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Regularization Without Preliminary Knowledge of Smoothness and Error Behavior

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Regularization without Preliminary Knowledge of Smoothness and Error Behavior

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Abstract

The mathematical formulation of many physical problems results in the task of inverting a compact operator. The only known sensible solution technique is regularization which poses a severe problem in itself. Classically one dealt with deterministic noise models and required both the knowledge of smoothness of the solution function and the overall error behavior.
We will show that we can guarantee an asymptotically optimal regularization for a physically motivated noise model under no assumptions for the smoothness and rather weak assumptions on the noise behavior which can mostly obtained out of two input data sets. An application to the determination of the gravitational field out of satellite data will be shown.

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1 Introduction

The primary objective of modern satellite missions like GOCE and CHAMP is determining the geopotential field precisely with high spatial resolution. In particular its knowledge is the base of further geoscientifical investigations like prospecting, exploration, solid earth physics or physical oceanography. For further information on this topic the reader is referred to [Fre99, FP01, Sch97] and the references therein.

A number of interesting mathematical problems is associated to this theme. We will concentrate on the following one [FGS98]. When we have approximated the geopotential field v at the height r of the satellite orbit $x \in \Omega_r$ (for reasons of simplicity now assumed as sphere) by

$$v(x) = \sum_{n=0}^{\infty} \sigma_n \sum_{k=-n}^{n} v^\wedge(n,k) Y_n^k \left(\frac{x}{r}\right)$$

then it reads on the height R of the earth's surface $x \in \Omega_R$ (also assumed as sphere)

$$v(x) = \sum_{n=0}^{\infty} \sum_{k=-n}^{n} v^\wedge(n,k) Y_n^k \left(\frac{x}{R}\right)$$

where $\sigma_n = \left(\frac{R}{r}\right)^n$ and Y_n^k denote the standard spherical harmonics. So the downward-continuation (i.e. determination of the geopotential field out of satellite data) is a severely ill-posed problems because the eigenvalues σ_n of the downward-continuation operator $\Lambda_{R/r}$ decrease with exponential rate.

In order to solve this problem we need to regularize it, i.e. perturbing $\Lambda_{R/r}$ slightly in order to get a continuous inverse. Because we are dealing with measurements it is sensible to assume that our data are biased with random noise [FP01], which makes this regularization procedure harder then the standard deterministic noise estimate. In this text we will concentrate on the spectral cut-off scheme as regularization procedure, i.e. our regularized solution v_N reads

$$v_N(x) = \sum_{n=0}^{N} \sum_{k=-n}^{n} v^\wedge(n,k) Y_n^k \left(\frac{x}{R}\right)$$

The important question is how big one should choose the regularization parameter N; if it is two low we are far away from the real solution even if there would be no noise at all, if it is two high the noise completely conceals the data. At this point we have to face a negative result by Bakushinskii [Bak84] which tells that we cannot find a good regularization parameter without preliminary knowledge of the smoothness of the solution or the size of the error. However in practice one normally never knows the actual smoothness of the solution and normally just has very rough estimates on the error level.

We will show that some knowledge concerning the error behavior is sufficient in order to regularize in an asymptotically near to optimal way. Furthermore we will present an algorithm telling how to deal with severely ill-posed problems occurring in reality and show it to be working using a particular example from satellite gradiometry.

2 Parameter Identification for Regularization

2.1 Preliminaries and Notation

From now on let $\mathcal{X}$ and $\mathcal{Y}$ be separable Hilbert spaces with inner products $< \cdot, \cdot >_{\mathcal{X}}$ and $< \cdot, \cdot >_{\mathcal{Y}}$ with basis $\{u_k\}_{k \in \mathbb{N}}$ and $\{v_k\}_{k \in \mathbb{N}}$ respectively. If no confusion is likely to arise we will denote the inner product just by $< \cdot, \cdot >$. Additionally assume $x \in \mathcal{X}$ and $y \in \mathcal{Y}$ if not stated otherwise.

Furthermore assume A is a map $A : \mathcal{X} \to \mathcal{Y}$ which is a continuous linear operator with infinite rank. A shall admit a singular value decomposition

$$Ax = \sum_{k=1}^{\infty} s_k v_k \langle u_k, x \rangle$$

where $s_k \geq s_{k+1} > 0$ for all $k \in \mathbb{N}$.

We will consider two different kinds of noise, namely the classical deterministic noise and the physically seen more sensible but also more difficult to treat stochastic noise case.

Definition 2.1 (Deterministic Noise)
The data y_δ are biased with deterministic noise (in comparison to y) if $||y - y_\delta|| \leq \delta$, i.e., there exists a vector ξ with $||\xi|| \leq 1$ such that $y_\delta = y + \delta\xi$.

Definition 2.2 (Stochastic Gaussian White Noise)
Let $(\Omega, \Sigma, \mathbb{P})$ be the ordinary probability space. Furthermore $y^\delta = y + \delta\xi$, where ξ is a random vector fulfilling

- *For all $y \in \mathcal{Y}$ we have that $\xi_y(\omega) = \langle y, \xi \rangle$, where $\xi_y(\omega) : \Omega \to \mathbb{R}$ is a random variable. Assume furthermore $\forall t : \{\omega \,|\, \omega \in \Omega, \xi_y(\omega) \leq t\} \in \Sigma$*
- $\mathbb{E}_\xi \langle y, \xi \rangle = 0$
- $\mathbb{E} \langle y, \xi \rangle^2 = ||y||^2$
- *ξ_y is normally distributed around 0.*

Then y^δ is called to be biased with stochastic Gaussian white noise.

