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**Models and Observations: Data
Assimilation in Hydrological and
Geological Sciences**

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Preface

There are many problems in the hydrologic and geologic sciences in which data need to be fused with models. There is often either the abundance of measurements which hampers interpretation or a deficit of information which leaves degrees of freedom in diagnosing a problem. In either case observations and models are elements that need to be combined in solving problems in fields such as hydrology and geology where the systems are inherently highly heterogeneous but nevertheless governed by known physical laws.

Observations are error-prone and they may represent indirect or under-sampled measures of model states and parameters. Furthermore there may be scattered or overlapping measurements from different sensors with varying observing scales (e.g. point sampling vs. areal mean remote sensing).

Models are imperfect representations of physical systems and they often include parameterizations that are unobservable directly. Nevertheless models are capable of imposing strong physical constraints in relating relevant variables in systems and may hence reduce the degrees of freedom in interpreting data. Multidimensional models, by virtue of their dynamic or spatial dependencies, may also serve to advect information from the observed domains of the data space to other unobserved portions.

Data assimilation is the process of merging measurements and models. It is essentially directed towards the determination of model variables based on measurements using statistical estimation and inverse solution techniques.

The report here represents notes from a short course held at the Faculty of Engineering of the University of Perugia in June 1998 under the auspices of the *Consiglio Nazionale delle Ricerche-Massachusetts Institute of Technology Cooperative Agreement on Climate Change and Hydrogeologic Hazards in the Mediterranean Area*. The notes are strictly restricted to the theoretical bases of data assimilation techniques applicable to hydrologic and geologic sciences. Furthermore mostly linear systems are considered in order to turn the focus on the impact of noise and sampling issues in data assimilation. The material contained herein is based on a number of different sources but there is some attempt to provide basic albeit theoretical interpretation of the similarities and differences between the various approaches.

The report is designed to introduce graduate students to the theoretical underpinning of data assimilation which is believed to be a powerful yet underutilized approach to hydrologic and geologic characterization and forecasting problems.

1 Estimation and Inverse Solution of Linear Systems

1.1 General Formulation of the Estimation Problem

Estimates $\hat{\mathbf{x}}$ of the the state \mathbf{x} are formed based on measurements/observations \mathbf{z} . The estimator $\hat{\mathbf{x}}=\hat{\mathbf{x}}(\mathbf{z})$ is:

- unbiased if its expectation is the same as the expectation of \mathbf{x} , i.e. $E[\hat{\mathbf{x}}] = E[\mathbf{x}]$,
- minimum-variance if the error variance is less than or equal to any other estimator, i.e. $var[\mathbf{x}-\hat{\mathbf{x}}(\mathbf{z})] \leq var[\mathbf{x}-\hat{\mathbf{x}}'(\mathbf{z})]$,
- consistent if it converges to the true value of \mathbf{x} as the number of measurements increase.

We will consider unbiased, minimum-variance and consistent estimators. In linear systems it is assumed that observations may be linearly combined to form estimates of the state, i.e.

$$\hat{\mathbf{x}}(\mathbf{z}) = \hat{\mathbf{x}} = \mathbf{W}\mathbf{z}$$

where \mathbf{W} is a matrix of linear weighting coefficients. The measurements or observations have additive noise or error as in

$$\mathbf{z} = \mathbf{H}\mathbf{x} + \mathbf{v}$$

where \mathbf{z} is an $(m \times 1)$ vector of measurements, \mathbf{x} is an $(n \times 1)$ vector of states, \mathbf{v} is an $(m \times 1)$ vector of measurement errors and \mathbf{H} is an $(m \times n)$ matrix of constants relating measurements to the states (see Appendix A for a basic review of probability and statistics concepts).

Three estimators will be derived based on successive sets of assumptions. They are:

1. Least-squares estimators (LSE): No assumptions on the distributions of \mathbf{z} , \mathbf{x} , and \mathbf{v} are made,
2. Maximum-likelihood estimators (MLE): Assume distributions for measurements \mathbf{z} ,
3. Bayesian estimators: Assume distributions for measurements \mathbf{z} and state \mathbf{x} .

1.2 General Formulation of the Inverse Problem

Where a model $\mathbf{f}(\mathbf{d}, \mathbf{m}) = [f_1(\mathbf{d}, \mathbf{m}), f_2(\mathbf{d}, \mathbf{m}), \dots, f_L(\mathbf{d}, \mathbf{m})]^T = 0$ consisting of L elements relate a data vector (length N) $\mathbf{d} = [d_1, d_2, \dots, d_N]^T$ and a parameters vector (length M) $\mathbf{m} = [m_1, m_2, \dots, m_M]^T$, then the forward and the inverse problems may be posed with the following definitions:

Forward problem: find estimates of the data \mathbf{d} given the model \mathbf{f} and estimates of the model parameters \mathbf{m} (and possibly some "prior" information on \mathbf{d}).

Inverse problem: find estimates of the model parameters \mathbf{m} given the model \mathbf{f} and estimates of the data \mathbf{d} (and possibly some "prior" information on \mathbf{m}).

A special case is the implicit linear form

$$\mathbf{f}(\mathbf{d}, \mathbf{m}) = 0 = \mathbf{F} \begin{bmatrix} \mathbf{d} \\ \mathbf{m} \end{bmatrix}$$

where \mathbf{F} is an $L \times (M + N)$ matrix
The explicit form would be

$$\mathbf{f}(\mathbf{d}, \mathbf{m}) = 0 = \mathbf{d} - \mathbf{g}(\mathbf{m})$$

for which the linear form is

$$\mathbf{f}(\mathbf{d}, \mathbf{m}) = 0 = \mathbf{d} - \mathbf{G}\mathbf{m}$$

where $L = N$ and \mathbf{G} is an $N \times (M + N)$ matrix.

1.3 Performance Criteria

In order to fit data to models for both the estimation and inverse problems, especially when measurements are noisy and/or the model is imperfect, metrics of performance need to be defined. Optimization of the metrics yield optimal estimators and optimal solutions to the inverse problem. The basic principle is to minimize the norm of the prediction error.

For the case of the inverse problem:

$$\mathbf{e} = \mathbf{d}^{obs} - \mathbf{d}^{pre}$$

where \mathbf{d}^{obs} are the observed data and $\mathbf{d}^{pre} = \mathbf{G}\mathbf{m}^{est}$ are the predicted data on the basis of the estimated model parameters \mathbf{m}^{est} .

For the case of estimation:

$$\mathbf{e} = \mathbf{z} - \mathbf{H}\hat{\mathbf{x}}(\mathbf{z})$$

where $\mathbf{H}\hat{\mathbf{x}}(\mathbf{z})$ is the predicted measurement based on the estimator.

Types of norm are:

$$L_1 \text{ norm: } \|\mathbf{e}\|_1 = \sum_i |e_i|$$

$$L_2 \text{ norm: } \|\mathbf{e}\|_2 = \left[\sum_i |e_i|^2 \right]^{1/2}$$

$$L_n \text{ norm: } \|\mathbf{e}\|_n = \left[\sum_i |e_i|^n \right]^{1/n}$$

$$L_\infty \text{ norm: } \|\mathbf{e}\|_\infty = \max_i |e_i|$$

The choice of the more appropriate norm depends on how much "weight" is to be given to "outliers" (more precisely, it depends on the probability distribution of the data, as discussed further on in the maximum likelihood view-point).

1.4 The Simple Least-Squares Estimator

If the measurement errors are zero-mean and no information on distributional features are available, then the best estimate of the state $\hat{\mathbf{x}}$ is found by considering the L_2 -norm of the predicted measurement errors as in

$$E = \mathbf{e}^T \mathbf{e} = (\mathbf{z} - \mathbf{H}\hat{\mathbf{x}})^T (\mathbf{z} - \mathbf{H}\hat{\mathbf{x}})$$

which should be minimized with respect to $\hat{\mathbf{x}}$. Expanding this expression

$$E = \mathbf{z}^T \mathbf{z} - \hat{\mathbf{x}}^T \mathbf{H}^T \mathbf{z} - \mathbf{z}^T \mathbf{H} \hat{\mathbf{x}} + \hat{\mathbf{x}}^T \mathbf{H}^T \mathbf{H} \hat{\mathbf{x}}$$

The function is minimized by taking its first derivative and setting it to zero as in

$$\begin{aligned} \frac{\partial E}{\partial \hat{\mathbf{x}}} &= \frac{\partial}{\partial \hat{\mathbf{x}}} (\mathbf{z}^T \mathbf{z}) - \frac{\partial}{\partial \hat{\mathbf{x}}} (\hat{\mathbf{x}}^T \mathbf{H}^T \mathbf{z}) - \frac{\partial}{\partial \hat{\mathbf{x}}} (\mathbf{z}^T \mathbf{H} \hat{\mathbf{x}}) + \frac{\partial}{\partial \hat{\mathbf{x}}} (\hat{\mathbf{x}}^T \mathbf{H}^T \mathbf{H} \hat{\mathbf{x}}) \\ &= \mathbf{0} - \mathbf{H}^T \mathbf{z} - (\mathbf{z}^T \mathbf{H})^T + \left[\mathbf{H}^T \mathbf{H} \hat{\mathbf{x}} + (\mathbf{H}^T \mathbf{H})^T \hat{\mathbf{x}} \right] \\ &= -2\mathbf{H}^T \mathbf{z} + 2\mathbf{H}^T \mathbf{H} \hat{\mathbf{x}} \\ &= \mathbf{0} \end{aligned}$$

whose solution for $\hat{\mathbf{x}}$ is

$$\hat{\mathbf{x}} = (\mathbf{H}^T \mathbf{H})^{-1} \mathbf{H}^T \mathbf{z}$$

Thus

$$\mathbf{W} = (\mathbf{H}^T \mathbf{H})^{-1} \mathbf{H}^T$$

in

$$\hat{\mathbf{x}} = \mathbf{W} \mathbf{z}$$

for least-squares estimators with no assumptions on the statistics and distributions of the states and the measurements.

1.5 The Least-Squares for Linear Inverse Problems

The general form for the "prediction error" is now

$$\begin{aligned} E &= \mathbf{e}^T \mathbf{e} = (\mathbf{d} - \mathbf{G}\mathbf{m})^T (\mathbf{d} - \mathbf{G}\mathbf{m}) = \\ &= \sum_{i=1}^N \left[d_i - \sum_{j=1}^M G_{ij} m_j \right] \left[d_i - \sum_{k=1}^M G_{ik} m_k \right] = \\ &= \sum_{j=1}^M \sum_{k=1}^M m_j m_k \sum_{i=1}^M G_{ij} G_{ik} - 2 \sum_{j=1}^M m_j \sum_{i=1}^N G_{ij} d_i + \sum_{i=1}^N d_i^2 \end{aligned}$$

Differentiating E (find the minimum) with respect to the generic parameter m_q , the various terms are (let δ_{ij} be the Kronecker delta):

$$\begin{aligned} \frac{\partial}{\partial m_q} \left[\sum_{j=1}^M \sum_{k=1}^M m_j m_k \sum_{i=1}^M G_{ij} G_{ik} \right] &= \sum_{j=1}^M \sum_{k=1}^M [\delta_{jq} m_k + m_j \delta_{kq}] \sum_{i=1}^M G_{ij} G_{ik} = \\ &= 2 \sum_{k=1}^M m_k \sum_{i=1}^M G_{iq} G_{ik} \end{aligned}$$

$$-2 \frac{\partial}{\partial m_q} \left[\sum_{j=1}^M m_j \sum_{i=1}^N G_{ij} d_i \right] = -2 \sum_{j=1}^M \delta_{jq} \sum_{i=1}^N G_{ij} d_i = -2 \sum_{i=1}^N G_{iq} d_i$$

$$\frac{\partial}{\partial m_q} \left[\sum_{i=1}^N d_i^2 \right] = 0$$

Then:

$$\frac{1}{2} \frac{\partial E}{\partial m_q} = \sum_{k=1}^M m_k \sum_{i=1}^M G_{iq} G_{ik} - \sum_{i=1}^N G_{iq} d_i = 0$$

In matrix notation:

$$\mathbf{G}^T \mathbf{G} \mathbf{m} - \mathbf{G}^T \mathbf{d} = 0$$

Note that $\mathbf{G}^T \mathbf{G}$ is a square $M \times M$ matrix and both \mathbf{m} and $\mathbf{G}^T \mathbf{d}$ are vectors of length M , so we have a linear algebraic system which, if $[\mathbf{G}^T \mathbf{G}]^{-1}$ exists (to be discussed later), gives the solution:

$$\mathbf{m}^{est} = [\mathbf{G}^T \mathbf{G}]^{-1} \mathbf{G}^T \mathbf{d}$$

Sometimes it is useful to "weight" differently the various prediction errors (i.e. some data are more "certain" than others). The following weighted error needs then to be minimized, given a $N \times N$ weight matrix \mathbf{W}_e :

$$E = \mathbf{e}^T \mathbf{W}_e \mathbf{e} = (\mathbf{d} - \mathbf{G} \mathbf{m})^T \mathbf{W}_e (\mathbf{d} - \mathbf{G} \mathbf{m})$$

The solution to this minimization problem is called weighted least squares and is given by:

$$\mathbf{m}^{est} = [\mathbf{G}^T \mathbf{W}_e \mathbf{G}]^{-1} \mathbf{G}^T \mathbf{W}_e \mathbf{d}$$

1.5.1 The Existence of the Least-Square Solution

In general, linear inverse problems may be classified as:

Overdetermined Problems - There is excess information in the equation $\mathbf{G} \mathbf{m} = \mathbf{d}$, in the sense that $N > M$ and $[\mathbf{G}^T \mathbf{G}]^{-1}$ exists. There is no solution with zero prediction error, and we may use the Least-Squares technique to select the one with minimum prediction error (in the Least-Squares sense).

Even-Determined Problems - There is exactly enough information to determine the parameters ($N = M$ and $[\mathbf{G}^T \mathbf{G}]^{-1}$ exists). Typical example

is fitting a line with two data points. There is only one solution with zero prediction error.

Underdetermined Problems - The equation $\mathbf{Gm} = \mathbf{d}$ does not provide enough information to determine uniquely all the model parameters. Typical example is the case of fitting a line with only 1 data point: there exist infinite solutions with zero prediction error. Underdetermined problems may occur when $N < M$ and all the model equations are "consistent", in this case they are called **Purely Undetermined Problems**. It may also be the case that $N \geq M$ but $[\mathbf{G}^T \mathbf{G}]^{-1}$ does not exist, in this case we have **Mixed Determined Problems**.

These cases are treated separately below.

1.5.2 The Purely Undetermined Problem

Suppose that a problem has been identified to be purely undetermined. To solve the problem, we need to define a criteria to single out one of the many (infinite) solutions with zero prediction error, that is we need to add to the problem some information which is not contained in the equation $\mathbf{Gm} = \mathbf{d}$. This type of information is called prior information. There are many kinds of prior information, which characterize the type of solution of the inverse problem.

One first kind of prior information is termed simplicity, quantified by some norm of the solution \mathbf{m} (i.e. the L_2 norm).

We can then consider the following constrained minimization problem: find the \mathbf{m}^{est} that minimizes $L = \mathbf{m}^T \mathbf{m}$ subject to the constraint $\mathbf{e} = \mathbf{d} - \mathbf{Gm} = 0$.

This problem can be solved using the method of Lagrange multipliers λ_i , minimizing the function:

$$\Phi(\mathbf{m}) = L + \boldsymbol{\lambda}^T \mathbf{e} = \mathbf{m}^T \mathbf{m} + \boldsymbol{\lambda}^T (\mathbf{d} - \mathbf{Gm})$$

Deriving with respect to the generic parameter m_q we obtain:

$$\frac{\partial \Phi}{\partial m_q} = \dots = 2m_q - \sum_{i=1}^N \lambda_i G_{iq} = 0$$

which in matrix notation is $2\mathbf{m} = \mathbf{G}^T \boldsymbol{\lambda}$. Substituting this in $\mathbf{Gm} = \mathbf{d}$ gives $\mathbf{d} = \mathbf{Gm} = \mathbf{G}\mathbf{G}^T \boldsymbol{\lambda}/2$. Note that $\mathbf{G}\mathbf{G}^T$ is a $N \times N$ square matrix (not $M \times M$ as $\mathbf{G}^T \mathbf{G}$). If $[\mathbf{G}\mathbf{G}^T]^{-1}$ exists (this is the meaning of the consistency of

the model equations), then we can solve for the unknown Lagrange multipliers $\lambda = 2 [\mathbf{G}\mathbf{G}^T]^{-1} \mathbf{d}$ and finally obtain:

$$\mathbf{m}^{est} = \mathbf{G}^T [\mathbf{G}\mathbf{G}^T]^{-1} \mathbf{d}$$

The one above is just a particular choice of priori information. The derived solution procedure can be however generalized to include both a priori parameter estimates $\langle \mathbf{m} \rangle$ (such as some knowledge of the parameters expected value) and some weighting matrix \mathbf{W}_m ($M \times M$):

$$L = [\mathbf{m} - \langle \mathbf{m} \rangle]^T \mathbf{W}_m [\mathbf{m} - \langle \mathbf{m} \rangle]$$

$$\mathbf{m}^{est} = \langle \mathbf{m} \rangle + \mathbf{W}_m \mathbf{G}^T [\mathbf{G}\mathbf{W}_m \mathbf{G}^T]^{-1} [\mathbf{d} - \mathbf{G} \langle \mathbf{m} \rangle]$$

1.5.3 The Mixed Determined Problem

In the mixed determined problem, the available information is redundant (overdetermining) for some of the parameters and insufficient (underdetermining) for some others. To clearly separate the overdetermined from the underdetermined ones, a particular technique is required (singular value decomposition, discussed in Appendix C). The general idea is to build a transform $\mathbf{G}'\mathbf{m}' = \mathbf{d}'$ of the original problem $\mathbf{G}\mathbf{m} = \mathbf{d}$ which can be cast in the form:

$$\begin{bmatrix} \mathbf{G}^{o'} & 0 \\ 0 & \mathbf{G}^{u'} \end{bmatrix} \begin{bmatrix} \mathbf{m}^{o'} \\ \mathbf{m}^{u'} \end{bmatrix} = \begin{bmatrix} \mathbf{d}^{o'} \\ \mathbf{d}^{u'} \end{bmatrix}$$

where $\mathbf{G}^{o'}\mathbf{m}^{o'} = \mathbf{d}^{o'}$ is purely overdetermined and $\mathbf{G}^{u'}\mathbf{m}^{u'} = \mathbf{d}^{u'}$ is purely underdetermined.

Another approach, less computational demanding but suitable only for slightly underdetermined problem, is based on directly "weighting" the least-squares and constrained minimization approaches without splitting the problem. This technique is called damped least squares and is based on the minimization of the function:

$$\Phi(\mathbf{m}) = E + \varepsilon^2 L = \mathbf{e}^T \mathbf{e} + \varepsilon^2 \mathbf{m}^T \mathbf{m}$$

where ε^2 is an ad-hoc (to be determined by trial and error in order to obtain a reasonably small value of E). The solution to the minimization of such a function is (let \mathbf{I} be the identity matrix):

$$\mathbf{m}^{est} = [\mathbf{G}^T \mathbf{G} + \varepsilon^2 \mathbf{I}]^{-1} \mathbf{G}^T \mathbf{d}$$

This can be again generalized, to account for prior information and weights, as:

$$\mathbf{m}^{est} = \langle \mathbf{m} \rangle + \mathbf{W}_m^{-1} \mathbf{G}^T [\mathbf{G} \mathbf{W}_m^{-1} \mathbf{G}^T + \varepsilon^2 \mathbf{W}_e^{-1}]^{-1} [\mathbf{d} - \mathbf{G} \langle \mathbf{m} \rangle]$$

1.6 Generalized Inverses

All the solution methods previously described may be cast in the form $\mathbf{m}^{est} = \mathbf{M} \mathbf{d} + \mathbf{v}$, where \mathbf{M} is a $M \times N$ matrix and \mathbf{v} is a vector, both independent of the data. Since the matrix \mathbf{M} solve (inverts) the problem $\mathbf{G} \mathbf{m} = \mathbf{d}$, it is called the generalized inverse \mathbf{G}^{-g} . Studying the properties of \mathbf{G}^{-g} one may obtain useful information on many aspects of the inverse problem.

