XIIth Meeting on Lattice Parton Physics from LaMET

Ill-Posedness in Limited Discrete Fourier Inversion for Quasi Distributions in LaMET

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Outline

- Motivation
- Ill-Posedness
- Inversion methods
- Conclusions

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Motivation

Inverse problem is everywhere

Input (Reason)	Process (Model)	Output (Result)

$$f \;\underset{\text{Inverse}}{\overset{\text{Forward}}{\rightleftarrows}}\; K \;\underset{\text{Inverse}}{\overset{\text{Forward}}{\rightleftarrows}}\; g$$

- Forward problem: know the input f and process K, solve the output g
- Inverse problem: know the output g and process K, solve the input f
- Applications: Medical imaging, geological exploration, image processing

Motivation

Key step in LaMET: **get the momentum-fraction quasi-DA from non-matrix elements computed in Euclidean lattice QCD**

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

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

$$C_2^m(z, \vec{P}, t) = \int d^3 y e^{-i\vec{P}\cdot\vec{y}} \times \langle 0|\mathcal{O}_{\Gamma_1}(z; \vec{y}, t)\bar{\psi}_2(0,0)\Gamma_2\psi_1(0,0)|0\rangle,$$

$$\int \frac{d\xi^-}{2\pi} e^{ixp^+\xi^-} \langle 0|\bar{\psi}_1(0)\not{n}\gamma_5 U(0,\xi^-)\psi_2(\xi^-)|M(P)\rangle = i f_M (p\cdot n)\phi_M(x),$$

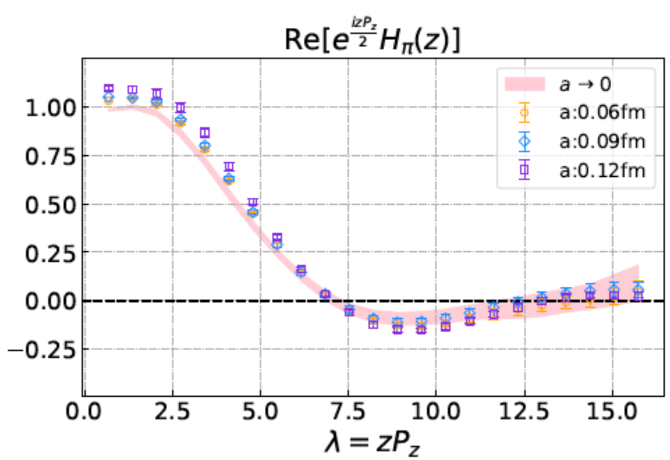
Equivalent to preforming a limited discrete Fourier transform

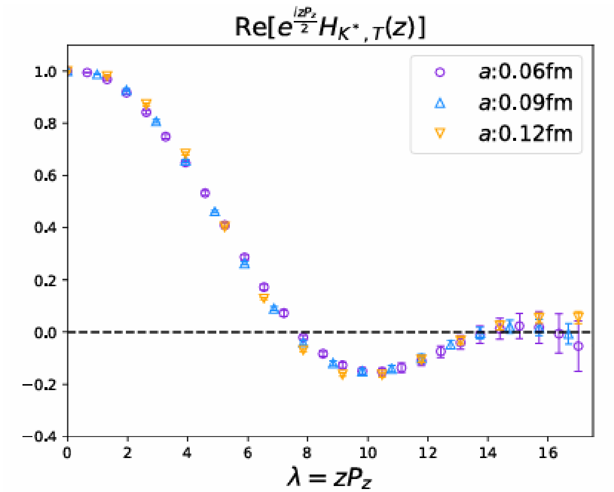
Motivation

Need to solve the limited inverse discrete Fourier transform rigorously and effectively

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

- $g(\lambda)$: discrete, finite and noisy data points in lattice calculation
- Direct inverse Fourier transform is failed

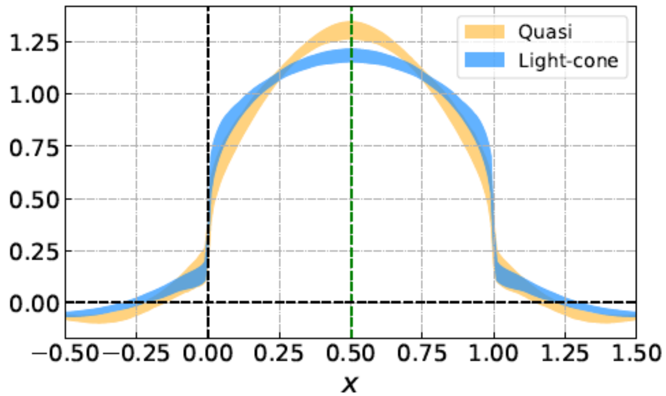


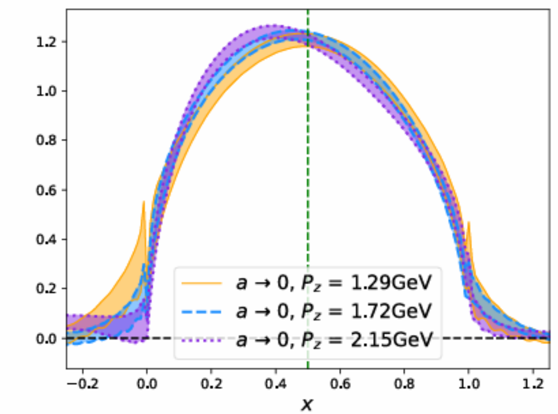


Physical extrapolation is good and effective

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

- Extrapolate the endpoints of $g(\lambda)$ base on physical analysis and perform the inverse Fourier transform to make it
- Have a long history of success, such as π, K^*





