



第二十一届全国重味物理与CP破坏研讨会

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# Inverse problem approach for non-perturbative QCD

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Based on [ASX, Ting Wei(魏婷), Fu-Sheng Yu(于福升) arXiv: 2211.13753;  
Yong Zheng (郑勇), Ao-Sheng Xiong, Ting Wei, Fu-Sheng Yu, in preparation]



# 目录

- 研究动机
- 反问题介绍与适定性研究
- 正则化方法
- 数值结果与物理运用
- 总结与展望

白強不息  
獨樹一幟



重大科学难题：非微扰物理量难以计算，  
是世纪难题

夸克禁闭和新物理……

现有的非微扰方法各有优缺点

格点QCD (LQCD)：第一性原理的计算方法，但需要  
超级计算机且对激发态等物理量计算难度大。

其他方法：如QCD求和规则、Dyson-Schwinger方程  
等在某些方面都很成功，但却有一定的模型依赖性。

唯象方法预言能力有限。

发展反问题方法计算非微扰物理量

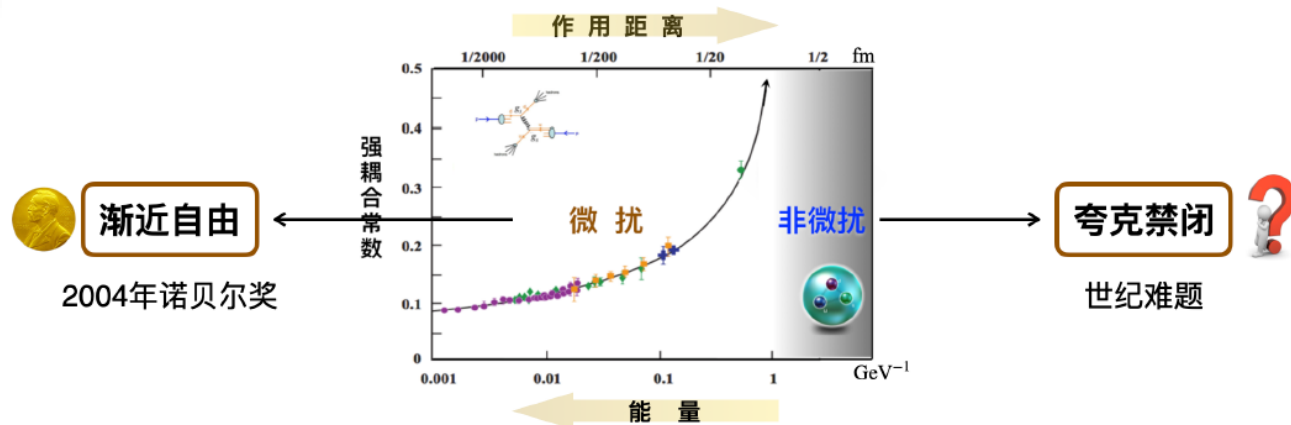
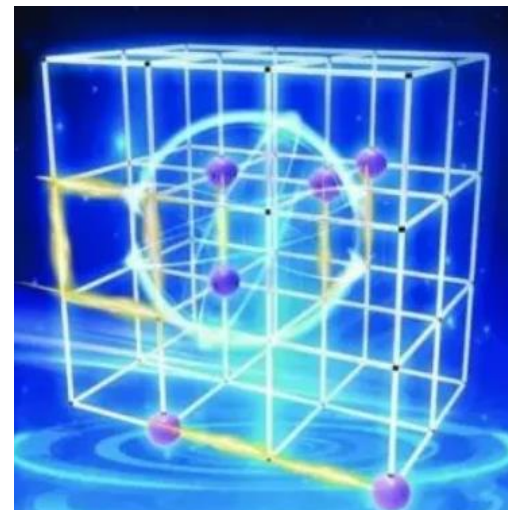


图1：高能微扰与低能非微扰



# 2 反问题介绍



基于量子场论的色散关系，通过已知的微扰计算反解未知的非微扰物理量：

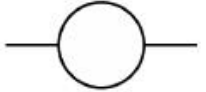
关联函数具有解析性；

复变函数的柯西公式；

以简单的色散关系为例，其余类似；

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

$$\text{Re}[\Pi(s)] = \frac{1}{\pi} \int_0^\infty \frac{\text{Im}[\Pi(s')]}{s - s'} ds'$$

  $\Pi(s)$

Dispersion Relation:

$$\text{Re}[\Pi(s)] = \frac{1}{\pi} \mathcal{P} \int_0^\infty \frac{\text{Im}[\Pi(s')]}{s - s'} ds'$$

$s$

$\infty$

Known : perturbation

$\Lambda \leq m_b^2$

Unknown : non-perturbation

0

If  $s > \Lambda$ ,

$$\mathcal{P} \int_0^\Lambda \frac{\text{Im}[\Pi(s')]}{s - s'} ds' = \pi \text{Re}[\Pi(s)] - \mathcal{P} \int_\Lambda^\infty \frac{\text{Im}[\Pi(s')]}{s - s'} ds'$$

To be solved

calculable

已知积分结果求被积函数需要用到反问题理论。

H.N.Li, H.U, F.R.Xu, F.S.Yu, Phys.Lett.B 810(2020)



反问题理论是成熟的数学分支领域：

与反问题对比的是正问题；

1950年左右发展至今；

在众多重要的前沿科学领域中广泛运用；

线性方程组的求解、地质探勘、缪子成像、CT……

$$\text{If } s > \Lambda, \quad \mathcal{P} \int_0^\Lambda \frac{\text{Im}[\Pi(s')]}{s-s'} ds' = \pi \text{Re}[\Pi(s)] - \mathcal{P} \int_\Lambda^\infty \frac{\text{Im}[\Pi(s')]}{s-s'} ds'$$

To be solved
calculable

反问题理论处处可见，且具有独特的性质：

线性方程组求解问题；解存在唯一？

正问题：  $Kx = y$ ;

反问题：  $x = K^{-1}y$ ;

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



$$x_1 = 1, x_2 = 1$$

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



$$x_1 = -59, x_2 = 41$$

输入数据存在一点点误差就会导致解发生巨大变化！解不稳定！

# 3 适定性研究



色散关系的算子方程:  $K: F \rightarrow G$

$$\int_a^b \frac{f(x)}{y-x} dx = g(y), y \in [c, d], c > b$$

正问题:  $Kf = g$

反问题:  $f = K^{-1}g$

**适定性**是研究反问题的基础:

**Define:** *The operator equation (3.1) is called well-posed if the following holds [8]:*

*1.Existence: For every  $g \in G$  there is (at least one)  $f \in F$  such that  $Kf = g$ ;*

*2.Uniqueness: For every  $g \in G$  there is at most one  $f \in F$  with  $Kf = g$ ;*

*3.Stability: The solution  $f$  depends continuously on  $g$ ; that is, for every sequence  $(f_n) \subset F$  with  $Kf_n \rightarrow Kf(n \rightarrow \infty)$ , it follows that  $f_n \rightarrow f(n \rightarrow \infty)$*

若上述有一个条件不满足, 就称该问题是**不适定问题**。



解的存在性:



R(K) is the analytic functions

$$\int_a^b \frac{f(x)}{y-x} dx = g(y), y \in [c, d], c > b$$

$$\begin{aligned} Kf &= \int_a^b \frac{f(x)}{y-x} dx = \int_a^b \frac{1}{y} \frac{f(x)}{1-\frac{x}{y}} dx \\ &= \frac{1}{y} \int_a^b \sum_{k=0}^{\infty} \left(\frac{x}{y}\right)^k f(x) dx = \sum_{k=0}^{\infty} \frac{1}{y^{k+1}} \int_a^b x^k f(x) dx \end{aligned}$$

where the last equal sign uses the control convergence theorem:

$$\begin{aligned} \sum_{k=0}^{\infty} \frac{1}{y^{k+1}} \int_a^b x^k f(x) dx &\leq \sum_{k=0}^{\infty} \frac{1}{y^{k+1}} \int_a^b x^{2k} dx \|f(x)\|_{L^2(a,b)} \\ &\leq \sum_{k=0}^{\infty} \frac{1}{y^{k+1}} b^k \sqrt{b-a} \|f(x)\|_{L^2(a,b)} \\ &\leq \sum_{k=0}^{\infty} \frac{1}{y^{k+1}} \left(\frac{b}{c}\right)^k \|f(x)\|_{L^2(a,b)} \leq \infty \end{aligned}$$

Thus, the R(K) is the analytic functions  $\in [c, d]$

# 3 适定性研究



解的存在性: 😊

解的唯一性: 😊

$$\int_a^b \frac{f(x)}{y-x} dx = g(y), y \in [c, d], c > b$$

**Theorem 3.3.** Suppose that  $f_1(x), f_2(x) \in L^2(a, b)$ . If  $Kf_1 = Kf_2 = g(y), y \in [c, d]$ , then we have  $f_1(x) = f_2(x)$ , a. e.  $x \in [a, b]$ .