1.6.1 The Resolution and Unit-Covariance Matrices

A basic question in inverse problems is how well the estimated parameters \mathbf{m}^{est} fits the data. Using the generalized inverse we obtain:

$$\mathbf{d}^{pre} = \mathbf{G} \mathbf{m}^{est} = \mathbf{G} \mathbf{G}^{-g} \mathbf{d}^{obs} = \mathbf{N} \mathbf{d}^{obs}$$

The $N \times N$ matrix $\mathbf{N} = \mathbf{G} \mathbf{G}^{-g}$ is called data resolution matrix. The case where the data are perfectly predicted would be simply $\mathbf{N} = \mathbf{I}$. A measure of how well the data are predicted (without knowing the data in advance!) may be then defined through the Dirichlet spread function:

$$spread(\mathbf{N}) = \|\mathbf{N} - \mathbf{I}\|_2^2$$

Suppose that a "perfect" parameter set \mathbf{m}^{true} exists such that $\mathbf{G} \mathbf{m}^{true} = \mathbf{d}^{obs}$. One may ask how well the given solution to the inverse problem approximates such true parameters. Using again the generalized inverse we obtain:

$$\mathbf{m}^{est} = \mathbf{G}^{-g} \mathbf{d}^{obs} = \mathbf{G}^{-g} \mathbf{G} \mathbf{m}^{true} = \mathbf{M} \mathbf{m}^{true}$$

The $M \times M$ matrix $\mathbf{M} = \mathbf{G}^{-g} \mathbf{G}$ is called model Resolution Matrix. The case where the parameters are perfectly guessed would be simply $\mathbf{M} = \mathbf{I}$. A measure of how well the parameters are guessed (without knowing the data in advance!) may be then defined again through the Dirichlet Spread Function:

$$spread(\mathbf{M}) = \|\mathbf{M} - \mathbf{I}\|_2^2$$

The covariance of the model parameters depends on the covariance of the data and the way in which error is mapped from data to model. The degree of error amplification in this mapping may be characterized by the unit-covariance matrix (equal to the correlation matrix in case the normalizing factor is the variance):

$$[cov_u \mathbf{m}] = \mathbf{G}^{-g} [cov_u \mathbf{d}] \mathbf{G}^{-gT}$$

whose measure is given by the sum of the diagonal elements:

$$trace([cov_u \mathbf{m}]) = \sum_{i=1}^M [cov_u \mathbf{m}]_{ii}$$

In the case of uncorrelated data, it is simply $[cov_u \mathbf{d}] = \mathbf{I}$, so that $[cov_u \mathbf{m}] = \mathbf{G}^{-g} \mathbf{G}^{-gT}$.

1.6.2 The General Generalized Inverse

A general Generalized Inverse may be obtained by minimization of:

$$\alpha_1 spread(\mathbf{N}) + \alpha_2 spread(\mathbf{M}) + \alpha_3 size([cov_u \mathbf{m}])$$

Where the α s are arbitrary constants. It may be demonstrated (with some involved algebra) that minimization of the above sum gives the following implicit equation for the Generalized Inverse:

$$\alpha_1 [\mathbf{G}^T \mathbf{G}] \mathbf{G}^{-g} + \mathbf{G}^{-g} \{ \alpha_2 \mathbf{G} \mathbf{G}^T + \alpha_3 [cov_u \mathbf{d}] \} = (\alpha_1 + \alpha_2) \mathbf{G}^T$$

Explicit solutions can be found for special cases only for uncorrelated data, such as:

Least Squares: $(\alpha_1, \alpha_2, \alpha_3) = (1, 0, 0)$

$$[\mathbf{G}^T \mathbf{G}] \mathbf{G}^{-g} = \mathbf{G}^T$$

$$\mathbf{G}^{-g} = [\mathbf{G}^T \mathbf{G}]^{-1} \mathbf{G}^T$$

$$\mathbf{N} = \mathbf{G}\mathbf{G}^{-g} = \mathbf{G} [\mathbf{G}^T\mathbf{G}]^{-1} \mathbf{G}^T$$

$$\mathbf{M} = \mathbf{G}^{-g}\mathbf{G} = [\mathbf{G}^T\mathbf{G}]^{-1} \mathbf{G}^T\mathbf{G} = \mathbf{I}$$

$$[cov_u\mathbf{m}] = \mathbf{G}^{-g}\mathbf{G}^{-gT} = [\mathbf{G}^T\mathbf{G}]^{-1} \mathbf{G}^T\mathbf{G} [\mathbf{G}^T\mathbf{G}]^{-1} = [\mathbf{G}^T\mathbf{G}]^{-1}$$

Minimum Length: $(\alpha_1, \alpha_2, \alpha_3) = (0, 1, 0)$

$$\mathbf{G}^{-g} [\mathbf{G}\mathbf{G}^T] = \mathbf{G}^T$$

$$\mathbf{G}^{-g} = \mathbf{G}^T [\mathbf{G}\mathbf{G}^T]^{-1}$$

$$\mathbf{N} = \mathbf{G}\mathbf{G}^{-g} = \mathbf{G}\mathbf{G}^T [\mathbf{G}\mathbf{G}^T]^{-1} = \mathbf{I}$$

$$\mathbf{M} = \mathbf{G}^{-g}\mathbf{G} = \mathbf{G}^T [\mathbf{G}\mathbf{G}^T]^{-1} \mathbf{G}$$

$$[cov_u\mathbf{m}] = \mathbf{G}^{-g}\mathbf{G}^{-gT} = \mathbf{G}^T [\mathbf{G}\mathbf{G}^T]^{-1} [\mathbf{G}\mathbf{G}^T]^{-1} \mathbf{G}^T$$

Damped Least Squares: $(\alpha_1, \alpha_2, \alpha_3) = (1, 0, \varepsilon^2)$

$$[\mathbf{G}^T\mathbf{G}] \mathbf{G}^{-g} + \mathbf{G}^{-g} [\varepsilon^2\mathbf{I}] = \mathbf{G}^T$$

$$\mathbf{G}^{-g} = [\mathbf{G}^T\mathbf{G} + \varepsilon^2\mathbf{I}]^{-1} \mathbf{G}^T$$

1.6.3 The Backus-Gilbert Spread Function and its Generalized Inverse

When there is a natural ordering of the data and model parameters, the Dirichlet spread function may not be an appropriate measure, since the off-diagonal elements of the resolution matrix are all weighted equally. One could prefer to have large elements of the resolution matrix as close as possible to the main diagonal, implementing what is call a local averaging.

To achieve this, the following Backus-Gilbert spread function may be used in the place of the Dirichlet one:

$$spread(\mathbf{M}) = \sum_{i=1}^M \sum_{j=1}^M w(i, j) (M_{ij} - I_{ij})^2$$

where the weights $w(i, j)$ depends on the "physical distance" between m_i and m_j . As an example, for linearly ordered parameters, one could simply choose $w(i, j) = (i - j)^2$.

Similar expressions apply for the data resolution matrix.

As an example of the use of the Backus-Gilbert spread function, we consider again the purely underdetermined problem. This is analogous to deriving the minimum length solution using the Dirichlet spread function, using the Backus-Gilbert spread function instead. We also require that $\sum_{j=1}^M M_{ij} = 1$, so that the rows of model resolution matrix \mathbf{M} are unit averaging functions acting on the true model parameters. The solution is now more involved because of the presence of the weights $w(i, j)$. After some algebra, the following expression for the generalized inverse is obtained:

$$G_{kl}^{-g} = \frac{\sum_{i=1}^N [S_{il}]_k^{-1} u_i}{\sum_{i=1}^N \sum_{j=1}^N u_i u_j [S_{il}]_k^{-1}}$$

$$[S_{ij}]_k = \sum_{l=1}^M w(l, k) G_{il} G_{jl}$$

$$u_i = \sum_{j=1}^M G_{ij}$$

1.7 The Maximum Likelihood Approach

If we know that the data in the linear inverse problem have a multivariate Gaussian distribution $f(\mathbf{d})$ with known covariance matrix $[covid]$. The quantity \mathbf{Gm} gives our estimate (prediction) of the data expected value, so that our estimate of $f(\mathbf{d})$ is:

$$f(\mathbf{d}) \propto \exp \left[-\frac{1}{2} (\mathbf{d} - \mathbf{Gm})^T [covid]^{-1} (\mathbf{d} - \mathbf{Gm}) \right]$$

This estimate clearly depends on the values of the parameters \mathbf{m} .

For the estimation problem, we would have a multivariate Gaussian distribution for measurements \mathbf{z} given \mathbf{x} , $f(\mathbf{z}|\mathbf{x})$, with mean $\mathbf{H}\mathbf{x}$:

$$f(\mathbf{z}|\mathbf{x}) \propto \exp \left[-\frac{1}{2} (\mathbf{z} - \mathbf{H}\mathbf{x})^T [\text{cov}\mathbf{z}]^{-1} (\mathbf{z} - \mathbf{H}\mathbf{x}) \right]$$

The **Maximum Likelihood** principle states that the best parameters estimate or estimator is (the) one that maximizes the probability of actually observing the data, that is (the) one that maximizes either $f(\mathbf{d})$ with respect to \mathbf{m} or $f(\mathbf{z}|\mathbf{x})$ with respect to \mathbf{x} .

1.8 The Maximum-Likelihood Estimator

The same objective function as for least squares may be posed but instead a weighting matrix is included to weight the contributions of various measurement errors to the estimation. For \mathbf{S}^{-1} being an $(m \times m)$ symmetric and positive-definite weighting matrix (otherwise arbitrary), then the estimation becomes:

$$E = (\mathbf{z} - \mathbf{H}\hat{\mathbf{x}})^T \mathbf{S}^{-1} (\mathbf{z} - \mathbf{H}\hat{\mathbf{x}})$$

The estimator that minimizes this objective function in this case becomes:

$$\hat{\mathbf{x}} = (\mathbf{H}^T \mathbf{S}^{-1} \mathbf{H})^{-1} \mathbf{H}^T \mathbf{S}^{-1} \mathbf{z}$$

There is no probabilistic interpretation of the arbitrary matrix \mathbf{S}^{-1} so far. However one may adopt a maximum likelihood viewpoint in which the value of the estimator $\hat{\mathbf{x}}$ is inferred from the assumption that, given the value of the state \mathbf{x} , the measurements \mathbf{z} will arrange themselves to form a mode in the probability distribution. In this case given \mathbf{x} , the probability of \mathbf{z} occurring is maximized, i.e. maximize $f(\mathbf{z} | \mathbf{x})$.

Here we need to introduce assumptions on the distribution of the measurements. If it is assumed that the measurements are gaussian distributed, then the conditional probability density function $f(\mathbf{z} | \mathbf{x})$ may be characterized by its mean and variance. Given

$$\mathbf{z} = \mathbf{H}\mathbf{x} + \mathbf{v}$$

with $E[\mathbf{v}] = \mathbf{0}$ and $E[\mathbf{v}\mathbf{v}^T] = \mathbf{R}$, i.e. the measurement errors are zero-mean additive errors with covariance \mathbf{R} , then the conditional mean $E(\mathbf{z} | \mathbf{x})$

and variance $var(\mathbf{z} | \mathbf{x})$ may be developed to yield the conditional probability density function $f(\mathbf{z} | \mathbf{x})$. If \mathbf{x} is given, then it is treated as a constant in $\mathbf{z} = \mathbf{H}\mathbf{x} + \mathbf{v}$ and

$$E(\mathbf{z} | \mathbf{x}) = \mathbf{H}\mathbf{x}$$

since $E[\mathbf{v}] = \mathbf{0}$. Since $\mathbf{H}\mathbf{x}$ is a constant when statistics are conditioned on \mathbf{x} , then

$$var(\mathbf{z} | \mathbf{x}) = \mathbf{R}$$

Thus the gaussian probability density function may be written as

$$f(\mathbf{z} | \mathbf{x}) = \frac{1}{(2\pi)^{m/2} |\mathbf{R}|^{1/2}} \exp \left\{ -\frac{1}{2} (\mathbf{z} - \mathbf{H}\mathbf{x})^T \mathbf{R}^{-1} (\mathbf{z} - \mathbf{H}\mathbf{x}) \right\}$$

Maximizing $f(\mathbf{z} | \mathbf{x})$ is equivalent to minimizing the exponent of the exponentiation $\left\{ -\frac{1}{2} (\mathbf{z} - \mathbf{H}\mathbf{x})^T \mathbf{R}^{-1} (\mathbf{z} - \mathbf{H}\mathbf{x}) \right\}$. This will be identical to the *weighted* least-squares estimator if $\mathbf{S}^{-1} = \mathbf{R}^{-1}$. Thus the maximum-likelihood linear estimator that assumes gaussian measurement error distribution is

$$\hat{\mathbf{x}} = (\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})^{-1} \mathbf{H}^T \mathbf{R}^{-1} \mathbf{z}$$

Note that if the measurement errors are uncorrelated and have equal variance (equivalent to having no information on the relative weight of the measurement errors), then

$$\mathbf{R} = r\mathbf{I}$$

which, when substituted yields the previous simpler least-squares estimator

$$\begin{aligned} \hat{\mathbf{x}} &= (\mathbf{H}^T r\mathbf{I}\mathbf{H})^{-1} \mathbf{H}^T r\mathbf{I}^{-1} \mathbf{z} \\ &= \frac{r}{r} (\mathbf{H}^T \mathbf{H})^{-1} \mathbf{H}^T \mathbf{z} \\ &= (\mathbf{H}^T \mathbf{H})^{-1} \mathbf{H}^T \mathbf{z} \end{aligned}$$

1.9 Maximum Likelihood for Inverse Problems

Given the gaussian distribution $f(\mathbf{d})$ for the data in the inverse problem, its maximization corresponds to the minimization of $(\mathbf{d} - \mathbf{G}\mathbf{m})^T [\text{covd}]^{-1} (\mathbf{d} - \mathbf{G}\mathbf{m})$.

The solution is then just a weighted least squares. Note that the hypothesis of Gaussian distribution of the data is necessary to obtain the least-squares solution from the maximum likelihood principle!

As before, such a solution is unique only if the problem is not undetermined.

1.9.1 The Underdetermined Problem and A Priori Distributions

When the linear inverse problem is undetermined, $f(\mathbf{d})$ has no distinct maximum with respect to variations in the model parameters. Some prior information is needed to solve the problem, which in probabilistic terms may be represented as an a priori probability distribution $f_A(\mathbf{m})$ for the model parameters. Analogously, instead of defining directly $f(\mathbf{d})$, we can summarize our knowledge about the data in the a priori data distribution $f_A(\mathbf{d})$. An a priori data distribution simply summarizes the observations, so its mean is \mathbf{d}^{obs} and its variance is equal to the expected variance of the data. Since $f_A(\mathbf{d})$ and $f_A(\mathbf{m})$ are independent, we can define the joint a priori distribution $f_A(\mathbf{m}, \mathbf{d}) = f_A(\mathbf{m}) f_A(\mathbf{d})$.

If the model $\mathbf{G}\mathbf{m} = \mathbf{d}$ may be regarded as exact, it defines a surface in the space (\mathbf{m}, \mathbf{d}) , where also $f_A(\mathbf{m}, \mathbf{d})$ is defined. The maximum likelihood principle then translate into finding the maximum of $f_A(\mathbf{m}, \mathbf{d})$ on the $\mathbf{G}\mathbf{m} = \mathbf{d}$ surface.

If the model $\mathbf{G}\mathbf{m} = \mathbf{d}$ may be regarded as inexact, that is there are errors associated also with the matrix \mathbf{G} , we may regard it, rather than as a surface, as a (conditional) distribution $f_g(\mathbf{d}|\mathbf{m})$ which is centered on the surface $\mathbf{G}\mathbf{m} = \mathbf{d}$ and whose spread around this surface depends on the uncertainty of the model. Because the model is assumed to be independent of the actual values of data and parameters, the maximum likelihood principle translates in simply finding the maximum, with respect to \mathbf{m} , of a total probability distribution defined as $f_T(\mathbf{m}, \mathbf{d}) = f_A(\mathbf{m}, \mathbf{d}) f_g(\mathbf{d}|\mathbf{m})$. To find the maximum with respect to \mathbf{m} only, we must "sum" all the probabilities along surfaces with constant \mathbf{m} in the (\mathbf{m}, \mathbf{d}) space, that is we need to find the minimum of the "projected" probability distribution:

$$f_P(\mathbf{m}) = \int f_T(\mathbf{m}, \mathbf{d}) d\mathbf{d}$$

1.9.2 The General Linear Gaussian Case

We assume the following gaussian multivariate distribution in the linear problem $\mathbf{G}\mathbf{m} = \mathbf{d}$:

$$\begin{aligned} f_A(\mathbf{m}) &\propto \exp \left[-\frac{1}{2} (\mathbf{m} - \langle \mathbf{m} \rangle)^T [\text{covm}]^{-1} (\mathbf{m} - \langle \mathbf{m} \rangle) \right] \\ f_A(\mathbf{d}) &\propto \exp \left[-\frac{1}{2} (\mathbf{d} - \mathbf{d}^{obs})^T [\text{covd}]^{-1} (\mathbf{d} - \mathbf{d}^{obs}) \right] \\ f_g(\mathbf{d}|\mathbf{m}) &\propto \exp \left[-\frac{1}{2} (\mathbf{d} - \mathbf{G}\mathbf{m})^T [\text{covg}]^{-1} (\mathbf{d} - \mathbf{G}\mathbf{m}) \right] \end{aligned}$$

The total distribution $f_T(\mathbf{m}, \mathbf{d})$, product of the baove three, may be proved to be again a multivariate gaussian distribution. After projection to obtain $f_P(\mathbf{m})$ and its maximization, the following general linear gaussian maximum likelihood solution is obtained:

$$\mathbf{m}^{est} = \langle \mathbf{m} \rangle + \mathbf{G}^{-g} [\mathbf{d}^{obs} - \mathbf{G} \langle \mathbf{m} \rangle]$$

where \mathbf{G}^{-g} may be written as:

$$\begin{aligned} \mathbf{G}^{-g} &= [\text{covm}] \mathbf{G}^T \{ [\text{covd}] + [\text{covg}] + \mathbf{G} [\text{covm}] \mathbf{G}^T \}^{-1} \\ &\text{if } [\mathbf{G}\mathbf{G}^T]^{-1} \text{ exists} \end{aligned}$$

or:

$$\begin{aligned} \mathbf{G}^{-g} &= \{ \mathbf{G}^T [[\text{covd}] + [\text{covg}]]^{-1} \mathbf{G} + [\text{covm}]^{-1} \}^{-1} \mathbf{G}^T \{ [\text{covd}] + [\text{covg}] \}^{-1} \\ &\text{if } [\mathbf{G}^T \mathbf{G}]^{-1} \text{ exists} \end{aligned}$$

1.9.3 Limiting cases with uncorrelated quantities

For uncorrelated a priori model parameters ($[\text{covm}] = \sigma_m^2 \mathbf{I}$), data ($[\text{covd}] = \sigma_d^2 \mathbf{I}$) and model ($[\text{covg}] = \sigma_g^2 \mathbf{I}$), we obtain:

$$\begin{aligned} \mathbf{G}^{-g} &= \sigma_m^2 \mathbf{G}^T \{ (\sigma_d^2 + \sigma_g^2) \mathbf{I} + \sigma_m^2 \mathbf{G}\mathbf{G}^T \}^{-1} \\ &\text{if } [\mathbf{G}\mathbf{G}^T]^{-1} \text{ exists} \end{aligned}$$

or:

$$\mathbf{G}^{-g} = \left\{ (\sigma_d^2 + \sigma_g^2)^{-1} \mathbf{G}^T \mathbf{G} + (\sigma_m^2)^{-1} \mathbf{I} \right\}^{-1} \mathbf{G}^T (\sigma_d^2 + \sigma_g^2)^{-1}$$

if $[\mathbf{G}^T \mathbf{G}]^{-1}$ *exists*

For exact data and model, setting $\sigma_d^2 = \sigma_g^2 = 0$ we simply obtain:

$$\mathbf{G}^{-g} = \mathbf{G}^T [\mathbf{G}\mathbf{G}^T]^{-1}$$

if $[\mathbf{G}\mathbf{G}^T]^{-1}$ *exists*

that is the constrained-minimization solution for the purely undetermined problem, or:

$$\mathbf{G}^{-g} = [\mathbf{G}^T \mathbf{G}]^{-1} \mathbf{G}^T$$

if $[\mathbf{G}^T \mathbf{G}]^{-1}$ *exists*

that is the least-squares solution for the overdetermined problem.

