Wave-Selection Techniques for Partial-Wave Analysis in Light-Meson Spectroscopy

Hadron 2019, Guilin, China

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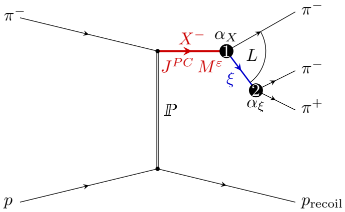
Physics Motivation

Diffractive Dissociation

can produce light-meson resonances



diffractive dissociation into 3-pion final state [1]

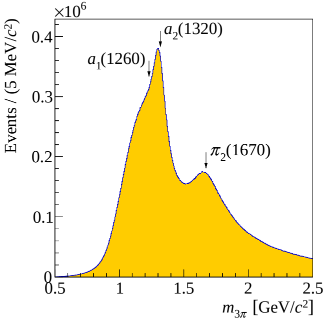
[1] C. Adolph et al. "Resonance production and $\pi\pi$ S-wave in $\pi^- + p \to \pi^-\pi^-\pi^+ + p_{\text{recoil}}$ at $190\ \text{GeV}/c$". In: *Phys. Rev. D* 95 (3 Feb. 2017), p. 032004. DOI: 10.1103/PhysRevD.95.032004. URL: https://link.aps.org/doi/10.1103/PhysRevD.95.032004

Diffractive Dissociation

can produce light-meson resonances

Interfering Resonances

can be disentangled by partial-wave decomposition



m_X spectrum [1]

[1] C. Adolph et al. "Resonance production and $\pi\pi$ S-wave in $\pi^- + p \to \pi^-\pi^-\pi^+ + p_{\text{recoil}}$ at $190\ \text{GeV}/c$". In: *Phys. Rev. D* 95 (3 Feb. 2017), p. 032004. DOI: `10.1103/PhysRevD.95.032004`. URL: `https://link.aps.org/doi/10.1103/PhysRevD.95.032004`

Diffractive Dissociation

can produce light-meson resonances

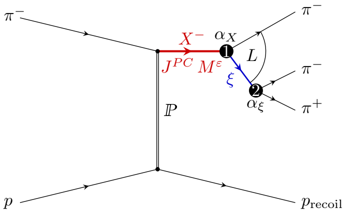
Interfering Resonances

can be disentangled by partial-wave decomposition

Extended Likelihood Fit

model with hundreds to thousands of parameters!

(actually ∞ number of partial waves)



diffractive dissociation into 3-pion final state [1]

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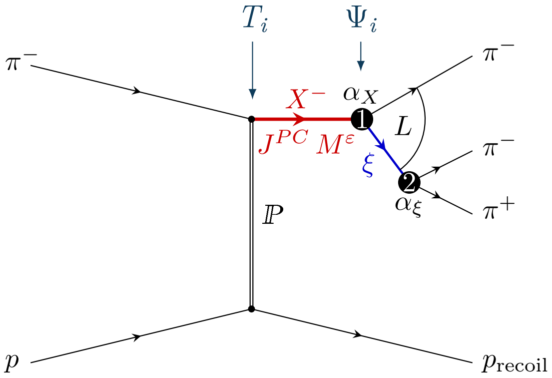
Intensity: (simplified)

$$\mathcal{I}(\tau; m_{3\pi}) = \Big| \sum_{i \in \{\text{waves}\}} T_i(m_{3\pi}) \Psi_i(\tau; m_{3\pi}) \Big|^2 + \Big| T_{\text{flat}}(m_{3\pi}) \Big|^2$$

$m_{3\pi}$ dependence unknown → narrow bins in $m_{3\pi}$



diffractive dissociation into three pions in the isobar model [2]

(extended) logLikelihood from intensity:

$$\log(\mathcal{L}) = \log\left(\frac{\bar{n}^n}{n!}\,e^{-\bar{n}}\prod_j^n \frac{\mathcal{I}(\tau_j)}{\int_\Omega \mathcal{I}(\tau)\,d\mathsf{LIPS}(\tau)}\right)$$

Maximize $\log\mathcal{L}$ to obtain estimate for complex transition amplitudes T_i (= Fit)

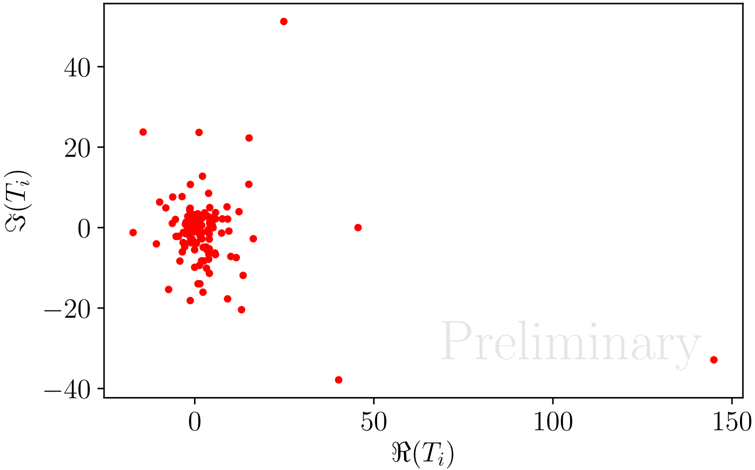
Transition amplitudes T_i:

Complex number: Phase and intensity ($|T_i|^2$)

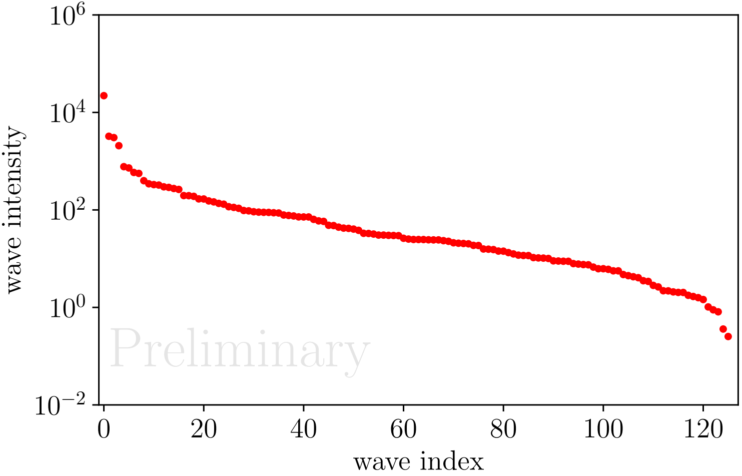
Two Monte Carlo Mock Datasets for 3π diffraction

- Generated mock-data sets with a few thousands events
- 3π-mass regions 1.00 GeV - 1.02 GeV with 19 waves and 1.80 GeV - 1.82 GeV with 126 waves (include only sensible isobars)

Every dot represents one amplitude T_i in the complex plane ...



… representation of their sorted intensities $|T_i|^2$ strong hierachy!



Model Selection

Different Fit Models:

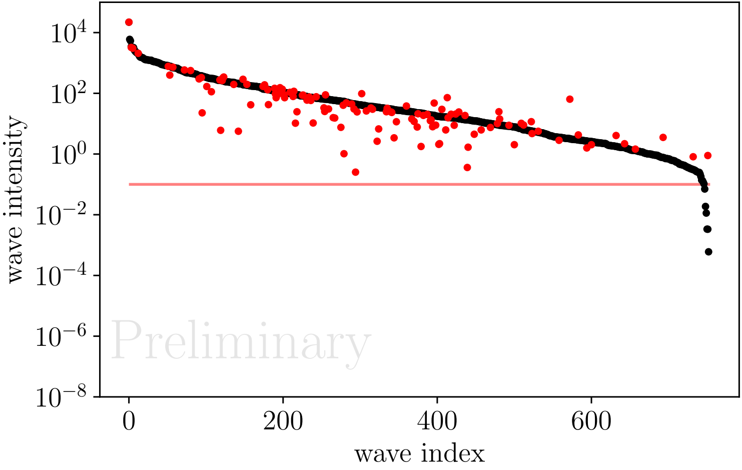
- selection of relevant subset of waves (we cannot fit a very large or even infinite number of waves) $\rightarrow$ model selection
- different parametrizations of decay amplitudes Ψ_i
- model for background
- ...

All aspects are interdependent $\rightarrow$ model selection required!

Model Selection:

- An objective way to select a subset of contributing waves
- Here:
  1. wave pool (= all waves up to certain QN & isobars)
  2. regularization

Fit of full 753 wave pool without regularization at 1.8 GeV. Black intensities of pool. Red intensities of reference fit. → Fails!



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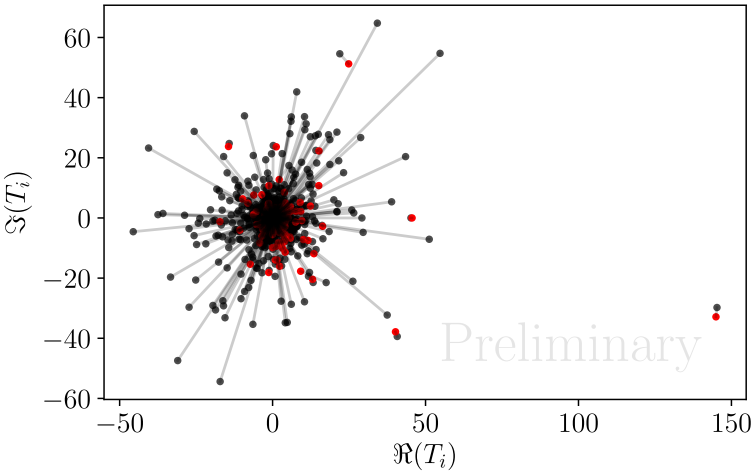


(Sparse) Regularization:

- Use large pool of 'all possible' waves and add regularization term to $\log \mathcal{L}$ that pushes T_i towards zero during the fit
  $\rightarrow T_i = 0$ equivalent to exclusion
- Probably the most famous: LASSO[3]

$$\log \mathcal{L} - \frac{1}{\Gamma} \sum_i |T_i|$$

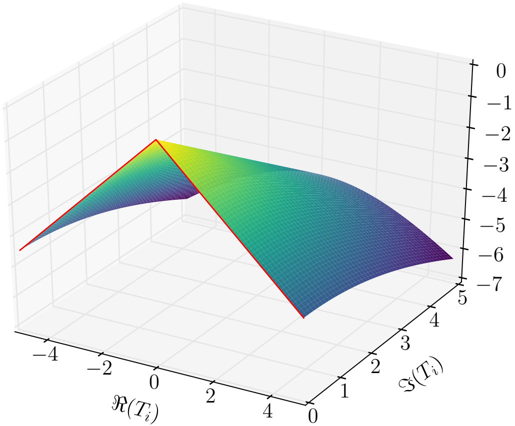
  Suggested for and applied to amplitude analysis by Guegan et al.[4] and for pion photo production by Landay et al.[5] also used for analysis of CLEO-c D-decay data (P. d'Argent et al.) and other analyses in the field!
  $\rightarrow$ established

[3] Robert Tibshirani. "Regression Shrinkage and Selection via the Lasso". In: *Journal of the Royal Statistical Society. Series B (Methodological)* 58.1 (1996), pp. 267–288. ISSN: 00359246. URL: http://www.jstor.org/stable/2346178.

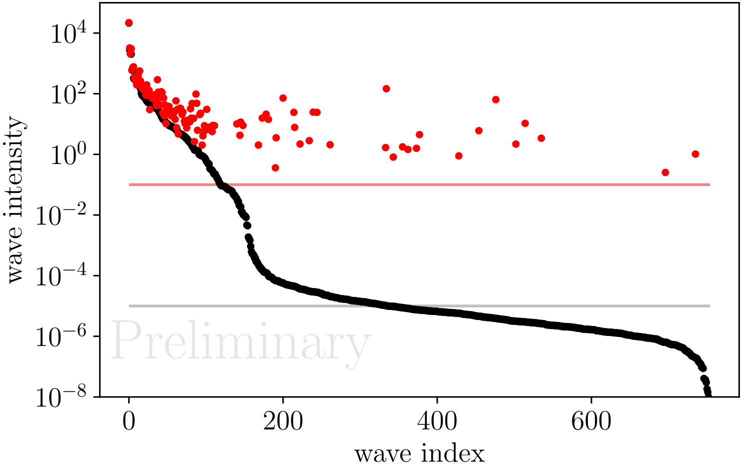
[4] Baptiste Guegan et al. "Model selection for amplitude analysis". In: *JINST* 10.09 (2015), P09002. DOI: 10.1088/1748-0221/10/09/P09002. arXiv: 1505.05133 [physics.data-an].

[5] J. Landay et al. "Model selection for pion photoproduction". In: *Physical Review C* 95.1 (Jan. 2017). DOI: 10.1103/physrevc.95.015203.

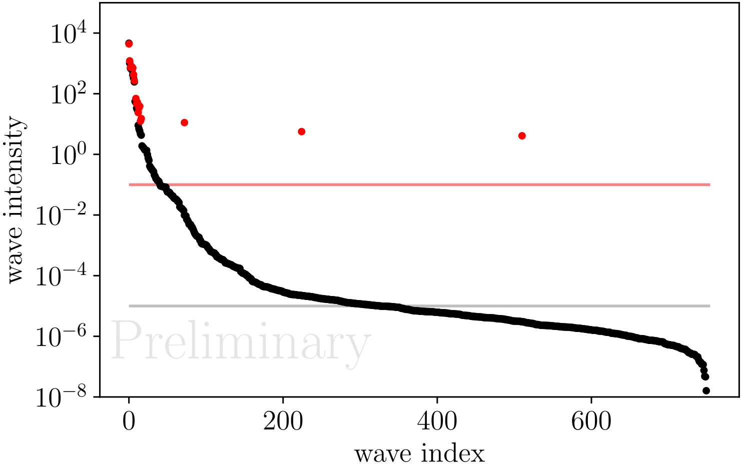
LASSO penalty is cone in the complex plane. For our fits: 'smooth' absolute value via $\sqrt{(x^2+\epsilon)}$ to remove non-differentiability at zero



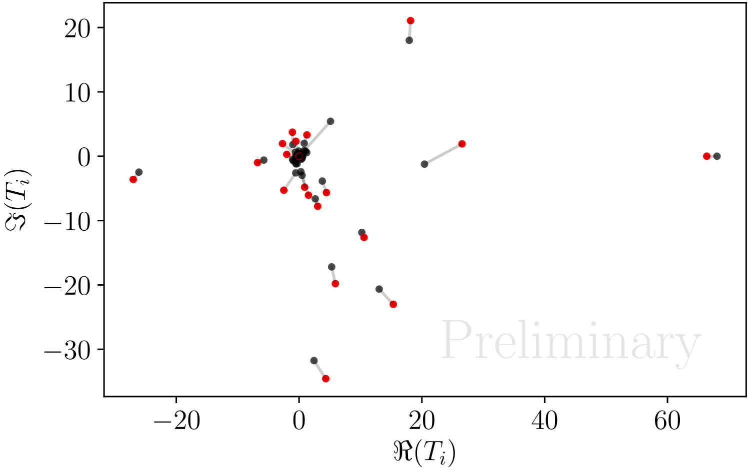
Sorted intensities of waves with LASSO regularization for $\Gamma_{\text{LASSO}} = 0.3$ and smoothing of $\epsilon = 10^{-5}$ for the high mass bin:



Sorted intensities of waves with LASSO regularization for $\Gamma_{\text{LASSO}} = 0.4$ and smoothing of $\epsilon = 10^{-5}$ for the low mass bin:



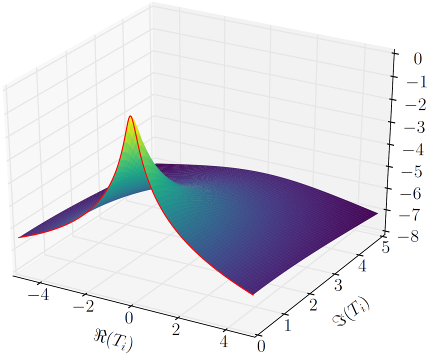
Amplitudes of waves with LASSO regularization for $\Gamma_{\text{LASSO}} = 0.4$ and smoothing of $\epsilon = 10^{-5}$ for the low mass bin:



BCM/Cauchy Regularization:

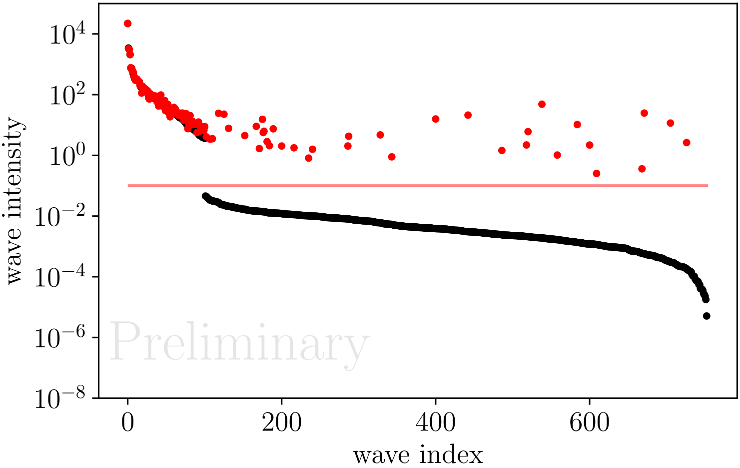
Model selection Ansatz by K. Bicker[6] 'Biggest Conceivable Model':

$$\log \mathcal{L} + \sum_i \log \left(1/(1 + |T_i|^2/\Gamma^2)\right)$$

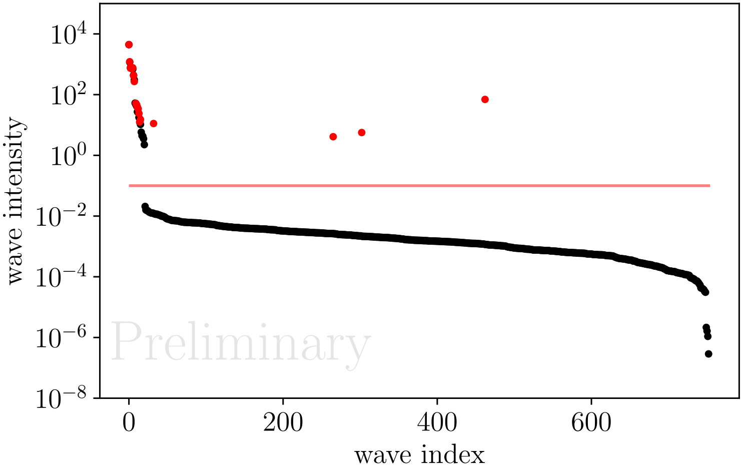


[6] Karl Bicker. "Model Selection for and Partial-Wave Analysis of a Five-Pion Final State at the COMPASS Experiment at CERN". PhD Thesis. Technische Universität München, Apr. 19, 2016, Oliver Drotleff. "Model Selection of $\pi^- + p \to \pi^-\pi^+\pi^- + p$ at the COMPASS Experiment at CERN". Diploma Thesis. Technische Universität München, Nov. 2, 2015.

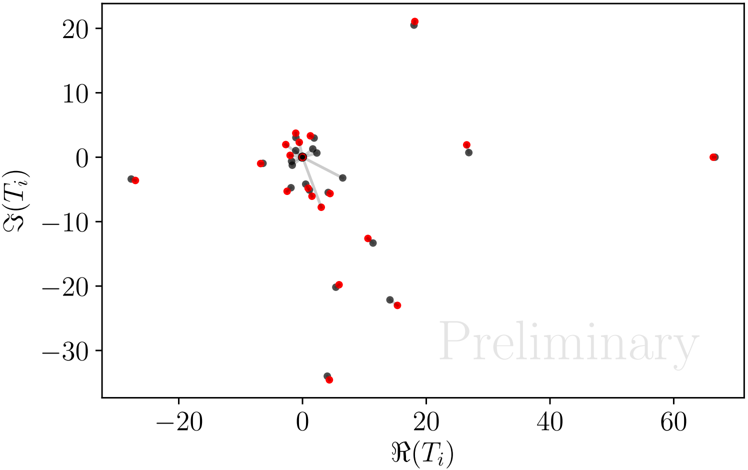
Sorted intensities of waves with BCM regularization for $\Gamma_{\text{BCM}} = 0.2$:



Sorted intensities of waves with BCM regularization for $\Gamma_{\text{BCM}} = 0.25$:



Amplitudes of waves with BCM regularization for $\Gamma_{\mathrm{BCM}} = 0.25$:



LASSO Properties:

- LASSO is convex $\rightarrow$ less problems with multimodality
- Pushes deselected wave intensities to zero (or smoothing scale ϵ)
- Stronger bias on large intensity waves

BCM Properties:

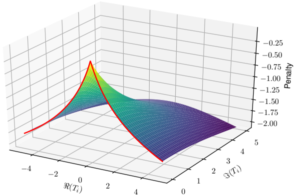
- BCM is NOT convex $\rightarrow$ many minima
- Does not push deselected waves all the way to zero
- Less bias on large intensity waves $\rightarrow$ bad at constraining destructive inference

$\rightarrow$ Invesitgate alternatives that combine advantages of both!

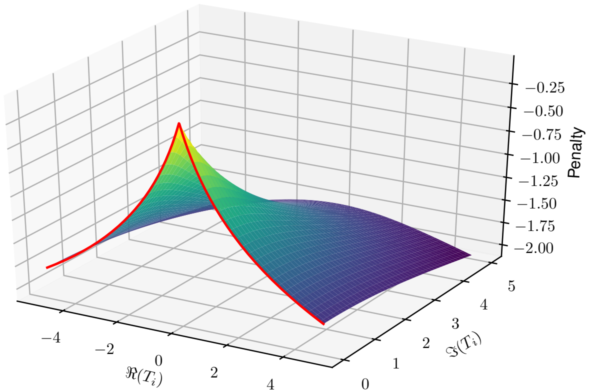
Generalized Pareto[7]:

- Logarithmic behavior for large intensities
- LASSO-like behavior for small intensities
- In the limit $\zeta \to 0$ this regularization falls back to the LASSO

$$\log \mathcal{L} - \frac{1}{\zeta} \sum_i \log\left(1 + \zeta \left| T_i \right| / \Gamma\right)$$



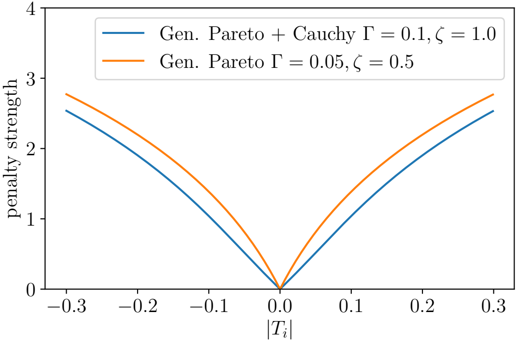
[7] Artin Armagan, David B. Dunson, and Jaeyong Lee. "Generalized double Pareto shrinkage". In: *Statistica Sinica* (2013). DOI: 10.5705/ss.2011.048.


−0.25
−0.50
−0.75
−1.00
−1.25
−1.50
−1.75
−2.00
Penalty
−4
−2
0
2
4
$\Re(T_i)$
0
1
2
3
4
5
$\Im(T_i)$

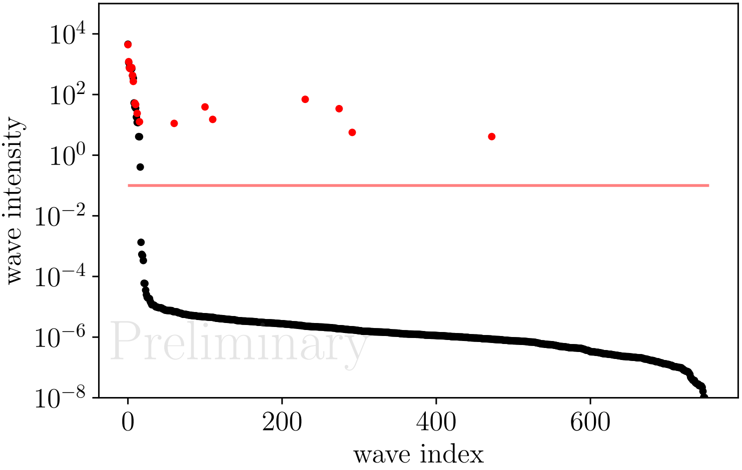
Generalized Pareto + Cauchy Smoothing:

Like generalized Pareto, but convex near minimum!

$$\log \mathcal{L} - \left(\sum_i \frac{1}{\zeta} \log \left(1 + \zeta \left| T_i \right| / \Gamma \right) + 0.5 \zeta \log \left(1 + \left| T_i \right|^2 / \Gamma^2 \right) \right)$$



Generalized Pareto + Cauchy smoothing in low mass bin.