Motivation

New perspective: inverse problem approach

- Given the integral $g(\lambda)$, find the function $f(x)$
- Solving integral equation is a classic inverse problem
- 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)

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A classic example of an inverse problem

- Solve a system of linear equations: $A_{m\times n}x_{n\times 1} = b_{m\times 1}$
- Example one: no solution (over-determined)
- Example two: non-unique solutions (under-determined)
- Example three: a unique solution but unstable (a small change in input leads to a large change in the output)

$$\begin{cases} x_1 + x_2 + x_3 = 1 \\ x_1 + x_2 + x_3 = 2 \end{cases}$$

$$\begin{cases} x_1 + x_2 = 1 \\ 2x_1 + 2x_2 = 2 \\ 3x_1 + 3x_2 = 3 \end{cases}$$

$$\begin{cases} 2x_1 + 3x_2 = 5 \\ 1.9999x_1 + 3.0001x_2 = 5 \end{cases} \quad \begin{cases} x_1 = 1 \\ x_2 = 1 \end{cases}$$

$$\begin{cases} 2x_1 + 3x_2 = 5 \\ 1.9999x_1 + 3.0001x_2 = 5.01 \end{cases} \quad \begin{cases} x_1 = -59 \\ x_2 = 41 \end{cases}$$

Ill-posedness is the key to inverse problems

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

- Can not take it for granted
- Study the mathematical properties carefully
- Not every inverse problem is inherently ill-posed

The ill-posedness of limited discrete Fourier inversion

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

- 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
- Instability: tiny change in the input $g(\lambda)$ can lead to a big changes in the output $f(x)$

The rigorous proof of the uniqueness

Theorem A.1 (The Uniqueness of the Limited Fourier Transform). *Suppose that $f_1(x), f_2(x) \in L^2(x_{\min}, x_{\max})$, with $-\infty < x_{\min} < x_{\max} < \infty$. If $\int_{x_{\min}}^{x_{\max}} e^{-ix\lambda} f_1(x)dx = \int_{x_{\min}}^{x_{\max}} e^{-ix\lambda} f_2(x)dx = g(\lambda), \lambda \in [\lambda_{\min}, \lambda_{\max}]$ (or a sequence of points converging to this interval), with $-\infty < \lambda_{\min} < \lambda_{\max} < \infty$, then we have $f_1(x) = f_2(x)$, a. e. $x \in [x_{\min}, x_{\max}]$.*

Proof. Since the integral equation is linear, we know that

$$\int_{x_{\min}}^{x_{\max}} e^{-ix\lambda} \left(f_1(x) - f_2(x)\right) dx = 0. \tag{A1}$$

Setting $f(x) = f_1(x) - f_2(x)$, we just need to prove that

$$\int_{x_{\min}}^{x_{\max}} e^{-ix\lambda} f(x)dx = 0, \ \ \lambda \in [\lambda_{\min}, \lambda_{\max}] \tag{A2}$$

implies $f(x) = 0$, a. e. $x \in [x_{\min}, x_{\max}]$.
First, we prove the analyticity of the complex function

$$\phi(z) = \int_{x_{\min}}^{x_{\max}} e^{-ixz} f(x)dx, z \in \mathbb{C}. \tag{A3}$$

It is known that e^{-ixz} is analytic for $z \in \mathbb{C}$ to $x \in \mathbb{R}$, and $e^{-ixz} = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} z^n x^n$. Then we have

$$\phi(z) = \int_{x_{\min}}^{x_{\max}} e^{-ixz} f(x)dx = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} z^n \int_{x_{\min}}^{x_{\max}} x^n f(x)dx, \tag{A4}$$

For $f \in L^1(x_{\min}, x_{\max})$, we have

$$\left| \int_{x_{\min}}^{x_{\max}} x^n f(x)dx \right| \le \left(\max\{|x_{\min}|, |x_{\max}|\}\right)^n \int_{x_{\min}}^{x_{\max}} |f(x)|dx. \tag{A5}$$

The coefficients in the series $\phi(z)$ satisfy

$$\lim_{n\to\infty} \left(\frac{1}{n!}\right)^{1/n} \left| \int_{x_{\min}}^{x_{\max}} x^n f(x)dx \right|^{1/n} \le \lim_{n\to\infty} \left(\frac{1}{n!}\right)^{1/n} \left(\int_{x_{\min}}^{x_{\max}} |f(x)|dx \right)^{1/n} \left(\max\{|x_{\min}|, |x_{\max}|\}\right) \to 0, \tag{A6}$$

by $\lim_{n\to\infty}(n!)^{1/n} = \infty$. Therefore the convergence radius of the series $\phi(z)$ is ∞, that means the complex function $\phi(z)$ is analytic in the complex plane. By the property of analytic function, from Eq. (A2), we have $\phi(z) = 0, \ z \in \mathbb{C}$, namely

$$\int_{x_{\min}}^{x_{\max}} f(x)dx + (-i)z \int_{x_{\min}}^{x_{\max}} x f(x)dx + (-i)^2 \frac{z^2}{2} \int_{x_{\min}}^{x_{\max}} x^2 f(x)dx + \cdots + (-i)^n \frac{z^n}{n!} \int_{x_{\min}}^{x_{\max}} x^n f(x)dx + \cdots = 0, \ z \in \mathbb{C}. \tag{A7}$$

