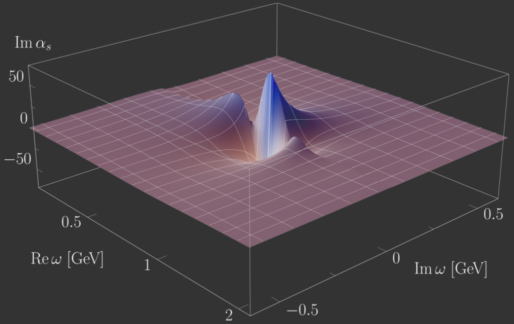
Fredholm inversion with Gaussian processes

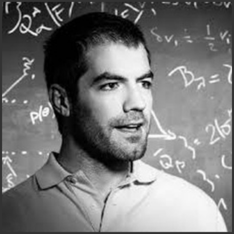


Julian M. Urban lettucefield.org

MIT / IAIFI

Collaborators

J. M. Pawlowski



S. Zafeiropoulos

J. Rodríguez-Quintero

N. Wink

C. S. Schneider

J. Horak

J. Turnwald

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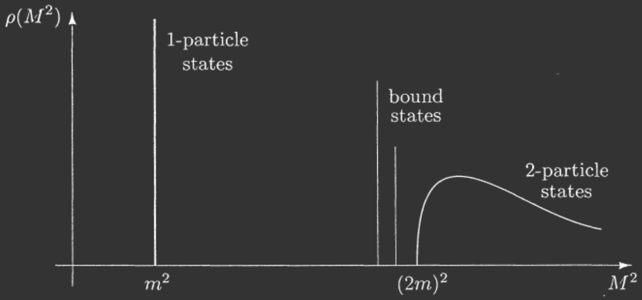

Figure 7.2. The spectral function $\rho(M^2)$ for a typical interacting field theory. The one-particle states contribute a delta function at m^2 (the square of the particle's mass). Multiparticle states have a continuous spectrum beginning at $(2m)^2$. There may also be bound states.

Analogous expressions hold for the case $y^0 > x^0$. Both cases can be summarized in the following general representation of the two-point function (the *Källén-Lehmann spectral representation*):

$$\langle\Omega| T\phi(x)\phi(y) |\Omega\rangle = \int_0^\infty \frac{dM^2}{2\pi}\, \rho(M^2)\, D_F(x-y; M^2), \tag{7.6}$$

where $\rho(M^2)$ is a positive *spectral density* function,

$$\rho(M^2) = \sum_\lambda (2\pi)\delta(M^2 - m_\lambda^2)\big|\langle\Omega| \phi(0) |\lambda_0\rangle\big|^2. \tag{7.7}$$

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- Computing spectral function $\rho(\omega)$ from noisy data $\mathbf{G}$ is an ill-posed linear inverse problem (Fredholm inversion)

Outline

- Motivation for probabilistic ansatz
- Gaussian process regression (GPR)
- Fredholm inversion with GPR
- Related & original work
- Application 1: bound state masses
- Incorporating asymptotic constraints
- Application 2: S-matrix building blocks

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- For $f[\rho] \equiv \int \mathrm{d}\omega\, K(p,\omega)\rho(\omega) = G(p),\ \mathcal{G}, \mathcal{R}$ are *function* spaces
- Determination of $\rho(\omega)$ from $G(p)$ is well-posed in principle

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- Desirable: incorporation of additional prior information in the form of constraints and biases

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- Analogy: free scalar field theory $\sim$ ∞-dim. multivariate normal

$\longrightarrow$ mean $\mu(\omega)$ $\sim$ vacuum expectation value

$\longrightarrow$ covariance $C(\omega, \omega')$ $\sim$ propagator

Gaussian processes

- Finite-dim. multivariate normal for any finite set of points:

$$\begin{pmatrix} \rho(\omega_1) \\ \vdots \\ \rho(\omega_N) \end{pmatrix} \sim \mathcal{N}\begin{pmatrix} \mu(\omega_1) & & C(\omega_1, \omega_1) & \dots & C(\omega_1, \omega_N) \\ \vdots & , & \vdots & \ddots & \vdots \\ \mu(\omega_N) & & C(\omega_N, \omega_1) & \dots & C(\omega_N, \omega_N) \end{pmatrix}$$

$$= (2\pi)^{-\frac{N}{2}} \det(\mathbf{C})^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\boldsymbol{\rho} - \boldsymbol{\mu})^T \mathbf{C}^{-1} (\boldsymbol{\rho} - \boldsymbol{\mu})\right)$$

