Inverse Problem Approach

——A novel non-perturbative QCD method

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Lanzhou University

Based on [A.-S. Xiong, F.-S. Yu, Y. Zheng, T. Wei, arXiv:2211.13753;

and more in preparations]

The 8th Heavy Flavor Physics and QCD Conference @ Chongqing University，2026.4.25

前言

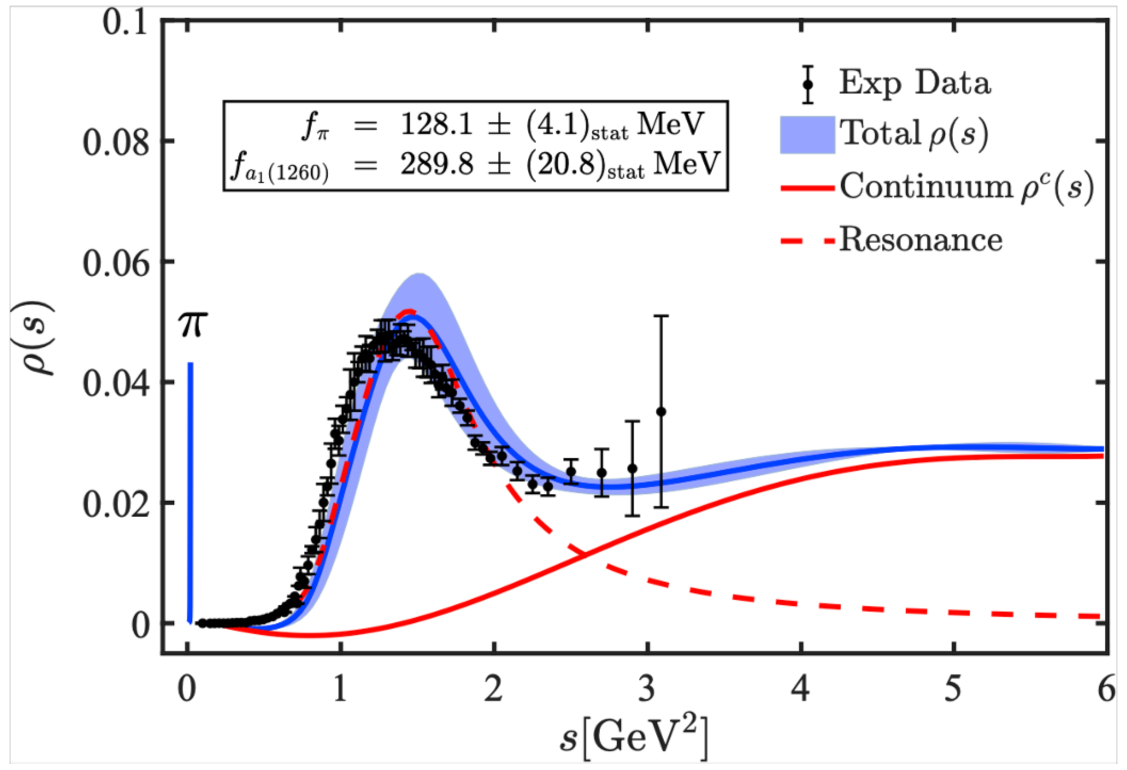
1. 感谢很多前辈、同仁多年来的关心和支持！

2. 方法仍在发展过程中，截至目前仍坚持严谨的数学框架；希望听取大家任何批判性的或建设性的意见，让它更完善；

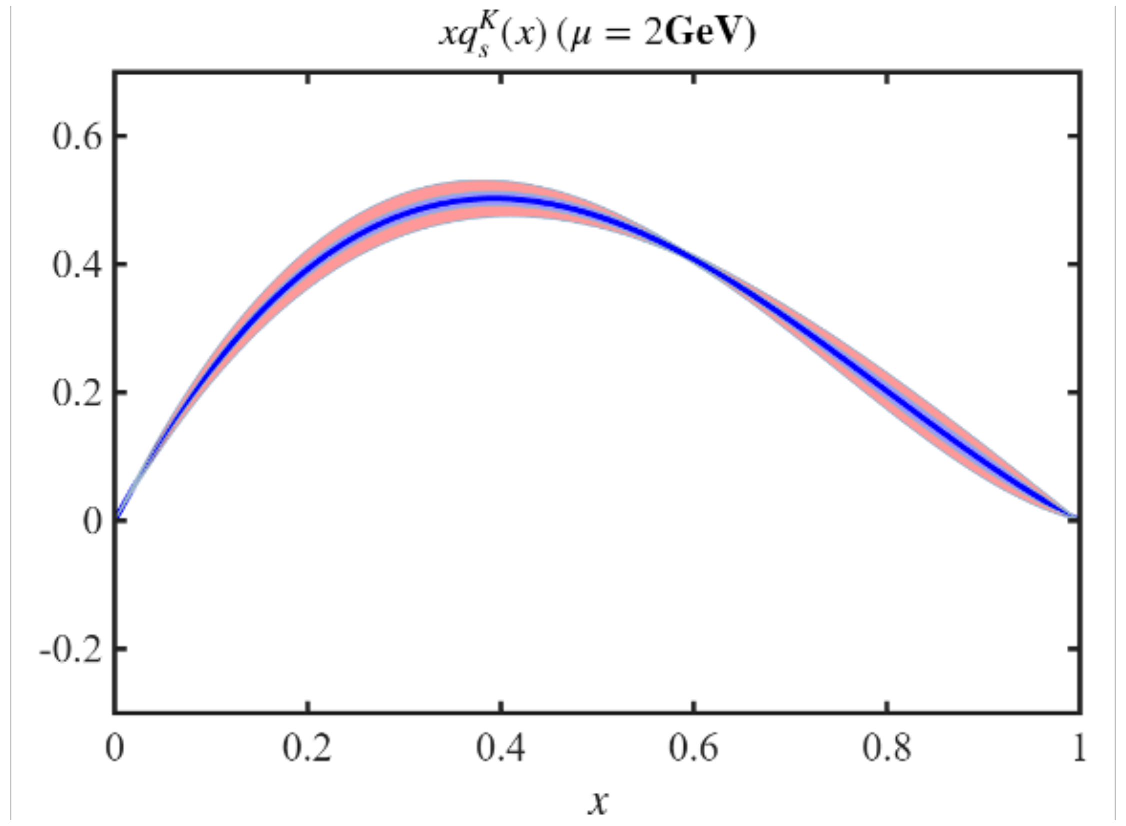
3. 反问题方法解决病态问题，有点反直觉；但对粒子物理来说是个新思路，可以期待前景广阔。

Physical Applications

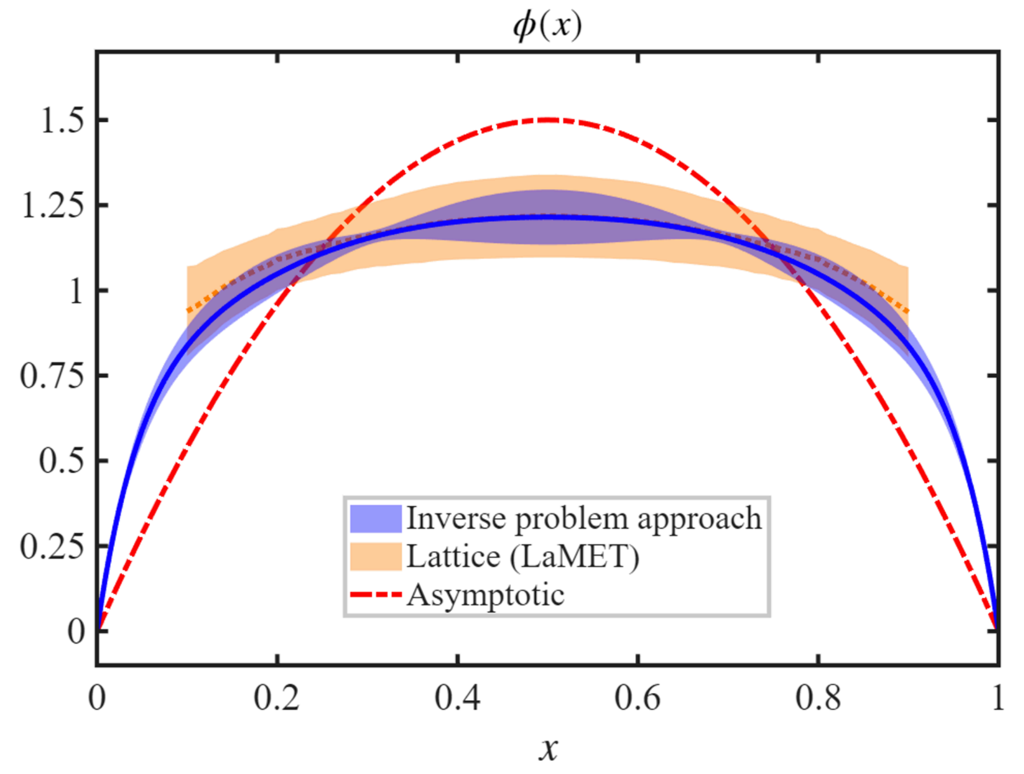
1. f_π and spectrum



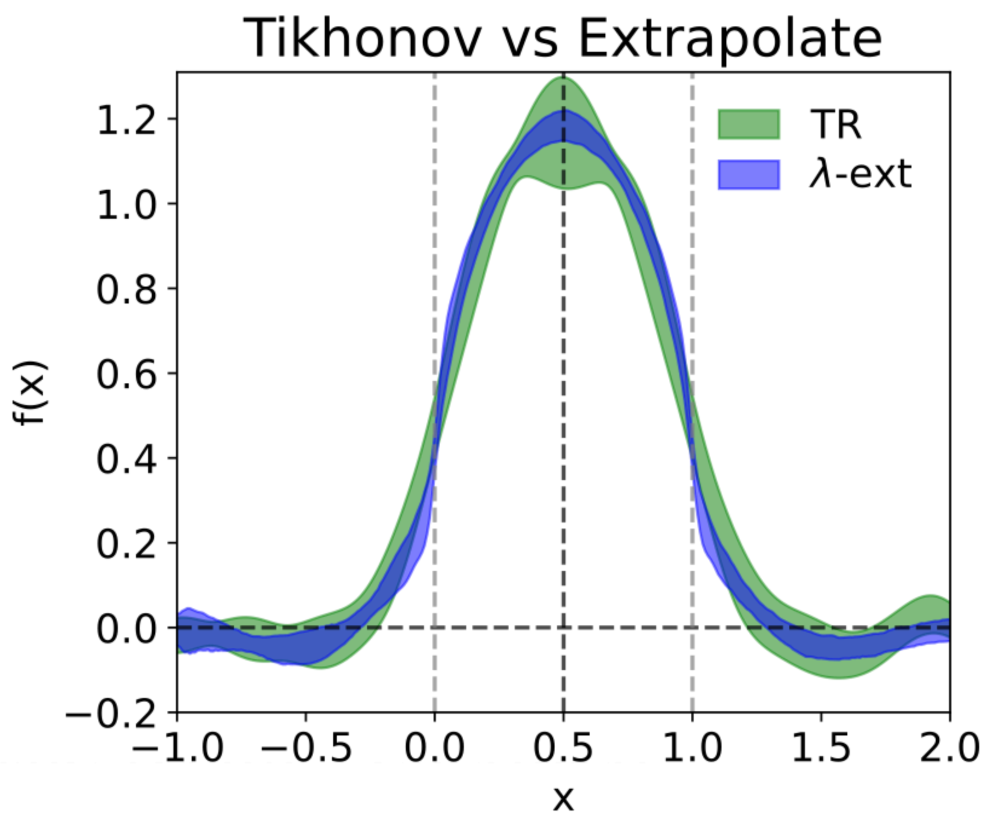
2. Parton Distribution Functions



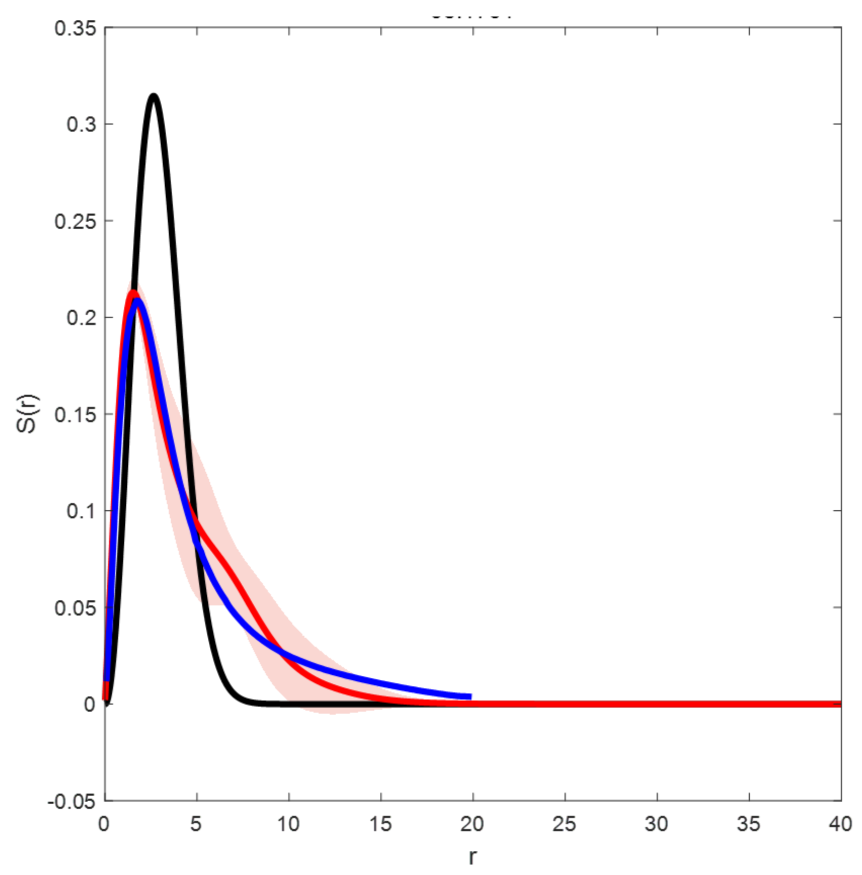
3. Distribution Amplitudes



4. Fourier transformation（LaMET）



5. Source function in femtoscopy



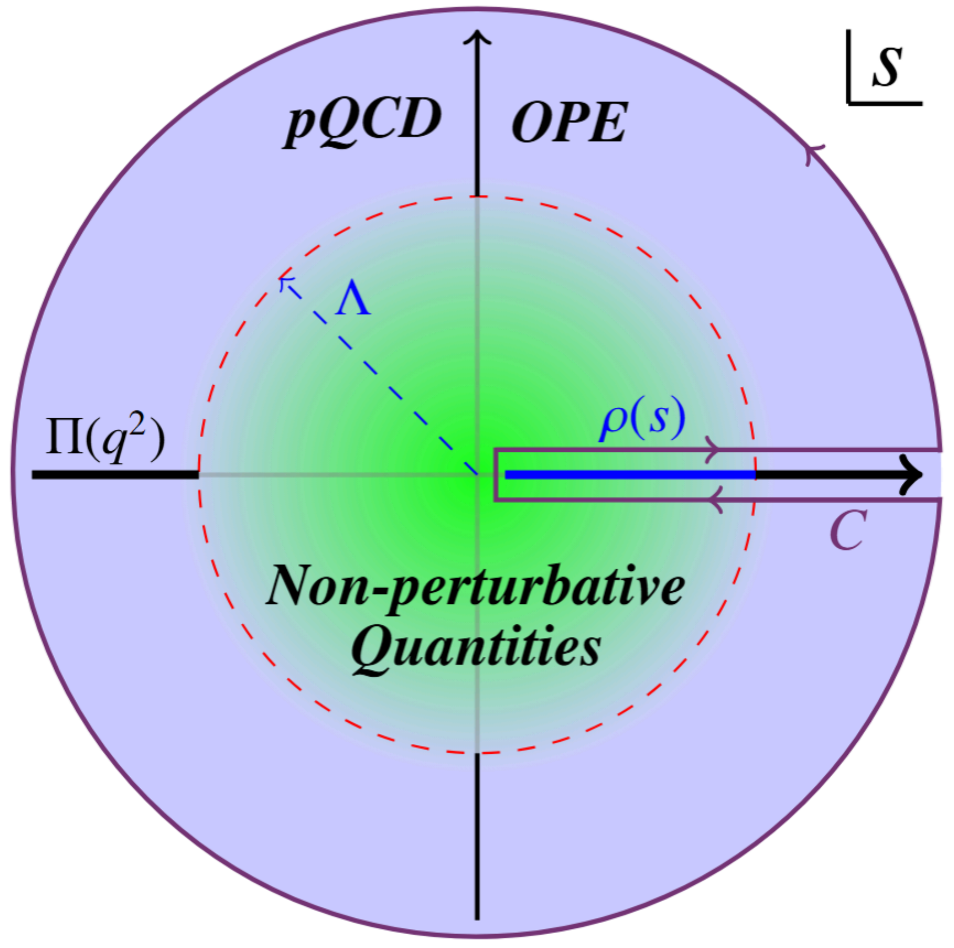
Dispersion Relation and Inverse Problem

- Based on Quantum Field Theory and correlation functions

$$\Pi(q^2) = i \int \mathrm{d}^4x\, e^{iqx} \langle \Omega | T\{\mathcal{O}_1(x)\mathcal{O}_2(0)\} | \Omega \rangle$$

- Analyticity of QFT $\Longrightarrow$ Dispersion Relation

$$\Pi(q^2) = \frac{1}{\pi} \int_{t_{min}}^{\infty} \mathrm{d}s\, \frac{\mathrm{Im}\,\Pi(s)}{s - q^2}$$



- Any dispersion relation would be studied similarly.

- Inverse Problem:

$$\int_{t_{\min}}^{\Lambda} \mathrm{d}s\, \frac{\mathrm{Im}\,\Pi(s)}{s - q^2} = \pi \Pi(q^2) - \int_{\Lambda}^{\infty} \mathrm{d}s\, \frac{\mathrm{Im}\,\Pi(s)}{s - q^2} \qquad q^2 \ll 0$$

Non-perturbative objective

Perturbative input

Illustration of Inverse Problem Approach

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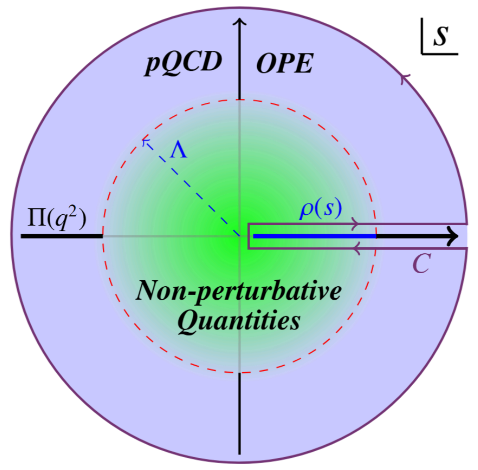

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c) Ill-posedness

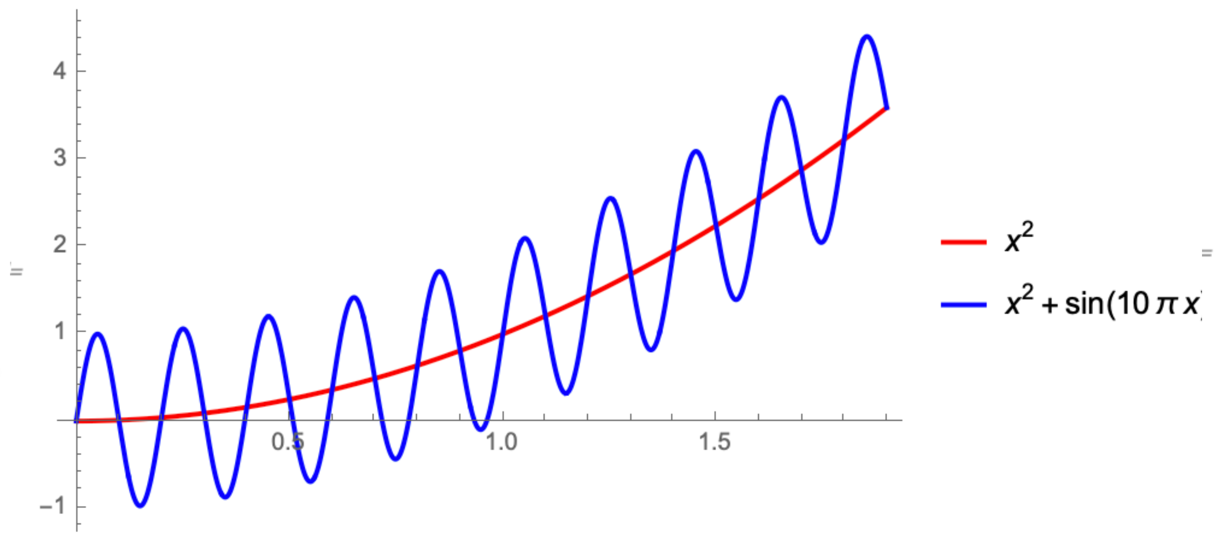
$$\int_a^b dx \, \frac{f(x)}{x-y} = g(y)$$

$$\Rightarrow \quad Kf = g$$

Solutions:

- existence ✓
- uniqueness ✓
- stability ✗

$f(x)$



Instabilit

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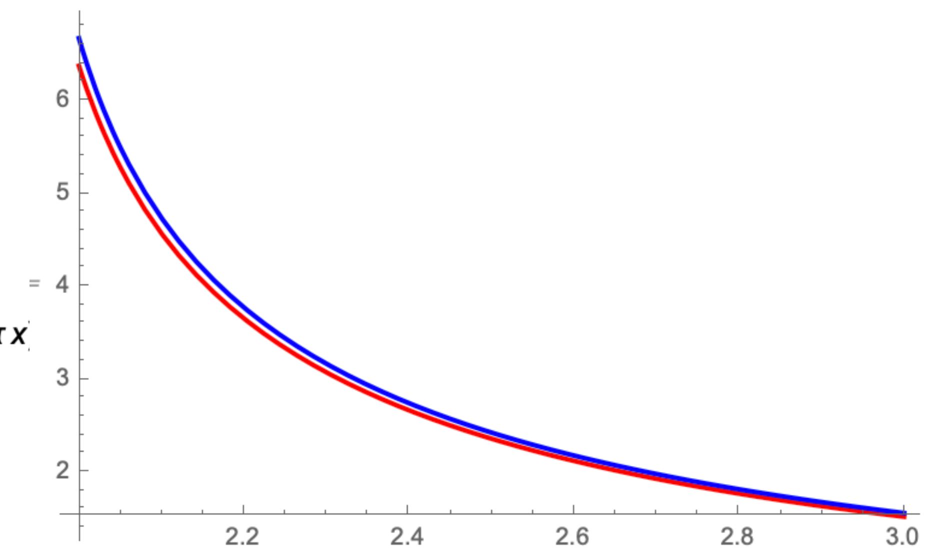

uniquenes

- No regularization $\Longrightarrow$ Unstable solution $\Longrightarrow$ Necessity of regularization

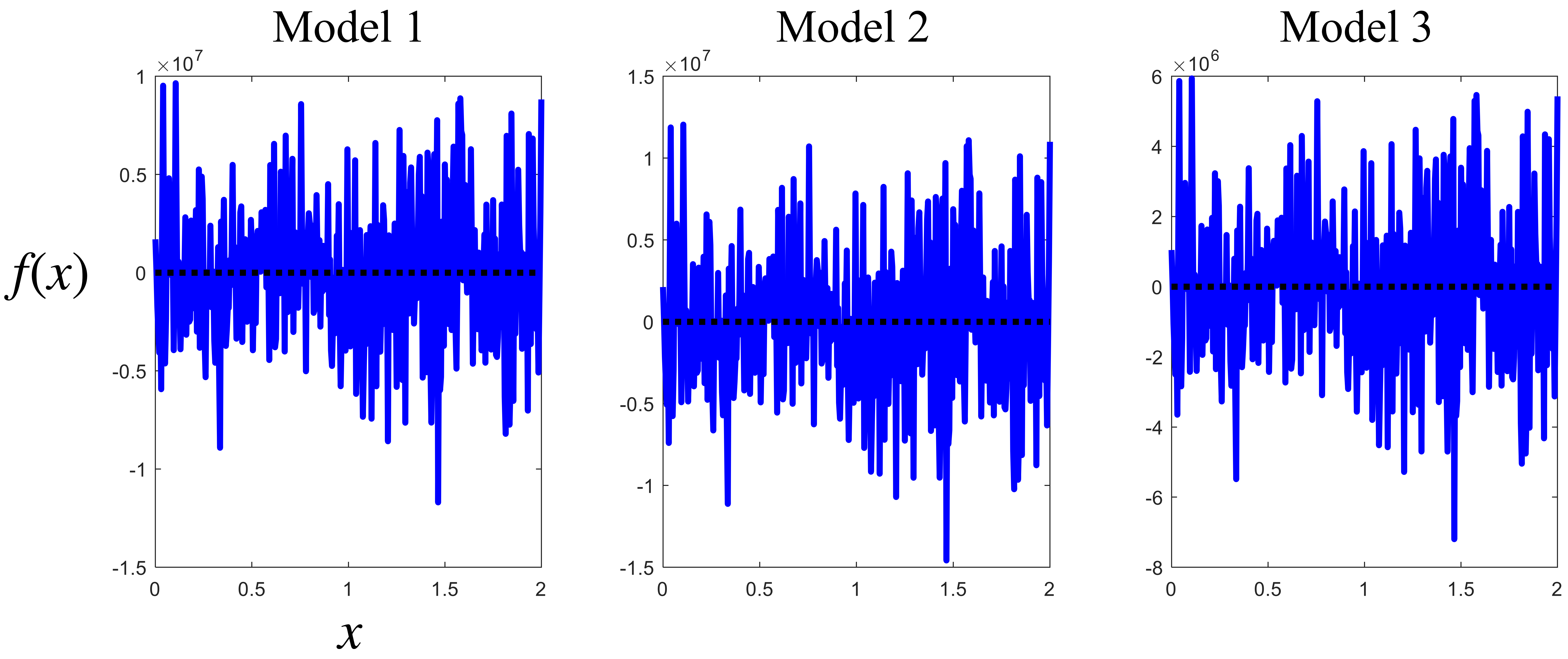

Illustration of Regularization Methods

a) Regularization strategy

- Nearby well-posed approximation

$$Kf = g \quad \Rightarrow \quad \text{bounded } \; R_\alpha \sim K^{-1}$$

- Regularization strategy:

$$\lim_{\alpha \to 0} R_\alpha K f = f, \qquad f_\alpha^\delta = R_\alpha g^\delta$$

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b) Tikhonov regularization

- Regularization operator

$$R_\alpha = (K^* K + \alpha I)^{-1} K^*$$

- Equivalent to minimize the functional

$$f_\alpha^\delta = \arg\min \left\{ \|Kf - g^\delta\|_G^2 + \alpha \|f\|_F^2 \right\}$$

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c) Convergence of solution

- Error estimation in a priori condition

$$\|f_\alpha^\delta - f\| \leqslant \alpha E + \delta/(2\sqrt{\alpha})$$

- Convergence of solution, $\alpha = (\delta/E)^{2/3}$

$$\|f_\alpha^\delta - f\| \leqslant 3/2 \, \delta^{2/3} E^{1/3} \to 0, \text{ as } \delta \to 0$$

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d) Interpretability by SVD

- Singular Value Decomposition (SVD)

$$\mu_1 \geqslant \mu_2 \geqslant \mu_3 \geqslant \cdots > 0$$

- Convergence by the leading terms

$$f_\alpha^\delta = \sum_i \frac{\mu_i}{\mu_i^2 + \alpha} \, (g^\delta, g_i) \, f_i$$

Ability to Uncertainty Analysis and Systematical Improvement of Precision

- Based on rigorous mathematics without artificial assumptions
- Be able to analyze statistical and systematic uncertainties and improve the precision

a) Uncertainty Analysis

$$\|f_\alpha^\delta - f\| \leqslant \delta\,\|R_\alpha\| + \|R_\alpha K f - f\|$$

$\delta\,\|R_\alpha\|$ ↓ statistical uncertainty

$\|R_\alpha K f - f\|$ ↓ systematic uncertainty

b) Improvement of precision

1. Input errors
2. Priori information and regularization methods
3. Combination with experiments or lattice QCD

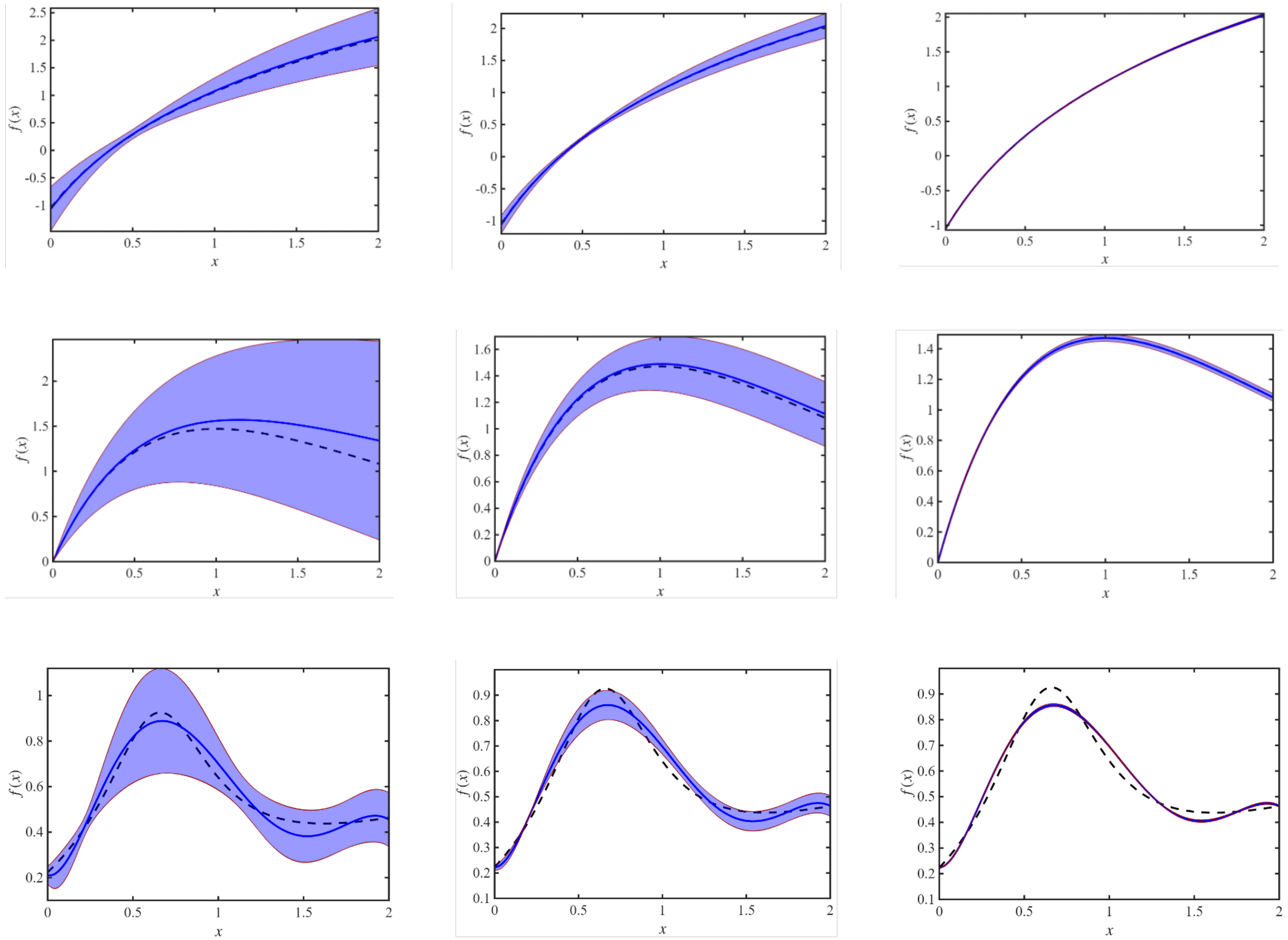
Systematically improve precision: Input Errors

$\delta = 30\,\%$ | $\delta = 10\,\%$ | $\delta = 1\,\%$

Model 1

Model 2

Model 3

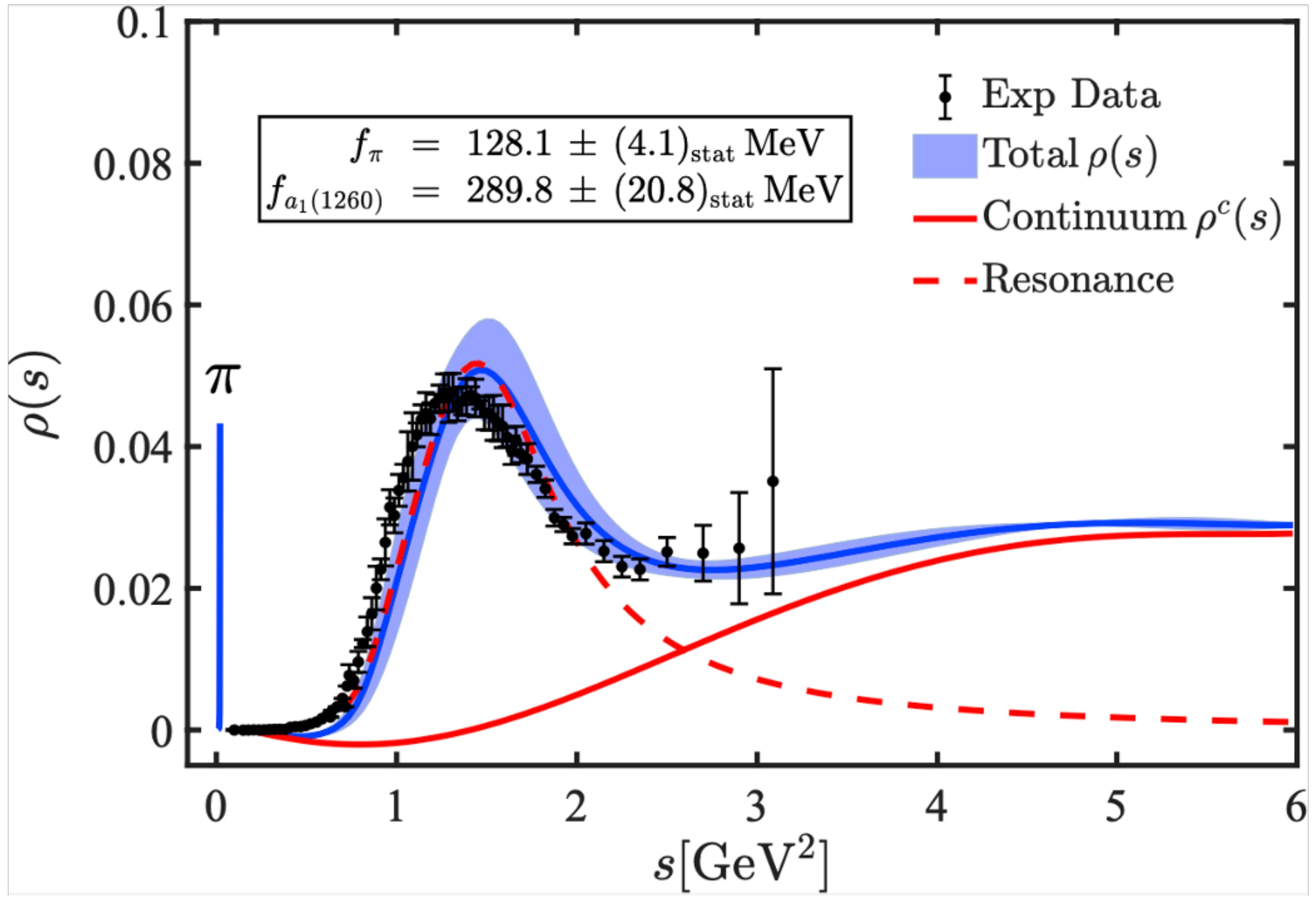


Physical Application: f_π and spectrum

$$\Pi_q(q^2) = \Pi_q(\sigma_0) + (q^2 - \sigma_0)\left[\int_0^\Lambda \frac{\rho(s)\,ds}{(s-\sigma_0)(s-q^2)} + \int_\Lambda^\infty \frac{\frac{1}{\pi}\mathbf{Im}\Pi_q^{\text{pert}}(s)\,ds}{(s-\sigma_0)(s-q^2)}\right]$$

$$\rho(s) = f_\pi^2\delta(s - M_\pi^2) + f_{a_1(1260)}^2\mathbb{BW}\left(s, M_{a_1(1260)}, \Gamma_{a_1(1260)}\right) + \rho^c(s)$$

$$\begin{aligned}\Pi_q(q^2) = &-\frac{1}{4\pi^2}\left(1+\frac{\alpha_s(\mu)}{\pi}\right)\ln\left(\frac{-q^2}{\mu^2}\right) + \frac{1}{12\pi}\frac{\langle\alpha_s G^2\rangle}{(q^2)^2}\\ &+\frac{m_u\langle\bar{u}u\rangle + m_d\langle\bar{d}d\rangle}{(q^2)^2} + \frac{1}{9}\frac{m_u\langle g_s\bar{u}\sigma TGu\rangle + m_d\langle g_s\bar{d}\sigma TGd\rangle}{(q^2)^3}\\ &-\frac{4}{81}\frac{\langle g_s\bar{u}u\rangle^2 + \langle g_s\bar{d}d\rangle^2}{(q^2)^3} - \frac{\left[105 + 50\ln\left(\frac{-q^2}{\mu^2}\right)\right]}{243\pi^2}\frac{\sum_{\psi=u,d,s}\langle g_s^2\bar{\psi}\psi\rangle^2}{(q^2)^3}\end{aligned}$$



Solving Problem of Quark-Hadron Duality in Sum Rules

Quark-hadron duality: $$\mathrm{Im}\Pi(q^2) = \pi f_V^2 \delta(q^2 - m_V^2) + \pi \rho^h(q^2)\theta(q^2 - s_h)$$

$$\rho^h(s) = \frac{1}{\pi}\mathrm{Im}\Pi^{\mathrm{pert}}(s)\theta(s - s_0)$$

$$\int_{s_h}^{\infty} ds \frac{\rho^h(s)}{s - q^2} = \frac{1}{\pi}\int_{s_0}^{\infty} ds \frac{\mathrm{Im}\Pi^{\mathrm{pert}}(s)}{s - q^2}$$

- Uncertainty sources: quark-hadron duality. Results are sensitive to s_0

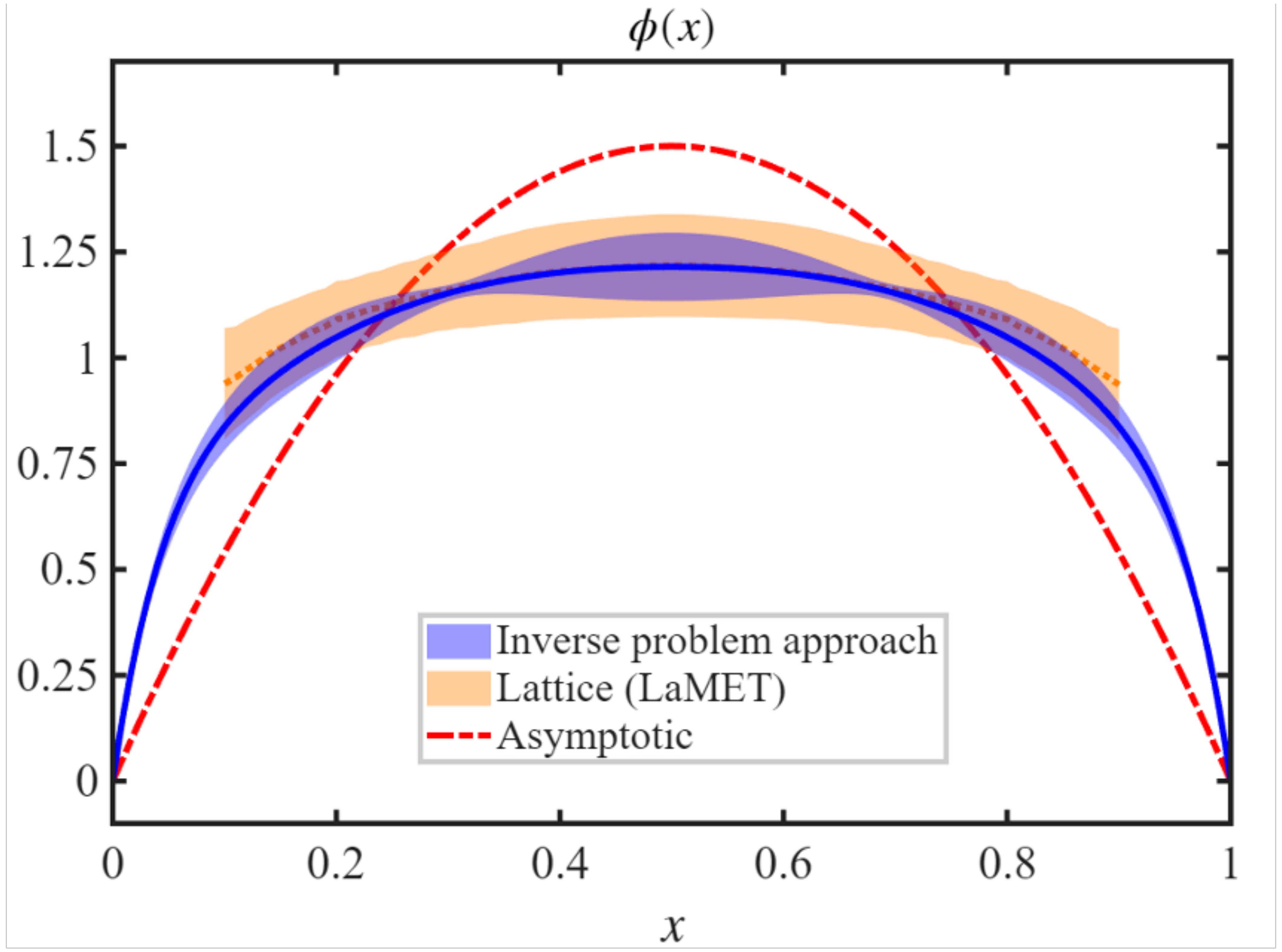
- Inverse Problem : Excited states and continuum spectrum can be directly solved.
- Avoid the quark-hadron duality

Physical Application: Moment Problem

LCDAs by moments from Dispersion Relation

$$\int_0^1 (2u-1)^n \varphi(u)\,\mathrm{d}u = \langle \xi^n \rangle, \quad \xi = 2u-1$$