1.9.4 The General Linear Problem with Exponential Distributions

Consider the linear inverse problem $\mathbf{G}\mathbf{m} = \mathbf{d}$ with uncorrelated data and parameters, known means \mathbf{d}^{obs} and $\langle \mathbf{m} \rangle$ and known standard deviations σ_d and σ_m . The joint distribution is assumed to be exponential:

$$f(\mathbf{d}, \mathbf{m}) = 2^{-(N+M)/2} \prod_{i=1}^N \sigma_{di}^{-1} \prod_{i=1}^M \sigma_{mi}^{-1} \exp \left[-\frac{1}{\sqrt{2}} \sum_{i=1}^N \frac{|e_i|}{\sigma_{di}} - \frac{1}{\sqrt{2}} \sum_{i=1}^M \frac{|l_i|}{\sigma_{mi}} \right]$$

where $\mathbf{e} = \mathbf{d} - \mathbf{G}\mathbf{m}$ is the prediction error and $\mathbf{l} = \mathbf{m} - \langle \mathbf{m} \rangle$ is the solution length. Finding the maximum likelihood is equivalent to finding the minimum of the argument of the exponential, that is minimizing the sum of the weighted L_1 norms of the prediction error and solution length:

$$E + L = \sum_{i=1}^N \frac{|e_i|}{\sigma_{di}} + \sum_{i=1}^M \frac{|l_i|}{\sigma_{mi}}$$

Note that now the weights are proportional to the inverse of the standard deviation, not to the inverse of the variance as in the gaussian case!

The above, apparently non-linear, minimization problem can be transformed in a linear programming problem of the form:

Find the vector \mathbf{x} that maximizes (or minimizes) $z = \mathbf{c}^T \mathbf{x}$ subject to the constraints $\mathbf{Ax} \begin{bmatrix} \geq \\ = \\ \leq \end{bmatrix} \mathbf{b}$ and $\mathbf{x} \geq \mathbf{0}$.

Let us consider, for the sake of simplicity, the purely undetermined problem with a priori model parameters $\langle \mathbf{m} \rangle$ and σ_m , so that we want to minimize the weighted L_1 norm of the solution length:

$$L = \sum_{i=1}^M \frac{|l_i|}{\sigma_{mi}}$$

subject to the constraint $\mathbf{Gm} = \mathbf{d}$.

We then introduce 5 new vectors \mathbf{m}' , \mathbf{m}'' , α , \mathbf{x} , \mathbf{x}' , each of length M , and consider the following linear programming problem

(let also $\mathbf{s} = [\sigma_{m1}^{-1}, \sigma_{m2}^{-1}, \dots, \sigma_{mM}^{-1}]^T$):

$$\begin{aligned} & \text{Minimize } z = \mathbf{s}^T \alpha \\ & \text{subject to the constraints:} \\ & \quad \mathbf{G} [\mathbf{m}' - \mathbf{m}''] = \mathbf{d} \\ & \quad \mathbf{m}' - \mathbf{m}'' + \mathbf{x} - \alpha = \langle \mathbf{m} \rangle \\ & \quad \mathbf{m}' - \mathbf{m}'' - \mathbf{x}' + \alpha = \langle \mathbf{m} \rangle \\ & \quad \mathbf{m}' \geq \mathbf{0}; \quad \mathbf{m}'' \geq \mathbf{0}; \quad \alpha \geq \mathbf{0}; \quad \mathbf{x} \geq \mathbf{0}; \quad \mathbf{x}' \geq \mathbf{0} \end{aligned}$$

If one makes the identification $\mathbf{m} = \mathbf{m}' - \mathbf{m}''$, signs of \mathbf{m} are not constrained, while the ones of \mathbf{m}' and \mathbf{m}'' are (as required by linear programming). Then two of the constraints are equivalent to:

$$\begin{aligned} \alpha - \mathbf{x} &= [\mathbf{m} - \langle \mathbf{m} \rangle] \\ \alpha - \mathbf{x}' &= -[\mathbf{m} - \langle \mathbf{m} \rangle] \end{aligned}$$

Now if $[\mathbf{m} - \langle \mathbf{m} \rangle]$ is positive, the first equation requires $\alpha \geq [\mathbf{m} - \langle \mathbf{m} \rangle]$ since \mathbf{x} is non-negative, while the second can be satisfied by some appropriate \mathbf{x}' . If $[\mathbf{m} - \langle \mathbf{m} \rangle]$ is negative, the second equation requires $\alpha \geq -[\mathbf{m} - \langle \mathbf{m} \rangle]$ since \mathbf{x}' is non-negative, while the first can be satisfied by some appropriate

\mathbf{x} . Then these two equations are equivalent to the constraint $\boldsymbol{\alpha} \geq |\mathbf{m} - \langle \mathbf{m} \rangle|$, and minimizing $\mathbf{s}^T \boldsymbol{\alpha}$ is equivalent to minimizing L .

Similar procedures may be easily developed for the overdetermined and the mixed-determined problems.

1.10 The Bayesian Estimator

1.10.1 Cost Function with Complete Prior Information

When there is knowledge of the distributional features of both measurements and states, a superior estimator may be constructed using Bayes theorem. The Bayesian estimators states that the optimal estimate of $\hat{\mathbf{x}}$ should minimize the cost function

$$C(\hat{\mathbf{x}}(\mathbf{z}), \mathbf{x}) = C(\hat{\mathbf{x}}, \mathbf{x}) = (\mathbf{x} - \hat{\mathbf{x}})^T \mathbf{S}^{-1} (\mathbf{x} - \hat{\mathbf{x}})$$

over all possible values of \mathbf{x} and \mathbf{z} given their distributional assumptions. The Bayes risk function may thus be defined

$$B(\hat{\mathbf{x}}(\mathbf{z}), \mathbf{x}) = B(\hat{\mathbf{x}}, \mathbf{x}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (\mathbf{x} - \hat{\mathbf{x}})^T \mathbf{S}^{-1} (\mathbf{x} - \hat{\mathbf{x}}) f(\mathbf{x}, \mathbf{z}) d\mathbf{x}$$

where $f(\mathbf{x}, \mathbf{z})$ is the joint probability density function of \mathbf{x} and \mathbf{z} . This expression may be re-written as

$$B(\hat{\mathbf{x}}, \mathbf{x}) = \int_{-\infty}^{\infty} \left\{ \int_{-\infty}^{\infty} (\mathbf{x} - \hat{\mathbf{x}})^T \mathbf{S}^{-1} (\mathbf{x} - \hat{\mathbf{x}}) f(\mathbf{x} | \mathbf{z}) d\mathbf{x} \right\} f(\mathbf{z}) d\mathbf{z}$$

using

$$f(\mathbf{x}, \mathbf{z}) = f(\mathbf{x} | \mathbf{z}) f(\mathbf{z})$$

Since $B(\hat{\mathbf{x}}, \mathbf{x})$ is being minimized with respect to \mathbf{x} and the terms outside of the brackets $\{\cdot\}$ are independent of \mathbf{x} , then minimizing $B(\hat{\mathbf{x}}, \mathbf{x})$ is equivalent to minimizing the conditional Bayes risk function

$$\begin{aligned} B(\hat{\mathbf{x}} | \mathbf{z}) &= \int_{-\infty}^{\infty} (\mathbf{x} - \hat{\mathbf{x}})^T \mathbf{S}^{-1} (\mathbf{x} - \hat{\mathbf{x}}) f(\mathbf{x} | \mathbf{z}) d\mathbf{x} \\ &= E[C(\hat{\mathbf{x}}, \mathbf{x}) | \mathbf{z}] \end{aligned}$$

Taking derivative and setting to zero

$$\begin{aligned}\frac{\partial B(\hat{\mathbf{x}} | \mathbf{z})}{\partial \hat{\mathbf{x}}} &= 2 \int_{-\infty}^{\infty} \mathbf{S}(\mathbf{x} - \hat{\mathbf{x}}) f(\mathbf{x} | \mathbf{z}) d\mathbf{x} \\ &= \mathbf{0}\end{aligned}$$

has the solution

$$\hat{\mathbf{x}} \int_{-\infty}^{\infty} f(\mathbf{x} | \mathbf{z}) d\mathbf{x} = \int_{-\infty}^{\infty} \mathbf{x} f(\mathbf{x} | \mathbf{z}) d\mathbf{x}$$

The left-hand and right-hand sides of this expression are simply

$$\hat{\mathbf{x}} = E[\mathbf{x} | \mathbf{z}]$$

i.e. the Bayesian estimator is the conditional expectation of the state \mathbf{x} given measurements \mathbf{z} . In order to complete this derivation by evaluating $E[\mathbf{x} | \mathbf{z}]$, the conditional probability density function $f(\mathbf{x} | \mathbf{z})$ needs to be developed. The Bayes theorem may now be used to identify the conditional distribution $f(\mathbf{x} | \mathbf{z})$ based on the statistics of the state \mathbf{x} and the measurements \mathbf{z} . Bayes theorem states that

$$f(\mathbf{x} | \mathbf{z}) = \frac{f(\mathbf{z} | \mathbf{x}) f(\mathbf{x})}{f(\mathbf{z})}$$

1.10.2 The Case of Gaussian Distributions

Now \mathbf{x} and \mathbf{z} are assumed to be gaussian distributed. Since gaussian distributions may be characterized through the mean and variance only, we seek to develop the statistics for the probability density functions $f(\mathbf{x})$, $f(\mathbf{z})$, and $f(\mathbf{z} | \mathbf{x})$. We assume

$$E[\mathbf{x}] = \mathbf{m}$$

$$\text{var}[\mathbf{x}] = E[(\mathbf{x} - \mathbf{m})(\mathbf{x} - \mathbf{m})^T] = \mathbf{P}$$

The statistics of the measurements may similarly be established

$$\begin{aligned}E[\mathbf{z}] &= E[\mathbf{H}\mathbf{x} + \mathbf{v}] \\ &= E[\mathbf{H}\mathbf{x}] + E[\mathbf{v}] \\ &= \mathbf{H}E[\mathbf{x}] = \mathbf{H}\mathbf{m}\end{aligned}$$

and

$$\begin{aligned}
var [\mathbf{z}] &= E [\mathbf{z}\mathbf{z}^T] = \mathbf{E} \left[(\mathbf{H}\mathbf{x} + \mathbf{v}) (\mathbf{H}\mathbf{x} + \mathbf{v})^T \right] \\
&= \mathbf{E} \left[\mathbf{H}\mathbf{x}\mathbf{x}^T\mathbf{H}^T + 2\mathbf{H}\mathbf{x}\mathbf{v}^T + \mathbf{v}\mathbf{v}^T \right] \\
&= \mathbf{H}E [\mathbf{x}\mathbf{x}^T] \mathbf{H}^T + E [\mathbf{v}\mathbf{v}^T] \\
&= \mathbf{H}\mathbf{P}\mathbf{H}^T + \mathbf{R}
\end{aligned}$$

since the measurement errors and the state are not correlated, i.e. $E [\mathbf{H}\mathbf{x}\mathbf{v}^T] = \mathbf{0}$.

We have further established that if \mathbf{x} is given, then it is treated as a constant in $\mathbf{z} = \mathbf{H}\mathbf{x} + \mathbf{v}$ and

$$E(\mathbf{z} | \mathbf{x}) = \mathbf{H}\mathbf{x}$$

since $E[\mathbf{v}] = \mathbf{0}$. Since $\mathbf{H}\mathbf{x}$ is a constant when statistics are conditioned on \mathbf{x} , then

$$var(\mathbf{z} | \mathbf{x}) = \mathbf{R}$$

Using these statistics ($E[\mathbf{x}]$, $var[\mathbf{x}]$, $E[\mathbf{z}]$, $var[\mathbf{z}]$, $E[\mathbf{z} | \mathbf{x}]$, $var[\mathbf{z} | \mathbf{x}]$) and the gaussian distributional assumptions, we may find the probability density function $f(\mathbf{x} | \mathbf{z})$. Using these moments of the distributions we write:

$$f(\mathbf{x}) = \frac{1}{(2\pi)^{n/2} |\mathbf{P}|^{\frac{1}{2}}} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \mathbf{m})^T \mathbf{P}^{-1} (\mathbf{x} - \mathbf{m}) \right\}$$

$$f(\mathbf{z} | \mathbf{x}) = \frac{1}{(2\pi)^{m/2} |\mathbf{R}|^{\frac{1}{2}}} \exp \left\{ -\frac{1}{2} (\mathbf{z} - \mathbf{H}\mathbf{x})^T \mathbf{R}^{-1} (\mathbf{z} - \mathbf{H}\mathbf{x}) \right\}$$

and

$$f(\mathbf{z}) = \frac{1}{(2\pi)^{m/2} |\mathbf{H}\mathbf{P}\mathbf{H}^T + \mathbf{R}|^{\frac{1}{2}}} \exp \left\{ -\frac{1}{2} (\mathbf{z} - \mathbf{H}\mathbf{m})^T (\mathbf{H}\mathbf{P}\mathbf{H}^T + \mathbf{R})^{-1} (\mathbf{z} - \mathbf{H}\mathbf{m}) \right\}$$

Use these distributions in Bayes theorem:

$$f(\mathbf{x} | \mathbf{z}) = \frac{f(\mathbf{z} | \mathbf{x}) f(\mathbf{x})}{f(\mathbf{z})}$$

to write

$$f(\mathbf{x} | \mathbf{z}) = \frac{|\mathbf{H}\mathbf{P}\mathbf{H}^T + \mathbf{R}|^{\frac{1}{2}}}{(2\pi)^{n/2} |\mathbf{P}|^{\frac{1}{2}} |\mathbf{R}|^{\frac{1}{2}}} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \hat{\mathbf{x}})^T (\boldsymbol{\Sigma})^{-1} (\mathbf{x} - \hat{\mathbf{x}}) \right\}$$

where

$$\hat{\mathbf{x}} = (\mathbf{P}^{-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})^{-1} (\mathbf{H}^T \mathbf{R}^{-1} \mathbf{z} + \mathbf{P}^{-1} \mathbf{m})$$

and

$$\boldsymbol{\Sigma}^{-1} = \mathbf{P}^{-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H}$$

have been defined. The estimator alternately be written as

$$\hat{\mathbf{x}} = \boldsymbol{\Sigma} (\mathbf{H}^T \mathbf{R}^{-1} \mathbf{z} + \mathbf{P}^{-1} \mathbf{m})$$

The Bayes estimator is a most general estimator in this context. If nothing is known about the state \mathbf{x} , i.e. $\mathbf{P} \rightarrow \infty \mathbf{I}$ or $\mathbf{P}^{-1} \rightarrow \mathbf{0}$, then the Bayesian estimator collapses into the MLE estimator

$$\hat{\mathbf{x}} = (\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})^{-1} \mathbf{H}^T \mathbf{R}^{-1} \mathbf{z}$$

consistent with the distributional assumptions. If furthermore the measurement errors are uncorrelated and characterized by equal variance, i.e. $\mathbf{R} = r\mathbf{I}$, the MLE estimator further reduces to the LSE estimator

$$\hat{\mathbf{x}} = (\mathbf{H}^T \mathbf{H})^{-1} \mathbf{H}^T \mathbf{z}$$

The Bayesian estimator weights the prior estimates of the state from the distribution of the state with the measurements.

For further interpretation of the Bayesian estimator take $\mathbf{H} = \mathbf{I}$ which gives

$$\begin{aligned} \hat{\mathbf{x}} &= (\mathbf{P}^{-1} + \mathbf{R}^{-1})^{-1} (\mathbf{R}^{-1} \mathbf{z} + \mathbf{P}^{-1} \mathbf{m}) \\ &= (\mathbf{P}^{-1} + \mathbf{R}^{-1})^{-1} \mathbf{R}^{-1} \mathbf{z} + (\mathbf{P}^{-1} + \mathbf{R}^{-1})^{-1} \mathbf{P}^{-1} \mathbf{m} \\ &= (\mathbf{R} (\mathbf{P}^{-1} + \mathbf{R}^{-1}))^{-1} \mathbf{z} + (\mathbf{P} (\mathbf{P}^{-1} + \mathbf{R}^{-1}))^{-1} \mathbf{m} \\ &= ((\mathbf{R}\mathbf{P}^{-1} + \mathbf{I}))^{-1} \mathbf{z} + ((\mathbf{I} + \mathbf{P}\mathbf{R}^{-1}))^{-1} \mathbf{m} \\ &= ((\mathbf{R} + \mathbf{P}) \mathbf{P}^{-1})^{-1} \mathbf{z} + ((\mathbf{R} + \mathbf{P}) \mathbf{R}^{-1})^{-1} \mathbf{m} \\ &= ((\mathbf{R} + \mathbf{P}) \mathbf{P}^{-1})^{-1} \mathbf{z} + ((\mathbf{R} + \mathbf{P}) \mathbf{R}^{-1})^{-1} \mathbf{m} \\ &= \mathbf{P} (\mathbf{R} + \mathbf{P})^{-1} \mathbf{z} + \mathbf{R} (\mathbf{R} + \mathbf{P})^{-1} \mathbf{m} \end{aligned}$$

Now if measurements are more trustworthy than the prior estimates of the state, i.e. \mathbf{R} is smaller than \mathbf{P} , then estimate of $\hat{\mathbf{x}}$ will mostly rely on the measurements \mathbf{z} . On the other hand if the measurements are exceedingly noisy, then \mathbf{R} is larger than \mathbf{P} , then the prior estimate of the mean of the state (\mathbf{m}) forms the best estimate of the state $\hat{\mathbf{x}}$. In reality both the prior and the measurements are needed to form the estimate $\hat{\mathbf{x}}$ and they are weighted in proportion to their uncertainty through the variance matrices. If a weight

$$\mathbf{K} = \mathbf{P} (\mathbf{R} + \mathbf{P})^{-1}$$

is defined, then

$$\begin{aligned} \mathbf{I} - \mathbf{K} &= \mathbf{I} - \mathbf{P} (\mathbf{R} + \mathbf{P})^{-1} \\ &= ((\mathbf{R} + \mathbf{P}) - \mathbf{P}) (\mathbf{R} + \mathbf{P})^{-1} \\ &= \mathbf{R} (\mathbf{R} + \mathbf{P})^{-1} \end{aligned}$$

so that

$$\hat{\mathbf{x}} = \mathbf{K}\mathbf{z} + (\mathbf{I} - \mathbf{K}) \mathbf{m}$$

The weights sum to unity.

2 Estimation in Time and Inverse Dynamic Problems

2.1 Estimation in Dynamic Systems

2.1.1 State-space Formulation of Forced Dynamical Systems

A linear dynamic system consisting of an $n \times 1$ state vector $\mathbf{x}(t)$ is propagated in time according to

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}(t) \mathbf{x}(t)$$

Given an initial condition $\mathbf{x}(t_0)$, the solution to this equation is

$$\mathbf{x}(t) = \mathbf{\Phi}(t, t_0) \mathbf{x}(t_0)$$

The linear transition matrix $\mathbf{\Phi}(t, t_0)$ itself obeys

$$\begin{aligned} \frac{d\mathbf{\Phi}}{dt} &= \mathbf{F}(t) \mathbf{\Phi}(t, t_0) \\ \text{subject to } \mathbf{\Phi}(t_0, t_0) &= \mathbf{I} \end{aligned}$$

It is also possible to relate values of the state at successive time periods to the initial state as in

$$\begin{aligned}\mathbf{x}(t_2) &= \Phi(t_2, t_1) \mathbf{x}(t_1) \\ &= \Phi(t_2, t_1) \Phi(t_1, t_0) \mathbf{x}(t_0)\end{aligned}$$

When the system is time-invariant meaning that \mathbf{F} is not a function of time, then the transition depends only on the time separation, i.e.

$$\Phi(t_2, t_1) = \Phi(t_2 - t_1)$$

For this case the solution to the dynamic system is obtained by first expanding the state into a Taylor series around the initial state

$$\mathbf{x}(t) = \mathbf{x}(t_0) + \frac{d\mathbf{x}}{dt}(t - t_0) + \frac{d^2\mathbf{x}}{dt^2} \frac{(t - t_0)^2}{2!} + \dots$$

Notice that for the time-invariant case

$$\begin{aligned}\frac{d\mathbf{x}}{dt} &= \mathbf{F}\mathbf{x}(t_0) \\ \frac{d^2\mathbf{x}}{dt^2} &= \mathbf{F}^2\mathbf{x}(t_0) \\ \frac{d^3\mathbf{x}}{dt^3} &= \mathbf{F}^3\mathbf{x}(t_0)\end{aligned}$$

and so on so that

$$\begin{aligned}\mathbf{x}(t) &= \left[\mathbf{I} + \mathbf{F}(t - t_0) + \mathbf{F}^2 \frac{(t - t_0)^2}{2!} + \dots \right] \mathbf{x}(t_0) \\ &= e^{\mathbf{F}(t - t_0)} \mathbf{x}(t_0)\end{aligned}$$

so that $\Phi(t, t_0) = e^{\mathbf{F}(t - t_0)}$.