From Eq. (A7) we obtain for $z = 0$

$$\int_{x_{\min}}^{x_{\max}} f(x)dx = 0 \tag{A8}$$

and

$$(-i)z \int_{x_{\min}}^{x_{\max}} x f(x)dx + (-i)^2 \frac{z^2}{2} \int_{x_{\min}}^{x_{\max}} x^2 f(x)dx + \cdots + (-i)^n \frac{z^n}{n!} \int_{x_{\min}}^{x_{\max}} x^n f(x)dx + \cdots = 0, \ z \in \mathbb{C}. \tag{A9}$$

Dividing both sides of Eq. (A9) by $-iz$, and then set $z = 0$, one obtain

$$\int_{x_{\min}}^{x_{\max}} x f(x)dx = 0. \tag{A10}$$

Repeating above process, one can obtain that

$$\int_{x_{\min}}^{x_{\max}} x^n f(x)dx = 0, \ \ n = 0, 1, 2, \cdots \tag{A11}$$

Since $C[x_{\min}, x_{\max}]$ is dense in $L^2(x_{\min}, x_{\max})$, then for $f(x) \in L^2(x_{\min}, x_{\max})$ and any $\epsilon > 0$, there exists $\bar{f}(x) \in C[x_{\min}, x_{\max}]$, such that

$$\|f - \bar{f}\|_{L^2(x_{\min}, x_{\max})} < \epsilon. \tag{A12}$$

On the other hand, for $\bar{f}(x) \in C[x_{\min}, x_{\max}]$, there exists a polynomial $Q_n(x)$ of degree $n \in \mathbb{N}$, such that

$$\|\bar{f} - Q_n\|_{C[x_{\min}, x_{\max}]} < \epsilon, \tag{A13}$$

by the Weierstrass theorem. Therefore, one have

$$\begin{aligned} \|f - Q_n\|_{L^2(x_{\min}, x_{\max})} &\le \|f - \bar{f}\|_{L^2(x_{\min}, x_{\max})} + \left\|\bar{f} - Q_n\right\|_{L^2(x_{\min}, x_{\max})} \\ &\le \epsilon + \sqrt{x_{\max} - x_{\min}} \left\|\bar{f} - Q_n\right\|_{C[x_{\min}, x_{\max}]} \\ &< \epsilon + \epsilon\sqrt{x_{\max} - x_{\min}}. \end{aligned} \tag{A14}$$

By using Eq. (A11), we know that

$$\int_{x_{\min}}^{x_{\max}} f(x) Q_n(x)dx = 0. \tag{A15}$$

Combined with the Cauchy inequality, we have

$$\begin{aligned} \|f\|^2_{L^2(x_{\min}, x_{\max})} &= \int_{x_{\min}}^{x_{\max}} f^2(x)dx = \int_{x_{\min}}^{x_{\max}} \left(f^2(x) - f(x)Q_n(x)\right) dx \\ &\le \int_{x_{\min}}^{x_{\max}} |f(x)| \cdot |f(x) - Q_n(x)|\, dx \\ &\le \left(\int_{x_{\min}}^{x_{\max}} f^2(x)dx \right)^{\frac{1}{2}} \left(\int_{x_{\min}}^{x_{\max}} |f(x) - Q_n(x)|^2 \, dx \right)^{\frac{1}{2}} \\ &= \|f\|_{L^2(x_{\min}, x_{\max})} \|f - Q_n\|_{L^2(x_{\min}, x_{\max})} \\ &\le (\epsilon + \epsilon\sqrt{x_{\max} - x_{\min}}) \|f\|_{L^2(x_{\min}, x_{\max})}, \end{aligned} \tag{A16}$$

which implies that

$$\|f\|_{L^2(x_{\min}, x_{\max})} \le \epsilon + \epsilon\sqrt{x_{\max} - x_{\min}}. \tag{A17}$$

Letting $\epsilon \to 0$, we finally have

$$\|f\|_{L^2(x_{\min}, x_{\max})} = 0, \tag{A18}$$

i. e. $f(x) = 0$, a. e. $x \in [x_{\min}, x_{\max}]$. The proof is completed.

□

The source of instability

- 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

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

$$\boldsymbol{g}_k = \sum_j \boldsymbol{K}_{kj} \boldsymbol{f}_j,$$

$$\boldsymbol{K}_{kj} = e^{-i\lambda_k x_j} \Delta x,$$

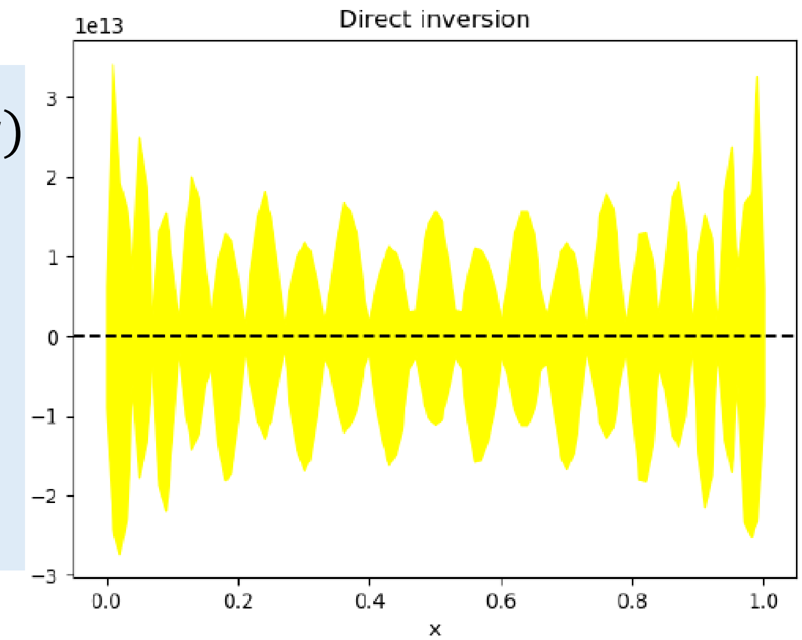
$$\boldsymbol{K}_{\text{re}} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T = \sum_{i=1}^{n} \boldsymbol{u}_i \sigma_i \boldsymbol{v}_i^T,$$

