Nevanlinna-Pick interpolation from uncertain Euclidean correlation functions

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Outline

- Lattice QCD and the inverse problem
- Nevanlinna–Pick interpolation
- Euclidean correlation functions
- Generating synthetic data and sample set
- Validation of approach
- Propagating computational errors through NP interpolation
- Conclusions and discussion

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The inverse problem

- The decay width we are ultimately interested in depends on a collection of the densities of hadronic states, $\rho(\omega)$:

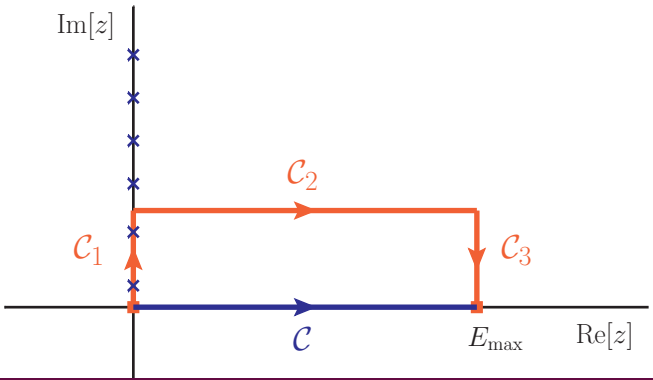
$$\Gamma = \int_0^{E_{\text{max}}} W(\omega)\rho(\omega)d\omega$$

$W(\omega) = (1 - \frac{\omega^2}{m_\tau^2})^2(1 + 2\frac{\omega^2}{m_\tau^2})$ is the corresponding weight function for the τ that vanishes $\omega = E_{\text{max}} = m_\tau$

- Using $\rho(\omega) = \frac{1}{\pi}\ \text{Im}\ G(\omega + i\epsilon)\big|_{\epsilon=0^+}$ where $G_i(\omega) = i\omega \int_0^\infty d\omega'\ \frac{\rho(\omega')}{\omega'(\omega' - i\omega)}$ this becomes:

$$\Gamma = \frac{1}{\pi}\int_0^{E_{\text{max}}} W(\omega)\,\text{Im}\left[G(\omega + i\epsilon)\right]\big|_{\epsilon=0^+}\, d\omega$$

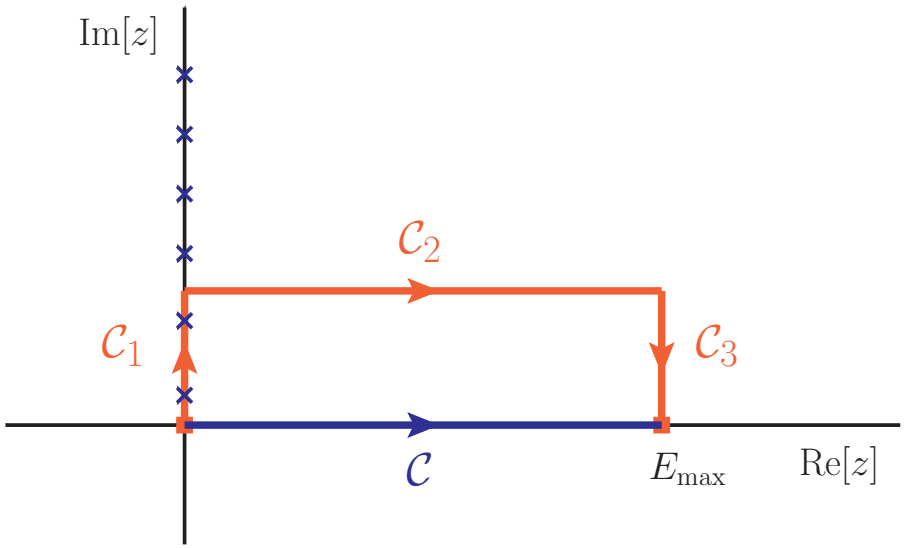
- Physical decay width $\Longrightarrow$ $G(\omega)$ evaluated on the positive real axis
- Real axis evaluation of $G(\omega)$ is inaccessible to lattice QCD. Using Cauchy's theorem, we deform the integral into the complex plane:



$$\Gamma = \text{Im}\left[\frac{1}{\pi}\int_{\mathcal{C}'} W(z)G(z)\,dz\right]$$

$$\mathcal{C}' = \mathcal{C}_1 \cup \mathcal{C}_2 \cup \mathcal{C}_3$$

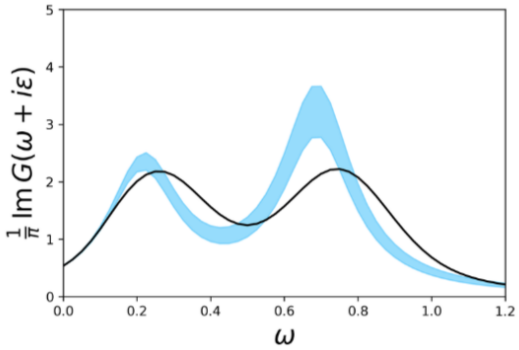
Inverse problem



- Evaluation of $\mathcal{C}_1$ is directly accessible with lattice QCD
- Evaluation of $\mathcal{C}_2$ requires $G(z)$ known elsewhere in the complex plane
- $\mathcal{C}_3$ potentially dangerous $\Rightarrow$ errors from interpolation blow up as the real axis is approached $\Rightarrow$ suppressed by the weight function

Nevanlinna-Pick Interpolation

- Nevanlinna–Pick incorporates the interpolation uncertainty by providing bounds (Wertevorrat) that constrain the interpolation function
- A Cayley transformation maps the complex energy plane into the complex unit disk where Nevanlinna–Pick interpolation can be applied
- By recursively applying Möbius transformations (mapping circles into circles), the interpolation constraints are imposed one at a time, progressively restricting the allowed region for the functions
- Vital element of Nevanlinna–Pick interpolation is the Pick criterion, matrix to the right is positive semi-definite $\Rightarrow$ condition guarantees the interpolation problem defined by the initial constraints is mathematically consistent



$$\begin{pmatrix} \frac{1-\Gamma_1\overline{\Gamma_1}}{1-\zeta_1\overline{\zeta_1}} & \cdots & \frac{1-\Gamma_1\overline{\Gamma_N}}{1-\zeta_1\overline{\zeta_N}} \\ \vdots & & \vdots \\ \frac{1-\Gamma_N\overline{\Gamma_1}}{1-\zeta_N\overline{\zeta_1}} & \cdots & \frac{1-\Gamma_N\overline{\Gamma_N}}{1-\zeta_N\overline{\zeta_N}} \end{pmatrix}$$

Nevanlinna-Pick interpolation

Our Previous Work

- Developed a method for the propagation of errors through Nevanlinna-Pick interpolation
- Began with **energy-dependent Euclidean Green's function values** as the input lattice data
- With a simple example, showed that the interpolation could preserve the scale of the original lattice uncertainties

This Work

- Uses more realistic spectral density with physically motivated high energy behavior
- Starts from **lattice two-point Euclidean space-time correlator** and introduces required discrete Laplace transform
- Extends the reconstruction with relevant weight function and evaluates the full contour integral required for decay calculation

Euclidean correlation functions

- From lattice QCD we get the Euclidean two-point current-current correlator,

$$C(t) = \sum_{\vec{x}} \sum_{\mu=1}^{3} \left\langle J_\mu(\vec{x}, t)\, J_\mu^\dagger(\vec{0}, 0) \right\rangle .$$

- Using the spectral representation, this correlator can be written as

$$C(t) = \int_0^\infty d\omega\, \rho(\omega)\, \omega^2 e^{-\omega t}$$

where the factor of ω^2 arises from the Lorentz structure of the vector current correlator after projecting onto zero spatial momentum

- the three-times subtracted Laplace transform of the Euclidean time correlator extending the prescription in [Bernecker and Meyer, arXiv:1107.4388]:

$$G^{(3)}(\omega) = \frac{-1}{\omega^2} \int_0^\infty dt\; C(t) \left(e^{i\omega t} - 1 - i\omega t + \frac{1}{2}(\omega t)^2 \right)$$

where the subtractions remove the low-order polynomial contributions eliminating unphysical divergence and improving dispersion relation convergence

Generating synthetic data

- The target spectral density is based on the R ratio in [Bernecker and Meyer, arXiv:1107.4388]:

$$\begin{aligned} R(\omega) =& \theta(\omega - 2m_\pi)\theta(4.4m_\pi - \omega)[\frac{1}{4}(1 - \frac{4m_\pi^2}{\omega^2})^{\frac{3}{2}}(0.6473 + f_0(\omega)] \\ &+ \theta(\sqrt{s} - 4.4m_\pi)\theta(M_3 - \sqrt{s})[f_1(\omega) + f_2(\omega)] \\ &+ \theta(\omega - M_3)[f_3(\omega) + 3((\frac{2}{3})^2 + 2(\frac{1}{3})^2)] \end{aligned}$$

$$f_i(\omega) = \frac{C_i \Gamma_i^2}{4(\omega - M_i)^2 + \Gamma_i^2}$$

- Relation $\rho(\omega) = \frac{R(\omega)}{12\pi^2}$ is used to get synthetic correlator data from this known spectral density:

$$C(t_n) = \int_0^{\omega_{max}} d\omega\, \rho(\omega)\, \omega^2 e^{-\omega t_n}$$

where $t_n = n * a$

- The spectral integral is truncated at $\omega_{\max} = 6$ as higher energy contributions are exponentially suppressed by $e^{-\omega t_n}$, $N = 48$ time slices and a lattice spacing of $0.5\mathrm{GeV}^{-1}$

