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Ill-posed inverse problems and their optimal regularization

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Abstract

The regularization of ill-posed systems of equations is carried out by corrections of the data or the operator. It is shown how the efficiency of regularizations can be calculated by statistical decision principles. The efficiency of nonlinear regularizations depends on the distribution of the admitted disturbances of the data. For the class of linear regularizations optimal corrections are given.

Keywords: Ill-posed problems, regularizations, efficiency, smoothing.

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1 Introduction

If it is not possible to measure certain properties of an object directly and one has to draw conclusions about these properties from indirect observations instead, then this is called an *inverse problem* or *problem of identification*. Denoting the measurable observation by g and the parameters describing the desired properties by φ we model the problem mathematically by a mapping A and write

$$A(\varphi) = g. \quad (1)$$

Let the data g be a deterministic quantity or the realization of a random variable. We require \mathcal{X} and \mathcal{Y} to be topological spaces with $\varphi \in \mathcal{X}$ and $g \in \mathcal{Y}$. Further we assume the operator A to be Frechét differentiable and compact. Our problem now is to determine φ in equation (1). Hadamard introduced the following terminology.

Definition 1.1. The problem (1) is said to be *well-posed* if

- (1) has a solution $\varphi \in \mathcal{X}$ for each $g \in \mathcal{Y}$,
- this solution is unique, and
- this solution depends on g continuously.

If at least one of these conditions is violated, (1) is termed *ill-posed*.

Different kinds of equations can be treated by problem (1). Having $\mathcal{X} \subseteq \mathbb{R}^k$ and $\mathcal{Y} \subseteq \mathbb{R}^n$ then $A(\varphi)$ is a n -vector of components that are functions of the k -dimensional parameter φ . If $A(\varphi) = A\varphi$ is a linear function of φ , then A is a $n \times k$ -matrix and (1) is a linear system of equations. \mathcal{X} or \mathcal{Y} can be function spaces so that parametric or nonparametric problems are included, too. Mostly problem (1) occurs in the setting of differential or integral equations. Also in linear and nonlinear statistics we find such equations.

Many inverse problems turn out to be ill-posed and the "true" solution is objectively not determinable. Then it is necessary to find approximative equations to (1) that are well-posed with calculable solutions. This need arises from deriving stable methods of identification and calculation of the solution of (1). Such *regularizations* of (1) lead to well-posed equations. These often can be reduced to data corrections as

$$A(\varphi) = F(g) \quad . \quad (2)$$

It is the objective of this work to describe the goodness of regularizations and to determine optimal regularizations. We consider an F optimal if disturbances of g lead to as small as possible changes in the solution of equation (2).

We describe the admitted disturbances by a random variable Y with mean g . For the solution $\hat{\varphi}_F$ of $A(\varphi) = F(Y)$ the calculation of the resulting mean squared error

MSE $\hat{\varphi}_F$ enables us to value regularizations F . So we find in linear models optimal linear regularizations \tilde{F} with a minimal MSE $\hat{\varphi}_{\tilde{F}}$. It turns out that optimal regularizations depend essentially on the distribution of Y . Thus the type of disturbance of the data has an influence on the right choice of the regularization. In the special case of linear operators A and F the optimal regularizations depend on the distribution of Y only via the first two moments. From calculations of the efficiency of nonlinear regularizations by using medians one obtains that their goodness differs considerably for normal and double-exponential distributions. So here the chosen family of distributions of Y is substantial, too.

With the exposition in this work it is not intended to describe the regularization of ill-posed problems in general, but to reveal the possibility of an optimal choice of the regularization. Therefore the chosen statistical access is appealing. A similar background for the determination of optimal regularizations is found in the works of Chow/Khasminski (1996) and Khasminski (1996), where the optimal rate of convergence is taken as the basis for the regularization of dynamical inverse problems.

There are many analogies between the regularization of ill-posed problems and descriptive statistical methods. In both fields methods of solution and description are sought that remain insensitive to random distractions. Of the statistical literature especially the papers of Tukey (1977), Mallows (1980a,b), Wahba (1977), Utreras (1981), Läuter/Pincus (1989) and Härdle (1990) are to be mentioned. Here linear methods of smoothing are examined for their optimality and goodness. Some of these results are extended in this paper.

Notations. For an operator A we denote its domain by $\mathcal{D}(A)$, the range by $\mathcal{R}(A) = \{A(\varphi) \mid \varphi \in \mathcal{X}\}$ and the null space by $\mathcal{N}(A)$. Let $\overline{\mathcal{R}(A)}$ be the topological closure of $\mathcal{R}(A)$.

If A is a linear operator, we write A^* for the adjoint and A^+ for the Moore-Penrose inverse operator. $P_{\mathcal{L}}$ stands for the orthogonal projection onto the closed space \mathcal{L} . We always require \mathcal{X} and \mathcal{Y} to be separable Hilbert spaces with inner products (\cdot, \cdot) and norms $\|\cdot\|$ respectively.

