Approaches to the Inverse Fourier Transformation with Limited and Discrete Data

Speaker: Yu-Fei Ling

Joint work with Jun Hua, Jian Liang, Ao-Sheng Xiong, and Qi-An Zhang

South China Normal University, Guangzhou, China

Outline

- Motivation
- Ill-posedness
- Inversion methods
  - Tikhonov regularization
  - Backus-Gilbert
  - Bayesian approach
  - Artificial neurons network (ANN)
  - Results
- Conclusions&Outlook

Motivation

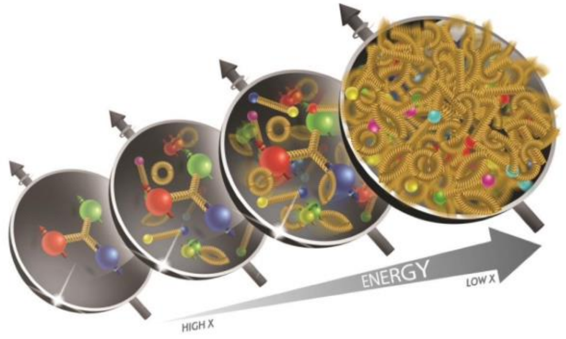
The partonic structure of hadron—the fundamental goal

- Lattice QCD is formulated in Euclidean space-time.

Mismatch

- light-cone PDFs/DAs are formulated in Mikowski space-time.

- Direct calculation of light-cone PDFs/DAs from first principles remained a major challenge for a long time.



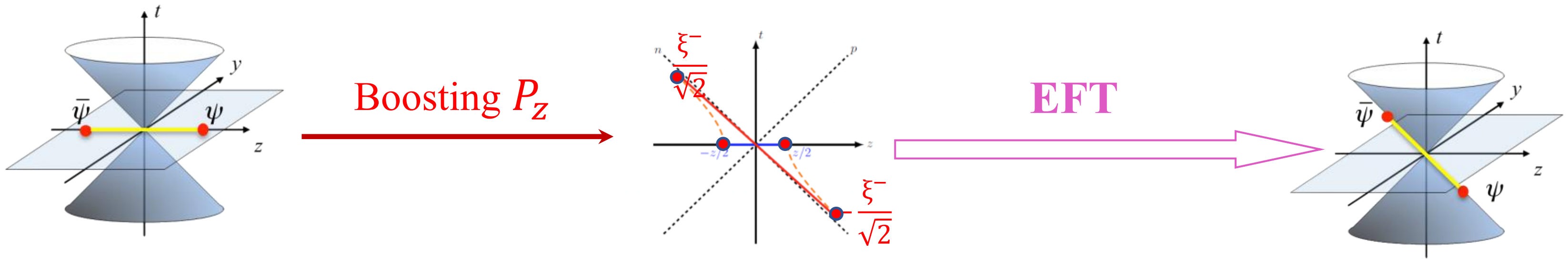
Motivation

LaMET—transformative progress

- A direct pathway to access light-cone observables

- We can define an equal-time, spatial separated quasi-DA which can be calculated by lattice QCD.

- Quasi-DA and LCDA are related by a rigorous factorization formula. (Matching)



Motivation

Key numerical step in LaMET: obtain the momentum-fraction quasi-DA from non-local matrix elements computed in Euclidean lattice

- $g(\lambda)$ and $f(x)$ are related by a Fourier transform

$$\underbrace{g(\lambda)}_{\text{We have}} = \int dx e^{-i\lambda x} \underbrace{f(x)}_{\text{Our target}},$$

- $g(\lambda)$ is the renormalized matrix element of non-local Euclidean operator
- $f(x)$ is the corresponding quasi-DA in momentum space

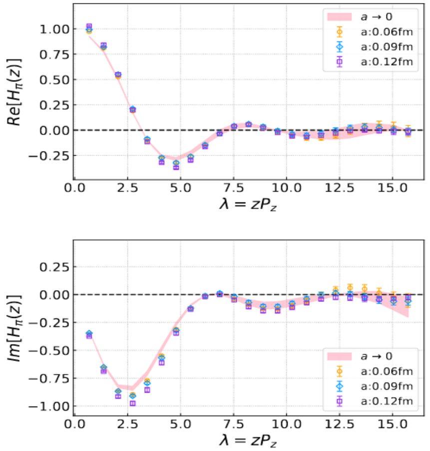
Motivation

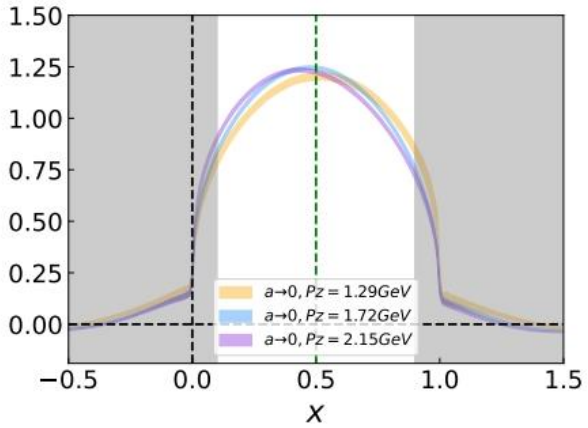
Physics-driven λ-extrapolation is good and effective

