The inverse problem: can we provide unbiased results?

hep-lat/2409.04413

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NGT Algorithm Workshop

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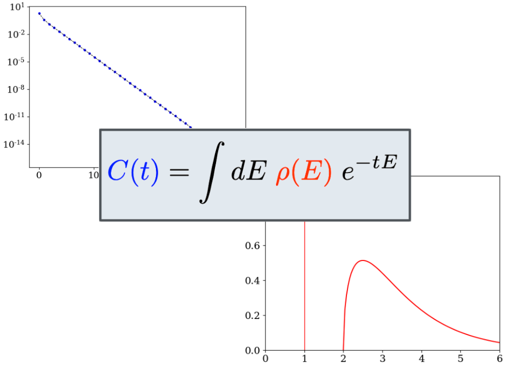
The inverse problem

- Concerns the calculation of the spectral density $\rho(E)$ associated to a lattice correlator $C(t)$
- Ill-posed in presence of a finite set of noisy data
- Ill-conditioned because the Euclidean signal is exponentially suppresed in time.
- There are ways to regularise the problem, with a price to pay.
- Methods can rely on very different assumptions. We will focus on method for which:

$$\rho_\sigma(E) = \sum_t g_t(\sigma; E)\, C(t)$$

$$\rho(E) = \lim_{\sigma \to 0} \rho_\sigma(E)$$

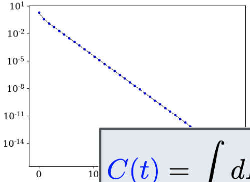


$$C(t) = \int dE\ \rho(E)\ e^{-tE}$$

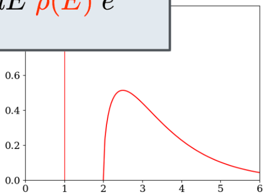
Difficulties

- Finite set of measurements vs function with potentially continuous support
- Target function is a distribution
- Information is suppressed by $\exp(-tE)$
- We work we data that is affected by errors

▶ Two regulators are enough!



$$C(t) = \int dE \; \rho(E) \; e^{-tE}$$



Smearing

- Smearing must be introduced to have a function that is smooth even in a finite volume

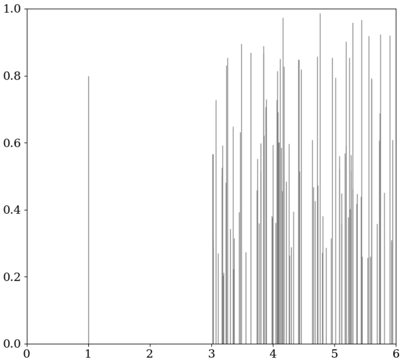
$$\rho_\sigma(\omega) = \int dE\, \mathcal{S}_\sigma(E,\omega)\, \rho(E)$$

- Linear combinations of correlators automatically produce a smeared SD

$$\rho_\sigma(\omega) = \sum_t g_t(\sigma;\omega)\; C(t)$$
$$= \sum_t g_t(\sigma;\omega) \int dE\; e^{-tE} \rho(E)$$

- We can now take the infinite volume limit

$$\lim_{L\to\infty} \rho_L(E) = 🚫$$
$$\lim_{\sigma\to 0} \lim_{L\to\infty} \rho_L(\sigma;E) = \rho(E)$$



Bayesian Inference

Y. Burnier and A. Rothkopf [1307.6106]

J. Horak et al. [2107.13464]

A.P. Valentine and M. Sambridge 2019

L. Del Debbio, T. Giani and M. Wilson [2111.05787]

FASTSUM collaboration

and more!

Bayesian Inference with Gaussian Processes

- Aim for a probability distribution over a functional space of possible spectral densities

- Consider the stochastic field $\mathcal{R}(E)$ Gaussian-distributed around the prior value $\rho^{\text{prior}}(E)$ with covariance $\mathcal{K}^{\text{prior}}(E, E')$.

$$\mathcal{GP}\left(\rho^{\text{prior}}(E), \mathcal{K}^{\text{prior}}(E, E')\right)$$

- Similarly, assume that observational noise is Gaussian: $\eta(t)$

$$\mathbb{G}\left(\eta, \text{Cov}_d\right) = \exp\left(-\frac{1}{2}\vec{\eta}^T \ \text{Cov}_d^{-1} \ \vec{\eta}\right)$$