2 Methods of regularization

The starting point of the following considerations is the relation

$$A(\varphi) = g, \varphi \in \mathcal{X}, g \in \mathcal{Y} \quad (3)$$

where a solution $\varphi_g \in \mathcal{X}$ is sought for arbitrary $g \in \mathcal{Y}$. Ill-posedness in this setting means that either

$$\mathcal{Y} \not\subseteq \mathcal{R}(A)$$

holds or

$\mathcal{Y} \subseteq \mathcal{R}(A)$ and there exists a $\tilde{g} \in \mathcal{Y}$ such that the map $g \mapsto \varphi_g$ is not continuous at \tilde{g} .

The second case includes the possibility that the solution is not unique. Sometimes an ill-posed problem may be transformed into a well-posed one by choosing an extension $\mathcal{X}' \supseteq \mathcal{X}$ and a restriction $\mathcal{Y}' \subseteq \mathcal{Y}$ such that the problem

$$A(\varphi) = g, \quad \varphi \in \mathcal{X}', \quad g \in \mathcal{Y}'$$

is well-posed. This is often possible, but there are more general constructions that in the following will be called regularizations by correction of the data or of the operator.

2.1 Regularization by data correction

If one wants to transform an ill-posed relation (3) by approximation of the equation into a well-posed problem, then the choice of a map $F : \mathcal{Y} \rightarrow \mathcal{R}(A)$ and the solution of the equation

$$A(\varphi) = F(g), \quad \varphi \in \mathcal{X}, \quad g \in \mathcal{Y} \tag{4}$$

must be considered.

Definition 2.1. Let $F : \mathcal{Y} \rightarrow \mathcal{R}(A)$ be a continuous operator such that

$$A(\varphi) = F(g), \quad \varphi \in \mathcal{X}, \quad g \in \mathcal{Y} \tag{5}$$

is well-posed. Then (5) is called a *regularization by data correction*.

Such regularizations are often used according to suitable interpretations. So one thinks of smoothing or projection when changing from g to $F(g)$. For characterization of the admitted transformations let \mathcal{S}_R and \mathcal{S}_E be subsets of \mathcal{Y} such that for positive constants c_1, c_2 with $c_2 < c_1$ it holds

$$F(\mathcal{S}_R) \subseteq \mathcal{S}_R \quad \text{and} \quad \|F(g)\| \geq c_1 \|g\| \quad \text{for all } g \in \mathcal{S}_R, \tag{6}$$

$$\|F(g)\| \leq c_2 \|g\| \quad \text{for all } g \in \mathcal{S}_E. \tag{7}$$

Here \mathcal{S}_R describes a subset of \mathcal{Y} that is mapped into itself by F , or in other words, that is reproduced. The case $F(g) = g$ for all $g \in \mathcal{S}_R$ has a special meaning here. The elements of \mathcal{S}_E are functions that are almost eliminated by F . For example one can think of \mathcal{S}_R as a set of low-frequency or monotone functions and of \mathcal{S}_E as high-frequency signals. Now we consider some special cases.

2.1.1 Projection of the data

Let A be a linear operator and $\mathcal{S}_R = \overline{\mathcal{R}(A)}$. With $F = P_{\overline{\mathcal{R}(A)}}$ equation (5) then becomes

$$A\varphi = P_{\overline{\mathcal{R}(A)}}g. \quad (8)$$

Theorem 2.1. *Problem (8) is well-posed if $\mathcal{X} = \mathcal{R}(A^*)$, and if the generalized inverse A^+ is bounded in \mathcal{Y} , i.e. if there exists a constant $c > 0$ with*

$$\|A^+g\| \leq c\|g\| \text{ for all } g \in \mathcal{Y} \quad (9)$$

Proof. A solution of (8) in $\mathcal{R}(A^*)$ is a solution of the equivalent equation

$$A^*A\varphi = A^*g$$

and this is $\varphi_g = A^+g$. It follows from (9) that g lies in the domain of A^+ . Also from (9) one deduces the continuous dependence of φ_g on g . \square

The main assumption in this theorem is (9), which amounts to a serious restriction on \mathcal{Y} if A^+ is an unbounded operator. Herefore, let λ_j be the eigenvalues of AA^* with eigenvectors u_j respectively. Further denote by e_j the eigenvectors of A^*A belonging to λ_j , then we can write

$$\varphi_g = \sum_{\lambda_j > 0} \lambda_j^{-\frac{1}{2}} e_j(u_j, g).$$

From this follows

$$\|\varphi_g\|^2 = \sum_{\lambda_j > 0} \lambda_j^{-1} (u_j, g)^2$$

and this norm is finite if (9) holds, that is if

$$\sum_{\lambda_j > 0} \lambda_j^{-1} (u_j, g)^2 \leq c^2 \|g\|^2. \quad (10)$$

This means that for $\lambda_j \rightarrow 0$ the Fourier coefficients (u_j, g) must converge to zero fast enough, that is g has to be necessarily smooth compared to the operator A . If $\{\lambda_j^{-1}\}$ is bounded, then (10) is no restriction. In Louis (1989), as an example for the linear equation $A\varphi = g$, one finds the integral equation of the first kind

$$A\varphi(x) = \int_0^x \varphi(\xi) d\xi \quad (11)$$

for $\mathcal{X} = \mathcal{Y} = L_2(0, 1)$. The problem

$$\int_0^x \varphi(\xi) d\xi = g(x), \quad x \in [0, 1] \quad (12)$$

is ill-posed. Here we have $\lambda_j = [(j + \frac{1}{2})\pi]^{-2}$ and $u_j(x) = \sqrt{2} \sin((j + \frac{1}{2})\pi x)$ and thus (10) becomes

$$\sum_j \lambda_j^{-1} \left(\int_0^1 u_j(\xi) g(\xi) d\xi \right)^2 \leq c^2 \int_0^1 g^2(\xi) d\xi \quad .$$