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- Sampling similar to pseudofermion generation in LQCD:

  1. Cholesky decomposition: $\mathbf{C} = \mathbf{A}\mathbf{A}^T$
  2. $\boldsymbol{\rho} = \mathbf{A}\boldsymbol{\eta}$ with $\boldsymbol{\eta} \sim \mathcal{N}(\mathbf{0}, \mathbb{1})$

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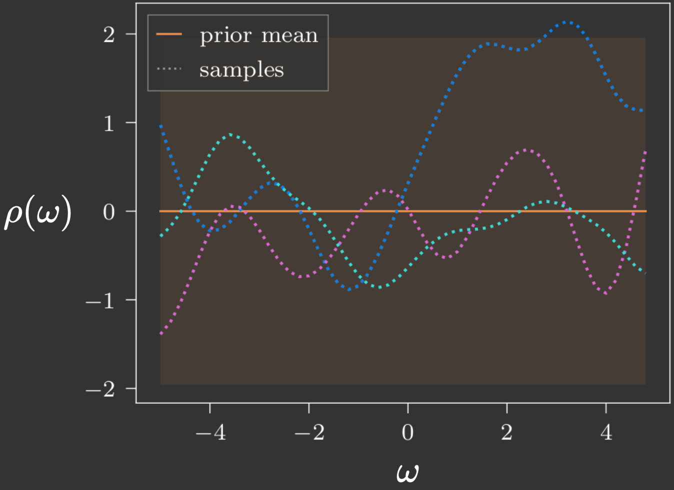

Gaussian process regression

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- Joint distribution of *observed* $\boldsymbol{\rho}$ and *unobserved* $\rho(\omega)$:

$$\begin{pmatrix} \rho(\omega) \\ \boldsymbol{\rho} \end{pmatrix} \sim \mathcal{N}\left(\begin{matrix} \mu(\omega) \\ \boldsymbol{\mu} \end{matrix} \, , \, \begin{matrix} C(\omega,\omega') & \mathbf{C}^T(\omega) \\ \mathbf{C}(\omega') & \mathbf{C} + \sigma_n^2 \mathbb{1} \end{matrix} \right)$$

$$\boldsymbol{\mu}_i = \mu(\omega_i),\ \mathbf{C}_i(\omega) = C(\omega_i, \omega),\ \mathbf{C}_{ij} = C(\omega_i, \omega_j)$$

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- Closed-form expression for conditional posterior:

$$\rho(\omega)|\boldsymbol{\rho} \sim \mathcal{N}\left(\mu(\omega) + \mathbf{C}^T(\omega)\left(\mathbf{C} + \sigma_n^2 \cdot \mathbb{1}\right)^{-1}(\boldsymbol{\rho} - \boldsymbol{\mu}),\ C(\omega,\omega') - \mathbf{C}^T(\omega)\left(\mathbf{C} + \sigma_n^2 \cdot \mathbb{1}\right)^{-1}\mathbf{C}(\omega') \right)$$

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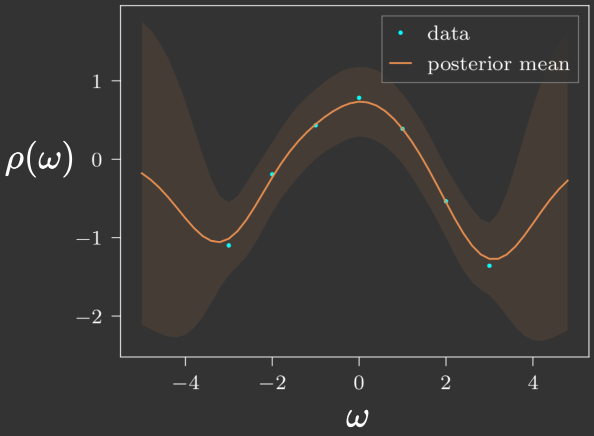