$$\boldsymbol{f} = \sum_{i=1}^{n} \frac{\boldsymbol{u}_i^T \boldsymbol{g}}{\sigma_i} \boldsymbol{v}_i.$$

$$||\boldsymbol{f}^{\delta} - \boldsymbol{f}_{\text{true}}||_2^2 = \sum_{i=1}^{n} \left(\frac{\boldsymbol{u}_i^T (\boldsymbol{g}^{\delta} - \boldsymbol{g}_{\text{true}})}{\sigma_i} \boldsymbol{v}_i\right)^2 = \sum_{i=1}^{n} \left(\frac{\boldsymbol{u}_i^T \boldsymbol{\delta}}{\sigma_i} \boldsymbol{v}_i\right)^2,$$

The numerical show of instability

- 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 $g^\delta(\lambda)$ using SVD
- The reconstructed $f^\delta(x)$ on the right



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

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- **Inversion methods**
- Conclusions

Regularization methods overcome the ill-posedness

- Regularization method: a process of getting a stable, approximate solution to an ill-posed problem
- Restore well-posedness: existence, uniqueness and stability
- Convergence: the regularized solution converges to the true solution as the noise level decreases

Four popular inversion methods

- Tikhonov regularization: the most standard method in mathematics
- Bayesian method: probability distribution
- Backus-Gilbert method (BG): used widely in inversion for spectral function
- Artificial neural network (ANN): universal approximation theorem

Use Tikhonov regularization as an example to see how to overcome the ill-posedness

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

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

- Using variational method, the regularized solution is given by

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

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

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

- Regularization parameter α can be obtained by mathematical method

Mathematical properties of Tikhonov regularization

- Well-posedness: convert the original ill-posed problem to well-posed approximation
- Convergence: Tikhonov solution converges to the true answer as the noise in the put decrease. δ is the noise level in the data ($\delta = ||g^{\delta} - g_t||_{l^2}$), E is the upper bound for the true solution ($||f_t||_{l^2} \le E$)

$$\|f_\alpha^\delta - f_t\|_{l^2} \le \frac{\delta}{2\sqrt{\alpha}} + \frac{\sqrt{\alpha}E}{2}, \qquad \alpha = \delta/E,$$

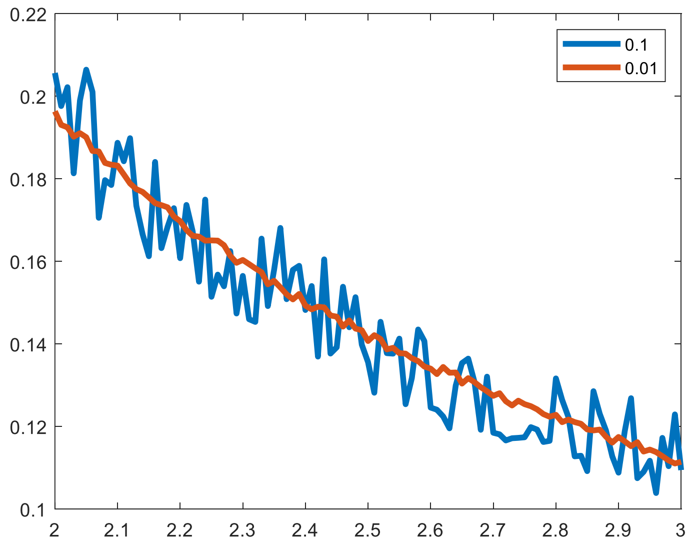
$$\|f_\alpha^\delta - f_t\|_{l^2} \le \sqrt{\delta E} \overset{\delta\to 0}{\longrightarrow} 0,$$

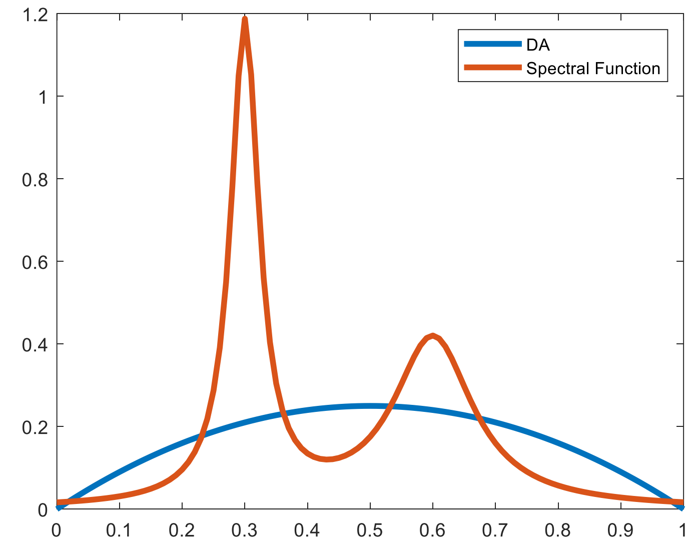
The regularized solution converges to the true answer in a stable and controlled manner as the noise level δ goes to zero