When the system is forced by a deterministic signal $\mathbf{u}(t)$ as in

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}(t) \mathbf{x}(t) + \mathbf{L}(t) \mathbf{u}(t)$$

then the transition is given by the linear state propagation and a convolution of past deterministic forcing,

$$\mathbf{x}(t) = \Phi(t, t_0) \mathbf{x}(t_0) + \int_{t_0}^t \Phi(t, \tau) \mathbf{L}(\tau) \mathbf{u}(\tau) d\tau$$

When there is also a stochastic forcing $\mathbf{w}(t)$ present, then

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}(t) \mathbf{x}(t) + \mathbf{L}(t) \mathbf{u}(t) + \mathbf{G}(t) \mathbf{w}(t)$$

and

$$\mathbf{x}(t) = \Phi(t, t_0) \mathbf{x}(t_0) + \int_{t_0}^t \Phi(t, \tau) \mathbf{L}(\tau) \mathbf{u}(\tau) d\tau + \int_{t_0}^t \Phi(t, \tau) \mathbf{G}(\tau) \mathbf{w}(\tau) d\tau$$

If the expression is evaluated for discrete time increments $t = k \cdot \Delta t$ and the convolution is simplified in terms of matrices $\Lambda_k = \int_{t_k}^{t_{k+1}} \Phi(t_k, \tau) \mathbf{L}(\tau) \mathbf{u}(\tau) d\tau$ and $\Gamma_k = \int_{t_k}^{t_{k+1}} \Phi(t_k, \tau) \mathbf{G}(\tau) \mathbf{w}(\tau) d\tau$, then

$$\mathbf{x}_{k+1} = \Phi_k \mathbf{x}_k + \Lambda_k \mathbf{u}_k + \Gamma_k \mathbf{w}_k$$

2.1.2 Propagation of Expectations and Covariances

The dynamic state (mean-removed) with system uncertainty is given by

$$\mathbf{x}_{k+1} = \Phi_k \mathbf{x}_k + \Gamma_k \mathbf{w}_k$$

If the estimate of the state at time k includes all the measurements up to that time, then the latest estimate of the state is the conditional mean denoted by $\hat{\mathbf{x}}_{k|k}$. The mean square error of this state is also given by $\mathbf{P}_{k|k}$ and it is known. A forecast of the state conditional on past observations is performed by taking the expectation of the system equation (conditional expectation given past observations):

$$\hat{\mathbf{x}}_{k+1|k} = \Phi_k \hat{\mathbf{x}}_{k|k}$$

The error of forecast is

$$\begin{aligned} \delta \mathbf{x}_{k+1|k} &= \hat{\mathbf{x}}_{k+1|k} - \mathbf{x}_{k+1} \\ &= \Phi_k \hat{\mathbf{x}}_{k|k} - (\Phi_k \mathbf{x}_k + \Gamma_k \mathbf{w}_k) \\ &= \Phi_k (\hat{\mathbf{x}}_{k|k} - \mathbf{x}_k) - \Gamma_k \mathbf{w}_k \\ &= \Phi_k \delta \mathbf{x}_{k|k} - \Gamma_k \mathbf{w}_k \end{aligned}$$

The error covariance matrix is

$$\begin{aligned} \mathbf{P}_{k+1|k} &= E [\delta \mathbf{x}_{k+1|k} \delta \mathbf{x}_{k+1|k}^T] \\ &= \Phi_k E [\delta \mathbf{x}_{k|k} \delta \mathbf{x}_{k|k}^T] \Phi_k^T - \Phi_k E [\delta \mathbf{x}_{k|k} \mathbf{w}_k^T] \Gamma_k^T \\ &\quad - \Gamma_k E [\mathbf{w}_k \delta \mathbf{x}_{k|k}^T] \Phi_k^T + \Gamma_k E [\mathbf{w}_k \mathbf{w}_k^T] \Gamma_k^T \end{aligned}$$

When the system errors and forecasts errors are uncorrelated (i.e. $E [\delta \mathbf{x}_{k|k} \mathbf{w}_k^T] = E [\mathbf{w}_k \delta \mathbf{x}_{k|k}^T] = \mathbf{0}$) and the system noise covariance is $E [\mathbf{w}_k \mathbf{w}_k^T] = \mathbf{Q}_k$, then

$$\mathbf{P}_{k+1|k} = \Phi_k \mathbf{P}_{k|k} \Phi_k^T + \Gamma_k \mathbf{Q}_k \Gamma_k^T$$

This equation is used to propagate the uncertainty of forecasts given observations until time k . Once an observation of the form

$$\mathbf{z}_{k+1} = \mathbf{H}_{k+1} \mathbf{x}_{k+1} + \mathbf{v}_{k+1}$$

becomes available, it must be combined with the conditional forecasts of the state $\hat{\mathbf{x}}_{k+1|k}$. The observation noise is characterized by $E [\mathbf{v}_k \mathbf{v}_k^T] = \mathbf{R}_k$.

This may be achieved by considering the two values that must be merged to form a new (updated) estimate of the state. The first is the forecast $\hat{\mathbf{x}}_{k+1|k}$ and it has covariance $\mathbf{P}_{k+1|k}$. The second is the observation \mathbf{z}_{k+1} . These two should be linearly weighted to obtain the updated state $\hat{\mathbf{x}}_{k+1|k+1}$ as in

$$\hat{\mathbf{x}}_{k+1|k+1} = \mathbf{K}'_{k+1} \hat{\mathbf{x}}_{k+1|k} + \mathbf{K}_{k+1} \mathbf{z}_{k+1}$$

Since

$$\begin{aligned} \delta \mathbf{x}_{k+1|k+1} &= \hat{\mathbf{x}}_{k+1|k+1} - \mathbf{x}_{k+1} \\ &= [\mathbf{K}'_{k+1} \hat{\mathbf{x}}_{k+1|k} + \mathbf{K}_{k+1} \mathbf{z}_{k+1}] - \mathbf{x}_{k+1} \\ &= [\mathbf{K}'_{k+1} [\mathbf{x}_{k+1} + \delta \mathbf{x}_{k+1|k}] + \mathbf{K}_{k+1} [\mathbf{H}_{k+1} \mathbf{x}_{k+1} + \mathbf{v}_{k+1}]] - \mathbf{x}_{k+1} \\ &= [\mathbf{K}'_{k+1} + \mathbf{K}_{k+1} \mathbf{H}_{k+1} - \mathbf{I}] \mathbf{x}_{k+1} + \mathbf{K}'_{k+1} \delta \mathbf{x}_{k+1|k} + \mathbf{K}_{k+1} \mathbf{v}_{k+1} \end{aligned}$$

Since $E [\delta \mathbf{x}_{k+1|k}] = E [\delta \mathbf{x}_{k+1|k+1}] = \mathbf{0}$ due to the unbiasedness condition and $E [\mathbf{v}_{k+1}] = \mathbf{0}$, then

$$[\mathbf{K}'_{k+1} + \mathbf{K}_{k+1} \mathbf{H}_{k+1} - \mathbf{I}] = \mathbf{0}$$

and therefore

$$\mathbf{K}'_{k+1} = \mathbf{I} - \mathbf{K}_{k+1} \mathbf{H}_{k+1}$$

Thus the update of the conditional mean is

$$\begin{aligned} \hat{\mathbf{x}}_{k+1|k+1} &= [\mathbf{I} - \mathbf{K}_{k+1} \mathbf{H}_{k+1}] \hat{\mathbf{x}}_{k+1|k} + \mathbf{K}_{k+1} \mathbf{z}_{k+1} \\ &= \hat{\mathbf{x}}_{k+1|k} + \mathbf{K}_{k+1} [\mathbf{z}_{k+1} - \mathbf{H}_{k+1} \hat{\mathbf{x}}_{k+1|k}] \end{aligned}$$

Substituting for \mathbf{z}_{k+1} gives

$$\begin{aligned}\widehat{\mathbf{x}}_{k+1|k+1} &= \widehat{\mathbf{x}}_{k+1|k} + \mathbf{K}_{k+1} [\mathbf{H}_{k+1}\mathbf{x}_{k+1} + \mathbf{v}_{k+1} - \mathbf{H}_{k+1}\widehat{\mathbf{x}}_{k+1|k}] \\ &= [\mathbf{I} - \mathbf{K}_{k+1}\mathbf{H}_{k+1}] \widehat{\mathbf{x}}_{k+1|k} + \mathbf{K}_{k+1}\mathbf{H}_{k+1}\mathbf{x}_{k+1} + \mathbf{K}_{k+1}\mathbf{v}_{k+1}\end{aligned}$$

Subtract the true state at time $k + 1$ to derive the forecast error after update

$$\begin{aligned}\widehat{\mathbf{x}}_{k+1|k+1} - \mathbf{x}_{k+1} &= \delta\mathbf{x}_{k+1|k+1} \\ &= [\mathbf{I} - \mathbf{K}_{k+1}\mathbf{H}_{k+1}] \widehat{\mathbf{x}}_{k+1|k} - [\mathbf{I} - \mathbf{K}_{k+1}\mathbf{H}_{k+1}] \mathbf{x}_{k+1} + \mathbf{K}_{k+1}\mathbf{v}_{k+1} \\ &= [\mathbf{I} - \mathbf{K}_{k+1}\mathbf{H}_{k+1}] \delta\mathbf{x}_{k+1|k} + \mathbf{K}_{k+1}\mathbf{v}_{k+1}\end{aligned}$$

The update of the covariance is achieved by noting that

$$\begin{aligned}\mathbf{P}_{k+1|k+1} &= E [\delta\mathbf{x}_{k+1|k+1}\delta\mathbf{x}_{k+1|k+1}^T] \\ &= E \left[[\mathbf{I} - \mathbf{K}_{k+1}\mathbf{H}_{k+1}] \widehat{\mathbf{x}}_{k+1|k} \left[\widehat{\mathbf{x}}_{k+1|k}^T [\mathbf{I} - \mathbf{K}_{k+1}\mathbf{H}_{k+1}]^T + \mathbf{v}_{k+1}^T \mathbf{K}_{k+1}^T \right] \right] \\ &\quad + \mathbf{K}_{k+1}\mathbf{v}_{k+1} \left[\widehat{\mathbf{x}}_{k+1|k}^T [\mathbf{I} - \mathbf{K}_{k+1}\mathbf{H}_{k+1}]^T + \mathbf{v}_{k+1}^T \mathbf{K}_{k+1}^T \right]\end{aligned}$$

Since $\mathbf{P}_{k+1|k} = E [\delta\mathbf{x}_{k+1|k}\delta\mathbf{x}_{k+1|k}^T]$ and $E [\mathbf{v}_{k+1}\mathbf{v}_{k+1}^T] = \mathbf{R}_{k+1}$, then the error covariance update equation is

$$\mathbf{P}_{k+1|k+1} = [\mathbf{I} - \mathbf{K}_{k+1}\mathbf{H}_{k+1}] \mathbf{P}_{k+1|k} [\mathbf{I} - \mathbf{K}_{k+1}\mathbf{H}_{k+1}]^T + \mathbf{K}_{k+1}\mathbf{R}_{k+1}\mathbf{K}_{k+1}^T$$

given $E [\delta\mathbf{x}_{k+1|k}\mathbf{v}_{k+1}^T] = \mathbf{0}$.

The remaining question is the optimum choice for \mathbf{K}_{k+1} . The optimal choice is once that minimizes the cost function

$$J = E [\delta\mathbf{x}_{k+1|k+1}^T \mathbf{S}^{-1} \delta\mathbf{x}_{k+1|k+1}]$$

where \mathbf{S} is an arbitrary positive-definite matrix. If we choose $\mathbf{S} = \mathbf{I}$, then

$$J = \text{trace} [\mathbf{P}_{k+1|k+1}]$$

Taking partial derivative with respect to the unknown matrix \mathbf{K}_{k+1} and setting to zero yields

$$-2 [\mathbf{I} - \mathbf{K}_{k+1}\mathbf{H}_{k+1}] \mathbf{P}_{k+1|k} \mathbf{H}_{k+1}^T + 2\mathbf{K}_{k+1}\mathbf{R}_{k+1} = \mathbf{0}$$

Solve for \mathbf{K}_{k+1} ,

$$\mathbf{K}_{k+1} = \mathbf{P}_{k+1|k} \mathbf{H}_{k+1}^T [\mathbf{H}_{k+1} \mathbf{P}_{k+1|k} \mathbf{H}_{k+1}^T + \mathbf{R}_{k+1}]^{-1}$$

This matrix is known as the Kalman gain matrix and the collection of forecast and update equations below represent the Kalman-Bucy filter for estimation of state in noisy dynamic linear systems with noisy measurements:

$$\begin{aligned} \text{Forecast} &: \hat{\mathbf{x}}_{k+1|k} = \Phi_k \hat{\mathbf{x}}_{k|k} \\ \mathbf{P}_{k+1|k} &= \Phi_k \mathbf{P}_{k|k} \Phi_k^T + \Gamma_k \mathbf{Q}_k \Gamma_k^T \\ \text{Update} &: \hat{\mathbf{x}}_{k+1|k+1} = \hat{\mathbf{x}}_{k+1|k} + \mathbf{K}_{k+1} [\mathbf{z}_{k+1} - \mathbf{H}_{k+1} \hat{\mathbf{x}}_{k+1|k}] \\ \mathbf{P}_{k+1|k+1} &= [\mathbf{I} - \mathbf{K}_{k+1} \mathbf{H}_{k+1}] \mathbf{P}_{k+1|k} [\mathbf{I} - \mathbf{K}_{k+1} \mathbf{H}_{k+1}]^T + \mathbf{K}_{k+1} \mathbf{R}_{k+1} \mathbf{K}_{k+1}^T \\ \text{with } \mathbf{K}_{k+1} &= \mathbf{P}_{k+1|k} \mathbf{H}_{k+1}^T [\mathbf{H}_{k+1} \mathbf{P}_{k+1|k} \mathbf{H}_{k+1}^T + \mathbf{R}_{k+1}]^{-1} \end{aligned}$$

In order to interpret the effects of system noise and observation noise on measurements, suppose that $\mathbf{H}_{k+1} = \mathbf{I}$ so

$$\begin{aligned} \text{Update} &: \hat{\mathbf{x}}_{k+1|k+1} = \hat{\mathbf{x}}_{k+1|k} + \mathbf{K}_{k+1} [\mathbf{z}_{k+1} - \hat{\mathbf{x}}_{k+1|k}] \\ &= [\mathbf{I} - \mathbf{K}_{k+1}] \hat{\mathbf{x}}_{k+1|k} + \mathbf{K}_{k+1} \mathbf{z}_{k+1} \\ \mathbf{P}_{k+1|k+1} &= [\mathbf{I} - \mathbf{K}_{k+1}] \mathbf{P}_{k+1|k} [\mathbf{I} - \mathbf{K}_{k+1}]^T + \mathbf{K}_{k+1} \mathbf{R}_{k+1} \mathbf{K}_{k+1}^T \\ \text{with } \mathbf{K}_{k+1} &= \mathbf{P}_{k+1|k} [\mathbf{P}_{k+1|k} + \mathbf{R}_{k+1}]^{-1} \end{aligned}$$

In the update of the state $\hat{\mathbf{x}}_{k+1|k+1}$, the forecast $\hat{\mathbf{x}}_{k+1|k}$ and the measurements \mathbf{z}_{k+1} are weighted by $[\mathbf{I} - \mathbf{K}_{k+1}]$ and \mathbf{K}_{k+1} . As in a Bayesian estimator the weighting matrix is composed of the covariance matrices, i.e. similar to the Bayesian estimator, the Kalman gain matrix itself is the ratio of the covariances associated with the forecast and the observations. If the measurements are exceedingly noisy, i.e. $\mathbf{R}_{k+1} \rightarrow \infty \mathbf{I}$, then $\mathbf{K}_{k+1} \rightarrow \mathbf{0}$ and in the update of $\hat{\mathbf{x}}_{k+1|k+1}$ the system forecast $\hat{\mathbf{x}}_{k+1|k}$ is favored. On the other hand if the measurements are perfect, i.e. $\mathbf{R}_{k+1} \rightarrow \mathbf{0}$, then $\mathbf{K}_{k+1} \rightarrow \mathbf{I}$ and the new observations form the updated system states. Similarly for the updated covariance, if the measurements are exceedingly noisy, i.e. $\mathbf{R}_{k+1} \rightarrow \infty \mathbf{I}$, then $\mathbf{K}_{k+1} \rightarrow \mathbf{0}$ and $\mathbf{P}_{k+1|k+1} = \mathbf{P}_{k+1|k}$. However if the measurements are perfect, i.e. $\mathbf{R}_{k+1} \rightarrow \mathbf{0}$, then $\mathbf{K}_{k+1} \rightarrow \mathbf{I}$ and the updated state covariance is the measurement covariance.

In the forecast step, the interpretation is simplified if we assume that $\Phi_k = \rho \mathbf{I}$ where $\rho < 1$ (e.g. first-lag autocorrelation in an autoregressive model) and $\Gamma_k = \mathbf{I}$. The forecast equations now become

$$\begin{aligned} \text{Forecast} & : \quad \hat{\mathbf{x}}_{k+1|k} = \rho \hat{\mathbf{x}}_{k|k} \\ \mathbf{P}_{k+1|k} & = \quad \rho^2 \mathbf{P}_{k|k} + \mathbf{Q}_k \end{aligned}$$

and with N -step ahead forecasts

$$\begin{aligned} \text{Forecast} & : \quad \hat{\mathbf{x}}_{k+N|k} = \rho^N \hat{\mathbf{x}}_{k|k} \\ \mathbf{P}_{k+N|k} & = \quad \rho^{2N} \mathbf{P}_{k|k} + \sum_{i=0}^{N-i-1} \rho^{2(N-i-1)} \mathbf{Q}_{k+i} \end{aligned}$$

For $\mathbf{Q}_{k+i} = \mathbf{Q}$, i.e. the system noise level is constant in time, then as $N \rightarrow \infty$ the conditional mean $\hat{\mathbf{x}}_{k+N|k}$ approaches zero or the unconditional mean and the covariance approaches $\mathbf{P}_{k+N|k} = \frac{1}{1-\rho^2} \mathbf{Q}$ owing to $\sum_{i=0}^{\infty} a^i = \frac{1}{1-a}$ for $a < 1$. Thus the forecast error in this illustration asymptotically approaches the unconditional variance of an autoregressive model forced by white noise with covariance \mathbf{Q} .

So far the system equation is assumed to be forced only with stochastic inputs. If deterministic inputs are also present, then

$$\mathbf{x}_{k+1} = \Phi_k \mathbf{x}_k + \Lambda_k \mathbf{u}_k + \Gamma_k \mathbf{w}_k$$

and only the forecast and update equations for the state itself are affected as in

$$\begin{aligned} \text{Forecast} & : \quad \hat{\mathbf{x}}_{k+1|k} = \Phi_k \hat{\mathbf{x}}_{k|k} + \Lambda_k \mathbf{u}_k \\ \text{Update} & : \quad \hat{\mathbf{x}}_{k+1|k+1} = \hat{\mathbf{x}}_{k+1|k} + \Lambda_k \mathbf{u}_k \\ & \quad + \mathbf{K}_{k+1} [\mathbf{z}_{k+1} - \mathbf{H}_{k+1} \hat{\mathbf{x}}_{k+1|k} - \mathbf{H}_{k+1} \Lambda_k \mathbf{u}_k] \end{aligned}$$

The equations for \mathbf{P} and \mathbf{K} are unchanged because they are based on errors $\delta \mathbf{x}$ that do not contain deterministic inputs. This is due to the fact that the deterministic inputs are subtracted out when forming $\delta \mathbf{x}$.

2.2 The Variational Approach to the Dynamic Inverse Problem

2.2.1 Optimization of Dynamic Systems

As the simplest case, we consider a single-stage dynamic system. The initial state of the system is described by a n -dimensional state vector $\mathbf{x}(0)$, while

an m -dimensional control vector $\mathbf{u}(0)$ determines the transition to a new state $\mathbf{x}(1)$ through the equation:

$$\mathbf{x}(1) = \mathbf{f}^0[\mathbf{x}(0), \mathbf{u}(0)]$$

We wish to choose $\mathbf{u}(0)$ to minimize a performance index J of the form:

$$J = \phi[\mathbf{x}(1)] + L^0[\mathbf{x}(0), \mathbf{u}(0)]$$

conditional to the transition equation.