Laplace transforming synthetic data

- With discrete correlator data $C(t_n)$ we evaluate a standard discrete Laplace transforming:

$$G^{(3)}(\omega_k) = \frac{-1}{\omega_k^2} \sum_{t_n=0}^{N} dt\ C(t_n) \left(e^{i\omega_k t_n} - 1 - i\omega_k t_n + \frac{1}{2}(\omega_k t_n)^2 \right)$$

- For the choice of frequencies

$$\omega_k = \frac{2\pi}{N} \frac{1}{a}(k + \frac{1}{2})$$

for $0 \leq k \leq 8$

- We assign Parisi-Lepage based uncertainties to the correlators and sample within these errors to generate mock ensembles and the corresponding covariance matrix

The goal is then to find sample sets of $G(\omega_k)$ for $0 \leq k \leq 8$ that are **both** Pick-consistant and are consistent with the assigned uncertainties, quantified by χ^2

Obtaining Samples

In practice, doing this led to a covariance matrix that was extremely ill-conditioned...

Alternative approach

$$G^{(3)}(\omega) = \frac{-1}{\omega^2} \sum_{t_n=0}^{N} dt\ C(t_n) \left(e^{i\omega t_n} - 1 - i\omega t_n + \frac{1}{2}(\omega t_n)^2 \right)$$

- Instead consider the twice-subtracted descrete Laplace transform:

$$G^{(2)}(i\omega) = \frac{-1}{\omega^2} \left[\sum_{t_n=1}^{N} C(t_n) \left[e^{i\omega t_n} - 1 - i\omega t_n \right] \right] + 2 \left(\frac{1}{3} \right)^2 \left(\frac{i\omega}{4\pi^2} \right) \leftarrow$$

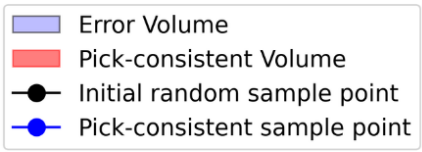
The contribution from $C(0^+)$ taken from perturbation theory needed for the trapezoidal rule

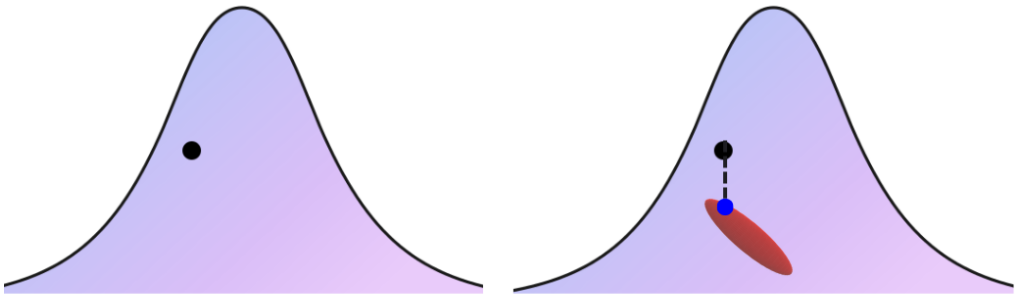
- The Green's function which determines the decay rate would be this $G^{(2)}$, and the real constant c_2 which we will omit:

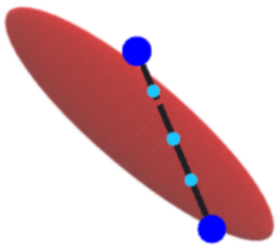
$$G^{(3)}(\omega) = G^{(2)}(\omega) - c_2$$

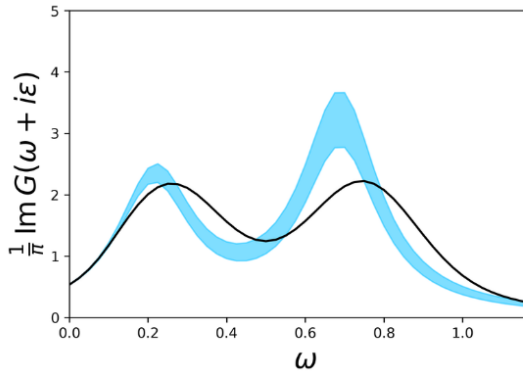
- c_2 does not impact the Pick-consistency requirement, automorphisms of the disk commute in Nevanlinna-Pick interpolation
- In addition, this shift will drop out of the finial contour integration
- We can then take advantage of the fact that the twice subtracted Laplace transform results in a covariance matrix that is better conditioned!

