Combination of Bayesian Inference with Truncated Partial-Wave Analysis (TPWA)

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Motivation

Classification

Polarization observables

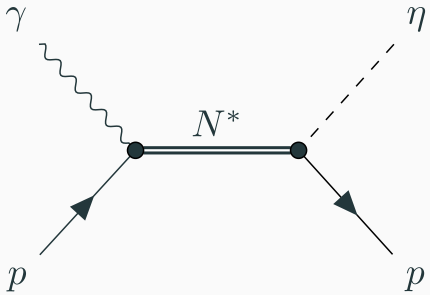
(Truncated) partial-wave analysis

Electromagnetic multipoles

Resonance parameters

Physical motivation

- model-independent approach
- estimation of multipole parameters
- prediction of yet unmeasured polarization observables



[Chew et al., 1957]

$$\hat{T} \overset{\mathrm{CMF}}{:=} \sum_{i=1}^{4} \boldsymbol{a}_i \cdot \mathcal{F}_i(W,\theta)$$

- $\hat{T}$: transition operator
- $\boldsymbol{a}_i$: spin-matrix
- $\mathcal{F}_i(W,\theta)$: complex spin amplitude

$$\mathcal{F}_i(W,\theta) \propto \sum_{\ell}^{\infty} h_i(\ell, M(W)) \times g_i(\theta)$$

$\Rightarrow$ Truncated Partial-Wave Analysis: $\sum_{\ell}^{\infty} \longrightarrow \sum_{\ell}^{\ell_{\mathrm{max}}}$

ℓ: angular momentum

ℓ_{max}: maximal angular momentum

$M(W)$: multipole parameters

(W, θ): CMF-(total energy, scattering angle)

Utilized polarization observables ($\gamma p \rightarrow \eta p$)

Complete set: $\sigma_0, T, F, \Sigma, E, G$

Observable	Number of data points	E_γ^{lab} / MeV	$\cos(\theta)$	Facility	References
σ_0	5736	$[723, 1571]$	$[-0.958, 0.958]$	MAMI	Kashevarov et al. [Kashevarov et al., 2017]
T, F	144	$[725, 1350]$	$[-0.917, 0.917]$	MAMI	Akondi et al. [Akondi et al., 2014]
Σ	140	$[724, 1472]$	$[-0.946, 0.815]$	GRAAL	Bartalini et al. [Bartalini et al., 2007]
E	84	$[750, 1350]$	$[-0.917, 0.917]$	MAMI	Afzal et al. [Afzal, 2019, obs,]
G	47	$[750, 1250]$	$[-0.889, 0.667]$	CBELSA/TAPS	Müller et al. [Müller et al., 2020]

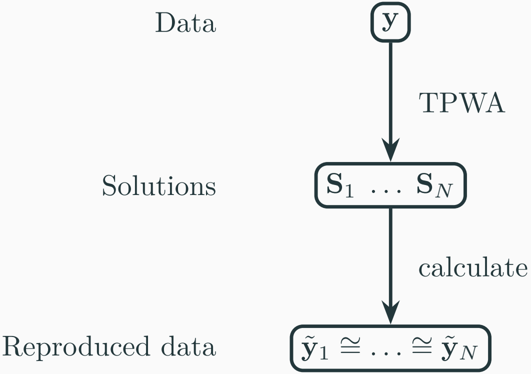
Fits @ $E_\gamma^{\text{lab}} = [750,\ 850,\ 950,\ 1050,\ 1150,\ 1250]$ MeV

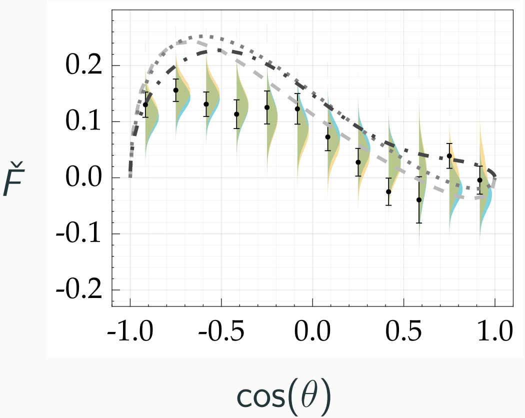
Bayes theorem

$$\underbrace{p(\mathbf{model} \mid \mathbf{data})}_{\text{posterior}} \propto \underbrace{p(\mathbf{data} \mid \mathbf{model})}_{\text{likelihood}} \times \underbrace{p(\mathbf{model})}_{\text{prior}}$$

- everything is a distribution
- integration instead of differentiation
- unprecedented uncertainty estimation
- marginal parameter distributions rather than point estimates