- The stochastic variable associated to the correlator, $\mathcal{C}$, is related to $\mathcal{R}$ and η via

$$\mathcal{C}(t) = \int dE \, e^{-tE} \mathcal{R}(E) + \eta(t)$$

- The joint, posterior distribution is again Gaussian, centred around ρ^{post} centre and variance:

$$\rho^{\text{post}}(\omega) = \rho^{\text{prior}}(\omega) + \sum_{t=1}^{t_{\max}} g_t^{\text{GP}}(\omega) \left(C(t) - \int_0^{\infty} dE\, e^{-tE} \rho^{\text{prior}}(E) \right)$$

$$\mathcal{K}^{\text{post}}(\omega,\omega) = \left(\mathcal{K}^{\text{prior}}(\omega,\omega) - \sum_{t=1}^{t_{\max}} g_t^{\text{GP}}(\omega)\, f_t^{\text{GP}}(\omega) \right)$$

Bayesian Inference with Gaussian Processes

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- The coefficients can be written as

$$\vec{g}^{\text{GP}}(\omega) = \left(\Sigma^{GP} + \lambda \text{Cov}_{\text{d}}\right)^{-1} \vec{f}^{\text{GP}}$$

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- With the following ingredients:

$$\Sigma^{\text{GP}}{}_{tr} = \int dE_1 \int dE_2\, e^{-tE_1}\, \mathcal{K}^{\text{prior}}(E_1, E_2)\, e^{-rE_2} \quad \text{ill cond}$$

$$f_t^{\text{ GP}}(\omega) = \int dE\, \mathcal{K}^{\text{prior}}(\omega, E)\, e^{-tE}$$

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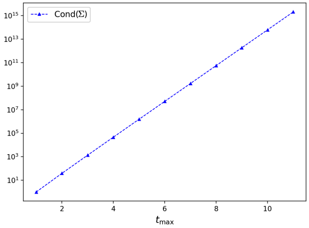
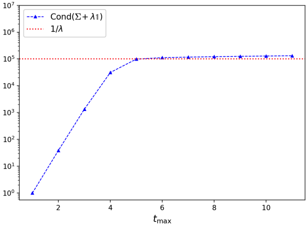
- What is λ? Hyper-parameter that enters as normalisation of the prior ($\mathcal{K}^{\text{prior}}/\lambda$).





HLT

M. Hansen, AL, N. Tantalo [1903.06476]

Related literature:

G. Backus and F. Gilbert 1968

C.A. Barata and K. Fredenhagen 1990

F.P. Pijpers and M.J. Thompson 1994

M.T. Hansen, H.B. Meyer, D. Robaina [1704.08993]

In an ideal world...

- (HLT) Fix and target an appropriate smearing kernel such that when $\sigma \to 0$ we recover $S_\sigma(E,\omega) \to \delta(E-\omega)$
- We need to find the set of coefficients spanning $S_\sigma(E,\omega)$:

$$\sum_{\tau=1}^{\infty} g_\tau^{\text{true}}(\sigma, E)\, e^{-a\tau\omega} = S_\sigma(E,\omega)$$

- We can find the coefficients by minimising

$$A[g(\omega)] = \int_{E_0}^{\infty} dE\; e^{\alpha E} \left| \sum_{\tau=1}^{\infty} g_\tau(\sigma, E)\, e^{-a\tau\omega} - S_\sigma(E,\omega) \right|^2$$

- Without errors on $C(t)$ and infinitely many points, this is the solution.

$$\sum_{\tau=1}^{\infty} g_\tau^{\text{true}}(\sigma, E)\, C(t) = \rho_\sigma(E)$$

Slightly less ideal world

- In reality, the correlator is known at a finite number of points. This translates into a systematic error in the reconstructed kernel and therefore in the reconstructed SD

$$\sum_{\tau=1}^{\tau_{\max}} g_\tau(\sigma, E) C(a\tau) = \rho_\sigma(E) + r(\tau_{\max}, \sigma; E)$$

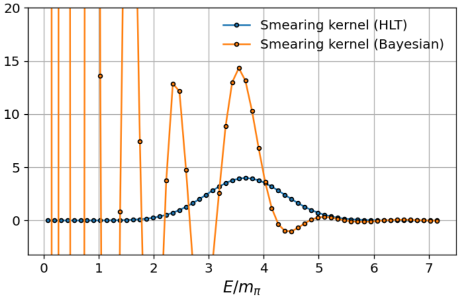
- The sum truncated to $\tau_{\max}$ is however well-defined and define unambiguously a given smearing kernel

- In fact, let us look at an example for both HLT and GP. For the latter, we shall choose a prior:

$$\mathcal{K}_\epsilon^{\text{prior}}(E, E') = \frac{e^{-(E-E')^2/2\epsilon^2}}{\lambda} \,, \qquad \rho^{\text{prior}} = 0$$

