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STOCHASTIC REGULARIZATION FOR THERMAL PROBLEMS WITH UNCERTAIN PARAMETERS

by

A. F. Emery University of Washington, Seattle WA National Science Foundation, Arlington VA emery@u.washington.edu

Abstract

Usually when determining parameters with an inverse method, it is assumed that parameters or properties, other than those being sought, are known exactly. When such *known* parameters are uncertain, the inverse solution can be very sensitive to the degree of uncertainty. The stochastic regularization method can be modified to reduce this sensitivity. This paper presents such a modification. In addition, the relationship between Tikhonov-Phillips regularization and stochastic regularization is described. Because of this relationship, it is possible to modify the usual Tikhonov-Phillips regularization to account for such uncertainties.

Nomenclature

A	discretized form of $F(\theta)$
b	uncertain $known$ parameters
E[]	expected value
$F(\theta)$	system model response
Η	discretized form of $\Phi(\theta)$
Ι	Identity matrix
Κ	number of uncertain $known$ parameters
L	quantity to be minimized
М	number of sought parameters
Ν	number of data points
t	time
V	extended covariance matrix
W	weighting matrix
Х	spatial location
z	measurements
α	regularizing parameter
δ	rms value of ϵ
ϵ	stochastic variable
σ	standard deviation

 Σ covariance matrix

- θ parameters
- $\hat{\theta}$ estimated parameter
- $\Phi(\theta)$ penalty function

subscripts

- T Tikhonov
- P Phillips
- sr stochastic regularization

Introduction

The usual determination of parameters by inverse analysis assumes that the parameters are deterministic, that is that they are unknown but constants. The Bayesian approach to estimating parameters assumes that the parameters are random and that some knowledge of their statistical properties is known via a prior probability density distribution. Statistical regularization is the name given to a form of Bayesian estimation which resembles the usual Tikhonov-Phillips regularization method in which the regularization parameter is related to the variance of the prior.

In both approaches, it is usual to assume that the only unknowns are the parameters sought and, with the exception of noise or uncertainty in the measured data, that all other parameters of the problem are known. In reality, boundary conditions, initial conditions, or other properties may have uncertainty. We will term the parameters other than those sought as known parameters. In this paper we develop the foundation of an extension to the usual identification problem to consider uncertainty in these known parameters and the inclusion of their uncertainties in the stochastic regularization method.

Although details of Tikhonov-Phillips and statistical regularization are available in very complete form in a variety of sources (Engl, Hoffman, Groetsch), it is worthwhile to recap their development to emphasize their inter-relationships. Because of this inter-relation- ship, it is possible to incorporate the extension developed for stochastic regularization into the standard Tikhonov-Phillips regularization method.

Tikhonov Regularization

Consider a system whose response can be characterized by $z = F(x,t,\theta,b)$ where $F(x,t,\theta,b)$ includes the parameters sought, θ , and the *known* parameters, b, both of which may represent properties, boundary conditions or initial conditions. Suppose that we make N measurements of the response, z, which are contaminated with a stochastic variable, ϵ , which has a zero mean and a covariance of Σ_{ϵ} . ϵ may be interpreted as noise in the data or departures of the data from the model predictions. From the measurements we want to estimate the M parameters, θ . The usual approach is to minimize a weighted least square error, L, where

$$L = (z - F)^T W(z - F)$$
(1)

in which the superscript T indicates the transpose. For many inverse problems, the error of the parameter estimate, $\hat{\theta}$, first decreases as the number of data points, N, increases and then increases. Such behavior is characteristic of "illposed" problems which are usually associated with determining the kernel of a Fredholm equation of the first kind as encountered in inverse heat transfer, computerized tomography and many other situations. The usual approach for estimating the parameters in this case is to modify the function L to include a smoothing function, $\Phi(\theta)$

$$L = (z - F)^T W(z - F) + \alpha \Phi(\theta)$$
(2)

