Approximate Covariance of the Nonlinear Implicit Normal Inverse Problem

Bill Menke, April 6, 2024

Eqn. 11.28 of Menke (2024) is a formula for the solution to the nonlinear implicit Normal inverse problem. Here, I provide a supplementary (and approximate) formula for the posterior covariance of the solution:

$$\left[\operatorname{cov}\mathbf{x}^{(n)}\right] \approx (\mathbf{I} - [\operatorname{cov}\mathbf{x}]\mathbf{F}^T[\mathbf{F}[\operatorname{cov}\mathbf{x}]\mathbf{F}^T]^{-1}\mathbf{F})[\operatorname{cov}\mathbf{x}]$$

(where the notation is explained below).

We consider a Normal prior pdf $p(\mathbf{x}) \propto \exp\{-½E(\mathbf{x})\}$ with

$$E(\mathbf{x}) = (\mathbf{x} - \bar{\mathbf{x}})^T[\operatorname{cov}\mathbf{x}]^{-1}(\mathbf{x} - \bar{\mathbf{x}})^T$$

where $\mathbf{x}$ is a concatenation of data and model parameters. The mean $\bar{\mathbf{x}}$ is a concatenation of the observed data and the prior model parameters and has covariance $[\operatorname{cov}\mathbf{x}]$. The implicit nonlinear problem has solution $\mathbf{x}^{(n)}$ that maximizes $p(\mathbf{x})$ with the constraint that the theory $\mathbf{f}(\mathbf{x}) = 0$ is satisfied (here $\mathbf{f}$ is of length L). The problem is to compute the posterior covariance $\left[\operatorname{cov}\mathbf{x}^{(n)}\right]$ of the solution $\mathbf{x}^{(n)}$. The superscript (n) is a reminder that the solution is determined iteratively by n iterations of the method.

The steps that we shall use are:

(1) Transform $\mathbf{x}$ to a new coordinate system $\mathbf{y}$ which has its origin at $\mathbf{x}^{(n)}$ and for which $[\operatorname{cov}\mathbf{y}]$ is the identity matrix (Fig. 1).

(2) Approximate $\mathbf{f}(\mathbf{x}) = 0$ as a hyperplane in the vicinity of $\mathbf{x}^{(n)}$ and identify two subspaces of $\mathbf{y}$, one of which is in the plane (the null space y_0) and the other which is normal to the plane (the p-space y_p). Singular value decomposition is used to identify the subspaces.

(3) The part of $\left[\operatorname{cov}\mathbf{y}^{(n)}\right]$ in the p-space must be is zero, as a perturbation would cause it leave the plane, which is forbidden by the constraint. The part of $\left[\operatorname{cov}\mathbf{y}^{(n)}\right]$ in null space equals the corresponding part of $[\operatorname{cov}\mathbf{y}]$, as the plane does not constrain perturbations within it. Consequently, $\left[\operatorname{cov}\mathbf{y}^{(n)}\right]$ is just the part of $[\operatorname{cov}\mathbf{y}]$ in the null space.

(4) Finally, $\left[\operatorname{cov}\mathbf{y}^{(n)}\right]$ is transformed back to $\left[\operatorname{cov}\mathbf{x}^{(n)}\right]$.

Step 1. We use the linear transformation rule for Normally-distributed random variables: Let $\mathbf{x}$ be Normally-distributed with mean $\bar{\mathbf{x}}$ and covariance $[\operatorname{cov}\mathbf{x}]$ and let $\mathbf{y} = \mathbf{A}\mathbf{x} + \mathbf{b}$. Then $\mathbf{y}$ is Normally-distributed with mean $\bar{\mathbf{y}} = \mathbf{A}\bar{\mathbf{x}} + \mathbf{b}$ and covariance $[\operatorname{cov}\mathbf{y}] = \mathbf{A}[\operatorname{cov}\mathbf{x}]\mathbf{A}^T$.

