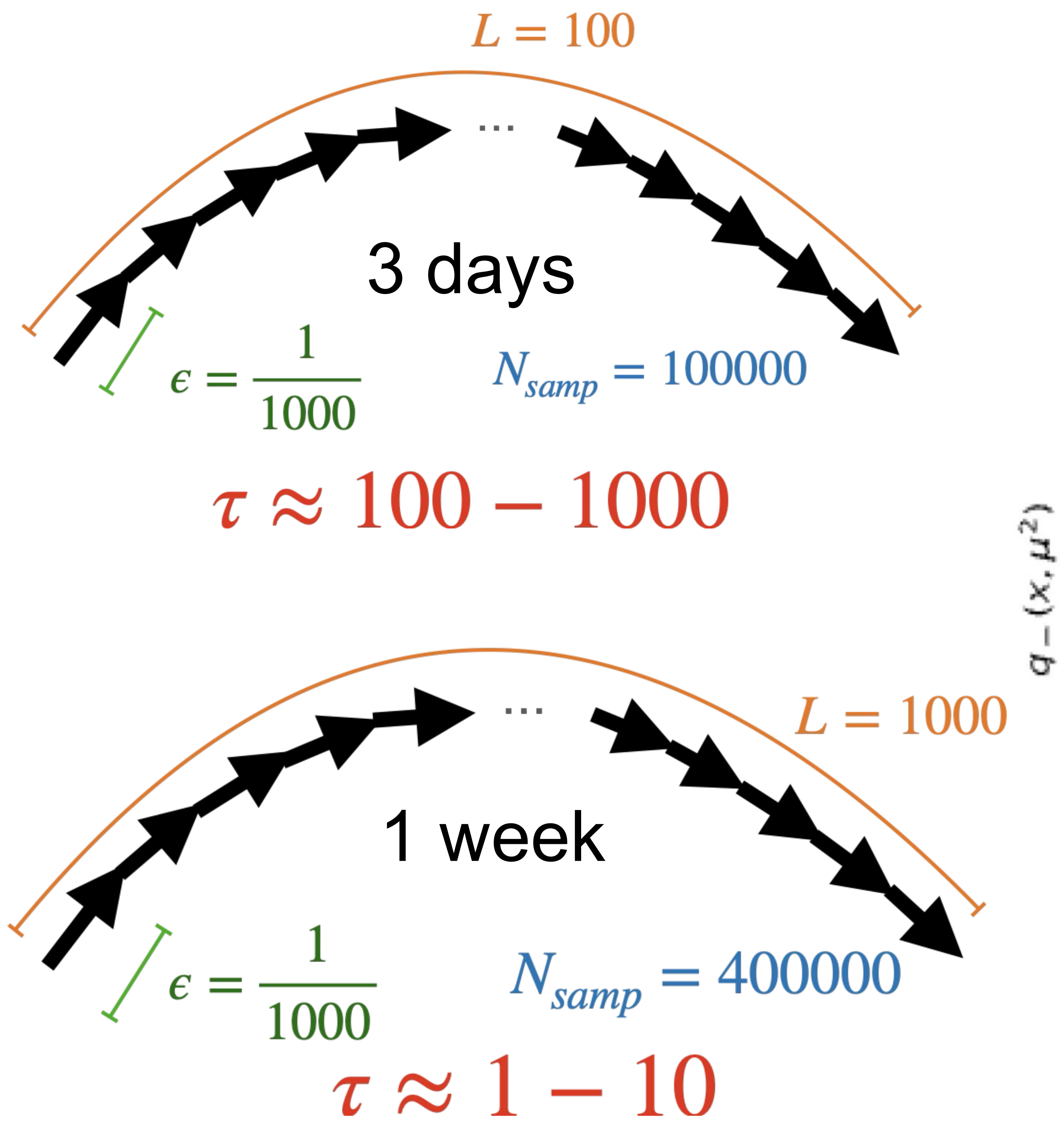


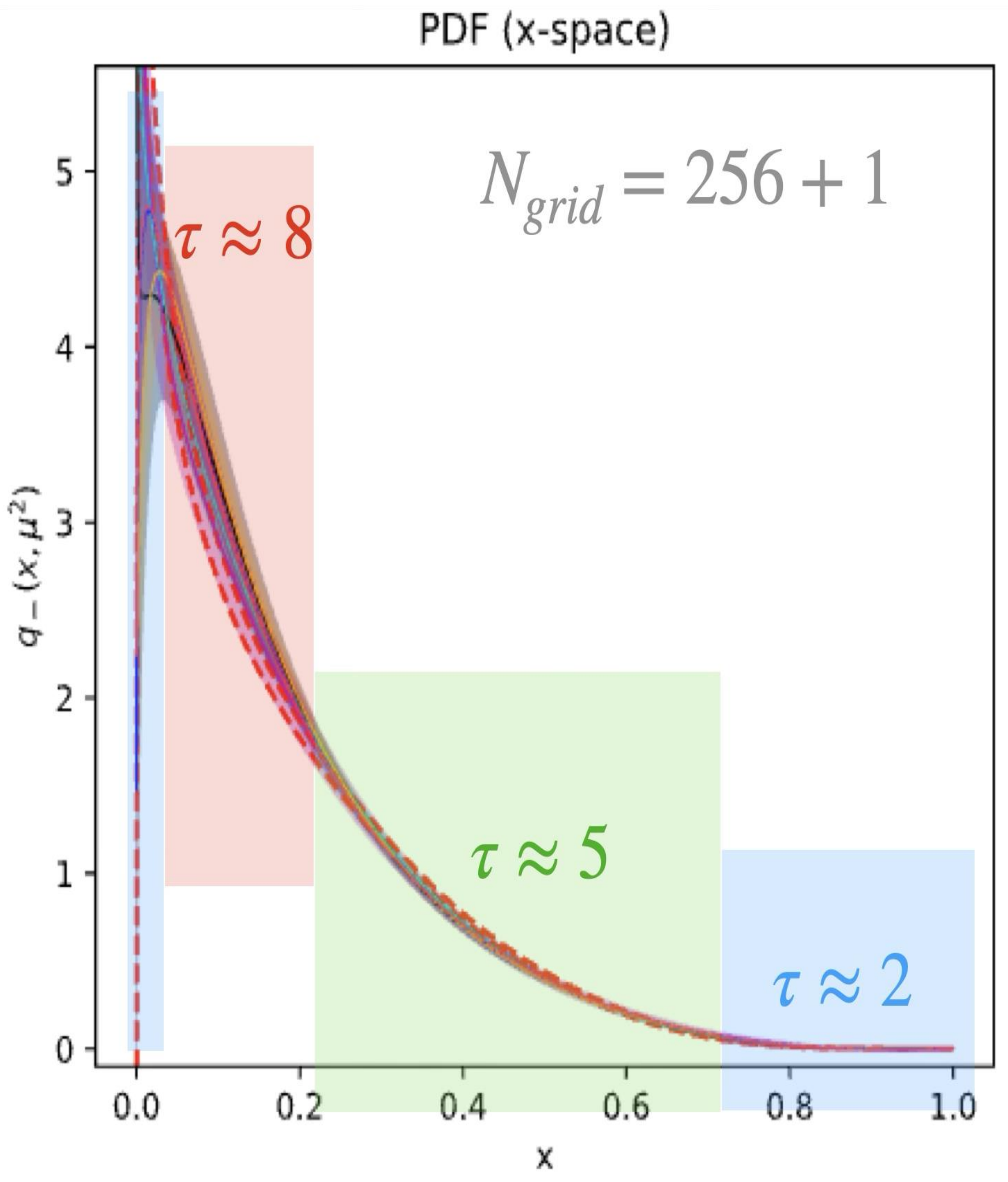
2^{nd} Level of inference

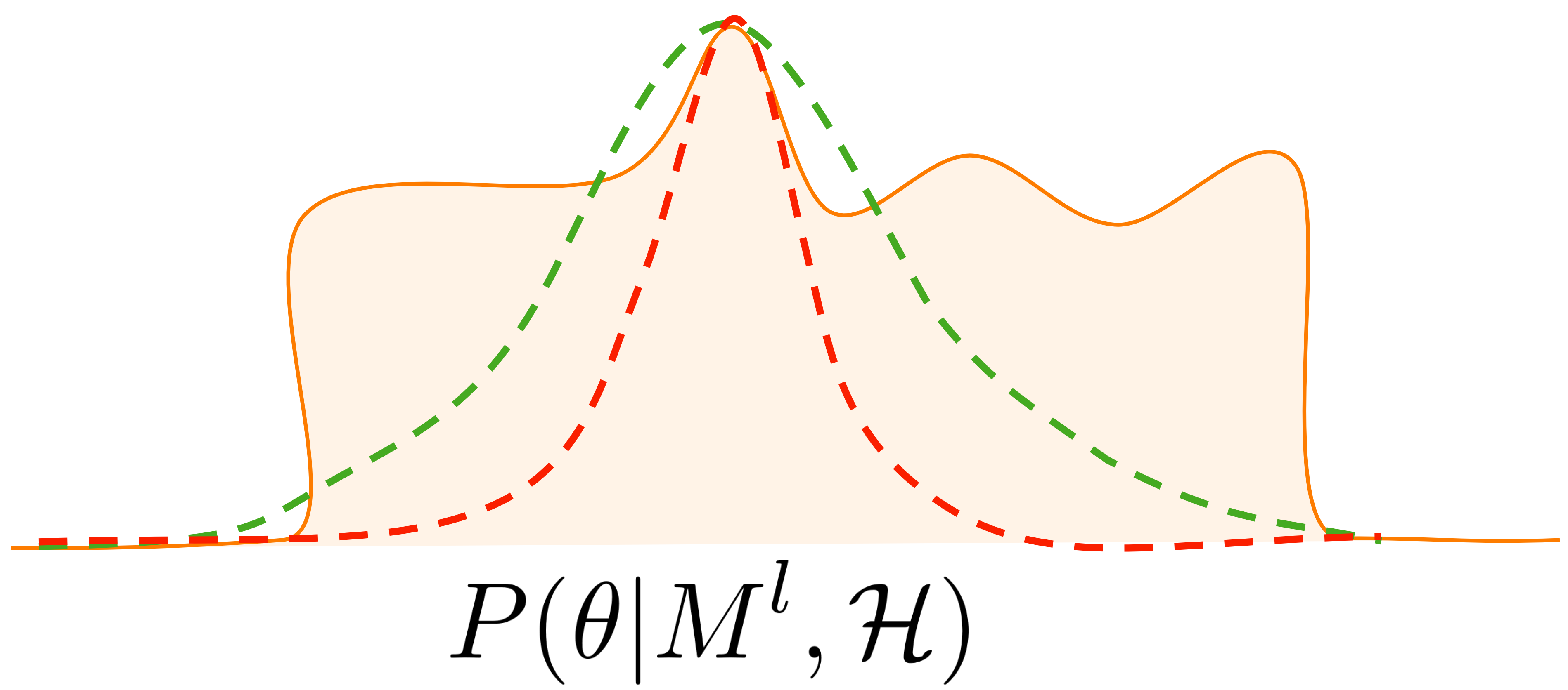
HMC -> Importance Sampling

$$P(\theta|M^l,\mathcal{H}) = \frac{P(M^l|\theta,\mathcal{H})P(\theta|\mathcal{H})}{P(M^l|\mathcal{H})}$$

$$< q(x) >= \int P(\theta|M^l,\mathcal{H})\bar{q}(x;\theta)d\theta \qquad < q(x)q(x) >\equiv \int (\bar{q}(x;\theta)- < q(x) >)^2 P(\theta,|M^l,\mathcal{H})d\theta$$





