

Problems in parameter estimation with nonlinear models

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1. Introduction

The dominating theory for estimation of unknown parameters from observations corrupted by random noise is the linear theory, which is linear in two respects:

- (a) The deterministic mathematical model connecting unknown parameters with the observables, i.e., the observed parameters, is linear.
- (b) The provided estimates are linear functions of the observations.

Here we will elaborate on the case where the first of the assumptions is violated, which is the usual case in physical applications, where linear mathematical models are rather the exception.

We will also compare two different traditions where the linear model is applied: The first is the classical one of applications in physical sciences, in particular astronomy and geodesy. It starts with the least squares method of Gauss and Legendre and it culminates in the statistical justification of the choice of weight matrix as a scalar multiple of the inverse of the error covariance matrix. According to the celebrated Gauss-Markov theorem with this choice the least squares solution provides Best Linear Uniformly Unbiased Estimates (BLUUE or simply BLUE) for all linear functions of the parameters, which are estimable, i.e. functions of the observables only.

The linear model $\mathbf{y} = \mathbf{A}\mathbf{x}$, that relates observables \mathbf{y} with other unknown parameters \mathbf{x} , is usually the result of linearization, and it is an approximation to a nonlinear model $\mathbf{y} = \mathbf{f}(\mathbf{x})$, while observations $\mathbf{b} = \mathbf{y} + \mathbf{e}$ are corrupted by noise (errors) \mathbf{e} which are considered random variables with zero mean and known covariance matrix (up to a scalar).

The second tradition has been developed in applications within the human sciences, where the processes involved are too complicated to be expressed by simple physical laws and mathematical relations with unquestionable validity. Instead, a set of attributes y, x_1, x_2, \dots, x_m is observed over a set of n different entities to produce values $y_i, X_{i1}, X_{i2}, \dots, X_{im}, i = 1, 2, \dots, n$. If a close to linear relation holds between these values a model of the form $y_i = X_{i1}\beta_1 + X_{i2}\beta_2 + \dots + X_{im}\beta_m + e_i$ is

used, where the “error” term e_i does not express imperfections in the measuring process but rather the inability of the linear model to absolutely express the relation between the $m+1$ attributes. In matrix form, the “regression model” $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e}$ has the same form as the “observation equations” model $\mathbf{b} = \mathbf{A}\mathbf{x} + \mathbf{e}$ of the physical sciences, but they are based on quite different grounds.

Nonlinear models $\mathbf{b} = \mathbf{f}(\mathbf{x}) + \mathbf{e}$ appear in both physical sciences, by avoiding the linearization step as, as well as in human sciences when the linear relation produces large discrepancies e_i . Since the formal model in its algebraic form and probabilistic properties is the same in both situations, the problems of estimation with nonlinear models are pretty much the same though with different interpretations. We will discuss these problems from the point of view of the physical sciences and in particular that of geodesy and surveying, which have significantly contributed to the development of the linear model theory.

Before doing so, it is worthwhile to mention a particular nonlinear model, which emerged in the regression framework when the error e_i is interpreted not as an overall discrepancy but rather as a result of “observation imperfection”. They are not though of the same nature as in physical sciences where errors are attributed to the inadequacies of the measuring devices and processes (though some contribution from modelling errors always exist). In such a case it is recognized that the observed values X_{ik} also contain observation errors, so that $X_{ik} = \bar{X}_{ik} + E_{ik}$, in matrix form $\mathbf{X} = \bar{\mathbf{X}} + \mathbf{E}$, where E_{ik} are the errors and \bar{X}_{ik} their error-free counterparts. This is the so called Errors-In-Variables (EIV) model which gave rise to the “total least squares” approach, where not only the errors \mathbf{e} of \mathbf{y} but also the errors \mathbf{E} of \mathbf{X} are minimized. The nonlinearity in the model $\mathbf{y} = \bar{\mathbf{X}}\boldsymbol{\beta} + \mathbf{e}$, $\mathbf{X} = \bar{\mathbf{X}} + \mathbf{E}$ is with respect to both unknown parameter $\bar{\mathbf{X}}$ and $\boldsymbol{\beta}$, although the model is linear with respect to each set separately. The clarity of the model is usually obscured by the elimination of the implicit deterministic unknown parameters $\bar{\mathbf{X}}$, by writing the EIV model in the form $\mathbf{y} = (\mathbf{X} - \mathbf{E})\boldsymbol{\beta} + \mathbf{e}$. Setting $\bar{\mathbf{y}} = \bar{\mathbf{X}}\boldsymbol{\beta}$, the model is in fact a linear (Gauss-Markov) model $\mathbf{y} = \bar{\mathbf{y}} + \mathbf{e}$, $\mathbf{X} = \bar{\mathbf{X}} + \mathbf{E}$, subject to the nonlinear constraints $\bar{\mathbf{y}} = \bar{\mathbf{X}}\boldsymbol{\beta}$. From our point of view, the Gauss-Markov linear model with nonlinear constraints is the basic generic model for the treatment of observations in order to estimate unknown parameters.

2. Alternative models in the physical sciences

Returning to the physical sciences, when we perform a redundant number of n observations \mathbf{b} , the observables \mathbf{y} are the fundamental set of unknown parameters although they may not appear explicitly in the model. In the presence of zero-mean random errors \mathbf{e} the basic linear model is $\mathbf{b} = \mathbf{y} + \mathbf{e}$. Nevertheless what we “ob-

serve”, in a more general sense of the word, is not the observables themselves but rather a natural “system” in the sense of an isolated part of the whole nature. In such a system, the existing interactions with the rest of the physical reality are ignored with the use of simple mathematical models based on an abstract simplified view of the physical word. Since reality cannot be circumvented or bypassed, nature hits back through discrepancies between observations and observables, to which we attribute the character of observation errors. Any system can be completely described by means of an intrinsic number of parameters r , which we will call the parametric rank of the system. Thus, the n observables are not independent but they must satisfy a number of $s = n - r$ conditions. The vector of the observables \mathbf{y} belongs to the n -dimensional space of reals R^n . The s conditions restrict the admissible values to an r -dimensional subset M of R^n , which we will call the manifold of the observables. We use the mathematical term “manifold” since in the general case this subspace will be a curved one (in the case of nonlinear models), rather than a flat one (as in the case of linear models). The most simple way (and in many sciences the only one in use) to describe the manifold M is as the image of r unknown parameters \mathbf{x} under a nonlinear mapping $\mathbf{y} = \mathbf{f}(\mathbf{x})$ called the “observation equations” model. In this case, the total number of unknown parameters (\mathbf{y}, \mathbf{x}) rises to $n + r$ and the $s = (n + r) - r = n$ independent conditions $\mathbf{y} = \mathbf{f}(\mathbf{x})$ restrict \mathbf{y} to lie to an r -dimensional manifold M . In geodesy M has been also described in different ways. The most traditional one is through the so-called $s = n - r$ “condition equations” $\mathbf{g}(\mathbf{y}) = \mathbf{0}$, without the use of any parameters other than the observables. An in-between description is that of the “mixed equations” or “condition equations with unknowns”, where a set of additional m unknown parameters \mathbf{x} is used, which interact with the observables \mathbf{y} through k nonlinear relations $\mathbf{h}(\mathbf{x}, \mathbf{y}) = \mathbf{0}$. The number of unknowns in this case is $n + m$ and the k conditions reduce them to $n + m - k = r$, so that the appropriate number of independent relations $\mathbf{h}(\mathbf{x}, \mathbf{y}) = \mathbf{0}$ must be $k = n + m - r$. Not all possibilities are yet exhausted. Two (at least) more descriptions arise by imposing d conditions $\mathbf{c}(\mathbf{x}) = \mathbf{0}$ on the m parameters \mathbf{x} . Thus we have the observation equations with constraints, namely $\mathbf{y} = \mathbf{f}(\mathbf{x})$, $\mathbf{c}(\mathbf{x}) = \mathbf{0}$, i.e. $n + d$ conditions which reduce the $n + m$ unknowns into $(n + m) - (n + d) = r$ ones and thus $d = m - r$ must hold. In the mixed equations with constraints, $\mathbf{h}(\mathbf{x}, \mathbf{y}) = \mathbf{0}$, $\mathbf{c}(\mathbf{x}) = \mathbf{0}$, $n + d$ conditions reduce the $n + m$ unknowns to $(n + m) - (k + d) = r$ ones and thus $k + d = n + m - r$ must hold.