*Proof.* Since  $K$  is a linear operator, we know that  $Kf_1 - Kf_2 = K(f_1 - f_2) = 0$ . Therefore, in order to prove  $f_1(x) = f_2(x)$ , a. e.  $x \in [a, b]$ , we just need to prove that  $Kf = 0$  implies  $f(x) = 0$ , a. e.  $x \in [a, b]$ .

It is easy to obtain that  $Kf = \int_a^b \frac{1}{y-x} f(x) dx = \int_a^b \left( \frac{1}{y} \sum_{k=0}^{\infty} \left(\frac{x}{y}\right)^k \right) f(x) dx$ . Since  $x \in [a, b], y \in [c, d], c > b$ , we know  $|\frac{x}{y}| \leq |\frac{b}{c}| < 1$ , which implies that  $|\sum_{k=0}^{\infty} (\frac{x}{y})^k f(x)| \leq \sum_{k=0}^{\infty} (\frac{b}{c})^k |f(x)|$  for all  $x \in [a, b]$ . Combined with  $\int_a^b |f(x)| dx < +\infty$  and the control convergence theorem, we have

$$y \int_a^b \frac{1}{y-x} f(x) dx = \sum_{k=0}^{\infty} \frac{1}{y^k} \int_a^b x^k f(x) dx = 0, \quad y \in [c, d]. \quad (3.4)$$

If  $d = +\infty$ , by using (3.4), we have

$$\int_a^b f(x) dx + \frac{1}{y} \int_a^b x f(x) dx + \dots + \frac{1}{y^k} \int_a^b x^k f(x) dx + \dots = 0, \quad y \in (c, +\infty). \quad (3.5)$$

Letting  $y \rightarrow +\infty$  in (3.5), we have  $\int_a^b f(x) dx = 0$ . Then multiplying  $y$  on both sides of (3.5) and letting  $y \rightarrow +\infty$ , we also have  $\int_a^b x f(x) dx = 0$ . Repeating above process, we can obtain that

$$\int_a^b x^k f(x) dx = 0, \quad k = 0, 1, 2, \dots \quad (3.6)$$

By using (3.6), we know that  $\int_a^b f(x) Q_n(x) dx = 0$ . Combined with the Cauchy inequality, we have

$$\begin{aligned} \|f\|_{L^2(a,b)}^2 &= \int_a^b f^2(x) dx = \int_a^b (f^2(x) - f(x) Q_n(x)) dx \\ &\leq \int_a^b |f(x)| \cdot |f(x) - Q_n(x)| dx \\ &\leq \left( \int_a^b f^2(x) dx \right)^{\frac{1}{2}} \left( \int_a^b |f(x) - Q_n(x)|^2 dx \right)^{\frac{1}{2}} \\ &= \|f\|_{L^2(a,b)} \|f - Q_n\|_{L^2(a,b)} \\ &\leq (\epsilon + \epsilon \sqrt{b-a}) \|f\|_{L^2(a,b)}, \end{aligned}$$

which implies that  $\|f\|_{L^2(a,b)} \leq \epsilon + \epsilon \sqrt{b-a}$ .

Letting  $\epsilon \rightarrow 0$ , we have  $\|f\|_{L^2(a,b)} = 0$ , i. e.  $f(x) = 0$ , a. e.  $x \in [a, b]$ . The proof is completed.  $\square$



# 3 适定性研究



解的存在性: 😊

解的唯一性: 😊

解的稳定性: 😞

We show the instability of the inverse problem of dispersion relation by the special case. Taking  $a = 0, b = 1, c = 2, d = 3, f_2(x) = f_1(x) + \sqrt{n} \cos(n\pi x)$ , and  $f_{1,2}$  are the solutions of  $g_{1,2}$  with  $g_i(y) = \int_0^1 \frac{1}{y-x} f_i(x) dx$ . As  $n \rightarrow \infty$ , it is obvious that

$$\|f_2 - f_1\|_{L^2(0,1)} = \left( \int_0^1 (\sqrt{n} \cos(n\pi x))^2 dx \right)^{1/2} = \frac{\sqrt{n}}{\sqrt{2}} \rightarrow \infty, \quad (3.7)$$

and

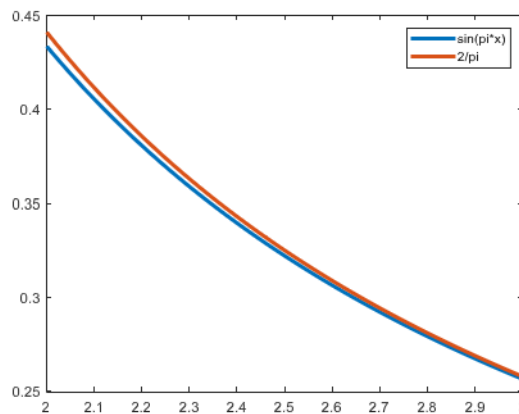
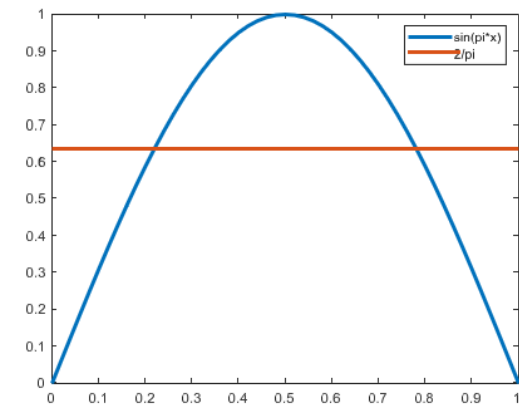
$$\|g_2 - g_1\|_{L^2(2,3)} = \frac{1}{\sqrt{n\pi}} \left( \int_2^3 \left( \int_0^1 \left( \frac{1}{y-x} \right)^2 \sin(n\pi x) dx \right)^2 dy \right)^{1/2} \leq \frac{M}{\sqrt{n\pi}} \rightarrow 0. \quad (3.8)$$

That means the solutions could be changed infinitely even though the noise of the input data is approaching to vanish. So the inverse problem is unstable.

实际物理中，数据一定存在误差:  $\|g^\delta - g\|_{L^2} \leq \delta$

不稳定性是求解该反问题的难题!

$$\int_a^b \frac{f(x)}{y-x} dx = g(y), y \in [c, d], c > b$$





## 4 正则化方法

目标：求解  $Kf = g$

数据一定存在误差且问题具有不稳定性，故不能直接求解  $f^\delta = K^{-1}g^\delta$

Andreas Kirsch.2011

正则化算子：

**Define:** A regularization strategy is a family of linear and bounded operators  $R_\alpha : G \rightarrow F, \alpha > 0$ , such that  $\lim_{\alpha \rightarrow 0} R_\alpha Kf = f$  for all  $f \in F$ , where the  $\alpha$  is the regularization parameter [8].