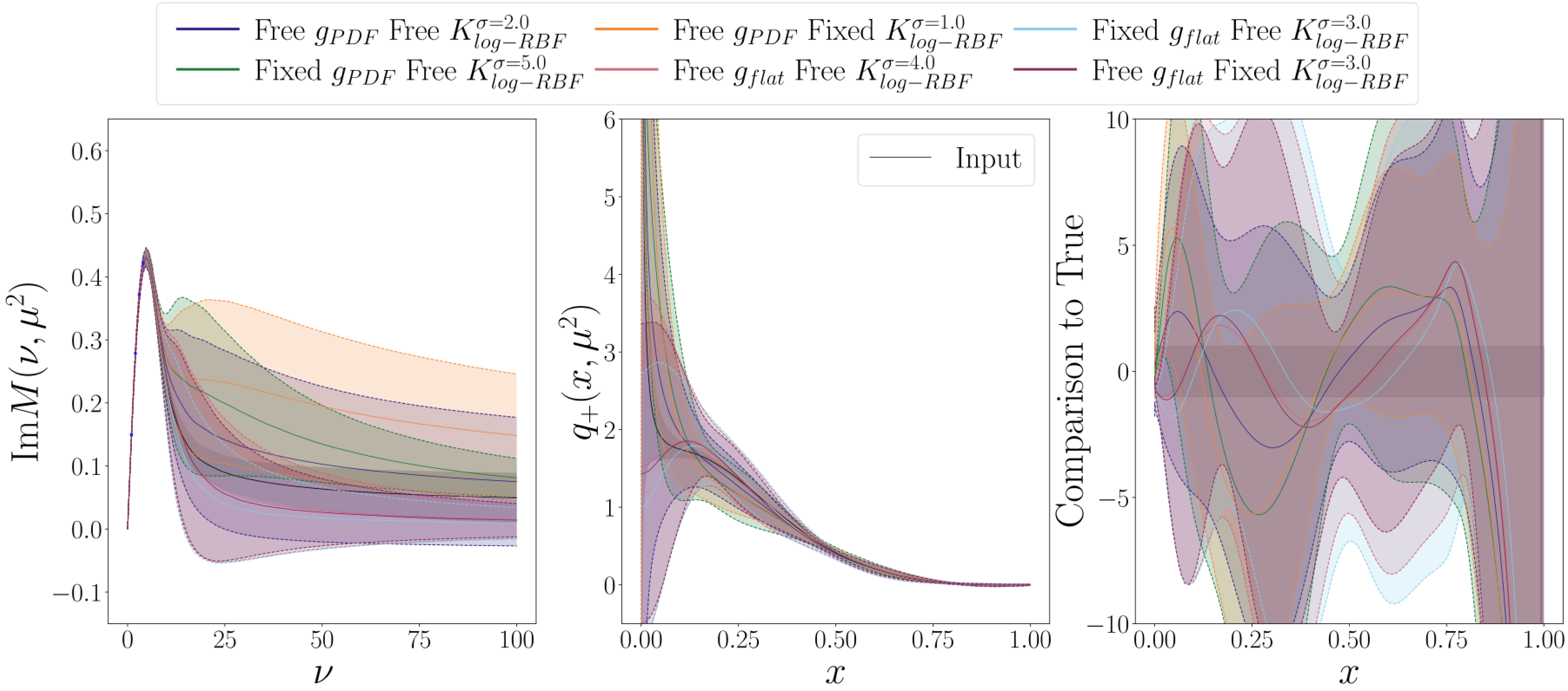


- HMC is effective but it can take a lot of computational resources and time to run.
- IS reduces the sampling process to 50 min per model

2^{nd} Level of inference

Sampled results

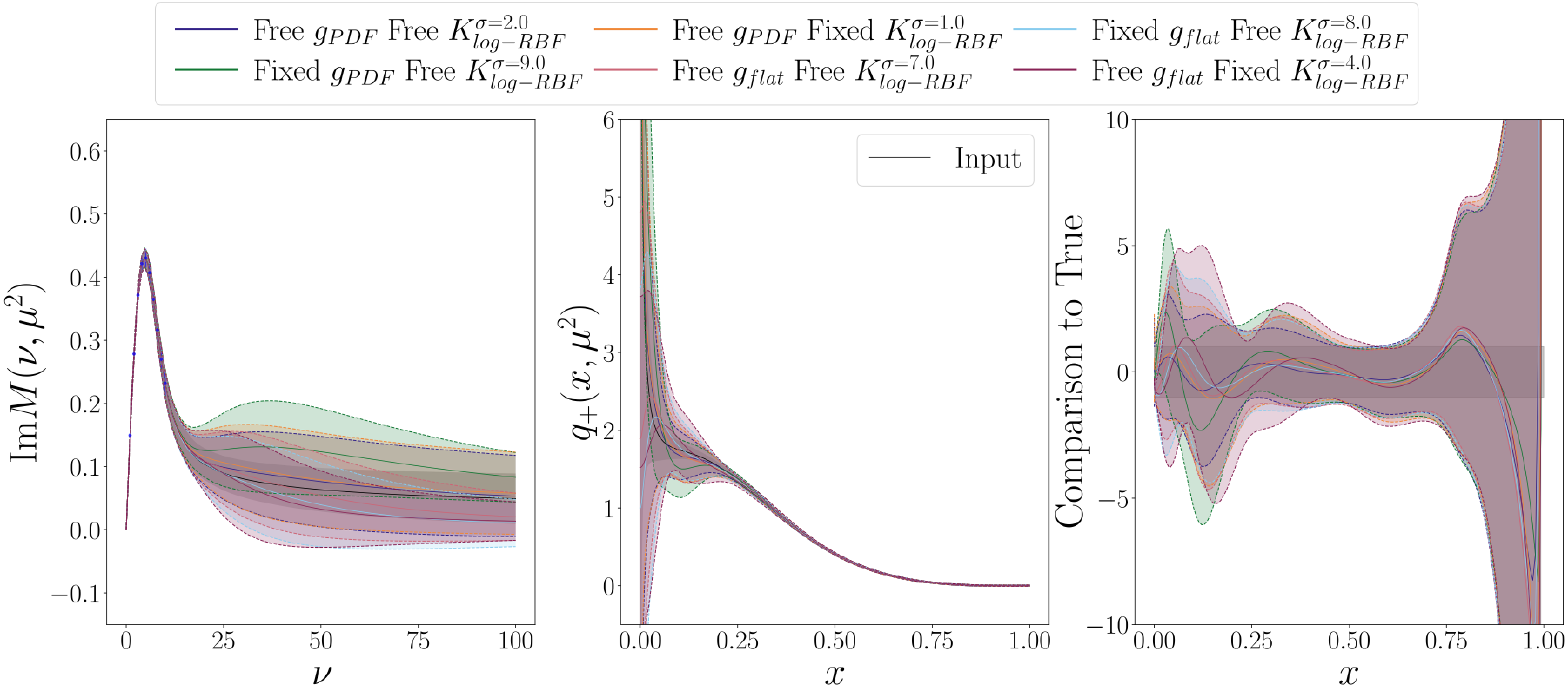
$$P(\theta|M^l,\mathcal{H}) = \frac{P(M^l|\theta,\mathcal{H})P(\theta|\mathcal{H})}{P(M^l|\mathcal{H})}$$



2nd Level of inference

Sampled results

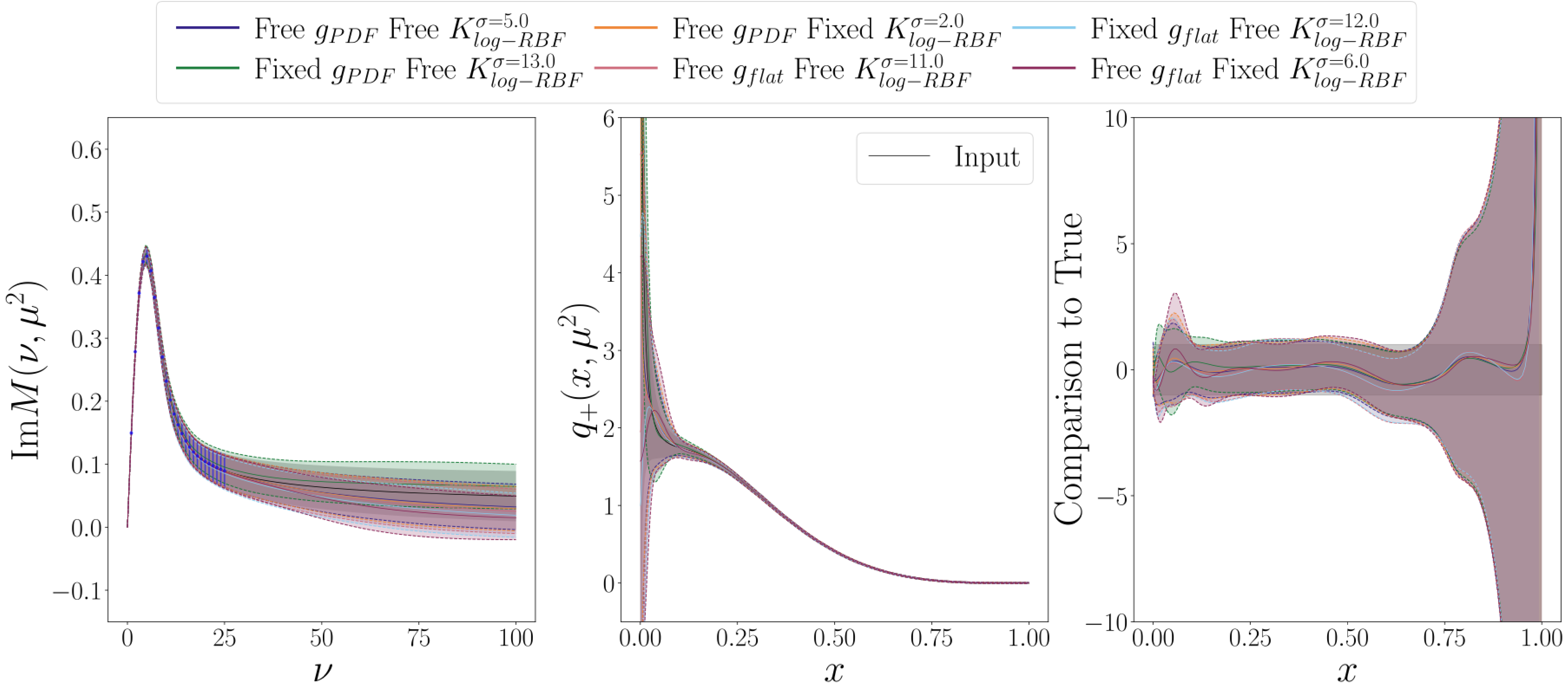
$$P(\theta|M^l,\mathcal{H}) = \frac{P(M^l|\theta,\mathcal{H})P(\theta|\mathcal{H})}{P(M^l|\mathcal{H})}$$



2nd Level of inference

Results…(we explore 30-ish models)

$$P(\theta|M^l,\mathcal{H}) = \frac{P(M^l|\theta,\mathcal{H})P(\theta|\mathcal{H})}{P(M^l|\mathcal{H})}$$



3rd Level of inference

Information criteria

$$P(\mathcal{H}_i|M^l) = \frac{P(M^l|\mathcal{H}_i)P(\mathcal{H}_i)}{P(M^l)}$$

$$-2\log(P(M^l|\mathcal{H}_i)) \approx \begin{cases} BAIC = -log(P(M^l|\theta_{min},\mathcal{H})P(\theta_{min}|\mathcal{H})) + 2k \\ BTIC = -log(P(M^l|\theta_{min},\mathcal{H})P(\theta_{min}|\mathcal{H})) + 2Tr(J^{-1}(\theta_{min})I(\theta_{min})) \\ PAIC = -<log(P(M^l|\theta,\mathcal{H})P(\theta|\mathcal{H}))> +2Tr(J^{-1}(\theta_{min})I(\theta_{min})) \end{cases}$$