where $\Phi(\theta)$ is sometimes referred to as a penalty, roughness or stabilizing function. We will employ the term *penalty* function because it better represents the action of the function. α is termed the regularizing parameter. This form of a regularized solution is usually referred to as Tikhonov regularization. A variety of such penalty functions can be used. The most common functions are the minimum square error of the estimator, $\theta^T \theta$, the differential operators of the 1st and 2nd derivatives employed by Beck in solving the inverse heat conduction problem, $(\theta')^T(\theta')$ and $(\theta'')^T(\theta'')$ where the primes denote differentiation, and the entropy information/theoretic function described by Engl. Sometimes the penalty function is implicit as in the iterative matrix solution methods for non-linear functions $F(\theta)$ where the iteration index plays the role of α . Depending upon the application, more than one penalty function can be employed.

Without loss of generality, let us consider the case of a discretized system and assume that $F(x, t, \theta, b)$ can be expressed in linear form as $A\theta$ where A is a NxM matrix, that the expected values of θ are zero, that the discretized penalty function $\Phi(\theta)$ can be expressed as $\theta^T H \theta$. The resulting form of Eq. 2 is then the more common form of Tikhonov regularization

$$L_T = (z - A\theta)^T W(z - A\theta) + \alpha \theta^T H\theta$$
(3)

Although a non-linear $F(\theta)$ can always be treated by linearization and non-zero expected values of θ can be absorbed into the equations easily and other weight functions considered, all almost trivially accommodated in the formulation of the equations, these effects may have very serious consequences in the numerical solution and they should not be treated cavalierly.

The solution to Eq. 3 can be expressed as

$$\hat{\theta}_T(\alpha) = (A^T W A + \alpha H)^{-1} A^T W z$$
(4a)

$$=H^{-1}A^{T}(AH^{-1}A^{T}+\alpha W^{-1})^{-1}z \qquad (4b)$$

where we have written $\hat{\theta}(\alpha)$ to emphasize that the estimate is a function of α . Eq. 4a is better suited for $N \geq M$ and Eq. 4b for N < M.

A full discussion of typical inverse problems, the different methods of regularization, the mathematical restrictions placed upon the regularization method, and procedures for the choice of α can be found in Engl and Groetsch. Since the method is essentially an extension of the usual least squares method of Gauss, it is common to impose the restriction that $N \geq M$, but cases where N < M can be treated using SVD, as long as sufficient conditions are met (Bjorck).

The regularization, Eqs. 3 or 4, can be viewed as a correction to the usual least squares method of estimating θ . The basic problem with Tikhonov regularization is the choice of α . Too small a value and, although the results display fidelity with the data, the erratic behavior of $\hat{\theta}$ persists; too large a value and the influence of the data is minimized. Probably the most common prescription for choosing α is Morozov's discrepancy principle which states that α should be such that the root mean square value of the residual should equal the estimated error in the data, that is choose α such that

$$(z - A\hat{\theta}(\alpha))^T (z - A\hat{\theta}(\alpha)) \approx \epsilon^T \epsilon \tag{4c}$$

The role of α can be seen by examining the error in the regularized solution, $\hat{\theta}(\alpha)$ which for W = I is given by (Hofmann, pg. 114)

$$\theta - \hat{\theta}_T(\alpha) = \sum_{i=1}^r \frac{\alpha}{\sigma_i^2 + \alpha} (\theta, u^{(i)}) u^{(i)} - \sum_{i=1}^r \frac{\sigma_i}{\sigma_i^2 + \alpha} (\epsilon, v^{(i)}) u^{(i)}$$
(5)

where we have neglected the error associated with the null space components that may not be resolved by the data z. In Eq. 5, r is the rank of A, $u^{(i)}$, $v^{(i)}$, are the column vectors of the orthogonal matrices U and V, σ_i^2 are the diagonal elements which arise from the SVD of A, $= VSU^T$, and (,) represents the dot product. The first term, which applies to exact data, makes the effect of α for ill-posed problems very clear: it provides a damping effect for singular values, σ_i which are close to zero. For components of θ associated with large values of σ_i , there is little effect. Clearly one wants to use as small a value of α as possible to reduce this error term. The second term shows the effect of contaminated data and we see that the larger α is, the more this effect is damped. It is this tradeoff between the first and second error terms which makes the choice of a "good" value of α difficult for treating ill-posed problems with noisy data.