Moments	Value
$\langle \xi^2 \rangle$	0.264 ± 0.022
$\langle \xi^4 \rangle$	0.107 ± 0.020
$\langle \xi^6 \rangle$	0.100 ± 0.012
$\langle \xi^8 \rangle$	0.067 ± 0.016
$\langle \xi^{10} \rangle$	0.083 ± 0.009
$\langle \xi^{12} \rangle$	0.064 ± 0.016



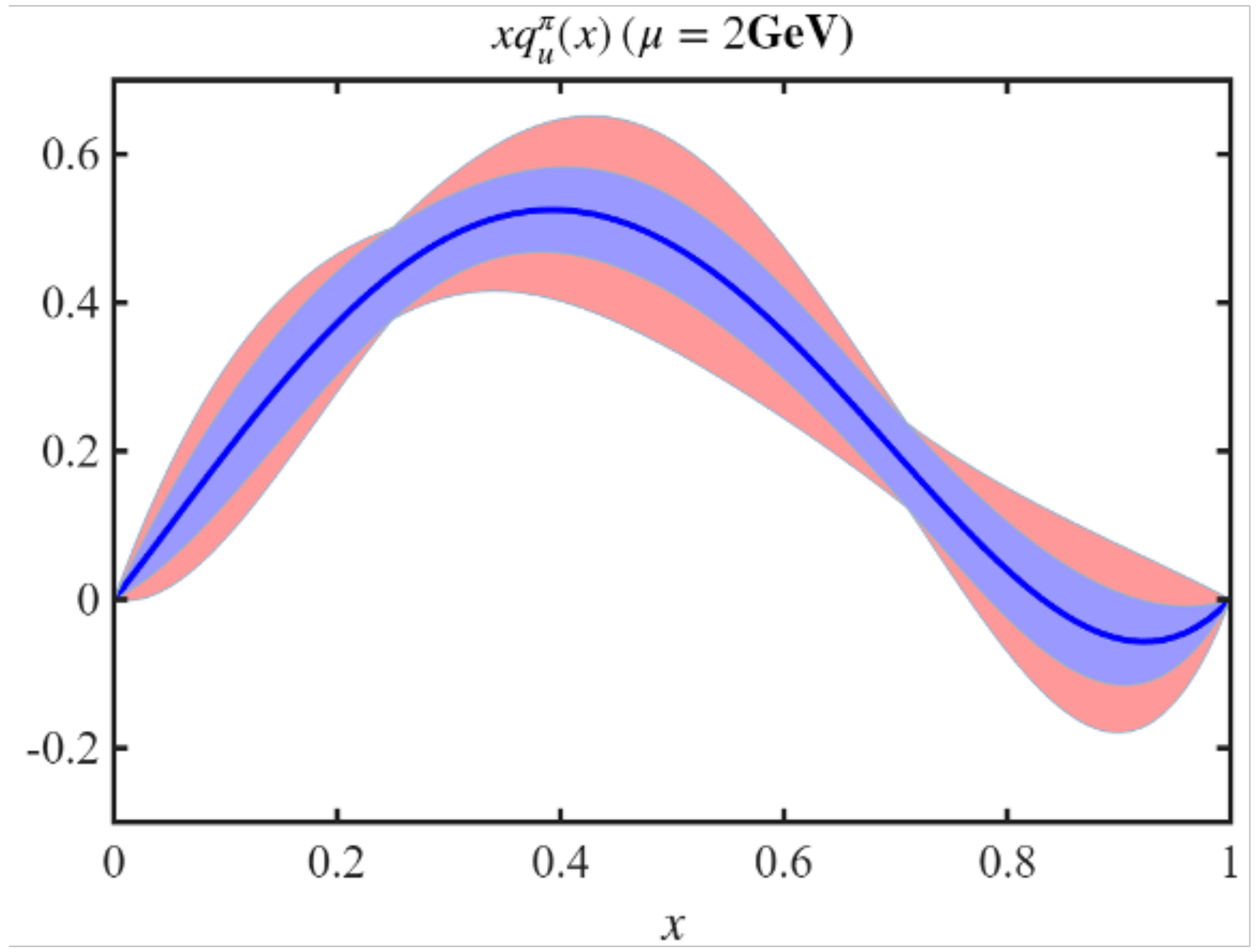
Physical Application: Moment Problem

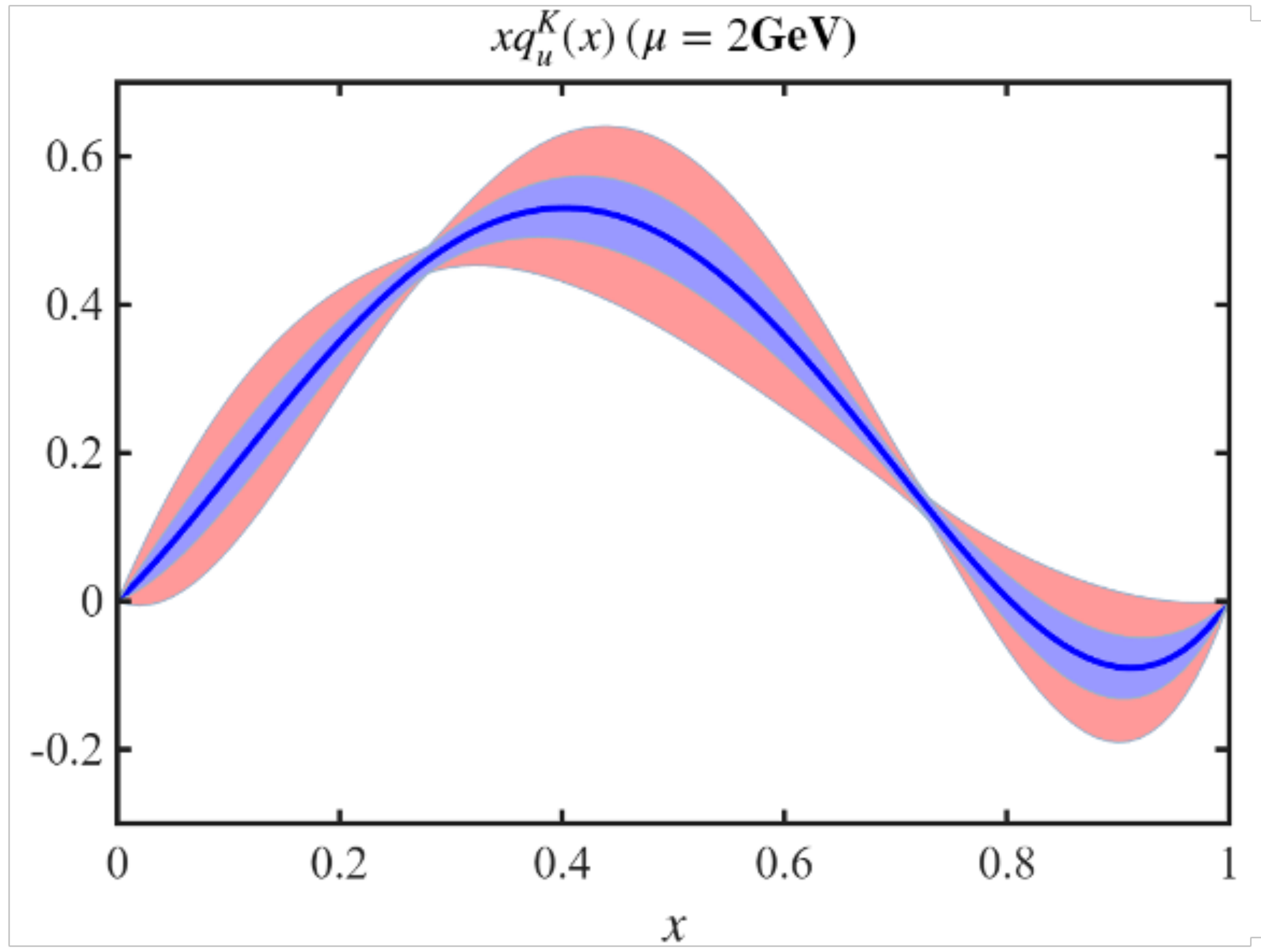
PDFs by moments from Lattice QCD

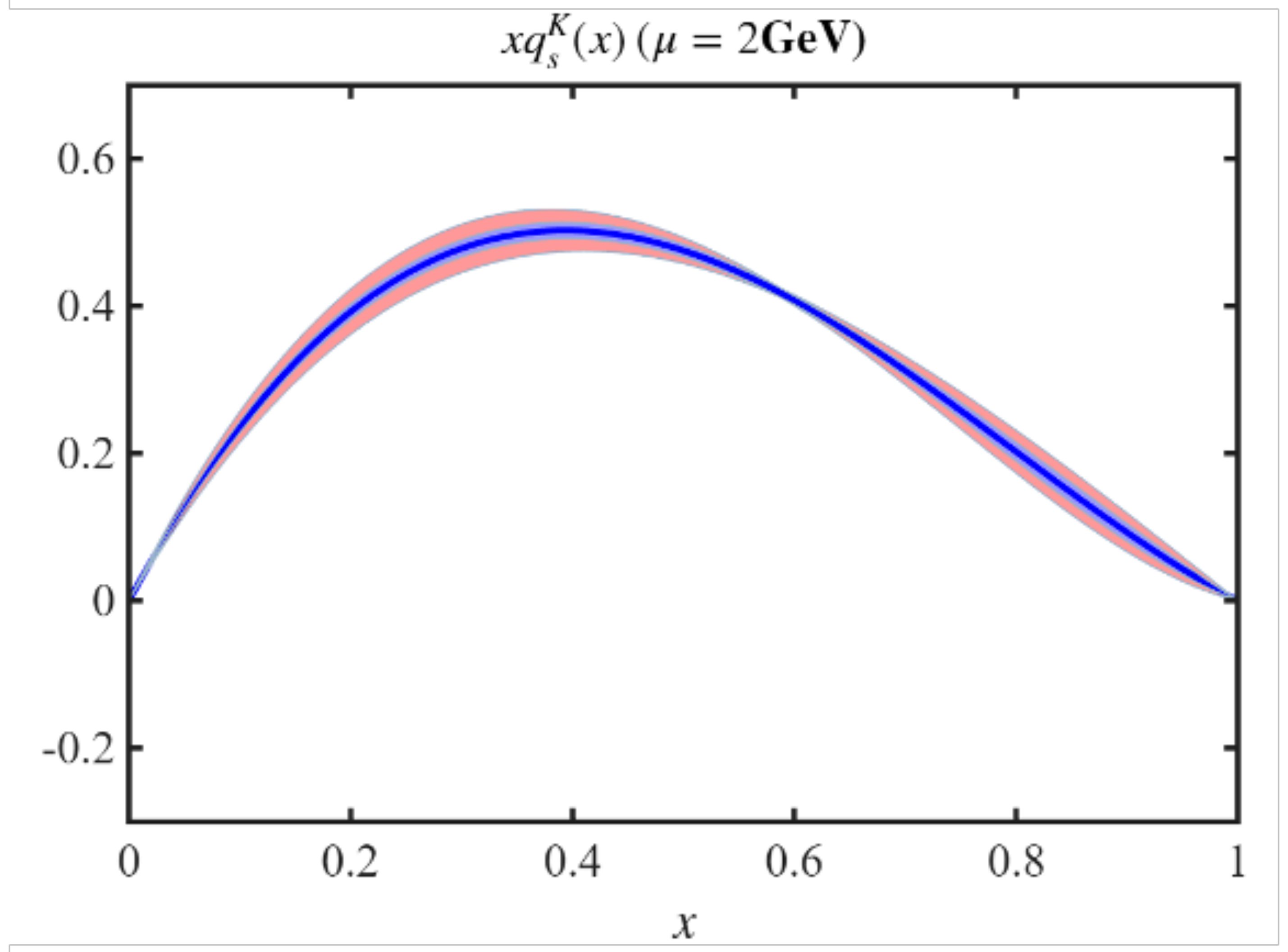
$$\int_0^1 x^n \varphi(x)\, \mathrm{d}x = \langle x^n \rangle$$

PDFs	$\langle x^1 \rangle$	$\langle x^2 \rangle$	$\langle x^3 \rangle$
$\pi^+(u^+)$	0.261(7)	0.110(14)	0.024(18)
$K^+(u^+)$	0.246(3)	0.096(3)	0.033(6)
$K^+(s^+)$	0.317(2)	0.139(2)	0.073(5)

Lattice QCD, PRD2021







Perspectives

- Firstly proposed to understand $D^0 - \overline{D}^0$ mixing by inversely solving dispersion relation [H.n.Li, H.Umeeda, **FSY**, F.Xu, 2001.04079]

- **Physical applications, with expansion of polynomials and inverse matrix method, by H.n.Li during 2020 - now:**
    - QCD related: muon g-2, ρ meson spectrum, glueballs, distribution amplitudes, neutral meson mixings, baryon spectrum
    - Determination of SM an NP: neutrino mass, EW scale, 4th generation quarks

- Its **mathematical framework** now provided with Tikhonov regularization method [A.S.Xiong, T.Wei, **FSY**, 2211.13753].
    - More applications in physics are expected.

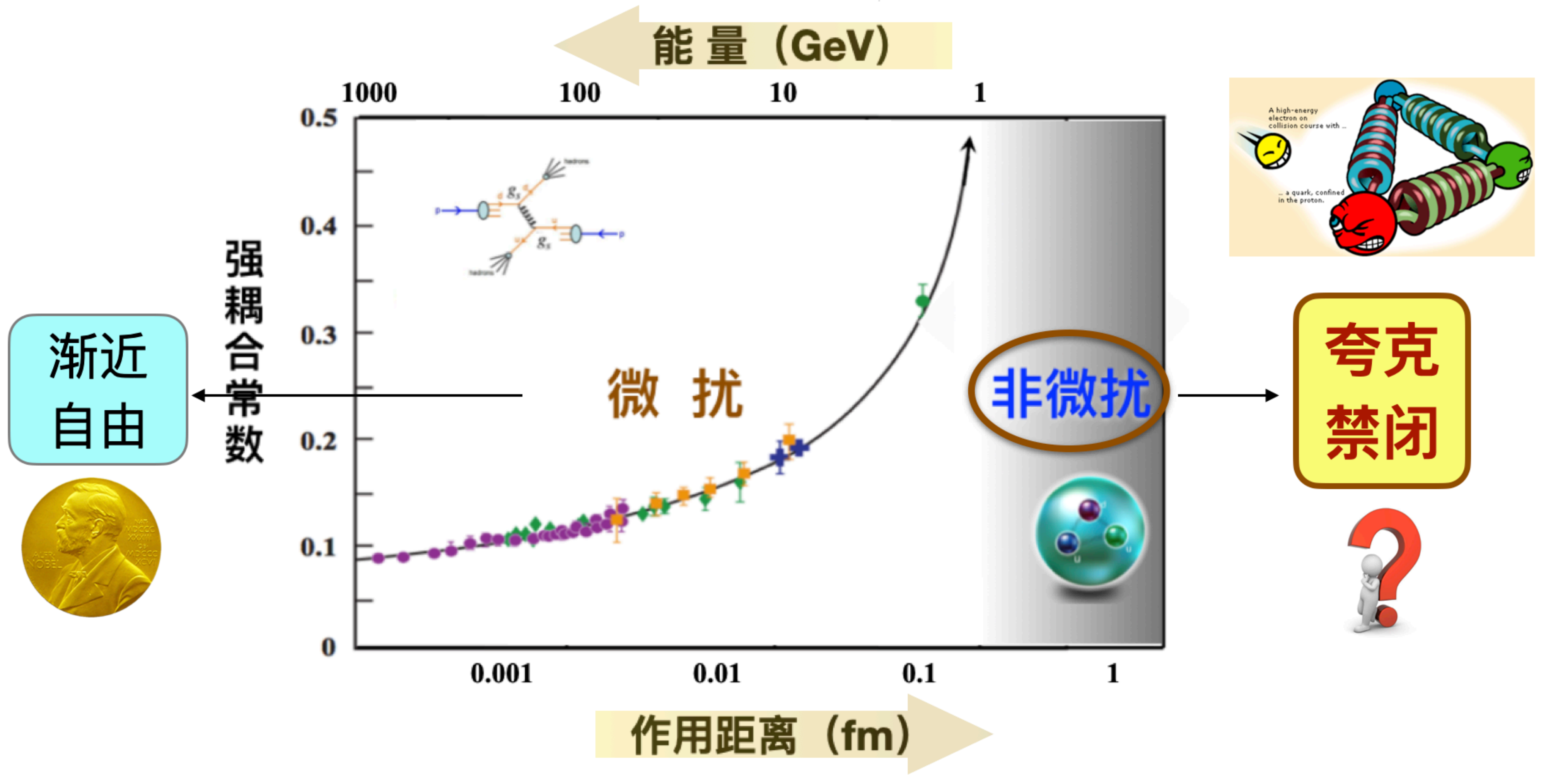
Summary

- We propose a novel method to calculate the non-perturbative quantities.
- With the **dispersion relation** of QFT, the non-perturbative quantities are obtained by solving the **inverse problem** with the perturbative calculations as inputs.
- The mathematical basis has been provided. The precision of the predictions can be systematically improved, without artificial assumptions.
- Physical applications are expected.

Thank you!

Backups

Problem of Non-Perturbation QCD



- **Particle physics:** color confinement
- **New physics**: muon g-2, $Br(B \to D^{(*)}\tau\nu)/Br(B \to D^{(*)}\ell\nu)$
- **Parton physics**: mass and spin of nucleon, PDF, GPD, TMD, LCDA
- **Hadron physics**: tetraquarks, pentaquark, glueballs
- **High energy nuclear physics**: QCD phase transition, critical point
- **Low energy nuclear physics**: nuclear force

How can we predict non-perturbative quantities from QCD?

Lattice QCD, Dyson-Schwinger Equation, QCD sum rules,
Holographic QCD, quark models, and so on

Advantages and disadvantages …

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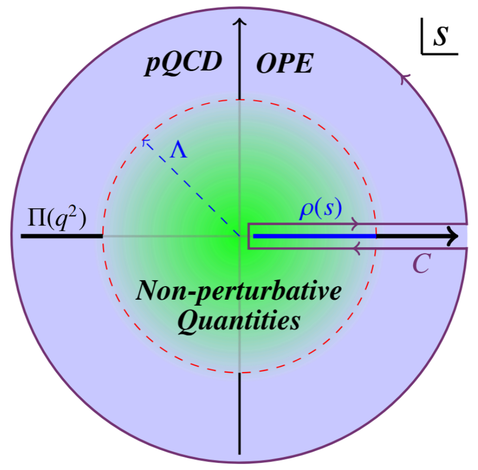
a) Dispersion relation



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Or subtraction formulas

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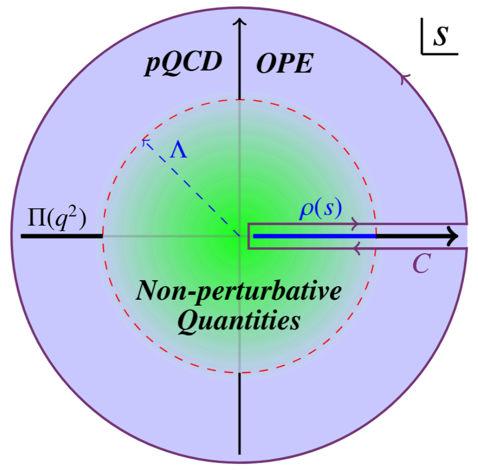

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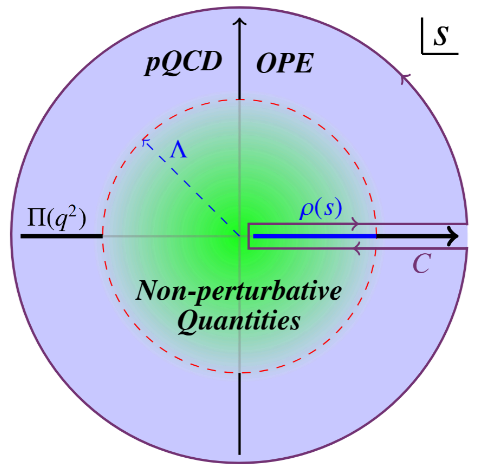

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$$\Rightarrow \quad Kf = g$$

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- uniqueness ✔
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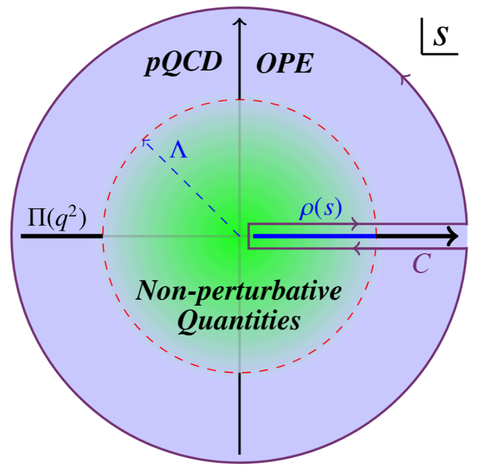

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Outline

1. Inverse problem of dispersion relation, and ill-posedness
2. Regularization strategy: Tikhonov regularization
3. Uncertainty analysis and systematical improvement of precision
4. Physical discussions and perspectives