It is customary to “eliminate” the observables and obtain models, which implement the observations and their errors, such as the “observation equations” $\mathbf{b} = \mathbf{f}(\mathbf{x}) + \mathbf{e}$, the “condition equations” $\mathbf{g}(\mathbf{b} - \mathbf{v}) = \mathbf{0}$ and the “condition equations with unknowns” $\mathbf{h}(\mathbf{x}, \mathbf{b} - \mathbf{v}) = \mathbf{0}$. The last ones in their linearized form have been introduced by the famous German geodesist F. R. Helmert (1907) and are widely

known in geodesy as the Gauss-Helmert (linear) model, a name suggesting a generalization of the linear Gauss-Markov model. The essential here is not how the r -dimensional observables manifold M is described, but rather how to select a point $\hat{\mathbf{y}} \in M$ on this manifold, which serves as an estimate of the unknown observables \mathbf{y} . Since errors ($\mathbf{e} = \mathbf{b} - \mathbf{y}$) are small a good idea is to obtain a $\hat{\mathbf{y}}$ close to the observations \mathbf{b} , by minimizing the distance $\|\mathbf{b} - \mathbf{y}\| = \|\mathbf{e}\| = \sqrt{\mathbf{e}^T \mathbf{P} \mathbf{e}}$ among all possible observables $\mathbf{y} \in M$. In other words, the error estimates are minimized in length and this is the basis of the least squares method, equivalently based on the minimization of the square distance $\|\mathbf{e}\|^2 = \mathbf{e}^T \mathbf{P} \mathbf{e} = \min$. The remaining question is how to choose the positive-definite weight matrix \mathbf{P} , and the answer is the provided in the linear model case, where M is a linear manifold, by the Gauss-Markov theorem.

3. The problem of the justification of the least squares solution for nonlinear models

Is it possible to extend the Gauss-Markov theorem to the nonlinear case? Unfortunately, the answer is negative! Linearity is an essential component of the Gauss-Markov model. In order to see why this is so, we will restrict ourselves to the estimation of the observables; once they are known, any other parameter of interest either can be computed from them, or they cannot be computed at all. This is the difference between estimable and non-estimable parameters, or more correctly between determinable and non-determinable ones. Let us see what the concept of uniform unbiased tells us. By modelling the errors \mathbf{e} as random parameters, we accept that each time we repeat the observations experiment an error value $\mathbf{e}(\omega)$ corresponding to the experiment ω is added to the fixed unknown deterministic observables \mathbf{y} to produce a value of the observations $\mathbf{b}(\omega) = \mathbf{y} + \mathbf{e}(\omega)$. The least squares solution assigns to $\mathbf{b}(\omega)$ its closest element $\hat{\mathbf{y}}(\omega)$ from M . In the linear case, this assignment is simply a projection on the linear manifold M . Under infinite conceivable repetitions of the experiment $\omega \in \Omega$ ($\Omega =$ set of all possible experiments) we have a “cloud” of observations $\mathbf{b}(\omega_1), \mathbf{b}(\omega_2), \dots$, which has a “center” (mean or expected value in statistical terminology) $E\{\mathbf{b}(\omega)\} = E\{\mathbf{y} + \mathbf{e}(\omega)\} = \mathbf{y} + E\{\mathbf{e}(\omega)\}$, which is the sum of the unknown true values of the observables and the “center” $E\{\mathbf{e}(\omega)\}$ of the errors. As a part of our stochastic model, we have assumed that the errors have zero mean, $E\{\mathbf{e}(\omega)\} = \mathbf{0}$ and hence of the errors $E\{\mathbf{b}(\omega)\} = \mathbf{y}$, i.e. the center (mean or expected value) of the observations is the true observables \mathbf{y} . For the linear case, the projection $\mathbf{b}(\omega) \rightarrow \hat{\mathbf{y}}(\omega)$ preserves the center of the observations cloud $\mathbf{b}(\omega)$ and thus the center of the observable estimates cloud $\hat{\mathbf{y}}(\omega)$ (a cloud within M) is simply \mathbf{y} . In statistical terminology, the estimates $\hat{\mathbf{y}}(\omega)$ are unbiased, i.e., their mean (expected) value equals the unknown

observables $E\{\hat{\mathbf{y}}(\omega)\} = \mathbf{y}$. In simple words, if we repeat the experiment ω (under the same conditions – whatever that may mean) infinite times and calculate the mean of the infinite obtained estimates $\hat{\mathbf{y}}(\omega)$, we will obtain the true value! Since infinite repetitions are impossible, in practice we are simply assured that a large number of repetitions provides a close to truth estimate, the larger the better. What is the value of this “unbiasedness” criterion when we hardly ever repeat the experiment a second time (one is costly enough already)? Well it simply says that when we put our hand in some bucket of estimates to draw out a single one, it is better to pick up a bucket where the estimates have the true value as mean. Of course unbiasedness is not a panacea and biased estimates have been proposed, when by allowing our cloud of estimates to be somewhat off-center we arrive to more dense clouds, where the chance to get closer to the truth increases. In statistical terms we give up unbiasedness for each observable y_i ($E\{\hat{y}_i\} \neq y_i$) for the sake of decreasing its mean square error $E\{(\hat{y}_i - y_i)^2\}$.

In the nonlinear case, the least squares solution projects each observation point $\mathbf{b}(\omega)$ into a corresponding point $\hat{\mathbf{y}}(\omega)$ on the nonlinear manifold. Since the manifold is curved, the center \mathbf{y} of the original cloud does not coincide with the center $E\{\hat{\mathbf{y}}(\omega)\}$ of the projected cloud! In the general case $E\{\hat{\mathbf{y}}(\omega)\}$ does not even belong to M , where \mathbf{y} lies. To visualize this, think of M as a sphere or a circle. The missing link for imposing unbiasedness in the nonlinear case is a new “intrinsic” definition of the mean, such that the mean of points on a nonlinear manifold remains always on the manifold.

There are two great advantages in the use of the Gauss-Markov theorem for the justification of the use of the weight matrix in linear models. The first is that the minimized target function for any linear function $q = \mathbf{a}^T \mathbf{y}$ of the observables \mathbf{y} is the mean square error $E\{(\hat{q} - q)^2\} = \min$, which suggest an intuitively attractive best concentration of the estimates $\hat{q}(\omega)$ for the various possible observation experiments ω around the unknown true value q . The second is that no knowledge of the complete probability density function of the observation errors is needed. In this respect, BLUE estimation is a “second order” theory requiring knowledge only of the first and second order statistics (means and covariances).

There are two ways for introducing statistical optimality in the case of nonlinear models. The first is to resort to the Bayesian approach where the unknown parameters are also consider as random variables with a known “prior” probability distribution. We will not examine further this approach here and the reader may consult Dermanis and Sanso (1995). The second is to resort to the maximum likelihood principle (see e.g. Seber and Wild, 2003). The likelihood is in our case the joint probability density function of the observations $p(\mathbf{b})$, defined in such a way that for any subset $S \subset R^n$, the probability of \mathbf{b} to belong to S is given by the integral