Method of getting samples in the Pick-consistent region



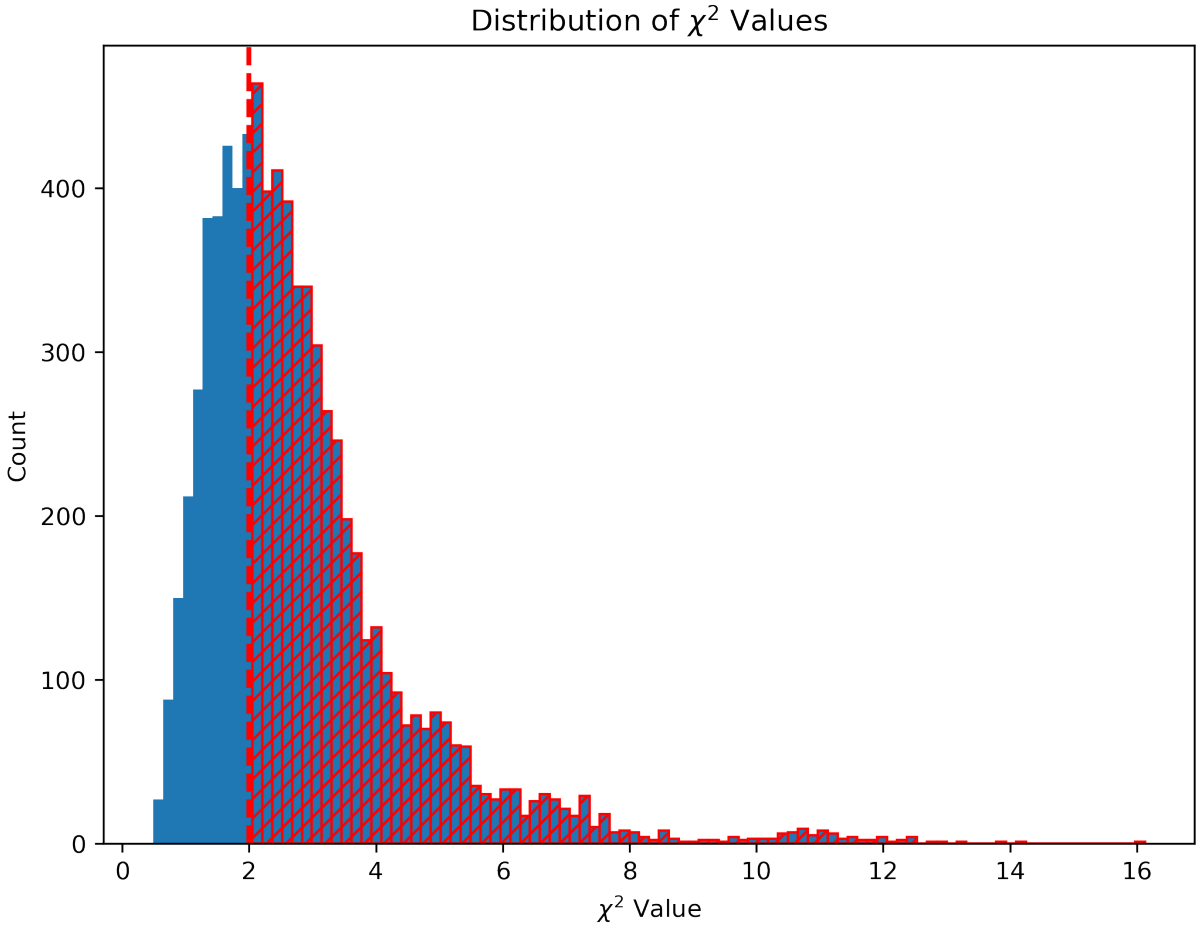






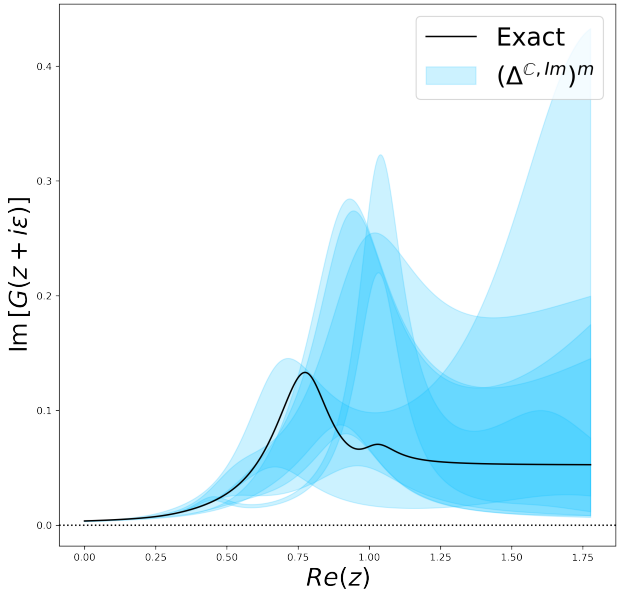
randomly distribute points within error → follow gradient ascent* to move to boundary points of the Pick-consistent volume → connect boundary points with lines and sample