Two factors influence the difficulty of solving ill-posedness

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

- Noise level in $g(\lambda)$: 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



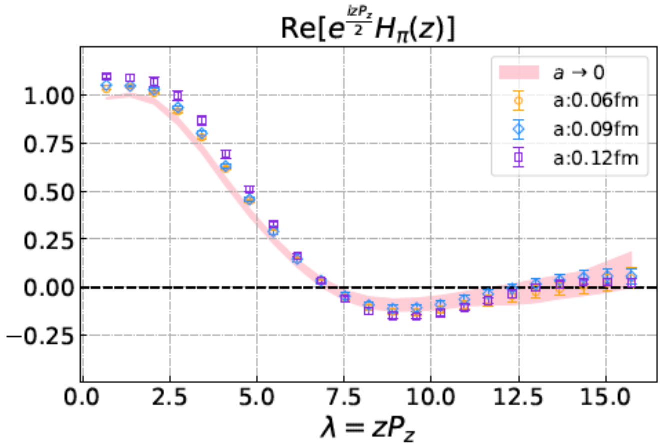


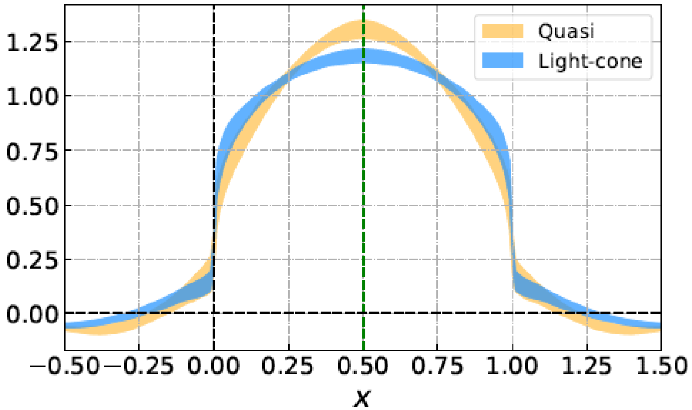
Inversion methods

The limited discrete Fourier transform is tractable

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

- Noise level in $g(\lambda)$: input data has low noise level, and measurement precision keeps getting better
- The behavior of the true $f(x)$: the quasi-DA in the momentum space has a simple form

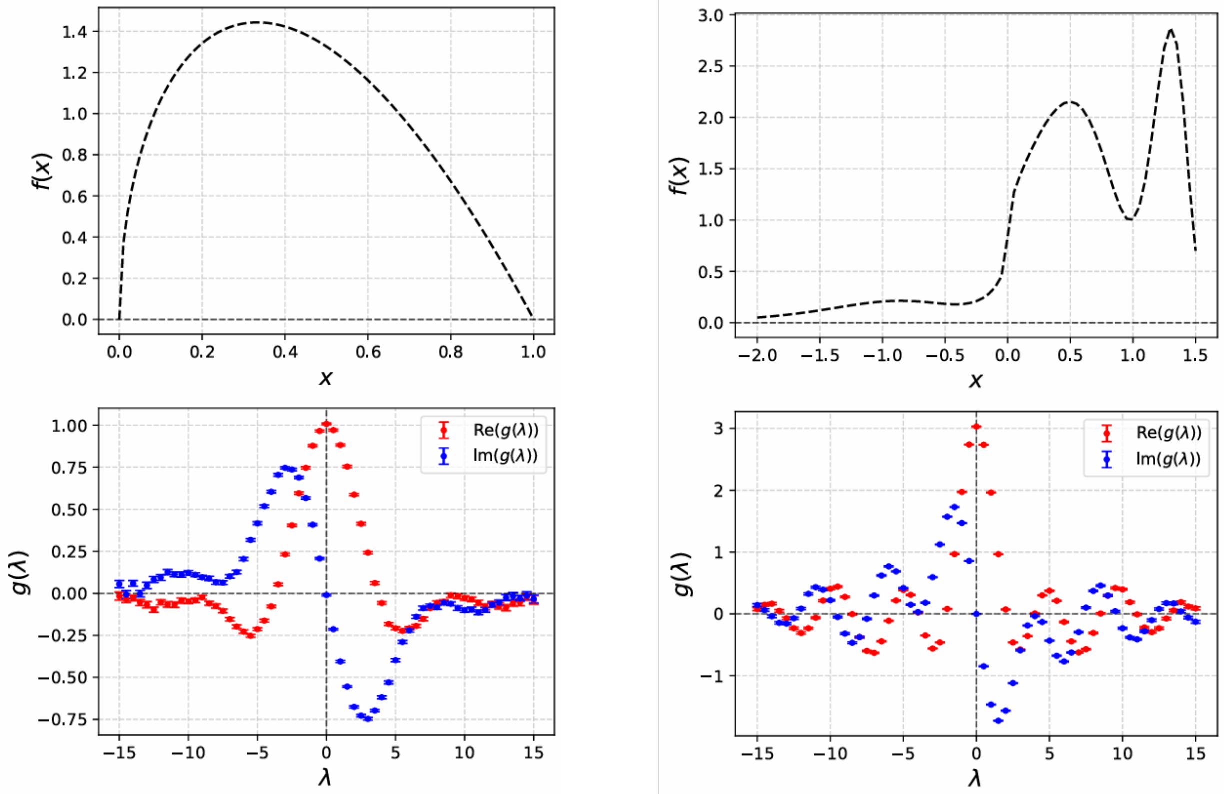




Toy models: show the effective of inversion methods

- Toy model I: universal behavior; Toy model II: more complex
- First row: the behavior of the true toys $f(x)$
- Second row: the input data $g(\lambda)$ (finite, discrete points with noise)