- Only a finite and discrete set of λ values is available, leading to a limited inverse discrete Fourier transform (L-IDFT)

$$f(x)=\int_{-\infty}^{\infty}\frac{d\lambda}{2\pi}e^{i\lambda x}g(\lambda)\rightarrow\sum_{-\lambda_{\rm cut}}^{\lambda_{\rm cut}}\frac{\Delta\lambda}{2\pi}e^{i\lambda x}g(\lambda).$$

- Extrapolate $g(\lambda)$ at large Euclidean separation based on physical constraint and perform the inverse Fourier transform to make it





(LPC)Jun Hua et.al. PRL129. 132001(2022)

Motivation

New perspective: inverse problem approach

- Given the integral $g(\lambda)$, find the function $f(x)$ (Inverse problem)
- Inverse problem is everywhere
- Inverse problem theory: mature mathematical field
- Strong foundation in mathematics
- Practical application in many field

$$g(\lambda) = \int dx e^{-i\lambda x} f(x),$$

Classic books on the inverse problem theory:

Solutions of Ill-Posed Problems (1977)
Computational Methods for Inverse Problems (2002)
Inverse Problem Theory and Methods for Model Parameter Estimation (2005)
Statistical and Computational Inverse Problems (2005)

Recovering image using inverse problem method

(T. Albert. Inverse Problem Theory and Methods for Model Parameter Estimation (2005), SIAM.)

Ill-posedness

Ill-posedness is the key to the inverse problem

- **Well-posedness:** satisfy the **existence**, **uniqueness** and **stability**
- **Ill-posedness:** fail to satisfy any one of the above condition

The ill-posedness of limited Fourier inversion problem

$$g(\lambda) = \int dx e^{-i\lambda x} f(x),$$

- **Existence**: guaranteed by the Wiener-Paley theorem
- **Uniqueness**: proven for the first time in our paper, provided that $g(\lambda)$ is a continuous function or a convergent sequence (Ao-Sheng Xiong et al. arXiv: 2506.16689)
- **Instability**: tiny change in the data $g(\lambda)$ can lead to a big changes in the output $f(x)$

Ill-posedness

Quantify the instability using SVD formulation

- Transform the integral equation into a system $Kf = g$
- Singular value decomposition (SVD) of the K reveals rapidly decaying singular values σ_i
- SVD provides a general solution
- the f^{δ} form noisy data g^{δ} diverges from the true solution f obtained with exact data g

$$g(\lambda) = \int dx e^{-i\lambda x} f(x),$$

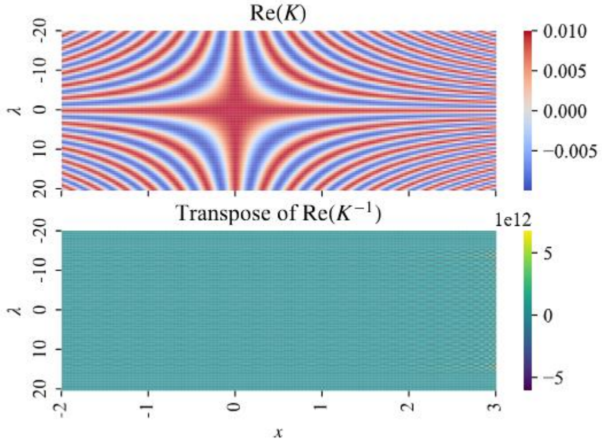
$$g_k = \sum_j K_{kj} f_j,$$

$$K_{kj} = e^{-i\lambda_k x_j} \Delta x,$$

$$K_{\mathrm{re}} = U \Sigma V^T = \sum_{i=1}^{n} u_i \sigma_i v_i^T,$$

$$\boxed{f = \sum_{i=1}^{n} \frac{u_i^T g}{\sigma_i} v_i.}$$

$$\boxed{\begin{aligned} \|f^{\delta} - f_{\mathrm{true}}\|_2^2 &= \sum_{i=1}^{n} \left(\frac{u_i^T (g^{\delta} - g_{\mathrm{true}})}{\sigma_i} v_i\right)^2, \\ &= \sum_{i=1}^{n} \left(\frac{u_i^T \delta}{\sigma_i} v_i\right)^2, \end{aligned}}$$