2.2 Regularization with all Information

Assume the sequence of operators $\{A_n\}_{n \in \mathbb{N}}$ converging to A. We will consider the following noisy solutions of our operator equation (noise element $\delta\xi$ with the standard formulation for a stochastical noise element ξ):

$$x_n^\delta = A_n^+(Ax + \delta\xi) = (A_n^* A_n)^{-1} A_n^*(Ax + \delta\xi) = x_n^0 + \delta\eta_n^\xi$$

where

$$\eta_n^\xi = A_n^+ \xi = (A_n^* A_n)^{-1} A_n^* \xi$$

is a Gaussian random element. (The spectral cut-off scheme fulfills this property, e.g.). From now on we assume that there exist functions ρ and ψ fulfilling:

Assumption 2.1
Assume that there exist decreasing functions $\rho, \psi : [1, \infty[\to [0, a]$, $\lim_{n\to\infty} \rho(n) = \lim_{n\to\infty} \psi(n) = 0$ which fulfill

- *$\rho(n+1) \geq c\rho(n)$ for a constant c*
- $\mathbb{E}_\xi ||\eta_n^\xi||^2 \leq \frac{1}{\rho^2(n)}$
- *$||x - x_n^0|| \leq \psi(n)$.*

Remark
The function ρ *may be associated with a kind of error spread by the operator* A *over the various frequencies, whereas the function* ψ *is determined by the smoothness of the solution. For deterministic noise we can actually use the same framework because then* $\mathbb{E}_\xi||\eta_n^\xi||^2 \leq ||\eta_n^\xi||^2 \leq \frac{1}{\rho^2(n)}$*. Therefore we will just do our proofs for the stochastic noise case.*
Please note that the condition $\rho(n+1) \geq c\rho(n)$ *just serves technical purposes and prevents* ρ *to decrease faster than an exponential function.*

Now we can determine the optimal regularization parameter via the following result which still needs the input of smoothness and error level but works for the stochastical noise case:

Lemma 2.1
When choosing

$$n_{opt} = \min\left\{n:\ \psi(n) \leq \frac{\delta}{\rho(n)}\right\}$$

we have

$$\sqrt{\mathbb{E}_\xi||x - x^\delta_{n_{opt}}||^2} \leq \frac{\sqrt{2}}{c}\psi\left((\psi\rho)^{-1}(\delta)\right)$$

The proof is taken from [Per03]:

Proof
We have:

$$\begin{aligned}
\mathbb{E}_\xi||x - x_n^\delta||^2 =& \mathbb{E}_\xi\left\langle x - x_n^0 - \delta\eta_n^\xi, x - x_n^0 - \delta\eta_n^\xi\right\rangle \\
=& \mathbb{E}_\xi\left\langle x - x_n^0, x - x_n^0\right\rangle - 2\delta\mathbb{E}_\xi\left\langle x - x_n^0, \eta_n^\xi\right\rangle \\
& + \delta^2\mathbb{E}_\xi\left\langle \eta_n^\xi, \eta_n^\xi\right\rangle \\
=& ||x - x_n^0||^2 - 2\delta\mathbb{E}_\xi\left\langle x - x_n^0, (A_n^*A_n)^{-1}A_n^*\xi\right\rangle \\
& + \delta^2\mathbb{E}_\xi||\eta_n^\xi||^2 \\
=& ||x - x_n^0||^2 - 2\delta\mathbb{E}_\xi\left\langle A_n(A_n^*A_n)^{-1}(x - x_n^0), \xi\right\rangle \\
& + \delta^2\mathbb{E}_\xi||\eta_n^\xi||^2 \\
=& ||x - x_n^0||^2 + \delta^2\mathbb{E}_\xi||\eta_n^\xi||^2 \\
\leq& \psi^2(n) + \frac{\delta^2}{\rho^2(n)}
\end{aligned}$$

The only non-obvious point in the above equation is

$$\mathbb{E}_\xi\left\langle A_n(A_n^*A_n)^{-1}(x - x_n^0), \xi\right\rangle = 0$$

which holds because of Definition 2.2. Balancing for the best possible order of accuracy yields that we need a n_0 fulfilling $\psi(n_0)\rho(n_0) = \delta$. On the one hand we have:

$$\psi(n_{opt})\rho(n_{opt}) \leq \delta = \psi(n_0)\rho(n_0)$$

On the other hand

$$\psi(n_{opt} - 1)\rho(n_{opt} - 1) > \delta = \psi(n_0)\rho(n_0)$$

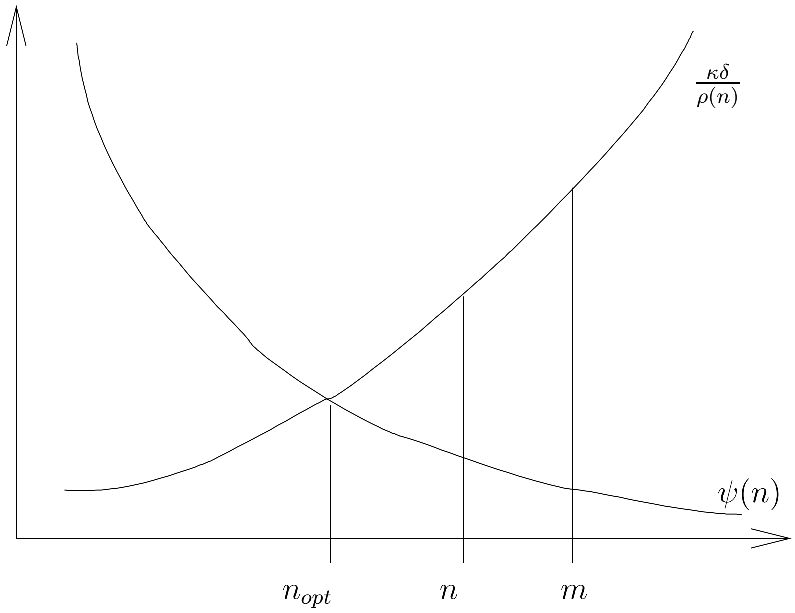
This yields

$$\begin{aligned}\mathbb{E}_\xi||x - x_{n_{opt}}^\delta||^2 \leq& \psi^2(n_{opt}) + \frac{\delta^2}{\rho^2(n_{opt})}\\ \leq& \frac{2\delta^2}{\rho^2(n_{opt})}\\ \leq& \frac{\psi^2(n_0)\rho^2(n_0)}{\rho^2(n_0+1)}\\ \leq& \frac{2}{c^2}\psi^2(n_0)\\ =& \frac{2}{c^2}\psi^2\left((\psi\rho)^{-1}(\delta)\right)\end{aligned}$$

q.e.d.