along them → perform Nevanlinna-Pick interpolation with each data sample set resulting in absolute bounds

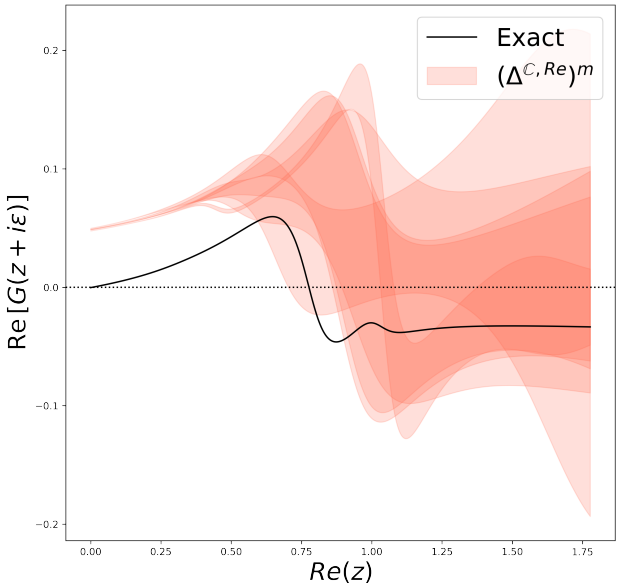
χ^2 distribution

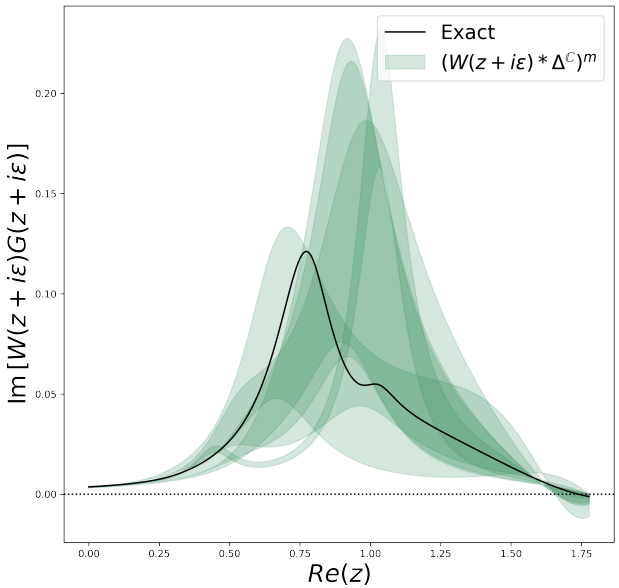


- Total samples generated: 7740
- Samples satisfying the selection criterion ($\chi^2 \leq 2$): **2625**