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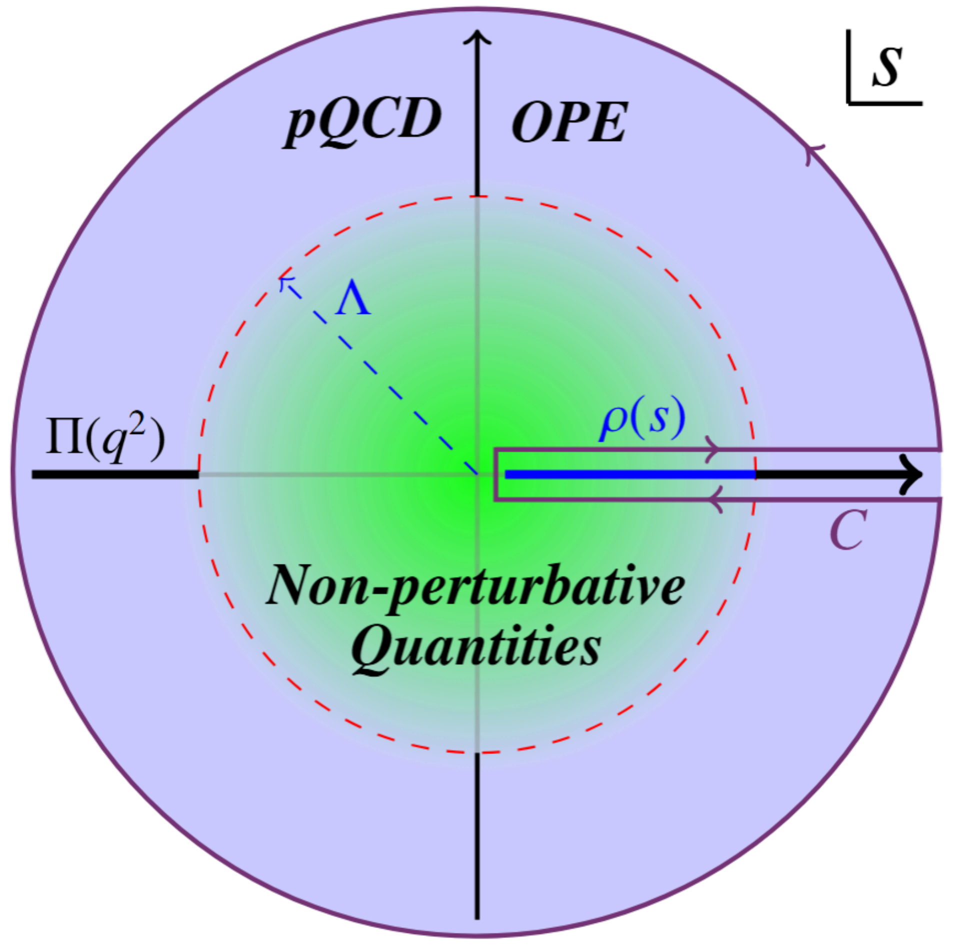

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Non-perturbative objective — Perturbative input

Integral Equation and Operator Equation

- Inverse problem of dispersion relation: $$\int_{t_{\min}}^{\Lambda} \mathrm{d}s \frac{\mathrm{Im}\,\Pi(s)}{s-q^2} = \pi\Pi(q^2) - \int_{\Lambda}^{\infty} \mathrm{d}s \frac{\mathrm{Im}\,\Pi(s)}{s-q^2}$$

$$\int_{t_{\min}}^{\Lambda} \frac{f(x)}{x-y}\,\mathrm{d}x = g(y)\,,$$ with $y \in [q^2_{\mathrm{low}}, q^2_{\mathrm{up}}]\,,$ $\Lambda > t_{\min} \geqslant 0$ and $q^2_{\mathrm{low}} < q^2_{\mathrm{up}} \ll 0.$

$$Kf = g\,,$$ with $f \in F\,,\ g \in G\,,$ $K : F \to G$ is the linear integral operator,

$F = L^2(t_{\min}, \Lambda)$ $\quad G = L^2(q^2_{\mathrm{low}}, q^2_{\mathrm{up}})$ $\quad \|f\|_{L^2(a,b)} = \left(\int_a^b |f(x)|^2\,\mathrm{d}x\right)^{1/2}$

ill-posedness

The inverse problem of dispersion relation is ill-posed

See 2211.13753

1) Existence ✓

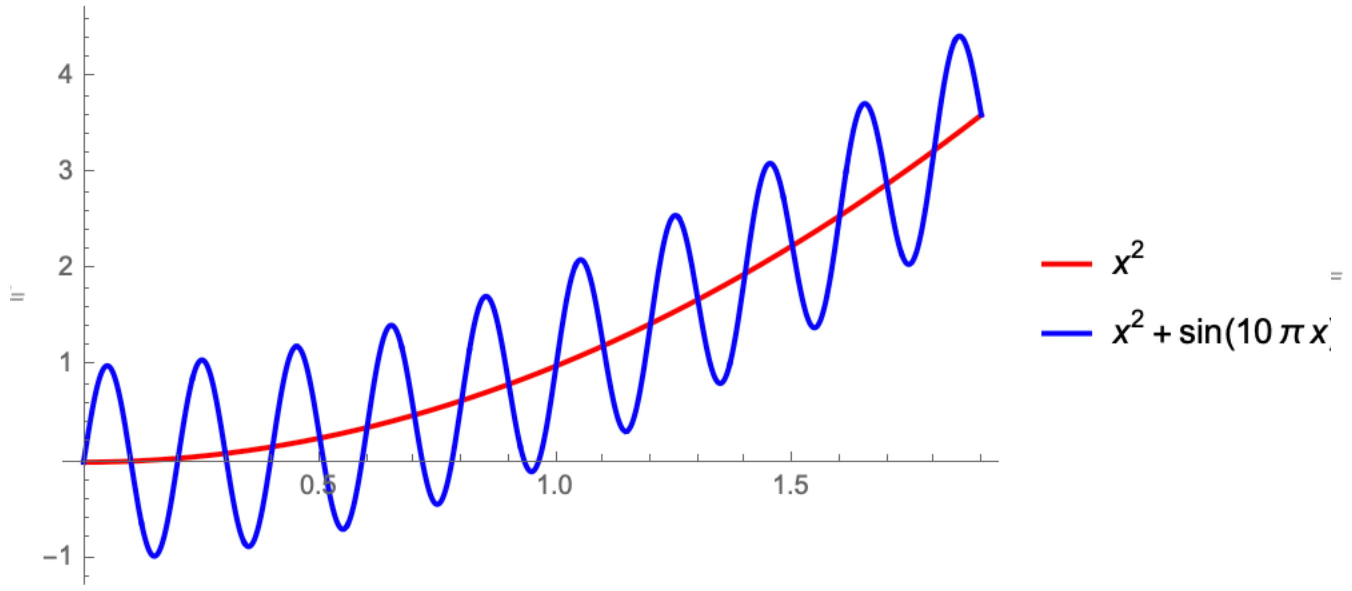
2) Uniqueness ✓

3) Stability ✗

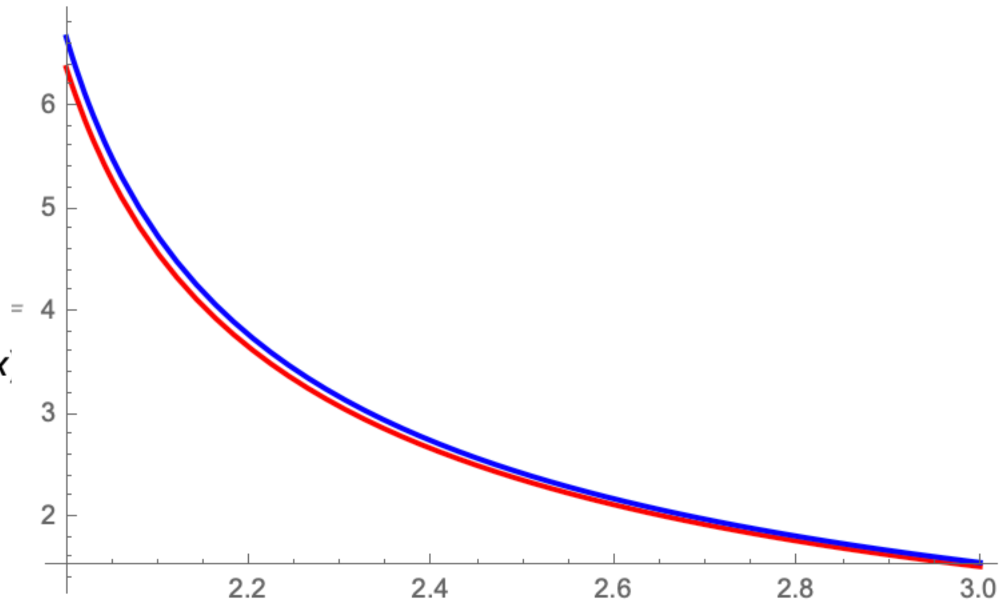
$$\int_{t_{\min}}^{\Lambda} \frac{f(x)}{x-y}\,\mathrm{d}x = g(y)\,, \qquad \text{with } y \in [q^2_{\mathrm{low}}, q^2_{\mathrm{up}}]\,,$$

$f(x)$

$g(y)$



Instability



uniqueness

Discrete problems do not even satisfy uniqueness

ill-posedness

- Discretization: $K_{ij}f_j = g_i\ ,\quad f_j = (K^{-1})_{ji}g_i\ .$ The problem is that K^{-1} diverges

- K is a compact operator, which cannot have a bounded inverse in an infinite-dimensional space

In the formula of matrix, $K^{-1} = \dfrac{K^*}{\det(K)}$ with K^* the conjugate of K

$\det(K) \to 0$, since K is a continuous operator

discretization dimensions: $n = 10\ ,\ \det(K) = 10^{-88}\ ;\quad n = 20\ ,\ \det(K) = 10^{-244}$

- K^{-1} diverges $\Longrightarrow$ A small error of g^δ would induce infinitely large error of solution

ill-posedness

- 算子方程：$Kf = g$ $$\int_a^b \frac{f(x)}{y-x}\mathrm{d}x = g(y),\ \ y \in [c,d],\ \ c > b,\ \ a > 0$$

- 离散成矩阵问题：$K_{ij}f_j = g_i$ ， $f_j = (K^{-1})_{ji}g_i$ ， 问题关键是K^{-1}发散

  - 补充数学知识：K是紧算子，无穷维时紧算子不存在有界的逆

    有界空间：$\|\phi\| \leqslant C,\ \ C > 0.$ 有界算子：$\|A\phi\| \leqslant C\|\phi\|,\ \ C > 0.$ 不发散的意思

    L^2范数：$\|f\|_2 = \sqrt{\int_a^b |f(x)|^2 dx}$

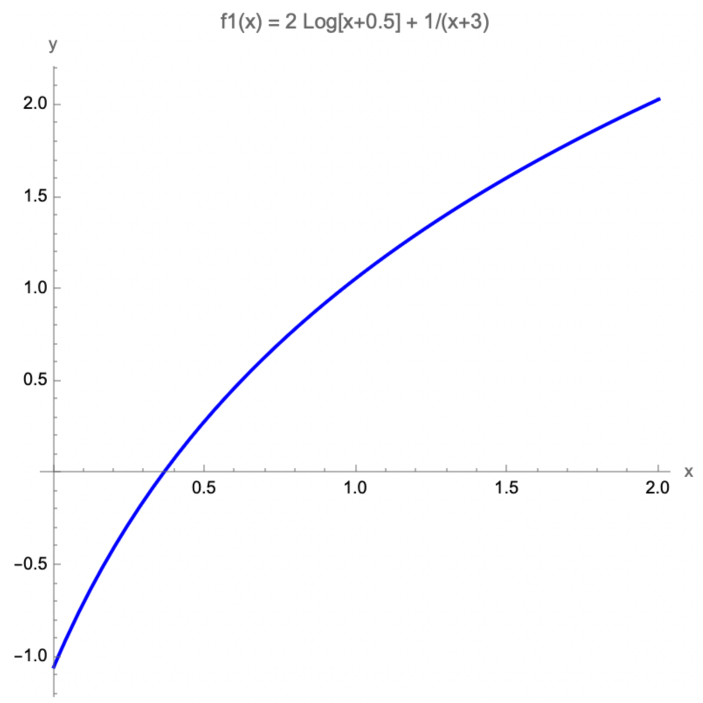
    无限维空间中的紧集对应于有限维空间的有界闭集。

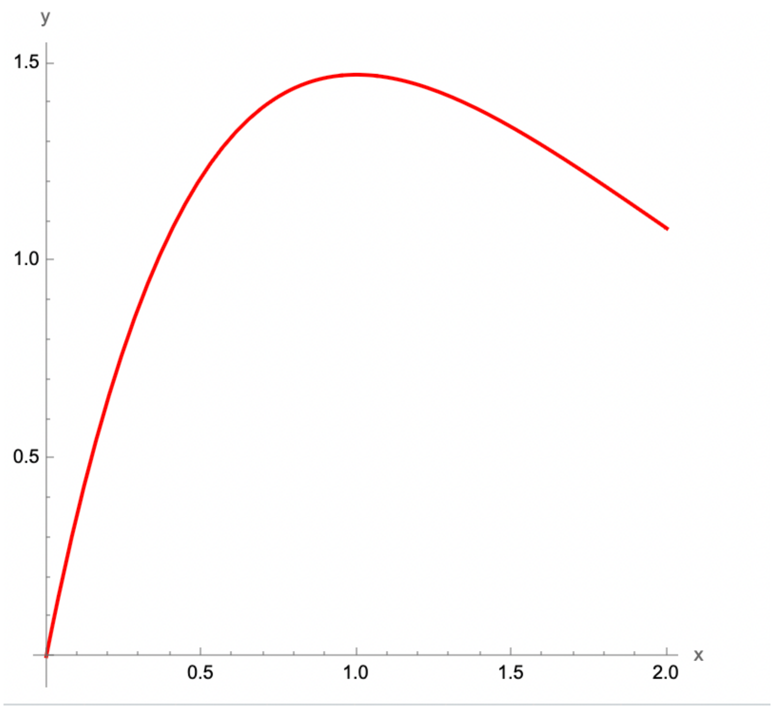
Toy Models

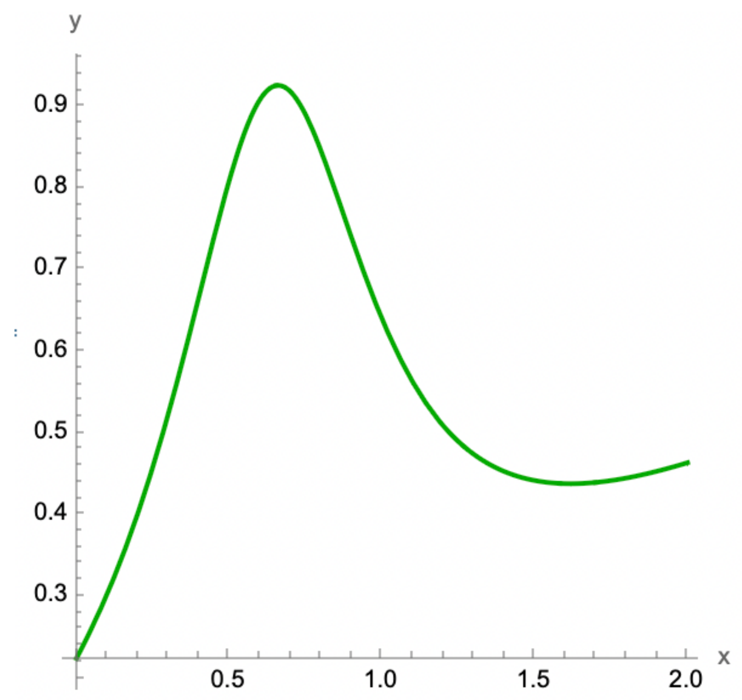
Model 1 (monotonic) : $f(x) = a_1 2\log(x+0.5) + \dfrac{a_2}{x+3}$,

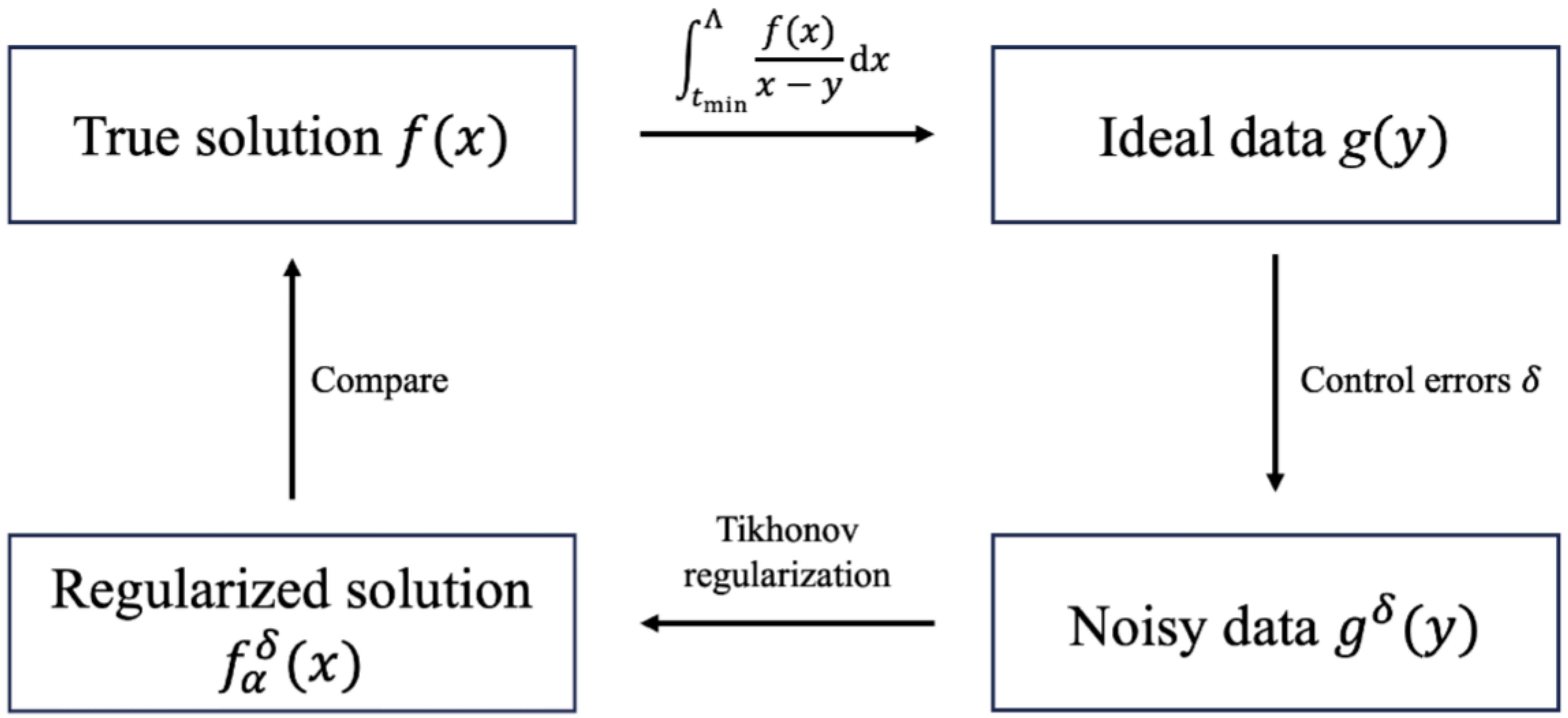
Model 2 (simple non-monotonic) : $f(x) = a_1 10 x e^{-a_2 2x}$,

Model 3 (resonance) : $f(x) = \dfrac{1}{\pi}\dfrac{0.4a_1}{(x-0.64)^2+(0.4a_1)^2} + a_2\dfrac{x}{5}$.