Hyperparameter optimization

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- Common selection approach: maximize likelihood

$$p(\boldsymbol{\rho}|\boldsymbol{\alpha}) = \left((2\pi)^N \det\left(\mathbf{C}_\alpha + \sigma_n^2 \mathbb{1}\right)\right)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\boldsymbol{\rho}-\boldsymbol{\mu})^T \left(\mathbf{C}_{\boldsymbol{\alpha}} + \sigma_n^2 \mathbb{1}\right)^{-1} (\boldsymbol{\rho}-\boldsymbol{\mu})\right)$$

or, conventionally, minimize negative log-likelihood (NLL)

$$-\log p(\boldsymbol{\rho}|\boldsymbol{\alpha}) = \frac{1}{2}(\boldsymbol{\rho}-\boldsymbol{\mu})^T \left(\mathbf{C}_{\boldsymbol{\alpha}} + \sigma_n^2 \mathbb{1}\right)^{-1} (\boldsymbol{\rho}-\boldsymbol{\mu}) + \frac{1}{2}\log\det\left(\mathbf{C}_\alpha + \sigma_n^2 \mathbb{1}\right) + \frac{N}{2}\log 2\pi$$

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- Ignores structure & unstable directions of posterior landscape

  $\longrightarrow$ stabilize or integrate out with suitable *hyperprior* $q(\boldsymbol{\alpha})$

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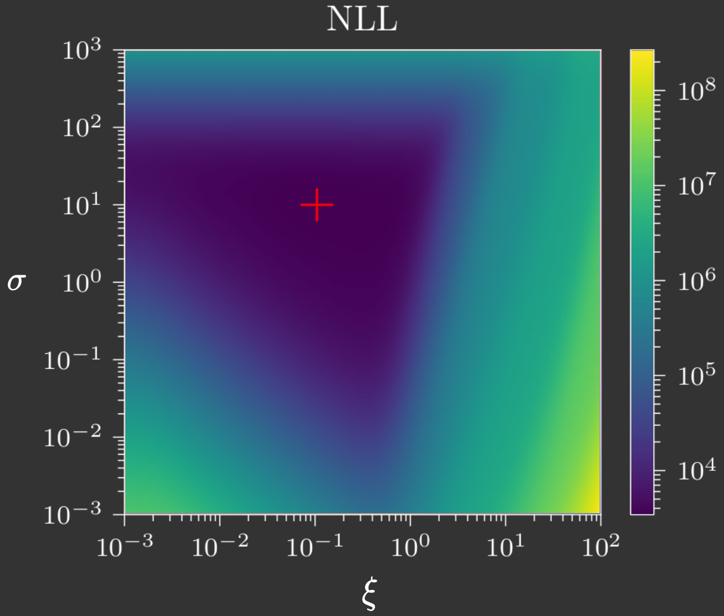

sklearn to the rescue

```
>>> from sklearn.datasets import make_friedman2
>>> from sklearn.gaussian_process import GaussianProcessRegressor
>>> from sklearn.gaussian_process.kernels import DotProduct, WhiteKernel
>>> X, y = make_friedman2(n_samples=500, noise=0, random_state=0)
>>> kernel = DotProduct() + WhiteKernel()
>>> gpr = GaussianProcessRegressor(kernel=kernel,
...         random_state=0).fit(X, y)
>>> gpr.score(X, y)
0.3680...
>>> gpr.predict(X[:2,:], return_std=True)
(array([653.0..., 592.1...]), array([316.6..., 316.6...]))
```
>>>

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- Closed-form posterior like before, with $\mathcal{K} \circ$ where necessary