This inequality holds if the Fourier coefficients $\int_0^1 u_j(\xi) g(\xi) d\xi$ are sufficiently small. As a remark, note that equation (8) will be solved when a least squares solution of (3) is calculated, or equivalently, if a $\hat{\varphi}$ minimizing $\|A\varphi - g\|^2$ is determined.

2.1.2 Linear smoothing of the data

Often the regularization consists in smoothing the data. Here the regularization F is defined by

$$(Fg)(x) = \int K(x, t) g(t) dt \quad (13)$$

with a suitably chosen kernel $K(x, t)$. The properties of the chosen kernel K have an influence on the properties of the smoothed data Fg . For the integral equation (12) the kernel must satisfy

$$\int_0^1 K(0, t) g(t) dt = 0$$

such that

$$\int_0^1 K(x, t) g(t) dt \text{ is absolutely continuous.}$$

A large class of linear smoothers is described by (13).

The choice of $K(x, t)$ determines the sets \mathcal{S}_R and \mathcal{S}_E . According to the preceding remarks \mathcal{S}_R and \mathcal{S}_E can be chosen as the spaces spanned by the eigenfunctions of F belonging to the largest or smallest eigenvalues respectively. On the other hand, for given sets \mathcal{S}_R and \mathcal{S}_E a kernel K can be found such that (6) and (7) are fulfilled.

2.1.3 Nonlinear smoothing of the data

Linear smoothing is not appropriate for the elimination of rough errors in the data. For this a well suited class of nonlinear smoothers is given by the *median smoothers*. Let (3) be given by

$$a(t_i, \varphi) = g(t_i), \quad i = 1, 2, \dots \quad (14)$$

for real-valued $g(t_i)$ and $t_i \leq t_{i+1}$ for all i . We now say that \tilde{g} emerges from g by median smoothing if

$$\tilde{g}(t_j) = \text{med}(g(t_{j-1}), g(t_j), g(t_{j+1})), \quad j = 2, \dots \quad (15)$$

and $\tilde{g}(t_1) = g(t_1)$ is defined. If $i = 1, \dots, J$ is only taken from a finite index set, we set $\tilde{g}(t_J) = g(t_J)$. More generally we speak of k -median smoothing if instead of (15)

$$\tilde{g}(t_j) = \text{med}(g(t_{j-k}), \dots, g(t_{j+k})), \quad j = k+1, \dots$$

is defined. Again the smoothing in the beginning and the end of the index set must be defined additionally.

Tightly connected with this is the median smoothing of the ε -closest neighbors. If (14) is given and the t_i are not necessarily ordered, then any closed sphere $U_\varepsilon(t_j)$ around t_j with radius ε shall contain at most finitely many of the other points t_i . Under this condition \tilde{g} is called *median smoothing of the ε -closest neighbors* if

$$\tilde{g}(t_j) = \text{med}\{g(t_i) \mid t_i \in U_\varepsilon(t_j)\}.$$

If now $A(\varphi) = \tilde{g}$ is a well-posed problem, this regularized equation will be solved. If not, another transformation F_1 of the data \tilde{g} must be defined such that $A(\varphi) = F(g)$ with $F(g) = F_1(\tilde{g})$ is well-posed. In any case F is now nonlinear since the median smoothing is so. The sets \mathcal{S}_R and \mathcal{S}_E depend on the median smoothing and on F_1 . For this nonlinear k -median smoothing monotone functions g are invariant since then $\tilde{g}(t_i) = g(t_i)$ always holds.

2.2 Regularization by operator correction

Another possibility for the regularization of (3) consists in a substitution of the operator A by \tilde{A} .

Definition 2.2. Let $\tilde{A} : \mathcal{X} \rightarrow \mathcal{Y}$ be an operator such that

$$\tilde{A}(\varphi) = g \tag{16}$$

is a well-posed problem. Such an approximation of equation (3) is called *regularization by operator correction*.

An \tilde{A} can be constructed in different manners.