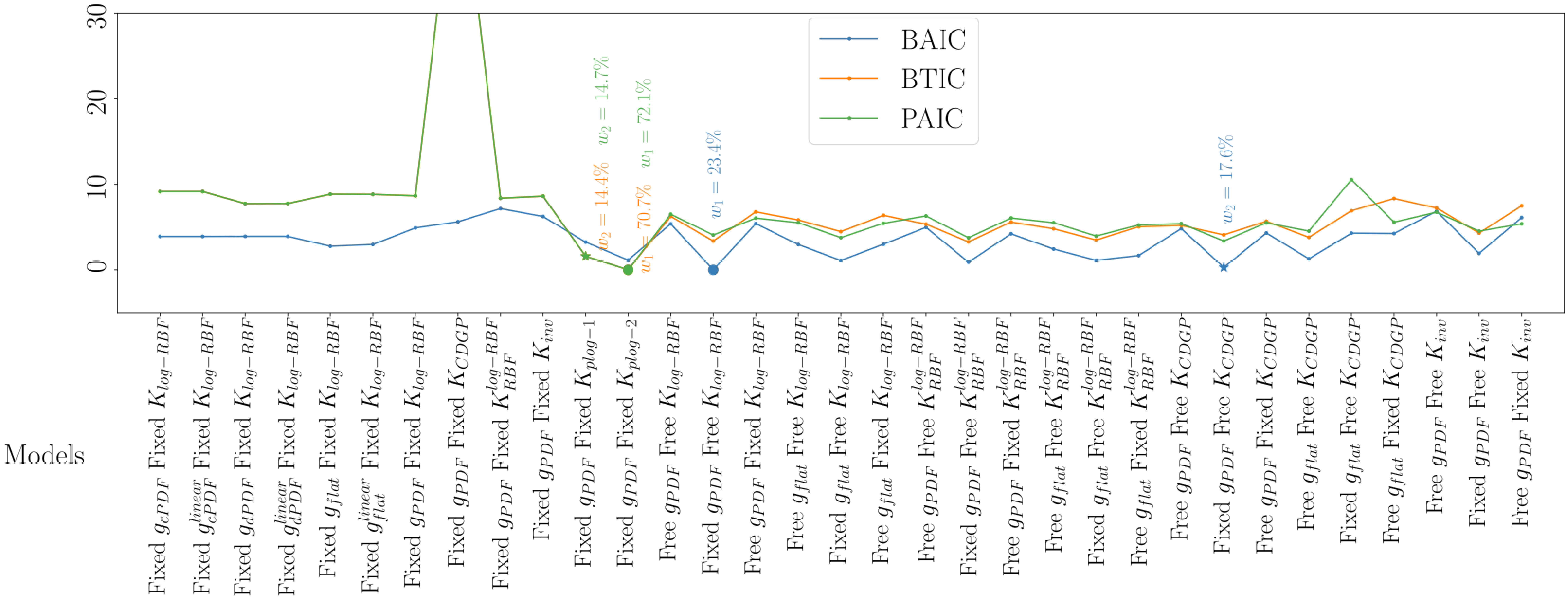
$$P(\mathcal{H}_i) = \frac{1}{N_{models}}$$

$$\mathfrak{q}(x) \equiv \sum_i^{models} P(\mathcal{H}_i|M^l) < q(x) >_i \qquad \mathfrak{q}(x)\mathfrak{q}(x) \equiv \sum P(\mathcal{H}_i|M^l)[< q(x) >_i -\mathfrak{q}(x)]^2$$

3rd Level of inference

Selection ~ Averaging

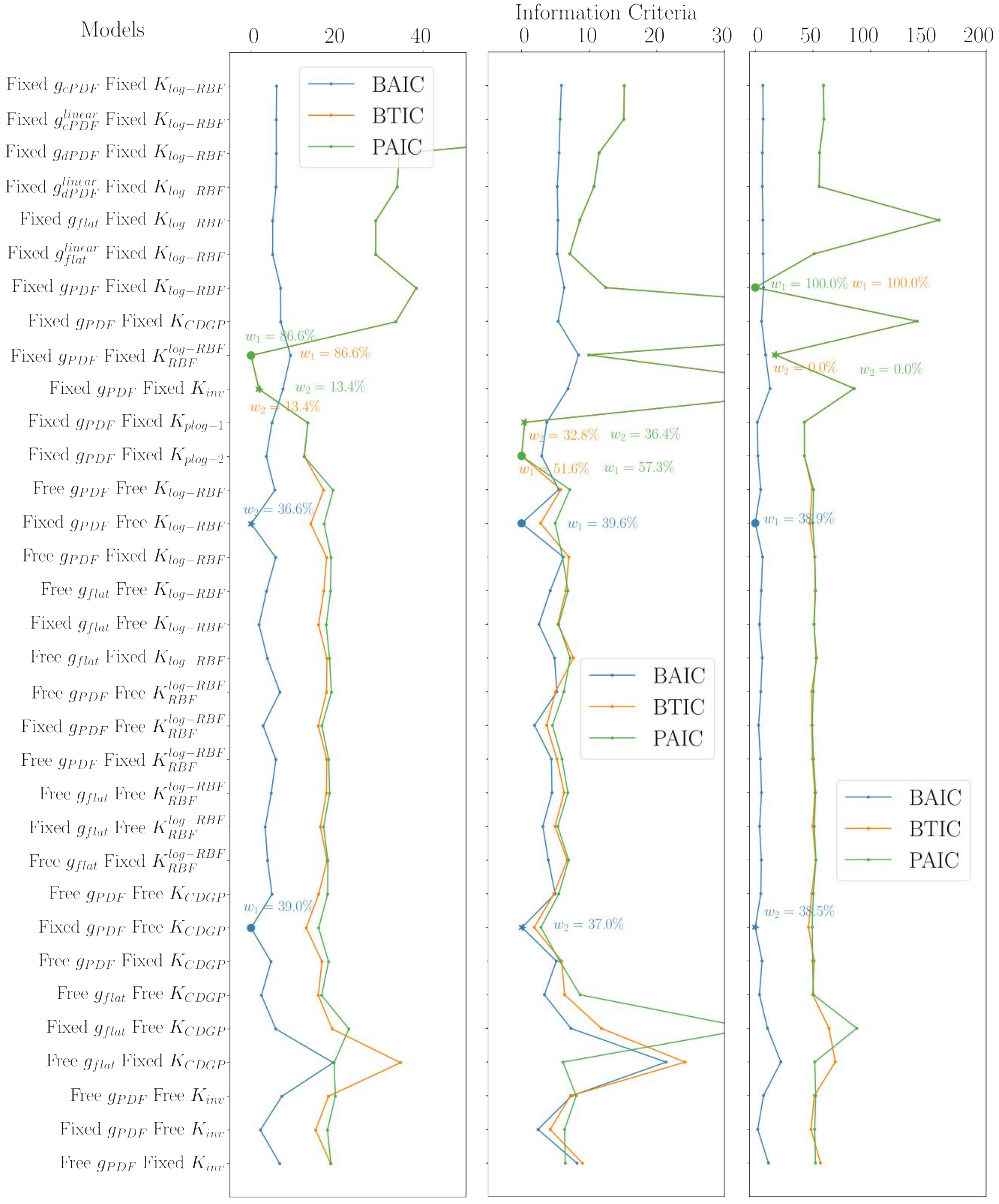
$$P(\mathcal{H}_i|M^l) = \frac{P(M^l|\mathcal{H}_i)P(\mathcal{H}_i)}{P(M^l)}$$

