Estimation of the Derivative and Fractional Derivative of a Function Specified by Noisy Data

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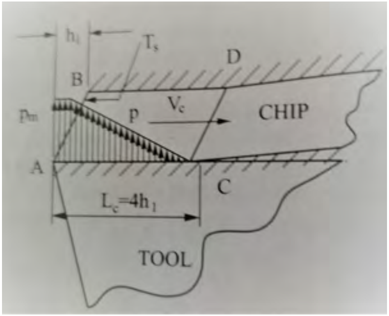
High-Speed Machining Application



Abel's Integral Equation

$$T(x) = T_s + \frac{\nu}{\sqrt{\pi}} \int_0^x \frac{p(y)}{\sqrt{x-y}} dy$$

Smooth function $T(x)$ defined by discrete data $\{T_1^\epsilon, \ldots, T_m^\epsilon\}$, corresponding to $0 < x_1 < x_2 < \cdots < x_m = L_c$, contaminated by random, zero-mean measurement errors $\{\epsilon_1, \ldots, \epsilon_m\}$. Estimate stress distribution $p(x)$ on $[0, L_c]$.

Inverse Problem $Af = g^\epsilon = g + \epsilon$.

- Given: Finite sequence of data measurements $\mathbf{g}^\epsilon = \{g_k^\epsilon\}$, determined by Abel's integral transform, contaminated by noise, with known statistical properties.
- Find: Source function f.
- Mathematical Problem: Estimate Fractional Derivative of Smooth Data Function Defined by Noisy Data.
- Regularize Data: $\mathbf{g}^\epsilon = \mathbf{g}_S^\epsilon + \mathbf{g}_N^\epsilon$.
- Finite-Dimensional Projection Method

$$\hat{\mathbf{f}} \approx \mathbf{A}^{-1}\mathbf{g}_S^\epsilon$$

based on known singular value decomposition (SVD) of compact infinite-dimensional Hilbert Space operator

$$A = U\Sigma V^T : \; X \to Y$$

SVD $A = U\Sigma V^T$

Injective compact $A : X \to Y$, Adjoint $A^* : Y \to X$

X, Y weighted L^2 spaces

Singular system $\{(\sigma_j,\ v_j,\ u_j),\ j = 1, 2, \ldots\}$

σ_j nonincreasing positive numbers $\to 0$ as $j \to \infty$

Orthonormal basis $v_j \subset X$, Orthonormal system $u_j \subset Y$

$$Av_j = \sigma_j u_j, \qquad A^* u_j = \sigma_j v_j, \qquad A^* A v_j = \sigma_j^2 v_j$$

For each $f \in X$, we have the Singular Value Decomposition

$$f = \sum_{j=1}^{\infty} (f, v_j)_X \, v_j, \qquad \text{and} \qquad Af = \sum_{j=1}^{\infty} (f, v_j)_X \, \sigma_j u_j$$

$$A = U \Sigma V^T, \quad V^T : X \to \ell^2, \quad \Sigma : \ell^2 \to \ell^2, \quad U : \ell^2 \to Y$$

$$Af = g \text{ has a solution } g \in Y \iff g = \sum_{j=1}^{\infty} (g, u_j)_Y \, u_j,$$

and

$$\sum_{j=1}^{\infty} \frac{1}{\sigma_j^{\,2}} |(g, u_j)_Y|^2 < \infty. \qquad \text{Picard Condition}$$

In this case, the unique solution is given by

$$f = \sum_{j=1}^{\infty} \frac{1}{\sigma_j} (g, u_j)_Y \, v_j.$$

Volterra Integral Equation of First Kind $Af = g$

Abel Transform $0 < \mu < 1$

$$A: \ L^2(\Omega, w_1) \to L^2(\Omega, w_2), \qquad \Omega = [a, b]$$

$$Af = \ I_a^{\mu} f(x) \ := \frac{1}{\Gamma(\mu)} \int_a^x (x-y)^{\mu-1} f(y) dy = g(x), \ \ g(a) = 0$$

Inverse Transform: Fractional Derivative of g

$$A^{-1} g = D_a^{\mu} g(x) := \frac{1}{\Gamma(1-\mu)} \int_a^x (x-y)^{-\mu} \frac{dg}{dy}(y) dy = f(x)$$

Case $\mu = 1$

Integration

$$A : \; L^2[a,b] \to L^2[a,b]$$

$$Af = I_a^1 f(x) := \int_a^x f(y)dy = g(x), \qquad g(a) = 0$$

Inverse: Differentiation $\qquad g \in H^1[a,b]$

$$A^{-1}g = D_a^1 g(x) := \frac{dg}{dx} = f(x)$$

For $\mu \in (0,1]$, I_a^μ is a compact linear operator acting on and into infinite-dimensional Hilbert spaces. Therefore, its inverse D_a^μ cannot be continuous.