Phillips' Regularization

A different point of view was formulated by Phillips in a paper which predated Tikhonov. Later work demonstrated that Phillips' method, in which the penalty function was a differential function of θ , was a special subset of Tikhonov's regularization (Groetsch, pg. 60). Subsequent to Phillips' work, many others have used differential functions, particularly in inverse heat conduction, but some care must be exercised to ensure satisfaction of all the conditions required to yield unique and properly convergent regularized solutions (Engl).

However, the fundamental idea behind Phillips' development differs from that of Tikhonov's. In Phillips' method the idea is to minimize a penalty function, but to subject the minimization to the requirement that the root mean square error of the data be less than or equal to some prescribed error magnitude, that is let the error in the signal be defined by

$$\epsilon^T \epsilon = N \delta^2 \tag{6a}$$

and choose θ to minimize

$$L_P = \Phi(\theta) + \lambda \{ \epsilon^T \epsilon - \delta^2 \}$$
(6b)

$$=\theta^T H\theta + \lambda \{z - A\theta\}^T (z - A\theta) - \delta^2\}$$
(6c)

where λ is a Lagrangian multiplier and we have substituted $\Phi(\theta) = \theta^T H \theta$. Since δ^2 is constant, the quantity to be minimized can be written as

$$L_P = \frac{1}{\lambda} \theta^T H \theta + (z - A\theta)^T (z - A\theta)$$
(7)

and comparing Eqs. 3 and 7, we see that $1/\lambda$ is equivalent to α . Although Eqs. 3 and 7 are identical, both minimizing the sum of the least squares error and a penalty function, there is a very fundamental difference in the underlying philosophy of the two methods. Tikhonov's regularization is based on reducing the ill-posedness of the least squares solution by adding a penalty function and assigning a weight of W to the errors and a weight of α to the penalty function. Phillips' method calls for the minimization of the penalty function with the mean square error of the data acting as a constraint, the penalty function being weighted by unity and the data by a weight of λ . Because λ is directly related to δ (i.e. specifying δ^2 defines the value of λ), Phillips' approach leads automatically and rather straightforwardly to Morozov's discrepancy principle (Engl, pg. 121).

(As an interesting aside, Phillips considered only the case where N = M and minimized Eq. 6b with respect to ϵ_i , not θ , and assumed values of λ and then determined the resulting value of δ^2 . He then investigated the effect of different values of λ on both δ^2 and the behavior of ϵ_i . His approach was in essence that of Tikhonov's in which α is assumed.)

Twomey extended Phillips' approach to the over-deter- mined case, generalized H to a range of penalty functions, and considered an initial estimate of the parameter. If an initial estimate of θ is taken to be p, then $\hat{\theta}_P$ is found from

$$\hat{\theta}_P = (H + \lambda A^T A)^{-1} (\lambda A^T z + Hp) \tag{8a}$$

$$=p + \lambda (H + \lambda A^T A)^{-1} A^T (z - Ap)$$
(8b)

If no initial estimate is assumed, i.e. p = 0, and W = I, Eq. 8 is identical to Eq. 4a with $1/\lambda = \alpha_P$. If u are the eigenvectors of $A^T A$ and β are the eigenvalues, so that $\theta = \gamma u$ and $\hat{\theta} = \hat{\gamma} u$, then the coefficients are related by

$$\hat{\gamma}_k = \left(1 + \frac{\alpha_P \xi_k}{\beta_k}\right)^{-1} \gamma_k \tag{9}$$

where ξ_k is a number equal to 1 if H = I, otherwise $|\xi_k| \leq 1$ and depends upon H. From Eq. 9 it is clear that α_P has the greatest effect on the components corresponding to the small eigenvalues (i.e. high frequency) and leaves the components corresponding to large β_k unaffected.