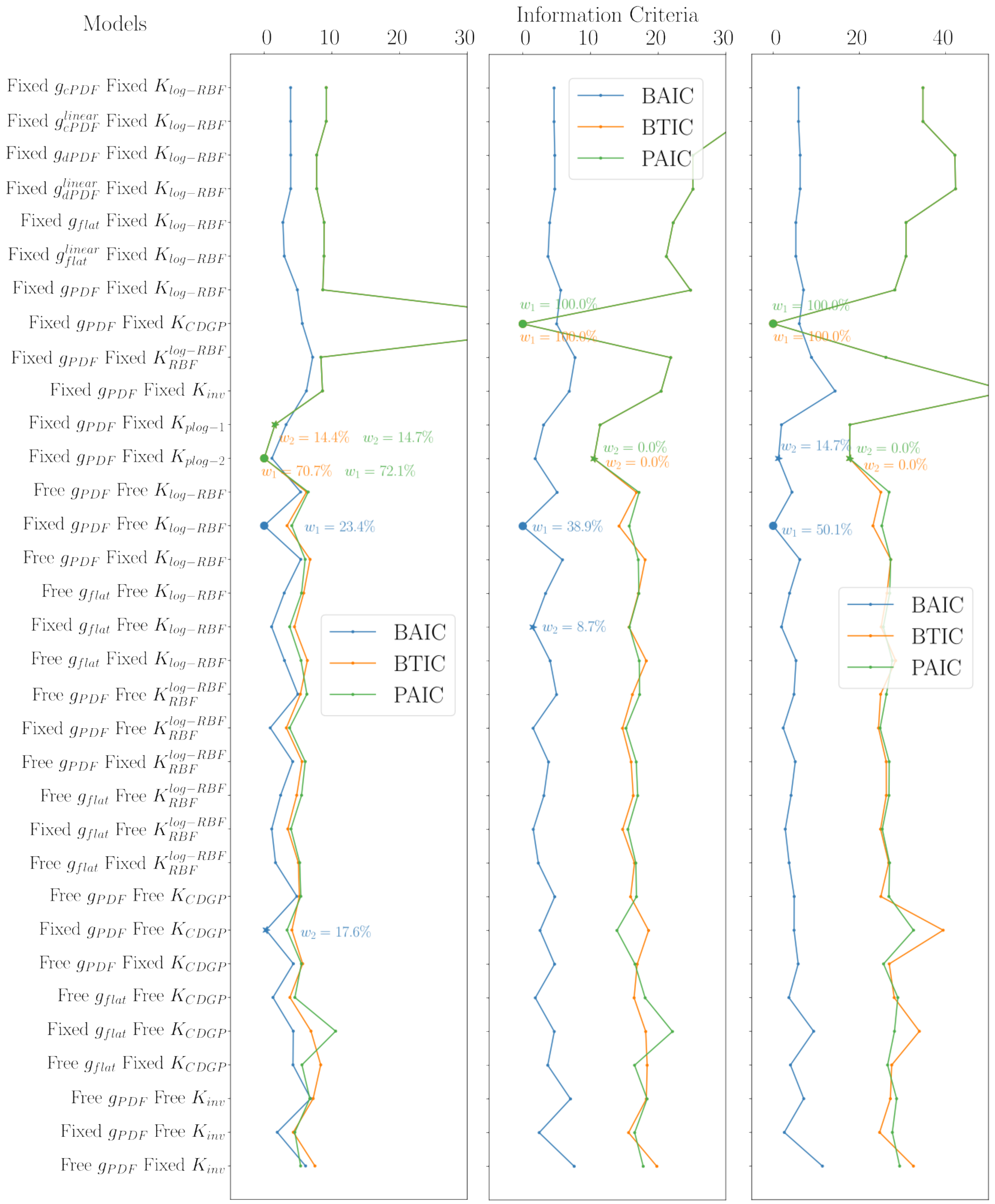


3rd Level of inference

Information criteria

$$P(\mathcal{H}_i|M^l) = \frac{P(M^l|\mathcal{H}_i)P(\mathcal{H}_i)}{P(M^l)}$$

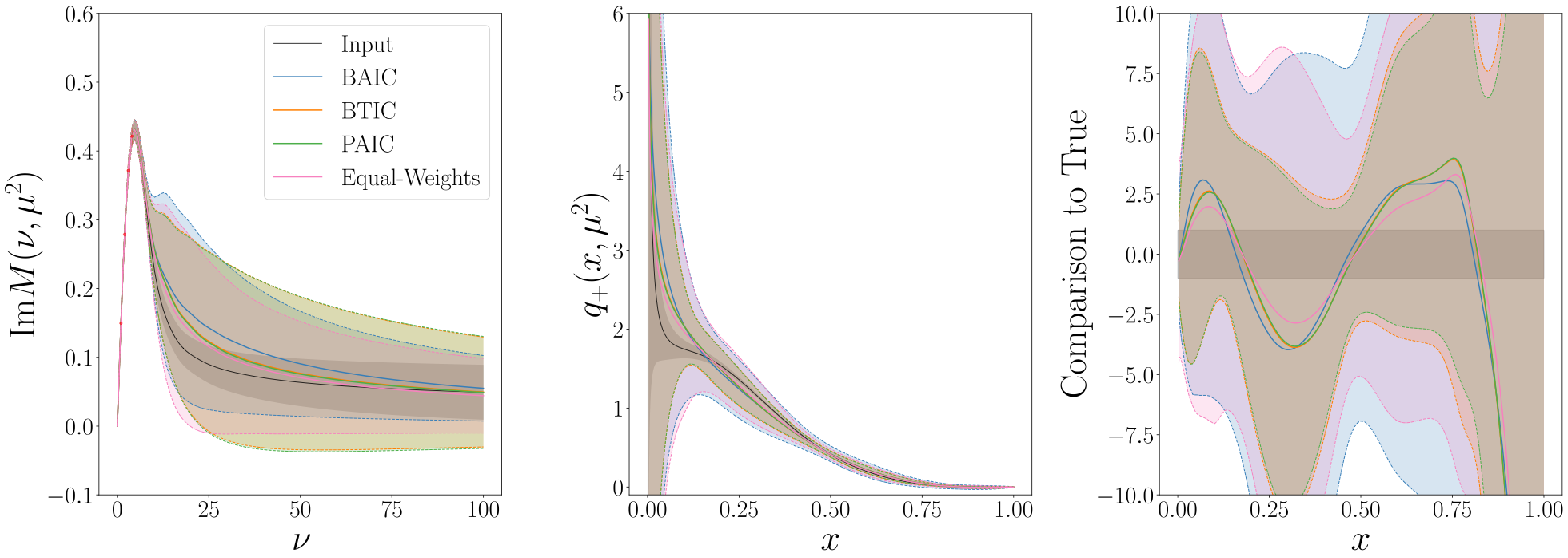




3rd Level of inference

Results

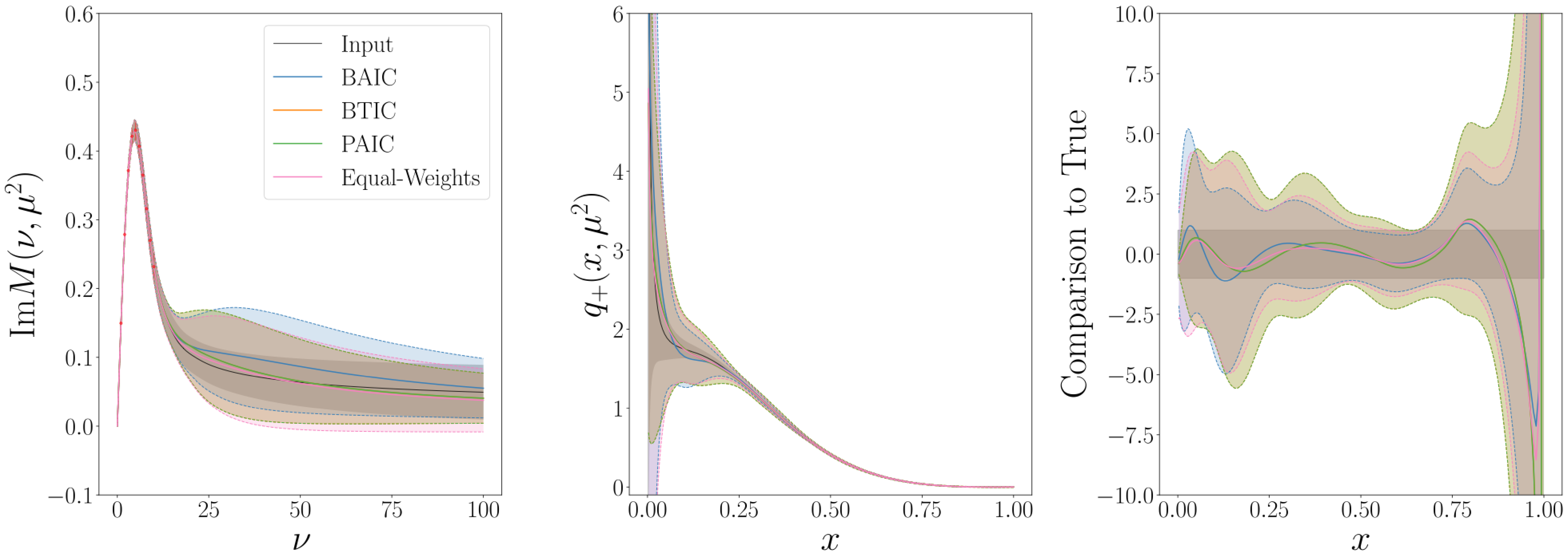
$$P(\mathcal{H}_i|M^l) = \frac{P(M^l|\mathcal{H}_i)P(\mathcal{H}_i)}{P(M^l)}$$



3^{rd} Level of inference

Results

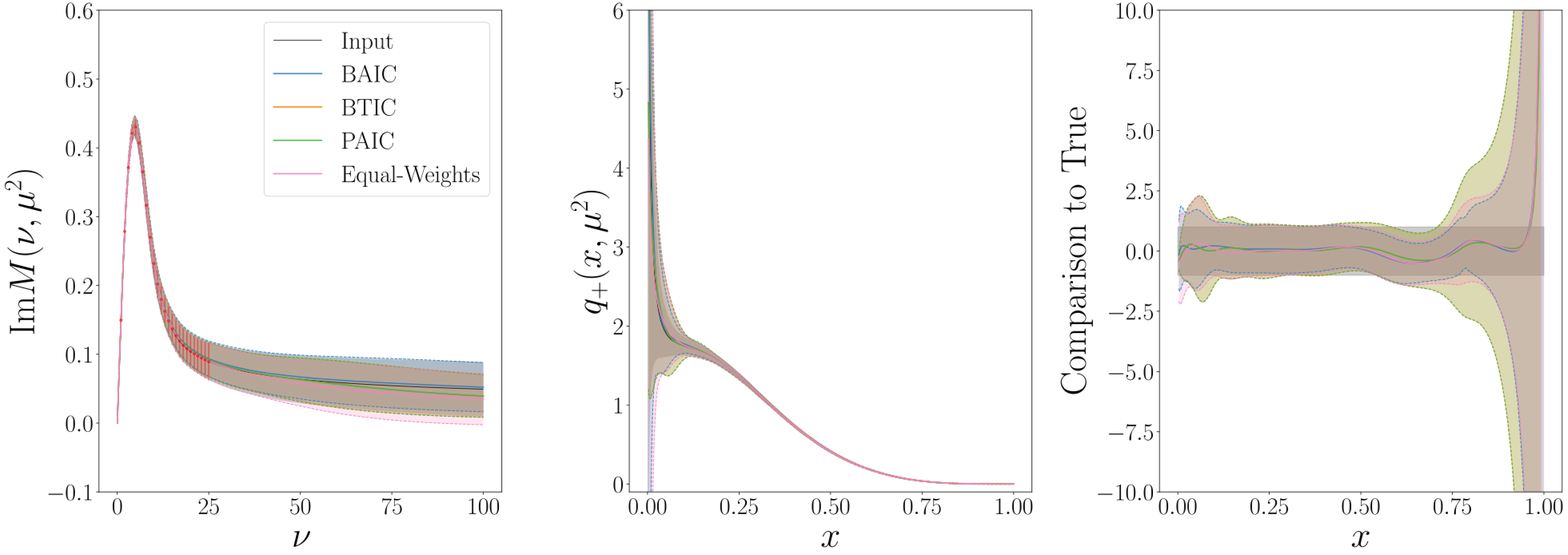
$$P(\mathcal{H}_i|M^l) = \frac{P(M^l|\mathcal{H}_i)P(\mathcal{H}_i)}{P(M^l)}$$



3rd Level of inference

Results

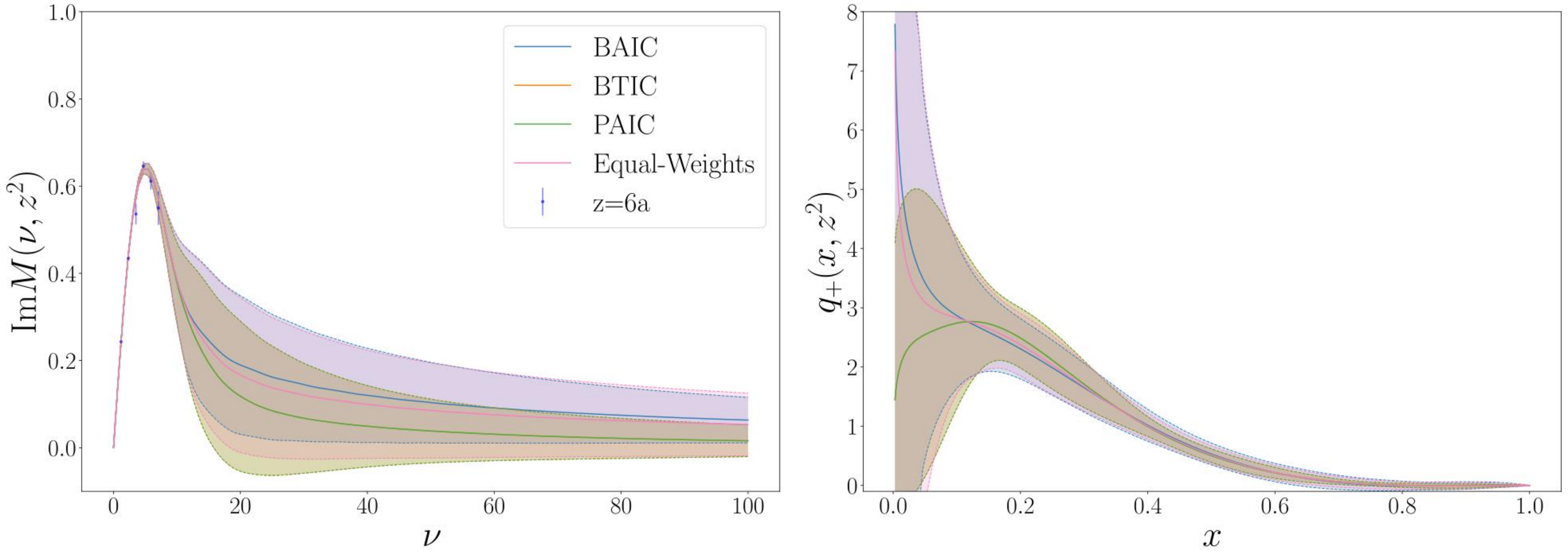
$$P(\mathcal{H}_i|M^l) = \frac{P(M^l|\mathcal{H}_i)P(\mathcal{H}_i)}{P(M^l)}$$