构造一族正则化算子  $R_\alpha$  去逼近  $K^{-1}$ ，即可克服不稳定性。

正则化解  $f_\alpha^\delta = R_\alpha g^\delta$  与真解  $f$  的估计：

$$\begin{aligned} \|f_\alpha^\delta - f\|_F &\leq \|R_\alpha g^\delta - R_\alpha g\|_F + \|R_\alpha g - f\|_F \\ &\leq \|R_\alpha\| \|g^\delta - g\|_G + \|R_\alpha Kf - f\|_F \\ &\leq \|R_\alpha\| \delta + \|R_\alpha Kf - f\|_F \propto O\left(\frac{\delta}{\alpha^{M_1}} + \alpha^{M_2}\right) \end{aligned}$$



Tikhonov正则化方法:

$$f_{\alpha}^{\delta} = \operatorname{argmin} \left\{ \frac{1}{2} \|Kf - g^{\delta}\|_{L^2}^2 + \frac{\alpha}{2} \|f\|_{L^2}^2 \right\}$$

Y. X. Zhang 2017

X. B. Yan 2018

X. B. Yan 2021

- 第一项可看作 $\chi^2$ 拟合，第二项是罚项；
- 罚项的形式可根据实际问题做改进： $H^1$ 、TV、 $L^1$ ……
- $\alpha > 0$ 是正则化参数，对结果有影响，不能过大或过小，但可被严格选取。

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

正则化解和真解的估计：先验信息： $f = K^*v, v \in G, \|v\|_G \leq E$

令 $\alpha = \delta/E$ ，则有 $\|f_{\alpha}^{\delta} - f\|_F \leq \sqrt{\delta E} \rightarrow 0, \text{ as } \delta \rightarrow 0$

离散正则化方法：选取合适的基底对积分方程做离散，并选取合适的离散维数，即可自动起到正则化效果。

- 当误差趋于零时，正则化解一定能收敛到真解；
- 误差可以系统性控制。



正则化参数选取方法：

先验选取：理论上清楚展示正则化方法的收敛性；

后验选取：实际计算中方便运用，知道输入数据或误差即可。

**L-curve法：**

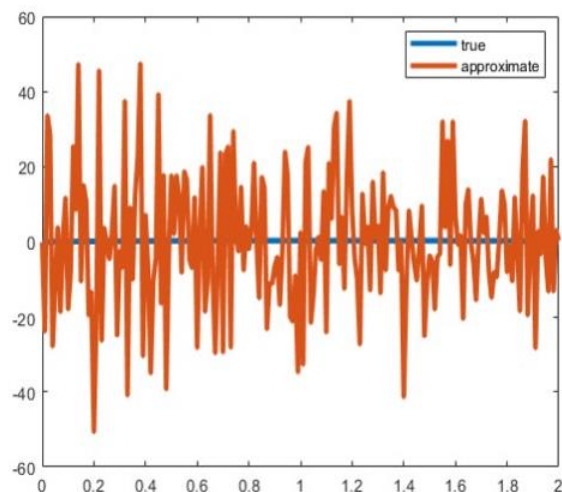
$$\alpha = \operatorname{argmin}\{\|f_\alpha^\delta\|_{L^2} \|Kf_\alpha^\delta - g^\delta\|_{L^2}\}$$

$\|f_\alpha^\delta\|_F$  和  $\|Kf_\alpha^\delta - g^\delta\|$  同时达到最小

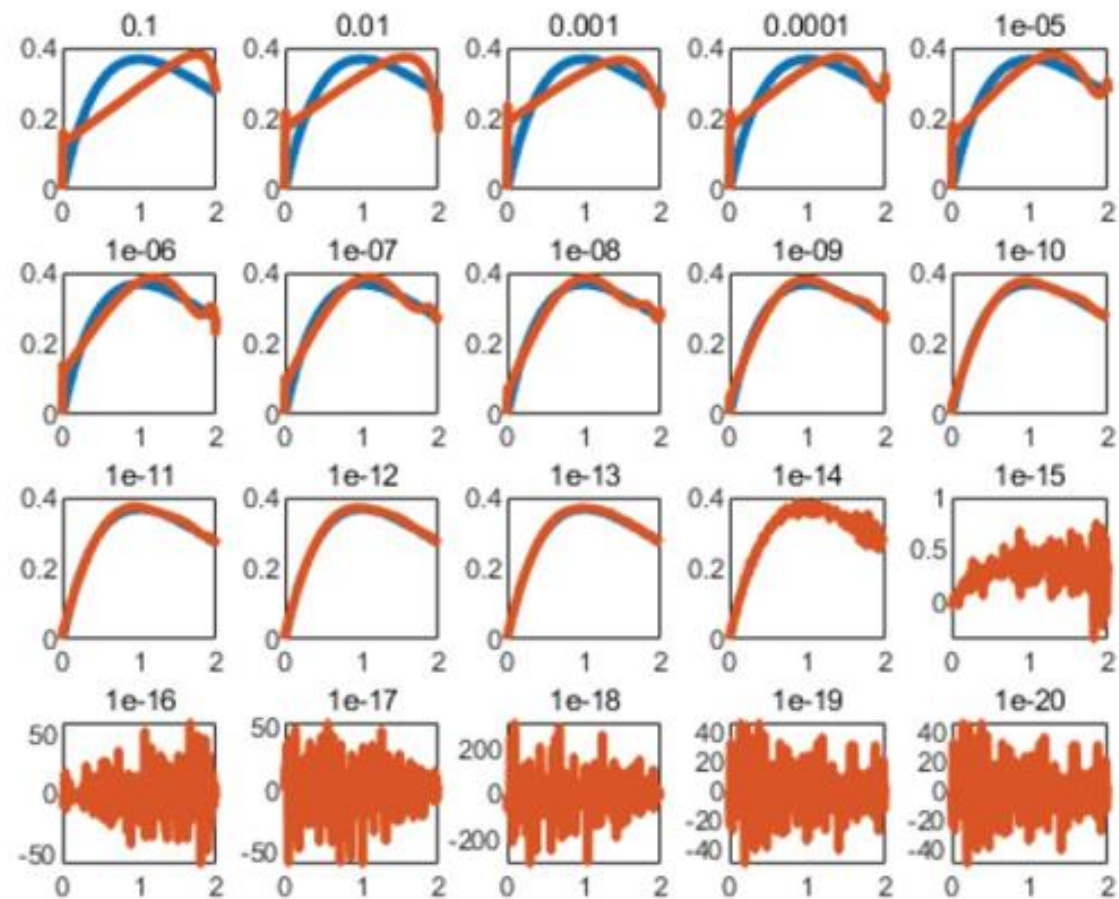


## 正则化方法的有效性

- 经典方法用有限元展开直接求逆，结果不稳定
- 正则化参数 $\alpha$ 的不能过大也不能过小，与理论预期一致；
- 正则化参数存在很大的平台，跨越多个量级；
- 正则化方法可以很好地解决色散关系的反问题。