Lemma 2.2. *Let $\tilde{A} : \mathcal{X} \rightarrow \mathcal{Y}$ be an operator with the Frechét derivative \tilde{H}_φ in $\varphi \in \mathcal{X}$. If $(\tilde{H}_\varphi^* \tilde{H}_\varphi)^{-1}$ is for every $\varphi \in \mathcal{X}$ a bounded operator, and if (16) has for every g exactly one solution, then the solution of $\tilde{A}(\varphi) = g$ depends on g continuously.*

Proof. By assumption we have in a neighborhood of an arbitrary but fixed $\varphi_0 \in \mathcal{X}$

$$\tilde{A}(\varphi) - \tilde{A}(\varphi_0) = \tilde{H}_{\varphi_0}(\varphi - \varphi_0) + o(\|\varphi - \varphi_0\|). \tag{17}$$

Hence

$$\|\tilde{A}(\varphi) - \tilde{A}(\varphi_0)\|^2 = \left(\varphi - \varphi_0, \tilde{H}_{\varphi_0}^* \tilde{H}_{\varphi_0}(\varphi - \varphi_0) \right) + o(\|\varphi - \varphi_0\|).$$

Since $\tilde{H}_{\varphi_0}^* \tilde{H}_{\varphi_0}$ has a bounded inverse and is linear and self-adjoint the statement follows. \square

With the help of this lemma a Tichonov operator correction can be constructed the following way: Let \tilde{A} be an operator whose Frechét derivative \tilde{H}_φ is a linear operator satisfying

$$H_\varphi^* H_\varphi \leq \tilde{H}_\varphi^* \tilde{H}_\varphi \quad \text{and} \quad \left(\tilde{H}_\varphi^* \tilde{H}_\varphi \right)^{-1} \text{ is bounded}$$

for all $\varphi \in \mathcal{X}$, where H_φ denotes the Frechét derivative of the original operator A . By the lemma the solutions of (16) depend continuously on g . The transfer from $A(\varphi) = g$ to $\tilde{A}(\varphi) = g$ is a *Tichonov regularization*. A frequently used construction of \tilde{H}_φ proceeds by

$$\tilde{H}_\varphi^* \tilde{H}_\varphi = H_\varphi^* H_\varphi + \kappa I, \quad \kappa > 0,$$

for the identity I .

2.3 Regularization by data and operator correction

Both proceeding methods of regularization can be combined in a straightforward manner.

Definition 2.3. Let $\tilde{A} : \mathcal{X} \rightarrow \mathcal{Y}$ be an operator and $F : \mathcal{Y} \rightarrow \mathcal{Y}$ a continuous mapping such that

$$\tilde{A}(\varphi) = F(g) \tag{18}$$

is a well-posed problem. Such an approximation of equation (3) is called *regularization by data and operator correction*.

Since \tilde{A} and F can be chosen in various ways this regularization, too, is only reasonable with concrete requirements on the solution and the special model. The best known example for such a regularization in a linear model, that is A linear, is the Tichonov regularization. The equation $A(\varphi) = g$ leads to

$$A^* A \varphi = A^* g \quad .$$

If here $A^* A$ is ill-conditioned, then one uses the regularized equation

$$(A^* A + B) \varphi = A^* g \tag{19}$$

with a self-adjoint linear operator B such that $(A^* A + B)^{-1}$ is bounded. If \tilde{A} is a linear operator with $\tilde{A}^* \tilde{A} = A^* A + B$, then (19) is of the form (18).

In regression one meets this type of formula in connection with the Ridge regression. The Tichonov regularization can be viewed as a regularization by data and operator correction. But easily one sees that (19) can be interpreted as a regularization by data correction only, since it is equivalent to

$$A \varphi = A(A^* A + B)^{-1} A^* g \quad .$$

For any regularization the question arises how good it works and if an optimal regularization exists.

2.4 Ill-posed and numerically stable problems

If an equation $A(\varphi) = g$ is uniquely soluble but the solution φ_g does not depend on g continuously, then the problem is ill-posed. The discontinuity can be viewed as a limiting case of a numerical instability in $A(\varphi) = g$. Here we call $A(\varphi) = g$ numerically instable of size ρ if g and \tilde{g} , $g \neq \tilde{g}$ exist with

$$\|\varphi_g - \varphi_{\tilde{g}}\| \geq \rho \|g - \tilde{g}\| \quad .$$

Problems with $\rho \geq 10^3$ are often difficult to solve numerically. The discontinuity would belong to $\rho = \infty$.

Example. *Growth curves*

Let $\varphi = (\alpha, \beta\gamma)$ and

$$a(t, \varphi) = \frac{\alpha}{1 + \beta e^{-\alpha\gamma t}} \quad , \quad 0 \leq t \leq 2.5 \quad .$$

Setting $\varphi_1 = (7.68, 3.68, -1.095)$, $\varphi_2 = (231271, 142711.7, -0.941)$, it results for $0 \leq t \leq 2.5$:

$$\frac{|\varphi_1 - \varphi_2|}{|a(t, \varphi_1) - a(t, \varphi_2)|} \geq 5.4 \cdot 10^6 \quad .$$

In this case $\rho \geq 5.4 \cdot 10^6$ so that these growth curves must be considered numerically instable. \diamond

We recognize numerical instability if $\frac{\partial}{\partial \varphi} a(t, \varphi) \rightarrow 0$ for $\|\varphi\| \rightarrow \infty$. With $A^{(n)}(\varphi) = (a(t_1, \varphi), \dots, a(t_n, \varphi))^*$ and if $G^{(n)}(\varphi) := \frac{\partial}{\partial \varphi} A^{(n)}(\varphi)$ exists, the ill-conditionedness of $G^{(n)}(\varphi)^* G^{(n)}(\varphi)$ is the reason for the instability.