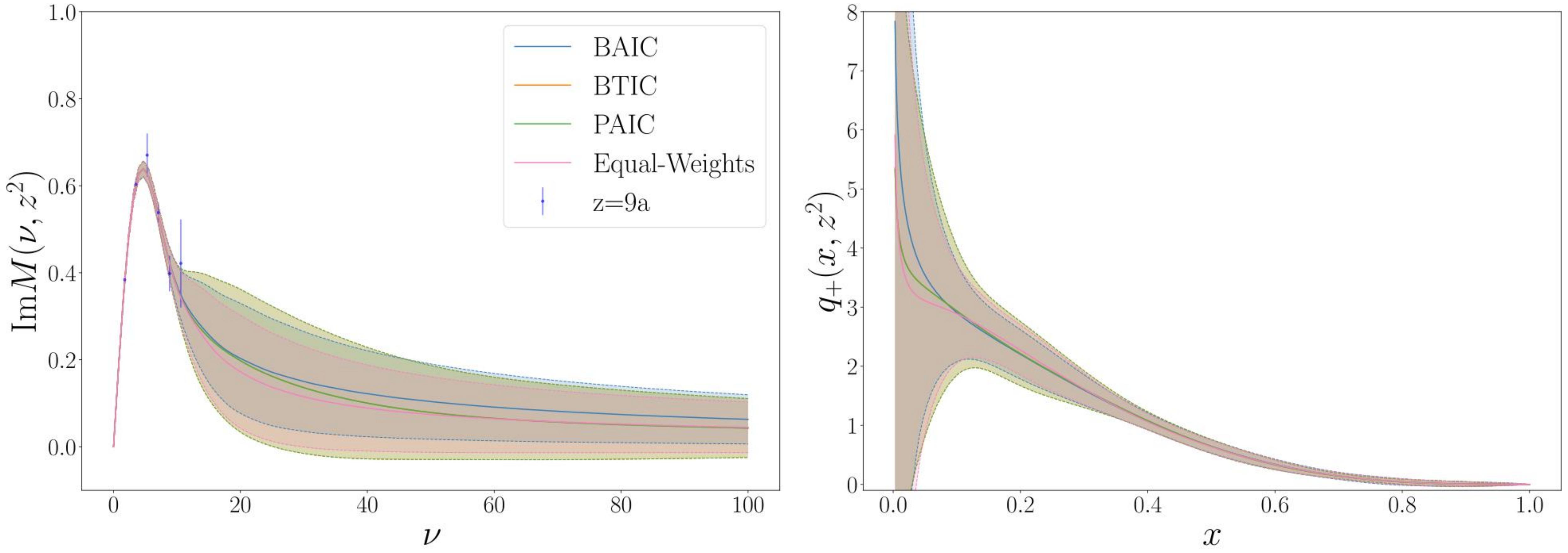


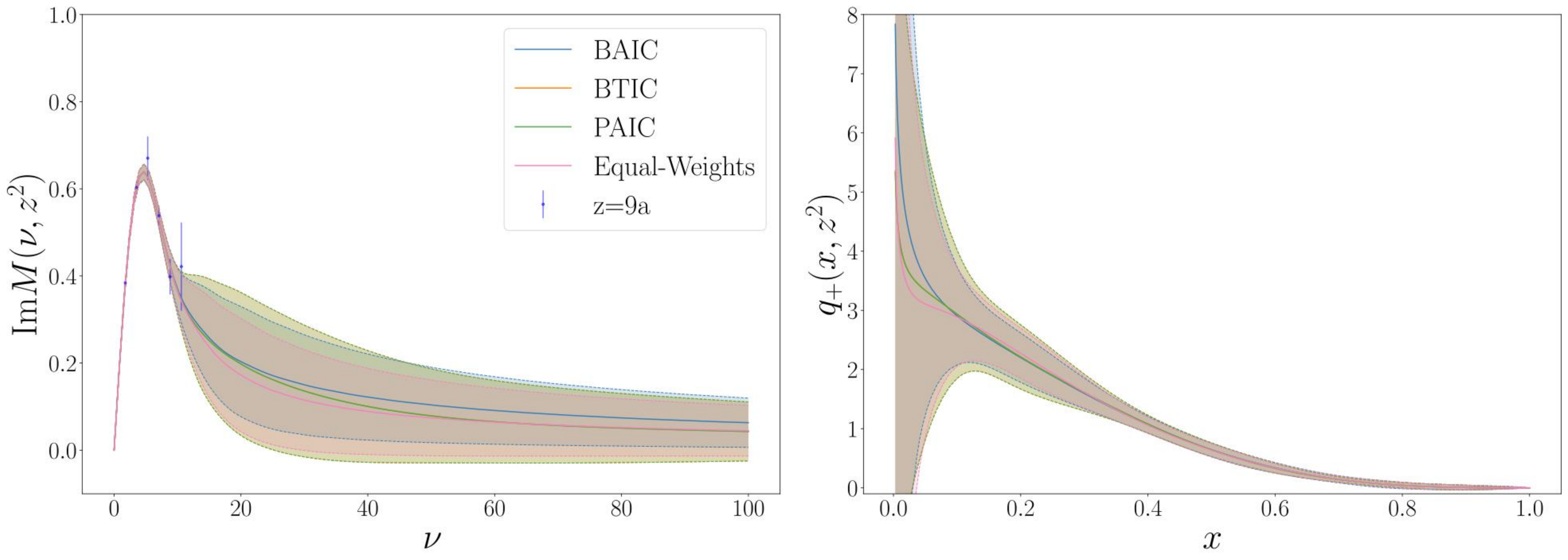
3rd Level of inference

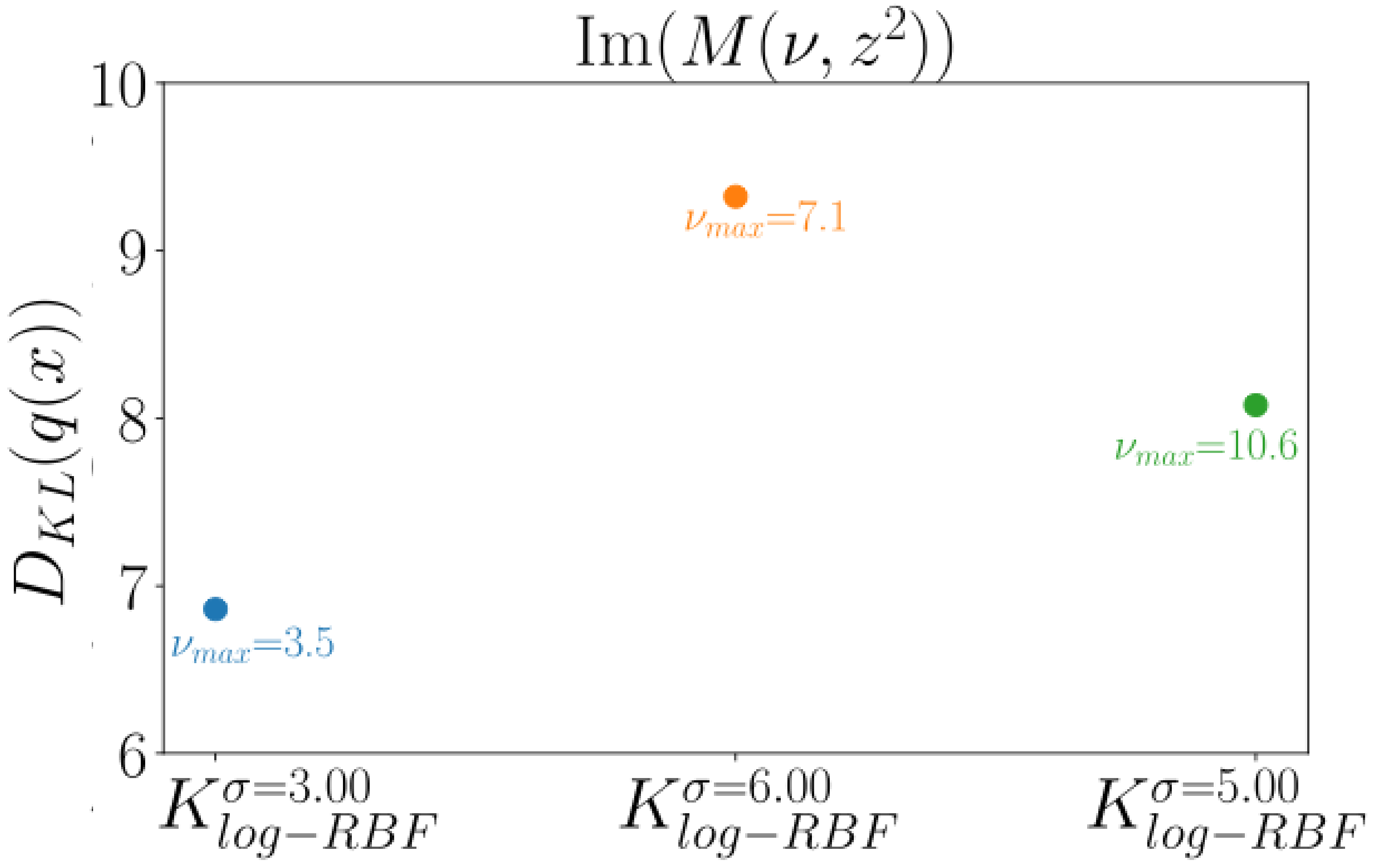
$$P(\mathcal{H}_i|M^l) = \frac{P(M^l|\mathcal{H}_i)P(\mathcal{H}_i)}{P(M^l)}$$

Lattice data (6 data points)





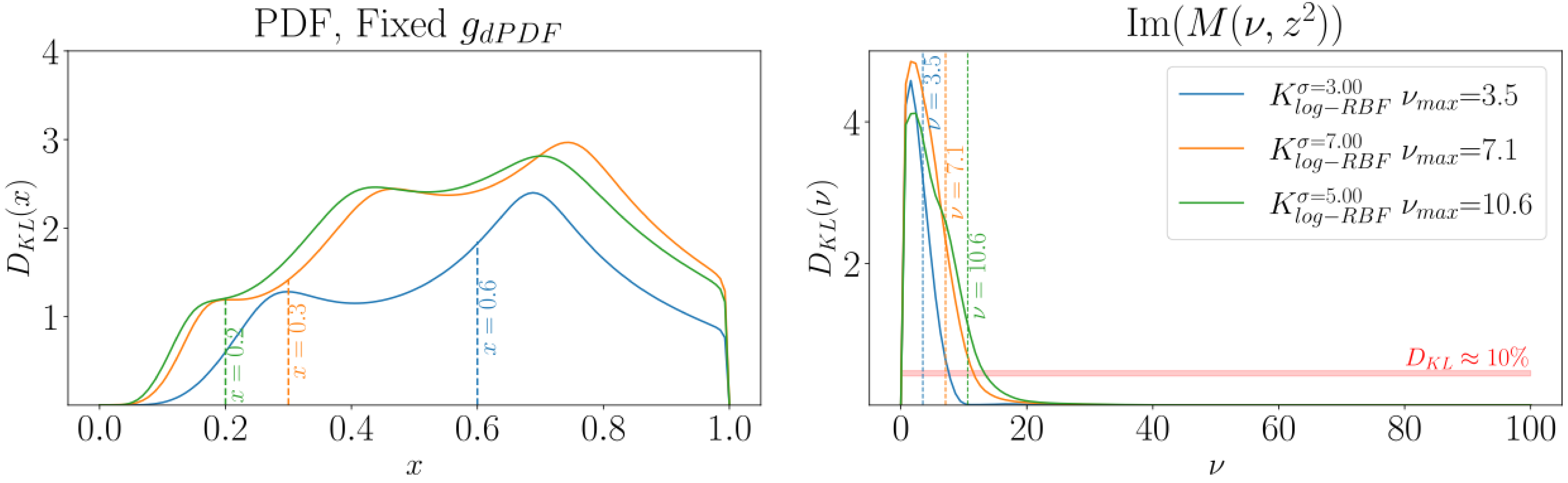




3rd Level of inference

KL divergence

$$P(\mathcal{H}_i|M^l) = \frac{P(M^l|\mathcal{H}_i)P(\mathcal{H}_i)}{P(M^l)}$$



Conclusions

Key points

- GP provides a systematic and flexible way to regulate the inverse problem
- Synthetic tests evaluate the reconstructed uncertainty bands.
- KL divergence shows information gained from synthetic and lattice data globally and locally.
- Results remain stable under changes in kernels, mean functions, and hyperparameters through model averaging.
- GPR reduces model bias and shows a transparent uncertainty quantification

Thanks!

yacahuanamedra@wm.edu

Back-up slides

Kernels and Models

Some equations…

$$K_{f-\mathrm{RBF}}(x,x';\theta=\{\sigma,l^2\}) = \sigma \exp\left(-\frac{||f(x)-f(x')||^2}{2l^2}\right),$$

$$K_{plog-1}(x,x') = \sigma \sum_{n=1}^{\infty}(1-x)^n(1-x')^n = \sigma\frac{(1-x)(1-x')}{1-(1-x)(1-x')}.$$

$$K_{plog-2}(x,x') = \sigma \sum_{n=1}^{\infty}\frac{(1-x)^n(1-x')^n}{n} = -\sigma\log\big(1-(1-x)(1-x')\big).$$

$$K_{\mathrm{combined}}\Big(x,x';\theta=\{\theta_1,\theta_2,s,x_0\}\Big) = \sigma(x;s,x_0)K_1\Big(x,x';\theta_1\Big)\sigma(x';s,x_0)+$$
$$(1-\sigma(x;s,x_0))K_2\Big(x,x';\theta_2\Big)(1-\sigma(x';s,x_0))$$

$$g_{\mathrm{flat}}(x;\theta=\{N\}) = N \quad ; \qquad g_{\mathrm{PDF}}(x;\theta=\{N,\alpha,\beta\}) = Nx^{\alpha}(1-x)^{\beta}$$

Introduce Mellin moments

Constraints in the 1st level

$$P_{const} = e^{-\frac{1}{2\lambda}\left(\int_0^1 dx q(x) - 1\right)^2 - \frac{1}{2\lambda_c}\left(\int_0^1 dx q(x) \delta(1-x)\right)^2}$$

$$P_{Mellin} = P_{const} e^{-\frac{1}{2\lambda_n}\left(\int_0^1 dx q(x) x^{n-1} - b_n\right)^2}$$

In this case…

$$b_n^{lattice} = b_n \pm \delta b_n$$

$$\lambda_n = \frac{1}{\delta b_n}$$

The equivalence of data points in the x space has been already implemented before, we just have to generalize it.