Differentiation and fractional differentiation of approximately specified functions are ill-posed problems.

Finite-Dimensional Projection Method – Collocation

$$\mathbf{g}^\epsilon = \mathbf{g} + \epsilon = \{g_1^\epsilon, \ldots, g_m^\epsilon\}, \quad a < x_1 < \cdots < x_m = b$$

$$X_m = \text{span}\{v_j : j = 1, \ldots, m\}, \qquad Y_m = \text{span}\{u_j : j = 1, \ldots, m\}$$

Unique $G(x) \in Y_m, \quad G(a) = 0$

$$G(x) = \sum_{j=1}^{m} \xi_j u_j(x)$$

$$g_k^\epsilon = G(x_k) = \sum_{j=1}^{m} \xi_j u_j(x_k), \quad k = 1, \ldots, m$$

By Picard, estimate of source function given by

$$\hat{f}(x) = \sum_{j=1}^{m} \frac{\xi_j}{\sigma_j} v_j(x), \qquad \mathbf{A}\hat{\mathbf{f}} \approx \mathbf{g}.$$

Closed-Form SVD: $\mu \in (0,1)$ Fractional Integration

Gorenflo & Tuan (1995)

$$A : X \to Y, \qquad X = L^2([-1,1], w_1), \qquad Y = L^2([-1,1], w_2)$$

$$w_1(x) = 1, \qquad w_2(x) = (1 - x^2)^{-\mu}$$

$$\sigma_j = \sqrt{\frac{\Gamma(j - \frac{1}{2} - \mu)}{\Gamma(j - \frac{1}{2} + \mu)}} \sim 1/j^{\mu}, \qquad j \to \infty$$

$$v_j(x) = \sqrt{2j-1} L_{j-1}(x), \qquad u_j(x) = c_j\,(1+x)^{\mu}\, P_{j-1}^{(-\mu,\mu)}(x)$$

L_{j-1} Legendre polynomials, $P_{j-1}^{(-\mu,\mu)}$ Jacobi polynomials

$$c_j = \sqrt{\frac{(j - \frac{1}{2})\ [\Gamma(j)]^2}{\Gamma(j-\mu)\Gamma(j+\mu)}}$$

Closed-Form SVD: $\mu = 1$ Integration

Z. Zhao, Z. Meng, G. He (2009)

$$Tg := \frac{dg}{dx}, \qquad \mathcal{D}(T) = H_0^1[0,1] = \{g \in H^1[0,1] : \ g(0) = g(1) = 0\}$$

$$Af := \int_0^x f(s)ds, \qquad A = T^{-1} : L^2[0,1] \cap \mathbb{R}^{\perp} \to L^2[0,1]$$

$$\sigma_j = \frac{1}{j\pi}, \quad v_j(x) = \sqrt{2}\cos(j\pi x), \quad u_j(x) = \sqrt{2}\sin(j\pi x), \quad j = 1, 2, \ldots$$

$$\bar{g}(x) = g(x) - g(0)(1-x) - g(1)x, \qquad \bar{g}'(x) = g'(x) + g(0) - g(1)$$

$$g \in H^2[0,1], \qquad \|\bar{g} - \bar{g}^\delta\| \le \delta, \qquad f^\delta = \bar{f}^\delta + g^\delta(1) - g^\delta(0)$$

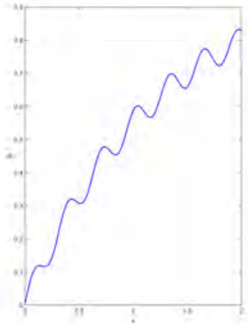
TSVD $$\bar{f}^\delta(x) = \sum_{i=1}^{k(\delta)} \frac{1}{\sigma_i}(\bar{g}^\delta, u_i)v_i \implies \|f^\delta - f\| = o(\delta^{\frac{1}{2}})$$