Accidental discrete ambiguities



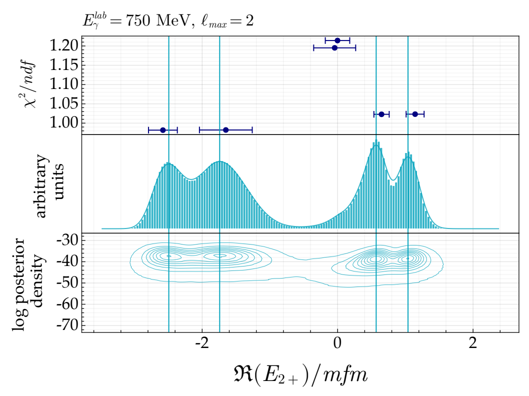


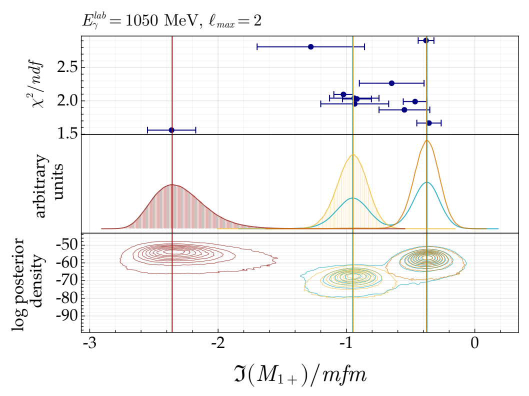
(dashed line) EtaMAID2018
[Tiator et al., 2018]

(dotted line) BnGa-2019
[Müller et al., 2020]

(dash-dotted line) JüBo-2022
[Rönchen et al., 2022]

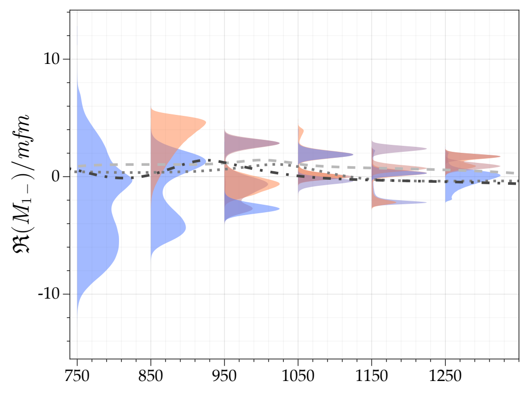
Electromagnetic multipoles



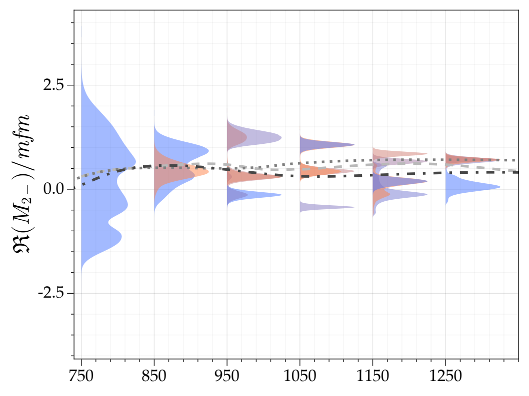


Multipoles vs. energy

- color coding: orange (less relevant) ⟶ blue (more relevant)



E_γ^{lab} / MeV



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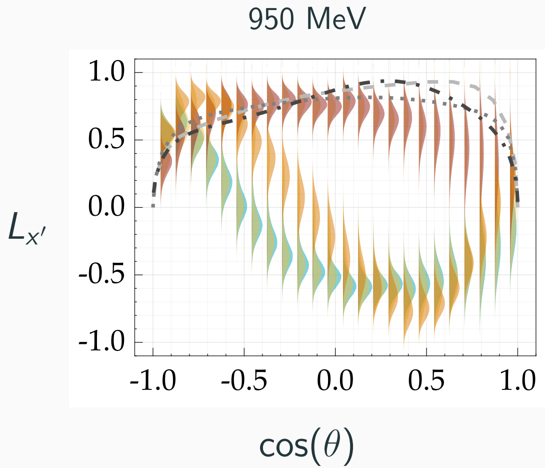
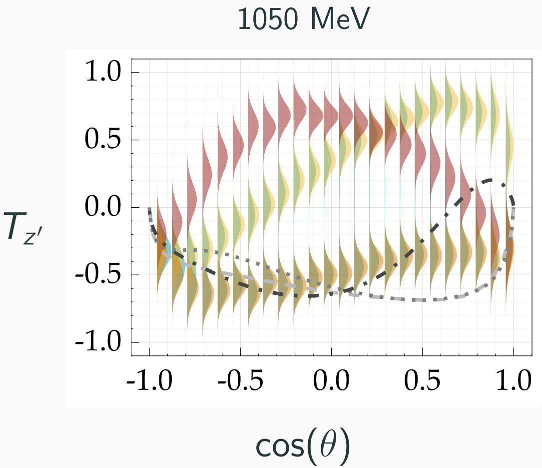
Predicted data distributions