$\Pr(\mathbf{b} \in S) = \int_S p(\mathbf{b}) d\mathbf{b}$. When the probability density function depends on some unknown parameters $\boldsymbol{\theta}$ (in our case \mathbf{x} and \mathbf{y}) then the likelihood function is the probability density function for fixed parameter values $L(\mathbf{b}|\boldsymbol{\theta})$. The maximum likelihood estimation criterion assigns to the unknown $\boldsymbol{\theta}$ the estimates $\hat{\boldsymbol{\theta}}$, which maximize the likelihood function $L(\mathbf{b}|\hat{\boldsymbol{\theta}}) = \max_{\boldsymbol{\theta}} L(\mathbf{b}|\boldsymbol{\theta})$. If the probability density is having a unique maximum then for the given outcomes $\mathbf{b}(\omega)$ we assign as maximum likelihood estimates the values $\hat{\boldsymbol{\theta}}(\omega)$ for which the value of $L(\mathbf{b}(\omega)|\boldsymbol{\theta})$ becomes maximal. Obviously, such an optimality criterion may well fit the statistician's way of thinking (and many times it is considered the best possible one!) but fails to gain the attraction of the applied scientist (at least the one who is not consuming statistical recipes unquestionably). It falls sort when facing the intuitive charm of the minimum mean square criterion and furthermore it necessitates knowledge of the observation probability distribution. Statistical theory is dominated by the use of the Gaussian or normal distribution, merely because of its mathematical convenience in producing easy to apply results. (By the way, the same is true for the use of the least squares principle instead of, e.g. $\|\mathbf{e}^T \mathbf{P} \mathbf{e}\|^p = \min$ with positive $p \neq 2$, e.g. $p=1$.) In our case, assuming that the observations $\mathbf{b} = \mathbf{y} + \mathbf{e}$ have mean $E\{\mathbf{b}\} = \mathbf{y}$, covariance matrix $\mathbf{C}_b = E\{(\mathbf{b} - \mathbf{y})(\mathbf{b} - \mathbf{y})^T\} = E\{\mathbf{e}\mathbf{e}^T\} = \mathbf{C}_e$ and follow the normal distribution, their probability density (likelihood) function is given by

$$(1) \quad L(\mathbf{b}|\mathbf{y}) = [(2\pi)^n \det \mathbf{C}_b]^{-1/2} e^{-\frac{1}{2}(\mathbf{b}-\mathbf{y})^T \mathbf{C}_b^{-1}(\mathbf{b}-\mathbf{y})} = [(2\pi)^n \det \mathbf{C}_e]^{-1/2} e^{-\frac{1}{2}\mathbf{e}^T \mathbf{C}_e^{-1} \mathbf{e}}.$$

Since maximum $L(\mathbf{b}|\mathbf{y})$ is equivalent to maximum $\ln L(\mathbf{b}|\mathbf{y}) = -\frac{1}{2} \ln[(2\pi)^n \det \mathbf{C}_e] - \frac{1}{2} \mathbf{e}^T \mathbf{C}_e^{-1} \mathbf{e}$ and the first term is constant, we may equivalently maximize $-\mathbf{e}^T \mathbf{C}_e^{-1} \mathbf{e}$, i.e. minimize $\mathbf{e}^T \mathbf{C}_e^{-1} \mathbf{e} = \min$. However, this is a least squares principle with weight matrix $\mathbf{P} = \mathbf{C}_e^{-1}$ or any positive scalar multiple, e.g. $\mathbf{P} = \mathbf{Q}_e^{-1}$ when $\mathbf{C}_e = \sigma^2 \mathbf{Q}_e$ with σ^2 unknown. Therefore, the (less attractive) maximum likelihood estimation principle leads to the same choice of weight matrix for nonlinear models as the Gauss-Markov theorem for linear models, but only when the additional assumption of Gaussian error distribution is true. Most geodesists have been so much brainwashed by reading statistical and other relevant texts that they have developed a firm belief that errors follow the Gaussian distribution. The practicing surveyor however, who has spent considerable time making repeated measurements under "the same conditions" knows that reality does not conform to such mathematical niceties. In fact, serious doubts about the reality of the Gaussian or normal distribution are already spread in the scientific community.

Here are some famous quotes:

"Normality is a myth; there never was, and never will be, a normal distribution."

Geary, R. C. (1947). 'Testing for normality', *Biometrika*, 34:209–242.

"Everybody believes in the exponential law of errors [i.e., the Normal distribution]: the experimenters, because they think it can be proved by mathematics; and the mathematicians, because they believe it has been established by observation."

Whittaker, E. T. and Robinson, G. (1967). "Normal Frequency Distribution." Ch. 8 in *The Calculus of Observations: A Treatise on Numerical Mathematics*, 4th Ed. New York: Dover, pp. 164-208, 1967. p. 179.

"...the statistician knows...that in nature there never was a normal distribution, there never was a straight line, yet with normal and linear assumptions, known to be false, he can often derive results which match, to a useful approximation, those found in the real world."

Box, George E. P. (1976). *Science and Statistics*. *Journal of the American Statistical Association*, Vol. 71, pages 791-799.

Recall that statistical inference (hypothesis testing) also requires knowledge of the probability distribution of the errors and relies greatly on the Gaussian distribution assumption.

We may still attempt to profit from the optimality of the BLUE estimates in the linear case. The least squares nonlinear estimate of the observables $\hat{\mathbf{y}}$ is not uniformly unbiased or best (does not have minimum mean square error) among other candidate estimates belonging to the curved manifold of the observables M , but has these optimality properties among estimates belonging to the linear manifold $T_{\hat{\mathbf{y}}}(M)$, which is tangent to M at the point $\hat{\mathbf{y}} \in M$. $T_{\hat{\mathbf{y}}}(M)$ is a very good approximation to M within a small neighborhood of $\hat{\mathbf{y}}$. One problem arises from the fact that the routinely used probability distributions for the errors \mathbf{e} , such as the Gaussian distribution, allow for outcomes in the domain $-\infty < e_i < +\infty$. Thus, very large values of outcomes $\mathbf{e}(\omega)$ are highly improbable but possible, thus leading to observations $\mathbf{b}(\omega)$ and estimates $\hat{\mathbf{y}}(\omega)$, which are far from the true value \mathbf{y} . However, this is a problem of the mathematical model and not of physical reality. Every geodesist is ready to bet his head over the fact that the measurement error does not exceed some relatively large value. Thus to comply with reality one should use instead bounded error distributions, in which case all possible estimates $\hat{\mathbf{y}}(\omega)$ lie in

a rather small neighborhood of the true value. Whether M can be sufficiently approximated by $T_{\hat{y}}(M)$ or even $T_y(M)$ depends mostly on the magnitude of the local mean curvature of M . Replacing $T_{\hat{y}}(M)$ with $T_y(M)$ as a local approximation to M , bypasses the problem that $T_{\hat{y}}(M)$ depends on the random estimate \hat{y} and is thus randomly defined.

4. Nonlinear normal equations and iterative solutions

Without a nonlinear analog of the Gauss-Markov theorem one has to refrain to the least squares solution, either by just imitating the linear model case, or by resorting to the maximum likelihood principle. Thus, the weight matrix is still taken to be the inverse of the covariance matrix of the errors (apart from a positive linear factor, which does not affect the values of the estimates). The application of the least squares principle leads to a set of “nonlinear normal equations” whose solution provides the least-squares parameter estimates. Various algorithms may implemented for solving these nonlinear equations. We will give as an example the nonlinear normal equations for the Gauss-Helmert model or, from our point of view, the trivial linear model $\mathbf{b} = \mathbf{y} + \mathbf{e}$ subject to nonlinear constraints $\mathbf{h}(\mathbf{y}, \mathbf{x}) = \mathbf{0}$. The minimization of $\mathbf{e}^T \mathbf{P} \mathbf{e} = (\mathbf{b} - \mathbf{y})^T \mathbf{P} (\mathbf{b} - \mathbf{y})$ subject to $\mathbf{h}(\mathbf{y}, \mathbf{x}) = \mathbf{0}$ is based on the formulation of the Lagrangean function $\Phi = (\mathbf{b} - \mathbf{y})^T \mathbf{P} (\mathbf{b} - \mathbf{y}) - 2\mathbf{k}^T \mathbf{h}(\mathbf{y}, \mathbf{x})$ and the vanishing of its derivatives with respect to \mathbf{y} , \mathbf{x} and the Lagrange multipliers \mathbf{k} .