Formally this is an optimization problem with equality constraints which may be solved through the Lagrange multipliers technique. We then introduce a n -dimensional vector $\boldsymbol{\lambda}$ of undetermined multipliers in the new index:

$$J' = J + \boldsymbol{\lambda}^T(1) \{ \mathbf{f}^0[\mathbf{x}(0), \mathbf{u}(0)] - \mathbf{x}(1) \}$$

Now, let:

$$H^0[\mathbf{x}(0), \mathbf{u}(0), \boldsymbol{\lambda}(1)] = L^0[\mathbf{x}(0), \mathbf{u}(0)] + \boldsymbol{\lambda}^T(1) \mathbf{f}^0[\mathbf{x}(0), \mathbf{u}(0)]$$

so that:

$$J' = \phi[\mathbf{x}(1)] + H^0[\mathbf{x}(0), \mathbf{u}(0), \boldsymbol{\lambda}(1)] - \boldsymbol{\lambda}^T(1) \mathbf{x}(1)$$

and consider the variations of J' with respect to infinitesimal variations in $\mathbf{x}(1)$ and $\mathbf{u}(0)$ ($\mathbf{x}(0)$ is given, so that $d\mathbf{x}(0) = 0$):

$$dJ' = \left[\frac{\partial \phi}{\partial \mathbf{x}(1)} - \boldsymbol{\lambda}^T(1) \right] d\mathbf{x}(1) + \frac{\partial H^0}{\partial \mathbf{u}(0)} d\mathbf{u}(0)$$

A convenient choice for $\boldsymbol{\lambda}$ is then:

$$\boldsymbol{\lambda}^T(1) = \frac{\partial \phi}{\partial \mathbf{x}(1)} \quad \Longrightarrow \quad dJ' = \frac{\partial H^0}{\partial \mathbf{u}(0)} d\mathbf{u}(0)$$

so that a stationary point of J' , and hence of J constrained to $\mathbf{x}(1) = \mathbf{f}^0[\mathbf{x}(0), \mathbf{u}(0)]$, is simply given by the system of $2 \times n + m$ equations for the unknowns $[\mathbf{x}(1), \boldsymbol{\lambda}(1), \mathbf{u}(0)]$:

$$\begin{aligned}
\mathbf{x}(1) &= \mathbf{f}^0[\mathbf{x}(0), \mathbf{u}(0)] \\
\boldsymbol{\lambda}^T(1) &= \frac{\partial \phi}{\partial \mathbf{x}(1)} \\
\frac{\partial H^0}{\partial \mathbf{u}(0)} &= 0
\end{aligned}$$

We consider next a multi-stage system which may be described by the nonlinear difference equation:

$$\mathbf{x}(i+1) = \mathbf{f}^i[\mathbf{x}(i), \mathbf{u}(i)]$$

where $\mathbf{x}(0)$ is given and $i = 1, \dots, N-1$. The performance index is now:

$$J = \phi[\mathbf{x}(N)] + \sum_{i=0}^{N-1} L^i[\mathbf{x}(i), \mathbf{u}(i)]$$

The problem is now to find a sequence of control vectors $\mathbf{u}(i)$ that maximizes (or minimizes) J . As before, we define the new index with a sequence of multipliers $\boldsymbol{\lambda}(i)$:

$$J' = J + \sum_{i=0}^{N-1} \boldsymbol{\lambda}^T(i+1) \{ \mathbf{f}^i[\mathbf{x}(i), \mathbf{u}(i)] - \mathbf{x}(i+1) \}$$

and the scalar sequence:

$$H^i[\mathbf{x}(i), \mathbf{u}(i), \boldsymbol{\lambda}(i+1)] = L^i[\mathbf{x}(i), \mathbf{u}(i)] + \boldsymbol{\lambda}^T(i+1) \mathbf{f}^i[\mathbf{x}(i), \mathbf{u}(i)]$$

so that (with a change of summation index):

$$J' = \phi[\mathbf{x}(N)] - \boldsymbol{\lambda}^T(N) \mathbf{x}(N) + \sum_{i=1}^{N-1} [H^i - \boldsymbol{\lambda}^T(i) \mathbf{x}(i)] + H^0$$

Taking variations (with $\mathbf{x}(0)$ given):

$$dJ' = \left[\frac{\partial \phi}{\partial \mathbf{x}(N)} - \boldsymbol{\lambda}^T(N) \right] d\mathbf{x}(N) + \frac{\partial H^0}{\partial \mathbf{u}(0)} d\mathbf{u}(0) + \sum_{i=1}^{N-1} \left\{ \left[\frac{\partial H^i}{\partial \mathbf{x}(i)} - \boldsymbol{\lambda}^T(i) \right] d\mathbf{x}(i) + \frac{\partial H^i}{\partial \mathbf{u}(i)} d\mathbf{u}(i) \right\}$$

and choosing the multipliers sequence as:

$$\begin{aligned} \frac{\partial H^i}{\partial \mathbf{x}(i)} - \boldsymbol{\lambda}^T(i) &= 0; \quad i = 0, \dots, N-1 \\ \boldsymbol{\lambda}^T(N) &= \frac{\partial \phi}{\partial \mathbf{x}(N)} \end{aligned}$$

the variation of J' reduces to:

$$dJ' = \sum_{i=1}^{N-1} \frac{\partial H^i}{\partial \mathbf{u}(i)} d\mathbf{u}(i)$$

For this to be zero (constrained minimization of J) for any arbitrary sequence $d\mathbf{u}(i)$, it must be:

$$\frac{\partial H^i}{\partial \mathbf{u}(i)} = 0; \quad i = 0, \dots, N-1$$

In summary, to find a control vector sequence $\mathbf{u}(i)$ that produces a stationary (minimum or maximum) value of the performance index J , we must solve the following two-point boundary value problem:

$$\mathbf{x}(i+1) = \mathbf{f}^i[\mathbf{x}(i), \mathbf{u}(i)]; \quad \mathbf{x}(0) \text{ given}$$

$$\boldsymbol{\lambda}(i) = \left[\frac{\partial \mathbf{f}^i}{\partial \mathbf{x}(i)} \right]^T \boldsymbol{\lambda}(i+1) + \left[\frac{\partial L^i}{\partial \mathbf{x}(i)} \right]^T; \quad \boldsymbol{\lambda}(N) = \left[\frac{\partial \phi}{\partial \mathbf{x}(N)} \right]^T$$

together with:

$$\frac{\partial L^i}{\partial \mathbf{u}(i)} + \boldsymbol{\lambda}^T(i+1) \left[\frac{\partial \mathbf{f}^i}{\partial \mathbf{u}(i)} \right] = 0$$

The numerical solution of this problem is computational demanding: note that boundary conditions are set at 0 for the first difference equation and at N for the second, and that such equations are coupled through $\mathbf{u}(i)$.

An iterative solution procedure may be constructed, known as sweep method (whose convergence is not guaranteed in general):

1. Guess an initial value for the sequence $\mathbf{u}(i)$
2. Integrate forward in time the first difference equation to find $\mathbf{x}(i)$
3. Compute the coefficients in the second difference equations (which depend on $\mathbf{u}(i)$ and $\mathbf{x}(i)$) and integrate it backward in time to find the multipliers sequence $\boldsymbol{\lambda}(i)$
4. Update the values of $\mathbf{u}(i)$ using the third equation
5. Go back to step 2 and iterate until some converge criterion is satisfied.

2.2.2 Quadratic performance index with linear system equations

Consider a performance index in the form:

$$J = \frac{1}{2} \mathbf{x}^T(N) \mathbf{A}(N) \mathbf{x}(N) + \sum_{i=0}^{N-1} \left[\frac{1}{2} \mathbf{x}^T(i) \mathbf{A}(i) \mathbf{x}(i) + \frac{1}{2} \mathbf{u}^T(i) \mathbf{B}(i) \mathbf{u}(i) \right]$$

where $\mathbf{A}(i)$ and $\mathbf{B}(i)$ are given positive definite matrices, with the linear system of equations ($\mathbf{x}(0)$ given):

$$\mathbf{x}(i+1) = \boldsymbol{\Phi}(i) \mathbf{x}(i) + \boldsymbol{\Gamma}(i) \mathbf{u}(i)$$

The H^i sequence for the problem is then:

$$H^i = \frac{1}{2} \mathbf{x}^T(i) \mathbf{A}(i) \mathbf{x}(i) + \frac{1}{2} \mathbf{u}^T(i) \mathbf{B}(i) \mathbf{u}(i) + \boldsymbol{\lambda}^T(i+1) [\boldsymbol{\Phi}(i) \mathbf{x}(i) + \boldsymbol{\Gamma}(i) \mathbf{u}(i)]$$

Setting $\partial H^i / \partial \mathbf{u}(i) = 0$ we then obtain:

$$\mathbf{u}(i) = -[\mathbf{B}(i)]^{-1} \boldsymbol{\Gamma}^T(i) \boldsymbol{\lambda}(i+1)$$

which substituted in the first equation gives:

$$\mathbf{x}(i+1) = \Phi(i) \mathbf{x}(i) - \Gamma(i) [\mathbf{B}(i)]^{-1} \Gamma^T(i) \boldsymbol{\lambda}(i+1); \quad \mathbf{x}(0) \text{ given}$$

to be solved with:

$$\boldsymbol{\lambda}(i) = \Phi^T(i) \boldsymbol{\lambda}(i+1) + \mathbf{A}(i) \mathbf{x}(i); \quad \boldsymbol{\lambda}(N) = \mathbf{A}(N) \mathbf{x}(N)$$

This linear two-point boundary value problem may be solved using a single sweep:

$$\boldsymbol{\lambda}(i) = \mathbf{S}(i) \mathbf{x}(i)$$

where $\mathbf{S}(i)$ is easily determined through the backward recursive relation:

$$\begin{aligned} \mathbf{S}(i) &= \Phi^T(i) [\mathbf{S}^{-1}(i+1) + \Gamma(i) \mathbf{B}^{-1}(i) \Gamma^T(i)]^{-1} \Phi(i) + \mathbf{A}(i) \\ \mathbf{S}(N) &= \mathbf{A}(N) \end{aligned}$$

2.2.3 Continuous systems with no terminal constraints

Consider the system described by the following nonlinear initial value problem:

$$\dot{\mathbf{x}} = \mathbf{f}[\mathbf{x}(t), \mathbf{u}(t), t]; \quad \mathbf{x}(t_0) = \mathbf{x}_0; \quad t_0 \leq t \leq t_f$$

where $\mathbf{x}(t)$ is a n -vector function and $\mathbf{u}(t)$ is a m -vector function.

Then consider a scalar performance index:

$$J = \psi[\mathbf{x}(t_f), t_f] + \int_{t_0}^{t_f} L[\mathbf{x}(t), \mathbf{u}(t), t] dt$$

The problem is to find $\mathbf{u}(t)$ that maximizes (or minimizes) J . To do this, adjoint the differential equations to J with Lagrange multiplier functions $\boldsymbol{\lambda}(t)$:

$$J' = \psi[\mathbf{x}(t_f), t_f] + \int_{t_0}^{t_f} \{L[\mathbf{x}(t), \mathbf{u}(t), t] + \boldsymbol{\lambda}^T(t) (\mathbf{f}[\mathbf{x}(t), \mathbf{u}(t), t] - \dot{\mathbf{x}})\} dt$$

The scalar function $H(t)$ (called Hamiltonian) is constructed as:

$$H[\mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\lambda}(t), t] = L[\mathbf{x}(t), \mathbf{u}(t), t] + \boldsymbol{\lambda}^T(t) \mathbf{f}[\mathbf{x}(t), \mathbf{u}(t), t]$$

After integration by parts, the adjoint performance index J' may be written as:

$$J' = \psi[\mathbf{x}(t_f), t_f] - \boldsymbol{\lambda}^T(t_f) \mathbf{x}(t_f) + \boldsymbol{\lambda}^T(t_0) \mathbf{x}(t_0) + \int_{t_0}^{t_f} \left\{ H[\mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\lambda}(t), t] + \dot{\boldsymbol{\lambda}}^T(t) \mathbf{x}(t) \right\} dt$$

Considering its variations with respect to $\mathbf{x}(t)$ and $\mathbf{u}(t)$ (note now the use of the symbol δ for function variation, which is "transparent" to integration (see calculus of variations) and being $\delta\mathbf{x}(t_0) = 0$:

$$\delta J' = \left[\left(\frac{\partial \psi}{\partial \mathbf{x}} - \boldsymbol{\lambda}^T \right) \delta \mathbf{x} \right]_{t=t_f} + \int_{t_0}^{t_f} \left[\left(\frac{\partial H}{\partial \mathbf{x}} + \dot{\boldsymbol{\lambda}}^T \right) \delta \mathbf{x} + \frac{\partial H}{\partial \mathbf{u}} \delta \mathbf{u} \right] dt$$

From this expression, it is evident that it is convenient to choose:

$$\dot{\boldsymbol{\lambda}}^T = -\frac{\partial H}{\partial \mathbf{x}} = -\frac{\partial L}{\partial \mathbf{x}} - \boldsymbol{\lambda}^T \frac{\partial \mathbf{f}}{\partial \mathbf{x}}$$

with boundary conditions:

$$\boldsymbol{\lambda}^T(t_f) = \left[\frac{\partial \psi}{\partial \mathbf{x}} \right]_{t=t_f}$$

so that:

$$\delta J' = \int_{t_0}^{t_f} \frac{\partial H}{\partial \mathbf{u}} \delta \mathbf{u} dt$$

Thus, for $\delta J'$ to be zero for any independent variation $\delta \mathbf{u}$, the following equation must hold:

$$\frac{\partial H}{\partial \mathbf{u}} = 0; \quad t_0 \leq t \leq t_f$$

Then again, we ended up with a two-point boundary value problem with an additional relation.

2.2.4 Inverse Problems as Optimized Dynamic Systems

Consider again the multi-stage dynamic model:

$$\mathbf{x}(i+1) = \mathbf{f}^i[\mathbf{x}(i), \mathbf{u}(i)]$$

where $\mathbf{x}(0)$ is given and $i = 1, \dots, N-1$.

Let $\mathbf{x}^{obs}(k_j)$ be a set of observations (data) with $0 \leq k_j \leq N$, $j = 1, \dots, M$ and $\max(k_j) = N$.

The inverse problem may be stated as follows: find the parameters sequence $\mathbf{u}^{est}(i)$ which minimizes the following weighted-damped least squares performance index:

$$J = \sum_{j=1}^M \frac{1}{2} [\mathbf{x}(k_j) - \mathbf{x}^{obs}(k_j)]^T \mathbf{A}(k_j) [\mathbf{x}(k_j) - \mathbf{x}^{obs}(k_j)] + \sum_{i=0}^{N-1} \frac{1}{2} [\mathbf{u}^{est}(i) - \langle \mathbf{u}(i) \rangle]^T \mathbf{B}(i) [\mathbf{u}^{est}(i) - \langle \mathbf{u}(i) \rangle]$$

constrained to:

$$\mathbf{x}(i+1) = \mathbf{f}^i[\mathbf{x}(i), \mathbf{u}^{est}(i)]; \quad \mathbf{x}(0) \text{ given}$$

where $\langle \mathbf{u}(i) \rangle$ is the a priori information on the parameters sequence. Note that the problem is generally a mixed determined one (Exactly determined if $M = N$ and $k_j = j$, purely undetermined if $M < N$).

The H^i sequence for the problem is then (δ is now the Kroneker delta):

$$H^i = \frac{1}{2} \sum_{j=1}^M [\mathbf{x}(k_j) - \mathbf{x}^{obs}(k_j)]^T \mathbf{A}(k_j) [\mathbf{x}(k_j) - \mathbf{x}^{obs}(k_j)] \delta(k_j - i) + \frac{1}{2} [\mathbf{u}^{est}(i) - \langle \mathbf{u}(i) \rangle]^T \mathbf{B}(i) [\mathbf{u}^{est}(i) - \langle \mathbf{u}(i) \rangle] + \boldsymbol{\lambda}^T(i+1) \mathbf{f}^i[\mathbf{x}(i), \mathbf{u}^{est}(i)]$$

The Lagrange multipliers are chosen such that:

$$\begin{aligned}\boldsymbol{\lambda}(i) &= \left[\frac{\partial \mathbf{f}^i}{\partial \mathbf{x}(i)} \right]^T \boldsymbol{\lambda}(i+1) + \sum_{j=1}^M \mathbf{A}(k_j) [\mathbf{x}(k_j) - \mathbf{x}^{obs}(k_j)] \delta(k_j - i) \\ \boldsymbol{\lambda}(N) &= \sum_{j=1}^M \mathbf{A}(k_j) [\mathbf{x}(k_j) - \mathbf{x}^{obs}(k_j)] \delta(k_j - N)\end{aligned}$$

While setting $\partial H^i / \partial \mathbf{u}^{est}(i) = 0$ we obtain:

$$\mathbf{B}(i) [\mathbf{u}^{est}(i) - \langle \mathbf{u}(i) \rangle] + \boldsymbol{\lambda}^T(i+1) \left[\frac{\partial \mathbf{f}^i}{\partial \mathbf{u}^{est}(i)} \right] = 0$$

The sweep method to solve the above two-point boundary value problem is then the following:

1. Obtain from a priori information a first estimate of the parameter sequence $\mathbf{u}^{est}(i) = \langle \mathbf{u}(i) \rangle$
2. Integrate forward in time the model to compute the sequence $\mathbf{x}(i)$
3. Integrate backward in time the adjoint equation to compute the sequence $\boldsymbol{\lambda}(i)$
4. Update the estimate of the parameter sequence as:

$$\mathbf{u}^{est}(i) = \langle \mathbf{u}(i) \rangle - \mathbf{B}^{-1}(i) \boldsymbol{\lambda}^T(i+1) \left[\frac{\partial \mathbf{f}^i}{\partial \mathbf{u}^{est}(i)} \right]$$

5. Consider the new estimate as a priori information $\langle \mathbf{u}(i) \rangle = \mathbf{u}^{est}(i)$, go back to step 2 and iterate until some converge criterion is satisfied.

Note that in an "exact model" with "exact data" the convergence should be:

$$[\mathbf{x}(k_j), \mathbf{u}^{est}(i), \boldsymbol{\lambda}(i)] \longrightarrow [\mathbf{x}^{obs}(k_j), \langle \mathbf{u}(i) \rangle, \mathbf{0}]$$

2.2.5 Extension to Continuous Systems

Consider again the initial value problem:

$$\dot{\mathbf{x}} = \mathbf{f}[\mathbf{x}(t), \mathbf{u}(t), t]; \quad \mathbf{x}(t_0) = \mathbf{x}_0; \quad t_0 \leq t \leq t_f$$

Now the state \mathbf{x} is a continuous function of time. Observations (data) of the state are not: they are always a discrete set $\hat{\mathbf{x}}_j^{obs}$, $j = 1, \dots, M$. Furthermore, they can be some "instantaneous" observations of the state, averages of the state over given limited time intervals, or combinations of both types.

Then, in order to "compare" observations with model predictions, a data parametrization needs to be introduced:

$$\hat{\mathbf{x}}_j = \int_{t_0}^{t_f} \mathbf{d}_j[\mathbf{x}(t), t] dt; \quad j = 1, \dots, M$$

In the case of instantaneous observations at discrete times $t_0 \leq t_j \leq t_f$ it is simply:

$$\hat{\mathbf{x}}_j = \int_{t_0}^{t_f} \mathbf{x}(t) \delta(t - t_j) dt = \mathbf{x}(t_j); \quad j = 1, \dots, M$$

while in the case of (generally weighted) averages over given intervals $t_0 \leq t_{0j} \leq t \leq t_{fj} \leq t_f$ it is (let h be the Heaviside step function):

$$\begin{aligned} \hat{\mathbf{x}}_j &= \int_{t_0}^{t_f} \mathbf{W}_j(t) \mathbf{x}(t) h(t - t_{0j}) h(t_{fj} - t) dt = \\ &= \int_{t_{0j}}^{t_{fj}} \mathbf{W}_j(t) \mathbf{x}(t) dt; \quad j = 1, \dots, M \end{aligned}$$

Assume that the given data parametrization may be expressed in the following linear form:

$$\hat{x}_j = \int_{t_0}^{t_f} G_j(t) x(t) dt; \quad j = 1, \dots, M$$

Suppose now that we want to gain as much information as possible about (estimate ?) $x(t)$ given the data \hat{x}_j . This is just a static continuous linear inverse problem, which is a natural limiting extension of the discrete case illustrated in part II. Note that such a problem is inherently underdetermined,

given that the number of data is finite while the "number" of "parameters" $x(t)$ to be estimated is infinite. Attempts to exactly estimate $x(t)$ at any specific time $t = t'$ are futile, so that a "local average" perspective must be used.