The numerical instability discussed here is, as a qualitative property, similar to the discontinuity of the solution, so that the regularization of ill-posed problems causes a higher numerical stability as well.

3 Optimal regularization

Two types of models for (1) are considered now that are not completely disjoint from each other but include different features. We admit deviations in the right hand side, which we describe by a probability law. We assume that g is disturbed additively by the errors, so that instead of $A(\varphi) = g$ the equation

$$A(\varphi) = g + \varepsilon \tag{20}$$

is to solve. The solutions $\varphi_{g+\varepsilon}$ then should lie as close as possible to φ_g .

Model I In (1) let $g \in \mathcal{Y}$ and A be an operator mapping into the Hilbert space \mathcal{Y} . Let g be disturbed additively by the random variable ε , whose realizations lie in \mathcal{Y} . It is

$$\mathbb{E}(\varepsilon) = 0 \text{ and } \text{Var } \varepsilon = \sigma^2 W$$

for a known positive definite linear operator W . The admitted deviations of the right hand side are described by ε .

Model II Equation (1) can be written equivalently as

$$a(t_i, \varphi) = g_i, \quad i = 1, 2, \dots \quad (21)$$

for design points t_1, t_2, \dots . The given admitted deviations in the data are described by additive disturbances ε_i . We assume that the ε_i are random variables with $\mathbb{E}(\varepsilon_i) = 0$ and equation (20) now corresponds to

$$a(t_i, \varphi) = g_i + \varepsilon_i, \quad i = 1, 2, \dots \quad (22)$$

We write the first n equations in (22) using the n -dimensional vector notation as

$$A^{(n)}(\varphi) = Y^{(n)} := g^{(n)} + \varepsilon^{(n)}.$$

The models I and II show many analogies. But while in model II the ε_i can be independent and identically distributed, for example, and so have a covariance matrix $\sigma^2 I_n$, in model I the covariance of ε always differs from $\sigma^2 I_n$, since we assumed the realizations of ε to lie in the Hilbert space \mathcal{Y} . It is essential in both models that the admitted deviations in the data, with respect to which the solutions should be stable, are described by ε and ε_i respectively.

3.1 Optimal regularizations in model I

Regularizations by data correction of equation (20) have the form

$$A(\varphi) = F(Y) \quad (23)$$

for a continuous operator F on $\{g + \varepsilon(\omega) \mid g \in \mathcal{Y}, \omega \in \Omega\}$. Since Y is random the solution of (23) becomes a random variable denoted by $\hat{\varphi}_F$. The aim now is to determine an operator F such that $\hat{\varphi}_F$ comes as close as possible to φ_g in the mean. The mean squared deviation of $\hat{\varphi}_F$ from φ_g is that linear operator $\text{MSE } \hat{\varphi}_F$ satisfying

$$(\varphi, (\text{MSE } \hat{\varphi}_F) \tilde{\varphi}) = \mathbb{E} \{ (\varphi, \hat{\varphi}_F - \varphi_g)(\tilde{\varphi}, \hat{\varphi}_F - \varphi_g) \} \quad (24)$$

for any $\varphi, \tilde{\varphi} \in \mathcal{X}$. Let Q be a nonnegative functional that is defined on the set of operators $\text{MSE } \hat{\varphi}_F$, $F \in \mathcal{F}$, for a set of admitted regularizations \mathcal{F} .

Definition 3.1. a) $\hat{F} \in \mathcal{F}$ is called an *optimal regularization* if

$$Q(\text{MSE } \hat{\varphi}_{\hat{F}}) = \inf_{f \in \mathcal{F}} Q(\text{MSE } \hat{\varphi}_F) .$$

b) The relative efficiency of F with respect to $F_1 \in \mathcal{F}$ is

$$\text{eff}(F, F_1) = \frac{Q(\text{MSE } \hat{\varphi}_{F_1})}{Q(\text{MSE } \hat{\varphi}_F)} .$$

It will turn out that an optimal regularization is determined by the operator A , the distribution of Y , the operator F and by Q . In general the whole distribution of the distraction ε is important here. In linear models - that is a linear operator A and a linear regularization F - from the distribution of Y only the first two moments determine the efficiency of F .

3.1.1 Linear models and linear regularizations

We consider equation (23) for linear bounded operators A and F , that is

$$A\varphi = FY , \quad (25)$$

and assume that F is chosen such that (25) is well-posed. Let $\text{Var } Y = \sigma^2 W$ be the covariance operator of Y with a known Hilbert-Schmidt operator W and an unknown factor σ^2 . Assuming $A^+FW^{1/2}$ to be bounded it follows that $\hat{\varphi}_F = (A^*A)^{-1}A^*FY$ is a solution of (25). If $A^+FA\varphi_g \in \mathcal{X}$ then

$$\begin{aligned} \mathbb{E}(\hat{\varphi}_F) &= (A^*A)^{-1}A^*FA\varphi_g , \\ \text{Var } \hat{\varphi}_F &= \sigma^2(A^*A)^{-1}A^*FWF^*A(A^*A)^{-1} \end{aligned}$$

and thus

$$\text{MSE } \hat{\varphi}_F = (A^*A)^{-1}A^*[\sigma^2FWF^* + (F - I)A\varphi_g\varphi_g^*A^*(F^* - I)]A(A^*A)^{-1} . \quad (26)$$

This representation makes clear that an optimal regularization depends on the distribution of Y only via the first two moments.