With $\mathbf{A} = \frac{\partial \mathbf{h}}{\partial \mathbf{x}}$, $\mathbf{B} = \frac{\partial \mathbf{h}}{\partial \mathbf{y}}$ the vanishing of the derivatives of the Lagrangean Φ with respect to \mathbf{y} , \mathbf{x} and \mathbf{k} leads to the system of nonlinear normal equations

$$(2a) \quad \hat{\mathbf{y}} = \mathbf{b} - \mathbf{P}^{-1} \mathbf{B}(\hat{\mathbf{y}}, \hat{\mathbf{x}})^T \hat{\mathbf{k}}$$

$$(2b) \quad \mathbf{A}(\hat{\mathbf{y}}, \hat{\mathbf{x}})^T \hat{\mathbf{k}} = \mathbf{0}$$

$$(2c) \quad \mathbf{h}(\hat{\mathbf{y}}, \hat{\mathbf{x}}) = \mathbf{0}.$$

Pope's iteration for the linear Gauss-Markov model with nonlinear constraints.

In geodetic applications, the same problem is solved in an ad hoc way by linearization and iteration using the estimates as new approximate values. Pope (1972) presented a corrected version of the linearization-iteration approach solving directly the above nonlinear normal equations (2) by replacing (2c) with its linear approximation. If \mathbf{x}_0 , \mathbf{y}_0 are approximate values to be used in a particular iteration step, then replacing $\mathbf{h}(\hat{\mathbf{y}}, \hat{\mathbf{x}})$ with its linear approximation we obtain the iteration scheme

$$(3a) \quad \delta \hat{\mathbf{y}} = \delta \mathbf{b} - \mathbf{P}^{-1} \mathbf{B}^T \hat{\mathbf{k}}$$

$$(3b) \quad \mathbf{A}^T \hat{\mathbf{k}} = \mathbf{0}$$

$$(3c) \quad \mathbf{h}(\hat{\mathbf{y}}, \hat{\mathbf{x}}) \approx \mathbf{h}_0 + \mathbf{A} \delta \hat{\mathbf{x}} + \mathbf{B} \delta \hat{\mathbf{y}} = \mathbf{0}$$

where $\mathbf{h}_0 = \mathbf{h}(\mathbf{x}_0, \mathbf{y}_0)$, $\mathbf{A} = \frac{\partial \mathbf{h}}{\partial \mathbf{x}}(\mathbf{x}_0, \mathbf{y}_0)$, $\mathbf{B} = \frac{\partial \mathbf{h}}{\partial \mathbf{y}}(\mathbf{x}_0, \mathbf{y}_0)$, $\delta \hat{\mathbf{x}} = \hat{\mathbf{x}} - \mathbf{x}_0$, $\delta \hat{\mathbf{y}} = \hat{\mathbf{y}} - \mathbf{y}_0$,

and $\delta \mathbf{b} = \mathbf{b} - \mathbf{y}_0$.

Replacing $\delta \hat{\mathbf{y}}$ from (3a) into (3c) gives $\mathbf{h}_0 + \mathbf{B} \delta \mathbf{b} + \mathbf{A} \delta \hat{\mathbf{x}} - \mathbf{B} \mathbf{P}^{-1} \mathbf{B}^T \hat{\mathbf{k}} = \mathbf{0}$ and $\hat{\mathbf{k}} = \mathbf{M}^{-1}(\mathbf{h}_0 + \mathbf{B} \delta \mathbf{b}) + \mathbf{M}^{-1} \mathbf{A} \delta \hat{\mathbf{x}}$, where $\mathbf{M} = \mathbf{B} \mathbf{P}^{-1} \mathbf{B}^T$, which replaced in the (3b) and (3a) yields

$$(4a) \quad \delta \hat{\mathbf{x}} = -(\mathbf{A}^T \mathbf{M}^{-1} \mathbf{A})^{-1} \mathbf{A}^T \mathbf{M}^{-1}(\mathbf{h}_0 + \mathbf{B} \delta \mathbf{b})$$

$$(4b) \quad \delta \hat{\mathbf{y}} = \delta \mathbf{b} - \mathbf{P}^{-1} \mathbf{B}^T \mathbf{M}^{-1}(\mathbf{A} \delta \hat{\mathbf{x}} + \mathbf{h}_0 + \mathbf{B} \delta \mathbf{b}),$$

$$(4c) \quad \hat{\mathbf{e}} = \mathbf{b} - \hat{\mathbf{y}} = \delta \mathbf{b} - \delta \hat{\mathbf{y}} = \mathbf{P}^{-1} \mathbf{B}^T \mathbf{M}^{-1}(\mathbf{A} \delta \hat{\mathbf{x}} + \mathbf{h}_0 + \mathbf{B} \delta \mathbf{b}).$$

The estimates $\hat{\mathbf{x}} = \mathbf{x}_0 + \delta \hat{\mathbf{x}}$, $\hat{\mathbf{y}} = \mathbf{y}_0 + \delta \hat{\mathbf{y}}$ are then used as approximate values in the next iteration step.

Pitfalls in iteration with the Gauss-Helmert model.

Let us compare the above iteration scheme with the usual geodetic (incorrect) linearization and iteration procedure. The Gauss-Helmert model of the form $\mathbf{h}(\mathbf{x}, \mathbf{y}) = \mathbf{h}(\mathbf{x}, \mathbf{b} - \mathbf{e}) = \mathbf{0}$, is linearized with respect to \mathbf{x}_0 and $\mathbf{e}_0 = \mathbf{0}$, as

$$(5) \quad \mathbf{h}(\mathbf{x}, \mathbf{b} - \mathbf{e}) = \mathbf{h}(\mathbf{x}_0, \mathbf{b}) + \bar{\mathbf{A}} \delta \mathbf{x} - \bar{\mathbf{B}} \mathbf{e} = \mathbf{w} + \bar{\mathbf{A}} \delta \mathbf{x} - \bar{\mathbf{B}} \mathbf{e} = \mathbf{0}$$

where $\bar{\mathbf{A}} = \frac{\partial \mathbf{h}}{\partial \mathbf{x}}(\mathbf{x}_0, \mathbf{b})$, $\bar{\mathbf{B}} = \frac{\partial \mathbf{h}}{\partial \mathbf{y}}(\mathbf{x}_0, \mathbf{b})$ and $\mathbf{w} = \mathbf{h}(\mathbf{x}_0, \mathbf{b})$ are the model misclosures.

The minimization of $\mathbf{e}^T \mathbf{P} \mathbf{e}$ subject to $\mathbf{w} + \bar{\mathbf{A}} \delta \hat{\mathbf{x}} - \bar{\mathbf{B}} \mathbf{e} = \mathbf{0}$ involves the Lagrangean $\bar{\Phi} = \mathbf{e}^T \mathbf{P} \mathbf{e} - 2\mathbf{k}^T(\mathbf{w} + \bar{\mathbf{A}} \delta \hat{\mathbf{x}} - \bar{\mathbf{B}} \mathbf{e})$. Setting the derivatives of $\bar{\Phi}$ with respect to \mathbf{e} , $\delta \hat{\mathbf{x}}$ and \mathbf{k} gives the solution system

$$(6a) \quad \hat{\mathbf{e}} = -\mathbf{P}^{-1} \bar{\mathbf{B}}^T \hat{\mathbf{k}},$$

$$(6b) \quad \bar{\mathbf{A}}^T \hat{\mathbf{k}} = \mathbf{0},$$

$$(6c) \quad \mathbf{w} + \bar{\mathbf{A}}\delta\hat{\mathbf{x}} - \bar{\mathbf{B}}\hat{\mathbf{e}} = \mathbf{0}.$$

Setting $\bar{\mathbf{M}} = \bar{\mathbf{B}}\mathbf{P}^{-1}\bar{\mathbf{B}}^T$ and replacing $\hat{\mathbf{e}}$ from (6a) to (6c) gives $\hat{\mathbf{k}} = -\bar{\mathbf{M}}^{-1}(\bar{\mathbf{A}}\delta\hat{\mathbf{x}} + \mathbf{w})$, which replaced in (6b) and (6a) leads to the estimates

$$(7a) \quad \delta\hat{\mathbf{x}} = -(\bar{\mathbf{A}}^T\bar{\mathbf{M}}^{-1}\bar{\mathbf{A}})^{-1}\bar{\mathbf{A}}^T\bar{\mathbf{M}}^{-1}\mathbf{w}, \quad (\bar{\mathbf{M}} = \bar{\mathbf{B}}\mathbf{P}^{-1}\bar{\mathbf{B}}^T),$$

$$(7b) \quad \hat{\mathbf{e}} = \mathbf{P}^{-1}\bar{\mathbf{B}}^T\bar{\mathbf{M}}^{-1}(\bar{\mathbf{A}}\delta\hat{\mathbf{x}} + \mathbf{w}), \quad \hat{\mathbf{y}} = \mathbf{b} - \hat{\mathbf{e}} = \mathbf{b} - \mathbf{P}^{-1}\bar{\mathbf{B}}^T\bar{\mathbf{M}}^{-1}(\bar{\mathbf{A}}\delta\hat{\mathbf{x}} + \mathbf{w}).$$