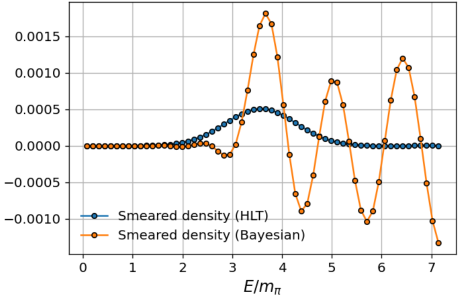
Example: no errors

- Blue should be a Gaussian
- Orange should be what it should be



Example: no errors

- Similarly for the reconstructed smeared density:



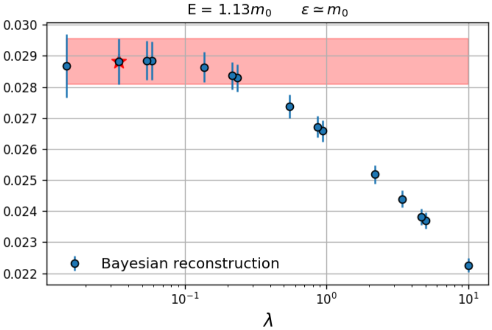
Real world: regulator is needed

- The main complication is that noisy data severely hinder this approach. Minimising $A[g]$ amounts to solve a massively ill-conditioned linear system
$$\vec{g} = \Sigma^{-1}\vec{f}$$
$$\Sigma_{tr} = \int dE_1 \, e^{-tE_1} \, e^{-rE_1}$$
- Backus-Gilbert regularisation:
$$\int_0^\infty dE \; e^{\alpha E} \left| \sum_{t=1}^{t_{\max}} g_t e^{-tE} - \mathcal{S}_\sigma(\omega, E) \right|^2 + \lambda \; \vec{g} \cdot \mathrm{Cov}_d \cdot \vec{g}$$
- The linear system is now
$$\vec{g} = (\Sigma + \lambda \mathrm{Cov_d})^{-1} \; \vec{f}$$
- We introduced a bias ($\lambda \neq 0$).

The bias

- In the HLT method we perform a "stability analysis" (Bulava et al. [2111.12774])
- We could do the same with the Bayesian reconstruction. Let us pick a prior:

$$\mathcal{K}_{\epsilon}^{\text{prior}}(E, E') = \frac{e^{-(E-E')^2/2\epsilon^2}}{\lambda} , \qquad \rho^{\text{prior}} = 0$$

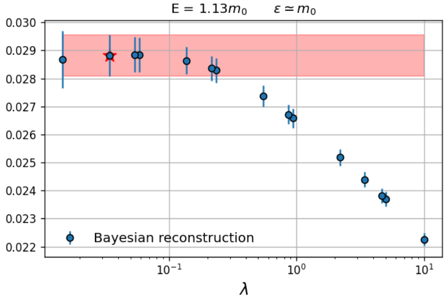


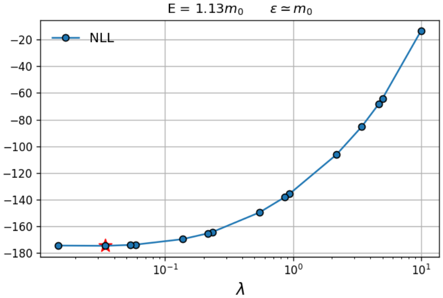
The bias

- In the Bayesian literature, hyperparameters are determined by minimising the negative log likelihood (NLL)

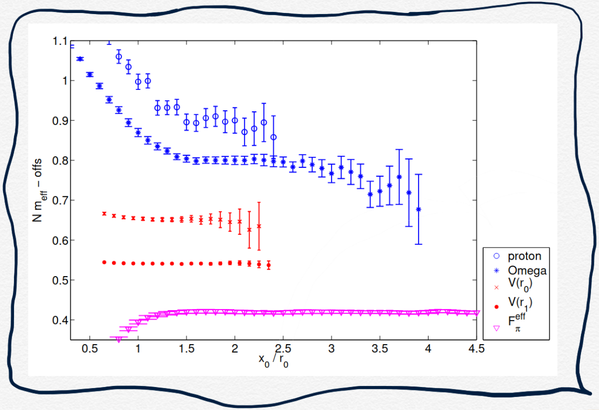
$$-\log P(\text{data}|\text{parameters})$$