Let B be a self-adjoint linear operator on \mathcal{X} , ρ_* a given constant and μ a measure on \mathcal{X} with

$$\mu\{\varphi \mid \varphi^*B\varphi \leq \sigma^2\rho_*^2\} = 1 \quad \text{and} \quad \int_{\varphi^*B\varphi \leq \sigma^2\rho_*^2} \varphi\varphi^*\mu(d\varphi) = \sigma^2\rho^2C \quad (27)$$

for a fixed linear self-adjoint operator C .

With (27) we calculate for the averaged risk

$$\begin{aligned} \int_{\varphi^*B\varphi \leq \sigma^2\rho_*^2} \text{MSE } \hat{\varphi}_F \mu(d\varphi_g) &= \\ &= (A^*A)^{-1}A^*[\sigma^2FWF^* + \sigma^2\rho^2(F - I)ACA^*(F^* - I)]A(A^*A)^{-1} . \end{aligned}$$

Defining $Q(\text{MSE } \hat{\varphi}_F) = \int_{\varphi_g^* B \varphi_g \leq \sigma^2 \rho_*^2} \text{MSE } \hat{\varphi}_F \mu(d\varphi_g)$ one obtains

$$Q(\text{MSE } \hat{\varphi}_F) = \sigma^2 \left[(A^* A)^{-1} A^* [F W F^* + \rho^2 (F - I) A C A^* (F^* - I)] A (A^* A)^{-1} \right]. \quad (28)$$

Let \mathcal{S}_R and \mathcal{S}_E be given linear spaces in $\mathcal{R}(W^{1/2}) \oplus \mathcal{N}(W)$. We denote the set of all linear operators F with

$$A^+ F W^{1/2} \text{ is bounded, } A^+ F g \in \mathcal{X} \text{ for } g \in \mathcal{R}(W^{1/2}) \oplus \mathcal{N}(W),$$

$$F g = g \text{ for all } g \in \mathcal{S}_R \text{ and } F g = 0 \text{ for all } g \in \mathcal{S}_E$$

by \mathcal{F} . Further we write P_R and P_E for the orthogonal projections onto \mathcal{S}_R and \mathcal{S}_E respectively.

For describing an optimal regularization, we denote $D = W + \rho^2 A C A^*$, $\mathcal{L} = (\mathcal{S}_R \oplus \mathcal{S}_E)^\perp$ and $\mathcal{K} = \mathcal{R}(D^{\frac{1}{2}} P_{\mathcal{L}})$.

The next theorem shows how an optimal regularization can be constructed from a given regularization $F \in \mathcal{F}$.

Theorem 3.1. *The operator*

$$\tilde{F} = F - P_{\overline{\mathcal{R}(A)}}(F D - \rho^2 A C A^*) D^{-\frac{1}{2}} P_{\mathcal{K}} D^{-\frac{1}{2}} \quad (29)$$

for any $F \in \mathcal{F}$ is an optimal regularization within \mathcal{F} .

Proof. With $F \in \mathcal{F}$ we have $\tilde{F} \in \mathcal{F}$ for \tilde{F} in (29) because $P_{\mathcal{K}} D^{-\frac{1}{2}} P_R = 0$, $P_{\mathcal{K}} D^{-\frac{1}{2}} P_E = 0$. We get for any H with $\tilde{F} + H \in \mathcal{F}$

$$\begin{aligned} Q(\text{MSE}_{\tilde{F}+H}) &= Q(\text{MSE}_{\tilde{F}}) + \sigma^2 A^+ H D H^* A^{+*} + \\ &+ \sigma^2 A^+ H [D \tilde{F}^* - \rho^2 A C A^*] A^{+*} + \sigma^2 A^+ [\tilde{F} D - \rho^2 A C A^*] H^* A^{+*}. \end{aligned} \quad (30)$$

Using $D^{-\frac{1}{2}} P_{\mathcal{K}} D^{-\frac{1}{2}} D P_{\mathcal{L}} = P_{\mathcal{L}}$ we compute

$$P_{\overline{\mathcal{R}(A)}}(\tilde{F} D - \rho^2 A C A^*) P_{\mathcal{L}} = 0. \quad (31)$$

From $\tilde{F}, \tilde{F} + H \in \mathcal{F}$ follow $H P_R = 0$ and $H P_E = 0$ which means that $H^* = P_{\mathcal{L}} H^*$ holds. So we get from (31) $A^+ [\tilde{F} D - \rho^2 A C A^*] H^* = 0$ and we obtain from (30)

$$Q(\text{MSE}_{\tilde{F}+H}) = Q(\text{MSE}_{\tilde{F}}) + \sigma^2 A^+ H D H^* A^{+*}$$

for any H with $\tilde{F} + H \in \mathcal{F}$. Any $G \in \mathcal{F}$ can be represented in this form $G = \tilde{F} + H$ and so the assertion is proved. \square

Conclusion 3.2. *If especially $\mathcal{S}_E = \{0\}$ and $I \in \mathcal{F}$, then*

$$\tilde{F} = I - P_{\overline{\mathcal{R}(A)}} D^{-\frac{1}{2}} P_{\mathcal{K}} D^{-\frac{1}{2}} \quad (32)$$

is an optimal regularization.