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[Rönchen et al., 2022]

Promising future measurements

- candidates to resolve the ambiguities for truncation order $\ell_{\text{max}} = 2$

E_{γ}^{lab} / MeV	Observables
750	$C_{z'}$, $C_{x'}$, $L_{x'}$, $L_{z'}$
850	$C_{z'}$, $C_{x'}$, $L_{x'}$, $L_{z'}$, $T_{x'}$, $T_{z'}$
950	$C_{z'}$, $C_{x'}$, $L_{x'}$, $L_{z'}$, $T_{z'}$
1050	$C_{z'}$, $C_{x'}$, $L_{x'}$, $O_{z'}$, $T_{z'}$
1150	$C_{z'}$, $O_{x'}$, $T_{x'}$, $T_{z'}$
1250	$C_{z'}$

Conclusion and outlook

Conclusion

- applied novel analysis technique to TPWA
- point estimates $\longrightarrow$ distributions
- model-independent:
  - estimation of electromagnetic multipole parameters
  - predictions for yet unmeasured polarization observables
- determination of promising future measurements

Outlook

- utilize priors to reduce ambiguities
- utilize priors to stabilize regression for $\ell_{\mathsf{max}} > 2$

1. Thank you for your attention!

2. Backup-Slides

[Wunderlich et al., 2017, Wunderlich, 2019]

Polarisation observables

$$\check{\Omega}^{\alpha}_{\text{theo}}(W,\theta) = \rho \sum_{k=\beta_\alpha}^{2\ell_{\text{max}}+\beta_\alpha+\gamma_\alpha} \mathcal{A}^{\alpha}_{k}(W)\, P^{\beta_\alpha}_{k}(\cos\theta) \quad (1)$$

Bilinear product

$$\mathcal{A}^{\alpha}_{k}(W) = \boldsymbol{M}^{\dagger}(W)\cdot \boldsymbol{\mathcal{C}}^{\alpha}_{k} \cdot \boldsymbol{M}(W) \quad (2)$$

Multipole vector (model parameters)

$$\boldsymbol{M}(W) = [E_{0+}, E_{1+}, M_{1+}, M_{1-}, E_{2+}, E_{2-}, M_{2+}, M_{2-}, \ldots] \quad (3)$$

Electromagnetic multipoles

- direct quote from page 1347 of the paper [Chew et al., 1957]:

"The energy-dependent amplitudes $M_{\ell\pm}$ and $E_{\ell\pm}$ refer to transitions initiated by magnetic and electric radiation, respectively, leading to final states of orbital angular momentum ℓ and total angular momentum $\ell \pm \frac{1}{2}$."

Origin is bilinear product

$$\check{\Omega}^{\alpha}(W,\theta) = \kappa \cdot \boldsymbol{b}^{\dagger}(W,\theta)\, \boldsymbol{\Gamma}^{\alpha}\, \boldsymbol{b}(W,\theta) \tag{4}$$

[Chiang and Tabakin, 1997, Pichowsky et al., 1996, Kroenert et al., 2021]

Suppose transformation T

$$b_i(W,\theta) \xrightarrow{T} \tilde{b}_i(W,\theta) \tag{5}$$

The Problem

$$\{\check{\Omega}^{\alpha_1}, \ldots, \check{\Omega}^{\alpha_n}\} \longrightarrow \boxed{\text{apply transf. } T} \longrightarrow \begin{cases} \text{not invariant,} & \text{good} \\ \text{invariant,} & \text{bad} \end{cases}$$

Complex roots representation

$$b_1(W,\theta) \propto \prod_{k=1}^{2\ell_{\max}} \left(\tan\frac{\theta}{2} + \beta_k(W)\right), \qquad b_2(W,\theta) \propto \prod_{k=1}^{2\ell_{\max}} \left(\tan\frac{\theta}{2} - \beta_k(W)\right) \tag{6}$$

$$b_3(W,\theta) \propto \prod_{k=1}^{2\ell_{\max}} \left(\tan\frac{\theta}{2} + \alpha_k(W)\right), \qquad b_4(W,\theta) \propto \prod_{k=1}^{2\ell_{\max}} \left(\tan\frac{\theta}{2} - \alpha_k(W)\right) \tag{7}$$

Constraint

$$\prod_{i=1}^{2\ell_{\max}} \alpha_i(W) = \prod_{j=1}^{2\ell_{\max}} \beta_j(W) \tag{8}$$

[Omelaenko, 1981, Wunderlich et al., 2014, Workman et al., 2017]

