

1. Initialize hydraulic parameters as ( $\mathbf{s}_0$ ) and structural parameters ( $\boldsymbol{\theta}_0$ ).
2. Solve for a new estimate of hydraulic parameters ( $\hat{\mathbf{s}}$ ) holding  $\boldsymbol{\theta}$  constant.
3. Solve for a new estimate of structural parameters ( $\hat{\boldsymbol{\theta}}$ ) holding  $\mathbf{s}$  constant.
4. Repeat steps 2 and 3 until the change in  $\boldsymbol{\theta}$  in two consecutive outer iterations of steps 2 and 3 decreases below a specified tolerance.

## Posterior Covariance

The posterior covariance can be calculated based on the inverse of the Hessian of the objective function (for example, Nowak and Cirpka, 2004). In closed form, the equation for the full posterior covariance matrix is:

$$\mathbf{V} = \mathbf{G}_{ss} - \mathbf{G}_{sy}\mathbf{G}_{yy}^{-1}\mathbf{G}_{sy}^T$$

where  $\mathbf{G}_{sy} = \mathbf{G}_{ss}\mathbf{H}^T$  and  $\mathbf{G}_{yy} = \mathbf{H}\mathbf{G}_{ss}\mathbf{H}^T + \mathbf{R}$ . In the case where compression of  $\mathbf{Q}$  is not used, the full matrix  $\mathbf{V}$  is calculated and reported. Where compression of  $\mathbf{Q}$  is used, however, the diagonal of  $\mathbf{V}$  is returned as a vector of variances on parameters. This information is reported in a separate file, but also used to calculate posterior 95% confidence intervals. The full matrix, when reported, can be used to calculate conditional realizations (Kitanidis, 1995, 1996).

## References Cited

- Box, G., and Cox, D. R., 1964, An analysis of transformations: Journal of the Royal Statistical Society, series B (Methodological), v. 26, no. 2, p. 211–252.
- D’Oria, M., 2010, Characterization of aquifer hydraulic parameters—From Theis to hydraulic tomography: Università degli Studi di Parma, Ph.D. Dissertation, 153 p.
- Fienen, M., Kitanidis, P., Watson, D., and Jardine, P., 2004, An application of Bayesian inverse methods to vertical deconvolution of hydraulic conductivity in a heterogeneous aquifer at Oak Ridge National Laboratory: Mathematical Geology, v. 36, no. 1, p. 101–126, doi:10.1023/B:MATG.0000016232.71993.bd.
- Fienen, M.N., Clemo, T.M., and Kitanidis, P.K., 2008, An interactive Bayesian geostatistical inverse protocol for hydraulic tomography: Water Resources Research, v. 44, W00B01, doi:10.1029/2007WR006730.
- Gaganis, P., and Smith, L., 2001, A Bayesian approach to the quantification of the effect of model error on the predictions of groundwater models: Water Resources Research, v. 37, no. 9, p. 2309–2322, doi:10.1029/2000WR000001.
- Gallagher, M.R., and Doherty, J., 2007, Parameter interdependence and uncertainty induced by lumping in a hydrologic model: Water Resources Research, v. 43, no. 5, W05421, doi:10.1029/2006wr005347.
- Gray, R., 2005, Toeplitz and circulant matrices—A review: Delft, The Netherlands: Kluwer Publishers, 90 p.
- Hoeksema, R.J., and Kitanidis, P.K., 1984, An application of the geostatistical approach to the inverse problem in two-dimensional groundwater modeling: Water Resources Research, v. 20, no. 7, p. 1003–1020, doi:10.1029/WR020i007p01003.
- Kitanidis, P.K., 1995, Quasi-linear geostatistical theory for inversing: Water Resources Research, v. 31, no. 10, p. 2411–2419, doi:10.1029/95WR01945.
- Kitanidis, P.K., 1996, Analytical expressions of conditional mean, covariance, and sample functions in geostatistics: Stochastic Hydrology and Hydraulics, v. 10, no. 4, p. 279–294, doi:10.1007/bf01581870.

The D should be lowercase.

Add p. here

- Kitanidis, P.K., and Vomvoris, E.G., 1983, A geostatistical approach to the inverse problem in groundwater modeling (steady state) and one-dimensional simulations: *Water Resources Research*, v. 19, no. 3, p. 677–690, doi:10.1029/WR019i003p00677.
- Li, W., and Cirpka, O.A., 2006, Efficient geostatistical inverse methods for structured and unstructured grids: *Water Resources Research*, v. 42, no. 6, W06402, doi:10.1029/2005WR004668.
- Li, W., Englert, A., Cirpka, O.A., Vanderborght, J., and Vereecken, H., 2007, Two-dimensional characterization of hydraulic heterogeneity by multiple pumping tests: *Water Resources Research*, v. 43, no. 4, W04433, doi:10.1029/2006WR005333.
- Nowak, W., and Cirpka, O.A., 2004, A modified Levenberg-Marquardt algorithm for quasi-linear geostatistical inversing: *Advances in Water Resources*, v. 27, no. 7, p. 737–750, doi:10.1016/j.advwatres.2004.03.004.
- Nowak, W., Tenkleve, S., and Cirpka, O.A., 2003, Efficient computation of linearized cross-covariance and auto-covariance matrices of interdependent quantities: *Mathematical Geology*, v. 35, no. 1, p. 53–66.
- Press, W.H., Teukolsky, S.A., Vetterling, W.T., and Flannery, B.O., 1992, *Numerical recipes in C—The art of scientific computing* (2d ed.): Cambridge, UK; New York; Cambridge University Press, 994 p.
- Rubin, Y., 2003, *Applied stochastic hydrogeology*, Oxford, UK; New York; Oxford University Press, 391 p.



Should be a colon