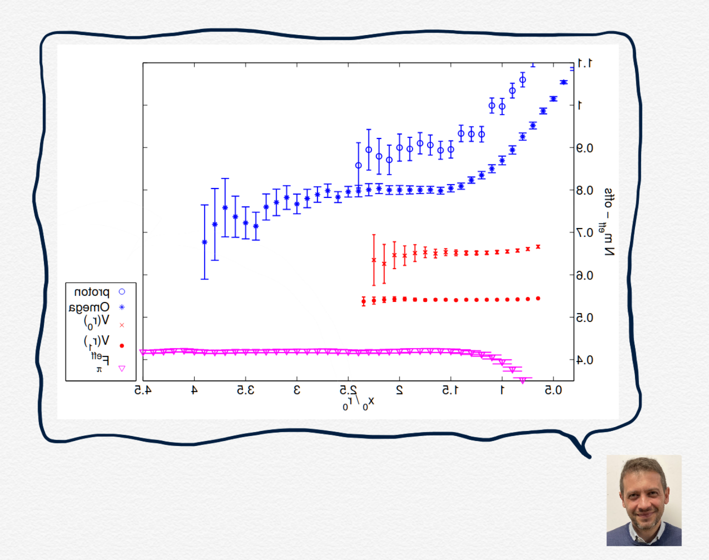
- The methods seem compatible



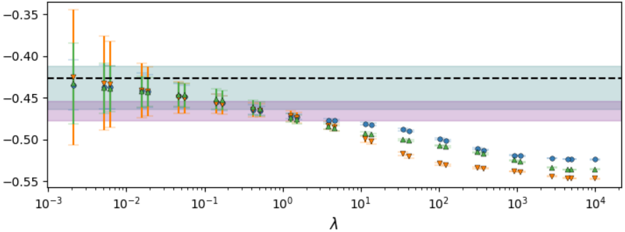


The plateau analysis




proton
Omega
V(r0)
V(r1)
Feff π
x0/r0
N meff − offs

The plateau analysis

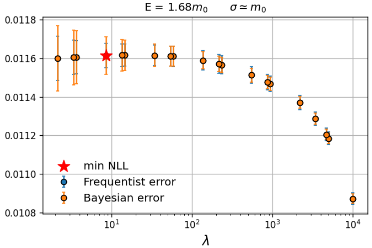


Bayesian inference with fixed smearing kernel

L. Del Debbio, AL, M. Panero, N. Tantalo [2409.04413]

Bayesian formulation of HLT

- Compute the posterior probability distribution for a spectral density smeared with a **fixed kernel** $G_\sigma(E, E') = \exp^{-(E-E')^2/2\sigma^2}$



❗ **Diagonal model covariance**

$$\mathcal{K}^{\text{prior}}(E, E') = \frac{\delta(E-E')}{\lambda} \ ,$$

- The solution is now given by the same coefficients as HLT
  $$g^{\text{GP}}(\sigma;\omega) = g(\sigma;\omega) \quad \text{even at finite } \sigma$$
- The only difference is in the error (averaged in frequentist methods)

$$\mathcal{K}^{\sigma}_{\text{post}}(\omega,\omega)^2 = \frac{1}{2}\int dE \left(\sum_t g_t(\sigma,\omega)e^{-tE} - G_\sigma(E,\omega)\right) G_\sigma(E,\omega)$$

Closure tests

Strategy

- Generate toys for spectral densities / correlators

$$C(t) = \sum_{n=0}^{n_{\max}-1} w_n \, e^{-|t| E_n} \,, \qquad E_0 < E_1 \leq \ldots \,,$$

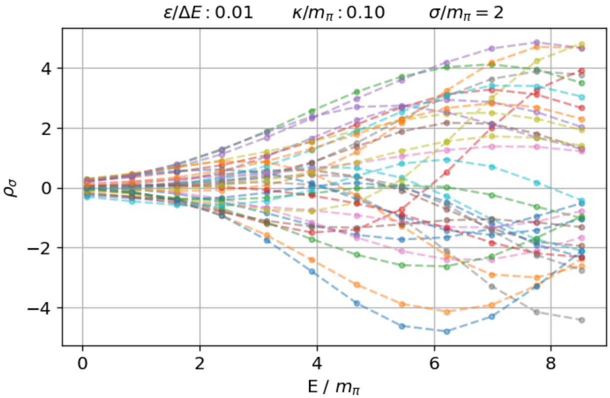
- We are generating instances of w_n with a multivariate normal distribution, centred around zero, and covariance

$$K_{\text{weights}}(n, n') = \kappa \; \exp\left(- \frac{(E_n - E_{n'})^2}{2\epsilon^2} \right) \,,$$