Phillips' approach lends itself naturally to the case when we have several heterogeneous sets of data, with each set representing different physical phenomena and having very different orders of magnitude, dimensional characteristics, and importance. It is very easy to accommodate this case by extending Eq. 6c to

$$L_P = \Phi(\theta) + \sum_{j=1}^J \lambda_j \{ (z - A_j \theta)^T (z - A_j \theta) - \delta_j^2 \}$$
(10)

where J represents the number of data sets and A_j is the appropriate matrix for each data set.

Stochastic Regularization

Stochastic regularization is another name for the minimum mean square estimator of a parameter which has a Gaussian distribution when the data is also Gaussian distributed. As such, this estimation process is unrelated to regularization. However, it is interesting to observe how we can develop the approach starting from regularization. Following Phillips' model of minimizing a penalty function, let us set the penalty function equal to the mean square error $E[(\theta - \hat{\theta})^T(\theta - \hat{\theta})]$. It is well known that the optimal estimator is the conditional mean of the parameter (Sorensen)

$$\hat{\theta} = E[\theta|z] \tag{11}$$

If both the parameters and the data have a normal distribution and are uncorrelated, then we obtain

$$\hat{\theta} = P A^T \Sigma_{\epsilon}^{-1} z \tag{12a}$$

where P is the covariance of the error given by

$$P = [\Sigma_{\theta}^{-1} + A^T \Sigma_{\epsilon}^{-1} A]^{-1}$$
(12b)

Comparing Eqs. 4a and 12b, we see that Σ_{θ}^{-1} plays the role of αH and Σ_{ϵ}^{-1} that of W. If both covariances are constant diagonal matrices, Eq. 12a can be written as

$$\hat{\theta}_{sr} = \left(\frac{\sigma_{\epsilon}^2}{\sigma_{\theta}^2}I + A^T A\right)^{-1} A^T z \tag{13}$$

Comparing Eq. 13 with Eq. 4a, we see that Eq. 13 is a form of generalized regularization and that $\sigma_{\epsilon}^2/\sigma_{\theta}^2$ can be considered to be the equivalent regularization parameters, α_{sr} . Unfortunately in many cases, Σ_{θ} has off diagonal elements and this choice may not be optimal. Letting $\overline{\theta} = E[\theta], \theta_{sr}$ minimizes

$$L_{sr} = (\theta - \overline{\theta})^T \Sigma_{\theta}^{-1} (\theta - \overline{\theta}) + (z - A\theta)^T \Sigma_{\epsilon}^{-1} (z - A\theta)$$
(14)

Because of the similarity of Eq. 14 to the usual regularization formulation, Eq. 3, and the relationship of α_{sr} to the statistical properties of the stochastic data and parameters, this subset of Bayesian estimation has been given the misnomer of *statistical regularization*. There is, however, a significant difference between regularization and statistical regularization. In the Tikhonov-Phillips regularization, α is chosen to alleviate the instability of an ill-posed problem, the ill-posedness existing irrespective of any noise in the data. In statistical regularization, α_{sr} is directly related to the ratio of the uncertainty in the data to that in the parameter and as our uncertainty of the parameter increases, i.e., as $\sigma_{\theta} \to \infty$, $\alpha_{sr} \to 0$ and the regularization term disappears. Since setting $\Sigma_{\theta} = \infty$ is equivalent to assuming that the parameter is deterministic. but unknown (Sorensen), the disappearance of the regularization term means that we must have some prior estimate of θ to use this approach. Statistical regularization has been used extensively by Twomey, Strand and Westwater and Turchin in determining the vertical temperature profile in the earth's atmosphere. In this case, there are sufficient data to provide reasonable estimates of σ_{θ} to make the approach useful.