2.3 Regularization without Known Smoothness

The above result cannot be used in the case when we do not know the smoothness of our solution. Therefore consider for $n < m$ and $n, m \in \{k:\ \psi(k) \leq \frac{\kappa\delta}{\rho(k)}\}$ the following picture:



Then we have in view of Assumption 2.1 for the "expected" behavior of the random variable $||\eta_n^\xi||$:

$$\begin{aligned}||x_n^\delta - x_m^\delta|| \leq& ||x - x_n^\delta|| + ||x - x_m^\delta||\\ \leq& \psi(n) + \delta||\eta_n^\xi|| + \psi(m) + \delta||\eta_m^\xi||\\ \leq& \frac{2\kappa\delta}{\rho(n)} + \frac{2\kappa\delta}{\rho(m)}\\ \leq& \frac{4\kappa\delta}{\rho(m)}\end{aligned}$$

Now we use an idea by Lepskij [Lep90] and take

$$n_* = \min\left\{n:\ ||x_n^\delta - x_m^\delta|| \leq \frac{4\kappa\delta}{\rho(m)},\ N = \rho^{-1}(\delta) > m > n\right\}$$

Remark
In real applications it might be better to choose

$$n_* = \min\left\{n:\ ||x_n^\delta - x_m^\delta|| \le \frac{2\kappa\delta}{\rho(n)} + \frac{2\kappa\delta}{\rho(m)},\ N = \rho^{-1}(\delta) > m > n\right\}$$

However, for the subsequent proofs we will use the simpler version.

Before starting with the main results we need the following supporting lemma:

Lemma 2.2
The following probability estimate holds:

$$\mathbb{P}_\xi\left\{||\eta_n^\xi||\rho(n) > \tau\right\} \le 4\exp\left(-\frac{\tau^2}{8}\right)$$

Proof
We have using $\mathbb{E}_\xi||\eta_n^\xi||^2 \le \frac{1}{\rho^2(n)}$ and the probability estimate for Gaussian random vectors [LT91]:

$$\begin{aligned}\mathbb{P}_\xi\left\{||\eta_n^\xi||\rho(n) > \tau\right\} =& \mathbb{P}_\xi\left\{||\eta_n^\xi|| > \frac{\tau}{\rho(n)}\right\}\\ \le& 4\exp\left(-\frac{\tau^2}{8\rho(n)^2\mathbb{E}_\xi||\eta_n^\xi||^2}\right)\\ \le& 4\exp\left(-\frac{\tau^2}{8}\right)\end{aligned}$$

q.e.d.

Theorem 2.3
Let n_* be chosen as above with $\kappa \ge 1$. Then we have:

$$\mathbb{E}_\xi||x - x_{n_*}^\delta||^2 \le C_1\rho^{-1}(\delta)\exp\left(-\frac{\kappa^2}{16}\right) + C_2\kappa^2\psi^2\left((\psi\rho)^{-1}(\delta)\right)$$

where C_1 and C_2 are constants.
In the deterministic noise case we additionally have $C_1 = 0$ from a certain δ onward.

Proof
Define

$$\Xi_\rho(\omega) = \max_{1\le n\le N} ||\eta_n^\xi||\rho(n)$$

and divide the probability space in two subspaces:

$$\Omega_\kappa = \{\omega : \Xi_\rho(\omega) \le \kappa\} \quad \text{and} \quad \overline{\Omega_\kappa} = \Omega \setminus \Omega_\kappa$$

The proof is mainly consisting of two different parts. The first one estimates the behavior for all "nice" cases Ω_κ. The second one deals with the "bad" cases, where the stochastic noise property produces results far away from the average. Therefore the second part has a strong emphasis on the probability when this case actually occurs.
Note that the second part has probability 0 as long as we are dealing with deterministic noise and δ is small enough.

Part 1: ("good" event $\omega \in \Omega_\kappa$)
Consider

$$n_{opt} = \min\left\{n: \ \psi(n) \leq \frac{\delta}{\rho(n)}\right\}$$

We want to show that $n_{opt} \geq n_*$. For all $n \geq n_{opt}$ we have (using $\frac{\kappa\delta}{\rho(n)} \geq \psi(n)$ and $\rho(n) < \rho(n_{opt})$ because $n \geq n_{opt}$):

$$\begin{aligned}
||x_n^\delta - x_{n_{opt}}^\delta|| \leq & ||x - x_n^\delta|| + ||x - x_{n_{opt}}^\delta|| \\
\leq & \psi(n) + \delta||\eta_n^\xi|| + \psi(n_{opt}) + \delta||\eta_{n_{opt}}^\xi|| \\
\leq & \psi(n) + \frac{\kappa\delta}{\rho(n)} + \psi(n_{opt}) + \frac{\delta}{\rho(n_{opt})} \\
\leq & \psi(n) + \frac{\kappa\delta}{\rho(n)} + \psi(n_{opt}) + \frac{\kappa\delta}{\rho(n_{opt})} \\
\leq & \frac{2\kappa\delta}{\rho(n)} + \frac{2\kappa\delta}{\rho(n_{opt})} \\
\leq & \frac{4\kappa\delta}{\rho(n)}
\end{aligned}$$

which tells that

$$n_* = \min\left\{n: ||x_n^\delta - x_m^\delta|| \leq \frac{4\kappa\delta}{\rho(n)}, \ N = \rho^{-1}(\delta) > m > n\right\} \leq n_{opt}$$

Then using $n_{opt} \geq n_*$ we have for all $\omega \in \Omega_\kappa$

$$\begin{aligned}
||x - x_{n_*}^\delta|| \leq & ||x - x_{n_{opt}}^\delta|| + ||x_{n_{opt}}^\delta - x_{n_*}^\delta|| \\
\leq & \psi(n_{opt}) + \frac{\delta}{\rho(n_{opt})} + \frac{4\kappa\delta}{\rho(n_{opt})} \\
\leq & \frac{2\delta}{\rho(n_{opt})} + \frac{4\kappa\delta}{\rho(n_{opt})} \\
\leq & \frac{2\kappa\delta}{\rho(n_{opt})} + \frac{4\kappa\delta}{\rho(n_{opt})} \\
\leq & 6\frac{\kappa}{c}\left(c\frac{\delta}{\rho(n_{opt})}\right) \\
\leq & 6\frac{\kappa}{c}\psi\left((\psi\rho)^{-1}(\delta)\right)
\end{aligned}$$

Hence we get

$$\int_{\Omega_\kappa} ||x - x_{n_*}^\delta||^2 d\mathbb{P}_\xi(\omega) \leq |\Omega_\kappa| \, ||x - x_{n_*}^\delta||^2 \leq 36\frac{\kappa^2}{c^2}\psi^2\left((\psi\rho)^{-1}(\delta)\right)$$