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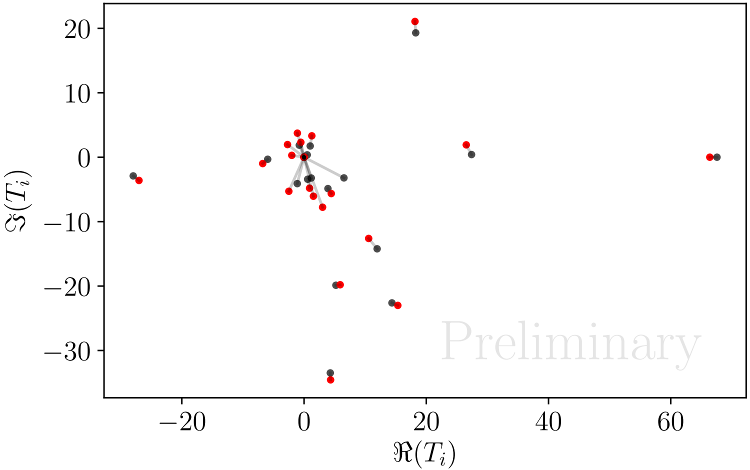
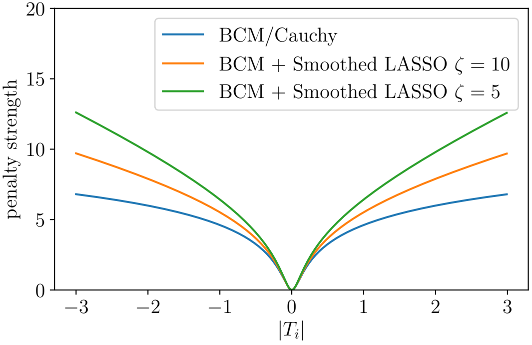


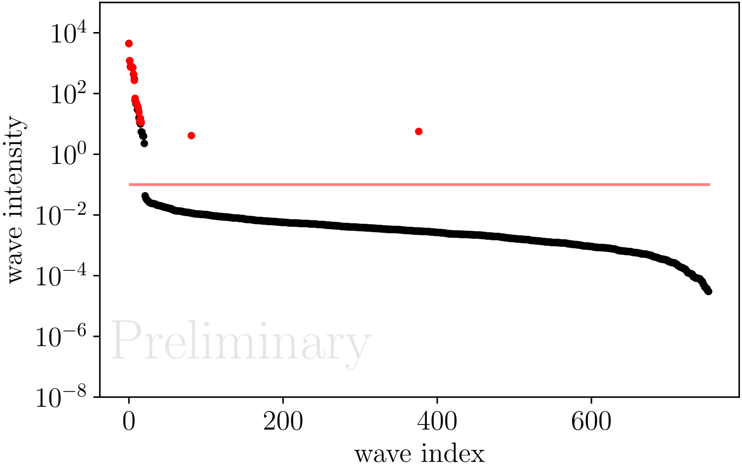
Cauchy + 'Smoothed LASSO':

ζ allows tuning of penalty tails towards LASSO

$$\log \mathcal{L} - \left(\sum_i \left(\sqrt{|T_i|^2 / \Gamma^2 + 1} \right) / \zeta + 2 \log \left(\sqrt{|T_i|^2 / \Gamma^2 + 1} \right) - 1/\zeta \right)$$



Sorted intensities of waves with BCM regularization for $\Gamma_{\text{BCM}} = 0.3$ and $\zeta = 100$:



PWA Fit: Start Value Generation

PWA fits oftentimes inherently multimodal: many different local optima

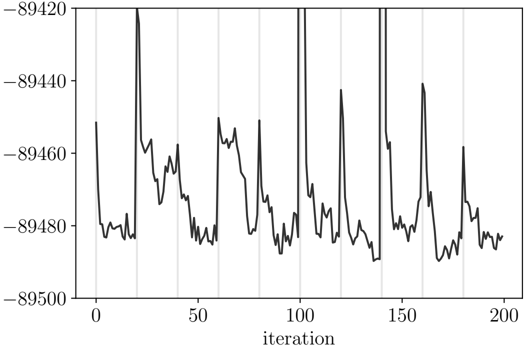
- Non-convex regularization cannot reduce fit to single optimum
- Situation similar to many Machine Learning problems: high-dimensional + many optima

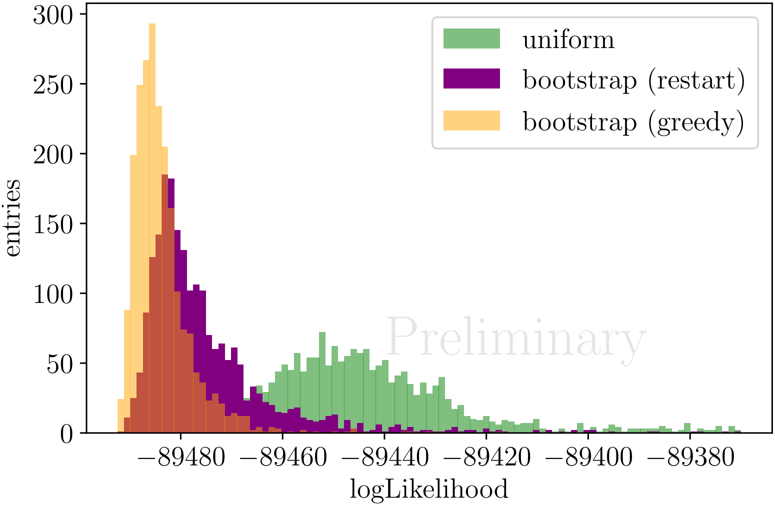
How to cope with multimodal and high-dimensional fits?