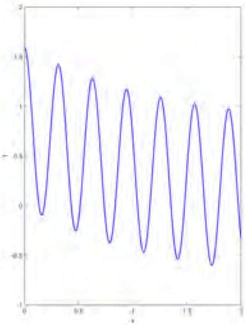
Need for Regularization (Differentiation $\mu = 1$)

Example: Craig & Brown

$$
\begin{aligned}
g(x) &= 1 - \exp(-\alpha x) + \beta \sin(\omega x), \qquad 0 \le x \le 2 \\
f(x) &= \alpha \exp(-\alpha x) + \beta\omega \cos(\omega x)
\end{aligned}
$$

$$\alpha = 0.8,\ \omega = 20,\ \beta = 0.04$$





Differentiation with Noisy Data

Transform domain to $[0, 1]$; compute $\mathbf{g} = (g_1, \ldots, g_m)^T$ on equally-spaced mesh $(x_1 = h,\ x_2 = 2h, \ldots, x_m = 1)$, with $m = 250$

Assume measurement errors statistically independent

Compute pseudo-random sample from standard multivariate normal distribution $\mathrm{N}(\mathbf{0}, \mathbf{I}_m)$, multiply each component by fixed standard deviation $s = 0.02$; get

$$\boldsymbol{\epsilon} = (\epsilon_1, \ldots, \epsilon_m)^T$$

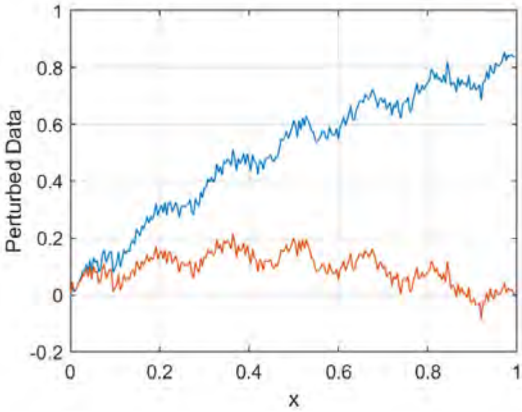
Create noisy data

$$\mathbf{g}^{\epsilon} = \mathbf{g} + \boldsymbol{\epsilon}$$

Transform Data to Periodic

$$\bar{\mathbf{g}}^{\epsilon} = \mathbf{g}^{\epsilon} - \mathbf{w}$$

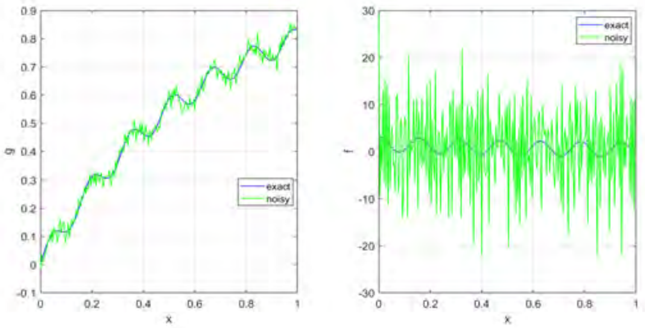
$$w_i = [1 - (i-1)\,h]\, g_1^{\epsilon} + [(i-1)\,h]\, g_m^{\epsilon}, \quad i = 1, \ldots, m$$



Must Separate Signal From Noise in Data

$$\bar{\mathbf{g}}^{\epsilon} = \mathbf{P}\xi, \qquad \mathbf{P} = \begin{pmatrix} u_1(x_1) & u_2(x_1) & \dots & u_m(x_1) \\ u_1(x_2) & u_2(x_2) & \dots & u_m(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ u_1(x_m) & u_2(x_m) & \dots & u_m(x_m) \end{pmatrix}$$

$$\hat{f}(x) = \sum_{j=1}^{m} \frac{\xi_j}{\sigma_j} v_j(x) + g_m^{\epsilon} - g_1^{\epsilon}, \qquad \|\hat{\mathbf{r}}\|_2^2 = \|\bar{\mathbf{g}}^{\epsilon} - \mathbf{A}\hat{f}\|_2^2 = 0$$



Abel Transform $Af = I_a^\mu f = g$ is Dissipative

$$g(x) \;=\; I_a^\mu f(x) \;= \frac{1}{\Gamma(\mu)} \int_a^x (x-y)^{\mu-1}\, f(y) dy, \quad g(a) = 0$$