1st level of inference

Important results

$$P(q(x)|M^l,\theta,\mathcal{H}) = \frac{P(M^l|q(x),\theta,\mathcal{H})P(q(x)|\theta,\mathcal{H})}{P(M^l|\theta,\mathcal{H})}$$

$$\overline{q}(x;\theta) = \int q(x)P(q(x)|M^l,\theta,\mathcal{H})D[q(x)]$$

Mean of the Posterior

$$\overline{q}(x;\theta) = q_{PDF}(x) + K \cdot B^{\perp}[C + BKB^{\perp}](M^l - B^l \cdot q_{PDF})$$

$$\overline{q(x)q(x)} = \int q(x)q(x)P(q(x)|M^l,\theta,\mathcal{H})D[q(x)]$$

Covariance of the Posterior

$$H(\theta) \equiv \overline{q(x)q(x')} = K(x,x') - KB^{\perp}[C + BKB^{\perp}]^{-1}BK$$

Effective evidence

$$E(\theta) \equiv -\log(P(M^l|\theta,\mathcal{H})) = \frac{1}{2}(M_i - Bq_{PDF})^{\perp}(C + BKB^{\perp})^{-1}(M_i - Bq_{PDF}) + \frac{1}{2}\log[det(C + BKB^{\perp})] + \frac{N_x}{2}\log(2\pi$$

2nd level of inference

Kernel and Mean functions

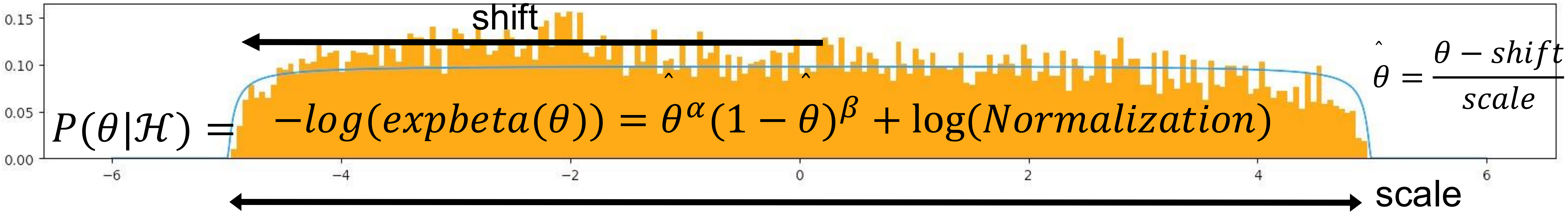
$$P(\theta|M^l,\mathcal{H}) = \frac{P(M^l|\theta,\mathcal{H})P(\theta|\mathcal{H})}{P(M^l|\mathcal{H})}$$

Where does this hyperparameter come from?

$$q_{PDF}(x) = Nx^{\alpha}(1-x)^{\beta} \quad + \quad K_{rbf}(x,x') = \sigma^2 e^{-\frac{|x-x'|^2}{2l^2}} \rightarrow \theta = \{N,\alpha,\beta,\sigma,l\}$$

How should we define the prior?

$$P(\theta|\mathcal{H}) = \{Normal(\theta), lognormal(\theta), expbeta(\theta)\}$$



$$P(\theta|\mathcal{H}) = -log(expbeta(\theta)) = \hat{\theta}^{\alpha}(1-\hat{\theta})^{\beta} + \log(Normalization)$$

$$\hat{\theta} = \frac{\theta - shift}{scale}$$

We use HMC/Important Sampling to obtain the posterior

$$P(M^l|\mathcal{H}) = \int d\theta P(M^l|\theta,\mathcal{H})P(\theta|\mathcal{H})$$

No functional variables anymore, we have to integrate over hyperparameters.

2nd level of inference

Important results

$$P(\theta|M^l,\mathcal{H}) = \frac{P(M^l|\theta,\mathcal{H})P(\theta|\mathcal{H})}{P(M^l|\mathcal{H})}$$

Mean of the Posterior

$$< q(x) >= \int P(\theta|M^l,\mathcal{H})\overline{q}(x;\theta)d\theta \qquad < q(x) >= \frac{\int e^{-E(\theta)}\overline{q}(x;\theta)d\theta}{\int e^{-E(\theta)}d\theta}$$

Covariance of the Posterior

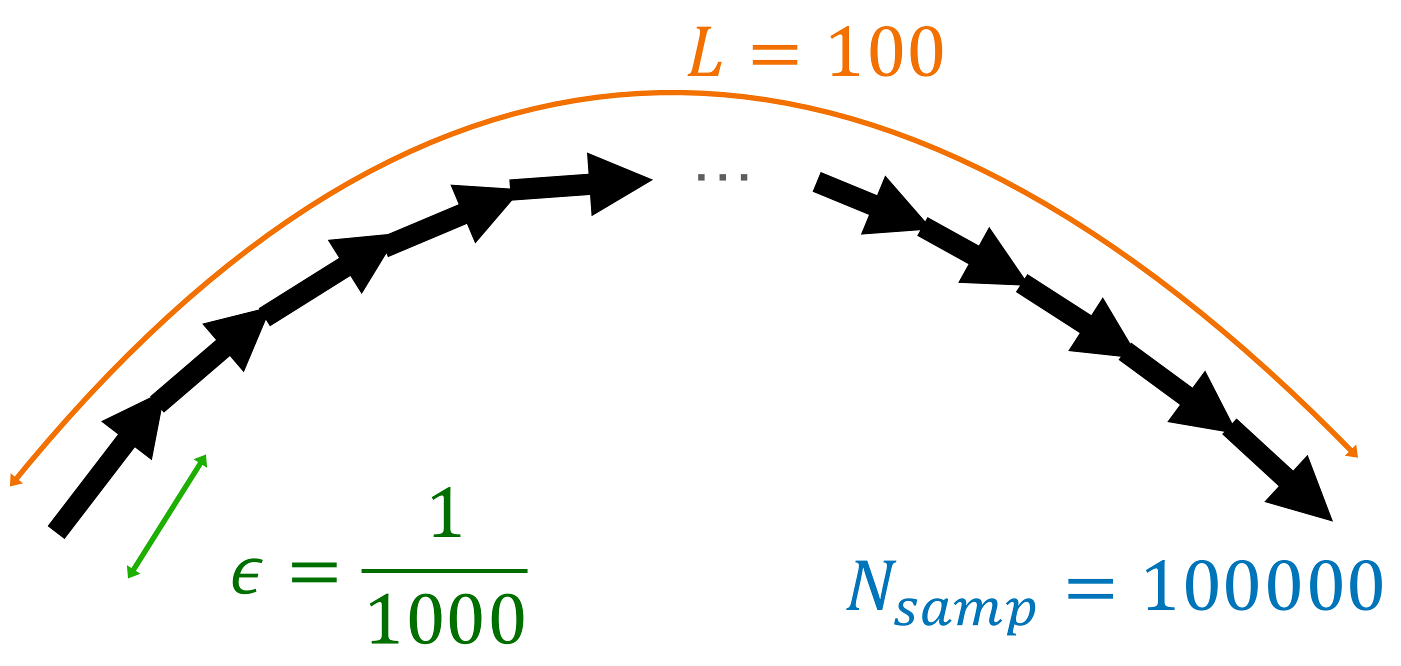
$$< q(x)q(x) >\equiv \int (\overline{q}(x;\theta) -< q(x) >)^2 P(\theta,|M^l,\mathcal{H})d\theta$$

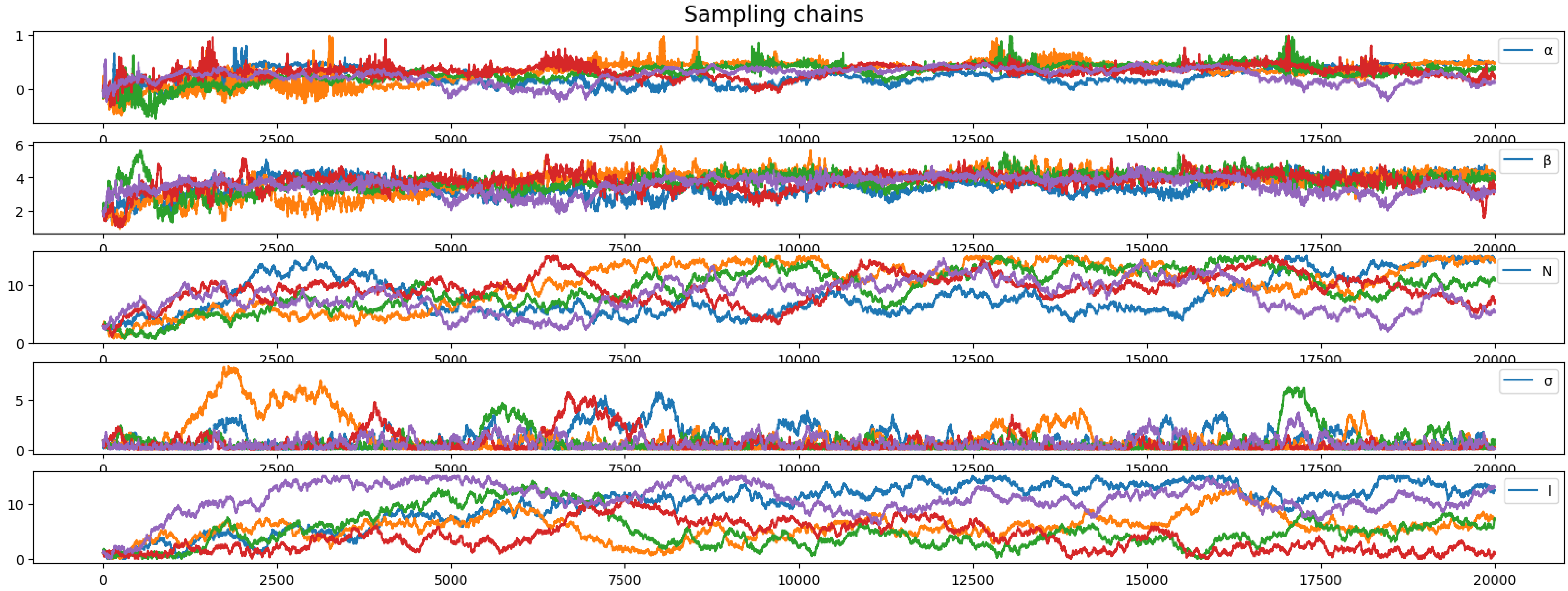
$$< q(x)q(x) >= \frac{\int e^{-E(\theta)}[H(\theta) + (\overline{q}(x;\theta) -< q(x) >)^2]P(\theta|\mathcal{H})d\theta}{\int e^{-E(\theta)}P(\theta|\mathcal{H})d\theta}$$

Hybrid Monte Carlo

Kernel and Mean functions

How does hyper parameters sampling looks like?