- Usual approach: Start with uniformly drawn parameters for each wave
- Alternative: Make use of boostrapping Ansatz[8]
- Fit on resampled data set to propose new start parameters → global structure should stay the same

[8] Simon N. Wood. “Minimizing Model Fitting Objectives That Contain Spurious Local Minima by Bootstrap Restarting”. In: *Biometrics* 57.1 (Mar. 2001), pp. 240–244. DOI: `10.1111/j.0006-341x.2001.00240.x`.

Boostrap restarting for 200 fit attempts with BCM regularization at 1.8 GeV: Potential to improve logLikelihood




300
250
200
150
100
50
0
entries
−89480
−89460
−89440
−89420
−89400
−89380
logLikelihood
uniform
bootstrap (restart)
bootstrap (greedy)
Preliminary

Model Comparison & Parameter Tuning

Regularization Parameters?

- Parameters of the regularization term influence number of selected waves: Every set of parameters yields a different model
- Compare these models to make a motivated choice of the parameter values!

Model Selection Critera:

- Try condensing the choice in a single number
- Penalize model complexity → counter likelihood improvement

→ different assumptions lead to different criteria

Guegan et al. and Landay et al. make use of the AIC[9] and BIC[10] information criteria

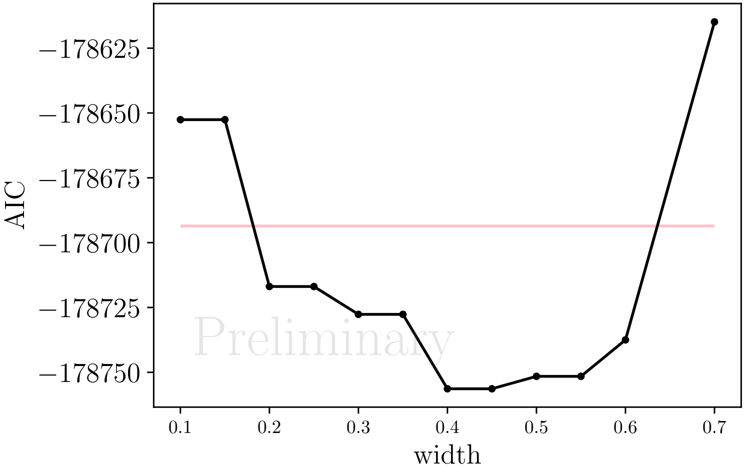
- AIC $= -2\log\mathcal{L} + 2k$
- BIC $= -2\log\mathcal{L} + k\log(n)$
- BIC is approximation of Bayesian evidence $\rightarrow$ Alternatively use Gaussian approximation to calculate evidence + prior defined by parameter volume with $\bar{n} = n$ [11]

[9] H. Akaike. "A new look at the statistical model identification". In: *IEEE Transactions on Automatic Control* 19.6 (Dec. 1974), pp. 716–723. ISSN: 0018-9286. DOI: `10.1109/TAC.1974.1100705`.

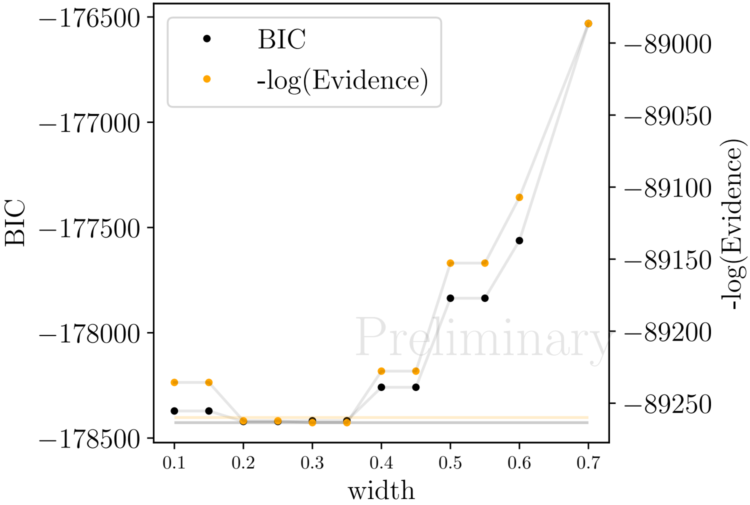
[10] Gideon Schwarz. "Estimating the Dimension of a Model". In: *Ann. Statist.* 6.2 (Mar. 1978), pp. 461–464. DOI: `10.1214/aos/1176344136`. URL: `http://dx.doi.org/10.1214/aos/1176344136`.

[11] Similar to what has been used for genetic model selection by [4]

AIC scan for BCM penalty at low mass bin



BIC and evidence scan for BCM penalty at low mass bin



Different Approach:

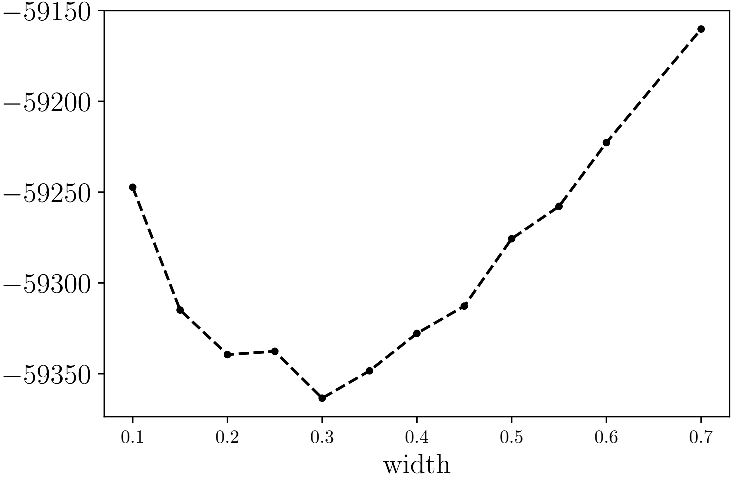
- AIC/BIC and the approximated Evidence are relatively easy to compute but require strong assumptions that might not be fulfilled on real data
- $\rightarrow$ Cross-Validation might be more robust
- Widely used in Machine Learning
- Used for example in Pion Photoproduction by Landay et al.[12]

K-Fold Cross-Validation:

- Split data in K sets, fit on K-1, evaluate 'loss' on the left out
- Repeat this procedure K times and add losses
- Here: Use $K = 20$

[12] J. Landay et al. "Model selection for pion photoproduction". In: *Physical Review C* 95.1 (Jan. 2017). DOI: 10.1103/physrevc.95.015203.

Parameter scan for BCM in the low mass bin. Summed loss of the 20 test sets:



Software

Framework Developments:

- ROOTPWA analysis framework currently undergoing changes towards Python implementation of PWA
- New interface makes use of the Autograd[13] package for automatic differentiation
- Autograd allows easy implementation of more complicated likelihoods/penalties: e.g. Penalty on fit fraction to reduce bias on total intensity

[13] Dougal Maclaurin et al. *Autograd*. URL: `https://github.com/HIPS/autograd`.

Summary

- Sparse regularization terms capable of selecting relevant partial waves (even for extremely many parameters)
- Can confirm usefulness of LASSO + parameter tuning
- LASSO experiences strong bias and includes additional (small) waves, but prevents destructive interference
- BCM/Cauchy reduces bias, but large destructive interference can overcome regularization
- Other approaches to combine desirable features of both penalties
- Use tools like bootstrap restart to find better optima …
- … and make cross validation feasible

Outlook

- Use more computational resources to study full CV scan of all the penalties
- Apply to real data

Thank you for your attention!

Acknowledgments

I would like to thank ...

Dr. Boris Grube, Dr. Fabian Krinner, Prof. Dr. Stephan Paul, Dr. Dmitri Ryabchikov and Stefan Wallner

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Questions?

C. Adolph et al. "Resonance production and $\pi\pi$ S-wave in $\pi^- + p \to \pi^-\pi^-\pi^+ + p_{\text{recoil}}$ at $190\ \mathrm{GeV}/c$". In: *Phys. Rev. D* 95 (3 Feb. 2017), p. 032004. DOI: 10.1103/PhysRevD.95.032004. URL: https://link.aps.org/doi/10.1103/PhysRevD.95.032004.

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Michael Droettboom et al. *matplotlib: matplotlib v1.5.0*. Oct. 2015. DOI: 10.5281/zenodo.32914. URL: https://doi.org/10.5281/zenodo.32914.

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Matthias Vogelgesang. *Metropolis Theme*. URL: `https://github.com/matze/mtheme`.

Simon N. Wood. "Minimizing Model Fitting Objectives That Contain Spurious Local Minima by Bootstrap Restarting". In: *Biometrics* 57.1 (Mar. 2001), pp. 240–244. DOI: `10.1111/j.0006-341x.2001.00240.x`.

Bayes' Theorem:

$$P(\theta|D,M) = \frac{P(D|\theta,M)\,P(\theta,M)}{P(D|M)} \tag{1}$$

Evidence: Probability of the data given the model can be used to compare models:

$$P(D|M) = \int P(D|\theta,M)\,P(\theta,M)\,d\theta \tag{2}$$

Select model with largest evidence

Reparametrization:

Reparametrization results in a Jacobian Determinant !!!

Problem:

- requires specification of prior and might be very sensitive to it
- computation prohibitively expensive for high-dimensional models $\rightarrow$ approximations needed!

Approximations:

- Laplace Approximation: $\log(\mathcal{L}) \approx$ Gaussian around maximum
  Bicker: prior is defined by parameter volume for which $\bar{n} = n$
  $\rightarrow$ defines Hyper-Ellipsoid
- BIC[14]: Asymptotic approximation $(n \rightarrow \infty) \rightarrow$ influence of prior negligible, results in "correction term" for $\log \mathcal{L}$ similar to AIC:
  $\text{BIC} = -2\log\mathcal{L} + k\log(n)$

[14] Gideon Schwarz. "Estimating the Dimension of a Model". In: *Ann. Statist.* 6.2 (Mar. 1978), pp. 461–464. DOI: 10.1214/aos/1176344136. URL: http://dx.doi.org/10.1214/aos/1176344136, Baptiste Guegan et al. "Model selection for amplitude analysis". In: *JINST* 10.09 (2015), P09002. DOI: 10.1088/1748-0221/10/09/P09002. arXiv: 1505.05133 [physics.data-an], J. Landay et al. "Model selection for pion photoproduction". In: *Physical Review C* 95.1 (Jan. 2017). DOI: 10.1103/physrevc.95.015203.

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