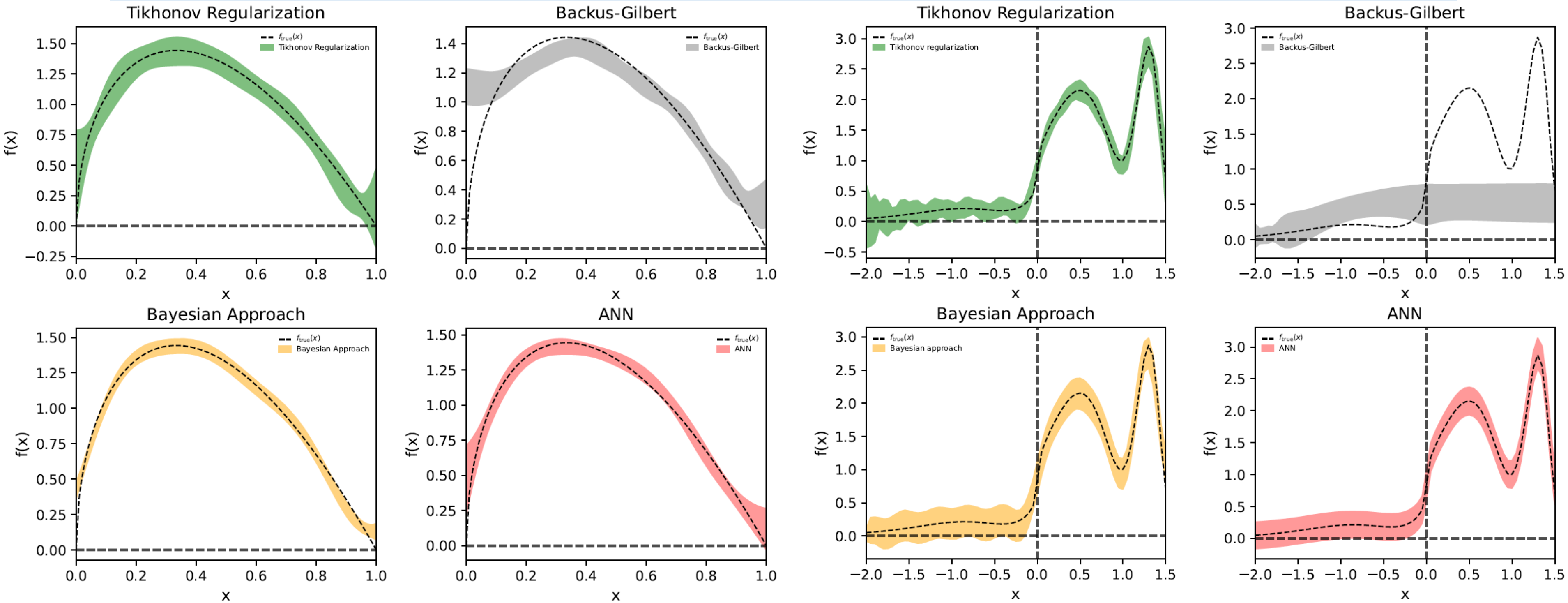
$$g(\lambda) = \int dx e^{-i\lambda x} f(x),$$



Inversion methods

The results of Toys obtained by four inversion methods

- Black line: the true solution; Colored lines: from four inversion ways
- Tikhonov, Bayesian, ANN gets good result
- BG performs poorly: mathematical foundation is weak, effective for simple models but breaking down with complex ones