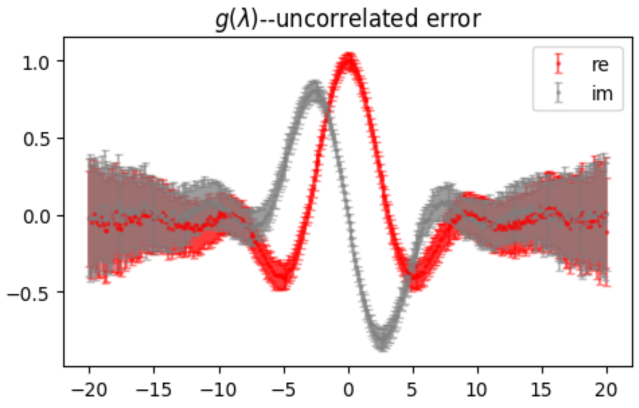
$$\sigma_1 = 0.3545 \geq \cdots \geq \sigma_n = 3.8 \times 10^{-18},$$

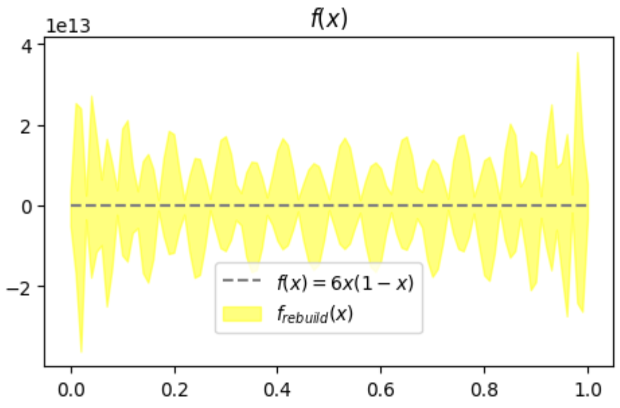
Ill-posedness

The instability of direct inversion

$$\boldsymbol{f} = (\boldsymbol{K}^{\dagger}\boldsymbol{K})^{-1}\boldsymbol{K}^{\dagger}\boldsymbol{g}$$

- A true solution is defined as $f_t(x) = 6x(1-x)$
- Get the noise-free data $g_t(\lambda)$ via integration
- Add noise to create the perturbed data $g^{\delta}(\lambda)$
- Reconstruct $f^{\delta}(x)$ from $g^{\delta}(\lambda)$ by direct inversion
- The reconstructed $f^{\delta}(x)$ on the right





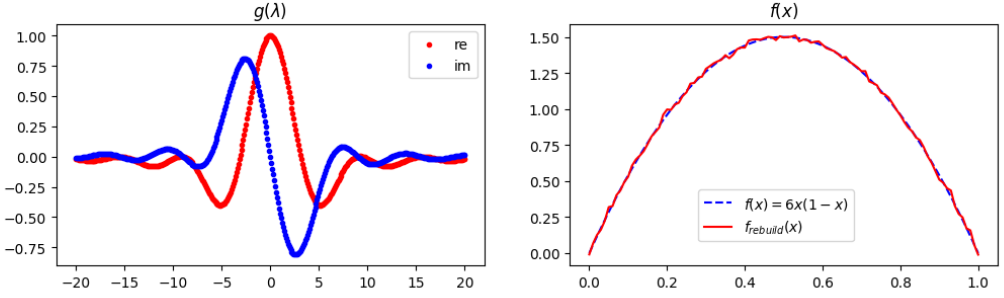
The inverse problem of limited discrete Fourier inversion is ill-posed: existence and uniqueness but instability

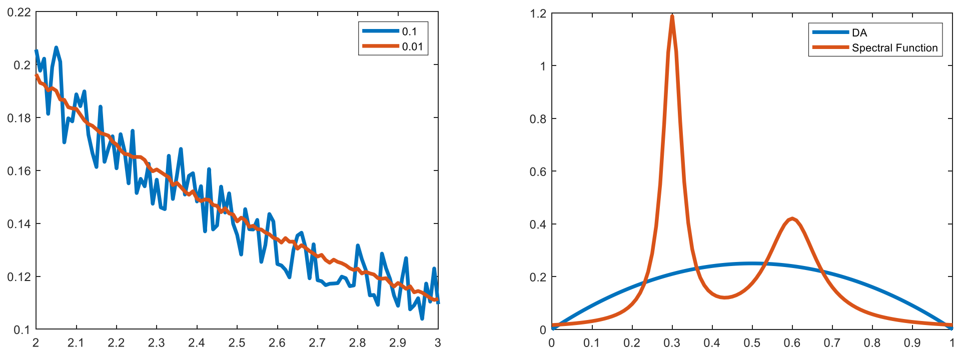
Ill-posedness

Factors influencing the difficulty of ill-posed problems:

- ➢ Error level: the lower noise the input has, the easier it is to solve

- ➢ Behavior of the true $f(x)$: the simpler and smoother the true solution is, the easier it is to reconstruct





The limited discrete Fourier inversion problem is tractable

- ➢ Error level: reconstruction quality improves with lower error in the quasi-DA
- ➢ Solution Nature: the DA has a simple form

Inversion methods—Tikhonov regularization

Tikhonov regularization is a standard technique for addressing ill-posed inverse problems