Observable definitions: pseudoscalar meson photoproduction

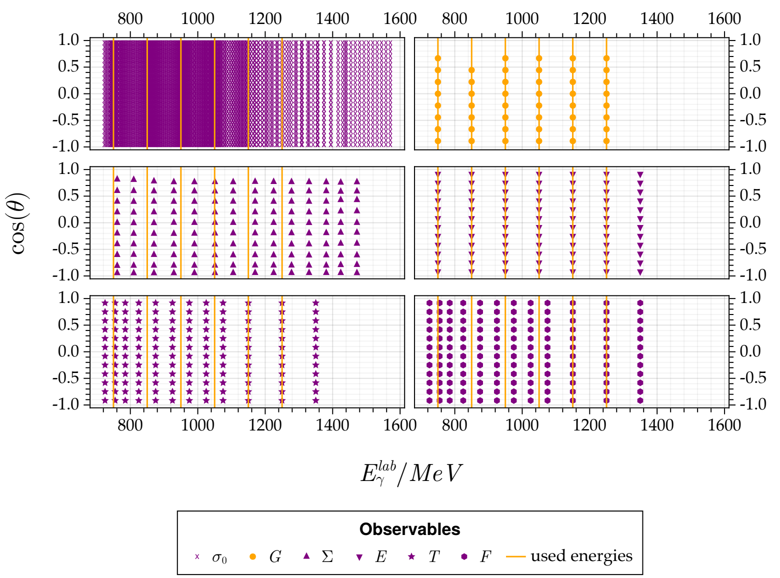
Observable	Beam polarisation	Direction of target-/recoil-nucleon polarisation
σ_0	unpolarized	—
Σ	linear	—
T	unpolarized	y
P	unpolarized	y'
H	linear	x
G	linear	z
F	circular	x
E	circular	z
$O_{x'}$	linear	x'
$O_{z'}$	linear	z'
$C_{x'}$	circular	x'
$C_{z'}$	circular	z'
$T_{x'}$	unpolarized	x, x'
$L_{x'}$	unpolarized	z, x'
$T_{z'}$	unpolarized	x, z'
$L_{z'}$	unpolarized	z, z'

[Sandorfi et al., 2011]

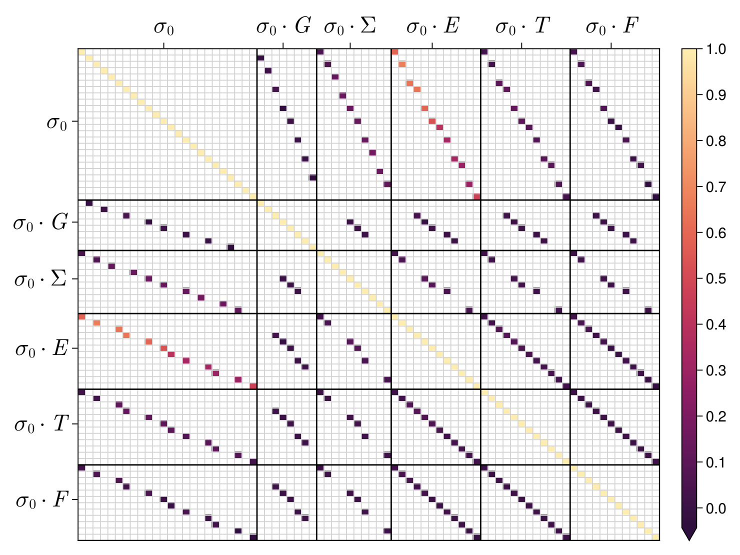
Observable	Transversity-representation / ρ	Type
$\check{\Omega}^1 = \sigma_0$	$\frac{1}{2}\left(\lvert b_1\rvert^2 + \lvert b_2\rvert^2 + \lvert b_3\rvert^2 + \lvert b_4\rvert^2\right)$	
$\check{\Omega}^4 = -\check{\Sigma}$	$\frac{1}{2}\left(\lvert b_1\rvert^2 + \lvert b_2\rvert^2 - \lvert b_3\rvert^2 - \lvert b_4\rvert^2\right)$	$\mathcal{S}$
$\check{\Omega}^{10} = -\check{T}$	$\frac{1}{2}\left(-\lvert b_1\rvert^2 + \lvert b_2\rvert^2 + \lvert b_3\rvert^2 - \lvert b_4\rvert^2\right)$	
$\check{\Omega}^{12} = \check{P}$	$\frac{1}{2}\left(-\lvert b_1\rvert^2 + \lvert b_2\rvert^2 - \lvert b_3\rvert^2 + \lvert b_4\rvert^2\right)$	
$\check{\Omega}^3 = \check{G}$	$\mathrm{Im}\left[-b_1 b_3^* - b_2 b_4^*\right]$	
$\check{\Omega}^5 = \check{H}$	$\mathrm{Re}\left[b_1 b_3^* - b_2 b_4^*\right]$	$\mathcal{BT}$
$\check{\Omega}^9 = -\check{E}$	$\mathrm{Re}\left[b_1 b_3^* + b_2 b_4^*\right]$	
$\check{\Omega}^{11} = \check{F}$	$\mathrm{Im}\left[b_1 b_3^* - b_2 b_4^*\right]$	
$\check{\Omega}^{14} = \check{O}_{x'}$	$\mathrm{Re}\left[-b_1 b_4^* + b_2 b_3^*\right]$	
$\check{\Omega}^7 = -\check{O}_{z'}$	$\mathrm{Im}\left[-b_1 b_4^* - b_2 b_3^*\right]$	$\mathcal{BR}$
$\check{\Omega}^{16} = -\check{C}_{x'}$	$\mathrm{Im}\left[b_1 b_4^* - b_2 b_3^*\right]$	
$\check{\Omega}^2 = -\check{C}_{z'}$	$\mathrm{Re}\left[b_1 b_4^* + b_2 b_3^*\right]$	
$\check{\Omega}^6 = -\check{T}_{x'}$	$\mathrm{Re}\left[-b_1 b_2^* + b_3 b_4^*\right]$	
$\check{\Omega}^{13} = -\check{T}_{z'}$	$\mathrm{Im}\left[b_1 b_2^* - b_3 b_4^*\right]$	$\mathcal{TR}$
$\check{\Omega}^8 = \check{L}_{x'}$	$\mathrm{Im}\left[-b_1 b_2^* - b_3 b_4^*\right]$	
$\check{\Omega}^{15} = \check{L}_{z'}$	$\mathrm{Re}\left[-b_1 b_2^* - b_3 b_4^*\right]$	