Extension to Uncertainty in the known Parameters

The only convenient way to incorporate uncertainty in the known parameters is to extend statistical regularization. If the sought after parameters, uncertain known parameters, and ϵ have Gaussian distributions, then the estimator satisfies

$$\hat{\theta}_{sre} = \Sigma_{\theta z} \Sigma_z^{-1} z \tag{15a}$$

where
$$\Sigma_z = E[\delta z \delta z^T]$$
 (15b)

By linearizing we have

$$\delta z = \frac{\partial F}{\partial b} \delta b + \frac{\partial F}{\partial \theta} \delta \theta + \delta \epsilon \tag{15c}$$

and evaluating $\Sigma_{\theta z}$ and Σ_z we obtain (Fadale)

$$\hat{\theta}_{sre} = (\Sigma_{\theta} + A^T V^{-1} A) A^T V^{-1} z \qquad (16a)$$

where the extended covariance matrix, V is

$$V = \Sigma_{\epsilon} + \sum_{k=1}^{K} \frac{\partial F}{\partial b_k} \Sigma_{b_k} \frac{\partial F}{\partial b_k}^T$$
(16b)

and we see that the effect of the uncertainty in b is to extend the definition of the variance of the measurement noise, Σ_{ϵ} . In most transient inverse heat transfer problems, it is usual to consider Σ_{ϵ} to be constant in time. This is not the case in this extended regularization because the sensitivities, $\partial F/\partial b$, are invariably strong functions of time and temperature, making V, the effective noise, time dependent.

Examples I

Consider an encapsulated microelectronic circuit (a die) bonded to an alumina substrate with a contact resistance \mathbf{R}_o between the die and the substrate. A convective heat transfer h_o exists at the interface between the encapsulated die and the ambient fluid. When powered, the die generates heat which is conducted into the substrate or through the cover to the ambient fluid whose temperature remains constant. We will determine \mathbf{R}_o from the temperature measured at the surface of the die, \mathbf{T}_f . (The measured temperatures are simulated by adding uncorrelated, random noise, with zero mean and a standard deviation of 1% of the maximum temperature of the chip)

We will examine two cases: 1) the lower surface of the substrate is insulated; 2) the lower surface is maintained at the ambient fluid temperature. The properties of the different materials are taken from Pecht and Agarwal for an alumina ceramic substrate ($k_s=25$, $\alpha_s=1.7$ 10⁶) and a highly conducting cover.

In calculating the contact resistance \mathbf{R} we assume that the convective coefficient h is not precisely known but has an uncertainty σ_h . Thus we solve for \mathbf{R} by assuming different values of h. Figure 1 illustrates the values of \mathbf{R} predicted for 3 different contact resistances defined in relation to the resistance across the substrate, \mathbf{R}_s , for two different thermal boundary conditions at the lower surface of the substrate. For an insulated substrate, we see that for $\mathbf{R}_o/\mathbf{R}_s$ equal to 0.1 and 10 that the predicted value of \mathbf{R} is unacceptably sensitive to our estimate of h and if there is any uncertainty about the value of \mathbf{R} .

The reason for this unacceptable sensitivity can be understood by examining the relation for the surface temperature \mathbf{T}_{f} which is given by

$$\mathbf{T}_f = Q_f / h \tag{17}$$

where Q_f is the heat transferred through the front surface. For the properties used in this example, little heat is stored in the encapsulating cover so that Q_f is essentially the difference between the heat generated in the die, Q_d , and that which flows through the attachment to the substrate. When \mathbf{R} is small compared to \mathbf{R}_s , the heat flow into the substrate is essentially independent of \mathbf{R} and thus Q_f is also insensitive to \mathbf{R} . From Eq. 17, \mathbf{T}_f is very sensitive to h, which must be known precisely to extract the correct value of \mathbf{R} . When \mathbf{R} is large in comparison to \mathbf{R}_s , essentially no heat flows into the substrate, all flowing into the ambient fluid and again there is no sensitivity to \mathbf{R} but a high sensitivity to h. When \mathbf{R} and \mathbf{R}_s are approximately the same, then the sensitivity of Q_f to \mathbf{R} is relatively high compared to the sensitivity to h and the prediction is better, but still not sufficiently independent of h to be acceptable.