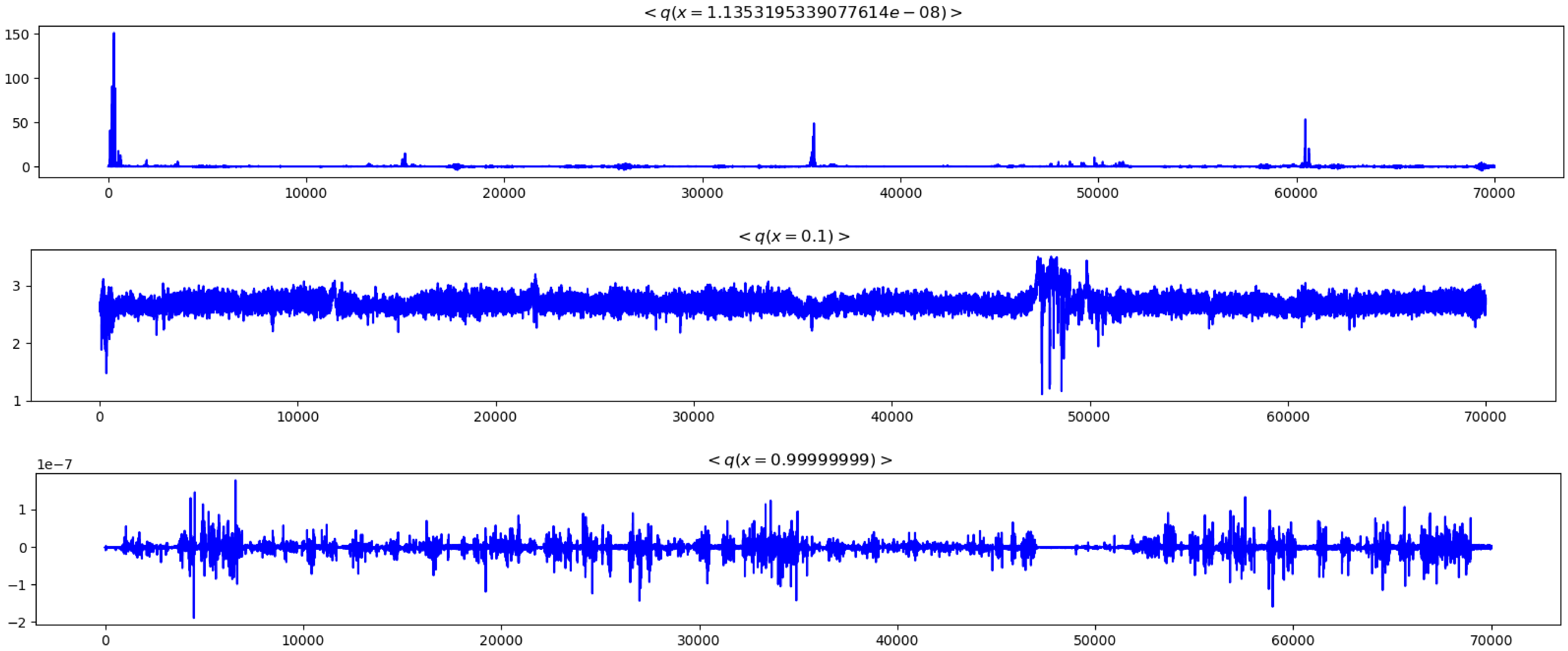
HMC observables

Kernel and Mean functions

$$P(\theta|M^l,\mathcal{H}) = \frac{P(M^l|\theta,\mathcal{H})P(\theta|\mathcal{H})}{P(M^l|\mathcal{H})}$$

How does <q(x)>, <q(x)q(x')> sampling looks like

$$< q(x) > \int d\theta P(\theta|M^l,\mathcal{H})\overline{q}(x)$$

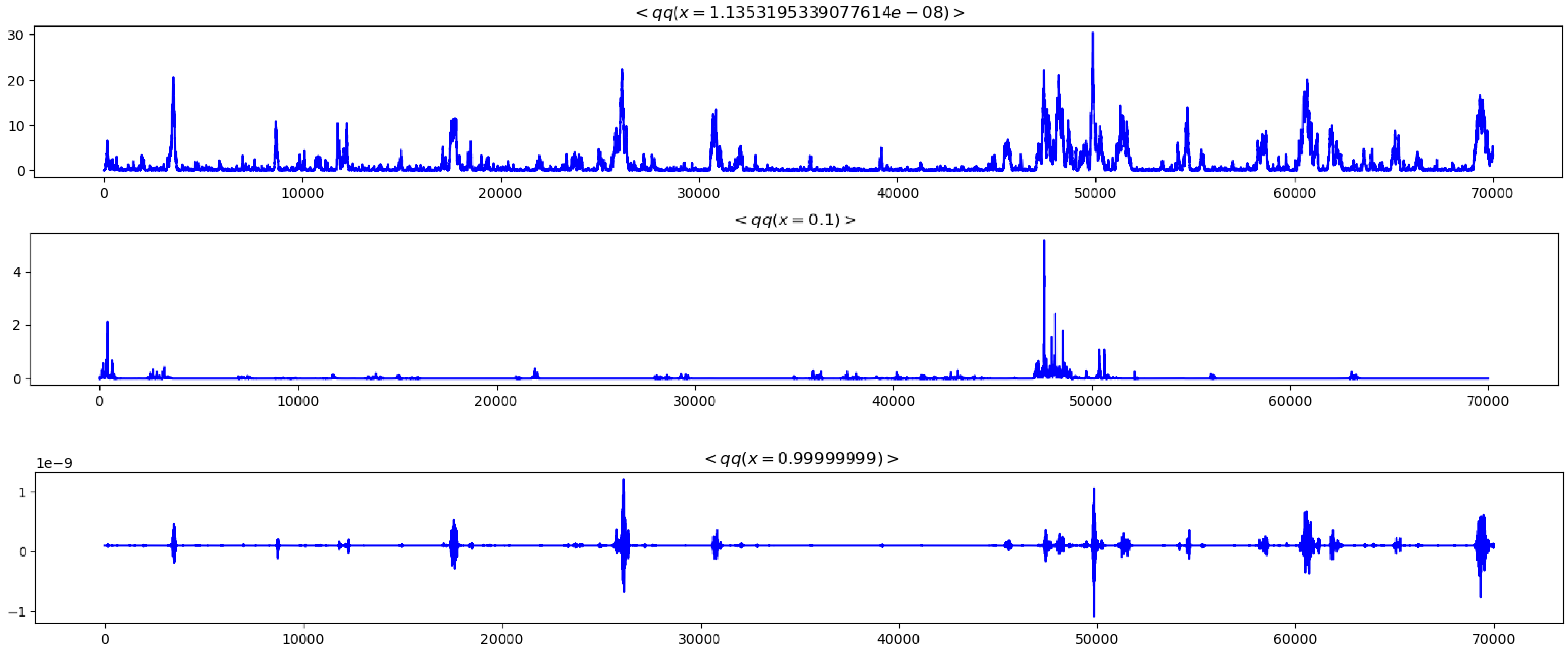


HMC observables

Kernel and Mean functions

$$P(\theta|M^l,\mathcal{H}) = \frac{P(M^l|\theta,\mathcal{H})P(\theta|\mathcal{H})}{P(M^l|\mathcal{H})}$$

How does <q(x)>, <q(x)q(x')> sampling looks like?