The estimates $\hat{\mathbf{x}} = \mathbf{x}_0 + \delta\hat{\mathbf{x}}$, are then used as approximate values \mathbf{x}_0 in the next iteration step. The failure to update the second part \mathbf{b} of the Taylor point in the linearization is the main pitfall pointed out by Pope (1972). The other differences between the first approach (nonlinear least squares and linear approximation of the nonlinear normal equations) from the second (linearization and linear least squares) are

- (a) the difference between the matrices \mathbf{A} , \mathbf{B} (evaluated at \mathbf{x}_0 , \mathbf{y}_0) and $\bar{\mathbf{A}}$, $\bar{\mathbf{B}}$ (evaluated at \mathbf{x}_0 , \mathbf{b}) and
- (b) the appearance of the misclosure \mathbf{w} in place of the term $\mathbf{h}_0 + \mathbf{B}\delta\mathbf{b}$.

With respect to (a) we note that the differences $\bar{\mathbf{A}} - \mathbf{A}$, $\bar{\mathbf{B}} - \mathbf{B}$ are very small and when multiplied with the small terms $\delta\hat{\mathbf{x}}$ and $\hat{\mathbf{e}}$ or $\delta\hat{\mathbf{y}}$ they produce second order negligible terms, e.g. $\mathbf{A}\delta\hat{\mathbf{x}} = \bar{\mathbf{A}}\delta\hat{\mathbf{x}} + (\bar{\mathbf{A}} - \mathbf{A})\delta\hat{\mathbf{x}} \approx \bar{\mathbf{A}}\delta\hat{\mathbf{x}}$. With respect to (b) we note that indeed in linear approximation

$$(8) \quad \mathbf{w} = \mathbf{h}(\mathbf{x}_0, \mathbf{b}) \approx \mathbf{h}(\mathbf{x}_0, \mathbf{y}_0) + \frac{\partial \mathbf{h}}{\partial \mathbf{y}}(\mathbf{x}_0, \mathbf{y}_0)(\mathbf{b} - \mathbf{y}_0) = \mathbf{h}_0 + \mathbf{B}\delta\mathbf{b}.$$

Pope's iteration applied to the Gauss-Helmert model.

A correct version for an iterative solution of the Gauss-Helmert model can be produced by updating also the error estimates, linearizing $\mathbf{h}(\mathbf{x}, \mathbf{b} - \mathbf{e}) = \mathbf{0}$ with respect to \mathbf{x}_0 and \mathbf{e}_0 , as

$$(9) \quad \mathbf{h}(\mathbf{x}, \mathbf{b} - \mathbf{e}) = \mathbf{h}(\mathbf{x}_0, \mathbf{b} - \mathbf{e}_0) + \bar{\mathbf{A}}\delta\mathbf{x} - \bar{\mathbf{B}}(\mathbf{e} - \mathbf{e}_0) = \bar{\mathbf{h}}_0 + \bar{\mathbf{B}}\mathbf{e}_0 + \bar{\mathbf{A}}\delta\mathbf{x} - \bar{\mathbf{B}}\mathbf{e} = \mathbf{0}$$

where $\bar{\mathbf{A}} = \frac{\partial \mathbf{h}}{\partial \mathbf{x}}(\mathbf{x}_0, \mathbf{b} - \mathbf{e}_0)$, $\bar{\mathbf{B}} = -\frac{\partial \mathbf{h}}{\partial \mathbf{e}}(\mathbf{x}_0, \mathbf{b} - \mathbf{e}_0)$ and $\bar{\mathbf{h}}_0 = \mathbf{h}(\mathbf{x}_0, \mathbf{b} - \mathbf{e}_0)$.

The minimization of $\mathbf{e}^T \mathbf{P} \mathbf{e}$ subject to $\bar{\mathbf{h}}_0 + \bar{\mathbf{B}}\mathbf{e}_0 + \bar{\mathbf{A}}\delta\mathbf{x} - \bar{\mathbf{B}}\mathbf{e} = \mathbf{0}$ involves the Lagrangean $\bar{\Phi} = \mathbf{e}^T \mathbf{P} \mathbf{e} - 2\mathbf{k}^T (\bar{\mathbf{h}}_0 + \bar{\mathbf{B}}\mathbf{e}_0 + \bar{\mathbf{A}}\delta\mathbf{x} - \bar{\mathbf{B}}\mathbf{e})$. Setting the derivatives of $\bar{\Phi}$ with respect to \mathbf{e} , $\delta\mathbf{x}$ and \mathbf{k} gives the solution system

$$(10a) \quad \hat{\mathbf{e}} = -\mathbf{P}^{-1}\bar{\mathbf{B}}^T\hat{\mathbf{k}},$$

$$(10b) \quad \bar{\mathbf{A}}^T\hat{\mathbf{k}} = \mathbf{0},$$

$$(10c) \quad \bar{\mathbf{h}}_0 + \bar{\mathbf{B}}\mathbf{e}_0 + \bar{\mathbf{A}}\delta\hat{\mathbf{x}} - \bar{\mathbf{B}}\hat{\mathbf{e}} = \mathbf{0}.$$

Setting $\bar{\mathbf{M}} = \bar{\mathbf{B}}\mathbf{P}^{-1}\bar{\mathbf{B}}^T$ and replacing $\hat{\mathbf{e}}$ from (10a) into (10c) gives $\hat{\mathbf{k}} = -\bar{\mathbf{M}}^{-1}(\bar{\mathbf{h}}_0 + \bar{\mathbf{B}}\mathbf{e}_0 + \bar{\mathbf{A}}\delta\hat{\mathbf{x}})$, which replaced in (10b) and (10a) leads to the estimates

$$(11a) \quad \hat{\mathbf{x}} = \mathbf{x}_0 - (\bar{\mathbf{A}}^T\bar{\mathbf{M}}^{-1}\bar{\mathbf{A}})^{-1}\bar{\mathbf{A}}^T\bar{\mathbf{M}}^{-1}(\bar{\mathbf{h}}_0 + \bar{\mathbf{B}}\mathbf{e}_0)$$

$$(11b) \quad \hat{\mathbf{e}} = \mathbf{P}^{-1}\bar{\mathbf{B}}^T\bar{\mathbf{M}}^{-1}(\bar{\mathbf{h}}_0 + \bar{\mathbf{B}}\mathbf{e}_0 + \bar{\mathbf{A}}\delta\hat{\mathbf{x}}),$$

$$(11c) \quad \hat{\mathbf{y}} = \mathbf{b} - \hat{\mathbf{e}} = \mathbf{b} - \mathbf{P}^{-1}\bar{\mathbf{B}}^T\bar{\mathbf{M}}^{-1}(\bar{\mathbf{h}}_0 + \bar{\mathbf{B}}\mathbf{e}_0 + \bar{\mathbf{A}}\delta\hat{\mathbf{x}}).$$

The estimates $\hat{\mathbf{x}} = \mathbf{x}_0 + \delta\hat{\mathbf{x}}$, $\hat{\mathbf{e}}$ are then used as approximate values \mathbf{x}_0 and \mathbf{e}_0 in the next iteration step.