[Chiang and Tabakin, 1997]

Phase space coverage



Example for correlations between profile functions



$$p(\boldsymbol{y} \mid \boldsymbol{\Theta}) = \frac{\exp\left(-\frac{1}{2}\boldsymbol{\Delta}^{\mathrm{T}}\boldsymbol{\Lambda}^{-1}\boldsymbol{\Delta}\right)}{\sqrt{(2\pi)^{N}|\boldsymbol{\Lambda}|}} \qquad \text{with} \qquad \boldsymbol{\Delta} := \boldsymbol{y} - \boldsymbol{\kappa} \times \boldsymbol{\mu}(\boldsymbol{x}, \boldsymbol{M}) \tag{9}$$

$\boldsymbol{y}$: values of polarization observables

$\boldsymbol{x}$: $\cos(\theta)$-values

N: number of data points

$\boldsymbol{\Lambda}$: covariance matrix

$\boldsymbol{\mu}$: prediction from TPWA

$\boldsymbol{\kappa}$: systematic parameter

$\boldsymbol{M}$: multipole parameters

Uninformative Prior for Multipoles $\boldsymbol{M}$

$$p(M) = \mathcal{U}(a, b) \tag{10}$$

$\mathcal{U}$: uniform distribution

a, b: physical limits

Priors for Systematic Parameters $\boldsymbol{\kappa}$

$$p(\kappa) = \mathcal{N}(1, f(\sigma_{\text{sys}})) \tag{11}$$

$\mathcal{N}$: normal distribution

σ_{sys}: systematic error of a data set

Example Stan model


```
functions {
  // Define functions

  vector expectation(vector x, real p){
    // ...
  }
}
data {
  // Define data structures which are imported via the interface

  // Number of total data points
  int<lower=1> N;

  // Data used for the regression
  vector[N] x;
  vector[N] y;

  // The covariance matrix for the data points
  matrix[N] CovarianceMatrix;
}
parameters {
  // Define Parameters
  real<lower=0> p;
}
model {
  // Define Prior Distributions
  p ~ normal(1, 100);

  // Define Likelihood Distribution
  y ~ multi_normal(expectation(x, p), CovarianceMatrix);
}
generated quantities {
  // Compute the posterior predictive distribution
  vector[N] y_rep;

  y_rep = multi_normal_rng(expectation(x, p), CovarianceMatrix);
}
```

- step $t-1$: starting point θ_{t-1}, $p(\theta_{t-1} \mid y) > 0$
- step t: predict new point θ^* via 'jumping distribution' J_t
- acceptance probability r:

$$r = \min(1, \frac{p(\theta^* \mid y) J_t(\theta_{t-1} \mid \theta^*)}{p(\theta_{t-1} \mid y) J_t(\theta^* \mid \theta_{t-1})}) \tag{12}$$

- next point of Markov chain

$$\theta_t = \begin{cases} \theta^* & , r \\ \theta_{t-1} & , 1 - r \end{cases} \tag{13}$$