We choose $\mathbf{A}$ and $\mathbf{b}$ in the transformation so that $\mathbf{y}^{(n)} \equiv \mathbf{y}\left(\mathbf{x}^{(n)}\right) = 0$ (that is, $\mathbf{y}^{(n)}$ is at the origin) and $[\operatorname{cov}\mathbf{y}] = \mathbf{I}$: (that is, $\mathbf{y}$ are uncorrelated and with unit variance):

$$\mathbf{y}\left(\mathbf{x}^{(n)}\right) = \mathbf{A}\mathbf{x}^{(n)} + \mathbf{b} = 0 \quad \text{and} \quad [\operatorname{cov}\mathbf{y}] \equiv \mathbf{A}[\operatorname{cov}\mathbf{x}]\mathbf{A}^T = \mathbf{I} \quad \text{and } [\operatorname{cov}\mathbf{x}] = \mathbf{A}^{-1}[\operatorname{cov}\mathbf{y}]\mathbf{A}^{-1\mathrm{T}}$$

which implies

$$\mathbf{A} = [\operatorname{cov}\mathbf{x}]^{-½} \quad \text{and} \quad \mathbf{b} = -[\operatorname{cov}\mathbf{x}]^{-½}\mathbf{x}^{(n)}$$

Then, various transformed and untransformed variables are

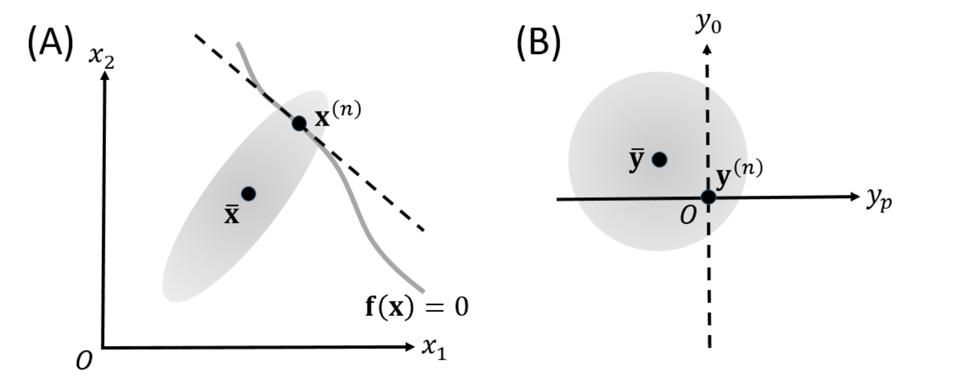

Fig. 1. (A) The solution $\mathbf{x}^{(n)}$ is the point on $\mathbf{f}(\mathbf{x}) = 0$ (curve) that maximizes the pdf $p(\mathbf{x})$ (shaded). A plane (dashed) is tangent to the curve at the solution. (B) A coordinate transformation takes $\mathbf{x}^{(n)}$ to $\mathbf{y}^{(n)} = 0$ and makes the prior pdf uncorrelated and with uniform variance.

$$\bar{\mathbf{y}} = [\mathrm{cov}\,\mathbf{x}]^{-½}\left(\bar{\mathbf{x}} - \mathbf{x}^{(n)}\right) \quad \text{and} \quad [\mathrm{cov}\,\mathbf{y}] = \mathbf{I}$$

$$\mathbf{y} = [\mathrm{cov}\,\mathbf{x}]^{-½}\left(\mathbf{x} - \mathbf{x}^{(n)}\right) \quad \text{and} \quad \mathbf{x} = \mathbf{x}^{(n)} + [\mathrm{cov}\,\mathbf{x}]^{½}\mathbf{y}$$

$$\mathbf{x} - \mathbf{x}^{(n)} = [\mathrm{cov}\,\mathbf{x}]^{½}\mathbf{y} \quad \text{and} \quad \mathbf{y} - \bar{\mathbf{y}} = [\mathrm{cov}\,\mathbf{x}]^{-½}(\mathbf{x} - \bar{\mathbf{x}})$$

(Step 2) Expanding the theory in a Taylor series and keeping the first two terms yields

$$\mathbf{f}(\mathbf{x}) = \mathbf{0} = \mathbf{f}\left(\mathbf{x}^{(n)}\right) + \mathbf{F}\left(\mathbf{x} - \mathbf{x}^{(n)}\right) \quad \text{with} \quad F_{ij} \equiv \left.\frac{\mathrm{d}f_i}{\mathrm{d}x_j}\right|_{\mathbf{x}^{(n)}}$$