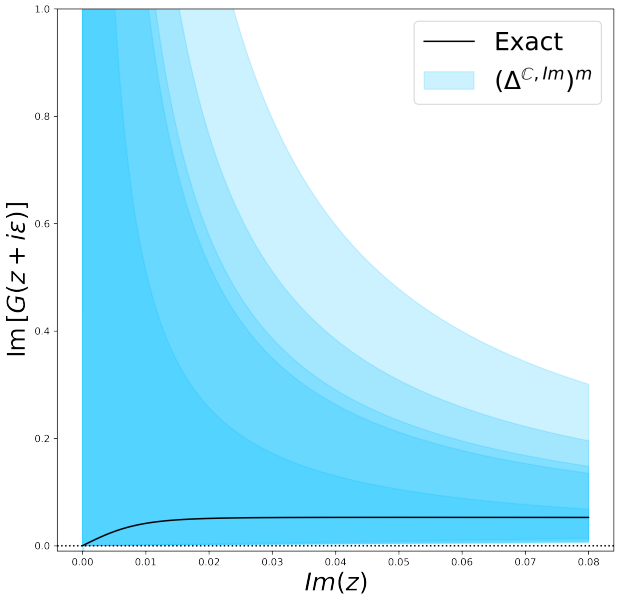
Validation of approach- $\mathcal{C}_2$

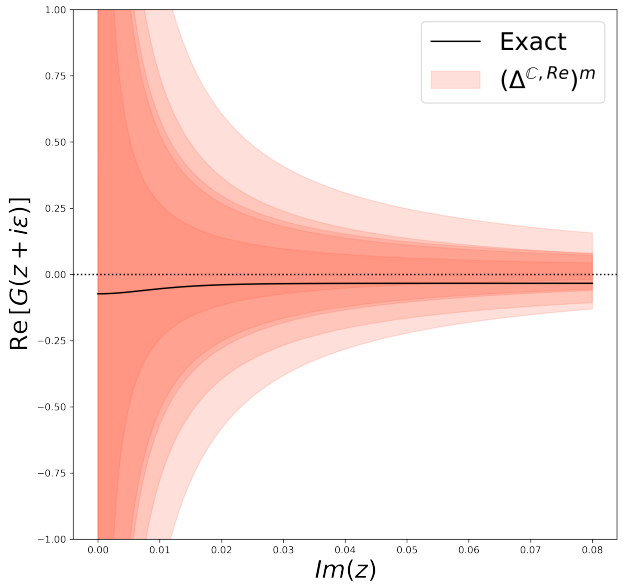


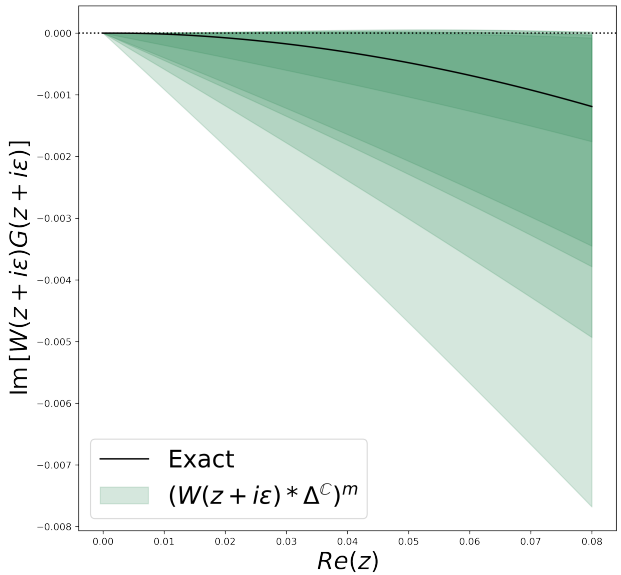




Validation of approach- $\mathcal{C}_3$







Validation of approach

	$\langle \mathcal{I}^{\mathrm{Im}}_{W,\mathrm{avg}} \rangle$	$\mathcal{I}^{\mathrm{Im}}_{W,\mathrm{Exact}}$	%error	error from avg fluctuations	error from widths
$\mathcal{C}_2$	0.0212 $\pm$ 0.0096	0.01899	45.28%	0.0024	0.0093
$\mathcal{C}_3$	1.6897e-06 $\pm$ 2.9248e-05	7.8320e-06	0.138%	6.1204e-06	2.8600e-05

- Note: 80% of the total error comes from the interpolation uncertainty which can be made much smaller if we interpolate from Green's function values at more than 8 energies

Conclusions, Discussion, and Future Work

- Presented a method that starts from synthetic Euclidean time correlator data and generates samples of Green's function values at a sample set of energies that are Pick-consistent and consistent with uncertainties through a χ^2 criteria

- For the $\mathcal{C}_2$ contour segment, the reconstructed contour integral agrees with the exact value within the estimated uncertainty

- Showed $\mathcal{C}_3$ contour segment can also be reconstructed using this approach, however it is negligible within error for choice of $\epsilon \Rightarrow$ another possible avenue for tuning to improve error

- Although relatively large uncertainties are obtained in these preliminary results, they can be reduced by increasing the number of frequencies at which the discrete Laplace transform is evaluated $\Rightarrow$ increase the number of interpolation conditions