- Aim to find the minimizer f_α^δ of the Tikhonov functional:

$$\begin{aligned} \boldsymbol{f}_{\text{reg}} &= \arg\min_{\boldsymbol{f}} L(\boldsymbol{f}), \\ &= \arg\min_{\boldsymbol{f}} [\underbrace{(\boldsymbol{K}\boldsymbol{f}-\boldsymbol{g})^T(\boldsymbol{K}\boldsymbol{f}-\boldsymbol{g})}_{\textbf{data fitness}} + \underbrace{\alpha||\boldsymbol{\Gamma}\boldsymbol{f}||_2^2}_{\textbf{regulator}}], \end{aligned}$$

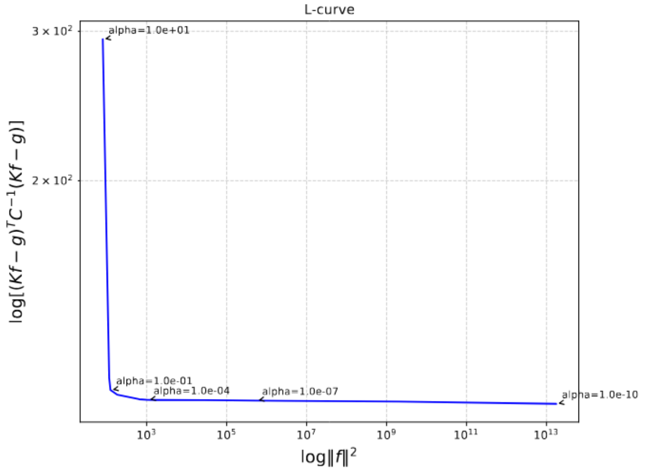
- Using variational principles, the solution is given by:

$$\boldsymbol{f}_{\text{reg}} = (\boldsymbol{K}^T\boldsymbol{K} + \alpha\boldsymbol{\Gamma}^T\boldsymbol{\Gamma})^{-1}\boldsymbol{K}^T\boldsymbol{g}.$$

- Overcome instability by slowing down the rapid decay of singular values

$$\frac{\sigma_1}{\sigma_n} \Rightarrow \frac{\sigma_1+\alpha}{\sigma_n+\alpha} \approx \frac{\sigma_1}{\alpha},$$

L-curve



- The regularization parameter α can be rigorously determined using L-curve criterion

Inversion methods—Backus-Gilbert

The Backus-Gilbert (BG) method and Tikhonov approach are conceptually similar

- Assumes the solution $f_{est}(x')$ can be expressed as a linear combination of the data $g(\lambda_i)$

$$f_{\rm est}(x') = \sum_i a_i(x')\boldsymbol{g}_i, \qquad \boldsymbol{g}_i \equiv g(\lambda_i) = \int_{x_{\min}}^{x_{\max}} dx\, K(x,\lambda_i) f_{\rm true}(x),$$

$$= \sum_i \int_{x_{\min}}^{x_{\max}} dx a_i(x') K(x,\lambda_i) f_{\rm true}(x),$$

$$= \int_{x_{\min}}^{x_{\max}} dx \rho(x-x') f_{\rm true}(x),$$

- A trade off between the width l of resolution function $\rho(x-x')$ and the solution stability, leading to minimizing the objective functional $L[\boldsymbol{a}]$

$$l(x') = \int_{x_{\min}}^{x_{\max}} dx (x-x')^2 (\rho(x-x'))^2.$$

$$1 = \int_{x_{\min}}^{x_{\max}} dx \rho(x-x').$$

normalized constraint

$$\boxed{L[\boldsymbol{a}] = \underbrace{\boldsymbol{a}^T \boldsymbol{H} \boldsymbol{a}}_{\textbf{width } l} + \underbrace{\alpha \boldsymbol{a}^T \boldsymbol{C}_{\boldsymbol{g}} \boldsymbol{a}}_{\textbf{regulator}} + \beta\underbrace{(\boldsymbol{a}^T \boldsymbol{m} - 1)}_{\textbf{normalized constraint}},}$$

- Using variational principles, the optimal vector $\boldsymbol{a}$ is given by:

$$\boldsymbol{a}_{\rm op} = \frac{1}{\boldsymbol{m}^T (\boldsymbol{H} + \alpha \boldsymbol{C}_{\boldsymbol{g}})^{-1} \boldsymbol{m}} (\boldsymbol{H} + \alpha \boldsymbol{C}_{\boldsymbol{g}})^{-1} \boldsymbol{m}.$$

Inversion methods—Bayesian approach

In the Bayesian framework, the unknown solution is modeled as a random variable characterized by a probability distribution

- The Bayesian approach is based on Bayes' theorem:

$$
\begin{aligned}
p(\boldsymbol{f}|\boldsymbol{g},I) &= \frac{p(\boldsymbol{g}|\boldsymbol{f},I)\cdot p(\boldsymbol{f}|I)}{\int_{\text{possible solutions}} p(\boldsymbol{g}|\boldsymbol{f},I)\cdot p(\boldsymbol{f}|I)d\boldsymbol{f}}, \\
&\propto p(\boldsymbol{g}|\boldsymbol{f},I)\cdot p(\boldsymbol{f}|I),
\end{aligned}
$$