It is then convenient, in order to solve this problem, to extend to the continuous case the Backus-Gilbert Generalized Inverse, defining a resolving kernel $R(t', t)$ (analogous to the model resolution matrix of the discrete case):

$$x^{avg}(t') = \sum_{j=1}^M G_j^{-g}(t') \hat{x}_j = \int_{t_0}^{t_f} R(t', t) x(t) dt;$$

where:

$$R(t', t) = \sum_{j=1}^M G_j^{-g}(t') G_j(t)$$

The average is localized around t' if the resolving kernel is peaked near t' . To optimize this, it is then convenient to use the Backus-Gilbert spread function:

$$J(t') = \int_{t_0}^{t_f} w(t', t) R^2(t', t) dt$$

where $w(t', t)$ is a non-negative function that is zero for $t = t'$ and that grows monotonically away from that point (such as $|t - t'|^2$). Minimization of such a spread function gives the following expression for the generalized inverse:

$$G_k^{-g}(t') = \frac{\sum_{j=1}^M [S_{jk}(t')]^{-1} u_j}{\sum_{j=1}^M \sum_{i=1}^M [S_{ji}(t')]^{-1} u_j u_i}$$

$$S_{ji}(t') = \int_{t_0}^{t_f} w(t', t) G_j(t) G_i(t) dt$$

$$u_i = \int_{t_0}^{t_f} G_i(t) dt$$

The procedure may be easily extended to vectorial cases to obtain:

$$\mathbf{x}^{avg}(t') = \sum_{j=1}^M \mathbf{G}_j^{-g}(t') \widehat{\mathbf{x}}_j$$

According to the above line of reasoning, we can define the following observation smoothing:

$$\mathbf{x}^{avg}(t) = \sum_{j=1}^M \mathbf{G}_j^{-g}(t) \widehat{\mathbf{x}}_j^{obs}$$

The (weighted damped least squares) performance index may be then generally expressed as:

$$\begin{aligned} J &= \frac{1}{2} \int_{t_0}^{t_f} [\mathbf{x}(t) - \mathbf{x}^{avg}(t)]^T \mathbf{A}(t) [\mathbf{x}(t) - \mathbf{x}^{avg}(t)] dt + \\ &+ \frac{1}{2} \int_{t_0}^{t_f} [\mathbf{u}^{est}(t) - \langle \mathbf{u}(t) \rangle]^T \mathbf{B}(t) [\mathbf{u}^{est}(t) - \langle \mathbf{u}(t) \rangle] dt + \\ &+ \frac{1}{2} [\mathbf{x}(t_f) - \mathbf{x}^{avg}(t_f)]^T \mathbf{C} [\mathbf{x}(t_f) - \mathbf{x}^{avg}(t_f)] \end{aligned}$$

The Hamiltonian:

$$\begin{aligned} H(t) &= \frac{1}{2} [\mathbf{x}(t) - \mathbf{x}^{avg}(t)]^T \mathbf{A}(t) [\mathbf{x}(t) - \mathbf{x}^{avg}(t)] + \\ &+ \frac{1}{2} [\mathbf{u}^{est}(t) - \langle \mathbf{u}(t) \rangle]^T \mathbf{B}(t) [\mathbf{u}^{est}(t) - \langle \mathbf{u}(t) \rangle] \\ &+ \boldsymbol{\lambda}^T(t) \mathbf{f}[\mathbf{x}(t), \mathbf{u}^{est}(t), t] \end{aligned}$$

And the adjointed performance index:

$$J' = J + \int_{t_0}^{t_f} \boldsymbol{\lambda}^T(t) (\mathbf{f}[\mathbf{x}(t), \mathbf{u}(t), t] - \dot{\mathbf{x}}) dt$$

which, after integration by parts, may be written as:

$$\begin{aligned} J' &= \frac{1}{2} [\mathbf{x}(t_f) - \mathbf{x}^{avg}(t_f)]^T \mathbf{C} [\mathbf{x}(t_f) - \mathbf{x}^{avg}(t_f)] - \\ &- \boldsymbol{\lambda}^T(t_f) \mathbf{x}(t_f) + \boldsymbol{\lambda}^T(t_0) \mathbf{x}(t_0) + \\ &+ \int_{t_0}^{t_f} \left\{ H[\mathbf{x}(t), \mathbf{u}^{est}(t), \boldsymbol{\lambda}(t), t] + \dot{\boldsymbol{\lambda}}^T(t) \mathbf{x}(t) \right\} dt \end{aligned}$$

Considering its variations with respect to $\mathbf{x}(t)$ and $\mathbf{u}^{est}(t)$ and being $\delta\mathbf{x}(t_0) = 0$:

$$\begin{aligned}\delta J' &= (\mathbf{C}[\mathbf{x}(t_f) - \mathbf{x}^{avg}(t_f)] - \boldsymbol{\lambda}^T) \delta\mathbf{x}(t_f) + \\ &+ \int_{t_0}^{t_f} \left[\left(\frac{\partial H}{\partial \mathbf{x}} + \dot{\boldsymbol{\lambda}}^T \right) \delta\mathbf{x} + \frac{\partial H}{\partial \mathbf{u}^{est}} \delta\mathbf{u}^{est} \right] dt\end{aligned}$$

From this expression, it is evident that it is convenient to choose:

$$\dot{\boldsymbol{\lambda}}^T = -\frac{\partial H}{\partial \mathbf{x}} = -\mathbf{A}(t) [\mathbf{x}(t) - \mathbf{x}^{avg}(t)] - \boldsymbol{\lambda}^T \frac{\partial \mathbf{f}}{\partial \mathbf{x}}$$

with boundary conditions:

$$\boldsymbol{\lambda}^T(t_f) = \mathbf{C}[\mathbf{x}(t_f) - \mathbf{x}^{avg}(t_f)]$$

so that:

$$\delta J' = \int_{t_0}^{t_f} \frac{\partial H}{\partial \mathbf{u}^{est}} \delta\mathbf{u}^{est} dt$$

Thus, for $\delta J'$ to be zero for any independent variation $\delta\mathbf{u}^{est}$, the following equation must hold:

$$\frac{\partial H}{\partial \mathbf{u}^{est}} = 0; \quad t_0 \leq t \leq t_f$$

that is:

$$\mathbf{u}^{est}(t) = \langle \mathbf{u}(t) \rangle - \mathbf{B}^{-1}(t) \boldsymbol{\lambda}^T(t) \frac{\partial \mathbf{f}[\mathbf{x}(t), \mathbf{u}^{est}(t), t]}{\partial \mathbf{u}^{est}(t)}$$

Then again, we ended up with a two-point boundary value problem with an additional relation, which can be solved analogously to the multi-stage discrete case.

3 Estimation and Inverse Solutions in Multi-dimensional Systems

3.1 Estimation in Space

Given scattered point measurements at locations \mathbf{u}_i , $i = 1, \dots, m$ in space $z(\mathbf{u}_i)$, the objective is to estimate the value of the field at a location \mathbf{u}_0 within the field by linearly weighting all the available measurements as in

$$\hat{x}(\mathbf{u}_0) = \sum_{i=1}^m \lambda(\mathbf{u}_i) z(\mathbf{u}_i)$$

where $\lambda(\mathbf{u}_i)$ are weights that need to be determined via estimation. The unbiasedness condition implies that

$$E[\hat{x}(\mathbf{u}_0)] = \sum_{i=1}^m \lambda(\mathbf{u}_i) E[z(\mathbf{u}_i)]$$

3.1.1 Stationary Fields

For a stationary field with a constant spatial mean m , the left- and right-hand sides become

$$m = \sum_{i=1}^m \lambda(\mathbf{u}_i) m$$

which implies

$$\sum_{i=1}^m \lambda_i(\mathbf{u}_i) = 1$$

The minimum-variance condition, here imposed as mean square error, implies that the estimation error

$$E[(x(\mathbf{u}_0) - \hat{x}(\mathbf{u}_0))^2]$$

must be minimized.

Estimators are developed assuming that the measurements of the state are direct (i.e. $\mathbf{H} = \mathbf{I}$) and error-free (i.e. $\mathbf{R} = \mathbf{0}$). Thus $z(\mathbf{u}_i) = x(\mathbf{u}_i)$,

$\forall i$. Expanding this expression and substituting $\hat{x}(\mathbf{u}_0) = \sum_{i=1}^m \lambda(\mathbf{u}_i) z(\mathbf{u}_i) = \sum_{i=1}^m \lambda(\mathbf{u}_i) x(\mathbf{u}_i)$

$$\begin{aligned}
& E[(x(\mathbf{u}_0) - \hat{x}(\mathbf{u}_0))^2] \\
&= E[x(\mathbf{u}_0)^2] - 2E[x(\mathbf{u}_0)\hat{x}(\mathbf{u}_0)] + E[\hat{x}(\mathbf{u}_0)^2] \\
&= E[x(\mathbf{u}_0)^2] - 2E\left[x(\mathbf{u}_0) \sum_{i=1}^m \lambda(\mathbf{u}_i) x(\mathbf{u}_i)\right] + E\left[\sum_{i=1}^m \lambda(\mathbf{u}_i) x(\mathbf{u}_i) \sum_{j=1}^m \lambda(\mathbf{u}_j) x(\mathbf{u}_j)\right] \\
&= E[x(\mathbf{u}_0)^2] - 2 \sum_{i=1}^m \lambda(\mathbf{u}_i) E[x(\mathbf{u}_0) x(\mathbf{u}_i)] + \sum_{i=1}^m \sum_{j=1}^m \lambda(\mathbf{u}_i) \lambda(\mathbf{u}_j) E[x(\mathbf{u}_i) x(\mathbf{u}_j)]
\end{aligned}$$

Using the definition of covariance

$$\begin{aligned}
cov[x(\mathbf{u}_i), x(\mathbf{u}_j)] &= E[(x(\mathbf{u}_i) - m)(x(\mathbf{u}_j) - m)] \\
&= E[x(\mathbf{u}_i)x(\mathbf{u}_j)] - E[x(\mathbf{u}_j)]m \\
&\quad - E[x(\mathbf{u}_i)]m + m^2 \\
&= E[x(\mathbf{u}_i)x(\mathbf{u}_j)] - 2m^2 + m^2 \\
&= E[x(\mathbf{u}_i)x(\mathbf{u}_j)] - m^2
\end{aligned}$$

Substitute

$$\begin{aligned}
& E[(x(\mathbf{u}_0) - \hat{x}(\mathbf{u}_0))^2] \\
&= cov[x(\mathbf{u}_0), x(\mathbf{u}_0)] - m^2 - 2 \sum_{i=1}^m \lambda(\mathbf{u}_i) cov[x(\mathbf{u}_0), x(\mathbf{u}_i)] + 2m^2 \sum_{i=1}^m \lambda(\mathbf{u}_i) \\
&\quad + \sum_{i=1}^m \sum_{j=1}^m \lambda(\mathbf{u}_i) \lambda(\mathbf{u}_j) cov[x(\mathbf{u}_i), x(\mathbf{u}_j)] - m^2 \sum_{i=1}^m \lambda(\mathbf{u}_i) \sum_{j=1}^m \lambda(\mathbf{u}_j) \\
&= cov[x(\mathbf{u}_0), x(\mathbf{u}_0)] - 2 \sum_{i=1}^m \lambda(\mathbf{u}_i) cov[x(\mathbf{u}_0), x(\mathbf{u}_i)] \\
&\quad + \sum_{i=1}^m \sum_{j=1}^m \lambda(\mathbf{u}_i) \lambda(\mathbf{u}_j) cov[x(\mathbf{u}_i), x(\mathbf{u}_j)]
\end{aligned}$$

using the unbiasedness condition $\sum_{i=1}^m \lambda_i(\mathbf{u}_i) = 1$. If the random field is second-order stationary, then the covariance depends only on distance $\mathbf{v}_{ij} =$

$\mathbf{u}_i - \mathbf{u}_j$

$$\begin{aligned} \text{cov} [z(\mathbf{u}_i), z(\mathbf{u}_j)] &= \text{cov} [\mathbf{u}_i - \mathbf{u}_j] \\ &= \text{cov} [\mathbf{v}_{ij}] \end{aligned}$$

or P_{ij} for short. The estimation error may now be written as

$$\begin{aligned} &E [(z(\mathbf{u}_0) - \hat{z}(\mathbf{u}_0))^2] \\ &= P_{00} - 2 \sum_{i=1}^m \lambda_i P_{i0} + \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j P_{ij} \end{aligned}$$

where the notation $\lambda_i = \lambda(\mathbf{u}_i)$ is used. This expression must be minimized with respect to the weights λ_i subject to the unbiasedness constraint $\sum_{i=1}^m \lambda_i = 1$. The constraint is added to a scalar objective function using lagrange multiplier 2β as in

$$E = \left[P_{00} - 2 \sum_{i=1}^m \lambda_i P_{i0} + \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j P_{ij} \right] + 2\beta \left[\sum_{i=1}^m \lambda_i - 1 \right]$$

Taking derivatives with respect to unknowns and setting to zero,

$$\begin{aligned} \frac{\partial E}{\partial \lambda_i} &= -2P_{i0} + 2 \sum_{j=1}^m \lambda_j P_{ij} + 2\beta = 0 \\ \frac{\partial E}{\partial \beta} &= \sum_{i=1}^m \lambda_i - 1 = 0 \end{aligned}$$

which yield $m+1$ linear equations for $m+1$ unknowns (β and $\lambda_i \quad i = 1 \dots m$)

$$\begin{aligned} \sum_{j=1}^m \lambda_j P_{ij} + \beta &= P_{i0} \\ \sum_{i=1}^m \lambda_i &= 1 \end{aligned}$$

In the first set of m equations, the estimation location is specified only in the right-hand side as a forcing. The left-hand side of these linear equations are the same for estimation at any location.

The optimal set of weights λ_i^* (known as kriging coefficients) result from the simultaneous solution of these $m + 1$ linear equations. The error of estimation may be found by multiplying the first m system of equations with λ_i^* and summing

$$\sum_{i=1}^m \sum_{j=1}^m \lambda_i^* \lambda_j^* P_{ij} = \sum_{i=1}^m \lambda_i^* P_{i0} - \beta \sum_{i=1}^m \lambda_i^*$$

When substituted for the last term in the existing expression

$$\begin{aligned} & E [(x(\mathbf{u}_0) - \hat{x}(\mathbf{u}_0))^2] \\ &= P_{00} - 2 \sum_{i=1}^m \lambda_i P_{i0} + \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j P_{ij} \\ &= \sigma_*^2 \end{aligned}$$

but with $\lambda_i = \lambda_i^*$, then the minimized error of estimation becomes

$$\sigma_*^2 = P_{00} - \sum_{i=1}^m \lambda_i^* P_{i0} - \beta$$

Thus for situations where the spatial field is noisy and lacks any covariance, i.e. $P_{i0} = 0$ for $i \neq 0$, then (neglecting β)

$$\sigma_*^2 \rightarrow P_{00}$$

or the variance of the field. On the other hand if there is strong covariance in the field and $P_{i0} \rightarrow P_{00} \forall i$, then

$$\sigma_*^2 \rightarrow 0$$

and the estimation is good.

For a simple illustration take $m = 2$ in which case

$$\begin{aligned} \lambda_1 P_{11} + \lambda_2 P_{12} + \beta &= P_{10} \\ \lambda_1 P_{21} + \lambda_2 P_{22} + \beta &= P_{20} \\ \lambda_1 + \lambda_2 &= 1 \end{aligned}$$

Substitute $\lambda_2 = 1 - \lambda_1$ in the first two equations and subtract to eliminate β

$$\lambda_1 (P_{11} - P_{21}) + (1 - \lambda_1) (P_{12} - P_{22}) = P_{10} - P_{20}$$

and solve for λ_1

$$\lambda_1 = \frac{P_{10} - P_{20} - P_{12} + P_{22}}{P_{11} - P_{21} - P_{12} + P_{22}}$$

If covariances $P_{22} = P_{11} = P$ and $P_{ij} = \rho_{ij}P$ and $\rho_{ij} = \rho_{ji}$ are correlation coefficients, then

$$\lambda_1 = \frac{\rho_{10} - \rho_{20} - \rho_{12} + 1}{1 - \rho_{21} - \rho_{12} + 1}$$

Furthermore take the measurements to be far apart and uncorrelated (i.e. $\rho_{12} = \rho_{21} = 0$), then

$$\lambda_1 = \frac{1 + \rho_{10} - \rho_{20}}{2}$$

Now if the measurements are equally distant to the estimation location (\mathbf{u}_0), then $\rho_{10} = \rho_{20}$ and $\lambda_1 = \lambda_2 = \frac{1}{2}$ or equal weight is given to each of the two measurements. However if $\rho_{10} = 1$ and $\rho_{20} = 0$, then $\lambda_1 = 1$ and $\lambda_2 = 0$ which weights only the first observation in forming an estimate. Conversely if the second measurement is closer to the estimation point, then $\rho_{20} = 1$ and $\rho_{10} = 0$, then $\lambda_2 = 1$ and $\lambda_1 = 0$.

3.1.2 Increment Stationary Fields

The assumptions of first-order stationarity ($E[x(\mathbf{u})] = m$) and second-order stationarity ($cov[x(\mathbf{u}_i), x(\mathbf{u}_j)] = cov[\mathbf{u}_i - \mathbf{u}_j]$) may be relaxed by requiring that only the increments of the field be stationary, i.e.

$$\begin{aligned} E[x(\mathbf{u}) - x(\mathbf{u} + \mathbf{v})] &= 0 \\ var[x(\mathbf{u}) - x(\mathbf{u} + \mathbf{v})] &= 2\gamma(\mathbf{v}) \end{aligned}$$

where $\gamma(\mathbf{v})$ is the semivariogram. For second-order stationary fields, as a function of separation h , $\gamma(h) = cov(0) - cov(h)$. But for increment stationary fields, the covariance may not exist but $\gamma(\mathbf{v})$ must exist. Again

considering the estimation error and using the fact that $\sum_{i=1}^m \lambda_i = 1$

$$\begin{aligned}
& E [(\hat{x}(\mathbf{u}_0) - x(\mathbf{u}_0))^2] \\
&= E \left[\left(\sum_{i=1}^m \lambda_i x(\mathbf{u}_i) - x(\mathbf{u}_0) \right) \left(\sum_{j=1}^m \lambda_j x(\mathbf{u}_j) - x(\mathbf{u}_0) \right) \right] \\
&= E \left[\left(\sum_{i=1}^m \lambda_i x(\mathbf{u}_i) - \sum_{i=1}^m \lambda_i x(\mathbf{u}_0) \right) \left(\sum_{j=1}^m \lambda_j x(\mathbf{u}_j) - \sum_{j=1}^m \lambda_j x(\mathbf{u}_0) \right) \right] \\
&= E \left[\left(\sum_{i=1}^m \lambda_i (x(\mathbf{u}_i) - x(\mathbf{u}_0)) \right) \left(\sum_{j=1}^m \lambda_j (x(\mathbf{u}_j) - x(\mathbf{u}_0)) \right) \right] \\
&= \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j E [(x(\mathbf{u}_i) - x(\mathbf{u}_0)) (x(\mathbf{u}_j) - x(\mathbf{u}_0))]
\end{aligned}$$

The expectation may be written as

$$\begin{aligned}
& E [(x(\mathbf{u}_i) - x(\mathbf{u}_0)) (x(\mathbf{u}_j) - x(\mathbf{u}_0))] \\
&= \frac{1}{2} E [(x(\mathbf{u}_i) - x(\mathbf{u}_0))^2 + (x(\mathbf{u}_j) - x(\mathbf{u}_0))^2 - (x(\mathbf{u}_i) - x(\mathbf{u}_j))^2]
\end{aligned}$$

which in terms of semivariograms $\gamma_{ij} = \gamma(\mathbf{u}_i - \mathbf{u}_j)$ is simply

$$E [(x(\mathbf{u}_i) - x(\mathbf{u}_0)) (x(\mathbf{u}_j) - x(\mathbf{u}_0))] = \gamma_{i0} + \gamma_{j0} - \gamma_{ij}$$

The estimator objective function now becomes

$$\begin{aligned}
& E [(\hat{x}(\mathbf{u}_0) - x(\mathbf{u}_0))^2] \\
&= \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j (\gamma_{i0} + \gamma_{j0} - \gamma_{ij}) \\
&= - \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j \gamma_{ij} + \sum_{i=1}^m \lambda_i \gamma_{i0} + \sum_{j=1}^m \lambda_j \gamma_{j0} \\
&= - \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j \gamma_{ij} + 2 \sum_{i=1}^m \lambda_i \gamma_{i0}
\end{aligned}$$

Minimizing this expression with respect to λ_i and imposing the unbiasedness constraint using lagrange multiplier 2β is performed on the objective

function

$$E = - \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j \gamma_{ij} + 2 \sum_{i=1}^m \lambda_i \gamma_{i0} - 2\beta \left(\sum_{i=1}^m \lambda_i - 1 \right)$$

that yields the $m + 1$ linear system of equations

$$\begin{aligned} \sum_{j=1}^m \lambda_i \lambda_j \gamma_{ij} + \beta &= \gamma_{i0} \\ \sum_{i=1}^m \lambda_i &= 1 \end{aligned}$$

for the $m + 1$ unknowns (β and $\lambda_i \quad i = 1 \dots m$).