Convolution Kernel

$$k(x-y) = \frac{1}{\Gamma(\mu)} (x-y)^{\mu-1}$$

Laplace Transform

$$\bar{g}(s) = \bar{k}(s) \bar{f}(s)\,, \qquad \bar{k}(s) = 1/s^\mu$$

Let $s = \gamma + i\omega$, where $\gamma > 0$ is a fixed real number

$$|\bar{k}(s)| \;\sim 1/|\omega|^\mu$$

Differentiation ($\mu = 1$) is most ill-posed case

Regularization of Data

Assume measurement errors ϵ are statistically independent samples from multivariate normal distribution, with respective estimated standard deviations s_j, so that covariance matrix is

$$\mathbf{S}^2 = \mathbf{diag}(s_1^2, \ldots, s_m^2)$$

Formulate problem as **semi-stochastic**

$$\bar{\mathbf{g}}^\epsilon = \mathbf{P}\tilde{\xi} + \epsilon, \qquad \epsilon \sim \mathrm{N}(\mathbf{0}, \mathbf{S})$$

$$\epsilon = (\epsilon_1, \ldots, \epsilon_m)^T, \qquad \mathcal{E}(\epsilon) = \mathbf{0}, \qquad \mathcal{E}\left(\epsilon\epsilon^T\right) = \mathbf{S}^2$$

Rescale problem so that errors are samples from standard multivariate normal distribution

$$\mathbf{b} = \mathbf{S}^{-1}\bar{\mathbf{g}}^\epsilon, \qquad \mathbf{W} = \mathbf{S}^{-1}\mathbf{P}, \qquad \eta = \mathbf{S}^{-1}\epsilon$$

$$\mathbf{b} = \mathbf{W}\tilde{\xi} + \eta, \qquad \eta \sim \mathrm{N}(\mathbf{0}, \mathbf{I}_m)$$

Key Idea: Morozov's Discrepancy Principle

Since

$$\eta = \mathbf{b} \; - \; \mathbf{W}\tilde{\xi}$$

an estimate $\hat{\xi}$ is acceptable only if

$$\hat{\mathbf{r}} = \mathbf{b} \; - \; \mathbf{W}\hat{\xi}$$

is a plausible sample from the η distribution.

If $\mathbf{b} \; - \; \mathbf{W}\tilde{\xi} \sim \mathrm{N}\left(\mathbf{0}, \mathbf{I}_m\right)$, then $\|\mathbf{b} \; - \; \mathbf{W}\tilde{\xi}\|_2^2 \sim \chi^2(m)$, and

$$\mathcal{E}\left(\|\mathbf{b} - \mathbf{W}\tilde{\xi}\|_2^2\right) = m, \qquad \mathrm{Var}\left(\|\mathbf{b} - \mathbf{W}\tilde{\xi}\|_2^2\right) = 2m$$

Sum of squared residuals of a reasonable estimate should be within two standard deviations of the expected value

$$m - 2\sqrt{2m} \leq \|\hat{\mathbf{r}}\|_2^2 \leq m + 2\sqrt{2m}$$

Separation of Signal from Noise $\bar{\mathbf{g}}^\epsilon = \bar{\mathbf{g}}^\epsilon_S + \bar{\mathbf{g}}^\epsilon_N$

Compute qr-factorization $\mathbf{W} = \mathbf{QR}$

$\mathbf{Q}$ orthogonal, $\mathbf{R}$ upper triangular

Project $\mathbf{b}$ onto orthonormal columns of $\mathbf{Q}$

$$\mathbf{a} = \mathbf{Q}^T\mathbf{b}, \qquad \|\mathbf{a}\|_2^2 = \|\mathbf{b}\|_2^2$$