- use geometry of the 'typical set'
- use therefore differential structure of $\pi(q)$
- introduce artificial momentum p for each q, i.e. $\pi(q,p) := \pi(p \mid q)\,\pi(q)$
- Hamiltonian equations of motion:

$$\frac{\mathrm{d}q_i}{\mathrm{d}t} = \frac{\partial H}{\partial p_i} \qquad \text{and} \qquad \frac{\mathrm{d}p_i}{\mathrm{d}t} = -\frac{\partial H}{\partial q_i} \qquad \text{with} \qquad H(q,p) := -\log(\pi(q,p)) \tag{14}$$

Hamiltonian Monte Carlo II

- current state: (q_0, p_0)
- solve Hamiltonian equations with leapfrog integrator (L steps with stepsize ϵ)
- proposed state: (q_L, p_L)
- acceptance probability:

$$\omega = \min[1, \exp(H(q_0, p_0) - H(q_L, p_L))] \tag{15}$$

Leapfrog integrator (reversible and preserves volume)

Step 1

$$p_i(t + \epsilon/2) = p_i(t) - \frac{\epsilon}{2}\frac{\partial V(q(t))}{\partial q_i}$$

Step 2

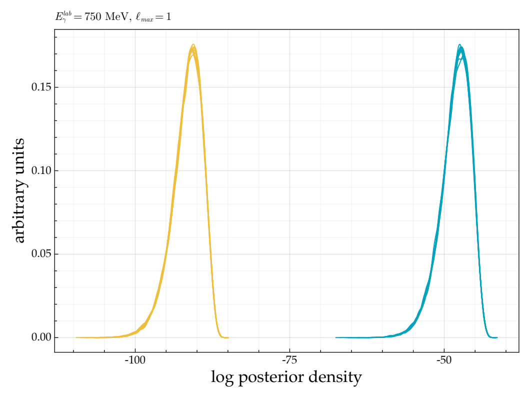
$$q_i(t + \epsilon) = q_i(t) + \frac{\epsilon}{m_i} p_i(t + \epsilon/2)$$

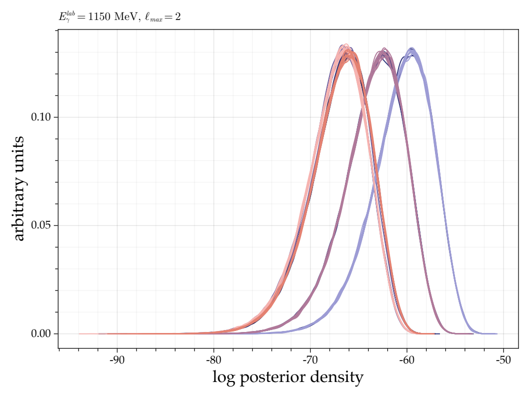
Step 3

$$p_i(t + \epsilon) = p_i(t + \epsilon/2) - \frac{\epsilon}{2}\frac{\partial V(q(t + \epsilon))}{\partial q_i}$$

- momentum p
- position q
- time t
- time-step ϵ
- 'potential energy' $V = -\log(\pi(q))$
- tuning parameter m

Examples of log posterior density distributions





No-U-Turn sampler

- automatically select number of steps L, step size ϵ of leapfrog integrator
- see [Hoffman and Gelman, 2014]

- Stan (https://mc-stan.org)
- Hamiltonian Monte Carlo (HMC)
- No-U-Turn Sampler (NUTS)
- Implemented in C++
- Runs on Linux, Mac, Windows
- Interfaces with:
  - R, Python, Shell, Matlab, **Julia**, Stata, Mathematica, Scala
  - For more information see: https://mc-stan.org/users/interfaces/

[Team, 2022]

Recap: Markov chain Monte Carlo (MCMC)

Target probability distribution $\pi(q)$
e.g. the posterior

↓

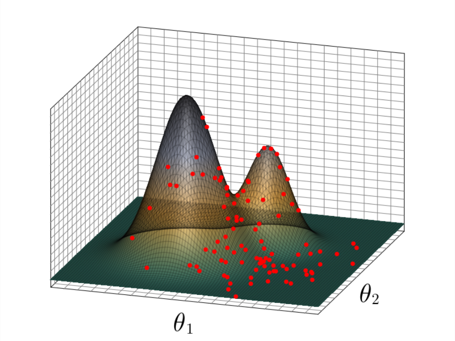
MCMC to approximate $\mu := \mathbb{E}_\pi[f]$ with $\hat{\mu} := \frac{1}{N}\sum_n^N f(q_n)$

↓

The 'typical set'