3.1.3 Estimation of Field Mean: Stationary Case

In the same way that the measurements and spatial covariance of the state may be used to estimate the value of the state at a point, the scheme may be used to estimate the field mean. For this case the estimator for

$$m = \frac{1}{A} \int_A x(\mathbf{u}) d\mathbf{u}$$

is

$$\hat{m} = \sum_{i=1}^m \lambda_i x(\mathbf{u}_i)$$

Since the field is stationary the condition $\sum_{i=1}^m \lambda_i = 1$ still applies. The mean error variance of estimation is

$$\begin{aligned} \sigma_m^2 &= E[(m - \hat{m})^2] \\ &= E[m^2] - 2E[m\hat{m}] + E[\hat{m}^2] \end{aligned}$$

After substitution

$$\begin{aligned} \sigma_m^2 &= \frac{1}{A^2} \int_A \int_A E[x(\mathbf{u}_1) x(\mathbf{u}_2)] d\mathbf{u}_1 d\mathbf{u}_2 - \frac{2}{A} \int_A \sum_{i=1}^m \lambda_i E[x(\mathbf{u}) x(\mathbf{u}_i)] d\mathbf{u} \\ &\quad + \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j E[x(\mathbf{u}_j) x(\mathbf{u}_i)] \end{aligned}$$

Given that the field is second-order stationary $cov(x(\mathbf{u}_1), x(\mathbf{u}_2)) = cov(\mathbf{u}_1 - \mathbf{u}_2)$ and

$$cov(\mathbf{u}_1 - \mathbf{u}_2) = E[x(\mathbf{u}_1)x(\mathbf{u}_2)] - m^2$$

Then

$$\begin{aligned} \sigma_m^2 &= \frac{1}{A^2} \int_A \int_A cov(\mathbf{u}_1 - \mathbf{u}_2) d\mathbf{u}_1 d\mathbf{u}_2 + \frac{m^2}{A^2} \int_A \int_A d\mathbf{u}_1 d\mathbf{u}_2 \\ &\quad - \frac{2}{A} \int_A \sum_{i=1}^m \lambda_i cov(\mathbf{u} - \mathbf{u}_i) d\mathbf{u} - \frac{2m^2}{A} \int_A d\mathbf{u} \sum_{i=1}^m \lambda_i \\ &\quad + \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j cov(\mathbf{u}_i - \mathbf{u}_j) + m^2 \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j \end{aligned}$$

The terms involving m^2 cancel to leave

$$\begin{aligned} \sigma_m^2 &= \frac{1}{A^2} \int_A \int_A cov(\mathbf{u}_1 - \mathbf{u}_2) d\mathbf{u}_1 d\mathbf{u}_2 \\ &\quad - \frac{2}{A} \int_A \sum_{i=1}^m \lambda_i cov(\mathbf{u} - \mathbf{u}_i) d\mathbf{u} \\ &\quad + \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j cov(\mathbf{u}_i - \mathbf{u}_j) \end{aligned}$$

which needs to be minimized with respect to the unknown kriging coefficients λ_i subject to the constraint $\sum_{i=1}^m \lambda_i = 1$. The objective function using lagrange multiplier 2β is

$$E = \sigma_m^2 + 2\beta \left(\sum_{i=1}^m \lambda_i - 1 \right)$$

Taking derivatives and setting them to zero,

$$\begin{aligned} \frac{\partial E}{\partial \lambda_i} &= -\frac{2}{A} \int_A cov(\mathbf{u} - \mathbf{u}_i) d\mathbf{u} + 2 \sum_{j=1}^m \lambda_j cov(\mathbf{u}_i - \mathbf{u}_j) + 2\beta = 0 \\ \frac{\partial E}{\partial \beta} &= \sum_{i=1}^m \lambda_i - 1 = 0 \end{aligned}$$

These $m + 1$ system of linear equations may be rewritten as

$$\sum_{j=1}^m \lambda_j \text{cov}(\mathbf{u}_i - \mathbf{u}_j) + \beta = \frac{1}{A} \int_A \text{cov}(\mathbf{u} - \mathbf{u}_i) d\mathbf{u}$$

$$\sum_{i=1}^m \lambda_i = 1$$

for the $m + 1$ unknowns (β and $\lambda_i \quad i = 1 \dots m$).

3.1.4 Estimation of Field Mean: Nonstationary Case

Fields with nonstationary drift may be characterized by linear combinations of basis functions $f_k(\mathbf{u})$ as in

$$m(\mathbf{u}) = \sum_{k=0}^L \alpha_k f_k(\mathbf{u})$$

The problem is to estimate the coefficients a_k , $k = 1 \dots L$. Estimators of the coefficients α_k are a_k which weight the error-free observations $z(\mathbf{u}_i) = x(\mathbf{u}_i)$, $i = 1 \dots m$. Thus

$$a_k = \sum_{i=1}^m \lambda_i x(\mathbf{u}_i)$$

After the coefficients λ_i are estimated based on observations, then the estimate mean ($M(\mathbf{u})$) is

$$M(\mathbf{u}) = \sum_{k=0}^L a_k f_k(\mathbf{u})$$

Unbiasedness condition requires that

$$E[a_k] = \alpha_k$$

which implies that

$$E \left[\sum_{i=1}^m \lambda_i x(\mathbf{u}_i) \right] = \sum_{i=1}^m \lambda_i E[x(\mathbf{u}_i)] = \alpha_k$$

which may be written as

$$\alpha_k = \sum_{i=1}^m \lambda_i \sum_{k=0}^L \alpha_k f_k(\mathbf{u}) = \sum_{k=0}^L \alpha_k \sum_{i=1}^m \lambda_i f_k(\mathbf{u})$$

This equation may only be satisfied if

$$\sum_{i=1}^m \lambda_i f_k(\mathbf{u}) = \delta(k, i) \text{ for } k = 0 \dots L$$

where $\delta(i, i) = 1$ and $\delta(i, j) = 0$ for $i \neq j$. These form $L + 1$ constraints. The variance of estimation, again in terms of mean squared deviations, is

$$\begin{aligned} & E[(a_k - \alpha_k)^2] \\ &= E[a_k^2] - 2E[a_k]E[\alpha_k] + E[\alpha_k^2] \\ &= E[a_k^2] - E[\alpha_k^2] \\ &= E\left[\left(\sum_{i=1}^m \lambda_i x(\mathbf{u}_i)\right)\left(\sum_{j=1}^m \lambda_j x(\mathbf{u}_j)\right)\right] - E[\alpha_k^2] \\ &= \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j E[x(\mathbf{u}_i)x(\mathbf{u}_j)] - E[\alpha_k^2] \\ &= \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j \text{cov}[\mathbf{u}_i - \mathbf{u}_j] + \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j m(\mathbf{u}_i)m(\mathbf{u}_j) - E[\alpha_k^2] \end{aligned}$$

Since $\alpha_k = \sum_{i=1}^m \lambda_i m(\mathbf{u}_i)$,

$$\begin{aligned} & E[(a_k - \alpha_k)^2] \\ &= \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j \text{cov}[\mathbf{u}_i - \mathbf{u}_j] + \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j m(\mathbf{u}_i)m(\mathbf{u}_j) - \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j m(\mathbf{u}_i)m(\mathbf{u}_j) \\ &= \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j \text{cov}[\mathbf{u}_i - \mathbf{u}_j] \end{aligned}$$

The constraints and this estimation error variance are combined in one scalar objective function using the lagrange multipliers $2\beta_k$

$$E = \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j \text{cov}[\mathbf{u}_i - \mathbf{u}_j] + 2 \sum_{k=0}^L \beta_k \sum_{i=1}^m (\lambda_i f_k(\mathbf{u}) - \delta(k, i))$$

Minimizing the function by taking the derivative and setting to zero yields $m + L + 1$ linear equations

$$\begin{aligned} \sum_{j=1}^m \lambda_j \text{cov} [\mathbf{u}_i - \mathbf{u}_j] - \sum_{k=0}^L \beta_k f_k(\mathbf{u}) &= 0 \\ \sum_{i=1}^m \lambda_i f_k(\mathbf{u}) &= \delta(k, i) \end{aligned}$$

for the $m + L + 1$ unknowns (β_k $k = 0 \dots L$ and λ_i $i = 1 \dots m$).

Since the estimation of the covariance $\text{cov} [\mathbf{u}_i - \mathbf{u}_j]$ requires knowledge of the mean drift $M(\mathbf{u})$, an iterative algorithm is required to estimate the covariance and the kriging coefficients together.

An alternate approach is to use increment and generalized covariances of order L . Take $\lambda_0 = -1$ so that $\sum_{i=0}^m \lambda_i = 0$. Also a two-dimensional field of order L has

$$\sum_{i=0}^m \lambda_i x_i^p y_i^q = 0 \quad \text{for } p \geq 0, q \geq 0, p + q \leq L$$

so that for $L = 1$

$$\sum_{i=0}^m \lambda_i = 0 \quad \sum_{i=0}^m \lambda_i x_i = 0 \quad \sum_{i=0}^m \lambda_i y_i = 0$$

and for $L = 2$, additionally

$$\sum_{i=0}^m \lambda_i x_i^2 = 0 \quad \sum_{i=0}^m \lambda_i y_i^2 = 0 \quad \sum_{i=0}^m \lambda_i x_i y_i = 0$$

and so on.

The mean squared error of estimation (here we take the example of estimation at a point) is

$$\begin{aligned} &E [(x(\mathbf{u}_0) - \hat{x}(\mathbf{u}_0))^2] \\ &= K_{00} - 2 \sum_{i=1}^m \lambda_i K_{i0} + \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j K_{ij} \end{aligned}$$

where K_{ij} is a generalized covariance of order L based on assumed spatial drift forms such as

$$K_{ij} = K(v_{ij}) = \theta_0 \delta + \theta_1 |v_{ij}| + \theta_2 |v_{ij}|^3 + \theta_3 |v_{ij}|^5$$

When $\theta_2 = \theta_3 = 0$, the generalized covariance corresponds to a constant drift situation. When $\theta_3 = 0$, the generalized covariance is for linear drift with x , and y components. With all the terms included, the basis functions include additional terms with x^2 , y^2 , and xy dependence for drift basis function. The value of θ_0 denotes a "nugget" effect.

Using the fact that $\lambda_0 = -1$, this expression is written as

$$\begin{aligned} & E [(x(\mathbf{u}_0) - \hat{x}(\mathbf{u}_0))^2] \\ &= (-1)^2 K_{00} - \lambda_0 \sum_{i=1}^m \lambda_i K_{i0} - \lambda_0 \sum_{j=1}^m \lambda_j K_{j0} + \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j K_{ij} \\ &= \sum_{i=0}^m \sum_{j=0}^m \lambda_i \lambda_j K_{ij} \end{aligned}$$

Adjoining the constraints $\sum_{i=0}^m \lambda_i x_i^p y_i^q = 0$ by lagrange multipliers and minimizing results in the system of linear equations

$$\begin{aligned} \sum_{j=1}^m \lambda_j K_{ij} - \sum_{p,q} \beta_k x_i^p y_i^q &= K_{i0} \\ \sum_{i=0}^m \lambda_i x_i^p y_i^q &= 0 \end{aligned}$$

For example if $L = 1$, then the system of equations are

$$\begin{aligned} \sum_{j=1}^m \lambda_j K_{ij} - \beta_1 - \beta_2 x_i - \beta_3 y_i &= K_{i0} \\ \sum_{i=0}^m \lambda_i &= 0 \quad \sum_{i=0}^m \lambda_i x_i = 0 \quad \sum_{i=0}^m \lambda_i y_i = 0 \end{aligned}$$

The variance of estimation is

$$var [x(\mathbf{u}_0) - \hat{x}(\mathbf{u}_0)] = \sigma_*^2 = K_{00} + \beta_1 + \beta_2 x_0 + \beta_3 y_0 - \sum_{j=1}^m \lambda_j^* K_{j0}$$

This function depends on the parameters of the generalized covariance function. An iteration scheme is implemented to estimate the parameters of the generalized covariance function K_{ij} . In the iteration cross-validation is used in which the error of cross-validation is

$$e_i = x(\mathbf{u}_0) - \hat{x}(\mathbf{u}_0)$$

where here $x(\mathbf{u}_0)$ is a measured value withheld from the estimation and $\hat{x}(\mathbf{u}_0)$ is its kriging estimate. Each of the m observations may be withheld individually. The estimation of the kriging coefficients along with the parameters of the generalized covariance minimizes the function

$$\left[\sum_{i=1}^m (e_i^2 - \sigma_*^2) \right]^2$$

with respect to the generalized covariance parameters. An unconstrained nonlinear minimization algorithm is used for solution procedure.

3.2 Inverse Problems in Multidimensional Dynamic Systems

Extension of the variational approach to the solution of inverse problems in multidimensional dynamic systems, such as those governed by partial differential equations in time and space, is not straightforward. The differential operator used in the previous dynamic case was first order and linear, that is d/dt . Common problems in the space-time domain present higher order and sometimes non-linear differential operators. This adds complexity to the treatment of the boundary values and the adjoining of the model's equation, which in the purely dynamical case was approached with a simple integration by parts.

A general method is not easy to develop, and each problem needs to be addressed with "problem-specific techniques". An example is given in the following section.

3.2.1 The Adjoint Problem for Groundwater Flow in Confined Aquifers

Two-dimensional groundwater flow in an isotropic and confined aquifer can be described by the following partial differential equation:

$$S \frac{\partial \phi}{\partial t} - \nabla \cdot (T \nabla \phi) - Q = 0; \quad (x, y) \in \Omega; \quad 0 \leq t \leq t_f$$

subject to initial and boundary conditions:

$$\begin{aligned} \phi(x, y, t)|_{t=0} &= f_0(x, y) \\ \phi(x, y, t)|_{(x, y) \in \Gamma_1} &= f_1(x, y, t) \\ [T \nabla \phi \cdot \mathbf{n}]|_{(x, y) \in \Gamma_2} &= f_2(x, y, t) \end{aligned}$$

where:

$\phi(x, y, t)$ = piezometric head (L);

$S(x, y)$ = storage coefficient (dimensionless);

$T(x, y)$ = transmissivity (L^2/T);

$\nabla = (\partial/\partial x, \partial/\partial y)$ = gradient operator vector (L^{-1})

Ω = flow region in the (x, y) plane with boundaries Γ_1 and Γ_2 ;

\mathbf{n} = unit vector normal to Γ_2 ;

f_1, f_2, f_3 = given functions;

Let the transmissivity T be the unknown parameter to be estimated. Consider a penalty function in the very general form (explicit reference to observation data is omitted for simplicity):

$$E(\phi, T) = \int_0^{t_f} \int_{\Omega} F(\phi, T; x, y, t) d\Omega dt$$

Then consider $\lambda(x, y, t)$ as an arbitrary function having continuous first derivative in time and second derivative in space, and build an adjoint penalty function as:

$$E'(\phi, T) = E(\phi, T) + \int_0^{t_f} \int_{\Omega} \lambda(x, y, t) \left[S \frac{\partial \phi}{\partial t} - \nabla \cdot (T \nabla \phi) - Q \right] d\Omega dt$$

Taking variations with respect to $\delta\phi$ and δT :

$$\begin{aligned} \delta E' &= \int_0^{t_f} \int_{\Omega} \left[\frac{\partial F}{\partial \phi} \delta\phi + \frac{\partial F}{\partial T} \delta T \right] d\Omega dt + \\ &+ \int_0^{t_f} \int_{\Omega} \lambda \left[S \frac{\partial \delta\phi}{\partial t} - \nabla \cdot (\delta T \nabla \phi) - \nabla \cdot (T \nabla \delta\phi) \right] d\Omega dt \end{aligned}$$

and:

$$\begin{aligned}\delta\phi(x, y, t)|_{t=0} &= 0 \\ \delta\phi(x, y, t)|_{(x,y)\in\Gamma_1} &= 0 \\ [(\delta T \nabla \phi + T \nabla \delta\phi) \cdot \mathbf{n}]|_{(x,y)\in\Gamma_2} &= 0\end{aligned}$$

After integration in time by parts, $\delta E'$ may be written as:

$$\begin{aligned}\delta E' &= \int_0^{t_f} \int_{\Omega} \left[\frac{\partial F}{\partial \phi} \delta\phi + \frac{\partial F}{\partial T} \delta T \right] d\Omega dt + \int_{\Omega} [S\lambda\delta\phi]_0^{t_f} d\Omega - \\ &\quad - \int_0^{t_f} \int_{\Omega} \left[S\delta\phi \frac{\partial \lambda}{\partial t} - \lambda \nabla \cdot (\delta T \nabla \phi) - \lambda \nabla \cdot (T \nabla \delta\phi) \right] d\Omega dt\end{aligned}$$

Such an integration allowed to drop the term $\lambda S \partial \delta\phi / \partial t$ in favour of $S \delta\phi \partial \lambda / \partial t$. This passage is needed to derive the adjoint equation fro λ . Analogously, we need to find a means of dropping $\lambda \nabla \cdot (T \nabla \delta\phi)$ in favour of partial derivatives in space of λ . To do this, let us start with the Gauss' divergence theorem for a continuous differentiable vector function $\mathbf{F}(x, y) = [F_x(x, y), F_y(x, y)]$ defined in an space domain Ω with boundary Γ :

$$\int_{\Omega} \nabla \cdot \mathbf{F} d\Omega = \int_{\Gamma} \mathbf{F} \cdot \mathbf{n} d\Gamma$$

When \mathbf{F} is defined by two scalar functions ψ and ϕ as $\mathbf{F} = \psi \nabla \phi$, the above relation gives the Green's first theorem:

$$\int_{\Omega} (\nabla \psi \cdot \nabla \phi + \psi \nabla^2 \phi) d\Omega = \int_{\Gamma} \psi \nabla \phi \cdot \mathbf{n} d\Gamma$$

Similarly, with $\mathbf{F} = \psi \nabla \phi - \phi \nabla \psi$, the Green's second theorem is obtained:

$$\int_{\Omega} (\psi \nabla^2 \phi - \phi \nabla^2 \psi) d\Omega = \int_{\Gamma} (\psi \nabla \phi - \phi \nabla \psi) \cdot \mathbf{n} d\Gamma$$

These can be extended to include either a scalar function u or a vector function \mathbf{v} , and combining them the following identities can be derived:

$$\begin{aligned}\int_{\Omega} \phi \nabla \cdot (u \nabla \psi) d\Omega &= - \int_{\Omega} u (\nabla \psi \cdot \nabla \phi) d\Omega + \int_{\Gamma} u \phi \nabla \psi \cdot \mathbf{n} d\Gamma \\ &= \int_{\Omega} \psi \nabla \cdot (u \nabla \phi) d\Omega - \int_{\Gamma} u (\phi \nabla \psi - \psi \nabla \phi) \cdot \mathbf{n} d\Gamma\end{aligned}$$

$$\int_{\Omega} \phi \nabla \cdot (\mathbf{v}\psi) d\Omega = \int_{\Omega} \psi \mathbf{v} \cdot \nabla \phi d\Omega + \int_{\Gamma} \phi \psi \mathbf{v} \cdot \mathbf{n} d\Gamma$$

Using these relations we may then write:

$$\begin{aligned} & \int_{\Omega} \left[S \delta \phi \frac{\partial \lambda}{\partial t} - \lambda \nabla \cdot (\delta T \nabla \phi) - \lambda \nabla \cdot (T \nabla \delta \phi) \right] d\Omega = \\ & = \int_{\Omega} \left[S \frac{\partial \lambda}{\partial t} + \nabla \cdot (T \nabla \lambda) \right] \delta \phi d\Omega - \int_{\Omega} (\nabla \lambda \cdot \nabla \phi) \delta T d\Omega \\ & \quad - \int_{\Gamma} \delta \phi T \nabla \lambda \cdot \mathbf{n} d\Gamma + \int_{\Gamma} \lambda T \nabla \delta \phi \cdot \mathbf{n} d\Gamma + \int_{\Gamma} \delta T \lambda \nabla \phi \cdot \mathbf{n} d\Gamma \end{aligned}$$

Using the homogeneous boundary conditions for $\delta \phi$ and defining:

$$\begin{aligned} \lambda(x, y, t)|_{(x, y) \in \Gamma_1} &= 0 \\ [T \nabla \lambda \cdot \mathbf{n}]|_{(x, y) \in \Gamma_2} &= 0 \end{aligned}$$

all the intergals along the boundary in the above expression vanish, hence:

$$\begin{aligned} \delta E' &= \int_0^{t_f} \int_{\Omega} \left[\frac{\partial F}{\partial \phi} \delta \phi + \frac{\partial F}{\partial T} \delta T \right] d\Omega dt + \int_{\Omega} [S \lambda \delta \phi]_0^{t_f} d\Omega - \\ & \quad - \int_0^{t_f} \int_{\Omega} \left[S \frac{\partial \lambda}{\partial t} + \nabla \cdot (T \nabla \lambda) \right] \delta \phi d\Omega dt + \int_0^{t_f} \int_{\Omega} (\nabla \lambda \cdot \nabla \phi) \delta T d\Omega dt \end{aligned}$$

If λ is selected to satisfy the following partial differential equation:

$$S \frac{\partial \lambda}{\partial t} + \nabla \cdot (T \nabla \lambda) - \frac{\partial F}{\partial \phi}$$

with boundary and final conditions:

$$\begin{aligned} \lambda(x, y, t)|_{t=t_f} &= 0 \\ \lambda(x, y, t)|_{(x, y) \in \Gamma_1} &= 0 \\ [T \nabla \lambda \cdot \mathbf{n}]|_{(x, y) \in \Gamma_2} &= 0 \end{aligned}$$

then the variation of the adjointed performance index reduces to (also using the homogeneous initial condition for $\delta\phi$):

$$\delta E' = \int_0^{t_f} \int_{\Omega} \left[\frac{\partial F}{\partial T} + (\nabla\lambda \cdot \nabla\phi) \right] \delta T d\Omega dt$$

Thus, for $\delta E'$ to be null for any independent variation of δT , the following equation must be satisfied:

$$\frac{\partial F}{\partial T} + (\nabla\lambda \cdot \nabla\phi) = 0$$

We have ended again with two coupled (partial) differential problems, one to be integrated forward in time to guess a prediction $\phi(\lambda, T)$ and one to be integrated backward in time to estimate $\lambda(\phi, T)$, plus a third equation to update $T(\lambda, \phi)$.