正则化方法



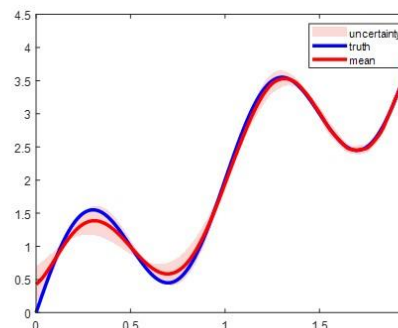
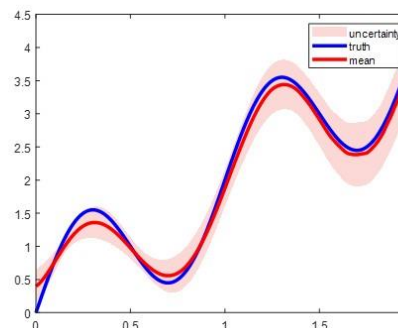
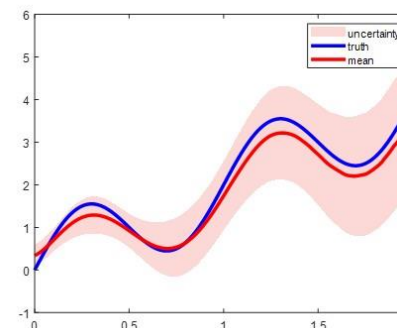
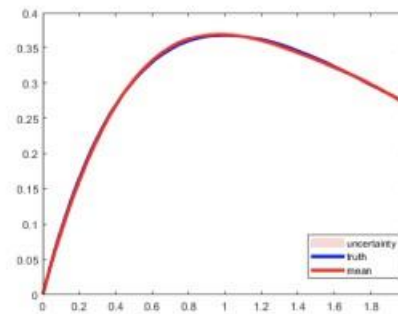
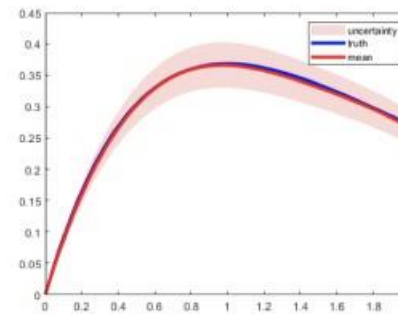
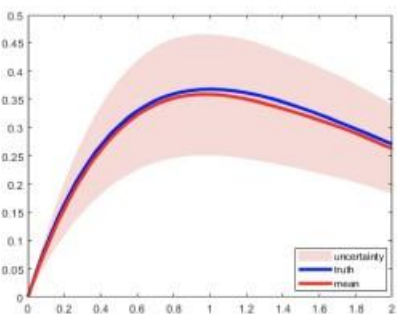
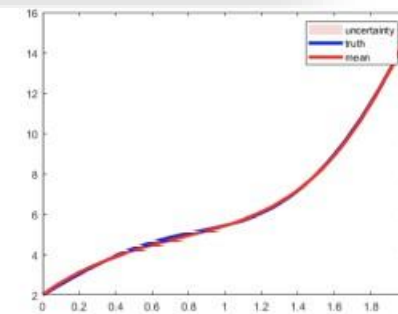
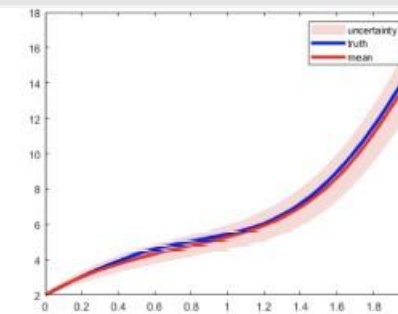
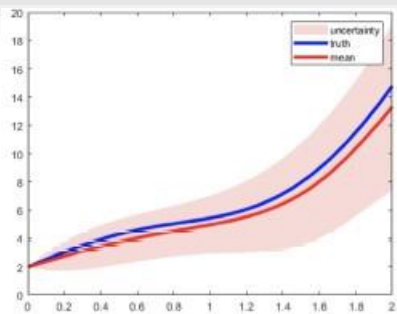


Tikhonov正则化方法和L-curve法的结果:

玩具模型均能够很好地反演;

输入误差分别为30%, 10%, 1%;

随着输入误差降低, 解的误差也  
逐渐降低, 误差水平基本一致





## 经典的QCDSR:

- 激发态难以计算
- 夸克强子对偶难以克服

$$\Pi_{\mu\nu}(q^2) = i \int d^4x e^{iq \cdot x} \langle 0 | T [J_\mu(x) J_\nu(0)] | 0 \rangle$$

$$\Pi(q^2) = \frac{1}{2\pi i} \oint ds \frac{\Pi(s)}{s - q^2} = \frac{1}{\pi} \int_{t_{min}}^{\infty} ds \frac{\text{Im} \Pi(s)}{s - q^2 - i\epsilon}$$

$$\text{Im} \Pi(q^2) = \pi f_V^2 \delta(q^2 - m_V^2) + \pi \rho^h(q^2) \theta(q^2 - s_h)$$

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

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

## 色散关系的反问题方法:

- 激发态和连续谱均能直接计算;
- 避免夸克强子对偶, 系统误差可被控制

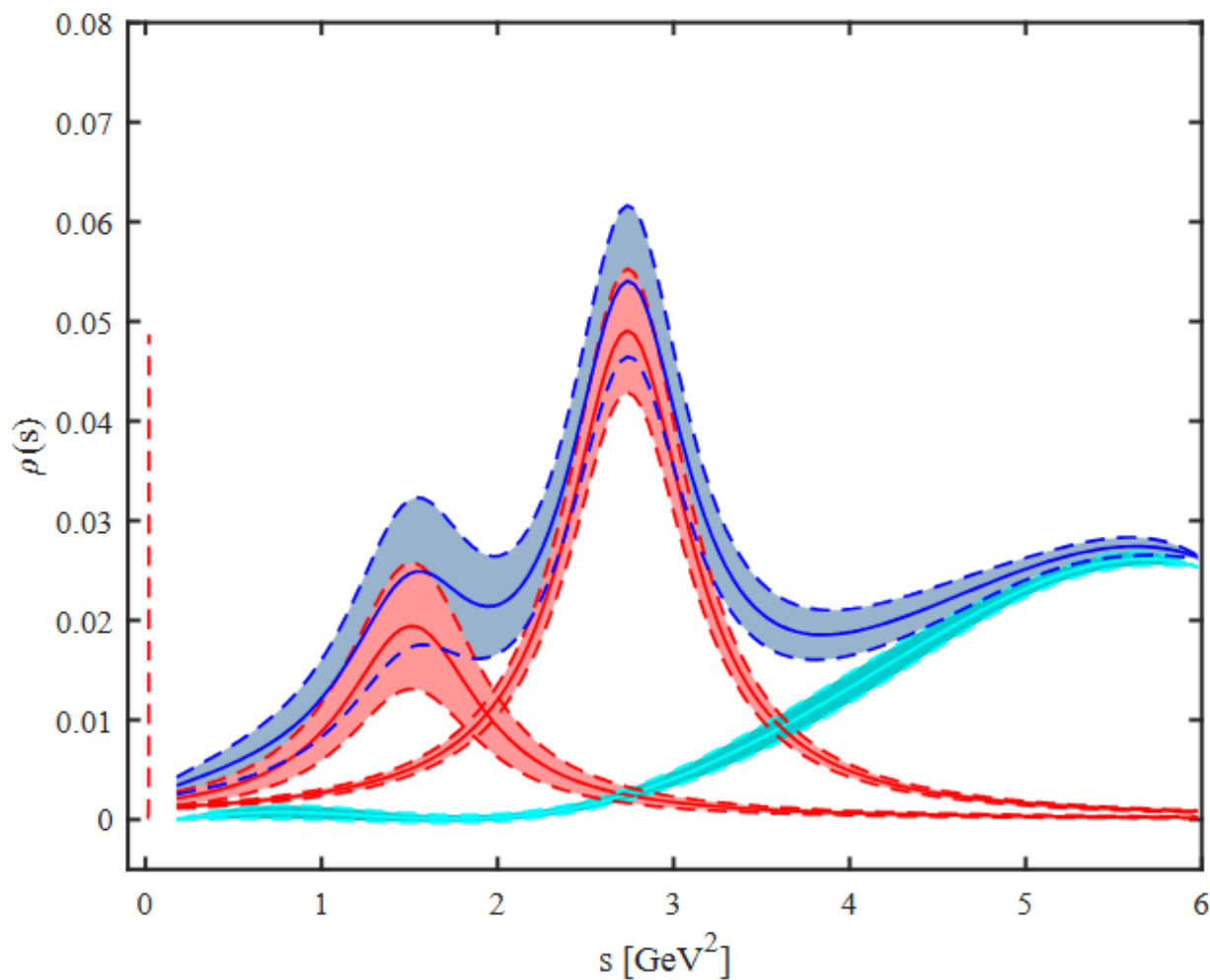
## 运用先验信息, 瞄准激发态衰变常数:

$$\text{Im} \Pi_q(s) = \pi f_\pi^2 \delta(s - m_\pi^2) + \pi f_{a_1(1260)}^2 \text{BW}(s, m_{a_1(1260)}) + \pi f_{a_1(1640)}^2 \text{BW}(s, m_{a_1(1640)}) + \pi \rho(s).$$