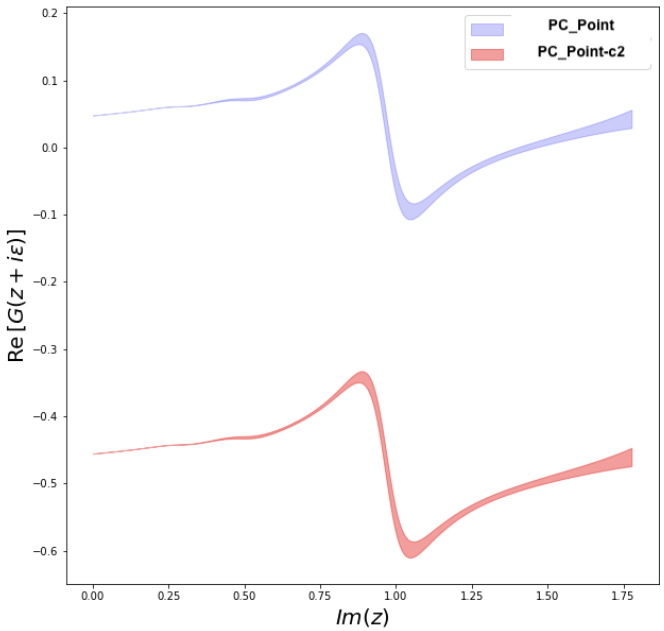
Backup Slides

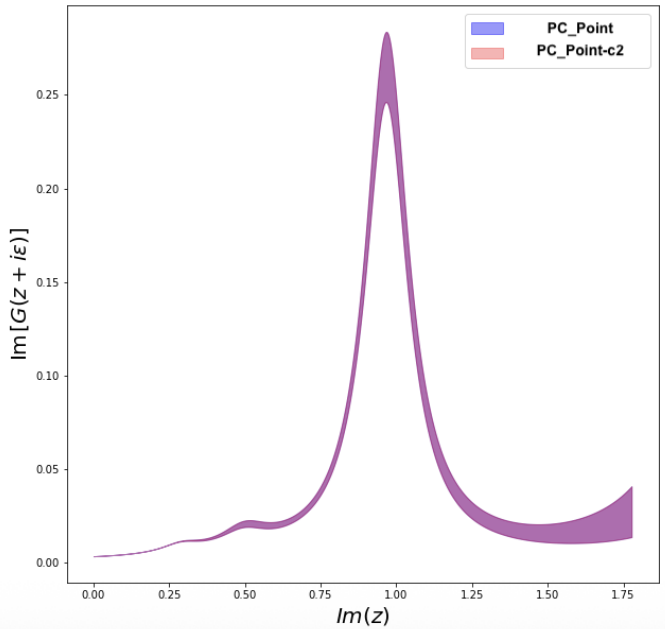
Table of Coefficients

The physical pion mass m_π used was 0.13957.

	C_i	M_i/GeV	Γ_i/GeV
0	655.5	0.7819	0.0358
1	8.5	0.765	0.130
2	11.5	0.7820	0.00829
3	50.0	1.0195	0.00426

Example





$$G(\omega) = \int_0^{E_{\max}} d\omega' \, \frac{\rho(\omega')\,\omega'^2}{\omega' - \omega} - c_0 - c_1\omega - c_2\omega^2$$

$$c_0 = \int_0^{E_{\max}} d\omega' \, \rho(\omega')\omega', \qquad c_1 = \int_0^{E_{\max}} d\omega' \, \rho(\omega'), \qquad c_2 = \int_0^{E_{\max}} d\omega' \, \rho(\omega') \, \frac{1}{\omega'}$$

Propagating computational errors through NP interpolation

– We use each of our M samples to calculate the integral:

$$\mathcal{I}_Y^{X,m} = \frac{1}{\pi} \int_{C_2} \left(\Delta_Y^X(z)\right)^m dz$$

Here $\Delta_Y^X(z)$ is the Wertevorrat, $Y =$ 'max', 'min', or 'avg', X is either 'Re' or 'Im', $1 \leq m \leq M$ where M is the number of samples

– The average of the M samples is then:

$$\left\langle \mathcal{I}_{\text{avg}}^X \right\rangle = \frac{1}{M} \sum_{m=1}^{M} \mathcal{I}_{\text{avg}}^{X,m}$$

– We can then study the error associated with the fluctuations of the sample averages around the mean:

$$\mathcal{E}_{\text{mean}}^X = \left[\frac{1}{M} \sum_m \left(\frac{\left(\mathcal{I}_{\text{max}}^X\right)^m + \left(\mathcal{I}_{\text{min}}^X\right)^m}{2} - \left\langle \mathcal{I}_{\text{avg}} \right\rangle \right)^2 \right]^{\frac{1}{2}}$$