Part 2: ("bad" event $\omega \in \overline{\Omega_\kappa}$)
Remember that we defined $n_{opt} \leq N = \rho^{-1}(\delta)$. Hence we get $\frac{\delta}{\rho(N)} = 1$ and $\psi(N) \leq \delta||\eta_N^\xi||$

and thus

$$\begin{aligned}||x-x_{n_*}^\delta|| \leq& ||x-x_N^\delta|| + ||x_N^\delta - x_{n_*}^\delta||\\ \leq& \psi(N) + \delta||\eta_N^\xi|| + \frac{4\kappa\delta}{\rho(N)}\\ \leq& 2\delta||\eta_N^\xi|| + \frac{4\kappa\delta}{\rho(N)}\\ \leq& 2\frac{\delta||\eta_N^\xi||\rho(N)}{\rho(N)} + 4\kappa\\ \leq& 2\Xi_\rho + 4\Xi_\rho = 6\Xi_\rho\end{aligned}$$

Using this result we obtain:

$$\begin{aligned}\int_{\overline{\Omega_\kappa}} ||x-x_{n_*}^\delta||^2 d\mathbb{P}_\xi(\omega) \leq& 36\int_{\overline{\Omega_\kappa}} \Xi_\rho^2(\omega) d\mathbb{P}_\xi(\omega)\\ \leq& 36\sqrt{\int_{\overline{\Omega_\kappa}} \Xi_\rho^4(\omega) d\mathbb{P}_\xi(\omega)}\sqrt{\int_{\overline{\Omega_\kappa}} 1 d\mathbb{P}_\xi(\omega)}\end{aligned}$$

Now we estimate the two parts separately:
Consider $F(\tau) = \mathbb{P}_\xi\{\Xi_\rho(\omega) \leq \tau\}$ for $\tau > \kappa$. Then

$$\begin{aligned}G(\tau) = 1 - F(\tau) =& \mathbb{P}_\xi\left\{\Xi_\rho(\omega) > \tau\right\}\\ \leq& \sum_{n=1}^N \mathbb{P}_\xi\left\{||\eta_n^\xi||\rho(n) > \tau\right\}\\ \leq& 4N\exp\left(-\frac{\tau^2}{8}\right)\end{aligned}$$

So we get:

$$\begin{aligned}\int_{\overline{\Omega_\kappa}} \Xi_\rho^4 d\mathbb{P}_\xi(\omega) =& -\int_\kappa^\infty \tau^4 d(1-F(\tau))\\ \leq& -\int_0^\infty \tau^4 dG(\tau)\\ =& -\tau^4 G(\tau)|_0^\infty + 4\int_0^\infty \tau^3 G(\tau)d\tau\\ =& 4\int_0^\infty \tau^3 G(\tau)d\tau\\ \leq& 4N\int_0^\infty \tau^3\exp\left(-\frac{\tau^2}{8}\right)d\tau\\ =& 2^9 N\int_0^\infty u\exp(-u)du\\ =& 2^9 N\end{aligned}$$

The other part gets:

$$\int_{\overline{\Omega_\kappa}} 1 d\mathbb{P}_\xi(\omega) \leq 4\exp\left(-\frac{\kappa^2}{8}\right)$$

Hence we get

$$\int_{\overline{\Omega_\kappa}} \Xi_\rho^2 d\mathbb{P}_\xi(\omega) \leq 2^{11/2} N \exp\left(-\frac{\kappa^2}{16}\right)$$
$$\leq 2^{11/2}\rho^{-1}(\delta)\exp\left(-\frac{\kappa^2}{16}\right)$$

This yields

$$\mathbb{E}_\xi ||x - x_{n_*}^\xi||^2 \leq 36 \cdot 2^{11/2}\rho^{-1}(\delta)\exp\left(-\frac{\kappa^2}{16}\right) + 36\frac{\kappa^2}{c^2}\psi^2\left((\psi\rho)^{-1}(\delta)\right)$$

This is exactly the proposition. q.e.d.

Now the main task will be choosing an appropriate κ for different possible scenarios.

As we have seen above the bound for the square of the total error consists of two parts. The second part $\psi^2((\psi\rho)^{-1}(\delta))$ is just the best order of accuracy we can reach. So we want that the first part $\rho^{-1}(\delta)\exp(-\frac{\kappa^2}{16})$ is negligible in comparison to the second one. It entered the equation when we considered the "bad" case $\omega \in \overline{\Omega_\kappa}$.

As remarked in the proof this part cancels automatically for deterministic noise. We will just consider the case of severely ill-posed problems with stochastical noise right now, a more thorough discussion of other cases can be found in [Bau04].

2.4 Remarks on Smoothness and Error Spread

Now we want to give some short remarks what the terms ρ^{-1} and $\psi((\rho\psi)^{-1})$ actually mean in practice. Assume that we have $\psi(n) = n^{-r}$ which means a finite smoothness of the solution.

Considering a severely ill-posed problem we have $\rho(n) = p(n)\exp(an^\beta)$, where $\ln p(n) \asymp \ln n^{-1}$. For reasons of simplicity we will assume $\rho(n) = n^{-\mu}\exp(an^\beta)$. Then we have:

$$\rho^{-1}(\delta) \approx \left(\frac{\ln\delta^{-1}}{a}\right)^{\frac{1}{\beta}}$$

$$\psi\left((\psi\rho)^{-1}(\delta)\right) \approx \left(\frac{\ln\delta^{-1}}{a}\right)^{-\frac{r}{\beta}}$$

The approximate sign means the equality in the sense of order.