Proof. This follows from theorem 3.1 with the possible choice $F = I \in \mathcal{F}$. \square

3.1.2 Nonlinear regularizations

We already mentioned that linear regularizations are not well suited for the elimination of rough errors in the data. But it turns out that for nonlinear regularizations no explicit expressions for the optimal regularizations are obtainable. In the following example we consider median smoothing and show how the efficiency of regularizations in simple models of the estimation of the mean is calculated.

Example. In the model $(\mathcal{X} = \mathbb{R}^1, \mathcal{Y} = \mathbb{R}^n)$, $Y = (Y_1, \dots, Y_n)'$ and

$$Y_i = \varphi + \varepsilon_i, \quad i = 1, \dots, n \quad (33)$$

φ is to be estimated. Here $\mathbf{1} = (1, \dots, 1)'$ is an n -vector. $\varepsilon_1, \dots, \varepsilon_n$ are independent and identically distributed. Equation (23) has the form

$$\varphi \cdot \mathbf{1} = F(Y), \quad (34)$$

the solution $\hat{\varphi}_F$ is one-dimensional, and

$$\text{MSE } \hat{\varphi}_F = \mathbb{E}(\hat{\varphi}_F - \varphi)^2.$$

Let $Q(a) = a$ for all $a \geq 0$.

a) Let $\varepsilon \sim \mathcal{N}(0, \sigma^2)$. Then $\hat{\varphi} = \bar{Y} = \frac{1}{n} \sum_{i=1}^n Y_i$ is the maximum likelihood estimation which is asymptotically optimal and a best unbiased estimation for φ . Also $\hat{\varphi}$ is a solution of (34) for $F(Y) = F_1(Y) = \bar{Y} \cdot \mathbf{1}$ and thus the regularization belonging to $\hat{\varphi}$ is the arithmetic average.

b) Let $Y_i + \varepsilon_i$ be distributed by the double exponential law with the density

$$h(y_i) = e^{-|y_i - \varphi|}.$$

Then $\tilde{\varphi} = \text{med}(Y_1, \dots, Y_n)$ is the asymptotically optimal maximum likelihood estimation. Also $\tilde{\varphi}$ is a solution of (34) for $F(Y) = F_2(Y) = \text{med}(Y_1, \dots, Y_n) \cdot \mathbf{1}$ and thus the regularization belonging to $\tilde{\varphi}$ is the median.

◇

In the next example we show which loss or gain in efficiency the median causes as a method of regularization. Here we use results from Lauter/Pincus (1989).

Example. We consider the model (33) and as a regularization we take the median smoothing :

$$F_3(Y) = \frac{1}{n} \sum_{i=1}^n U_i \cdot \mathbf{1} \quad \text{for } U_i = \text{med}(Y_{i-1}, Y_i, Y_{i+1}), \quad i = 2, \dots, n-1,$$

$$U_1 = U_n = \frac{1}{n-2} \sum_{i=2}^{n-1} U_i.$$

If G is the distribution of the Y_i , then the U_2, \dots, U_{n-1} are distributed identically and have the distribution $H(u) = 3G^2(u - \varphi) - 2G^3(u - \varphi)$. Whereas Y_1, \dots, Y_n are independent from each other this is not valid anymore for U_2, \dots, U_{n-1} . The setting of the initial and final values U_1 and U_n assures $\frac{1}{n} \sum_{i=1}^n U_i = \frac{1}{n-2} \sum_{i=2}^{n-1} U_i$ to hold so that by the regularization a reduction to a $(n-2)$ -dimensional model has happened. We obtain $\hat{\varphi}_{F_3} = \frac{1}{n-2} \sum_{i=2}^{n-1} U_i$. If $Y_i \sim \mathbf{N}(\varphi, \sigma^2)$, we get

$$\mathbf{E} \hat{\varphi}_{F_3} = \varphi, \quad \mathbf{Var} \hat{\varphi}_{F_3} = \frac{1.181n - 3.33}{(n-2)^2} \sigma^2.$$

If the Y_i are distributed double exponentially, we have

$$\mathbf{E} \hat{\varphi}_{F_3} = \varphi, \quad \mathbf{Var} \hat{\varphi}_{F_3} = \frac{0.775n - 2.16}{(n-2)^2} \sigma^2.$$