Particle	Mass	Width
$\pi$	0.140 GeV	
$a_1(1260)$	$(1.230 \pm 0.040)$ GeV	$[0.250, 0.600]$ GeV [4]
$a_1(1640)$	$(1.655 \pm 0.016)$ GeV	$(0.254 \pm 0.040)$ GeV



### 反问题方法计算 $\pi$ 介子及其激发态衰变常数：



Decay Constants	Our Prediction	Exp/Lattice
$f_\pi$	$130.2 \pm (6.6)_{stat} \pm (4.0)_{sys}$ MeV	$130.4 \pm 0.2$ MeV
$f_{a_1(1260)}$	$166.3 \pm (30.3)_{stat} \pm (21.6)_{sys}$ MeV	
$f_{a_1(1640)}$	$254.1 \pm (16.6)_{stat} \pm (17.7)_{sys}$ MeV	

- 结果与实验一致，使用L0输入
- 激发态可以被计算；
- 不确定性被系统性控制；
- 系统误差可被持续性改进：高阶修正。



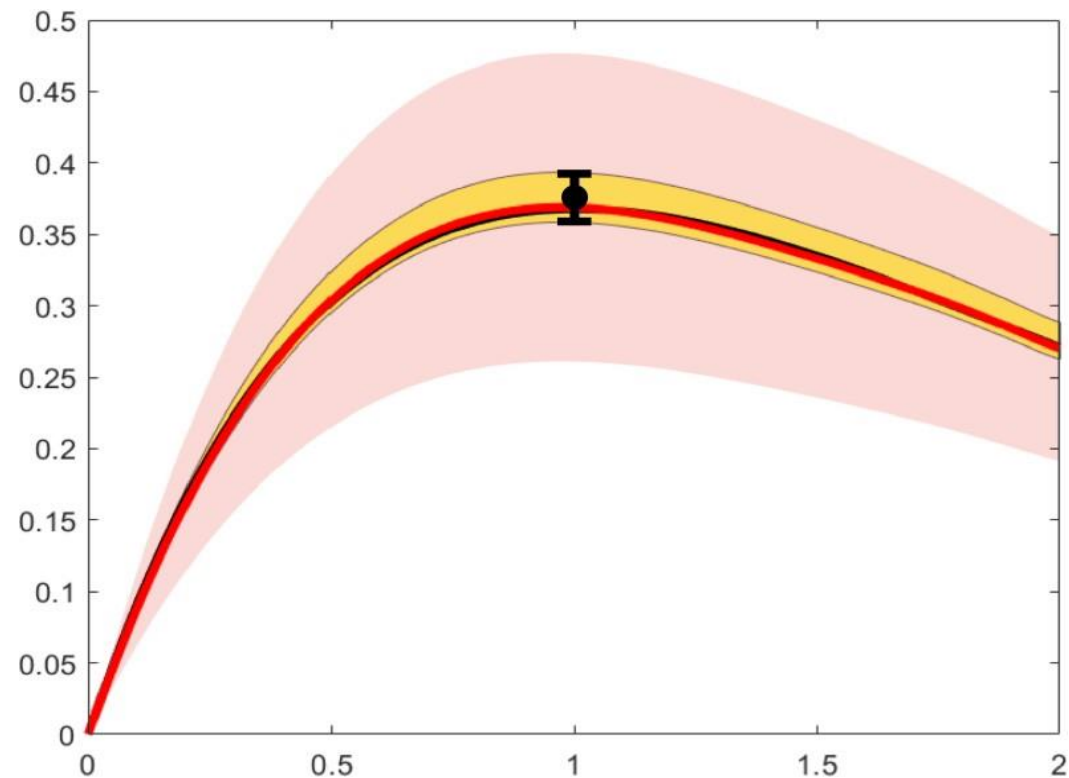


## 反问题方法的优势：

1. 基于严谨的数学框架，能够系统性地控制误差；
2. 不需要过大的计算资源；
3. 能够计算全部非微扰能区、激发态等；
4. 针对具体问题可进行改进；输入精度提高，结果会持续变好；选取不同的正则化方法针对不同问题
5. 可以与实验数据或格点QCD等其他方法结合并互补；

反问题方法的局限？ 输入误差和真解形状

方法正在起步，一切即将开始！



Thank  
you



## Toy Models:

$$\int_a^b \frac{f(x)}{y-x} dx = g(y), y \in [c, d], c > b$$

开始使用最简单的正则化方法：Tikhonov正则化方法和L曲线法。

数学和应用是简单清楚的，有助于后续进一步发展。

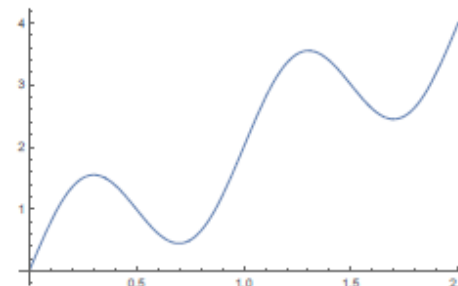
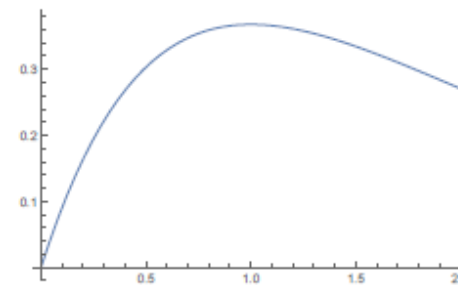
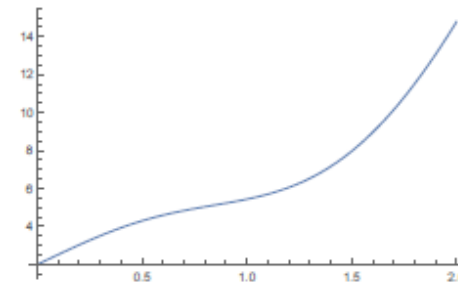
下述可展示反问题的性质并与真实的物理接近： $b_i = \mu_i \pm \sigma_i$

$$f(x) = a_1 f_1(x) + a_2 f_2(x) \quad g^\delta(y) = b_1 g_1(y) + b_2 g_2(y) \quad g_i(y) = \int_a^b \frac{f_i(x)}{y-x} dx.$$

**Model 1:** a monotonic function as  $f_1(x) = \sin(\pi x)$ ,  $f_2(x) = e^x$ ;

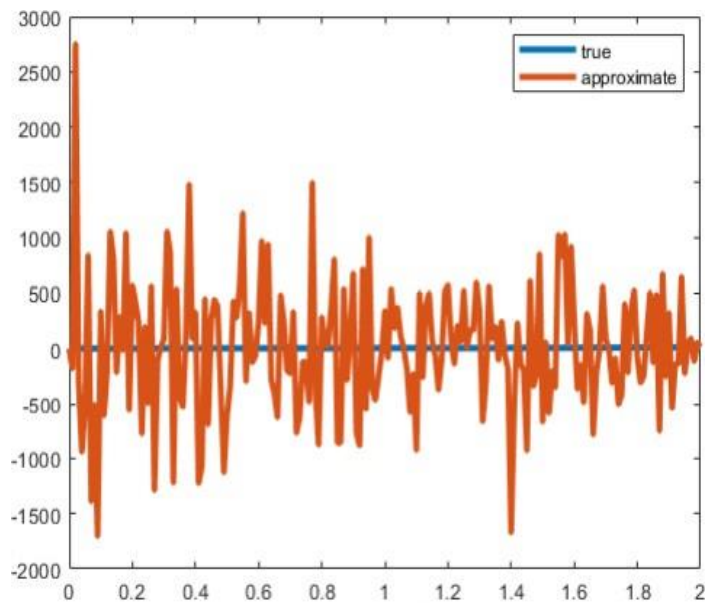
**Model 2:** a simple non-monotonic function as  $f_1(x) = x e^{-x}$ ,  $f_2(x) = 0$ ;