2.5 Relaxations

Now we may choose κ according to our needs. The factor $\chi > 0$ below should always be close to 1. We will do some balancing process:

Lemma 2.4
Assume that our problem is severely ill-posed with stochastical noise and polynomial behavior of the smoothness index function ψ. Now choose $\kappa = \chi 4 \ln\ln\delta^{-1}$.
Then we have

$$\mathbb{E}_\xi ||x - x_{n_*}^\delta||^2 \leq C\left(\ln\left(\delta^{-1}\right)\right)^{\frac{1}{\beta} - \chi^2 \ln\ln\delta^{-1}}$$
$$+ C\chi^2\left(\ln\ln\delta^{-1}\right)^2\psi^2\left((\psi\rho)^{-1}(\delta)\right)$$

Proof
Inserting κ we obtain

$$\begin{aligned} & C_1\rho^{-1}(\delta)\exp\left(-\frac{\kappa^2}{16}\right) + C_2\kappa^2\psi^2\left((\psi\rho)^{-1}(\delta)\right) \\ & \asymp \left(\ln\delta^{-1}\right)^{\frac{1}{\beta}}\left(\ln\delta^{-1}\right)^{-\chi^2\ln\ln\delta^{-1}} + \kappa^2\psi^2\left((\psi\rho)^{-1}(\delta)\right) \\ & \asymp \left(\ln\left(\delta^{-1}\right)\right)^{\frac{1}{\beta}-\chi^2\ln\ln\delta^{-1}} + \chi^2\left(\ln\ln\delta^{-1}\right)^2\psi^2\left((\psi\rho)^{-1}(\delta)\right) \end{aligned}$$

which yields the assertion. q.e.d.

Corollary 2.5
Assume that our problem is severely ill-posed with stochastical noise and polynomial behavior of the smoothness index function ψ*. Now choose* $\kappa = 4\ln\ln\delta^{-1}$*.*
Then we have if δ *small enough*

$$\sqrt{\mathbb{E}_\xi||x - x^\delta_{n_*}||^2} \le C\left(\ln\ln\delta^{-1}\right)\psi\left((\psi\rho)^{-1}(\delta)\right)$$

Proof
For a severely ill-posed problem with polynomial ψ we have as seen above

$$\rho^{-1}(\delta) \asymp \left(\frac{\ln\delta^{-1}}{a}\right)^{\frac{1}{\beta}}$$

and

$$\psi\left((\psi\rho)^{-1}(\delta)\right) \asymp \left(\frac{\ln\delta^{-1}}{a}\right)^{-\frac{r}{\beta}}$$

Hence using the fact that from some point onward

$$\ln\ln\delta^{-1} - \frac{1}{\beta} \ge 2\frac{r}{\beta}$$

we get (using $\chi = 1$):

$$\begin{aligned} & \left(\ln\left(\delta^{-1}\right)\right)^{\frac{1}{\beta}-\ln\ln\delta^{-1}} + \left(\ln\ln\delta^{-1}\right)^2\psi^2\left((\psi\rho)^{-1}(\delta)\right) \\ & \asymp \left(\ln\left(\delta^{-1}\right)\right)^{\frac{1}{\beta}-\ln\ln\delta^{-1}} + \left(\ln\ln\delta^{-1}\right)^2\left(\ln\left(\delta^{-1}\right)\right)^{-2\frac{r}{\beta}} \\ & \asymp \left(\ln\ln\delta^{-1}\right)^2\left(\ln\left(\delta^{-1}\right)\right)^{-2\frac{r}{\beta}} \\ & \asymp \left(\ln\ln\delta^{-1}\right)^2\psi^2\left((\psi\rho)^{-1}(\delta)\right) \end{aligned}$$

q.e.d.

Remark
In comparison to the theorem presented in [GP00] *we have replaced the factor* $\ln\delta^{-1}$ *by* $\ln\ln\delta^{-1}$ *which now guarantees convergence. For the other cases (i.e. ordinarily ill-posed with either noise type) we want to refer to* [Bau04, HPS02, MP02].

The Theorem 2.3 and its corollary tell that under certain conditions we just need the error (and error spread) and can obtain a (sometimes even order optimal) regularization procedure. This tells us further that the knowledge of δ is not just necessary as proposed in [Bak84] but also sufficient.

2.6 Regularization without Known Smoothness and Error Behavior

As we have seen the above results still hold even if we introduce an additional parameter χ. Of course, in no-one would like to obstruct our optimal κ by purpose. In practice we neither know the error level δ nor the error spread ρ. Now we will turn our attention on how one can obtain such information. Note that the lemma of Bakushinskii just tells that if we have *one* function as input data we cannot do anything. But in practice it is often possible to do get three sets y_1, y_2 and y of spectral data. (In particular the satellite missions generate enough data to justify such an idea).

So we will try the following ansatz; a more exhaustive discussion can be found in [Bau04]

- Invert the first two data sets, we get the sequences of regularized solutions $(x_{1,n})_{n\in\mathbb{N}}$ and $(x_{2,n})_{n\in\mathbb{N}}$ depending on the input data sets y_1 and y_2.
- Subtract pairwise the two sequences $(x_{1,n} - x_{2,n})_{n\in\mathbb{N}} = (x_{diff,n})_{n\in\mathbb{N}}$. This is now consisting of *pure* error $\delta A_n^+(\xi_1 - \xi_2) = \delta(\eta_n^{\xi_1} - \eta_n^{\xi_2})$.
- As we assumed the error is behaving like $\frac{\delta}{\rho(n)}$ for every $x_n^{diff} = ||x_{diff,n}||$.
- Under some further assumptions on ρ we can estimate the parameters which describe this function. In particular we will show that we can estimate every of these parameters with arbitrary precision.
- We choose the highest possible precision and regularize the third data set y with our resulting estimate for $\frac{\delta}{\rho}$.

For reasons of simplicity we will restrict ourselves to the spectral cut-off scheme as regularization procedure and our geoscientifical case where we exactly know the eigenvalues of the operator and hence ρ.

Now we want to estimate $\frac{\delta}{\rho}$ as good as possible. It is equivalent if we determine the behavior of either $\frac{\delta}{\rho(n)}$ or $\frac{\delta^2}{\rho(n)^2}$ or $\delta^2\widehat{\rho}(n)^2 := \frac{\delta^2}{\rho(n)^2} - \frac{\delta^2}{\rho(n-1)^2}$ because $\frac{\delta}{\rho(n)} = \sqrt{\sum_{i=1}^{n}\delta^2\widehat{\rho}(n)^2}$.

The particular advantage of the last method is that for the spectral cut-off scheme the errors of $(\widehat{x}_n^{diff})^2 := (x_n^{diff})^2 - (x_{n-1}^{diff})^2$ for each n are independent of each other and so do not impose practical difficulties for estimating $\delta\widehat{\rho}(n)$.

Now we assume that $\frac{\delta}{\rho}$ is behaving like $\delta f(k)$ (where f is assumed to be known). This is justified because for our gravity example we have an exact knowledge of the corresponding operator and its eigenvalues. So we get that $\delta\widehat{\rho}$ is behaving like $\delta\widehat{f}(k) = \delta\sqrt{f(k)^2 - f(k-1)^2}$.