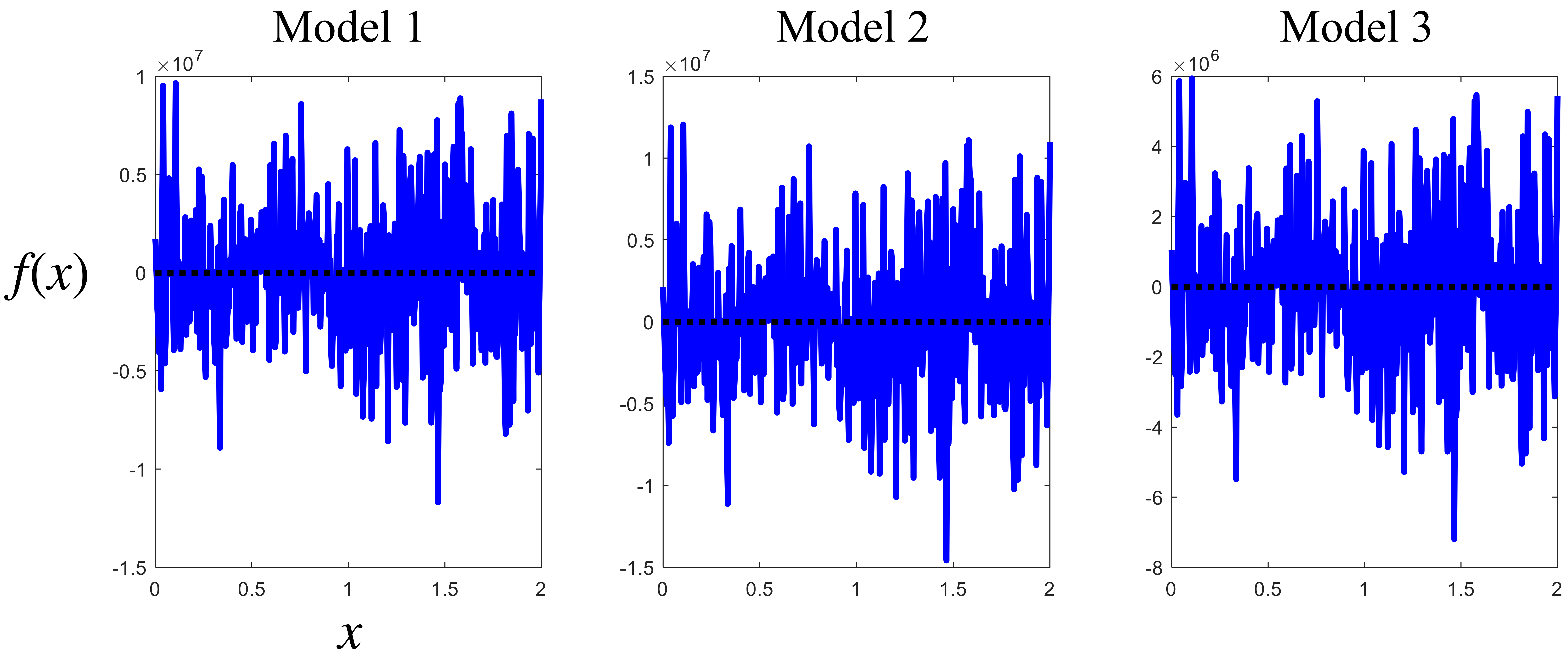






$a_1 = 1 \pm \sigma,\ a_2 = 1 \pm \sigma$

- No regularization $\Longrightarrow$ Unstable solution $\Longrightarrow$ Necessity of regularization



Outline

1. Inverse problem of dispersion relation, and ill-posedness
2. Regularization strategy: Tikhonov regularization
3. Uncertainty analysis and systematical improvement of precision
4. Physical discussions and perspectives

Illustration of Regularization Methods

a) Regularization strategy

- Nearby well-posed approximation

$$Kf = g \quad \Rightarrow \quad \text{bounded} \;\; R_\alpha \sim K^{-1}$$

- Regularization strategy:

$$\lim_{\alpha \to 0} R_\alpha K f = f, \qquad f_\alpha^\delta = R_\alpha g^\delta$$

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b) Tikhonov regularization

- Regularization operator

$$R_\alpha = (K^* K + \alpha I)^{-1} K^*$$

- Equivalent to minimize the functional

$$f_\alpha^\delta = \arg\min \left\{ \|Kf - g^\delta\|_G^2 + \alpha \, \|f\|_F^2 \right\}$$

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c) Convergence of solution

- Error estimation in a priori condition

$$\|f_\alpha^\delta - f\| \leqslant \alpha E + \delta/(2\sqrt{\alpha})$$

- Convergence of solution, $\alpha = (\delta/E)^{2/3}$

$$\|f_\alpha^\delta - f\| \leqslant 3/2 \, \delta^{2/3} E^{1/3} \to 0, \text{ as } \delta \to 0$$

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d) Interpretability by SVD

- Singular Value Decomposition (SVD)

$$\mu_1 \geqslant \mu_2 \geqslant \mu_3 \geqslant \cdots > 0$$

- Convergence by the leading terms

$$f_\alpha^\delta = \sum_i \frac{\mu_i}{\mu_i^2 + \alpha} (g^\delta, g_i) \, f_i$$

General Regularization Theory

- Basic idea: Approximate an ill-posed problem by a nearby well-posed problem
- Ensure that the approximate solution converges to true solution as $\delta \to 0$

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- Ensure that the approximate solution converges to true solution as $\delta \to 0$

- **Definition**: A regularization strategy is a family of linear and bounded operator

$R_\alpha : G \to F$, $\alpha > 0$, such that $\lim_{\alpha \to 0} R_\alpha K f = f$

- Condition 1: Boundedness. Not divergent, thus solvable.
- Condition 2: Convergence. As $\alpha \to 0$, $R_\alpha \to K^{-1}$, back to original problem

- $f_\alpha^\delta = R_\alpha g^\delta$ is an approximation of the solution of $Kf = g$

General Regularization Theory : Matrix Example

- 假如 A 是个半正定的方阵，它的一个简单近似是 $A + \alpha I$
- 当 $\alpha \to 0$ 时，$A + \alpha I \to A$，有收敛性
- A 不可逆 ⇔ A 奇异 ⇔ $\det(A) = 0$

  行列式等于特征值的乘积，$\det(A) = \Pi_i \lambda_i$

  $\det(A) \to 0 \Rightarrow$ 存在 $\lambda_i \to 0$

- 对于特征方程 $Ax = \lambda x$

  $(A + \alpha I)x = (\lambda + \alpha)x \quad \Rightarrow \quad (\lambda + \alpha)$ 是 $A + \alpha I$ 的特征值

  $\det(A + \alpha I) = \Pi_i(\lambda_i + \alpha) \neq 0, \quad \alpha > 0$

- 因此 $(A + \alpha I)^{-1}$ 是 A^{-1} 的有界、收敛的近似。

Tikhonov Regularization : Operator

- 对于 $Kf = g$，一般情况下 K 不是方阵，作用空间不同
  - 伴随算子：在Hilbert空间下，$(Kf, g) = (f, K^*g)$ $K : F \to G,\ K^* : G \to F$

$$Kf = g \quad \Rightarrow \quad K^*Kf = K^*g \quad \Rightarrow \quad f = (K^*K)^{-1}K^*g$$

- K^*K 是方阵，可以加正则化项：$f_\alpha = (K^*K + \alpha I)^{-1}K^*g$

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- K^*K 是方阵，可以加正则化项：$f_\alpha = (K^*K + \alpha I)^{-1}K^*g$

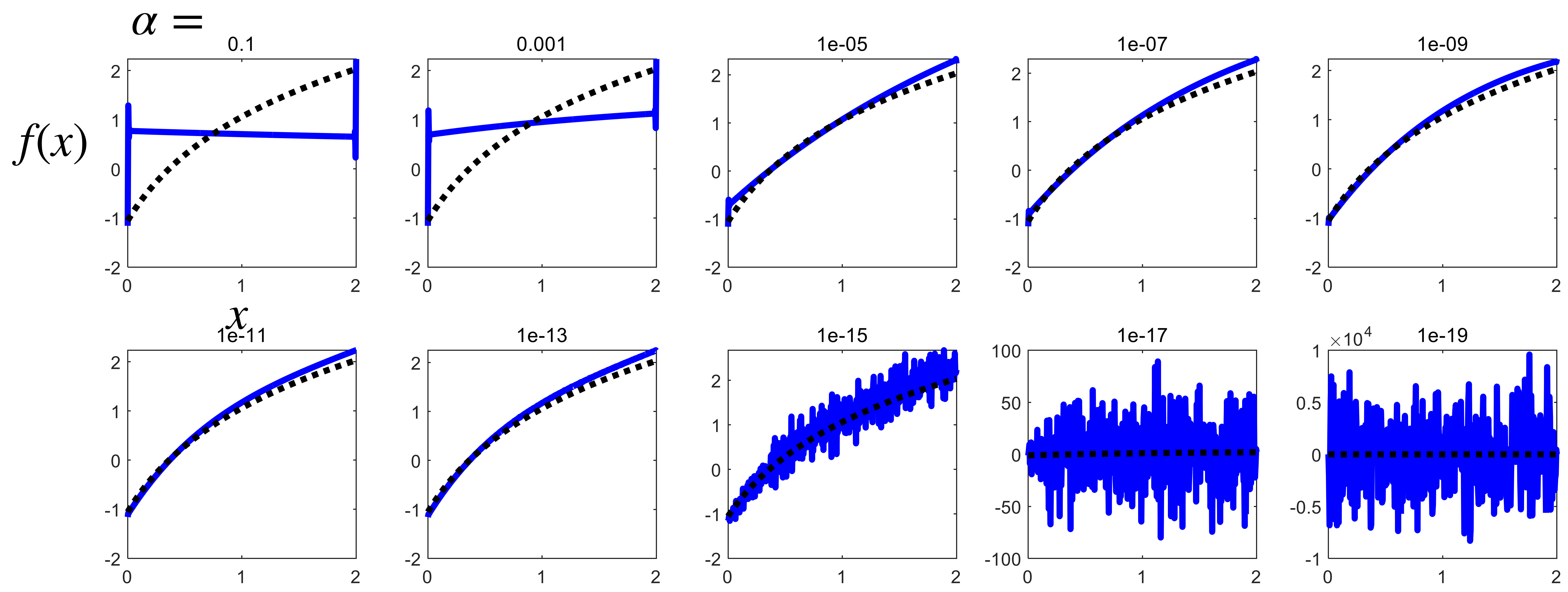
- Tikhonov正则化算子：$R_\alpha = (K^*K + \alpha I)^{-1}K^*$， $\quad f_\alpha^\delta = R_\alpha g^\delta$

  即 $f_\alpha^\delta = (K^*K + \alpha I)^{-1}K^*g^\delta$

- 它是 K^{-1} 最简单的有界近似，$\alpha \to 0$ 时，$R_\alpha \to K^{-1}$。R_α 有界、收敛，是正则化算子

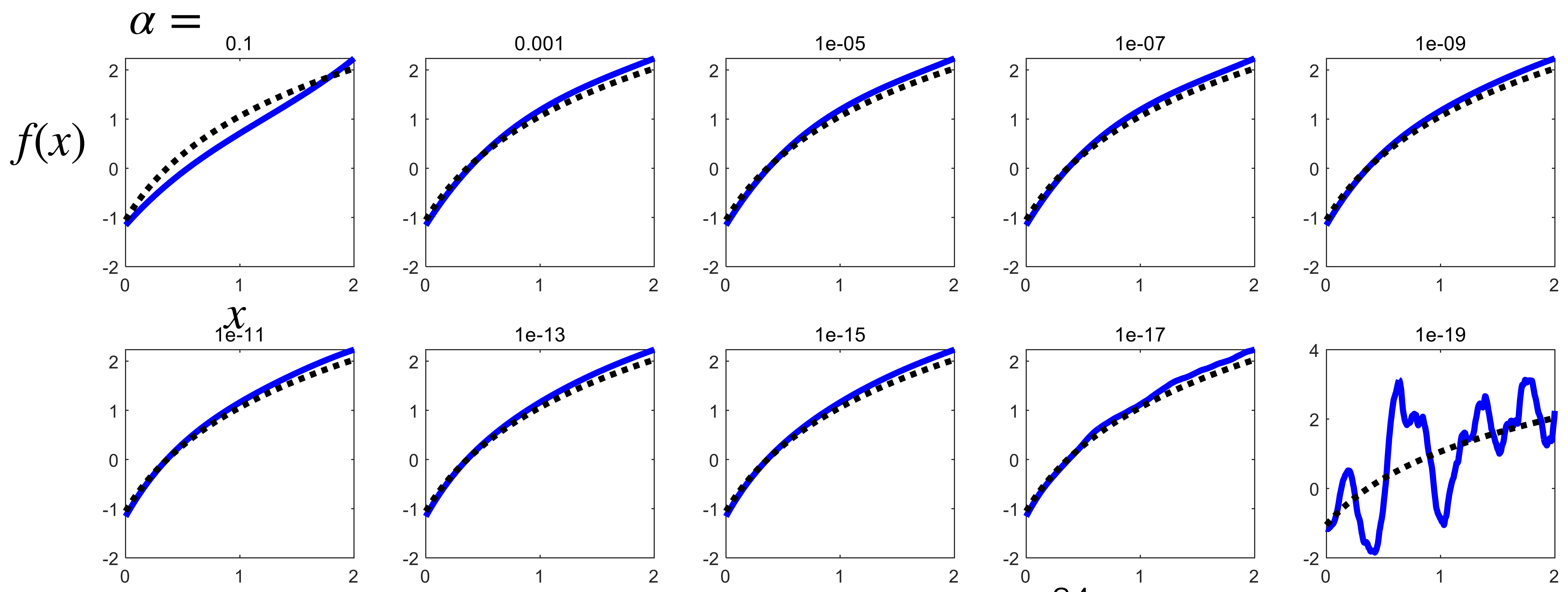
Numerical Results under Regularization

Model 1



- Tikhonov regularization in L^2 space

Model 1

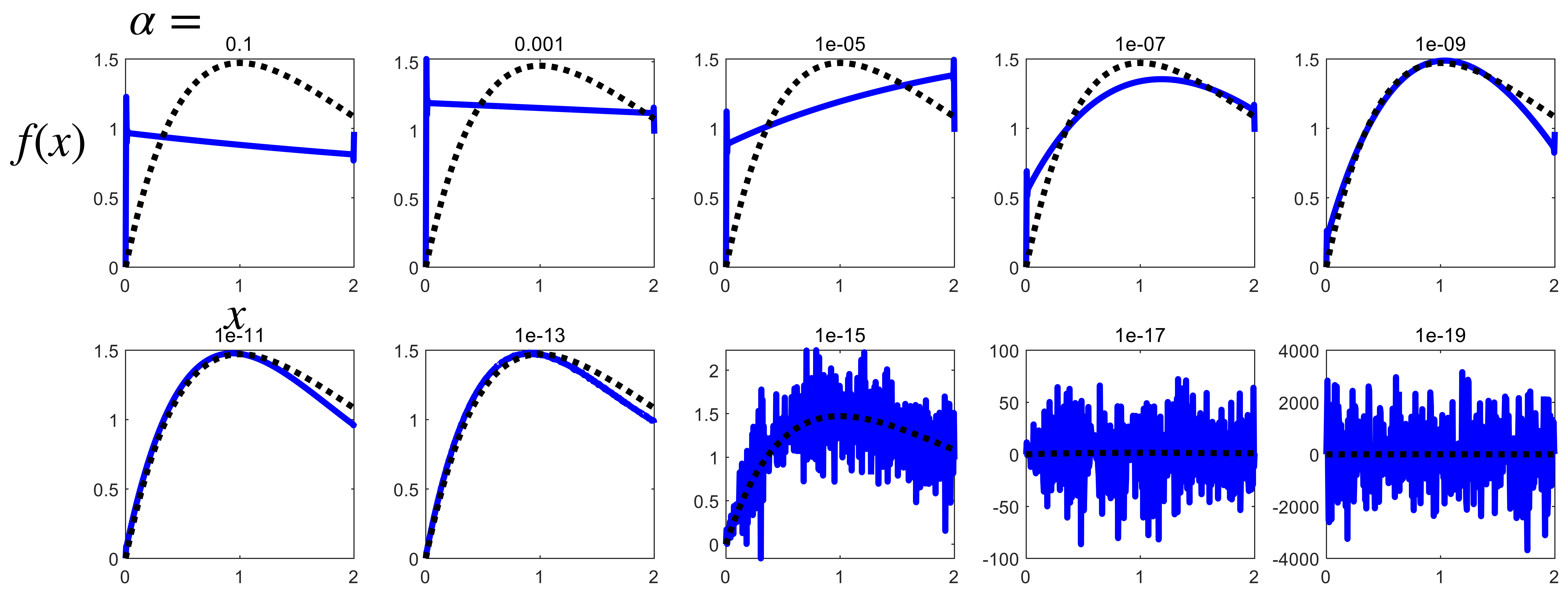


- Tikhonov regularization in H^1 space

$$\|f\|_{H^1(a,b)} = \left(\int_a^b \left(|f(x)|^2 + |f'(x)|^2 \right) \mathrm{d}x \right)^{1/2}$$

Numerical Results under Regularization

Model 2



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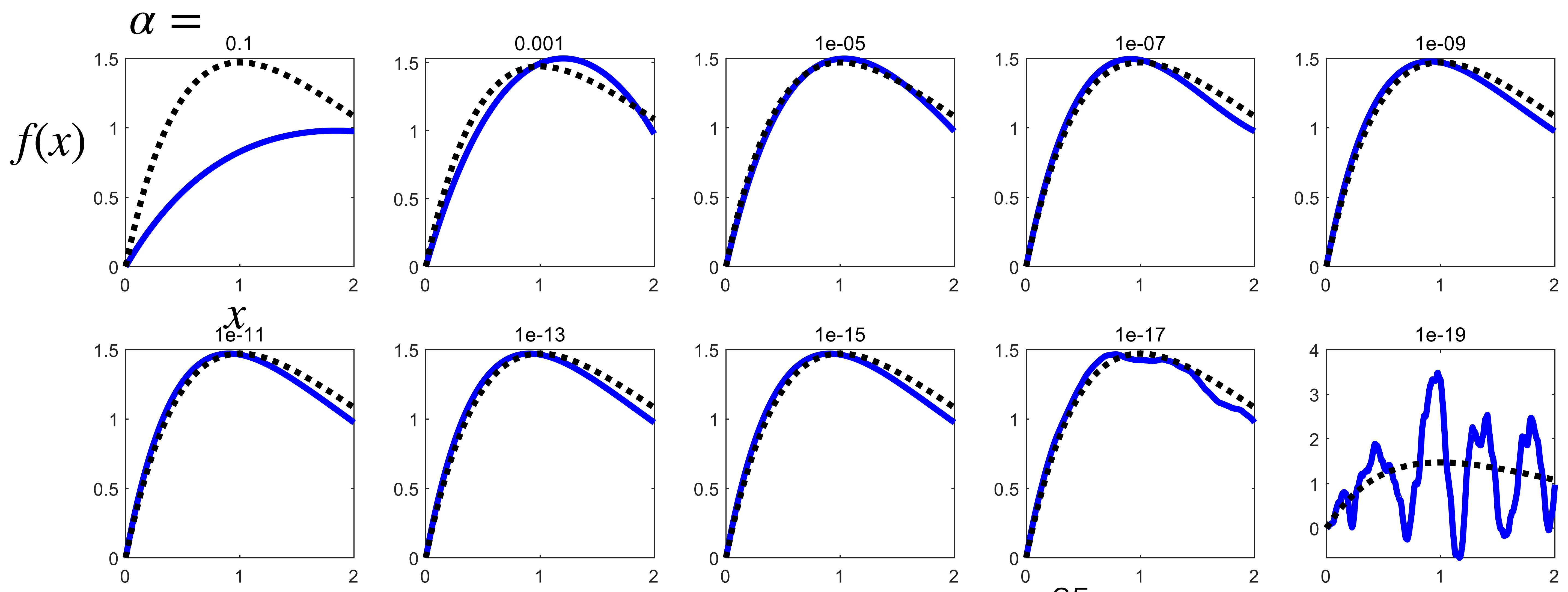
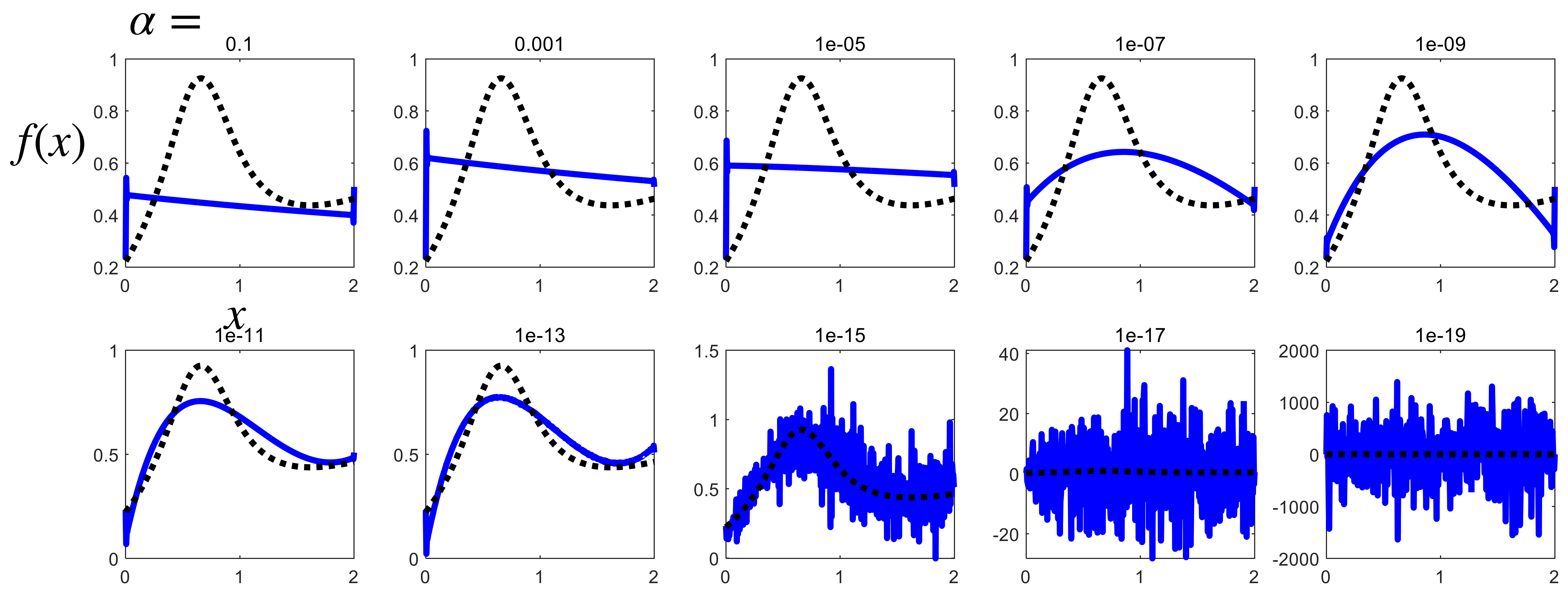
Model 2