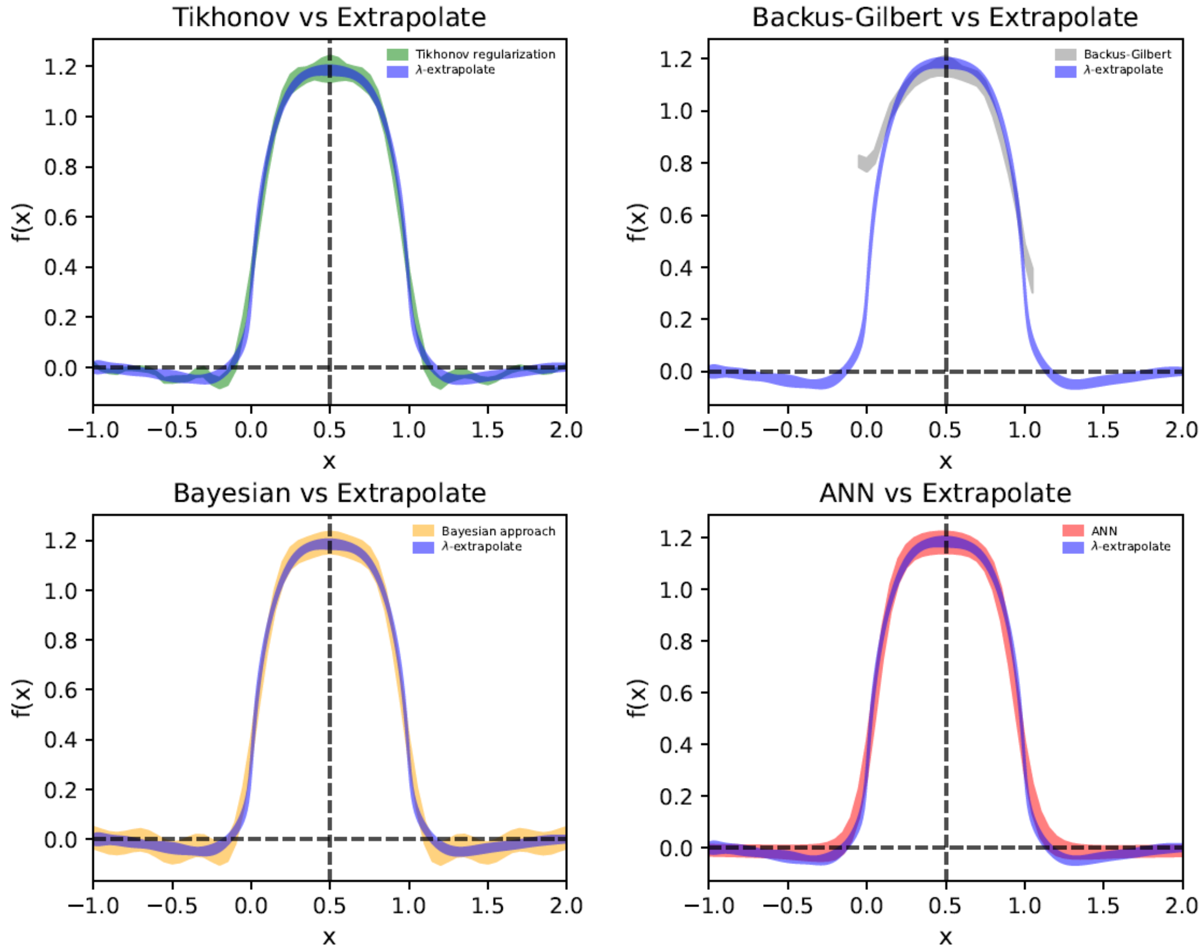


Inversion methods

The results of real physics obtained by inversion methods

- π meson quasi-DA
- The purple: λ extrapolation

  the colored: the inversion methods.
- Tikhonov, Bayesian, ANN: good results and consistent with λ extrapolation
- BG fails again



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Conclusions

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

Summary:

- The inverse 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)

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


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Thank you!


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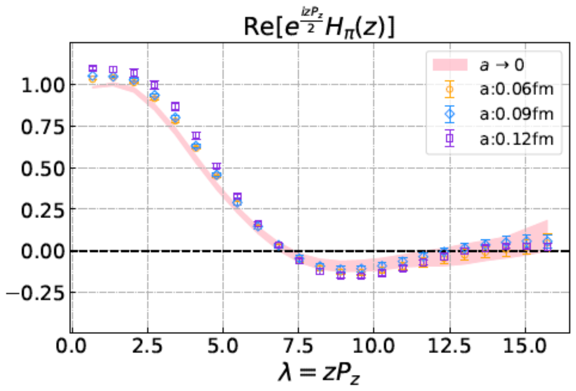
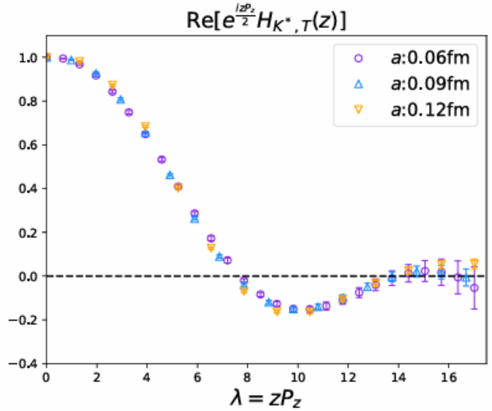
Back up

The uniqueness

- Finite set of discrete points undermine uniqueness
- In face of non-uniqueness, only the minimum norm solution can be obtained. No mathematical technique can compensate for the inherently ill-posed nature of the problem.
- Interpolation can be used to complete the data. Treating interpolation as a form of error, inverse problem theory tells us that as the error tends to zero, the solution converges to the true solution.





Regularization

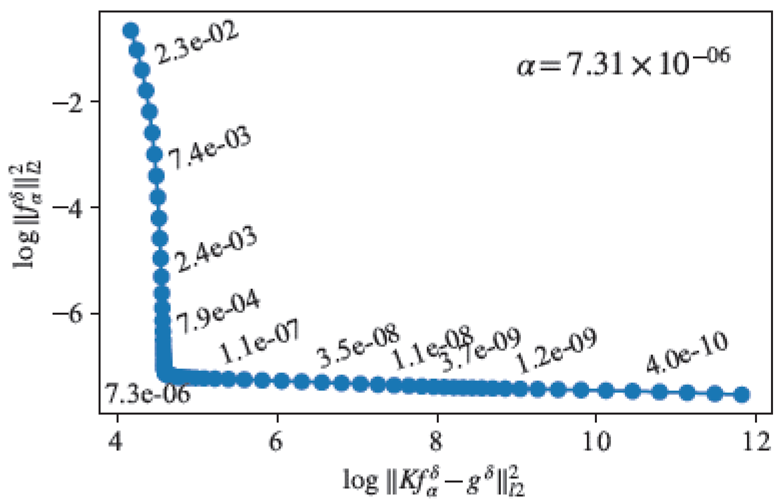
- The regularization in inverse problems is very similar to the regularization in physics. They both make unstable or ill-behaved problems more manageable
- Tikhonov regularization is similar to Pauli-Villars regularization