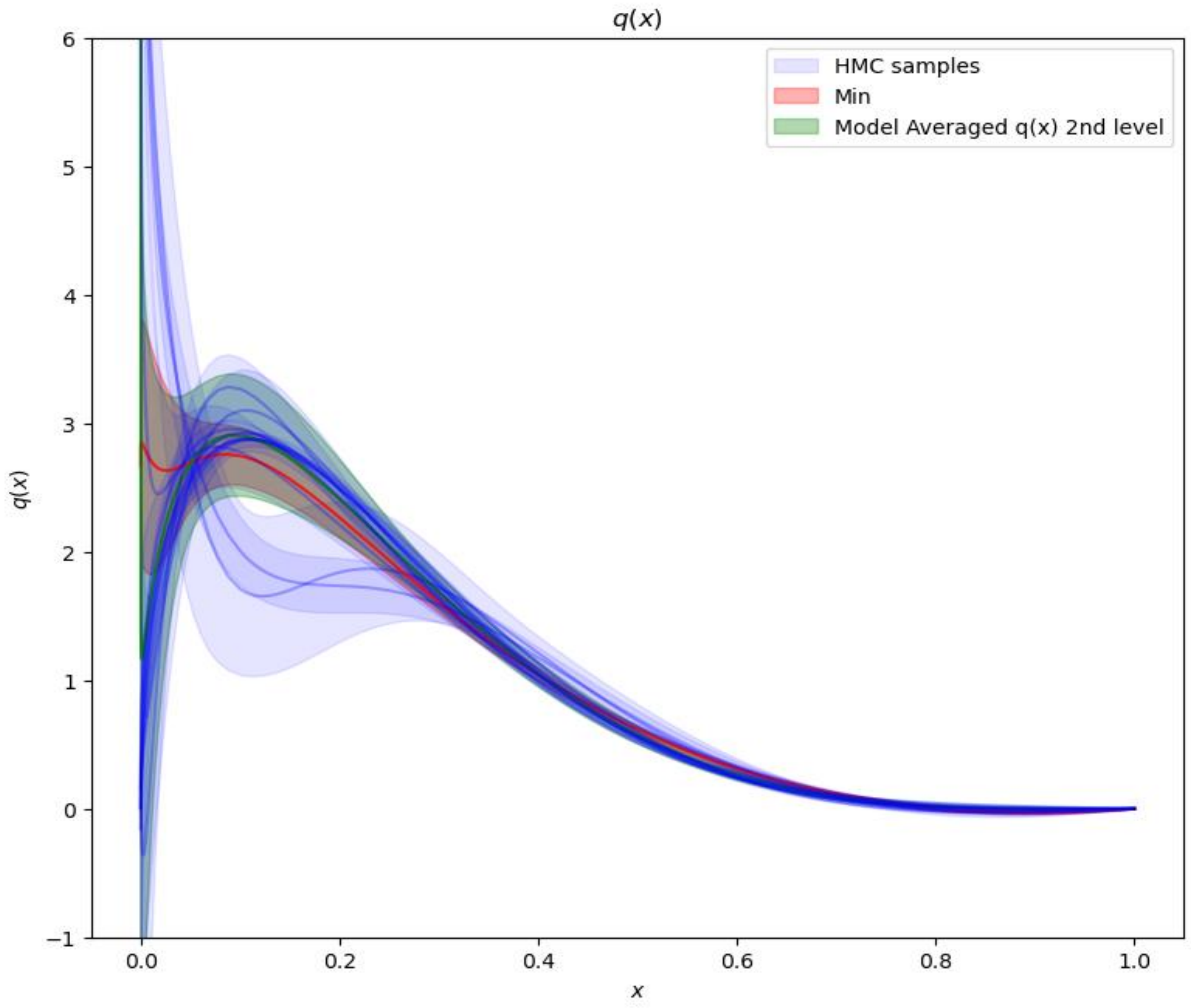


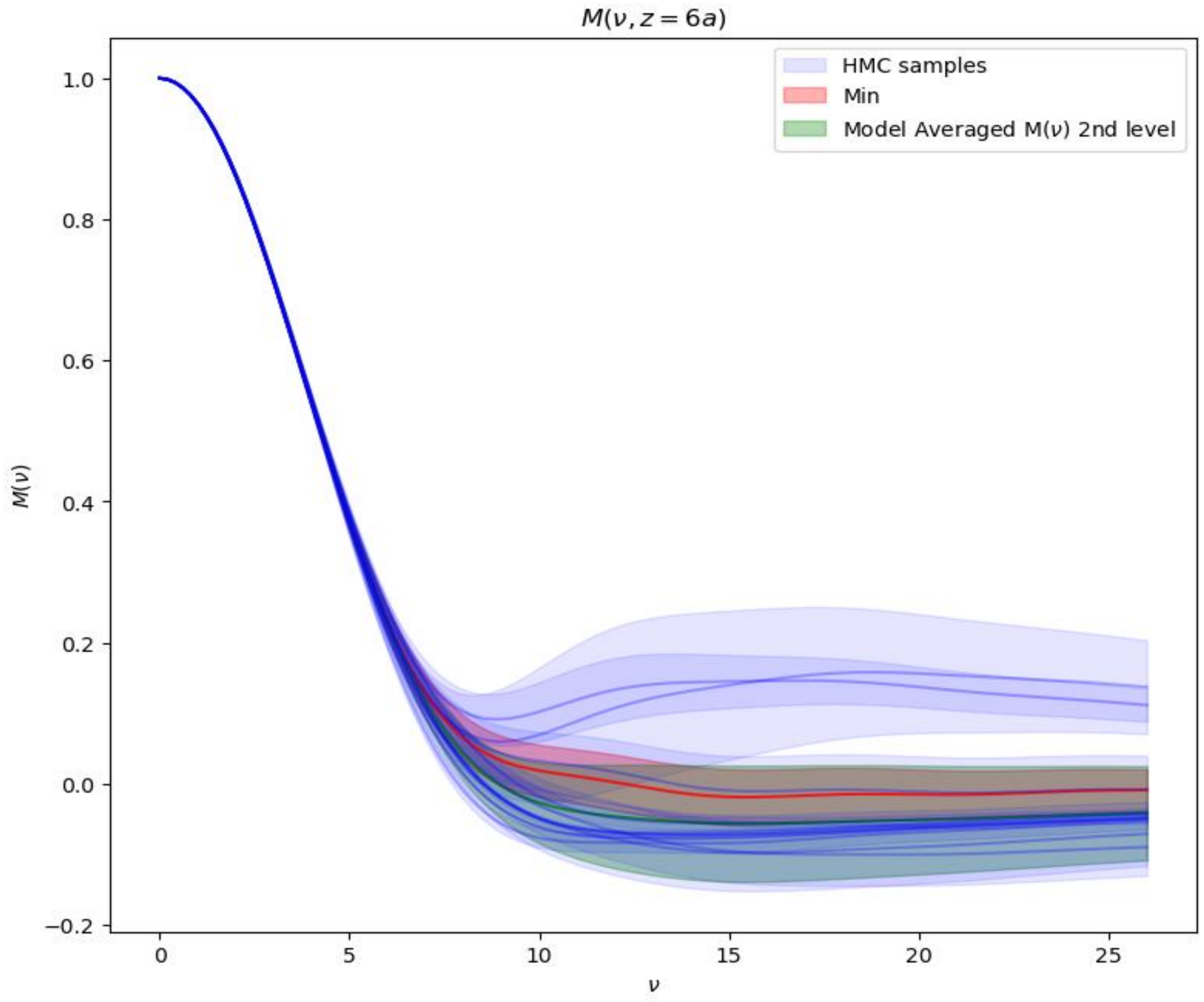
2nd level of inference

Model averaged results

$$P(\theta|M^l,\mathcal{H}) = \frac{P(M^l|\theta,\mathcal{H})P(\theta|\mathcal{H})}{P(M^l|\mathcal{H})}$$

How does <q(x)>, <q(x)q(x’)> sampling looks like?





3rd level of inference

Important results

$$P(\mathcal{H}_i|M^l) = \frac{P(M^l|\mathcal{H}_i)P(\mathcal{H}_i)}{P(M^l)}$$

Mean of the Posterior

$$\mathrm{q}(x) \equiv \sum_i^{models} P(\mathcal{H}_i|M^l) < q(x) >_i$$

$$\mathrm{q}(x) = \frac{\sum_i^{Models} e^{\frac{\Delta IC}{2}} < q(x) >_i}{\sum_i^{Models} e^{\frac{\Delta IC}{2}}}$$

Covariance of the Posterior

$$\mathrm{q}(x)\mathrm{q}(x) \equiv \sum P(\mathcal{H}_i|M^l)[< q(x) >_i - \mathrm{q}(x)]^2$$

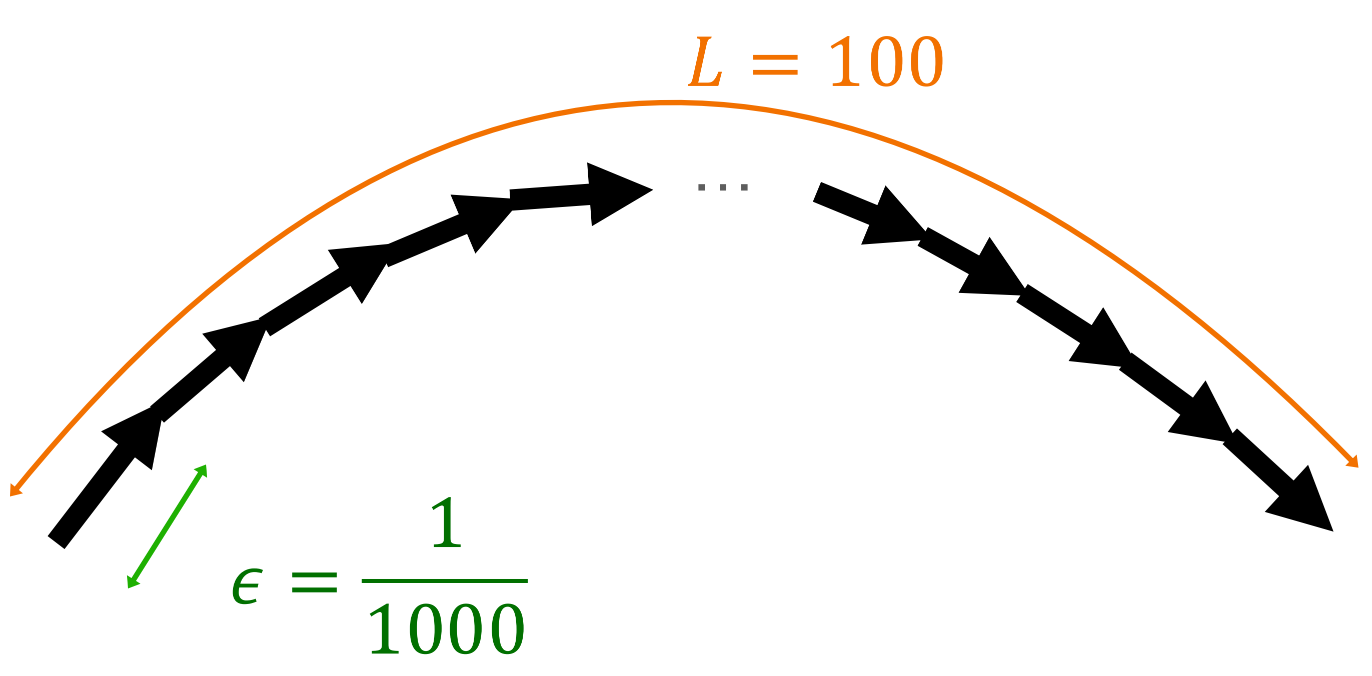
$$\mathrm{q}(x)\mathrm{q}(x) \equiv \frac{\sum_i^{Models} e^{\frac{\Delta IC}{2}} [< q(x)q(x) >_i + (< q(x) >_i - \mathrm{q}(x))^2]}{\sum_i^{Models} e^{\frac{\Delta IC}{2}}}$$

Hybrid Monte Carlo

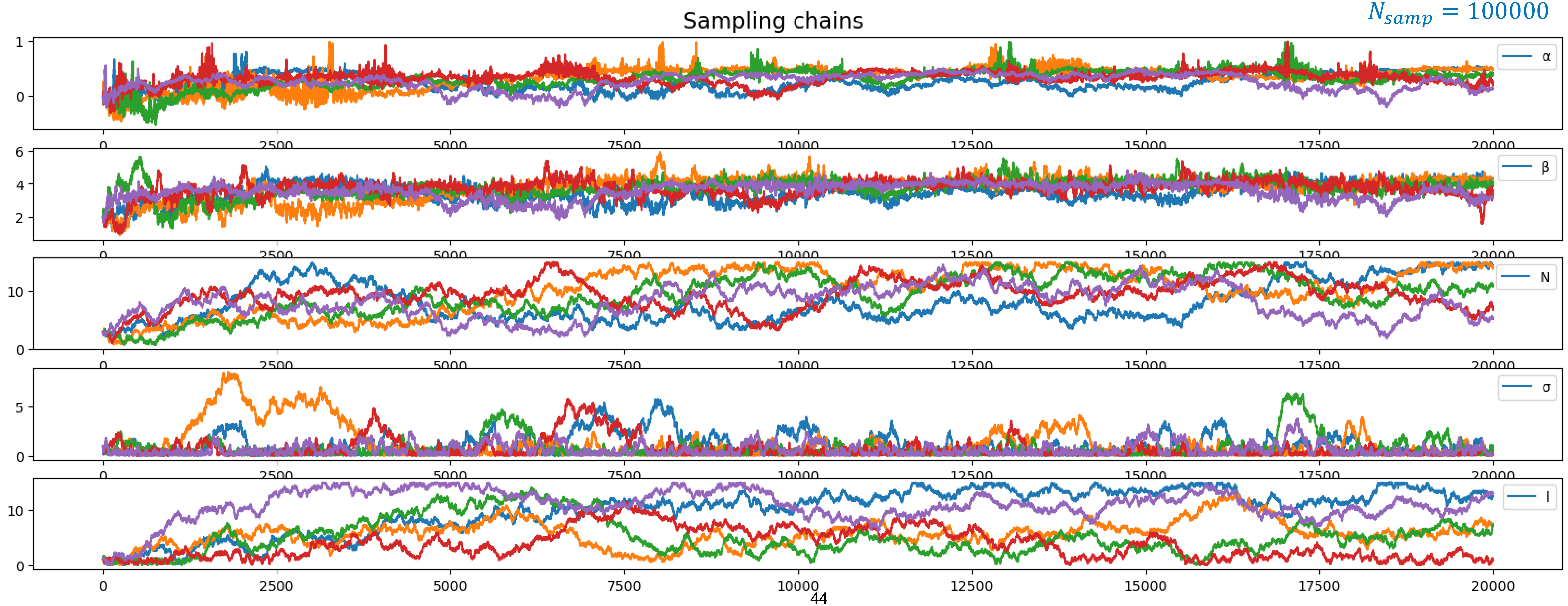
Sampling procedure

Skip 20 trajectories, 12 hours
(5 independent chains) —>

$\tau \approx 100 - 500$



$N_{samp} = 100000$



3rd level of inference

Counting Models

How many models do we actually explore?

$$P(\mathcal{H}_i|M^l) = \frac{P(M^l|\mathcal{H}_i)P(\mathcal{H}_i)}{P(M^l)}$$

Kernel

Mean

Grid in x

Sampling

$q_{PDF}(x)$

$q_{flat}(x) = N$

$K_{rbf}(x,x')$

$K_{debbio}(x,x')$

$K_{logrbf}(x,x')$

$K_{poly}(x,x')$

$K_{comb}(x,x')$

Linear

Log/Lin

mean

kernel

all

About 20-30 models, and we give equal prior factors $P(\mathcal{H}_i) = \frac{1}{N_{Models}}$

Bayesian approach

Bayes' Theorem (not that easy)

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

- How can we work with multiple conditions?

$$P(A|B,C,D) = ? \qquad P(A|B,C) = ?$$

- For now we can work with 2 conditions instead of 3

$$P(A,B|C) = P(A|B,C)P(B|C)$$

Textbook property

$$P(A,B) = P(B,A)$$

$$P(A|B,C) = \frac{P(A,B|C)}{P(B|C)} = \frac{P(B,A|C)}{P(B|C)} = \frac{P(B|A,C)P(A|C)}{P(B|C)}$$

$$C \rightarrow C,D$$

$$P(A|B,C,D) = \frac{P(B|A,C,D)P(A|C,D)}{P(B|C,D)}$$

2nd level of inference

Important results

$$P(\theta|M^l,\mathcal{H}) = \frac{P(M^l|\theta,\mathcal{H})P(\theta|\mathcal{H})}{P(M^l|\mathcal{H})}$$

Mean of the Posterior

$$< q(x) >= \int P(\theta|M^l,\mathcal{H})\overline{q}(x;\theta)d\theta \qquad < q(x) >= \frac{\int e^{-E(\theta)}\overline{q}(x;\theta)d\theta}{\int e^{-E(\theta)}d\theta}$$

Covariance of the Posterior

$$< (\overline{q}(x;\theta) -< q(x) >)^2 >= \int (\overline{q}(x;\theta) -< q(x) >)^2 P(\theta,|M^l,\mathcal{H})d\theta$$

$$< (\overline{q}(x;\theta) -< q(x) >)^2 >= \frac{\int e^{-E(\theta)}(\overline{q}(x;\theta) -< q(x) >)^2 P(\theta|\mathcal{H})d\theta}{\int e^{-E(\theta)}P(\theta|\mathcal{H})d\theta}$$