- Tikhonov regularization in H^1 space

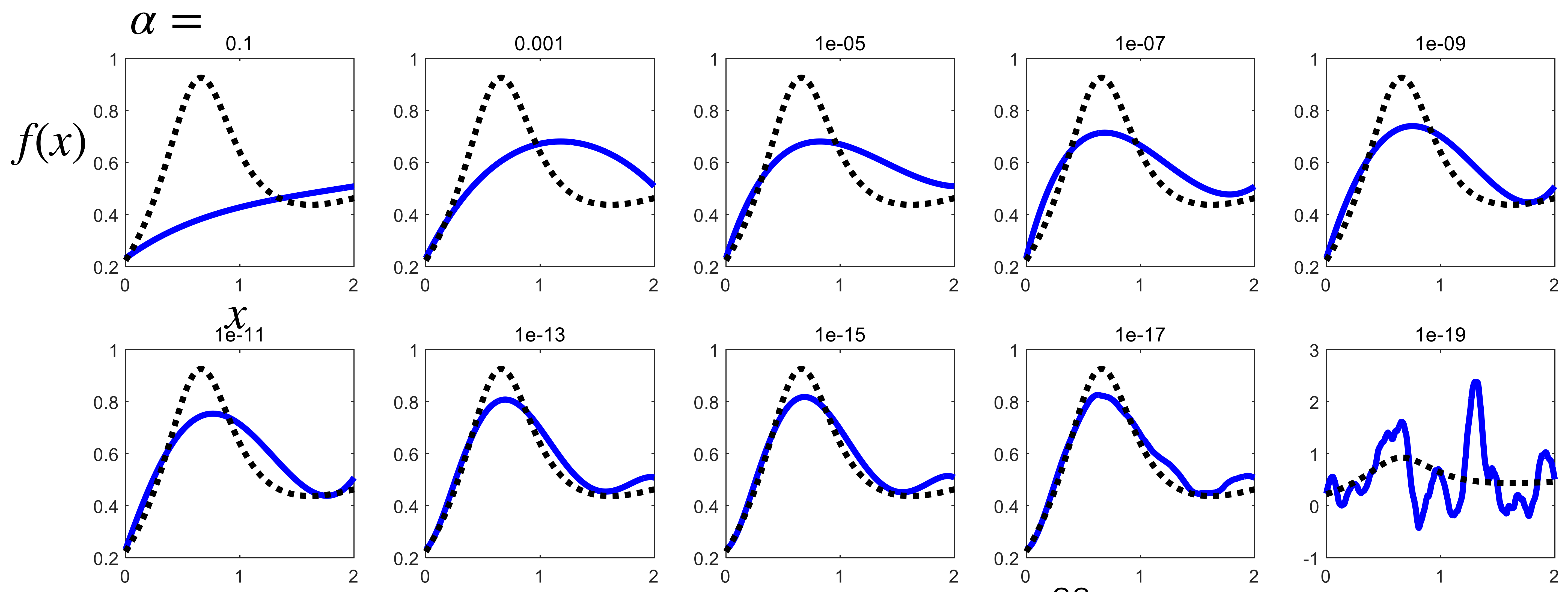
Numerical Results under Regularization

Model 3



- Tikhonov regularization in L^2 space

Model 3



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Outline

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Error Estimates

- 近似解是否接近真解？尤其是在输入误差 $\delta \to 0$ 时，近似解是否收敛到真解？
- 我们先看误差估计。已知 $\|g^\delta - g\| \leqslant \delta$，看解的误差 $\|f_\alpha^\delta - f\|$

$$
\begin{aligned}
\|f_\alpha^\delta - f\| &\leqslant \|f_\alpha^\delta - f_\alpha\| + \|f_\alpha - f\| \\
&= \|R_\alpha g^\delta - R_\alpha g\| + \|R_\alpha g - f\| \\
&\leqslant \|R_\alpha\| \|g^\delta - g\| + \|R_\alpha K f - f\| \\
&\leqslant \delta\, \|R_\alpha\| + \|R_\alpha K f - f\|
\end{aligned}
$$

Error Estimates

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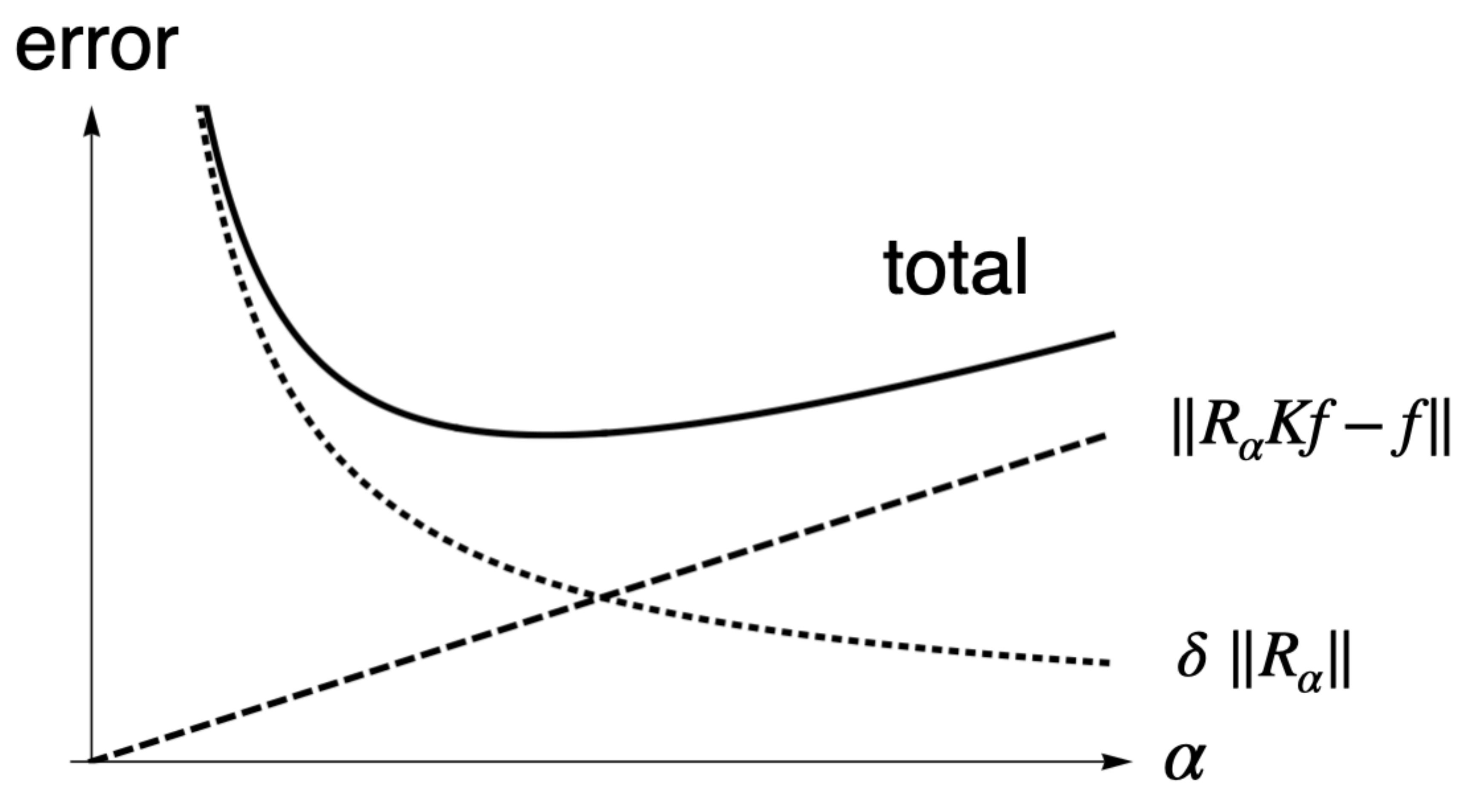
&\leqslant \|R_\alpha\|\|g^\delta - g\| + \|R_\alpha K f - f\| \\
&\leqslant \delta\,\|R_\alpha\| + \|R_\alpha K f - f\|
\end{aligned}
$$



- α 不能太大，也不能太小。α 的选取必须保持某种平衡。

Convergence of Solution

- 解的收敛性：要求 $\delta \to 0$ 时，$\|f_\alpha^\delta - f\| \to 0$，近似解收敛到真解。
- 解的误差：$\|f_\alpha^\delta - f\| \leqslant \|R_\alpha Kf - f\| + \delta \, \|R_\alpha\|$

(1)Tikhonov正则化下，$\|R_\alpha\| \leqslant 1/\left(2\sqrt{\alpha}\right)$

(2)在先验条件 $f = K^*Kz \in K^*K(F)$，$\|z\| \leqslant E$ 下，$\|R_\alpha Kf - f\| \leqslant \alpha E$

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- $\|f_\alpha^\delta - f\| \leqslant \dfrac{\delta}{2\sqrt{\alpha}} + \alpha E$ ， 取 $\alpha = \left(\dfrac{\delta}{E}\right)^{2/3}$，

$$\|f_\alpha^\delta - f\| \leqslant 3/2\ \delta^{2/3}\, E^{1/3} \to 0,\ \ \delta \to 0$$

Convergence of Solution

- $\|f_\alpha^\delta - f\| \leqslant \dfrac{\delta}{2\sqrt{\alpha}} + \alpha E$, 取 $\alpha = \left(\dfrac{\delta}{E}\right)^{2/3}$, $\|f_\alpha^\delta - f\| \leqslant 3/2\ \delta^{2/3}\ E^{1/3} \to 0,\ \ \delta \to 0$
- 解具有收敛性！$\delta \to 0$时能收敛到真解，这是最重要的性质！反问题方法可以系统性改进！
- 误差有上界，说明误差是可控的！
- 注(1)：α 不能太大也不能太小，α 的选取随 δ 变
- 注(2)：先验条件 $f = K^*Kz \in K^*K(F)$， $\|z\| \leqslant E$ ，其实就是 $\|f\|$ 有界。

  ✓ $\|f\|$ 有界是物理要求的，任何物理观测量都是有限的，因此解的收敛性必然满足

  ✓即使在实际应用中不方便使用上界条件，也不妨碍解的收敛性，无论实际应用中用什么 α 的选取方法，解的收敛性都是必须保证的

Choice of Regularization Parameter

- 正则化方法最重要的两步：第一，构造正则化算子；第二，选取正则化参数。
- $\delta \to 0$时近似解收敛到真解，但实际无法满足$\delta \to 0$，须在有限误差下选取α。
- 在物理上有个基本准则，物理结果不应依赖于参数的选取，即应该存在一个平台。

(1) 偏差原理：已知 $\|g^\delta - g\| \leqslant \delta$，取 $\|Kf_\alpha^\delta - g^\delta\| = \delta$ 时的α

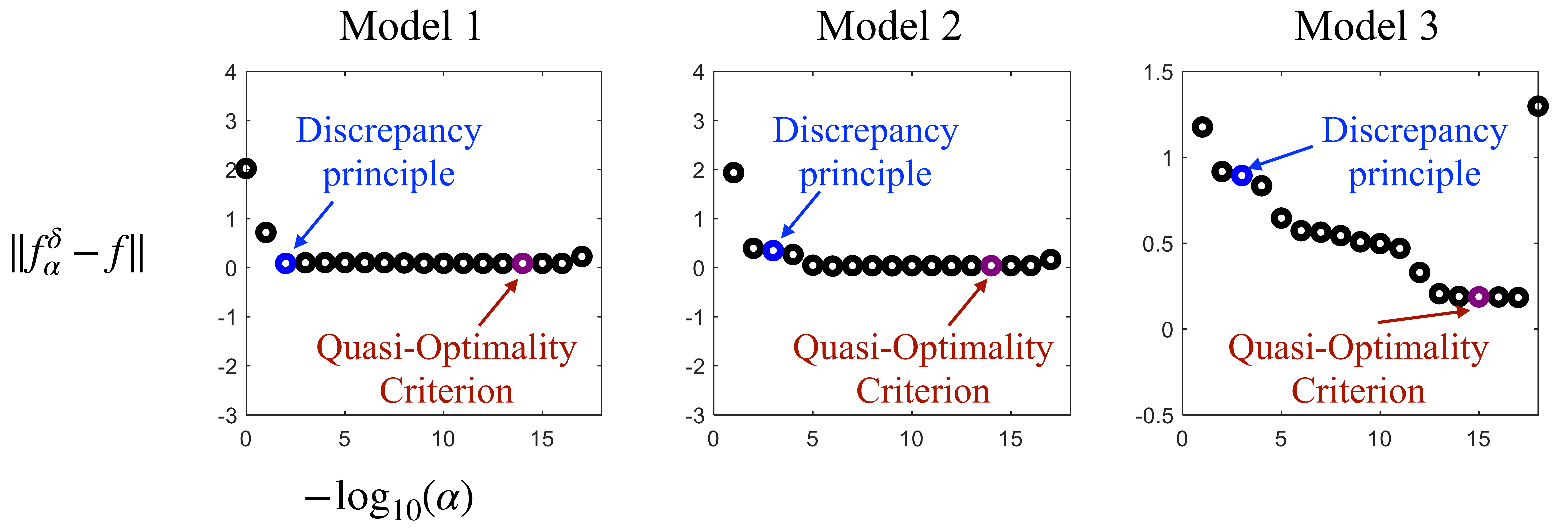
- $\|Kf - g^\delta\|$ 太小会过拟合，它稍大点 $\|f\|$ 更稳定。残差与噪声匹配，类似$\chi^2/\mathrm{dof} \sim 1$
- 偏差原理有严格的收敛性证明：$f^\delta \to f, \quad \delta \to 0$

(2) 拟最优准则：$\alpha_{\mathrm{opt}} = \arg\min_{\alpha>0} \left\{ \left\| \alpha \frac{\mathrm{d}f_\alpha}{\mathrm{d}\alpha} \right\| \right\}$. 找平台，以及选择相对小的$\alpha$

- 我们要求双保险：物理上对参数依赖的平台 + 数学方法。尽量提供α的鲁棒性

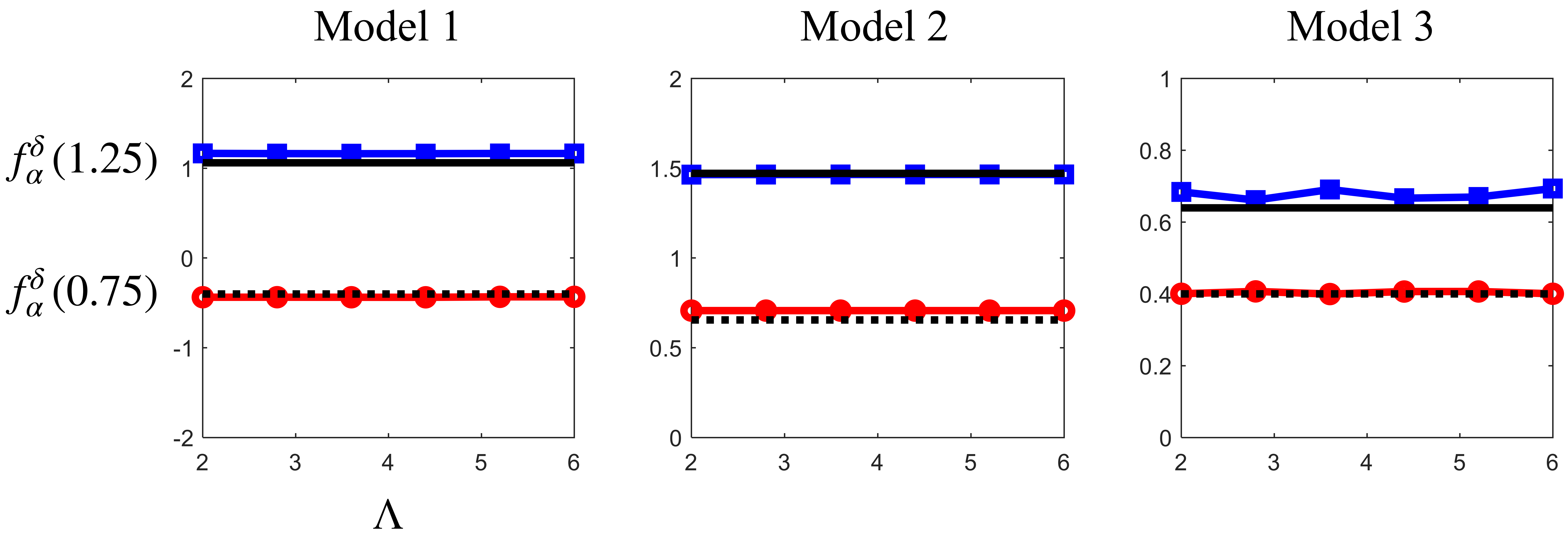
Numerical Results under Regularization

- Plateaus of regularization parameter



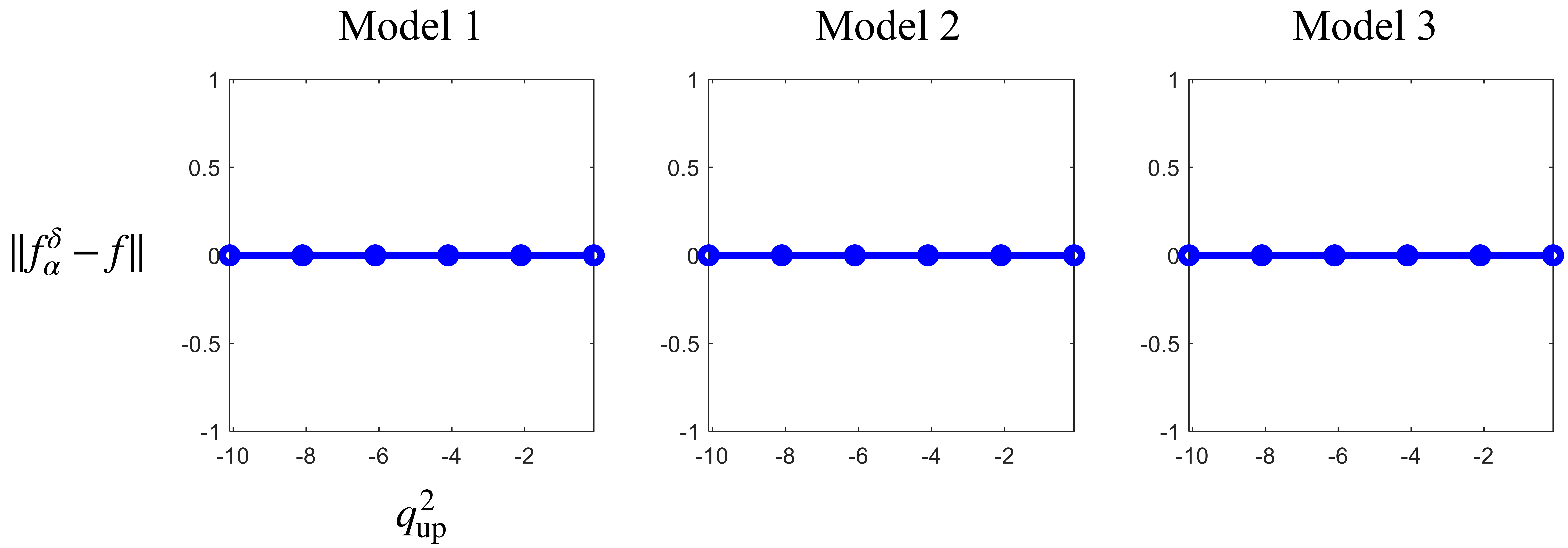
Numerical Results under Regularization

- Plateaus of Λ



Numerical Results under Regularization

- Plateaus of q_{up}^2



Uncertainty Analysis and Ability to Systematically improve Precision

a) Uncertainty Analysis

$$\|f_\alpha^\delta - f\| \leqslant \delta \, \|R_\alpha\| + \|R_\alpha K f - f\|$$