This value of δ can now be estimated by standard statistical procedures out of $(\widehat{x}_n^{diff})_{n\in\mathbb{N}}$ with arbitrary precision due to the fact that we assumed that we have an underlying Gaussian random vector. The estimation out of the first n values of $(\widehat{x}_n^{diff})_{n\in\mathbb{N}}$ shall be denoted by δ_n

However, when we work with estimated constants and functions, we automatically get different values for $\frac{4\kappa\delta}{\rho(m)}$ which are just due to the estimation process for ρ, κ, δ and hence influence the optimal regularization point heavily. Therefore we may consider the (multiplicative) difference between the actual and the estimated value exactly as the χ we have artificially introduced in Lemma 2.4.

If we write the estimated version of the various constants and functions with the index n of the corresponding estimate out of the first n values of $(\widehat{x}_n^{diff})_{n\in\mathbb{N}}$ we get the following equation. As we assume within this text ρ to be known exactly we have $\rho_n = \rho$.

$$\frac{4\chi_n(m)\kappa\delta}{\rho(m)} = \frac{4\kappa_n\delta_n}{\rho_n(m)} = \frac{4\kappa_n\delta_n}{\rho(m)}$$

which yields

$$\chi_n(m) = \frac{\frac{4\kappa_n\delta_n}{\rho(m)}}{\frac{4\kappa\delta}{\rho(m)}} = \frac{\kappa_n\delta_n}{\kappa\delta} = \frac{\delta_n \ln\ln\delta_n^{-1}}{\delta\ln\ln\delta^{-1}}$$

Now we have the bound

$$\overline{\chi}_n = \max_{m\in\{1\ldots\max\{N,N_n\}\}} \left\{\chi_n(m),\ \chi_n(m)^{-1}\right\} \le C\max\left\{(\delta/\delta_n)^{1+\varepsilon}, (\delta_n/\delta)^{1+\varepsilon}\right\}$$

where $1 > \varepsilon > 0$ and C an appropriate constant. This yields in particular that we have the following useful inequalities [Bau04]:

Lemma 2.6
For every constant $c_2 > 0$ there exists an n_0 such that for all $n > n_0$ every member $\overline{\chi}_n$ of the sequence $(\overline{\chi}_n)_{n\in\mathbb{N}}$ fulfills for $\tau > 1$:

$$\mathbb{P}_{\xi_1-\xi_2}\{\overline{\chi}_n > \tau\} \le c_1\exp\left(-c_2\left(\tau-1\right)\right)$$

and

$$\mathbb{P}_{\xi_1-\xi_2}\{\overline{\chi}_n^{-1} > \tau\} \le c_1\exp\left(-c_2\left(\tau-1\right)\right)$$

Furthermore c_1 is globally bounded from above.

Using this lemma and the previous result that

$$\mathbb{E}_\xi||x - x_{n_*}^\delta||^2 \le C\left(\ln\left(\delta^{-1}\right)\right)^{\frac{1}{\beta}-\chi^2\ln\ln\delta^{-1}} + C\chi^2\left(\ln\ln\delta^{-1}\right)^2\psi^2\left(\left(\psi\rho\right)^{-1}(\delta)\right)$$

we could show that we actually have [Bau04]:

$$\mathbb{E}_{\xi_1-\xi_2}\left(\mathbb{E}_\xi||x - x_{n_*}^\delta||^2\right) \le \overline{C}\left(\ln\ln\delta^{-1}\right)^2\psi^2\left(\left(\psi\rho\right)^{-1}(\delta)\right)$$

when the approximation of δ and the other variables is sufficiently good. A necessary condition in this proof is that y_1 and y_2 are independent random elements and that $y_1 - y_2$ is independent of y.

Remark
The usage of three different input data sets y_1, y_2 and additionally y in reality is inconvenient and impracticable. However we propose the following way out of this dilemma.
We use the following property of $y := \frac{1}{2}(y_1 + y_2)$:

$$\mathbb{E}\left\langle y_1 - y_2, y\right\rangle = \frac{1}{2}\left(\mathbb{E}||y_1||^2 - \mathbb{E}||y_2||^2\right) = 0$$

because we assumed the same distribution for the y_1 and y_2.
This implies that as long as y_1 and y_2 are biased with Gaussian white noise that y and $y_1 - y_2$ are independent.
In a real situation it would not be sensible to ignore the data sets y_1 and y_2 in order to generate a solution. Because we are dealing with linear problems the computation of $\frac{1}{2}(y_1 + y_2)$ and the corresponding regularized solutions can be done in a negligible time out of the ones of y_1 and y_2. Although the above argument is not rigorous the proposal seems to be the method of choice.

3 Numerics

We have tested our method using simulated satellite data. This has several particular advantages. Its a severely ill-posed problem where we exactly now the degree of ill-posedness as required in our theorems. Furthermore the use of simulated data allows to compute signal to error ratios which will enable us to compare and evaluate the method more easily.

We assumed our data to be given on an integration grid on a sphere. This has the advantage that we do not have to bother about the (ill-posed) problem of transferring data from a satellite track to such a grid and consequently evades several sources of additional error. Furthermore this enables us to study our new methods in an unbiased environment.

3.1 Technical Remarks

As data location we used a Driscoll-Healy grid [May01] at an orbit height of 3% and 6% of the Earth radius which roughly corresponds to an average satellite height of 200 km respectively 400 km. For approximation we used spherical harmonics up to degree 128 and we generated the data globally on a grid which allows exact integration up to degree 180 with a stable Clenshaw algorithm [Dea98]. The model EGM96 was always used as input and reference data. The noise level was chosen in a way such that theoretically the bias to variance ratio had to pass 1.0 around the degree of 80; we used a combination of correlated and uncorrelated noise in the space domain.

As regularization method we chose the spectral cut-off scheme cutting at each degree.

For the noise estimation we generated a small second data set of degrees 8–32 (i.e., about 900 actual data) and compared it with the biased approximation of our noisy data. Note that one could have also used a second noisy approximation. But this would have just increased computation time without giving any mathematical valuable information. We only need to consider more Fourier coefficients to obtain the same accuracy in the estimation (degrees 8–36).