- Prior distribution $p(\boldsymbol{f}|I)$: encodes the knowledge about the solution $\boldsymbol{f}$ without data

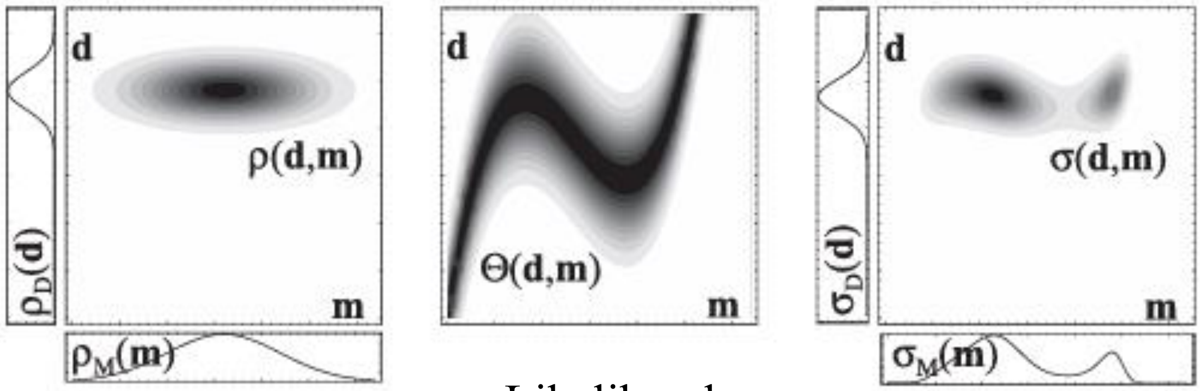
- Likelihood distribution $p(\boldsymbol{g}|\boldsymbol{f},I)$: quantifies how well the solution explain the data

- Posterior distribution $p(\boldsymbol{f}|\boldsymbol{g},I)$: The probability distribution of the final solution.

Inversion methods—Bayesian approach

Instability corresponds to a probability distribution with large uncertainty

- Prior distribution $p(\boldsymbol{f}|\boldsymbol{I})$ serves as a regulator to overcome instability



Prior

Likelihood
(large uncertainty)

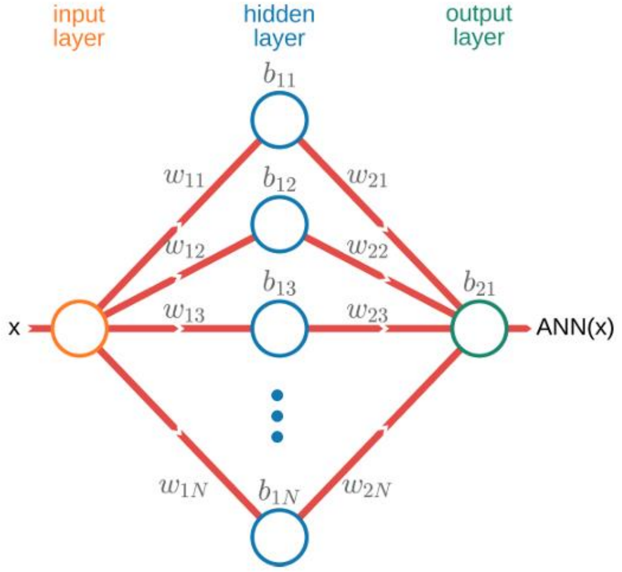
Posterior

(T. Albert. Inverse Problem Theory and Methods for Model Parameter Estimation (2005), SIAM.)

- The solution to the problem is determined from the posterior distribution using Maximum a posteriori (MAP) estimation or posterior mean estimation

Inversion methods—ANN

- ANN provides a powerful non-linear representation capacity which enables it to approximate highly complex mappings.



(Min-Huan Chu et.al. arXiv: 2506.16689)

- Minimizing the following loss function corresponds to finding a configuration of the network parameters that provides the optimal solution to the problem.

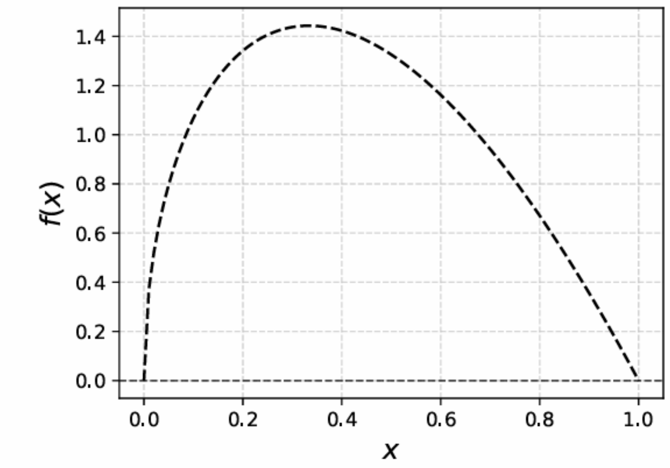
$$\chi^2(\{w\},\{b\}) = \left[(\boldsymbol{K}\boldsymbol{f}_{\{w\},\{b\}} - \boldsymbol{g})^T C_{\boldsymbol{g}}^{-1}(\boldsymbol{K}\boldsymbol{f}_{\{w\},\{b\}} - \boldsymbol{g})\right].$$