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$$G(p) \sim \mathcal{GP}\left(\int \mathrm{d}\omega\, K(p,\omega)\mu(\omega), \int \mathrm{d}\omega\, \mathrm{d}\omega' K(p,\omega)C(\omega,\omega')K(p',\omega')\right)$$

$$P(\rho(\omega)|\mathbf{G}) = \mathcal{N}\Bigg(\mu(\omega) + \int \mathrm{d}\eta' C(\omega,\eta')K(\mathbf{p}^T,\eta')$$

$$\left(\int \mathrm{d}\zeta\, \mathrm{d}\zeta' K(\mathbf{p},\zeta)C(\zeta,\zeta')K(\mathbf{p}^T,\zeta') + \sigma_n^2 \mathbb{1}\right)^{-1} \left(\mathbf{G} - \int \mathrm{d}\eta\, K(\mathbf{p},\eta)\mu(\eta)\right),$$

$$C(\omega,\omega') - \int \mathrm{d}\eta' C(\omega,\eta')K(\mathbf{p}^T,\eta')$$

$$\left(\int \mathrm{d}\zeta\, \mathrm{d}\zeta' K(\mathbf{p},\zeta)C(\zeta,\zeta')K(\mathbf{p}^T,\zeta') + \sigma_n^2 \mathbb{1}\right)^{-1} \int \mathrm{d}\eta\, K(\mathbf{p},\eta)C(\eta,\omega')\Bigg)$$

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- Closed-form posterior like before, with $\mathcal{K} \circ$ where necessary
- Generalizable to *arbitrary* derivative & integral constraints or known values of ρ by treating them as observations

Related/original work

- Krige, Danie G. (1951): *A statistical approach to some basic mine valuation problems on the Witwatersrand*. J. of the Chem., Metal. and Mining Soc. of South Africa. 52 (6): 119–139.

- Valentine, Andrew P. and Sambridge, Malcolm (2019): *Gaussian process models—I. A framework for probabilistic continuous inverse theory*. Geophysical Journal International, Volume 220, Issue 3, March 2020, Pages 1632–1647

- Del Debbio, Luigi and Giani, Tommaso and Wilson, Michael (2021): *Bayesian approach to inverse problems: an application to NNPDF closure testing.* arXiv:2111.05787 [hep-ph]

- Candido, Alessandro and Del Debbio, Luigi and Giani, Tommaso and Petrillo, Giacomo (2023): *Inverse problems in PDF determinations.* arXiv:2302.14731 [hep-lat]

Numerical Demo

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- Example with analytic solution: relativistic Breit-Wigner dist.

$$\rho(\omega) = \frac{4A\Gamma\omega}{4\Gamma^2\omega^2 + (M^2 + \Gamma^2 - \omega^2)^2},\ G(p) = \frac{A}{(p+\Gamma)^2 + M^2}$$

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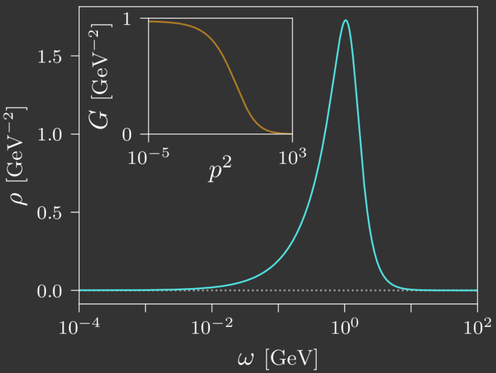
- Additive Gaussian noise: $\mathbf{G} + \boldsymbol{\epsilon},\ \epsilon \sim \mathcal{N}(0,\sigma^2),\ \sigma = 10^{-4}$

Numerical Demo

- Perfect data: $\boldsymbol{\rho} \approx \tilde{\mathbf{K}}^{-1}\mathbf{G}$



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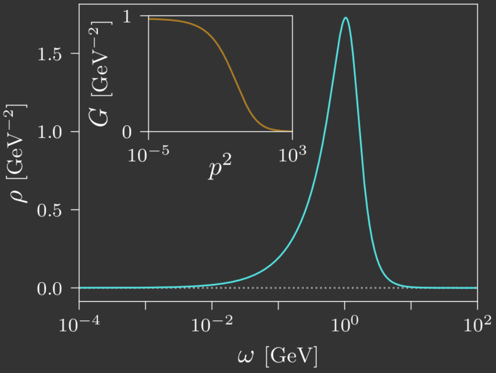
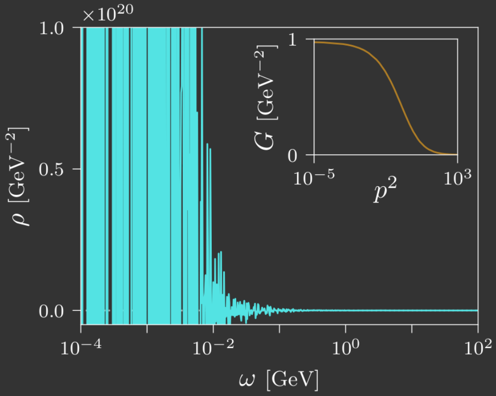