Since for the least squares estimation $\hat{\varphi}$ in (33) it holds $\mathbf{E} \hat{\varphi} = \varphi$ and $\mathbf{Var} \hat{\varphi} = \frac{1}{n} \sigma^2$ in both cases, we obtain for the relative efficiency of F_3 with respect to F_1 the following values :

$$\begin{aligned} \text{eff}^N(n) &:= \frac{(n-2)^2}{n(1.181n - 3.33)} && \text{(normal distribution)} \\ \text{eff}^{DE}(n) &:= \frac{(n-2)^2}{n(0.775n - 2.16)} && \text{(double exponential distribution)} \end{aligned}$$

Table 1: Efficiency of median smoothing for normal and double exponential distributions

n	5	10	20	50	100	∞
eff^N	.699	.755	.798	.827	.837	.847
eff^{DE}	1.05	1.14	1.21	1.26	1.27	1.29

Consequently, under normal distribution $\hat{\varphi}$ performs always better than $\hat{\varphi}_{F_3}$, and vice versa under double exponential distribution. \diamond

This example stands as a pattern for the questions that arise about regularizations. For being able to chose a proper regularization one has to know the model and, especially, the distribution of the variables.

3.2 Optimal regularizations in model II

Starting from model (22)

$$a(t_i, \varphi) = g_i + \varepsilon_i, \quad i = 1, 2, \dots,$$

or equivalently in n -dimensional vector notation as

$$A^{(n)}(\varphi) = Y^{(n)}, \quad (35)$$

the regularizations by data correction have the form

$$A^{(n)}(\varphi) = F^{(n)}(Y^{(n)}) \quad . \quad (36)$$

Here we consider $\mathcal{X} = \mathbb{R}^k$ only. For fixed n we can use the concepts of section 3.1 without change. Hence here we are interested mainly in statements on the solutions for $n \rightarrow \infty$. One of the properties of interest is the consistency of regularizations.

Definition 3.2. A sequence of regularizations $\{F^{(n)}\}$ is called *consistent* if the solutions of (36) converge weakly to the solution φ_g of (21).

It comes out that the consistency of regularizations is determined by the model and the design t_1, t_2, \dots (compare Auert/Läuter (1982)).

Theorem 3.3. *Let the linear equation*

$$A^{(n)}\varphi = g^{(n)}$$

be soluble for all n and assume $(A^{(n)}A^{(n)})^{-1} \rightarrow 0_{k \times k}$. Assuming $\mathbb{E} Y^{(n)} = g^{(n)}$, $\text{Var} Y^{(n)} = \sigma^2 I_n$. If the solutions of $A^{(n)}\varphi = F^{(n)}Y^{(n)}$ are asymptotically unbiased, and if $F^{(n)}F^{(n)*} \leq m \cdot I_n$ for a constant m , then $\{F^{(n)}\}$ is consistent.*

Proof. The solution $\hat{\varphi}_{F^{(n)}}$ of $A^{(n)}\varphi = F^{(n)}Y^{(n)}$ has the form

$$\hat{\varphi}_{F^{(n)}} = (A^{(n)*}A^{(n)})^{-1}A^{(n)*}F^{(n)}Y^{(n)}$$

and thus

$$\begin{aligned} \mathbb{E} \hat{\varphi}_{F^{(n)}} &= (A^{(n)*}A^{(n)})^{-1}A^{(n)*}F^{(n)}A^{(n)}\varphi_g^{(n)}, \\ \text{Var} \hat{\varphi}_{F^{(n)}} &= \sigma^2 (A^{(n)*}A^{(n)})^{-1}A^{(n)*}F^{(n)}F^{(n)*}A^{(n)}(A^{(n)*}A^{(n)})^{-1}. \end{aligned}$$

Because of $F^{(n)}F^{(n)*} \leq m \cdot I_n$ one obtains

$$\text{Var} \hat{\varphi}_{F^{(n)}} \leq m\sigma^2 (A^{(n)*}A^{(n)})^{-1}.$$

Together with $\mathbb{E} \hat{\varphi}_{F^{(n)}} \xrightarrow{p} \varphi$ the statement follows from this. \square

A necessary condition for $F^{(n)}F^{(n)*} \leq m \cdot I_n$ is given in Auert/Läuter (1982):

Theorem 3.4. *If $F^{(n)} = (f_{ij}^{(n)})$ and $\sum_{j=1}^n |f_{ij}^{(n)}| \leq \rho$ for all i and n , and if for $|i - j| > m_1 > 0$ the inequality*

$$|f_{ij}^{(n)}| \leq \frac{c}{|i - j|^{1+\alpha}}, \quad \alpha > 0, \quad c \geq 0$$

is fulfilled, then there exists a constant m with

$$F^{(n)}F^{(n)*} \leq m \cdot I_n \quad .$$

In Auert/Läuter (1982) general conditions for the asymptotic unbiasedness of the solutions of $A^{(n)}\varphi = F^{(n)}Y^{(n)}$ were formulated. These conditions affect the model, the design and the operator of regularization $F^{(n)}$. It turns out that, for example, polynomial smoothers and spline smoothers on tightening design points satisfy the conditions posed there.

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