The theory is satisfied at the solution point $\mathbf{x}^{(n)}$, implying that

$$\mathbf{F}\left(\mathbf{x} - \mathbf{x}^{(n)}\right) = 0$$

Rewriting in terms of $\mathbf{y}$

$$\mathbf{F}[\mathrm{cov}\,\mathbf{x}]^{½}\mathbf{y} = \mathbf{0}$$

We now introduce the singular value decomposition

$$\mathbf{U}_p\mathbf{\Lambda}_p\mathbf{V}_p^T = \mathbf{F}[\mathrm{cov}\,\mathbf{x}]^{½}$$

together with the null spaces $\mathbf{U}_0$ and $\mathbf{V}_0$, which satisfy $\mathbf{V}_p\mathbf{V}_p^T + \mathbf{V}_0\mathbf{V}_0^T = \mathbf{I}$. Note that the condition $\mathbf{F}[\mathrm{cov}\,\mathbf{x}]^{½}\mathbf{y} = \mathbf{U}_p\mathbf{\Lambda}_p\mathbf{V}_p^T\mathbf{y} = 0$ implies that $\mathbf{y}$ is the null space of $\mathbf{F}[\mathrm{cov}\,\mathbf{x}]^{½}$. Solving for $\mathbf{V}_p$

$$\mathbf{V}_p = [\mathrm{cov}\,\mathbf{x}]^{½}\mathbf{F}^T\mathbf{U}_p\mathbf{\Lambda}_p^{-1}$$

It follows that that

$$\mathbf{F}[\mathrm{cov}\,\mathbf{x}]\mathbf{F}^T = \left(\mathbf{F}[\mathrm{cov}\,\mathbf{x}]^{½}\right)\left(\mathbf{F}[\mathrm{cov}\,\mathbf{x}]^{½}\right)^T = \left(\mathbf{U}_p\mathbf{\Lambda}_p\mathbf{V}_p^T\right)\left(\mathbf{U}_p\mathbf{\Lambda}_p\mathbf{V}_p^T\right)^T = \mathbf{U}_p\mathbf{\Lambda}_p\mathbf{V}_p^T\mathbf{V}_p\mathbf{\Lambda}_p\mathbf{U}_p^T = \mathbf{U}_p\mathbf{\Lambda}_p^2\mathbf{U}_p^T$$

and that

$$[\mathbf{F}[\mathrm{cov}\,\mathbf{x}]\mathbf{F}^T]^{-1} = \mathbf{U}_p\mathbf{\Lambda}_p^{-2}\mathbf{U}_p^T$$

It also follows that

$$\mathbf{V}_p\mathbf{V}_p^T = [\text{cov}\,\mathbf{x}]^{½}\mathbf{F}^T\mathbf{U}_p\mathbf{\Lambda}_p^{-1}\mathbf{\Lambda}_p^{-1}\mathbf{U}_p^T\,\mathbf{F}[\text{cov}\,\mathbf{x}]^{½} = [\text{cov}\,\mathbf{x}]^{½}\mathbf{F}^T[\mathbf{F}[\text{cov}\,\mathbf{x}]\mathbf{F}^T]^{-1}\,\mathbf{F}[\text{cov}\,\mathbf{x}]^{½}$$

(Step 3) In the $\mathbf{y}$ coordinate system, the covariance matrix is $[\text{cov}\,\mathbf{y}] = \mathbf{I}$. The part of it in the null space is

$$\left[\text{cov}\,\mathbf{y}^{(n)}\right] = \mathbf{V}_0\mathbf{V}_0^T = \mathbf{I} - \mathbf{V}_p\mathbf{V}_p^T$$

(Step 4) Transforming back into the $\mathbf{y}$ coordinate system

$$\left[\text{cov}\,\mathbf{x}^{(n)}\right] = \mathbf{A}^{-1}\left(\mathbf{I} - \mathbf{V}_p\mathbf{V}_p^T\right)\mathbf{A}^{-1\text{T}} =$$

$$[\text{cov}\,\mathbf{x}]^{½}\left(\mathbf{I} - [\text{cov}\,\mathbf{x}]^{½}\mathbf{F}^T[\mathbf{F}[\text{cov}\,\mathbf{x}]\mathbf{F}^T]^{-1}\,\mathbf{F}[\text{cov}\,\mathbf{x}]^{½}\right)[\text{cov}\,\mathbf{x}]^{½} =$$

$$[\text{cov}\,\mathbf{x}] - [\text{cov}\,\mathbf{x}]\mathbf{F}^T[\mathbf{F}[\text{cov}\,\mathbf{x}]\mathbf{F}^T]^{-1}\,\mathbf{F}[\text{cov}\,\mathbf{x}]$$