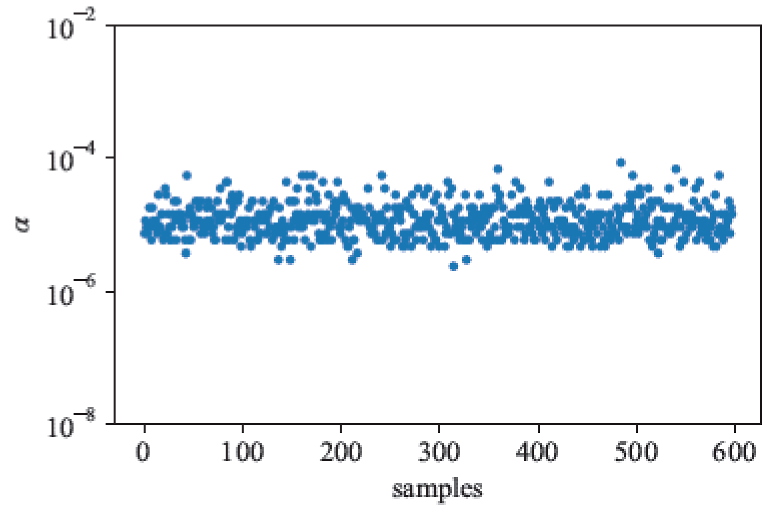
$$\frac{\sigma_1}{\sigma_n} \Rightarrow \frac{\sigma_1 + \alpha}{\sigma_n + \alpha} \approx \frac{\sigma_1}{\alpha},$$

$$\frac{i}{k^2 - m^2 + i\varepsilon} \to \frac{i}{k^2 - m^2 + i\varepsilon} + \sum_i^N \frac{iC_i}{k^2 - \Lambda_i^2 + i\varepsilon},$$

Select the regularization parameter α

- L-curve: compare the curves of $||Kf_\alpha^\delta - g^\delta||_{l^2}^2$ and $||f_\alpha^\delta||_{l^2}^2$ on a Log-Log scale to identify the regularization parameter
- Big platform and stable





Bayesian approach

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

- In dealing with an inverse problem, the Bayesian approach takes the form:

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

- Adopting a Gaussian Random Walk (GRW) prior as a regulator to characterize the smoothness property of solution

$$p(\bar{\boldsymbol{f}}|I) = \int p(\bar{\boldsymbol{f}}|\sigma,I)\cdot p(\sigma|I)d\sigma,$$

$$p(\bar{\boldsymbol{f}}|\sigma,I) = \frac{1}{\sqrt{2\pi}}e^{-\frac{\bar{f}_0^2}{2}}\cdot\prod_{j=1}^{m}\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{(\bar{f}_j-\bar{f}_{j-1})^2}{2\sigma^2}},$$

$$p(\sigma|I) = \begin{cases}\frac{2}{\sqrt{2\pi}\cdot 0.01}e^{-\frac{\sigma^2}{2\cdot 0.01^2}}, & \text{if} \quad \sigma>0,\\ 0, & \text{otherwise},\end{cases}.$$

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

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Backus-Gilbert

- BG assumes the solution to the problem can be expressed as a linear combination of the data $g(\lambda)$

$$
\begin{aligned}
f_{\mathrm{est}}(x') &= \sum_i a_i(x') \boldsymbol{g}_i, \\
&= \sum_i \int_{x_{\min}}^{x_{\max}} dx a_i(x') K(x, \lambda_i) f_{\mathrm{true}}(x), \\
&= \int_{x_{\min}}^{x_{\max}} dx \rho(x - x') f_{\mathrm{true}}(x),
\end{aligned}
$$

$$\boldsymbol{g}_i \equiv g(\lambda_i) = \int_{x_{\min}}^{x_{\max}} dx\, K(x, \lambda_i) f_{\mathrm{true}}(x),$$

- It aims to minimizes the width l of resolution function $\rho(x - x')$ under normalized constraint, leading to minimizing the objective functional $L[\boldsymbol{a}]$

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

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

$$\Rightarrow \quad L[\boldsymbol{a}] = \boldsymbol{a}^T \boldsymbol{H} \boldsymbol{a} + \alpha \boldsymbol{a}^T \boldsymbol{C_g} \boldsymbol{a} + \beta(\boldsymbol{a}^T \boldsymbol{m} - 1),$$

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

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

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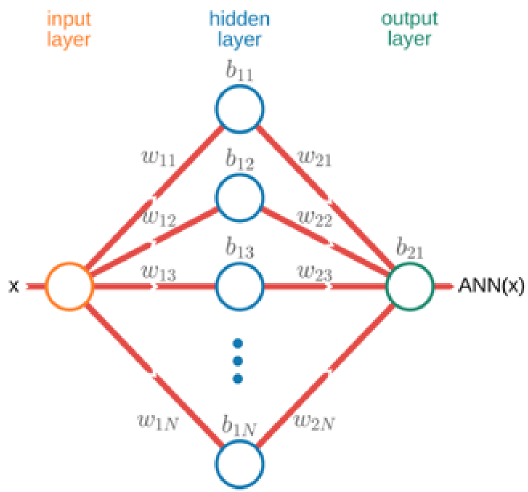
ANN

- 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.

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