4 APPENDIX A - Probability and Statistics Background

For a random variable X , the probability that its value is less than or equal to a certain magnitude x is given by the cumulative distribution function (cdf) $F(x)$:

$$F(x) = \text{prob}[X \leq x]$$

The properties of this function are

$$F(-\infty) = 0 \quad \text{and} \quad F(\infty) = 1$$

as well as $F(x_1) \leq F(x_2)$ for $x_1 \leq x_2$. If the cumulative distribution function is differentiable and continuous, the probability density function (pdf) $f(x)$ is defined as

$$f(x) = \frac{dF(x)}{dx}$$

The properties of $f(x)$ are

$$\begin{aligned} \int_{-\infty}^{\infty} f(y) dx &= 1 \\ F(x) &= \int_{-\infty}^x f(v) dv \\ f(x) &\geq 0 \end{aligned}$$

An example of a probability density function is the gaussian

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

Bivariate random variables are characterized by the cumulative distribution function

$$\begin{aligned} F(x, y) &= \text{prob}[X \leq x \text{ and } Y \leq y] \\ &= \int_{-\infty}^y \int_{-\infty}^x f(v, w) dv dw \end{aligned}$$

where the joint probability density function is

$$f(x, y) = \frac{\partial^2}{\partial x \partial y} F(x, y)$$

with the property that

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y) dx dy = 1$$

Marginal probability density function may be derived from the joint distribution by considering all possible values of the remainder random variables as in

$$f(x) = \int_{-\infty}^{\infty} f(x, y) dy$$

An example of a bivariate probability density function is the joint-gaussian

$$f(x, y) = \frac{1}{2\pi\sigma_x\sigma_y(1-\rho^2)} \cdot \exp \left\{ \frac{-1}{2(1-\rho^2)} \left(\left(\frac{x-\mu_x}{\sigma_x} \right)^2 - 2\rho \frac{(x-\mu_x)(y-\mu_y)}{\sigma_x\sigma_y} + \left(\frac{y-\mu_y}{\sigma_y} \right)^2 \right) \right\}$$

When the two random variables are independent

$$f(x, y) = f(x) f(y)$$

so in the example $\rho = 0$ and

$$\begin{aligned} f(x, y) &= \frac{1}{2\pi\sigma_x\sigma_y} \exp \left\{ -\frac{1}{2} \left(\left(\frac{x-\mu_x}{\sigma_x} \right)^2 - \left(\frac{y-\mu_y}{\sigma_y} \right)^2 \right) \right\} \\ &= \frac{1}{\sqrt{2\pi\sigma_x^2}} e^{-\frac{1}{2} \left(\frac{x-\mu_x}{\sigma_x} \right)^2} \frac{1}{\sqrt{2\pi\sigma_y^2}} e^{-\frac{1}{2} \left(\frac{y-\mu_y}{\sigma_y} \right)^2} \\ &= f(x) f(y) \end{aligned}$$

For more than two variables (say $\mathbf{x}^T = [x_1 x_2 \cdots x_n]$), this same probability density function becomes

$$f(\mathbf{x}) = \frac{1}{(2\pi)^{n/2} |\boldsymbol{\Sigma}|^{1/2}} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right\}$$

The moments of probability density functions are

$$m_k = \int_{-\infty}^{\infty} x^k f(x) dx$$

The central moments are defined as

$$m'_k = \int_{-\infty}^{\infty} (x - m_1)^k f(x) dx$$

For joint densities, the cross-moments are

$$m_{kl} = \int_{-\infty}^{\infty} x^k y^l f(x, y) dx dy$$

and

$$m'_{kl} = \int_{-\infty}^{\infty} (x - m_{10})^k (y - m_{01})^l f(x, y) dx dy$$

The first moment is the expectation

$$m_1 = E[x] = \int_{-\infty}^{\infty} x f(x) dx$$

which is a measure of central tendency. The operator $E[\cdot]$ is a linear operator so that

$$\begin{aligned} E[x + y] &= E[x] + E[y] \\ E[cx] &= cE[x] \quad c \text{ is a constant} \\ E[c] &= c \end{aligned}$$

The second central moment is a measure of spread and it is the variance

$$\begin{aligned} m'_2 &= var[x] = \int_{-\infty}^{\infty} (x - E[x])^2 f(x) dx \\ &= \int_{-\infty}^{\infty} (x^2 - 2xE[x] + E^2[x]) f(x) dx \\ &= E[x^2 - 2xE[x] + E^2[x]] \\ &= E[x^2] - 2E[x]E[x] + E^2[x] \\ &= E[x^2] - E^2[x] \end{aligned}$$

This is a nonlinear operator but has the following properties

$$\begin{aligned} var[cx] &= c^2 var[x] \\ var[c] &= 0 \\ var[x + y] &= var[x] + var[y] - cov[x, y] \end{aligned}$$

where

$$\begin{aligned} \text{cov}[x, y] &= m'_{11} \\ &= \int_{-\infty}^{\infty} (x - E[x]) (y - E[y]) f(x, y) dx dy \\ &= E[(x - E[x]) (y - E[y])] \end{aligned}$$

For bivariate random variables the covariance matrix (\mathbf{P}) consists of

$$\mathbf{P} = E \left[\begin{bmatrix} (x - E[x]) \\ (y - E[y]) \end{bmatrix} \begin{bmatrix} (x - E[x]) & (y - E[y]) \end{bmatrix} \right]$$

or in the multivariate case

$$\mathbf{P} = E \left[(\mathbf{x} - \mathbf{m})(\mathbf{x} - \mathbf{m})^T \right]$$

where \mathbf{x} is an $n \times 1$ vector of random variables and \mathbf{m} is the vector of expectations of the same. The $n \times n$ matrix \mathbf{P} is symmetric and the diagonal elements represent the variances.

Conditional probability density functions and moments (as well as cumulative distribution functions, expectations, variances and covariances, etc.) may also be defined. The conditional probability density function for x given the value of y is

$$f(x | y)$$

so that the joint density is

$$f(x, y) = f(x | y) f(y)$$

A property of the conditional probability density function is

$$\int_{-\infty}^{\infty} f(x | y) dx = 1$$

Using the definition of the conditional probability density function, the

Bayes theorem states that

$$\begin{aligned}
 f(x | y) &= \frac{f(x, y)}{f(y)} \\
 &= \frac{f(y | x) f(x)}{f(y)} \\
 &= \frac{f(y | x) f(x)}{\int_{-\infty}^{\infty} f(x, y) dx} \\
 &= \frac{f(y | x) f(x)}{\int_{-\infty}^{\infty} f(y | x) f(x) dx}
 \end{aligned}$$

based on

$$f(x) = \int_{-\infty}^{\infty} f(x, y) dy = \int_{-\infty}^{\infty} f(y | x) f(x) dy$$

The advantage of the Bayes theorem is that if $f(x | y)$ is the a posteriori probability of x given y and $f(y | x)$ is the a priori probability of y given x . Since a priori probabilities are estimate based on past measurements, Bayes theorem represents a method to estimate a posteriori probabilities based on past measurements.

For random function (random variables indexed on space \mathbf{x} or time t the process is said to be first-order stationary if its probability distribution function is not dependent on the index. Hence for a temporal process the probability density function

$$f(x(t_1)) = f(x(t_2))$$

The moments of this probability distribution function are also independent of the index so that $E[x]$ and $var[x]$ are constants.

Second order stationarity means that the joint distribution of the random function at two different index values, i.e.

$$f(x(t_1), x(t_2))$$

is dependent only on the relative separation so that $E[x]$ and $var[x]$ are constants and

$$cov[x(t_1), x(t_2)] = cov[x(t), x(t + v)]$$

5 APPENDIX B - The Singular Value Decomposition

5.1 Vector Spaces and Unitary Transformations

We may regard at the set \mathbf{d} as a generic vector in the vector-space $S(\mathbf{d})$, and at the model parameters \mathbf{m} as a generic vector in the vector space $S(\mathbf{m})$. Then, the linear model $\mathbf{Gm} = \mathbf{d}$ is a map from $S(\mathbf{d})$ to $S(\mathbf{m})$ and $\mathbf{m}^{est} = \mathbf{G}^{-g}\mathbf{d}$ is a map from $S(\mathbf{m})$ to $S(\mathbf{d})$.

One important property of vector spaces is the arbitrary choice of the coordinate system (basis vectors). If \mathbf{m} is the representation of a vector in one coordinate system and \mathbf{m}' is its representation in another, we can write the coordinate transformation in simple matrix notation as $\mathbf{m}' = \mathbf{Tm}$ and $\mathbf{m} = \mathbf{T}^{-1}\mathbf{m}'$. If the basis vectors of both coordinate systems are unit vectors, then \mathbf{T} represents simple rotations and reflections and, satisfying the property $\mathbf{T}^{-1} = \mathbf{T}^T$, it is called a unitary transformation.

If we apply this type of transformations to the linear inverse problem, we obtain:

$$\mathbf{d} = \mathbf{Gm} = \mathbf{GIm} = \mathbf{GT}^{-1}\mathbf{Tm} = \mathbf{G}'\mathbf{m}'$$

For the solution length we obtain:

$$L = \mathbf{m}^T\mathbf{m} = (\mathbf{T}^{-1}\mathbf{m}')^T (\mathbf{T}^{-1}\mathbf{m}') = \mathbf{m}'^T (\mathbf{T}^{-1T}\mathbf{T}^{-1}) \mathbf{m}' = \mathbf{m}'^T \mathbf{m}'$$

For the prediction error we obtain:

$$\mathbf{e}' = \mathbf{Te} = \mathbf{T}(\mathbf{d} - \mathbf{Gm}) = \mathbf{Td} - \mathbf{TGm} = \mathbf{d}' - \mathbf{G}'\mathbf{m}$$

Then, unitary transformations do not alter the properties of the linear inverse problem.

5.2 The Mixed-Determined Problem

If the problem is to some degree undetermined, than the equation $\mathbf{Gm} = \mathbf{d}$ contains information about only some combination of the model parameters which lies in the subspace $S_p(\mathbf{m})$ (contained in $S(\mathbf{m})$). No information is given for the rest of the parameter space, called null space $S_0(\mathbf{m})$. Analogously, if the problem is to some extent overdetermined, only a subspace

$S_p(\mathbf{d})$ of the data space can be span by $\mathbf{G}\mathbf{m}$, while no combination of data lying in $S_0(\mathbf{d})$ can be satisfied by any choice of the model parameters. If we are able to divide the data and parameters into parts that lie in the p and 0 subspaces, then we can write $\mathbf{G}\mathbf{m} = \mathbf{d}$ as:

$$\mathbf{G} [\mathbf{m}_p + \mathbf{m}_0] = [\mathbf{d}_p + \mathbf{d}_0]$$

$$L = [\mathbf{m}_p + \mathbf{m}_0]^T [\mathbf{m}_p + \mathbf{m}_0] = \mathbf{m}_p^T \mathbf{m}_p + \mathbf{m}_0^T \mathbf{m}_0$$

$$\begin{aligned} E &= [\mathbf{d}_p + \mathbf{d}_0 - \mathbf{G}\mathbf{m}_p]^T [\mathbf{d}_p + \mathbf{d}_0 - \mathbf{G}\mathbf{m}_p] = \\ &= [\mathbf{d}_p - \mathbf{G}\mathbf{m}_p]^T [\mathbf{d}_p - \mathbf{G}\mathbf{m}_p] + \mathbf{d}_0^T \mathbf{d}_0 \end{aligned}$$

where we have used the properties $\mathbf{G}\mathbf{m}_0 = 0$, $\mathbf{m}_p^T \mathbf{m}_0 = \mathbf{m}_0^T \mathbf{m}_p = 0$, $\mathbf{d}_p^T \mathbf{d}_0 = \mathbf{d}_0^T \mathbf{d}_p = 0$.

We can now define precisely what we mean by a solution to the mixed determined problem that minimizes prediction error while adding a minimum of a priori information: a priori information is added to specify only those linear combinations of the model parameters that reside in the null space $S_0(\mathbf{m})$, and the prediction error is reduced to only the portion in the null space $S_0(\mathbf{d})$ by satisfying $\mathbf{e}_p = [\mathbf{d}_p - \mathbf{G}\mathbf{m}_p]$ exactly. One possible choice of a priori information is $\mathbf{m}_0^{est} = 0$, which is called the natural solution of the mixed-determined problem.

The key step is then finding a coordinate transformation which "separate" the p and 0 components of data and parameters.

5.3 Singular-Value Decomposition and the Natural Generalized Inverse

Any $N \times M$ matrix \mathbf{G} can be written as the product of three matrices:

$$\mathbf{G} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^T$$

where:

- \mathbf{U} is a $N \times N$ matrix of eigenvectors that span the data space $S(\mathbf{d})$. The vectors are orthogonal to one another and can be chosen to be of unit length, so that $\mathbf{U}^T = \mathbf{U}^{-1}$.

- \mathbf{V} is a $M \times M$ matrix of eigenvectors that span the data space $S(\mathbf{m})$. The vectors are orthogonal to one another and can be chosen to be of unit length, so that $\mathbf{U}^T = \mathbf{U}^{-1}$.
- $\mathbf{\Lambda}$ is a $N \times M$ diagonal eigenvalue matrix whose diagonal elements are non-negative and are called singular values, usually arranged in order of decreasing size $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p > 0$:

$$\mathbf{\Lambda} = \begin{bmatrix} \mathbf{\Lambda}_p & 0 \\ 0 & 0 \end{bmatrix}$$

$$\mathbf{\Lambda}_p = \begin{bmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \lambda_p \end{bmatrix}$$

Denoting with \mathbf{U}_p and \mathbf{V}_p the first p columns of \mathbf{U} and \mathbf{V} , we obtain:

$$\mathbf{G} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^T = \mathbf{U}_p\mathbf{\Lambda}_p\mathbf{V}_p^T$$

Similarly denoting with \mathbf{U}_0 the columns $p+1, \dots, N$ of \mathbf{U} , and with \mathbf{V}_0 the columns $p+1, \dots, M$ of \mathbf{V} , we observe that the equation $\mathbf{G}\mathbf{m} = \mathbf{d} = \mathbf{U}_p\mathbf{\Lambda}_p\mathbf{V}_p^T\mathbf{m}$ contains no information about the part of model parameters in the space spanned by \mathbf{V}_0 because \mathbf{m} is multiplied by \mathbf{V}_p which is orthogonal to \mathbf{V}_0 . Then \mathbf{V}_p lies completely in $S_p(\mathbf{m})$ and \mathbf{V}_0 lies completely in $S_0(\mathbf{m})$. By analogous reasoning, we find that \mathbf{U}_p lies completely in $S_p(\mathbf{d})$ and \mathbf{U}_0 lies completely in $S_0(\mathbf{d})$.

It is then demonstrated that the above singular-value decomposition fully separates the null and p spaces of the given linear inverse problem. It also gives the natural solution of the linear inverse problem as:

$$\mathbf{m}^{est} = \mathbf{V}_p\mathbf{\Lambda}_p^{-1}\mathbf{U}_p^T\mathbf{d}$$

For this solution to be the natural one, we need to prove that \mathbf{m}^{est} has no component in $S_0(\mathbf{m})$ and the prediction error \mathbf{e} has no component in $S_p(\mathbf{d})$. These conditions are easily proven by observing that:

$$\mathbf{V}_0^T\mathbf{m}^{est} = \mathbf{V}_0^T(\mathbf{V}_p\mathbf{\Lambda}_p^{-1}\mathbf{U}_p^T\mathbf{d}) = (\mathbf{V}_0^T\mathbf{V}_p)\mathbf{\Lambda}_p^{-1}\mathbf{U}_p^T\mathbf{d} = 0$$

$$\begin{aligned}
\mathbf{U}_p^T \mathbf{e} &= \mathbf{U}_p^T [\mathbf{d} - \mathbf{G}\mathbf{m}^{est}] = \mathbf{U}_p^T [\mathbf{d} - \mathbf{U}_p \mathbf{\Lambda}_p \mathbf{V}_p^T \mathbf{V}_p \mathbf{\Lambda}_p^{-1} \mathbf{U}_p^T \mathbf{d}] = \\
&= \mathbf{U}_p^T [\mathbf{d} - \mathbf{U}_p \mathbf{\Lambda}_p \mathbf{\Lambda}_p^{-1} \mathbf{U}_p^T \mathbf{d}] = \mathbf{U}_p^T [\mathbf{d} - \mathbf{U}_p \mathbf{U}_p^T \mathbf{d}] = \\
&= \mathbf{U}_p^T [\mathbf{d} - \mathbf{d}] = 0
\end{aligned}$$

5.4 Derivation of the Singular-Value Decomposition

We first construct the following $(N + M) \times (N + M)$ square matrix:

$$\mathbf{S} = \begin{bmatrix} \mathbf{0} & \mathbf{G} \\ \mathbf{G}^T & \mathbf{0} \end{bmatrix}$$

We then solve the eigenvalue problem $\mathbf{S}\mathbf{w}_i = \lambda_i \mathbf{w}_i$, obtaining $(N + M)$ eigenvalues λ_i (only p non-null) and $(N + M)$ eigenvectors \mathbf{w}_i .

Then it can be demonstrated that choosing:

$$\begin{aligned}
\mathbf{u}_i &= [w_1, \dots, w_N]_i^T \\
\mathbf{v}_i &= [w_{N+1}, \dots, w_{N+M}]_i^T
\end{aligned}$$

and:

$$\mathbf{U} = [\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_N]$$

$$\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_M]$$

$$\mathbf{\Lambda}_p = \begin{bmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \lambda_p \end{bmatrix}$$

we have the sought singular-value decomposition $\mathbf{G} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^T$.

6 Bibliography

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