**Model 3:** an oscillating function as  $f_1(x) = \sin(2\pi x)$ ,  $f_2(x) = x$ .

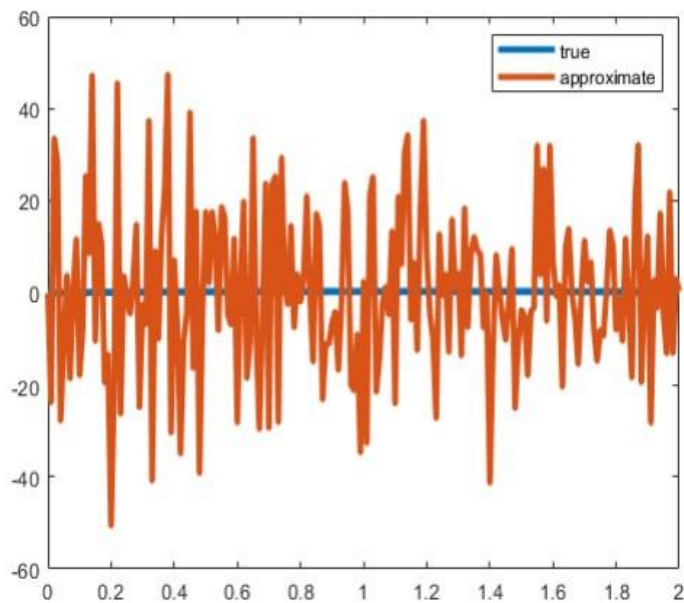




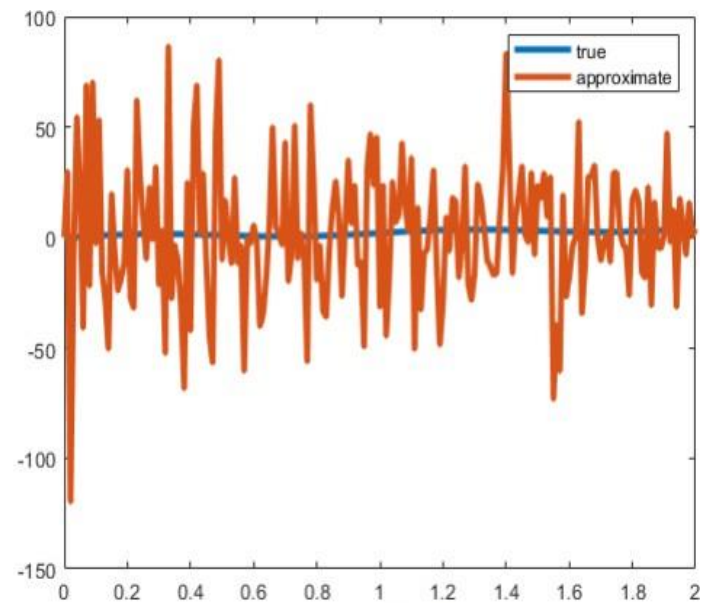
使用经典方法的结果：使用有限元展开求逆



model 1



model 2



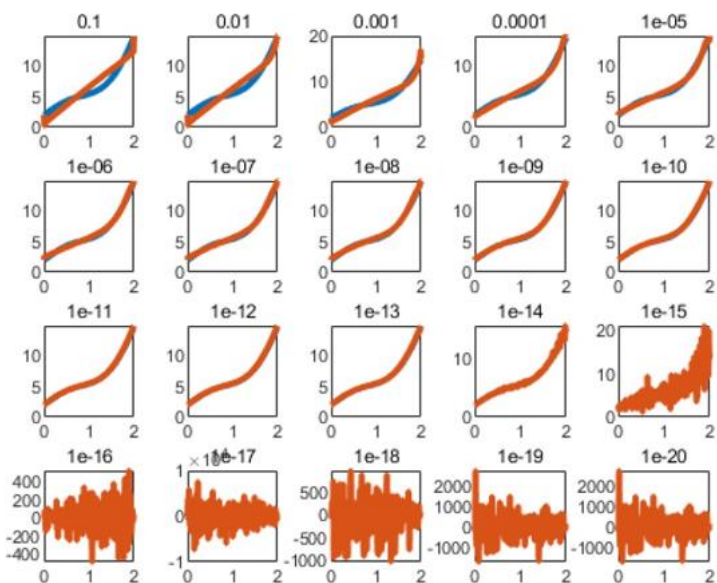
model 3

清楚地验证了问题的不稳定性；

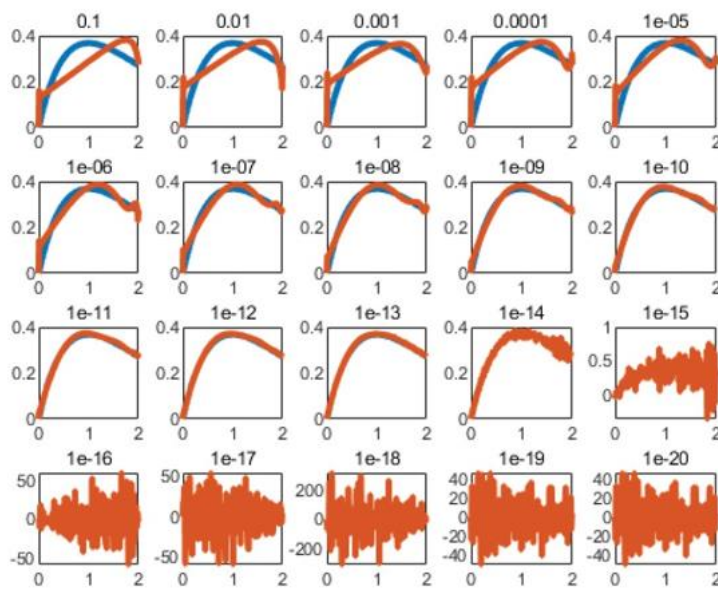
无法使用经典的方法求解，必须要使用正则化方法。



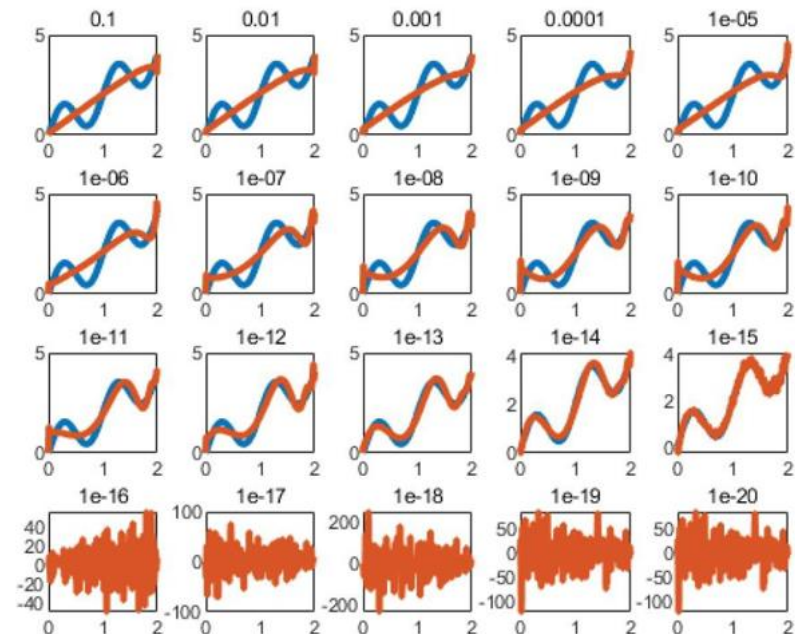
对正则化参数进行遍历：



model 1



model 2



model 3

正则化参数 $\alpha$ 的不能过大也不能过小，与理论预期一致；

正则化参数存在很大的平台，跨越多个量级；

L-curve曲线法可以较好地选取；

正则化方法可以很好地解决色散关系的反问题。



**不稳定：输入数据存在一点点误差就会导致解发生巨大变化！**

逆矩阵 $K^{-1}$ 会极大地放大误差；

在连续极限下， $K^{-1}$ 无界趋于无穷；

上述问题均称为**不适定问题**。

$$K = \begin{pmatrix} 2 & 3 \\ 1.9999 & 3.0001 \end{pmatrix}, \quad |K| = 0.0005,$$