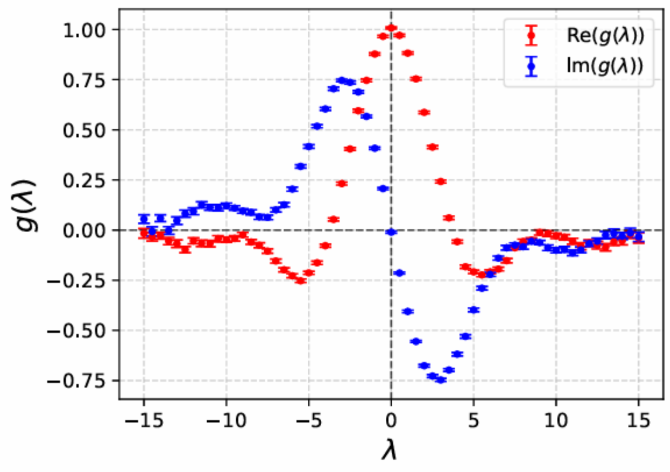
Inversion methods—Results

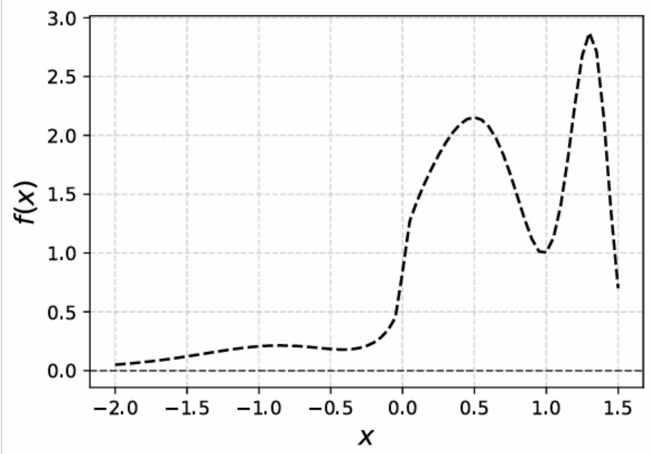
Toy models I&II：Include correlated errors and uncorrelated errors

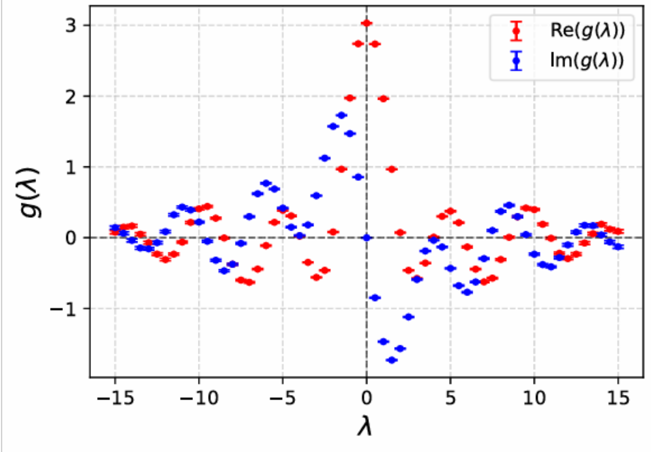
$$f(x)=\begin{cases}\frac{\Gamma(0.5+1+2)}{\Gamma(0.5+1)\Gamma(1+1)}x^{0.5}(1-x), & x\in[0,1]\\ 0, & \text{otherwise}\end{cases}.$$

$$f(x)=(\sqrt[3]{x}+x^2)e^{-x^2+x}+\sin(e^{\frac{\pi x}{2}}),\quad x\in[-2,1.5].$$