For our purposes we observed that a $\kappa = 0.25$ seems to be a good choice which corresponds (roughly) to an accepted Variance/Bias ratio of 1:1 at the cutting point. After having chosen this parameter we proceeded with our experiment.

3.2 Some Notation and the L-curve method

The given data at satellite height (projected to the space of spherical harmonics to the maximal degree of 128) shall be called d, our regularized solution x and the upward continuation operator A. Hence the size of x gets $||x||_2$ and the error occurring when choosing x gets $||Ax - d||_2$.

The L-curve method now tries to estimate the point, where the curvature of $(||x||_2, ||Ax - d||_2)$ is maximal. As we will see in the next pictures this point is rather hard to obtain, especially because there are a big number of possible points nearby. Within these limitations we want to see our guess for an appropriate regularization parameter using the L-curve method. The point $\circ$ marked in the following pictures could also mark another degree in the range of 35–45 without really changing too much. But this also signified that the choice of the regularization parameter via this method is sometimes made at random. Please note that the same (or even worse) problems occurred when we tried to use a log-log scale for determining the optimal regularization point via the L-curve method.

For a better readability of both the table and the pictures we rescaled the occurring values by a factor of $(10^5, 10^6)$.

The $\frac{\text{Bias}}{\text{Variance}}$ ratio is displayed for each degree of the solution. The optimal regularization point is, where it changes to values greater than 1.

3.3 Data

We present three different representations of the data: a table of data values where we chose the most interesting region due to space restrictions, the L-curves corresponding to our two input data sets and bias/variance behavior where we chose a log scale for better observability.

We displayed the optimal regularization point (i.e., $\frac{bias}{variance} = 1$) by $\bullet$, the regularization point proposed by the L-curve method by $\circ$ and the regularization point found by the auto-regularization method by $*$.

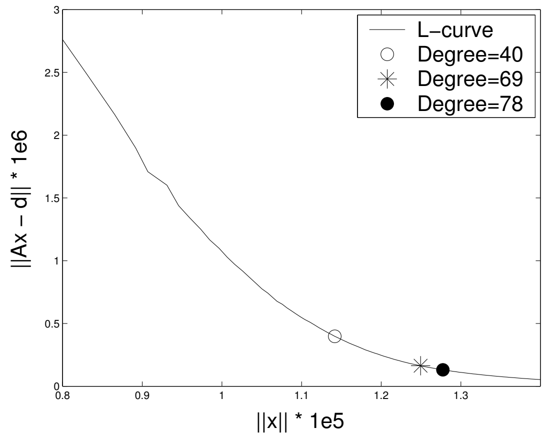


Figure 1: Data set at 200km

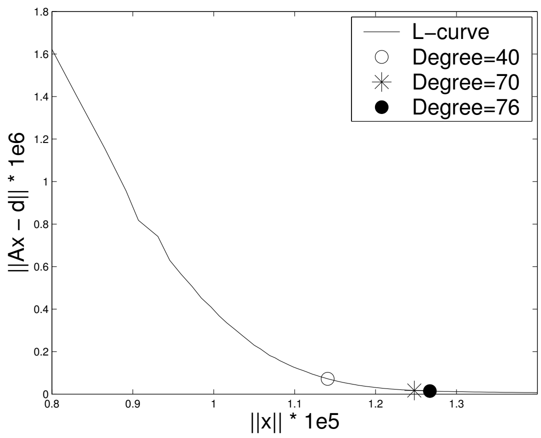


Figure 2: Data set at 400km

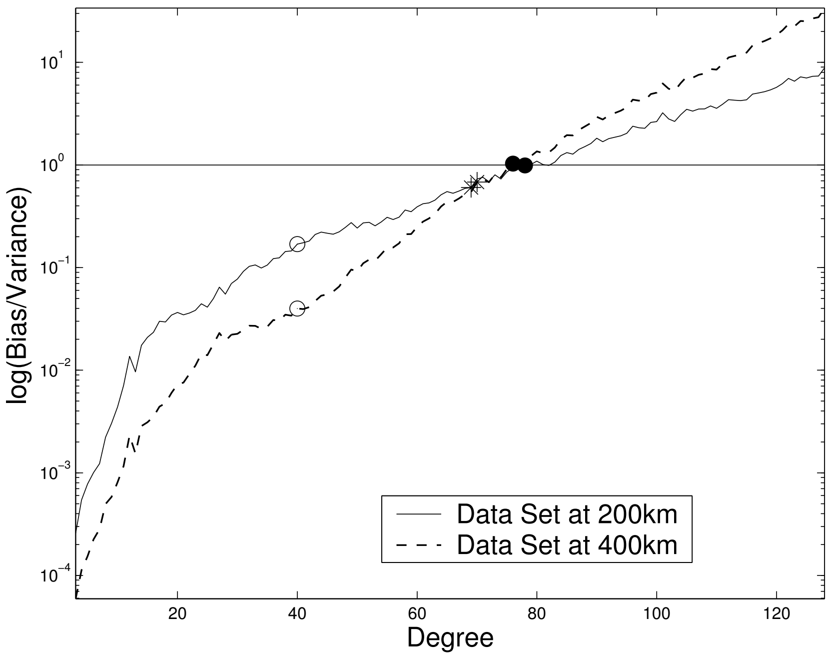


Figure 3: Bias/Variance ratio with respect to the degrees

3.3.1 Discussion

The data above indicate that the auto-regularization method is at least not worse and perhaps even superior to the L-curve method, which itself has been proven to be reliable in a wide