Projected data a_j are scaled to one standard deviation s_j

Separate signal from noise

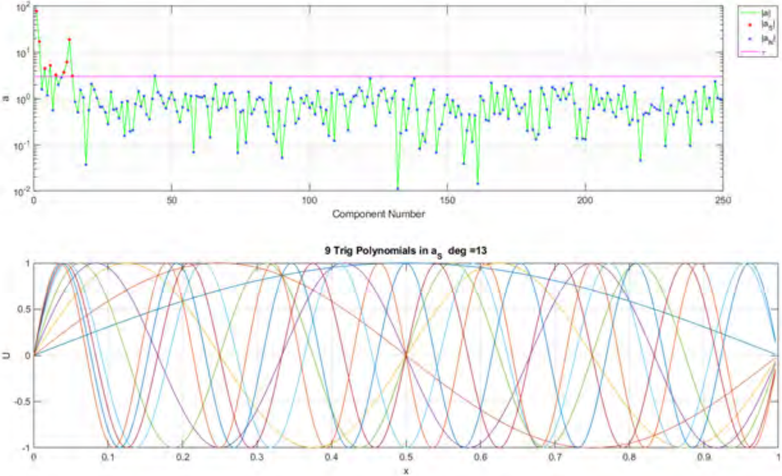
$$\mathbf{a} = \mathbf{a}_S + \mathbf{a}_N, \qquad \mathbf{b} = \mathbf{Q}\mathbf{a}_S + \mathbf{Q}\mathbf{a}_N, \qquad \bar{\mathbf{g}}^\epsilon = \mathbf{S}\mathbf{b}_S + \mathbf{S}\mathbf{b}_N$$

if $|a_j| > \tau$, and j "small", $a_j \in \mathbf{a}_S$; otherwise, $a_j \in \mathbf{a}_N$

Rule of Thumb: start with $\tau = 3$, and adjust up or down if necessary

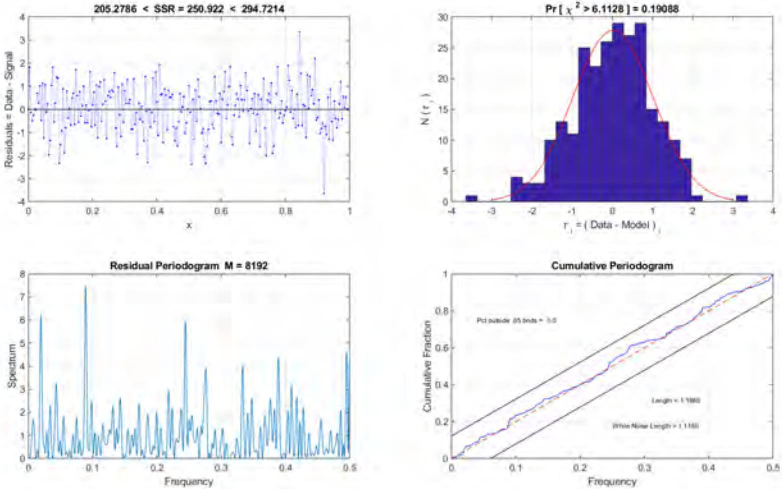
Differentiation $\mu = 1$, $s = 0.02$, $m = 250$, $\beta = 0.04$