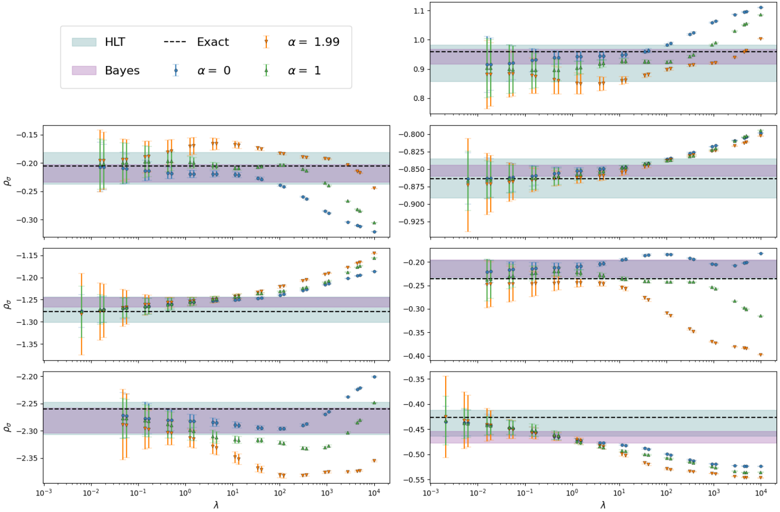
- with ϵ smaller than the spacing between states

- For the corresponding correlators, we inject noise from a covariance matrix measured on the lattice.

Toys

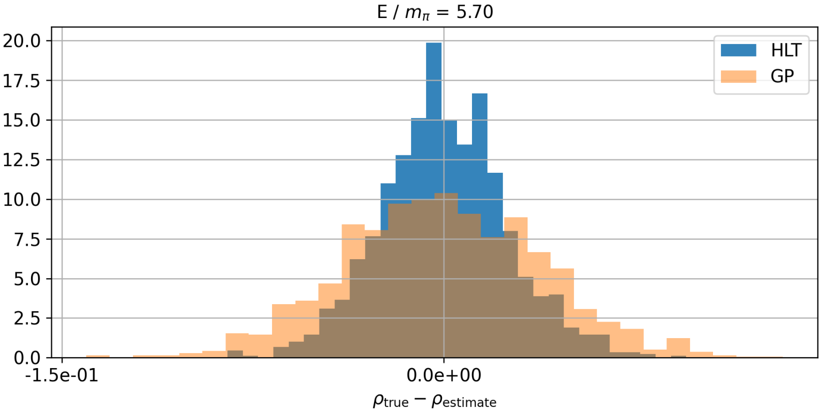


$\epsilon/\Delta E : 0.01$ $\kappa/m_\pi : 0.10$ $\sigma/m_\pi = 2$
ρ_σ
4
2
0
−2
−4
0
2
4
6
8
E / m_π


HLT
Exact
$\alpha = 1.99$
Bayes
$\alpha = 0$
$\alpha = 1$
ρ_σ
λ

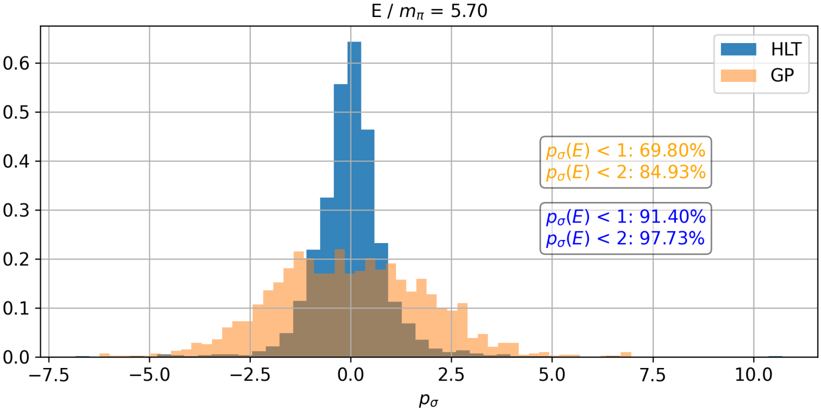
Results

- Results for $\delta_\sigma(E) = \rho_\sigma^{\text{true}}(E) - \rho_\sigma^{\text{estimate}}(E)$



Results

- Results for $p_\sigma(E) = \frac{\rho^{\text{true}}(E)_\sigma - \rho^{\text{estimate}}_\sigma(E)}{\Delta^{\text{tot}}_\sigma(E)}$



Thank you