↓

Markov chain central limit theorem
$\hat{\mu} = \mathcal{N}(\mu, \sigma_{MCSE})$



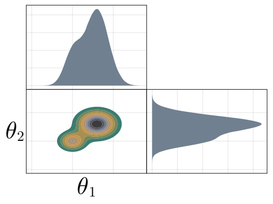
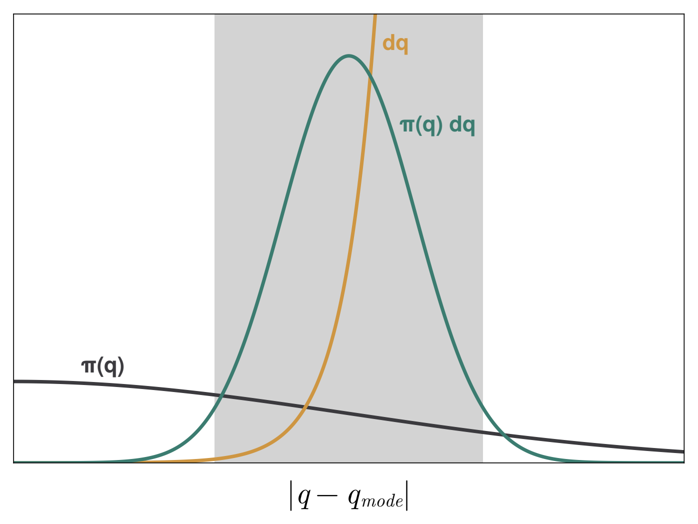


Illustration of the 'typical set'

- $\mathbb{E}_\pi[f] = \int_Q \mathrm{d}q\, \pi(q) f(q)$
- assume high dimensions
- probability density $\pi(q)$
- volume element $\mathrm{d}q$
- integrant $\pi(q)\,\mathrm{d}q$



Redrawn from [Betancourt, 2017]

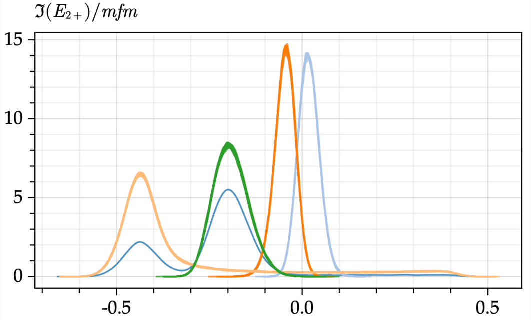
Challenges

- mathematical ambiguities $\longrightarrow$ multimodal posterior
- how to efficiently explore each marginal parameter distribution?
- MCMC diagnostics used to detect multimodality (normally a sign of not converged chains)
- how to verify MCMC diagnostics in this case?

Strategy for the regression

1. Monte Carlo maximum a posteriori estimation
2. Use the K solutions as starting values for HMC
3. Start N_c chains per solution, each with S sampling points
4. Perform Bayesian inference
5. Cluster the $K \cdot N_c$ chains
6. Look at MCMC diagnostics: $\hat{R}$, Monte Carlo standard error, trace plots, etc.
7. Adjust N_c, S if necessary

- dimensional reduction
- i.e. use [0.1,. . . ,0.9] - quantile vector
- DBSCAN algorithm [Ester et al., 1996]
- result are N_{cl} groups of chains



- alternative approach:
  - two-sample Kolmogorov-Smirnov test [Kolmogorov, 1933, Smirnov, 1939]
  - K-Sample Anderson–Darling test [Scholz and Stephens, 1987]

Functioning MCMC options

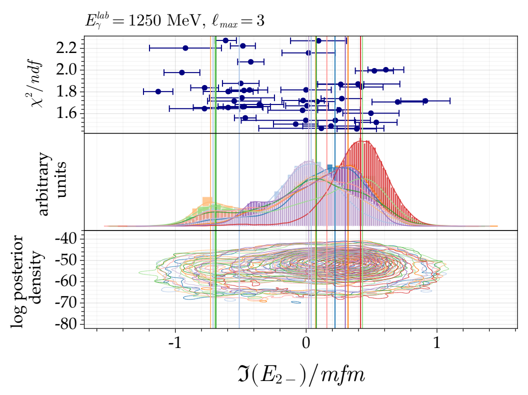
- aiming for MCMC diagnostics:
  - $\hat{R} < 1.01$
  - relative Monte Carlo standard error (MCSE) of a few percent
- chains started per posterior mode $N_c = 10$
- sampling points

  a. $\ell_{\text{max}} = 1 \longrightarrow \mathcal{S} = 1 \times 10^5$

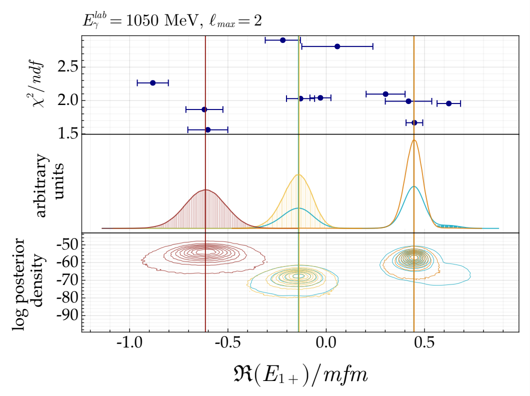
  b. $\ell_{\text{max}} = 2 \longrightarrow \mathcal{S} = 1.4 \times 10^5$
- warmup-phase $\equiv$ first 50%