$\delta \, \|R_\alpha\|$ ↓ statistical uncertainty

$\|R_\alpha K f - f\|$ ↓ systematic uncertainty

b) Ability to systematically improve precision

1. Input errors
2. Priori information and regularization methods
3. Combination with experiments or lattice QCD

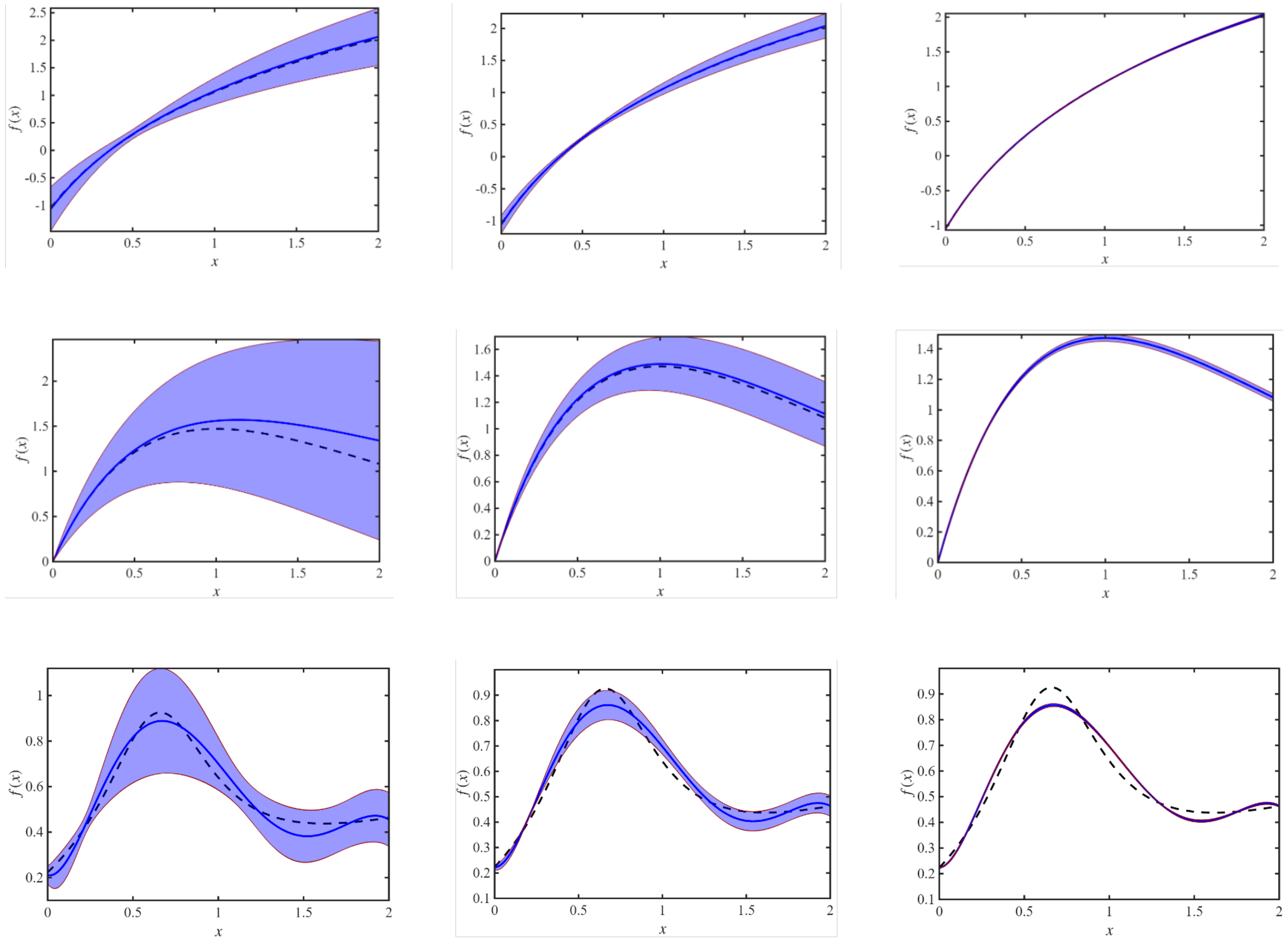
Systematically improve precision: Input Errors

$\delta = 30\,\%$ | $\delta = 10\,\%$ | $\delta = 1\,\%$

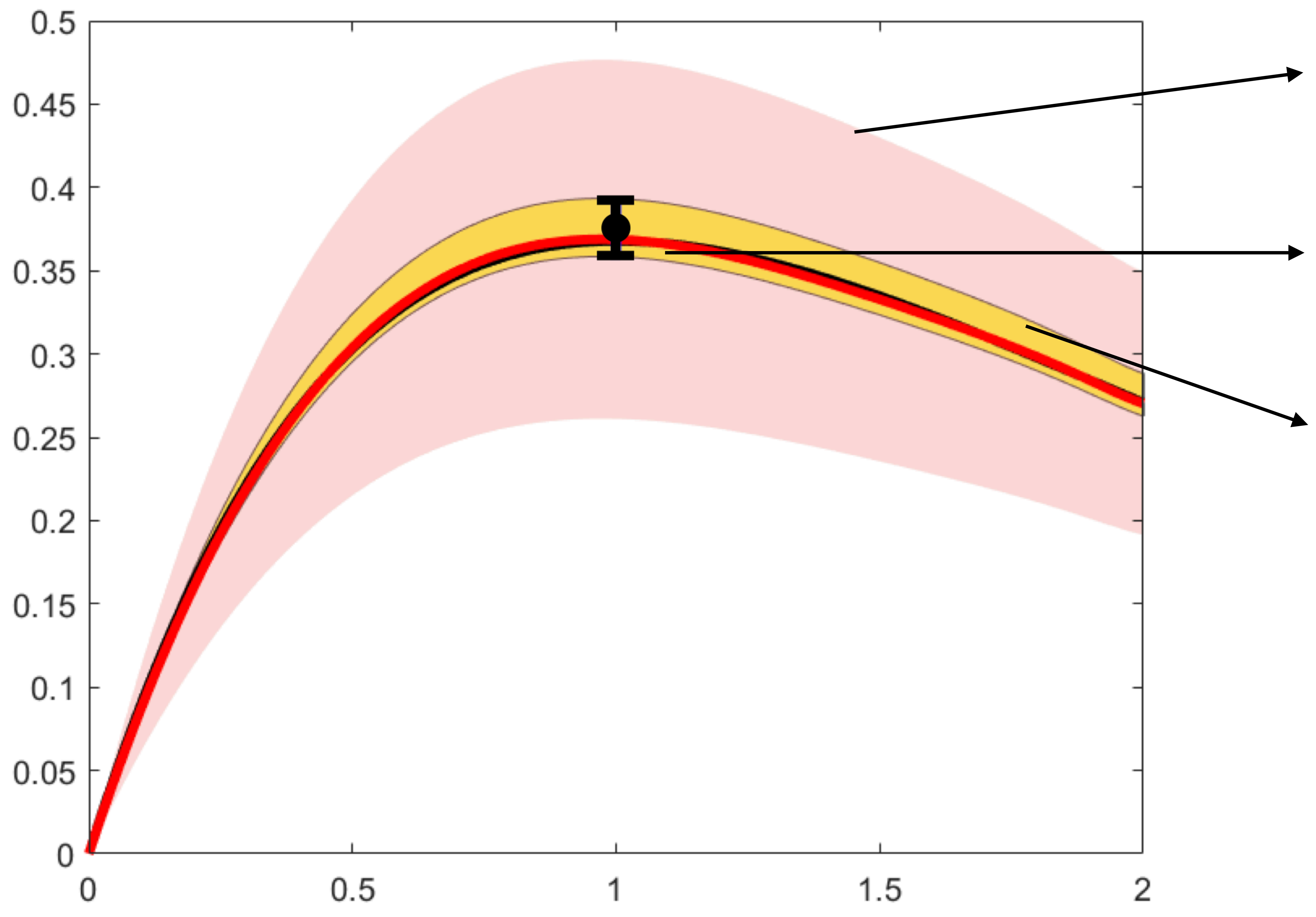
Model 1

Model 2

Model 3



Systematically improve precision: Constraints



Original uncertainty directly from inputs

Data from experiments or Lattice QCD

Improved uncertainty considering data

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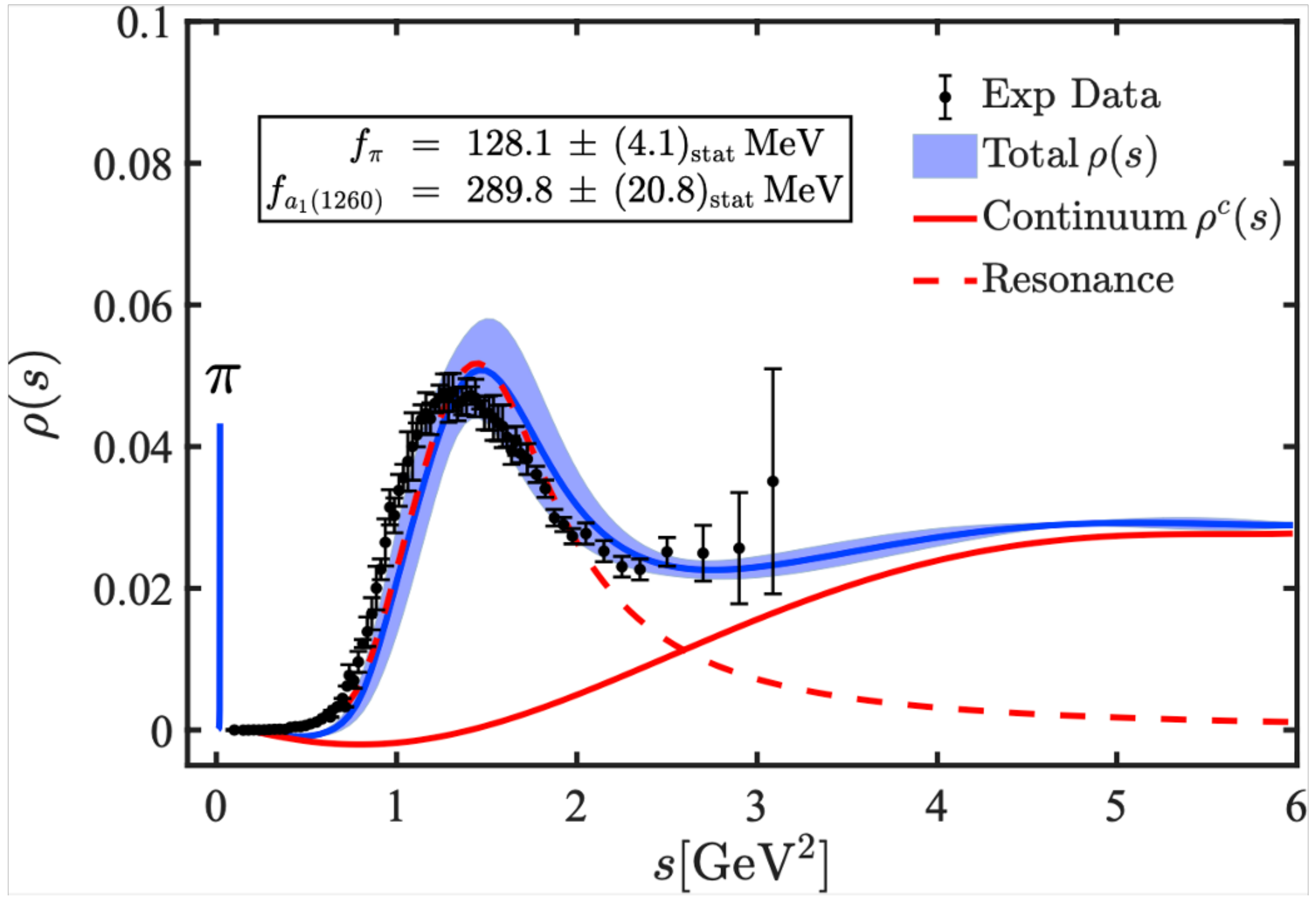
Physical Application: f_π and spectrum

$$\Pi_q(q^2) = \Pi_q(\sigma_0) + (q^2 - \sigma_0)\left[\int_0^\Lambda \frac{\rho(s)\,ds}{(s-\sigma_0)(s-q^2)} + \int_\Lambda^\infty \frac{\frac{1}{\pi}\mathbf{Im}\Pi_q^{\text{pert}}(s)\,ds}{(s-\sigma_0)(s-q^2)}\right]$$

$$\rho(s) = f_\pi^2\delta(s-M_\pi^2) + f_{a_1(1260)}^2\mathbb{BW}\left(s, M_{a_1(1260)}, \Gamma_{a_1(1260)}\right) + \rho^c(s)$$

$$\begin{aligned}\Pi_q(q^2) = &-\frac{1}{4\pi^2}\left(1+\frac{\alpha_s(\mu)}{\pi}\right)\ln\left(\frac{-q^2}{\mu^2}\right) + \frac{1}{12\pi}\frac{\langle\alpha_s G^2\rangle}{(q^2)^2} \\ &+ \frac{m_u\langle\bar{u}u\rangle + m_d\langle\bar{d}d\rangle}{(q^2)^2} + \frac{1}{9}\frac{m_u\langle g_s\bar{u}\sigma TGu\rangle + m_d\langle g_s\bar{d}\sigma TGd\rangle}{(q^2)^3} \\ &- \frac{4}{81}\frac{\langle g_s\bar{u}u\rangle^2 + \langle g_s\bar{d}d\rangle^2}{(q^2)^3} - \frac{\left[105+50\ln\left(\frac{-q^2}{\mu^2}\right)\right]}{243\pi^2}\frac{\sum_{\psi=u,d,s}\langle g_s^2\bar{\psi}\psi\rangle^2}{(q^2)^3}\end{aligned}$$



Solving Problem of Quark-Hadron Duality in Sum Rules

Quark-hadron duality: $\mathrm{Im}\Pi(q^2) = \pi f_V^2 \delta(q^2 - m_V^2) + \pi \rho^h(q^2)\theta(q^2 - s_h)$

$$\rho^h(s) = \frac{1}{\pi}\mathrm{Im}\Pi^{\mathrm{pert}}(s)\theta(s - s_0)$$

$$\int_{s_h}^{\infty} ds \frac{\rho^h(s)}{s - q^2} = \frac{1}{\pi}\int_{s_0}^{\infty} ds \frac{\mathrm{Im}\Pi^{\mathrm{pert}}(s)}{s - q^2}$$

- Uncertainty sources: quark-hadron duality. Results are sensitive to s_0

- Inverse Problem : Excited states and continuum spectrum can be directly solved.
- Avoid the quark-hadron duality

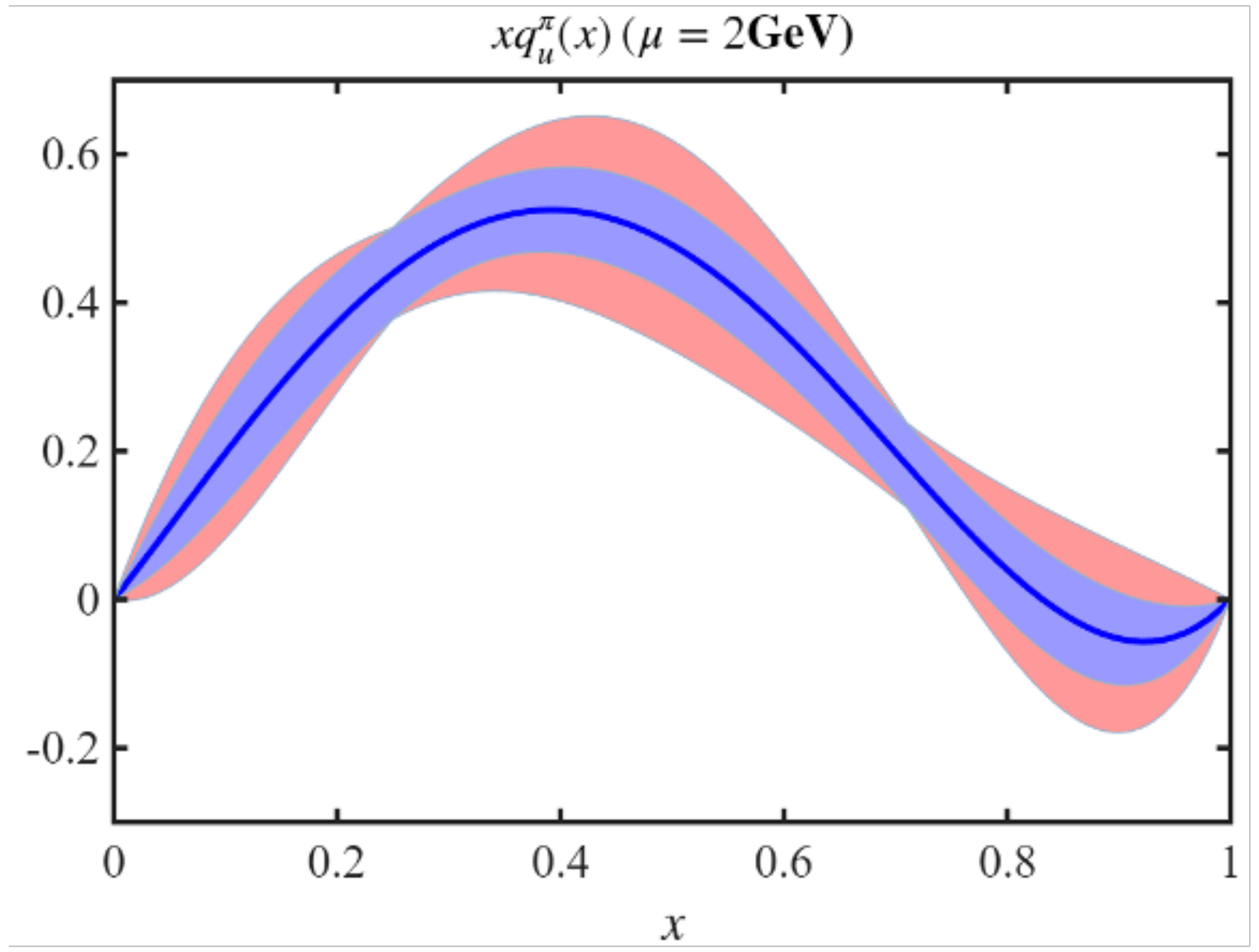
Physical Application: Moment Problem

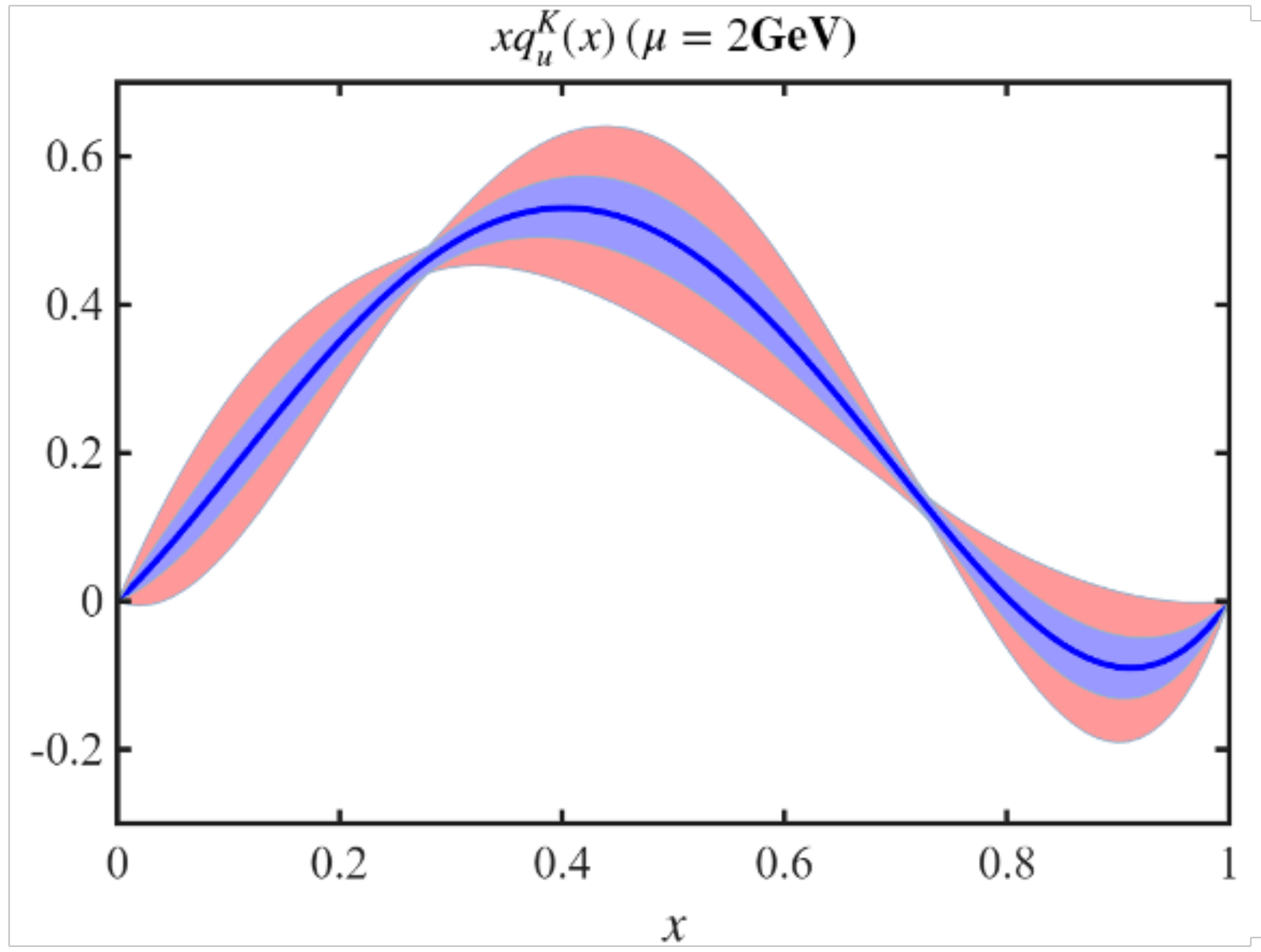
PDFs by moments from Lattice QCD

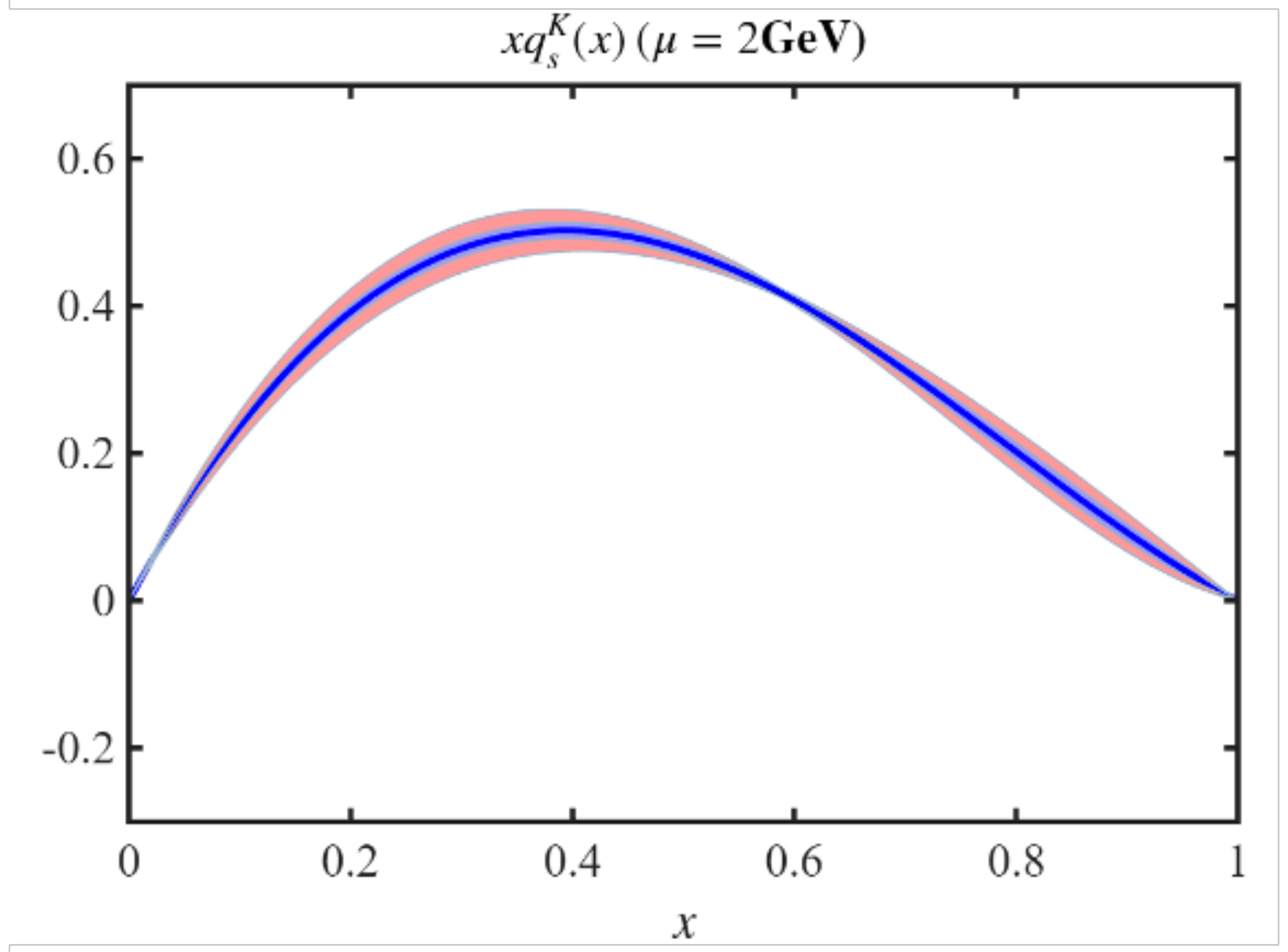
$$\int_0^1 x^n \varphi(x)\,\mathrm{d}x = \langle x^n \rangle$$