$$K^{-1} = \frac{K^*}{|K|} = \begin{pmatrix} 6000.2 & -6000 \\ -3999.8 & 4000 \end{pmatrix}$$

**色散关系的反问题：经典的反问题**

If  $s > \Lambda$ ,

$$\mathcal{P} \int_0^\Lambda \frac{\text{Im}[\Pi(s')]}{s - s'} ds' = \pi \text{Re}[\Pi(s)] - \mathcal{P} \int_\Lambda^\infty \frac{\text{Im}[\Pi(s')]}{s - s'} ds'$$

To be solved
calculable

$$\int_a^b \frac{f(x)}{y - x} dx = g(y), \quad y \in [c, d], \quad c > b, \quad a > 0$$

**色散关系的反问题是否为不适定问题！？！**



Tikhonov正则化方法和L-curve法的结果:

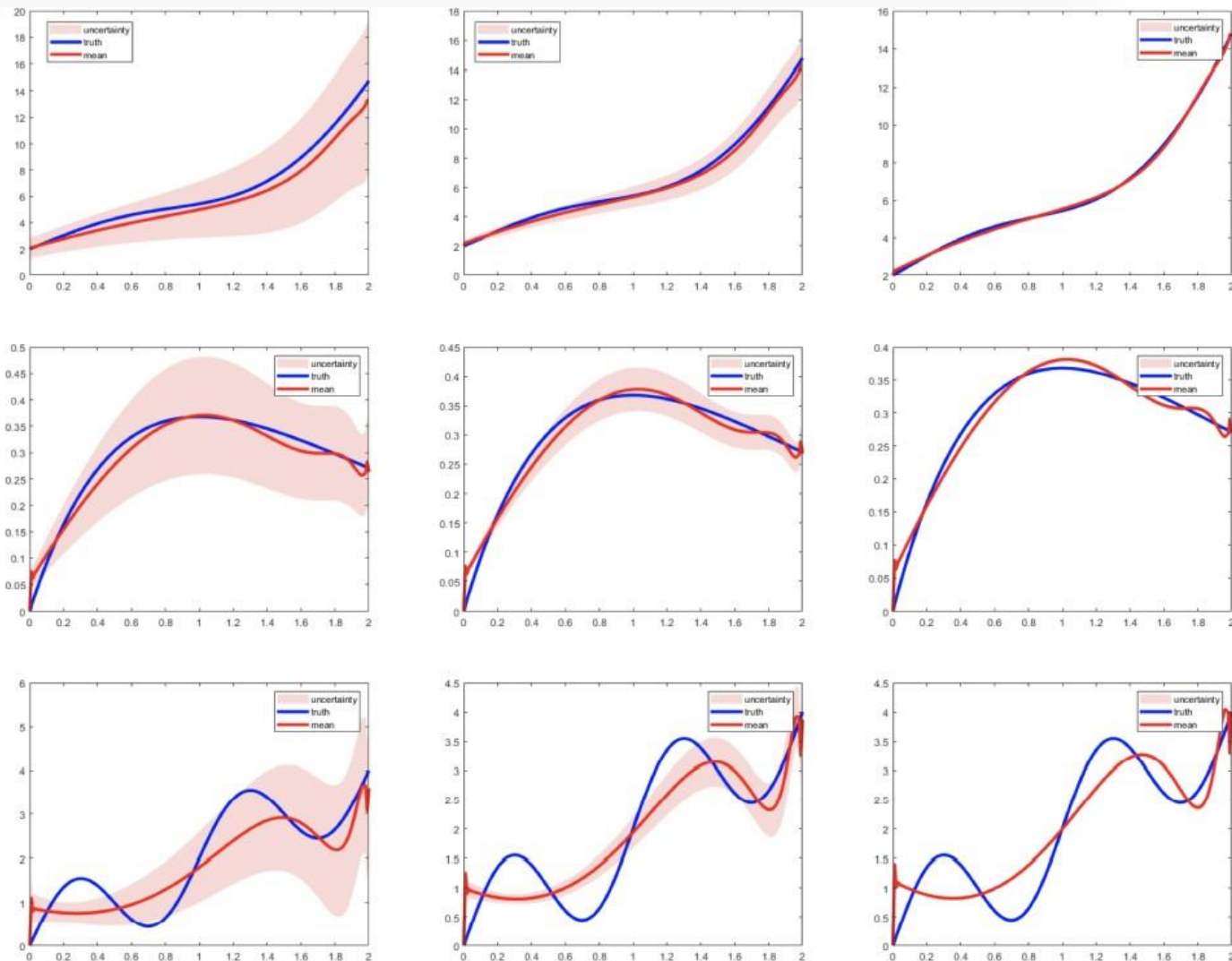
输入误差分别为30%, 10%, 1%;

随着输入误差降低, 解的误差也  
逐渐降低, 误差水平基本一致

Model 1能够很好地反演, 而Model 2和  
Model 3的反演效果不是特别好;