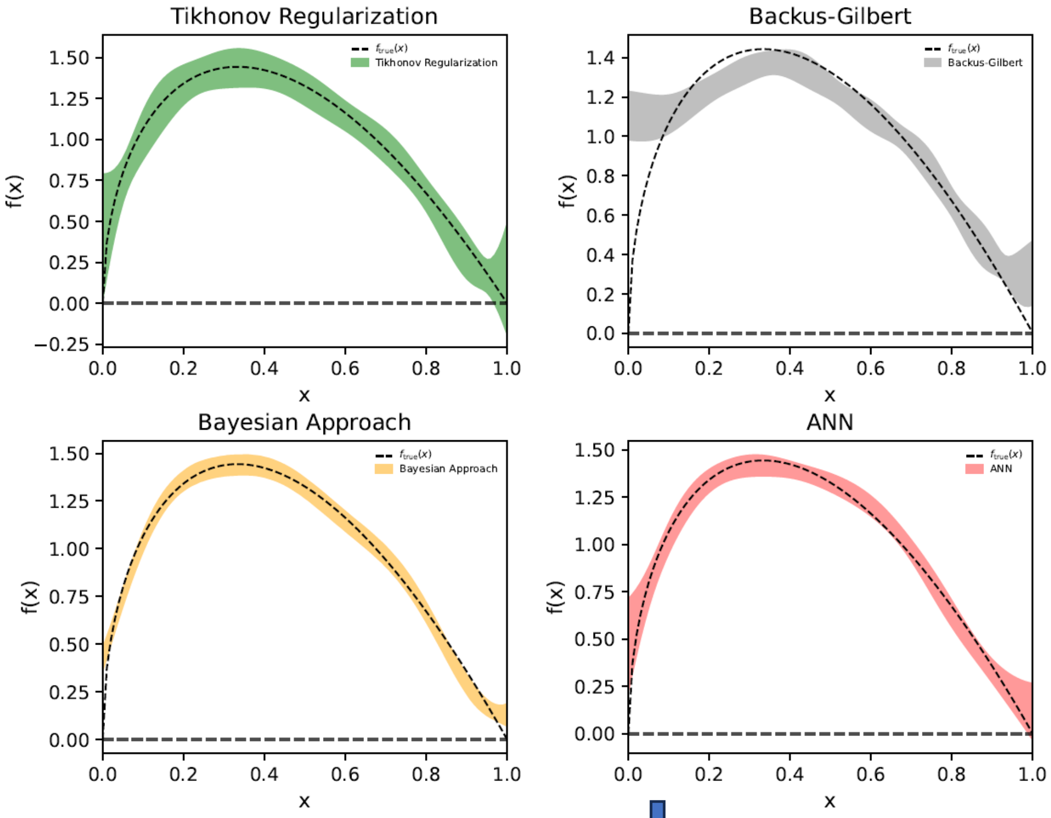


Inversion methods—Results

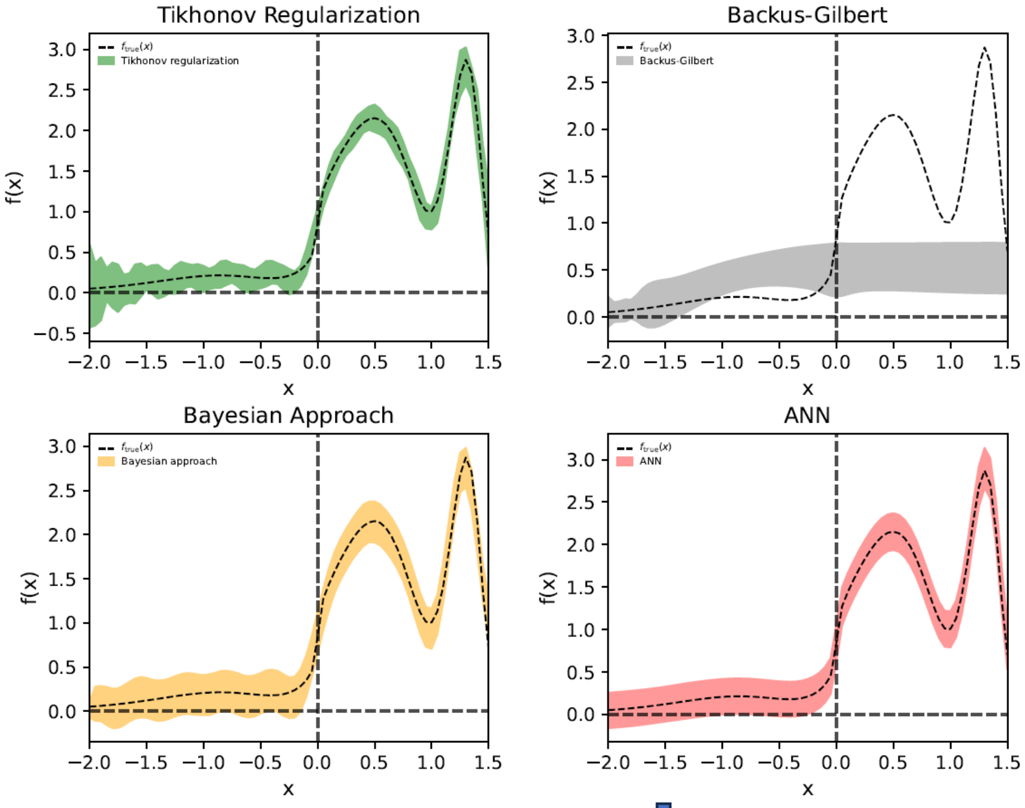
[1]Aster, R. C., Borchers, B., & Thurber, C. H. (2019). Parameter Estimation and Inverse Problems (3rdEdition), Elsevier, 135–149.