- Noisy data: $\boldsymbol{\rho} \approx \tilde{\mathbf{K}}^{-1}(\mathbf{G} + \boldsymbol{\epsilon})$



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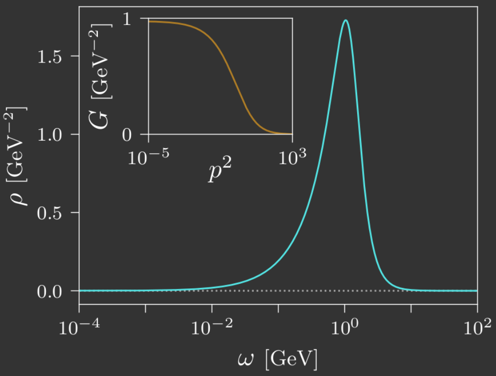

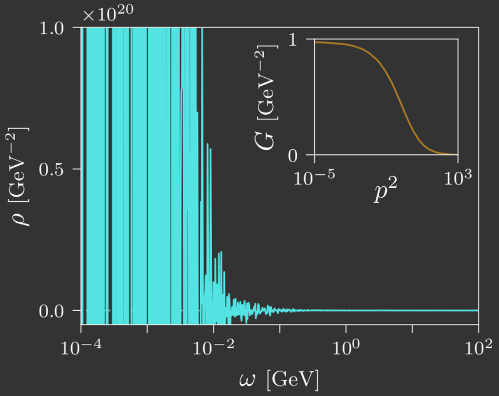

- Condition number $\kappa(\tilde{\mathbf{K}}) \approx \mathcal{O}(10^{33})$

  $\longrightarrow$ expect to lose $\sim$ 33 digits of accuracy with naive inversion

Numerical Demo

- GPR: $\boldsymbol{\rho} \approx \boldsymbol{\mu} + \mathbf{C}\tilde{\mathbf{K}}^T \left(\tilde{\mathbf{K}}\mathbf{C}\tilde{\mathbf{K}}^T + \sigma_n^2 \mathbb{1} \right)^{-1} \left((\mathbf{G} + \boldsymbol{\epsilon}) - \tilde{\mathbf{K}}\boldsymbol{\mu} \right)$

Numerical Demo

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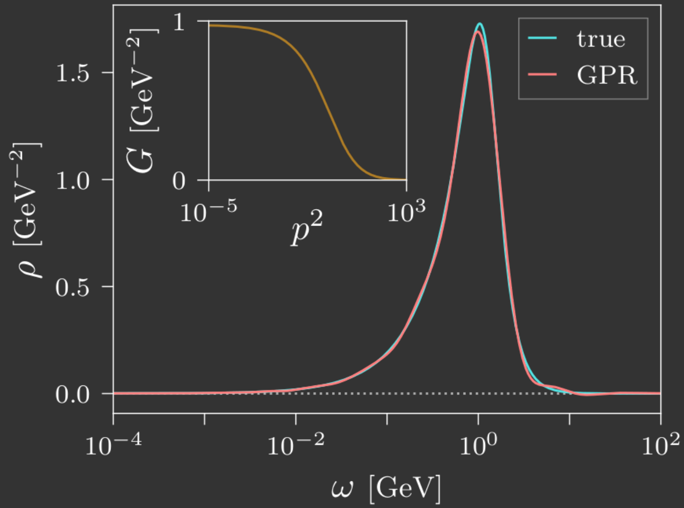
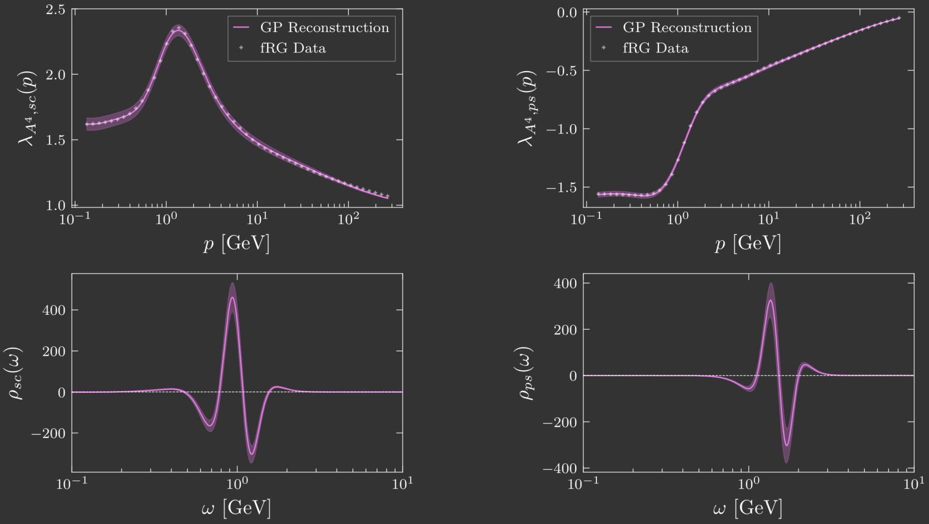