Table 1: Numerical Results

	Data Set 1			Data Set 2		
Degree	$\|\|x\|\|_2$	$\|\|Ax-d\|\|_2$	$\frac{\text{Bias}}{\text{Variance}}$	$\|\|x\|\|_2$	$\|\|Ax-d\|\|_2$	$\frac{\text{Bias}}{\text{Variance}}$
3	0.2970	9.3820	0.0003	0.2970	7.4766	0.0001
4	0.4557	6.6642	0.0005	0.4557	4.9830	0.0001
...	...	...	...	...	...	...
38	1.1321	0.4295	0.1433	1.1315	0.0823	0.0348
39	1.1372	0.4137	0.1452	1.1364	0.0771	0.0340
40	1.1417	0.3977	**0.1695**	1.1408	0.0721	**0.0399**
41	1.1462	0.3840	0.1747	1.1452	0.0679	0.0393
42	1.1508	0.3704	0.1817	1.1498	0.0638	0.0411
43	1.1552	0.3571	0.2100	1.1540	0.0598	0.0472
...	...	...	...	...	...	...
64	1.2335	0.1855	0.5121	1.2300	0.0211	0.3940
65	1.2365	0.1809	0.5500	1.2328	0.0204	0.4376
66	1.2397	0.1766	0.5301	1.2357	0.0197	0.4363
67	1.2429	0.1719	0.5576	1.2388	0.0191	0.4727
68	1.2460	0.1676	0.5925	1.2418	0.0185	0.5192
69	1.2495	0.1634	**0.6020**	1.2451	0.0179	0.5430
70	1.2523	0.1589	0.7311	1.2479	0.0173	**0.6805**
71	1.2553	0.1553	0.7592	1.2510	0.0169	0.7270
72	1.2586	0.1516	0.6886	1.2540	0.0164	0.6788
73	1.2616	0.1477	0.8026	1.2571	0.0159	0.8126
74	1.2648	0.1442	0.7290	1.2607	0.0155	0.7578
75	1.2681	0.1406	0.8573	1.2640	0.0150	0.9144
76	1.2711	0.1371	0.9374	1.2671	0.0146	**1.0299**
77	1.2742	0.1339	0.9501	1.2705	0.0142	1.0720
78	1.2774	0.1307	**0.9901**	1.2739	0.0138	1.1522
79	1.2806	0.1274	1.0123	1.2775	0.0135	1.2194
80	1.2838	0.1244	1.0903	1.2811	0.0131	1.3589
81	1.2872	0.1214	1.0126	1.2849	0.0128	1.3088
82	1.2905	0.1183	0.9891	1.2891	0.0124	1.3241
83	1.2943	0.1153	1.0683	1.2934	0.0121	1.4802
84	1.2976	0.1121	1.2364	1.2977	0.0117	1.7747
85	1.3010	0.1093	1.3210	1.3022	0.0114	1.9532
86	1.3045	0.1066	1.2775	1.3070	0.0111	1.9411
87	1.3080	0.1038	1.4173	1.3120	0.0108	2.1954
...	...	...	...	...	...	...
127	1.5560	0.0049	7.3559	1.9532	0.0005	27.5285
128	1.5666	0.0024	8.8348	1.9936	0.0002	33.8520

number of cases.

Furthermore we have observed that in almost all computations the method was reliable and we got a cutting point in the range of $\frac{bias}{variance} \in [0.5, 1.5]$ for the satellite case.

4 Outlook and General Situations

Now we want to summarize the results of the mathematical part of the article shortly and explain their relevance to satellite missions and other ill-posed problems. We have made the following points:

- It is reasonable to assume that our data in the frequency domain are biased with stochastical noise rather than deterministic noise. Our regularization method has to be suitable for this harder case.
- Out of one set of spectral data one cannot get an optimal regularization. (Lemma of Bakushinskii [Bak84]).
- If one adds some knowledge to one set of spectral data (e.g., error behavior) one can get an optimal regularization.
- Out of two sets of spectral data one can get a reasonable estimate on the overall error and error behavior in the spectral data.
- Using such an error model we obtain a regularization procedure which is asymptotically near to optimal, even under the hard assumption of stochastical noise.

As we have seen in the last section we can guarantee optimal regularization as long as we know the error spread function ρ sufficiently good. However this situation just holds for a very limited number of cases. In general one would like to have the following error spread functions:

$$\frac{\delta}{\rho(k)} = \delta k^{\mu} \exp(ak^{\beta}) f(k)$$

where f is assumed to be known and δ, μ, and a are parameters which need to be estimated. One of us was able to show that even for this very general situation the proposed regularization method works and that we can guarantee the same (up to a constant) speed of convergence as proposed beforehand [Bau04].

However the proofs are lengthy and very technical and therefore we omitted them in this article. Instead we want to propose a scheme for optimal regularization general ill-posed problems.

Please note that the situation is at some point different to the case we discussed in the proofs. We are not really interested in an asymptotically optimal solution but in an actual optimal solution because we do not have a sequence of input data with decreasing error. This means in particular that we should not take the κ which is proposed in the proofs but try to "guess" a good one. Additionally one sometimes does not like to find the point where the signal to noise ratio gets one but wants to stay above. So we end up with the following algorithm for practical applications:

1. Choose a sensible κ.
   (a) Solve the direct problem and add sensible noise.
   (b) Solve the inverse problem and choose a κ which gets a proper regularization point.

2. Generate two data sets of regularized data.

   (a) Partition the input into two data sets y_1 and y_2. It is necessary that the error of these two is as little correlated as possible.

   (b) Generate a solution family for each data set with respect to the (same) chosen regularization family $(A_n)_{n\in\mathbb{N}}$, i.e. $(x_{1,n})_{n\in\mathbb{N}}$ and $(x_{2,n})_{n\in\mathbb{N}}$.

3. Estimate a sensible error spread $\frac{\delta}{\rho}$.

   (a) Subtract the two solution families $(x_{1,n} - x_{2,n})_{n\in\mathbb{N}} = (x_{diff,n})_{n\in\mathbb{N}}$.

   (b) Fit an increasing function for $\frac{\delta}{\rho}$ using standard statistical methods for $x_n^{diff} = ||x_{diff,n}||$.

4. Regularize the data $y = \frac{1}{2}(y_1 + y_2)$, $x_n = A_n^+ y$ with the estimated parameter κ and the fitted error spread $\frac{\delta}{\rho}$ using

$$n_* = \min\left\{n : \ ||x_n - x_m|| \leq 2\kappa\left(\frac{\delta}{\rho(m)} + \frac{\delta}{\rho(n)}\right),\ m > n\right\}$$

The advantages and disadvantages of this procedure (from now on referred as our method) are obvious, especially when one compares it with the competing L-curve method and cross validation.

- Our method requires two independent input data sets, L-curve method and cross validation just one.
- Our method is comparably fast. Due to the necessity to compute two solutions we need double time of the L-curve method but considerably less time compared with cross validation.
- Our method can be automatized and does not require further human interaction, in comparison to the L-curve method, e.g..
- Our method is proven to work (in the mathematical sense!) for a wide number of special cases [Bau04]. This does not hold for the L-curve method and cross validation.

In our opinion our method could get the method of choice as long as one has broad basis of input data which allows the separation into two respectively three independent data sets.

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