Reconstruction results of Toy models I&II obtained by four inversion methods

- Tikhonov, Bayesian, ANN gets good result
- BG performs poorly: mathematical foundation is weak[1], effective for simple models but breaking down with complex ones



Single layer
5 neurons

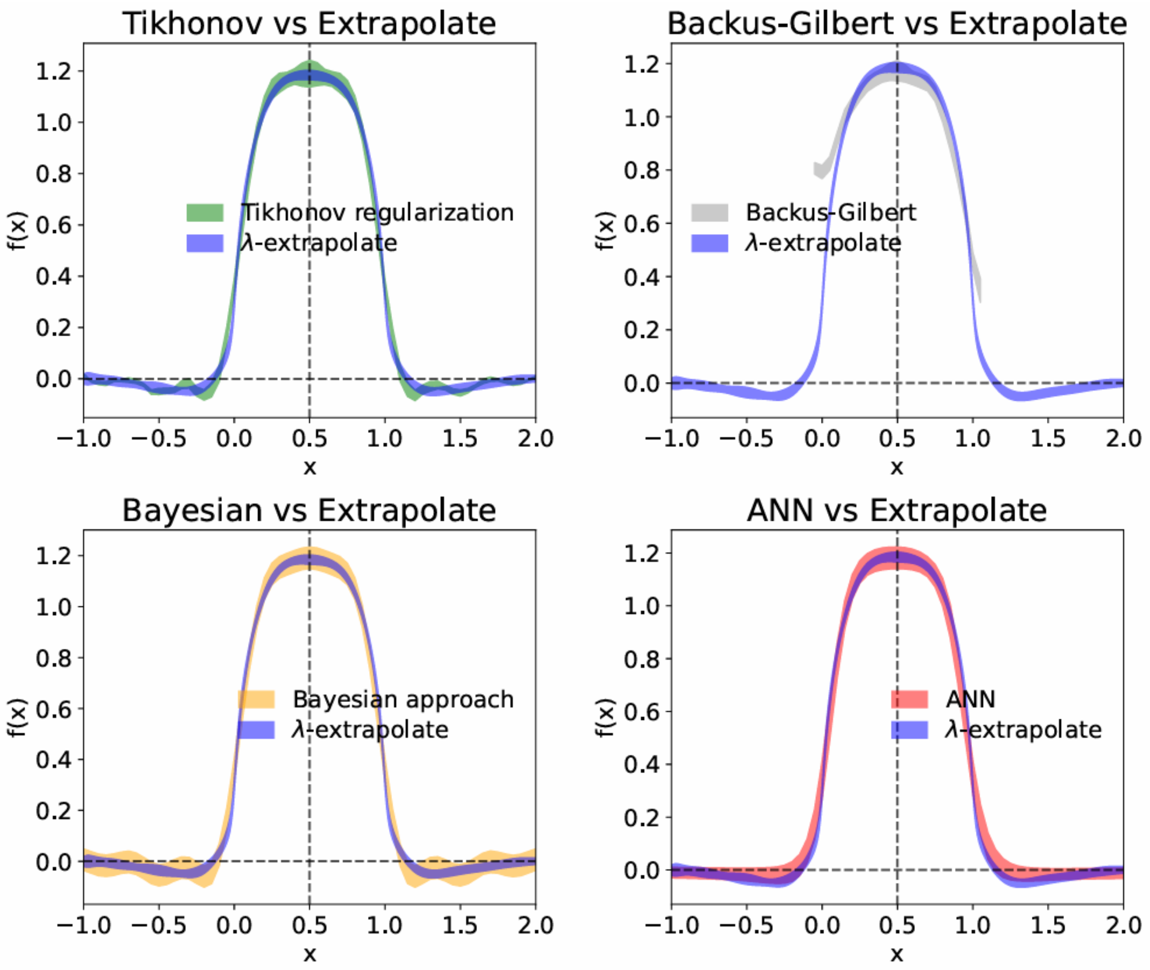


Multi-layers
300~400 neurons

Inversion methods—Results

Reconstruction results obtained by the four methods using real lattice QCD data as input

- Pion quasi-DA
- Tikhonov, Bayesian, ANN: good results and consistent with λ extrapolation.
- BG yields poorly result again.
- Preconditioned-BG (J. Karpie et al. JHEP 04, 057) is introduced to improve the result. However, it is heavily reliant on strong, specific priors, making it too inflexible and unreliable.



Conclusions&Outlook

New perspective: inverse problem approach to solve the limited discrete Fourier transform

Conclusions:

- The problem is ill-posed: existence and uniqueness, but instability
- This ill-posed problem is tractable: the input $g(\lambda)$ is precise and the behavior of the true solution $f(x)$ is simple
- Use four inversion methods: toy models and real physics (π meson)
- ANN has substantial potential for solving multi-peak spectral function reconstruction problem

Outlook:

- Input precision keeps better: the lattice is developing
- Work together: combine λ extrapolation and inverse problem approach
- Baryons quasi-DA: solve the two-dimensional integral equation

Thanks for watching