When the surface of the substrate is maintained at a fixed temperature, the heat flow into the substrate is much more sensitive to \mathbf{R} and the estimation of \mathbf{R} becomes essentially independent of the value of h.

Figure 2 illustrates the computation of \mathbf{R} using Σ_{ϵ} and V. It is clear that the extended method has succeeded in reducing the dependence of the estimated \mathbf{R} on our estimate of h.

Example II

For the second example let us estimate the conductivity of a homogenous material. This will be done by sampling the temperature of a one dimensional slab. The slab is of thickenss L=0.04m, has conductivity k = 1.0 W/(m-C) and volumetric heat capacity $\rho c = 1.0 \times 10^6 \text{ J}/(m^3 \text{ -C})$. It is initially at 0 temperature, has a convective heat transfer coefficient of $h_0 = 5 \mathrm{W}/(m^2$ -C) at x=0 and $h_L = 20 \mathrm{W}/(m^2$ -C) at x = L, and is immersed in a fluid of temperature 1000 at time zero. The temperature is measured at a fixed location at 10 equally spaced times over the duration of the experiment. The experimental temperatures are taken to be the analytical temperatures based upon a conductivity of k=1W/(m-C), corrupted by a Gaussian noise with zero mean and a standard deviation, σ_n of 1 degree, which corresponds to 0.1% of the maximum temperature. The heat transfer coefficient at x=L is distributed about the mean value h_L = 20 with a standard deviation of σ_h .

Measuring the temperature at x=L would normally be the best since it has the greatest sensitivity to **k**. However, it is precisely at x=L that h also has its greatest effect and the uncertainty in h seriously degrades the information available there. Figure 3 illustrates the result of estimating **k** using T(L) and the extended method has not had any effect. If one examines the information available, as measured by the Fisher information matrix (Emery), the effect of the uncertainty in h is to move the point of maximum information from x=L to x=0. Figure 4 illustrates the result of using T(0) to estimate **k** and here the extended estimator has reduced the dependence upon h; in this case almost totally eliminating its effect.

Summary

The extended theory has been shown to be able to account successfully for uncertainties in surface heat transfer coefficients when estimating the conductivity and the contact resistance. Although results are presented only for variations in h, we have found similar results for variations in fluid temperature, sensor locations, and other properties. We thus conclude that this extended theory is applicable in all cases in which some of the prescribed parameters, whether they be properties or boundary conditions, are uncertain. However, the success is achieved only when the sensor is placed at the position which is defined as optimal by the corresponding extended Fisher Information Matrix.

An extended method cannot be developed starting from the usual Tikhonov- Phillips regularization. However, since, under the restrictions of linear estimators with Gaussian distributions of noise and parameters, the stoch -astic and Tikhonov-Phillips regularizations satisfy the same equations, it is clear how to incorporate uncertainty in *known* parameters into the usual regularization by replacing Σ_{ϵ} by V.

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Figure 1: Estimated values of **R** based on 20 samples of \mathbf{T}_f equally spaced in time over the period $0.35 \leq Fo \leq 3.5$ using Σ_{ϵ}



Figure 2: Estimated Values of **R** using Σ_{ϵ} and V 1% noise and 10% Uncertainty in h



Figure 3: Estimated Conductivity for a sensor at x = L, for a Total Experiment Time (Fo) of 0.625), 0.1% noise and 10% Uncertainty in h_L



Figure 4: Estimated Conductivity using for a sensor at the Optimal Location, x = 0, for a Total Experiment Time (Fo) of 0.625, 0.1% noise, 10% Uncertainty in h_L