We introduce an approximate sign as a reminder that this formula is derived via a linear approcimation:

$$\left[\text{cov}\,\mathbf{x}^{(n)}\right] \approx [\text{cov}\,\mathbf{x}](\mathbf{I} - \mathbf{F}^T[\mathbf{F}[\text{cov}\,\mathbf{x}]\mathbf{F}^T]^{-1}\mathbf{F}[\text{cov}\,\mathbf{x}])$$

which is equal to

$$\left[\text{cov}\,\mathbf{x}^{(n)}\right] \approx (\mathbf{I} - [\text{cov}\,\mathbf{x}]\mathbf{F}^T[\mathbf{F}[\text{cov}\,\mathbf{x}]\mathbf{F}^T]^{-1}\mathbf{F})[\text{cov}\,\mathbf{x}]$$

We test this formula using a simple nonlinear implicit problem with $N = 20$ pairs of $\left(d_i^{obs}, z_i^{obs}\right)$ observations satisfying the "straight line" theory $f_i(\mathbf{x}) \equiv m_1 + m_2 z_i - d_i = 0$. The observed data scatter about the true values ($m_1 = 1, m_2 = 2$) with uncorrelated noise (σ_d=σ_z=0.1) and the prior information of (m_1, m_2) scatters about the true values with (σ_1=σ_2=1) (Fig. 2). The problem is solved 100,000 times, creating ensembles of $\mathbf{m}^{(i)}$ (estimated solutions) and $\left[\text{cov}\,\mathbf{x}^{(n)}\right]^{(i)}$ (linearized posterior covariance matrices, using $\mathbf{F}$ from the last iteration).

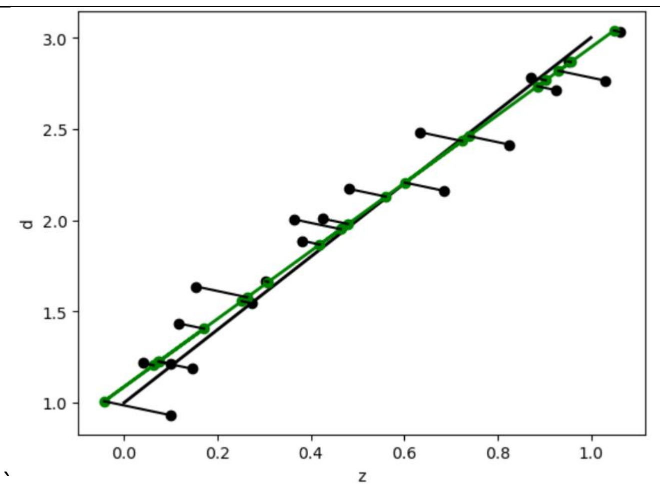

Fig. 2. Test using the theory $f_i(\mathbf{x}) \equiv m_1 + m_2 z_i - d_i = 0$, where both the observed zs and ds have error. The pdf $p(\mathbf{x}) \equiv p\left(\mathbf{d}^{obs}, \mathbf{z}^{obs}, \mathbf{m}^{pri}\right)$ is uncorrelated and Normal. True data (black line), observed data (black dots) and estimated data (green line and dots), with black bars connecting corresponding observations and predictions.

The sample covariance of the $\mathbf{m}^{(i)}$ ensemble is used as a proxy for the true posterior covariance of the ms. It is found to be:

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 [[ 0.00939108 -0.01379218]
 [-0.01379218  0.02768052]]
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The mean of the $\left[\text{cov}\,\mathbf{x}^{(n)}\right]^{(i)}$ ensemble is used as proxy for the linearized posterior covariance of the ms. It is found to be:

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[[ 0.00923739 -0.01342771]
 [-0.01342771  0.02692984]]
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These two estimates agree to within a few percent, giving us confidence that the linearized formula is a reasonably accurate approximation.

Reference

Menke, W. (2024), Geophysical Data Analysis and Inverse Theory with MATLAB(R) and Python, Fifth Edition, Academic Press, Elsevier (Amsterdam), 400pp.