Application 1: bound state masses

2212.01113 [hep-ph]

- Scalar glueball: $J^{PC} = 0^{++}$
- Pseudo-sc. glueball: $J^{PC} = 0^{-+}$



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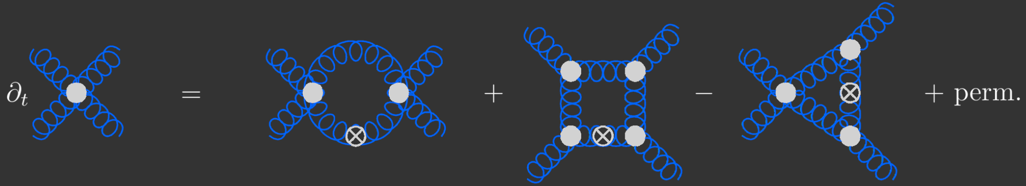

J^{PC}	lattice		DSE-BSE		this work
0^{++}	1760(70)	[9]	1850(130)	[18]	1870(75)
	1740(70)	[11]	1640	[15]	
	1651(23)	[12]			
	1618(26)(25)	[13]			
0^{-+}	2650(60)	[9]	2580(180)	[18]	2700(120)
	2610(70)	[11]	4530	[15]	
	2600(40)	[12]			
	2483(61)(55)	[13]			

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Mercer's theorem: $\forall$ continuous symmetric PSD kernels

$$C \ : \ [a, b] \times [a, b] \longrightarrow \mathbb{R}, \ C(x, y) = C(y, x) \, \forall \, x, y \in [a, b]$$

$\exists$ orthonormal basis of eigenfunctions $e_i(x)$ with non-negative eigenvalues λ_i s.t. $C(x, y) = \sum_{i=1} \lambda_i e_i(x) e_i(y)$.

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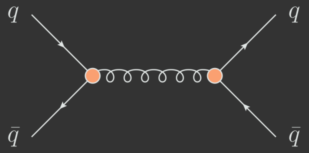
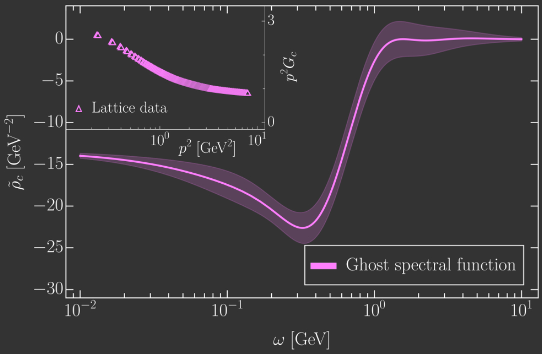
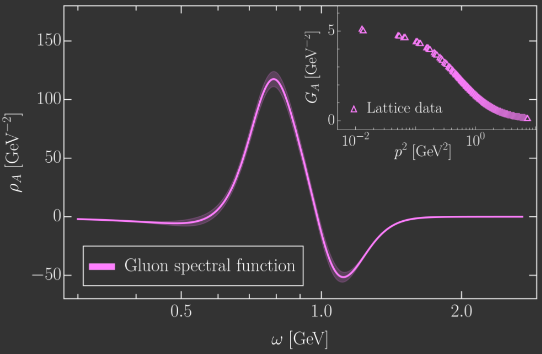
- E.g.: smooth transition from perturbative to non-pert. region