A problem with the Gauss-Helmert iteration without explicit use of the observables \mathbf{y} is the fact that as the coefficient matrices $\bar{\mathbf{A}}$ and $\bar{\mathbf{B}}$ are evaluated using the random observations \mathbf{b} they are themselves random variables and an Errors-In-Variables (EIV) type model should be used instead. A similar problem appears to be present in the first step of Pope's correct iteration scheme, where initial approximate values \mathbf{x}_0 , \mathbf{y}_0 are needed. Pope (1972) suggests using $\mathbf{y}_0 = \mathbf{b}$ in the first, but this will create also random coefficient matrices. In addition \mathbf{x}_0 must come either from some use of the observations \mathbf{b} , or from (random) estimates based on a previous data analysis and is therefore random. Furthermore, in the next iteration steps the approximate values are set equal to the random estimates of the previous step and are therefore random. However, this type of skepticism is easy to overcome. One must see the iteration process as a procedure leading to the final estimate $\hat{\mathbf{y}} \in M$, which is closer to the observations \mathbf{b} in the least squares sense. As far as the iteration converges, the departing point (approximate values at the first step) and the intermediate steps are of no direct importance. The iteration must be seen simply as a mathematical device for solving the nonlinear normal equations and not as a repeated application of a linear estimation process. As far as the same final value $\hat{\mathbf{y}}$ is obtained (allowing for insignificant variations due to different numerical errors), there exist no problem arising from the possible stochastic interpretation of the iteration steps. Recall that the same answer can be obtained by other iterative numerical methods such as the Gauss-Newton method, the method of steepest descent and the Levenberg-Marquardt method which a hybrid method between the previous two.

A final problem is the estimation of the covariance matrices of the parameters. In Pope's iteration, the covariance matrices resulting from the linear estimation model of the final iteration step are used as a good approximation. However the mapping from the observations \mathbf{b} to the estimates $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, as the solution of a system of nonlinear equations, is itself a nonlinear mapping. Therefore a nonlinear type of covariance propagation is needed which can only be realized by Monte-Carlo simulation methods. The problem again is that these methods require knowledge of the probability distribution of the observations, i.e. essentially of the observation errors.

5. Different solution algorithm generation for non-linear models.

The EIV example.

Apart from the use of different methods for solving the nonlinear normal equations (2), different algorithms may arise from different formulation of the normal equations and the order of elimination of all or some of the three sets of unknowns: unknown parameters $\hat{\mathbf{x}}$, observables $\hat{\mathbf{y}}$ or errors $\hat{\mathbf{e}}$ and Lagrange multipliers $\hat{\mathbf{k}}$. Strictly speaking, the term normal equations should be used for those remaining after all Lagrange multipliers are eliminated. For example elimination of $\hat{\mathbf{k}}$ will give the rather difficult to solve reduced set

$$(12) \quad \mathbf{A}(\hat{\mathbf{x}}, \hat{\mathbf{y}})^T \left[\mathbf{B}(\hat{\mathbf{x}}, \hat{\mathbf{y}}) \mathbf{P}^{-1} \mathbf{B}(\hat{\mathbf{x}}, \hat{\mathbf{y}})^T \right]^{-1} \mathbf{B}(\hat{\mathbf{x}}, \hat{\mathbf{y}}) (\mathbf{b} - \hat{\mathbf{y}}) = \mathbf{0}, \quad \mathbf{h}(\hat{\mathbf{x}}, \hat{\mathbf{y}}) = \mathbf{0}.$$

However, it is sometimes convenient to retain some of the Lagrange multipliers as part of the unknowns to be determined. The Errors-In Variables (EIV) model is a good example of how different algorithms may arise. We will apply the two iteration algorithms based on the linearization of either $\mathbf{h}(\mathbf{x}, \mathbf{y}) = \mathbf{0}$ or $\mathbf{h}(\mathbf{x}, \mathbf{b} - \mathbf{e}) = \mathbf{0}$, as well as Total Least Squares (TLS) algorithms based on the nonlinear equations $\mathbf{h}(\mathbf{x}, \mathbf{b} - \mathbf{e}) = \mathbf{0}$ without linearization.

We find convenient to depart from our standard convention of using bold letters for matrices, only for the EIV model. This will greatly help in distinguish the general case (in bold) from its application to the EIV model.

In the EIV model $y = (A - E_A)x + e_y$, where we set $e_A = \text{vec}E_A$, $a = \text{vec}A$, the observables are $\bar{y} = y - e_y$ and $\bar{a} \equiv \text{vec}\bar{A} = \text{vec}(A - E_A) = \text{vec}A - \text{vec}E_A \equiv a - e_A$, the observations are y and $a = \text{vec}A$, and the model is $h = y - (A - E_A)x - e_y = \bar{y} - \bar{A}x = 0$. We may apply directly the formulated nonlinear normal equations as well as the iterative solutions by simply replacing

$$(13) \quad \mathbf{h}(\mathbf{x}, \mathbf{y}) \rightarrow h(x, \bar{y}, \bar{a}) = \bar{y} - \bar{A}x = \bar{y} - (x^T \otimes I_n) \bar{a}$$

$$(14) \quad \mathbf{h}(\mathbf{x}, \mathbf{b} - \mathbf{e}) \rightarrow \\ \rightarrow h(x, y - e_y, A - E_A) = y - (A - E_A)x - e_y = y - Ax + (x^T \otimes I_n)e_A - e_y$$

$$(15) \quad \mathbf{b} \rightarrow \begin{bmatrix} y \\ a \end{bmatrix}, \quad \mathbf{y} \rightarrow \begin{bmatrix} \bar{y} \\ \bar{a} \end{bmatrix}, \quad \mathbf{e} \rightarrow \begin{bmatrix} e_y \\ e_A \end{bmatrix},$$

$$(16a) \quad \mathbf{A}(\mathbf{x}, \mathbf{y}) \rightarrow \frac{\partial h}{\partial x} = -\bar{A},$$

$$(16b) \quad \mathbf{B}(\mathbf{x}, \mathbf{y}) \rightarrow \frac{\partial h}{\partial \begin{bmatrix} \bar{y} \\ \bar{a} \end{bmatrix}} = \begin{bmatrix} \frac{\partial h}{\partial \bar{y}} & \frac{\partial h}{\partial \bar{a}} \end{bmatrix} = \begin{bmatrix} I_n & -(x^T \otimes I_n) \end{bmatrix}$$

$$(17a) \quad \mathbf{A}(\mathbf{x}, \mathbf{b} - \mathbf{e}) \rightarrow \frac{\partial h}{\partial x} = -(A - E_A),$$

$$(17b) \quad \mathbf{B}(\mathbf{x}, \mathbf{b} - \mathbf{e}) \rightarrow -\frac{\partial h}{\partial \begin{bmatrix} e_y \\ e_A \end{bmatrix}} = -\begin{bmatrix} \frac{\partial h}{\partial e_y} & \frac{\partial h}{\partial e_A} \end{bmatrix} = \begin{bmatrix} I_n & -(x^T \otimes I_n) \end{bmatrix}$$

Iteration of linear Gauss-Markov model with nonlinear constraints.

In this particular approach the matrices involved are

$$(18) \quad \mathbf{A}(\mathbf{x}_0, \mathbf{y}_0) \rightarrow -\bar{A}_0, \quad \mathbf{B}(\mathbf{x}_0, \mathbf{y}_0) \rightarrow \begin{bmatrix} I_n & -(x_0^T \otimes I_n) \end{bmatrix}, \quad \mathbf{P}^{-1} \rightarrow \begin{bmatrix} Q_y & 0 \\ 0 & Q_A \end{bmatrix}$$

$$(19) \quad \mathbf{M} = \mathbf{B}\mathbf{P}^{-1}\mathbf{B}^T \rightarrow M_0 = Q_y + (x_0^T \otimes I_n)Q_A(x_0 \otimes I_n)$$

$$(20) \quad \mathbf{h}_0 \rightarrow y_0 - \bar{A}_0 x_0 = y_0 - (x_0^T \otimes I_n)\bar{a}_0$$

$$(21) \quad \mathbf{B}\delta\mathbf{b} = \mathbf{B}(\mathbf{b} - \mathbf{y}_0) \rightarrow \begin{bmatrix} I_n & -(x_0^T \otimes I_n) \end{bmatrix} \begin{bmatrix} y - y_0 \\ a - \bar{a}_0 \end{bmatrix} = y - y_0 - (x_0^T \otimes I_n)(a - \bar{a}_0)$$