$$\tau = 3, \qquad \|\hat{\mathbf{r}}\|_2^2 = 250.922$$



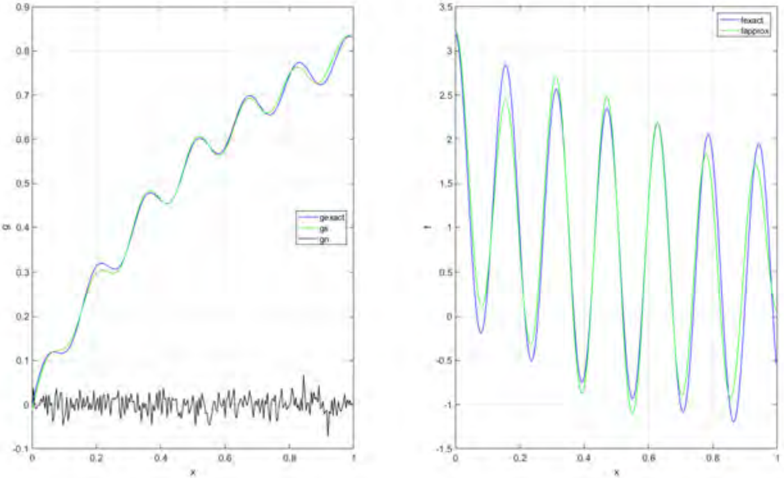
Differentiation

$$\mu = 1,\ s = 0.02,\ m = 250,\ \beta = 0.04$$



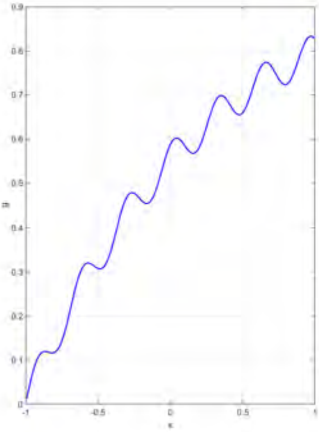
Differentiation

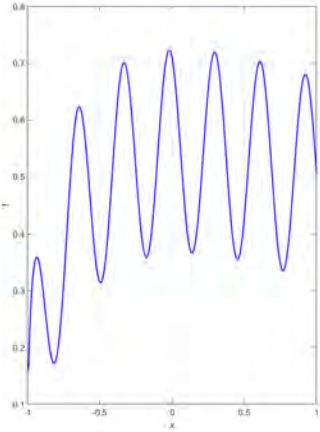
$$\mu = 1, \; s = 0.02, \; m = 250, \; \beta = 0.04$$



Fractional Differentiation – “Exact Solution"

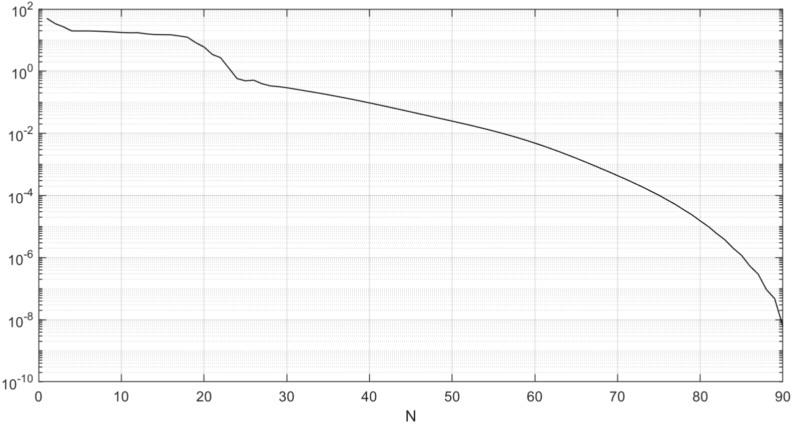
$$g(x) = 1 - e^{-\alpha x} + \beta \sin(\omega x) \approx G(x) = \sum_{j=1}^{90} \eta_j u_j, \qquad f(x) = \sum_{j=1}^{90} \eta_j \sigma_j^{-1} v_j$$





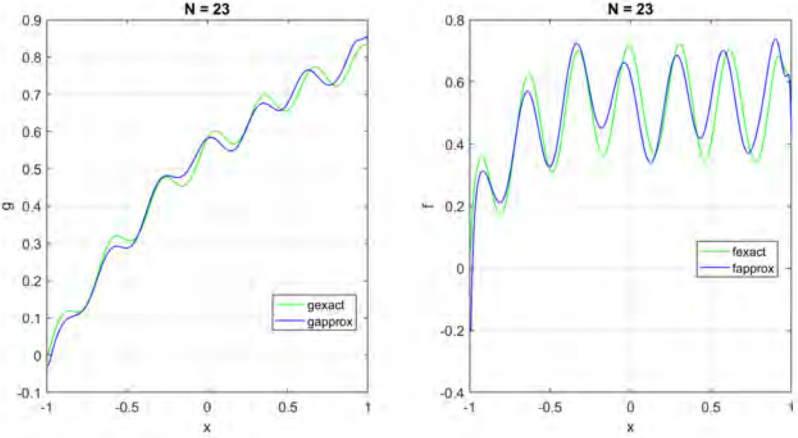
Estimate Fractional Derivative Using $\bar{\mathbf{g}}_S^{\epsilon}$ for $\mu = 1$

Scaled Collocation Residual $\frac{1}{s}\|G - \sum_{j=1}^{N} \xi_j u_j\|_2$



Estimate Fractional Derivative Using $\bar{\mathbf{g}}_S^{\epsilon}$ for $\mu = 1$

$$G(x) \approx \sum_{j=1}^{23} \xi_j u_j, \qquad \hat{f}(x) = \sum_{j=1}^{23} \xi_j \sigma_j^{-1} v_j$$



Summary

- Discrete data contaminated by noise with known statistical properties $\pm 2\sigma$
- Data generated by Abel Transform $g = Af$
- Smooth low-dimensional closed-form estimates of source f and data g functions
- Regularization method does not depend upon spectrum of operator A