Application 2: S-matrix building blocks

2107.13464 [hep-ph], 2301.07785 [hep-ph]







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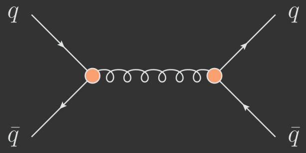

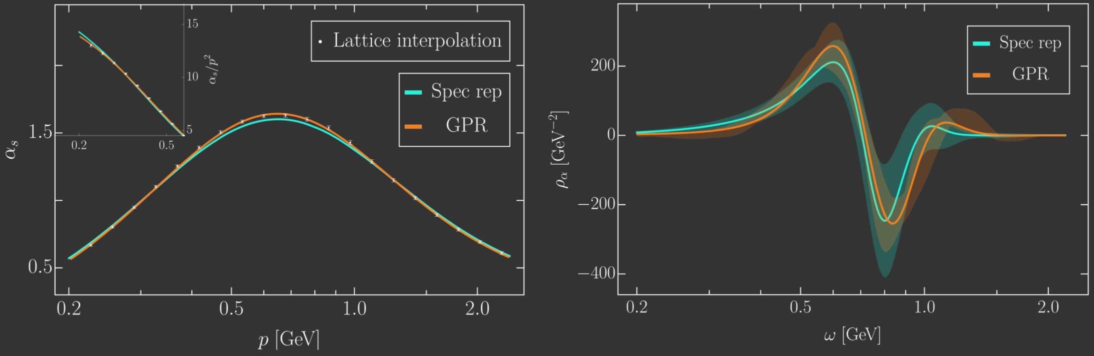

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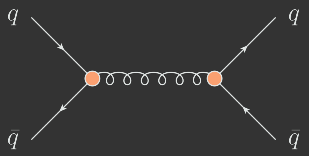
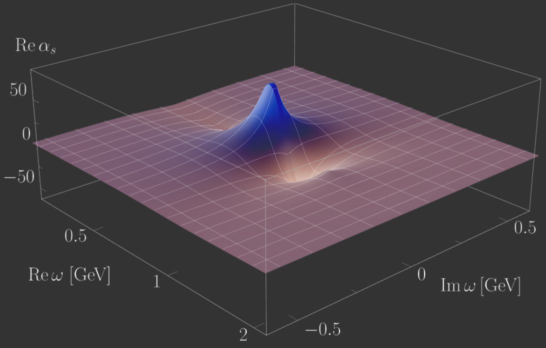
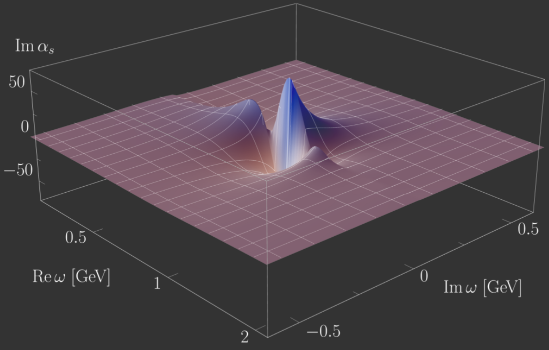
2107.13464 [hep-ph], 2301.07785 [hep-ph]







Outlook

- Algorithm:
  - Integrate out hyperparams via hyperpriors & HMC
  - Automatic kernel selection, hyperkernels, deep kernel learning
  - Inequality constraints like positivity & monotonicity
  - Smeared spectral densities from finite-volume correlators
- Data:
  - Increased resolution/precision of lattice & fRG results
  - Improved real-time constraints from spectral DSE
- Software:
  - **`fredipy`**: python package for Fredholm inversion, coming soon!
  - Couple to **`STAN-HMC`** for faster hyperparameter integration

Thanks!