$$(22) \quad \mathbf{h}_0 + \mathbf{B}\delta\mathbf{b} \rightarrow y_0 - (x_0^T \otimes I_n)\bar{a}_0 + y - y_0 - (x_0^T \otimes I_n)(a - \bar{a}_0) = y - Ax_0$$

$$(23) \quad \delta\hat{\mathbf{x}} = -(\mathbf{A}^T \mathbf{M}^{-1} \mathbf{A})^{-1} \mathbf{A}^T \mathbf{M}^{-1} (\mathbf{h}_0 + \mathbf{B}\delta\mathbf{b}) \rightarrow \delta\hat{x} = (\bar{A}_0^T M_0^{-1} \bar{A}_0)^{-1} \bar{A}_0^T M_0^{-1} (y - Ax_0)$$

$$(24) \quad \delta \hat{\mathbf{y}} = \delta \mathbf{b} - \mathbf{P}^{-1} \mathbf{B}^T \mathbf{M}^{-1} (\mathbf{A} \delta \hat{\mathbf{x}} + \mathbf{h}_0 + \mathbf{B} \delta \mathbf{b}) \rightarrow \\ \rightarrow \begin{bmatrix} \hat{y} - y_0 \\ \hat{a} - \bar{a}_0 \end{bmatrix} = \begin{bmatrix} y - y_0 \\ a - \bar{a}_0 \end{bmatrix} + \begin{bmatrix} -Q_y \\ Q_A(x_0 \otimes I_n) \end{bmatrix} M_0^{-1} (-\bar{A}_0 \delta \hat{\mathbf{x}} + y - Ax_0),$$

$$(25) \quad \hat{\mathbf{e}} = \mathbf{b} - \hat{\mathbf{y}} \rightarrow \begin{bmatrix} \hat{e}_y \\ \hat{e}_A \end{bmatrix} = \begin{bmatrix} y - \hat{y} \\ a - \hat{a} \end{bmatrix} = \begin{bmatrix} Q_y M_0^{-1} [y - \bar{A}_0 \hat{\mathbf{x}} + (\bar{A}_0 - A)x_0] \\ -Q_A(x_0 \otimes I_n) M_0^{-1} [y - \bar{A}_0 \hat{\mathbf{x}} + (\bar{A}_0 - A)x_0] \end{bmatrix}.$$

Therefore, the iteration solution is given by

$$(26a) \quad \hat{\mathbf{x}} = x_0 + (\bar{A}_0^T M^{-1} \bar{A}_0)^{-1} \bar{A}_0^T M_0^{-1} (y - Ax_0),$$

$$(26b) \quad \hat{y} = y - Q_y M_0^{-1} [y - \bar{A}_0 \hat{\mathbf{x}} + (\bar{A}_0 - A)x_0],$$

$$(26c) \quad \hat{e}_y = y - \hat{y} = Q_y M_0^{-1} [y - \bar{A}_0 \hat{\mathbf{x}} + (\bar{A}_0 - A)x_0],$$

$$(26d) \quad \hat{a} = a + Q_A(x_0 \otimes I_n) M_0^{-1} [y - \bar{A}_0 \hat{\mathbf{x}} + (\bar{A}_0 - A)x_0],$$

$$(26e) \quad \hat{e}_A = a - \hat{a} = -Q_A(x_0 \otimes I_n) M_0^{-1} [y - \bar{A}_0 \hat{\mathbf{x}} + (\bar{A}_0 - A)x_0].$$

Iteration of nonlinear Gauss-Helmert model.

In this particular approach the matrices involved are

$$(27a) \quad \bar{\mathbf{A}} = \mathbf{A}(\mathbf{x}_0, \mathbf{b} - \mathbf{e}_0) \rightarrow -(A - E_A^0),$$

$$(27b) \quad \bar{\mathbf{B}} = (\mathbf{x}_0, \mathbf{b} - \mathbf{e}_0) \rightarrow \begin{bmatrix} I_n & -(x_0^T \otimes I_n) \end{bmatrix},$$

$$(28) \quad \bar{\mathbf{h}}_0 = \mathbf{h}(\mathbf{x}_0, \mathbf{b} - \mathbf{e}_0) \rightarrow y - (A - E_A^0)x_0 - e_y^0, \quad \bar{\mathbf{B}}\mathbf{e}_0 \rightarrow e_y^0 - E_A^0 x_0$$

$$(29) \quad \bar{\mathbf{h}}_0 + \bar{\mathbf{B}}\mathbf{e}_0 \rightarrow y - Ax_0$$

$$(30) \quad \bar{\mathbf{M}} = \bar{\mathbf{B}}\mathbf{P}^{-1}\bar{\mathbf{B}}^T \rightarrow M_0 = Q_y + (x_0^T \otimes I_n)Q_A(x_0 \otimes I_n)$$

$$(31) \quad \delta \hat{\mathbf{x}} = -(\bar{\mathbf{A}}^T \bar{\mathbf{M}}^{-1} \bar{\mathbf{A}})^{-1} \bar{\mathbf{A}}^T \bar{\mathbf{M}}^{-1} (\bar{\mathbf{h}}_0 + \bar{\mathbf{B}}\mathbf{e}_0) \rightarrow \\ \rightarrow \delta \hat{\mathbf{x}} = \left[(A - E_A^0)^T M_0^{-1} (A - E_A^0) \right]^{-1} (A - E_A^0)^T M_0^{-1} (y - Ax_0)$$

$$(32) \quad \hat{\mathbf{e}} = \mathbf{P}^{-1} \bar{\mathbf{B}}^T \bar{\mathbf{M}}^{-1} (\bar{\mathbf{h}}_0 + \bar{\mathbf{B}} \mathbf{e}_0 + \bar{\mathbf{A}} \delta \hat{\mathbf{x}}) \rightarrow \\ \rightarrow \begin{bmatrix} \hat{e}_y \\ \hat{e}_A \end{bmatrix} = \begin{bmatrix} Q_y M_0^{-1} \\ -Q_A (x_0 \otimes I_n) M_0^{-1} \end{bmatrix} [y - Ax_0 - (A - E_A^0)(\hat{x} - x_0)].$$

Therefore, the iteration solution is given by

$$(33a) \quad \hat{x} = x_0 + \left[(A - E_A^0)^T M_0^{-1} (A - E_A^0) \right]^{-1} (A - E_A^0)^T M_0^{-1} (y - Ax_0)$$

$$(33b) \quad \hat{e}_y = Q_y M_0^{-1} [y - E_A^0 x_0 - (A - E_A^0) \hat{x}],$$

$$(33c) \quad \hat{e}_A = -Q_A (x_0 \otimes I_n) M_0^{-1} [y - E_A^0 x_0 - (A - E_A^0) \hat{x}].$$

Formulation of nonlinear normal equations and iterative solutions.

The general normal equations for the Gauss-Helmert model follow by simply replacing $\hat{\mathbf{y}} = \mathbf{b} - \hat{\mathbf{e}}$ in equations (2)

$$(34a) \quad \hat{\mathbf{e}} = -\mathbf{P}^{-1} \mathbf{B}(\hat{\mathbf{x}}, \mathbf{b} - \hat{\mathbf{e}})^T \hat{\mathbf{k}}$$

$$(34b) \quad \mathbf{A}(\hat{\mathbf{x}}, \mathbf{b} - \hat{\mathbf{e}})^T \hat{\mathbf{k}} = \mathbf{0}$$

$$(34c) \quad \mathbf{h}(\hat{\mathbf{x}}, \mathbf{b} - \hat{\mathbf{e}}) = \mathbf{0}$$