PDFs	$\langle x^1 \rangle$	$\langle x^2 \rangle$	$\langle x^3 \rangle$
$\pi^+(u^+)$	0.261(7)	0.110(14)	0.024(18)
$K^+(u^+)$	0.246(3)	0.096(3)	0.033(6)
$K^+(s^+)$	0.317(2)	0.139(2)	0.073(5)

Lattice QCD, PRD2021





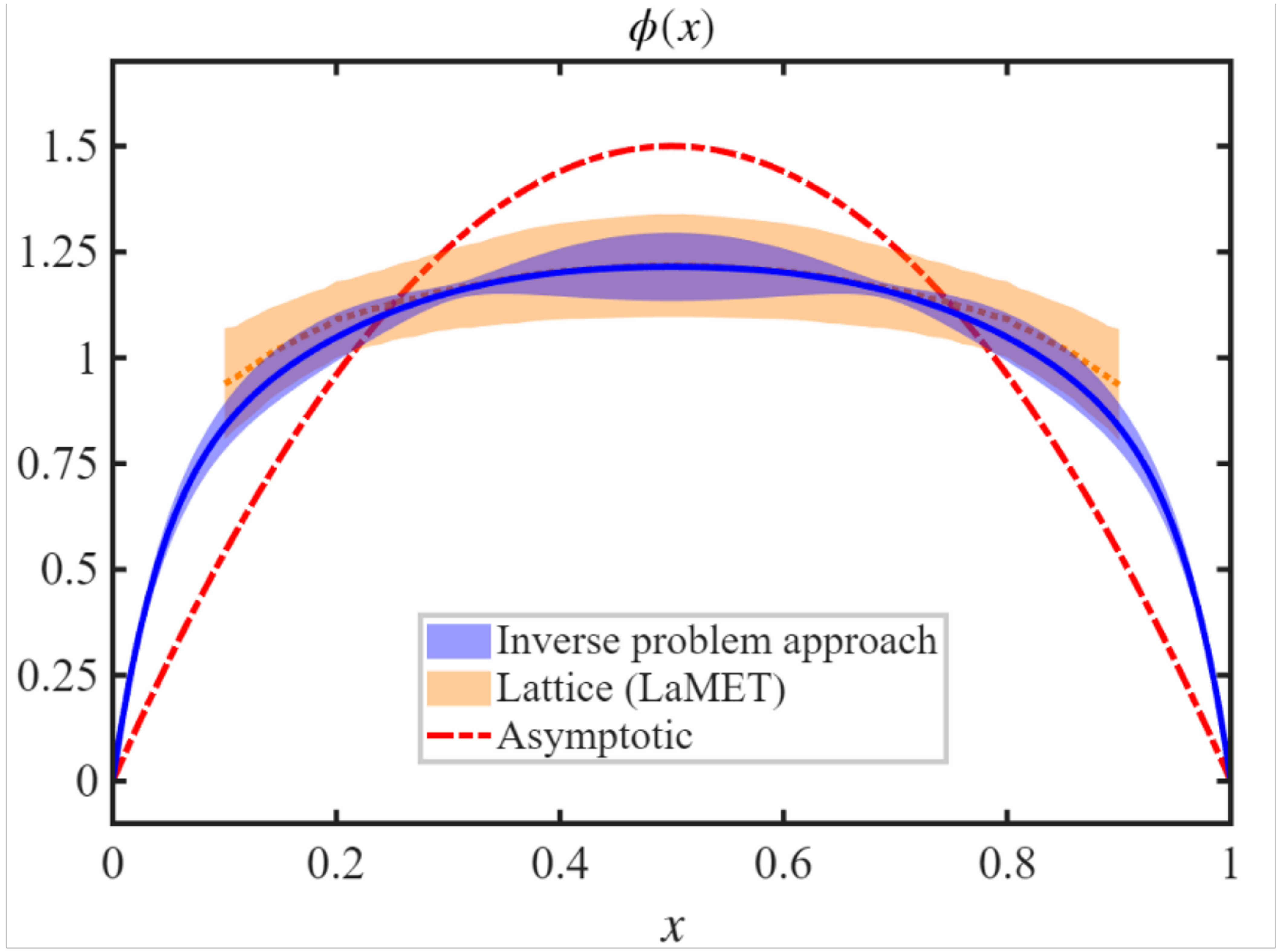


Physical Application: Moment Problem

LCDAs by moments from Dispersion Relation

$$\int_0^1 (2u-1)^n \, \varphi(u) \, \mathrm{d}u = \langle \xi^n \rangle, \quad \xi = 2u - 1$$

Moments	Value
$\langle \xi^2 \rangle$	0.264 ± 0.022
$\langle \xi^4 \rangle$	0.107 ± 0.020
$\langle \xi^6 \rangle$	0.100 ± 0.012
$\langle \xi^8 \rangle$	0.067 ± 0.016
$\langle \xi^{10} \rangle$	0.083 ± 0.009
$\langle \xi^{12} \rangle$	0.064 ± 0.016



正则化方法得到的近似解为什么接近真解?

- 用奇异值分解可以解释，是因为抓住了主要贡献!
- 特征方程 $Ax = \lambda x$，λ 是特征值，x 是特征向量。自伴算子$A^* = A$的所有特征值都是实数
- $K : X \to Y$，$K^* : Y \to X$。
- 自伴算子$K^*K : X \to X$ 的特征值 λ_j 的平方根 $\mu_j = \sqrt{\lambda_j}$ 称为 K 的奇异值。
- 满足 $Kx_j = \mu_j y_j$， $K^* y_j = \mu_j x_j$ 的系统 (μ_j, x_j, y_j) 称为 K 的奇异系统。
- 以 $\mu_1 \geqslant \mu_2 \geqslant \mu_3 \geqslant \cdots > 0$ 排序，这个排序很重要，抓住了主要贡献。

奇异值分解：$x = \sum_j (x, x_j)\, x_j$，$y = Kx = \sum_j \mu_j\, (x, x_j)\, y_j$

正则化方法得到的近似解为什么接近真解?

- Picard定理(1)：方程 $Kx = y$ 可解的充分必要条件是 $\sum_j \frac{1}{\mu_j^2} |(y, y_j)|^2 < \infty$
- 由 $y = \sum \mu_j (x, x_j)\, y_j$， 得 $\sum |(x, x_j)|^2 < \infty$
- 就是要求 (x, x_j) 收敛，$(x, x_j) \to 0, \ \ j \to \infty$

解的存在性 → (x, x_j) 收敛 → $x = \sum (x, x_j)\, x_j$ 在有限阶就可得到接近真解的近似解

- 不需要 $\{x_j\}$ 的完备集！即使解不唯一，也有可能得到比较好的近似解。

正则化方法得到的近似解为什么接近真解?

- Picard定理(2)：方程 $Kx = y$ 可解时，解 $x = \sum_j \frac{1}{\mu_j}(y, y_j)\, x_j$
- 解可以用奇异系统来表达。
- 它也直观反应了不适定性。$\|\delta x\|/\|\delta y\| = 1/\mu_n$ 可任意大，因为$\mu_n \to 0$， $n \to \infty$
- 构造正则化算子本质上就是找一种方法把算子 K 的小奇异值过滤掉

Tikhonov正则化下，$x_\alpha = \sum \frac{\mu_j}{\mu_j^2 + \alpha}(y, y_j)\, x_j$

前几项大奇异值 $\mu_j^2 \gg \alpha$，抓住主要贡献；对高阶项小奇异值 $\mu_j^2 \ll \alpha$， $x_\alpha \propto \mu_j/\alpha$ 可忽略

- 即使解不唯一，只要输入(y, y_j)抓住主要贡献，也可以得到接近真解的近似解！！！

正则化方法得到 … 么接近真解?

K矩阵奇异值的平方(离散步长0.01)

1.716942121
0.035495897
0.000472234
5.81415E-06
6.979E-08
8.27982E-10
9.75966E-12
1.1455E-13
2.03974E-15
1.41576E-15
1.29097E-15
8.80779E-16
8.63483E-16
5.58932E-16
4.86301E-16
3.25195E-16
3.13913E-16
2.33953E-16
2.2286E-16
2.14693E-16
1.75751E-16
1.63978E-16
1.61833E-16
1.48583E-16
1.4345E-16

- Picard定理(2)：方程 $Kx = y$ … $(y, y_j)\, x_j$
- 解可以用奇异系统来表达。
- 它也直观反应了不适定性。$\|\delta x$ … 大，因为$\mu_n \to 0$，$n \to \infty$
- 构造正则化算子本质上就是找 … 奇异值过滤掉

Tikhonov正则化下，$x_\alpha = \sum$ …

前几项大奇异值 $\mu_j^2 \gg \alpha$，抓住 … 奇异值 $\mu_j^2 \ll \alpha$，$x_\alpha \propto \mu_j/\alpha$ 可忽略

- 即使解不唯一，只要输入(y, y_j) … 得到接近真解的近似解！！！

正则化方法得到的近似解为什么接近真解?

- 唯一或不唯一通常是针对物理问题采用不同数学模型时的结果
  - 例如格点v.s.连续，有限矩v.s.无限矩

- α 参数选取的非平庸性，如同量子场论中正规化和重整化过程，重整化参数的确定需要重整化条件。

Numerical Method of Tikhonov Regularization

$$\varphi_i(x) = \begin{cases} \frac{x-x_{i-1}}{h}, x \in [x_{i-1}, x_i], \\ -\frac{x-x_{i+1}}{h}, x \in [x_i, x_{i+1}], \\ 0, otherwise, \end{cases}$$

$$\varphi_0(x) = \begin{cases} -\frac{x-x_1}{h}, x \in [x_0, x_1], \\ 0, otherwise, \end{cases}$$

$$\varphi_n(x) = \begin{cases} \frac{x-x_{n-1}}{h}, x \in [x_{n-1}, x_n], \\ 0, otherwise. \end{cases}$$

$$X_n = \text{span}\{\varphi_0, \varphi_1, \cdots, \varphi_n\}$$

$$f^\delta_{\alpha,n}(x) = \sum_{i=0}^n c_i \varphi_i(x)$$

$$f^\delta_\alpha = \underset{f\in L^2(a,b)}{\arg\min}\, J(f) = \underset{f\in L^2(a,b)}{\arg\min} \left(\frac{1}{2}\|Kf - g^\delta\|^2_{L^2(c,d)} + \frac{\alpha}{2}\|f\|^2_{L^2(a,b)} \right)$$

$$f^\delta_{\alpha,n}(x) = \sum_{i=0}^n c_i \varphi_i(x)$$

$$J(f^\delta_{\alpha,n}) = \frac{1}{2}\left\| \sum_{i=0}^n c_i K\varphi_i - g^\delta \right\|^2_{L^2(c,d)} + \frac{\alpha}{2}\left\| \sum_{i=0}^n c_i \varphi_i \right\|^2_{L^2(a,b)}$$

$$= \frac{1}{2}\sum_{i,j=0}^n c_i c_j (K\varphi_i, K\varphi_j)_{L^2(c,d)} - \sum_{i=0}^n c_i (K\varphi_i, g^\delta)_{L^2(c,d)} + \frac{1}{2}(g^\delta, g^\delta)_{L^2(c,d)} + \frac{\alpha}{2}\sum_{i,j=0}^n c_i c_j (\varphi_i, \varphi_j)_{L^2(a,b)}$$

$$A_{ij} = (K\varphi_i, K\varphi_j)_{L^2(c,d)} \qquad B_{ij} = (\varphi_i, \varphi_j)_{L^2(a,b)} \qquad C = (c_0, c_1, \cdots, c_n)^T$$

$$(A + \alpha B)C = D \qquad D_i = (K\varphi_i, g^\delta)_{L^2(c,d)}$$

Theorem 4.3. *If the noise δ and the regularization parameter α are fixed, we have $\|f^\delta_{\alpha,n} - f^\delta_\alpha\|_{L^2(a,b)} \to 0$, as $n \to \infty$.*

反问题方法应用举例

积分问题：已知积分结果，求被积函数 $$\int_a^b K(x,y)\,f(x)\,\mathrm{d}x = g(y)$$

1. 色散积分（谱分析）（连续）： $$\int_{t_{\min}}^{\Lambda} \mathrm{d}s\,\frac{\mathrm{Im}\,\Pi(s)}{s-q^2} = \pi\,\Pi(q^2) - \int_{\Lambda}^{\infty} \mathrm{d}s\,\frac{\mathrm{Im}\,\Pi(s)}{s-q^2}$$

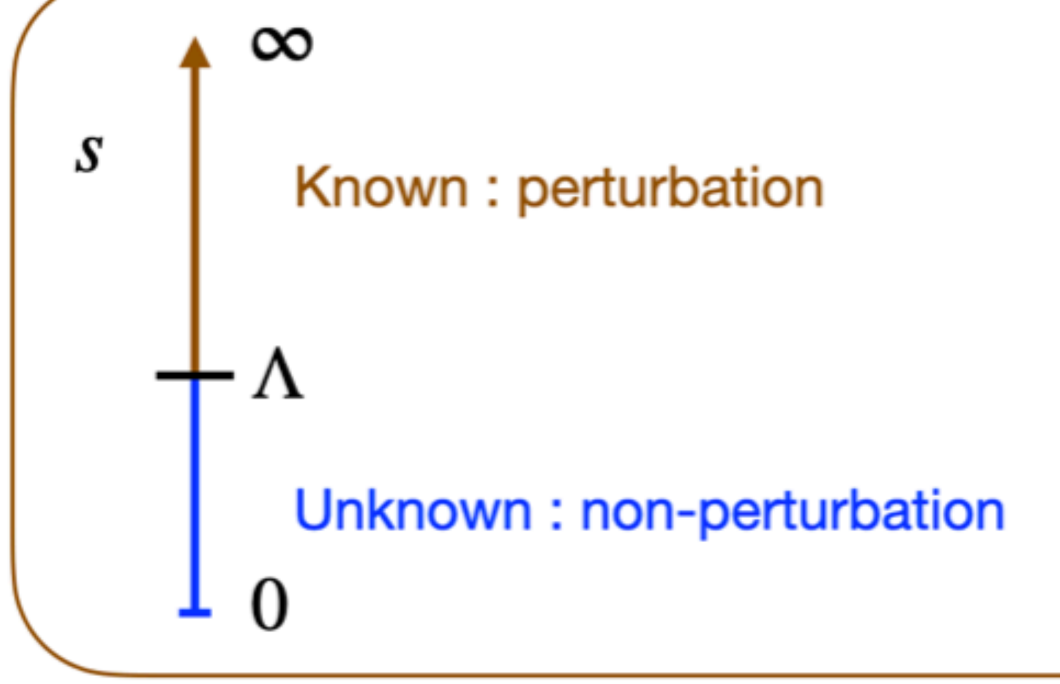
2. 矩（LCDA、PDF）（离散）： $$\int_0^1 x^n\,\varphi(x)\,\mathrm{d}x = \langle x^n \rangle \qquad \int_0^1 (2u-1)^n\,\varphi(u)\,\mathrm{d}u = \langle \xi^n \rangle, \quad \xi = 2u-1$$

3. 傅立叶变换（LaMET）（离散）： $$\int e^{-i\lambda x} f(x)\,\mathrm{d}x = g(\lambda)$$

4. 动量关联函数（强子强子相互作用）（离散）： $$\int \mathrm{d}^3 r\, S_{12}(r)\,|\Psi(r,k)|^2 = C(k)$$

Inverse problem approach

- 从量子场论的色散关系出发，通过已知的微扰计算反解未知的非微扰物理量
- 反问题：已知积分结果求被积函数
- 用正则化方法，得到近似稳定解，可以收敛于真解，精度可以系统性提高
- 基于严谨的数学理论和逻辑，不引入任何人为假设



$$\Pi(q^2) = i\int d^4x e^{iq\cdot x}\langle O(x)O(0)\rangle$$

Dispersion Relation:

$$\mathcal{R}e[\Pi(s)] = \frac{1}{\pi}\mathcal{P}\int_0^{\infty}\frac{\mathcal{I}m[\Pi(s')]}{s-s'}ds'$$

If $s > \Lambda$,

$$\mathcal{P}\int_0^{\Lambda}\frac{\mathcal{I}m[\Pi(s')]}{s-s'}ds' = \pi\mathcal{R}e[\Pi(s)] - \mathcal{P}\int_{\Lambda}^{\infty}\frac{\mathcal{I}m[\Pi(s')]}{s-s'}ds'$$

To be solved

calculable

A.S.Xiong, T.Wei, F.S.Yu, arXiv:2211.13753

Minimization of Tikhonov Functional

- 定理：泛函 $J_\alpha(f) = \|Kf - g\|_G^2 + \alpha\|f\|_F^2$ 的极小元与方程 $K^*Kf_\alpha + \alpha f_\alpha = K^*g$ 的解等价

$$f_\alpha^\delta = \arg\min J_\alpha(f),\quad J_\alpha(f) = \|Kf - g^\delta\|_G^2 + \alpha\|f\|_F^2$$

- 证明等价性：设 f_α 是泛函的极小元，对任意 f 有 $J_\alpha(f) - J_\alpha(f_\alpha) \geqslant 0$

$$\begin{aligned} J_\alpha(f) - J_\alpha(f_\alpha) &= \|Kf - g\|^2 + \alpha\|f\|^2 - \|Kf_\alpha - g\|^2 - \alpha\|f_\alpha\|^2 \\ &= \|K(f - f_\alpha)\|^2 + \alpha\|f - f_\alpha\|^2 + 2Re(K^*Kf_\alpha + \alpha f_\alpha - K^*g, f - f_\alpha) \geqslant 0 \end{aligned}$$

由于 f 的任意性，$f - f_\alpha$ 可正可负，只能 $K^*Kf_\alpha + \alpha f_\alpha - K^*g = 0$

- 第一项 $\|Kf - g\|^2$：是最小二乘法的χ^2项，它的极小化就是$Kf = g$的近似解。但它过小就会过拟合，结果 f 高度振荡，不适定了。它也叫残差项，代表原问题。
- 第二项 $\alpha\|f\|^2$：是控制 $\|f\|$ 不能太大，避免高度振荡，使解变稳定，得到正则化解。

Criteria of a good theoretical approach

(1) Well defined in mathematics $\longrightarrow$ Dispersion relation + proof of ill-posedness

(2) Realization in numerical calculations $\longrightarrow$ Regularization methods

(3) Can be systematically improved $\longrightarrow$ Errors converge to vanishing as $\delta \to 0$

(4) Simple at the beginning $\longrightarrow$ Tikhonov regularization