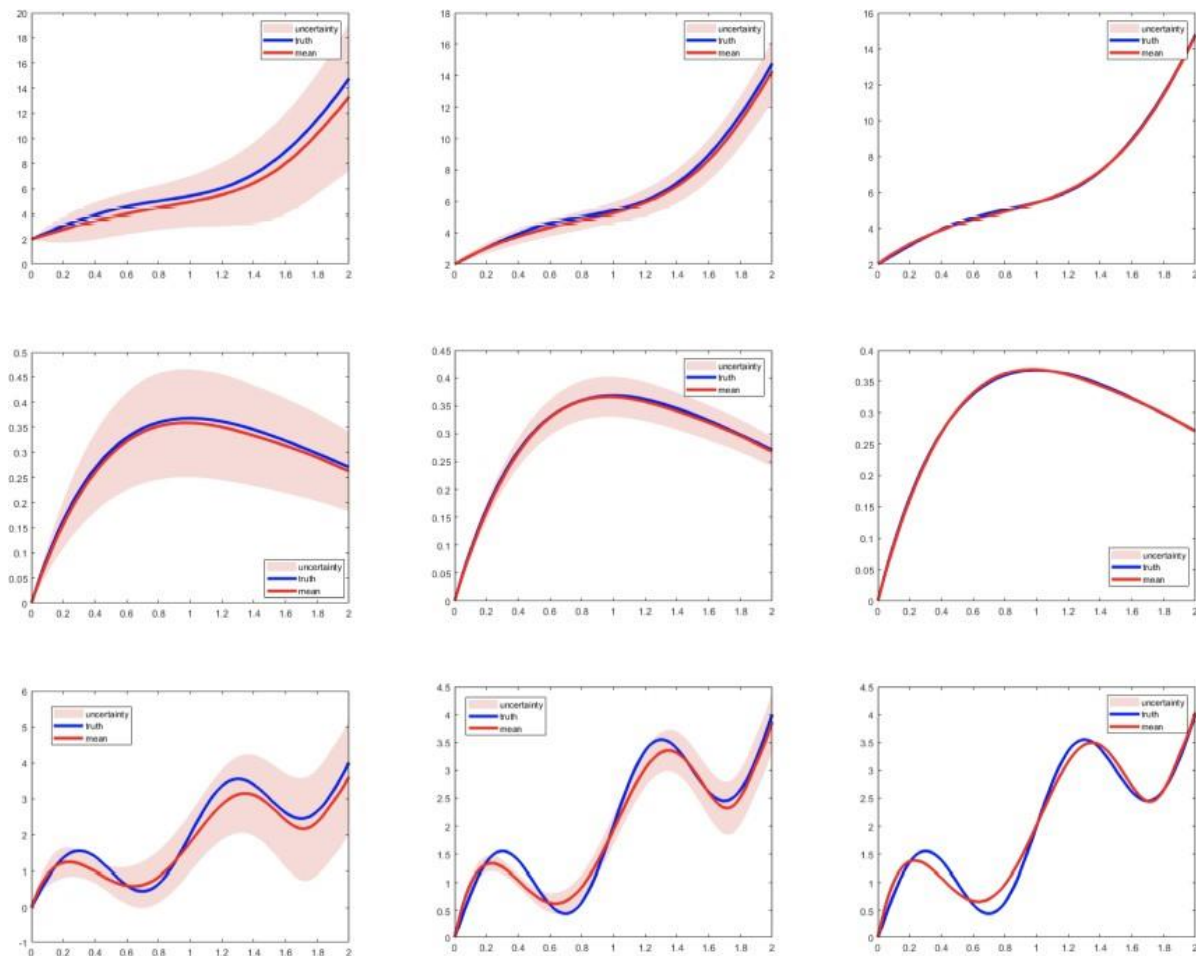
积分方程将解磨平

可对正则化方法进行不断改进。



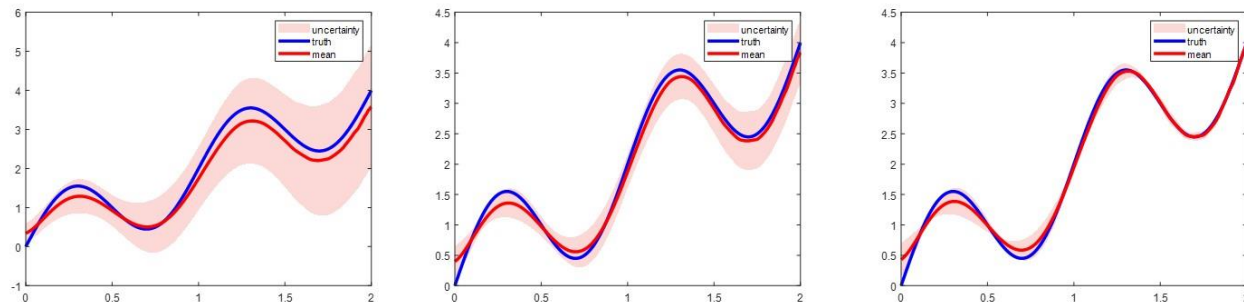


改进1: 限制解的空间:  $\|f\|_{L^2}^2 \rightarrow \|f\|_{H^1}^2$



改进2: 运用迭代, 将每次反演的结果保存并作为下次迭代的先验信息

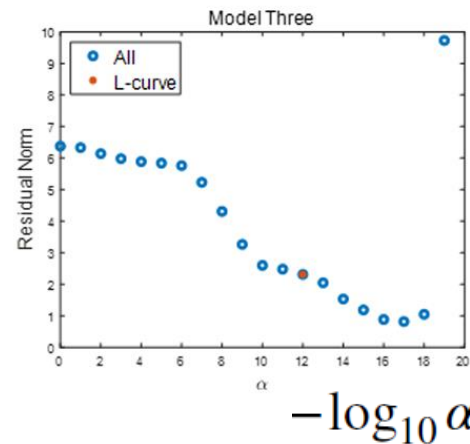
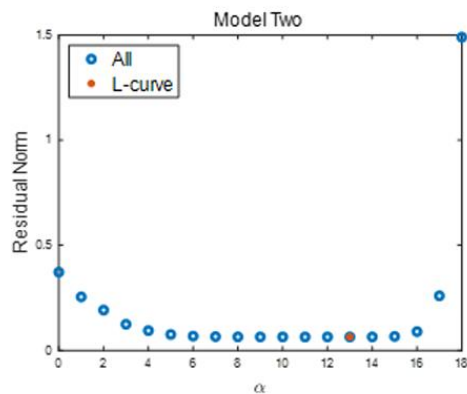
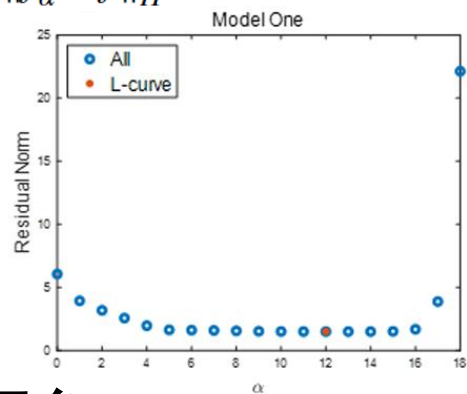
- (1) Compute  $r_k^\delta = g^\delta - Kf_k$
- (2) Solve  $h_k = \min\{\frac{1}{2}\|Kh - r_k^\delta\|_{L^2}^2 + \frac{\alpha_k}{2}\|h\|_{H^1}\}$
- (3) Update  $f_{k+1} = f_k + h_k$
- (4) Stop by the L-curve method





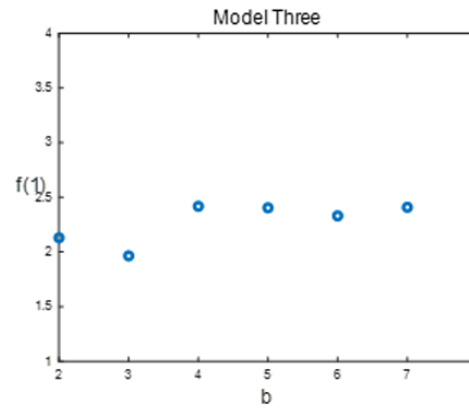
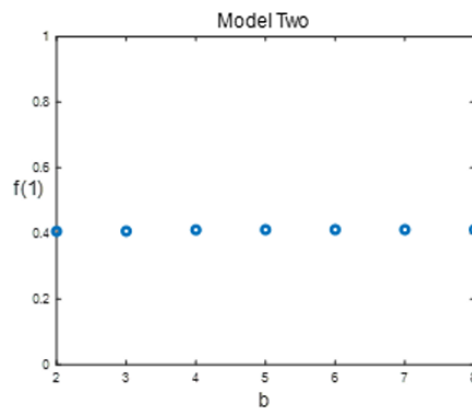
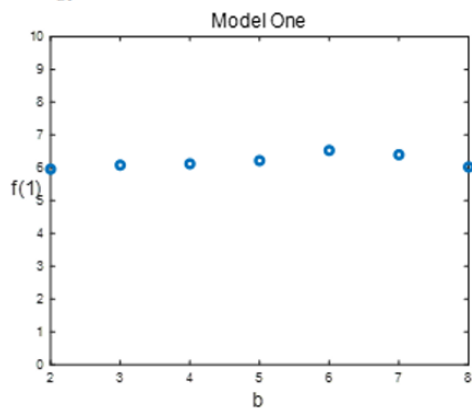
## 正则化参数 $\alpha$ 的平台

$$\|f_\alpha^\delta - f\|_{H^1}$$



## 阶段标度 $\Lambda$ 的平台

$$f_\alpha^\delta(1)$$


 $\Lambda$