For the particular case of the EIV model the matrices involved are

$$(35) \quad \mathbf{h}(\hat{\mathbf{x}}, \mathbf{b} - \hat{\mathbf{e}}) \rightarrow y - (A - \hat{E}_A) \hat{x} - \hat{e}_y = y - A \hat{x} + (\hat{x}^T \otimes I_n) \hat{e}_A - \hat{e}_y$$

$$(36) \quad \mathbf{b} \rightarrow \begin{bmatrix} y \\ a \end{bmatrix}, \quad \mathbf{y} \rightarrow \begin{bmatrix} \bar{y} \\ \bar{a} \end{bmatrix}, \quad \mathbf{e} \rightarrow \begin{bmatrix} e_y \\ e_A \end{bmatrix},$$

$$(37) \quad \mathbf{A}(\hat{\mathbf{x}}, \mathbf{b} - \hat{\mathbf{e}}) \rightarrow -(A - \hat{E}_A), \quad \mathbf{B}(\hat{\mathbf{x}}, \mathbf{b} - \hat{\mathbf{e}}) \rightarrow \begin{bmatrix} I_n & -(\hat{x}^T \otimes I_n) \end{bmatrix}$$

$$(38) \quad \hat{\mathbf{e}} = -\mathbf{P}^{-1} \mathbf{B}(\hat{\mathbf{x}}, \mathbf{b} - \hat{\mathbf{e}})^T \hat{\mathbf{k}} \rightarrow \begin{bmatrix} \hat{e}_y \\ \hat{e}_A \end{bmatrix} = - \begin{bmatrix} Q_y & 0 \\ 0 & Q_A \end{bmatrix} \begin{bmatrix} I_n \\ -(\hat{x} \otimes I_n) \end{bmatrix} \hat{\mathbf{k}}$$

$$(39) \quad \mathbf{A}(\hat{\mathbf{x}}, \mathbf{b} - \hat{\mathbf{e}})^T \hat{\mathbf{k}} = \mathbf{0} \rightarrow -(A - \hat{E}_A)^T \hat{\mathbf{k}} = \mathbf{0}$$

and the primary nonlinear normal equations become

$$(40a) \quad \hat{e}_y = -Q_y \hat{k}$$

$$(40b) \quad \hat{e}_A = Q_A(\hat{x} \otimes I_n) \hat{k}$$

$$(40c) \quad (A - \hat{E}_A)^T \hat{k} = 0$$

$$(40d) \quad y - (A - \hat{E}_A) \hat{x} - \hat{e}_y = y - A \hat{x} + (\hat{x}^T \otimes I_n) \hat{e}_A - \hat{e}_y = 0$$

Note that in the iteration solution based on the Gauss-Helmert model, the last rigorous equation $y - (A - \hat{E}_A) \hat{x} - \hat{e}_y = 0$ has been replaced by its linear approximation $y - (A - E_A^0) \hat{x} + (\hat{E}_A - E_A^0) x_0 - \hat{e}_y = 0$, after a Taylor expansion around the values (x_0, e_y^0, e_A^0) . The following iterative solutions are therefore superior in this respect. They are based on the possibility to convert a general nonlinear equation $f(\chi) = 0$ in the form $\chi = \varphi(\chi)$, such that the iteration $\chi_{i+1} = \varphi(\chi_i)$ converges. In the following will describe a single step of such a procedure as $\chi = \varphi(\chi_0)$.

Replacing $\hat{e}_y = -Q_y \hat{k}$ from the (40a) and $\hat{e}_A = Q_A(\hat{x} \otimes I_n) \hat{k}$ from (40b) into (40d) we obtain $y - A \hat{x} + M \hat{k} = 0$ where $M = M(\hat{x}) = Q_y + (\hat{x}^T \otimes I_n) Q_A(\hat{x} \otimes I_n)$ and

$$(41) \quad \hat{k} = M^{-1}(y - A \hat{x}).$$

Replacing this value in (40c), we obtain

$$(42) \quad (A - \hat{E}_A)^T M^{-1}(y - A \hat{x}) = 0,$$

which is the basic equation for obtaining \hat{x} . In an algorithm proposed by Fang (2011) the last equation is replaced by a symmetric counterpart

$$(43) \quad (A - \hat{E}_A)^T M^{-1}[y - (A - \hat{E}_A) \hat{x} - \hat{E}_A \hat{x}] = 0,$$

which takes the appropriate for iteration form $\hat{\chi} = \varphi(\hat{\chi})$

$$(44) \quad \hat{x} = \left[(A - \hat{E}_A)^T M^{-1} (A - \hat{E}_A) \right]^{-1} (A - \hat{E}_A)^T M^{-1} (y - \hat{E}_A \hat{x}).$$

Using the estimates of the previous step as approximate values in the right hand side of (44) the iteration of the form $\hat{\chi} = \varphi(\chi_0)$ is given by

$$(45) \quad \hat{x} = \left[(A - E_A^0)^T M_0^{-1} (A - E_A^0) \right]^{-1} (A - E_A^0)^T M_0^{-1} (y - E_A^0 x_0)$$

where now $M_0 = M(x_0) = Q_y + (x_0^T \otimes I_n) Q_A (x_0 \otimes I_n)$. The obtained value \hat{x} can be used to compute the Lagrange multipliers $\hat{k} = M(\hat{x})^{-1} (y - A\hat{x})$ and hence $\hat{e}_y = -Q_y \hat{k}$, $\hat{e}_A = Q_A (\hat{x} \otimes I_n) \hat{k}$ or directly

$$(46) \quad \hat{e}_y = -Q_y M(\hat{x})^{-1} (y - A\hat{x}), \quad \hat{e}_A = Q_A (\hat{x} \otimes I_n) M(\hat{x})^{-1} (y - A\hat{x}).$$

The obtained estimates \hat{x} , $\hat{e}_A = \text{vec} \hat{E}_A$ provide the approximate values x_0 , E_A^0 for the next step.

Equation (44) corresponds to equation (4.22) of Fang (2011), in the special case that $E\{e_A e_y^T\} = \sigma_0^2 Q_{Ay} = 0$, while Fang treats the more general case with $Q_{Ay} \neq 0$, which has little practical interest. Note that (44) also appears as formula (21) in Xu et al. (2012).

A slightly modified algorithm has been presented by Mahboub (2012). We will give here a much simpler than the original derivation based on the easy to verify property $\hat{E}_A^T \hat{k} = (I_m \otimes \hat{k}^T) \hat{e}_A$ (A is a $n \times m$ matrix).

Combining this with $(A - \hat{E}_A)^T \hat{k} = 0$ (40c), it follows that $A^T \hat{k} - (I_m \otimes \hat{k}^T) \hat{e}_A = 0$, which with $\hat{e}_A = -Q_A (\hat{x} \otimes I_n) \hat{k}$ (40b) gives $A^T \hat{k} + (I_m \otimes \hat{k}^T) Q_A (\hat{x} \otimes I_n) \hat{k} = 0$. Replacing in the last equation $\hat{k} = M^{-1} (y - A\hat{x})$ (41) we obtain $[A^T + (I_m \otimes \hat{k}^T) Q_A (\hat{x} \otimes I_n)] M^{-1} (y - A\hat{x}) = 0$, which solved for the last \hat{x} gives

$$(47) \quad \hat{x} = \left[A^T M^{-1} A - (I_m \otimes \hat{k}^T) Q_A (\hat{k} \otimes I_n) M^{-1} A \right]^{-1} \cdot \left[(I_m \otimes \hat{k}^T) Q_A (\hat{k} \otimes I_n) M^{-1} y + A^T M^{-1} y \right].$$

The last equation is identical with equation (24) of Mahboub (2012) which has the compact form $\hat{x} = (A^T R_1 A + R_2 A)^{-1} (R_2 y + A^T R_1 y)$ with $R_1 = M^{-1}$ and $R_2 = (I_m \otimes \hat{k}^T) Q_A (\hat{k} \otimes I_n) M^{-1}$.

This equation of the form $\hat{x} = \varphi(\hat{x})$ gives an iteration scheme of the form $\hat{x} = \varphi(x_0)$ by using approximate values from the previous step on the right side

$$(48) \quad \hat{x} = \left[A^T M_0^{-1} A - (I_m \otimes k_0^T) Q_A (k_0 \otimes I_n) M_0^{-1} A \right]^{-1} \cdot \left[(I_m \otimes k_0^T) Q_A (k_0 \otimes I_n) M_0^{-1} b + A^T M_0^{-1} y \right],$$

while $\hat{k} = M(\hat{x})^{-1}(y - A\hat{x})$ gives together with \hat{x} the approximate values k_0, x_0 to be used in the next iteration step.

Here we have only sketched the possibility of obtaining different solutions for nonlinear models using the EIV model as an example. For a more complete treatment of the EIV model see the review paper by Schaffrin (2013).

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