– There is also error associated the width of the bounds calculated from the Wertevorräte:

$$\mathcal{E}_{\mathrm{W}}^{X} = \left[\frac{1}{M} \sum_{m} \left(\frac{\left(\mathcal{I}_{\max}^{X}\right)^{m} - \left(\mathcal{I}_{\min}^{X}\right)^{m}}{2} \right)^{2} \right]^{\frac{1}{2}}$$

– An appealing definition of the total error is:

$$\mathcal{E}^{X} = \left[\frac{1}{2M} \sum_{m} \left(\left(\mathcal{I}_{\max}^{X}\right)^{m} - \langle \mathcal{I}_{\mathrm{avg}} \rangle \right)^{2} + \frac{1}{2M} \sum_{m} \left(\left(\mathcal{I}_{\min}^{X}\right)^{m} - \langle \mathcal{I}_{\mathrm{avg}} \rangle \right)^{2} \right]^{\frac{1}{2}}$$

– With a little algebra, this total error $\mathcal{E}$ can be written as:

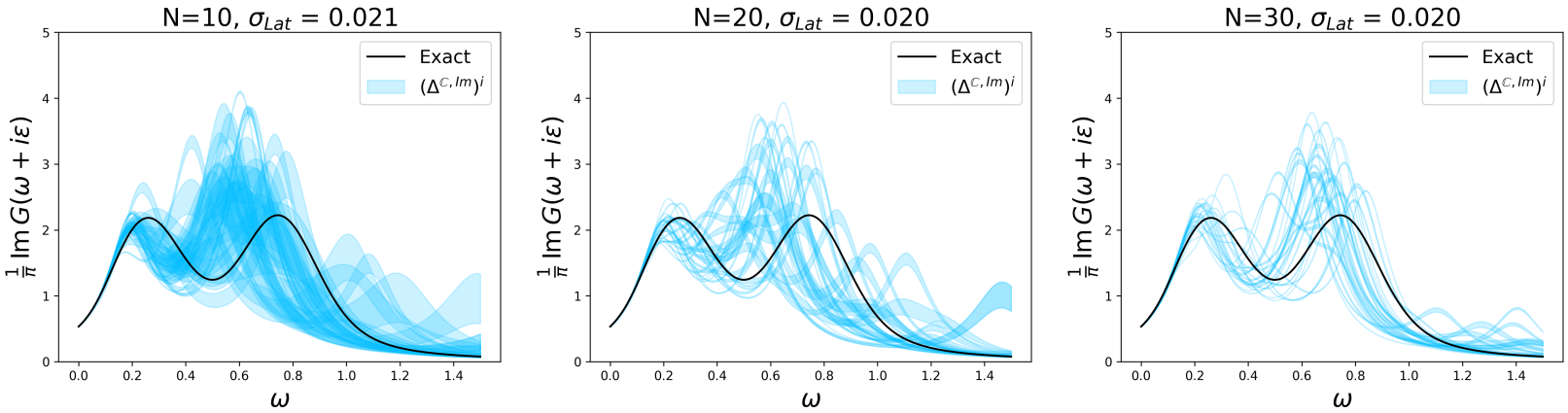
$$\mathcal{E}^{X} = \left[\left(\mathcal{E}_{\mathrm{W}}^{X}\right)^{2} + \left(\mathcal{E}_{\mathrm{mean}}^{X}\right)^{2} \right]^{\frac{1}{2}}$$

X is either ‘Re’ or ‘Im’ and $1 \leq m \leq M$ where M is the number of samples

Error form

$$\sigma_{\text{Lepage}}(n) = \frac{0.02 * C(3)}{e^{-3m_\pi}} e^{-m_\pi n}$$

Results - Dependence on N



N	$\left\langle \mathcal{I}^{lm}_{\mathrm{avg}} \right\rangle$	$\mathcal{E}^{lm}_{\mathrm{mean}}$	$\mathcal{E}^{lm}_{\mathrm{W}}$
10	1.682 ± 0.204	0.044	0.199
20	1.669 ± 0.059	0.034	0.048
30	1.671 ± 0.035	0.032	0.014
$\mathcal{I}^{lm}_{\mathrm{Exact}}$	1.706	-	-

The initial points z_n were chosen as equally spaced values along the interval $\{0.1i, 2.0i\}$ for the given number of points. The error scaling factor was 0.01 and the ϵ value was 0.1

Results - Dependence on N width distributions