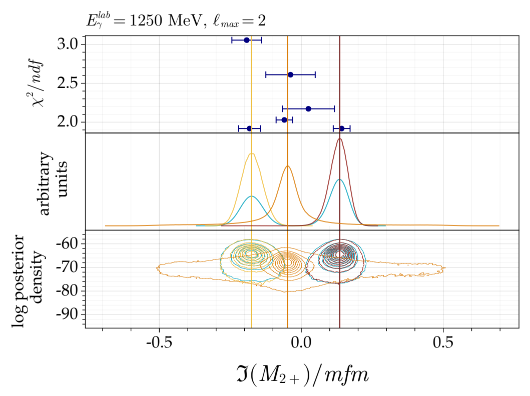
Example result for $\ell_{\text{max}} = 3$

- just for illustrative purposes!!!
- 43 maximum a posteriori solutions
- only one chain started for each
- sampling points $S = 2000$



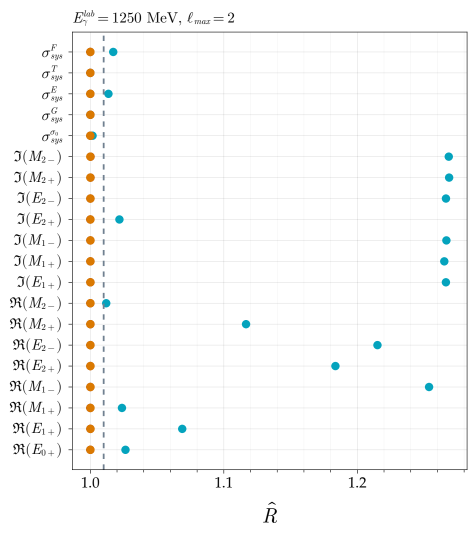
Special behaviour of MCMC I

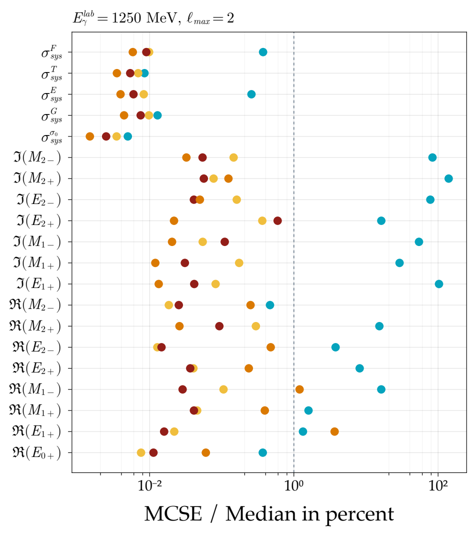




- more posterior modes than marginal modes
- chains can jump between marginal modes

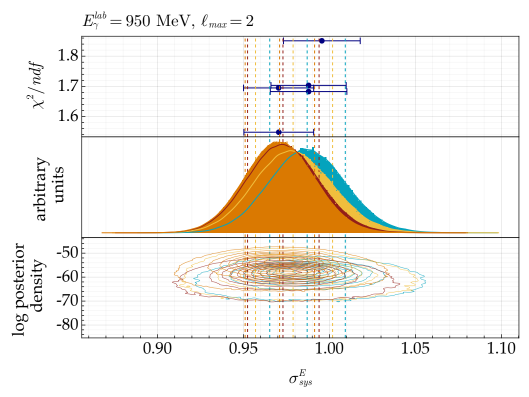
Special behaviour of MCMC II

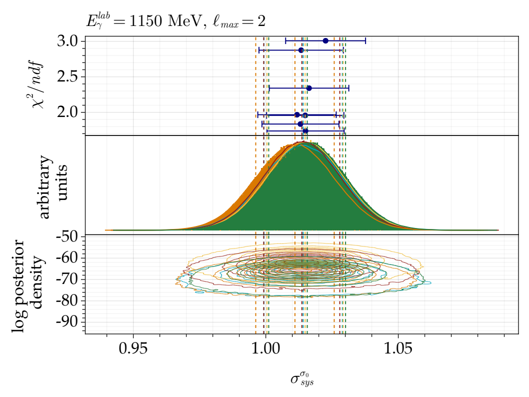




Systematic parameters

- exclusively unimodal distributions in all analyses





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