Rock Solid Inference: Bayesian Methods for Estimating Pressure, Temperature, and Other Parameters in Metamorphic Systems.

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Metamorphic studies often constrain the conditions of equilibration and evolution of a rock using qualitative to semi-quantitative comparisons between natural data and predicted values calculated using forward models. This is typically achieved by analysing the stable phase assemblage and/or the intersection point of key isopleths in Pressure (P) -Temperature (T) space, which has been effectively used to semi-quantitatively analysed the tectonothermal evolution of metamorphic terrains [1]. This method has well-understood issues, including the lack of consideration for uncertainty [2]. Constraining uncertainties is essential for extracting reliable insights from petrological studies and interpreting the data within a well-defined range of confidence. In addition, key parameters (x) such as XFe^{3+} and aH_2O are often assigned *a priori* despite their influence on the forward model.

In this study, we present a multi-dimensional inversion which calculates the model values $m = [T, P, x]$ from data such as phase composition, phase modal abundance and bulk rock properties. We apply Bayesian Inference to solve the inversion under a probabilistic framework. Bayesian Inference allows the calculation of the posterior probability distribution function of the model values given the observed data d_{obs} and prior knowledge $p(m)$, following Bayes' rule (Equation 1) [3].

$$p(m|d_{obs}) = \frac{p(d_{obs}|m)p(m)}{p(d_{obs})} \tag{1}$$

Where $p(d_{obs}|m)$ is the likelihood function which describes how well d_{obs} matches the forward model predicted data for a particular value of m**.** We estimate the Bayesian posterior distribution using Markov Chain Monte Carlo (MCMC) sampling [4], with the forward models being calculated in MAGEMin [5]. This approach enables a multi-dimensional inversion of metamorphic conditions within a robust probabilistic framework.

[1] Štípská, P., Powell, R., 2005. *J Metamorphic Geol*, 23, pp. 627-647.
[2] Green, E., Powell, R., 2021. *Metamorphic Studies Group RiP Meeting.*
[3] Bayes, T., 1763. LII. An essay towards solving a problem in the doctrine of chances. By the late Rev. Mr. Bayes, FRS communicated by Mr. Price, in a letter to John Canton, AMFR S. *Philosophical transactions of the Royal Society of London*, (53), pp.370-418.
[4] Metropolis, N., Rosenbluth, A.W., Rosenbluth, M.N., Teller, A.H., Teller, E., 1953. *The Journal of Chemical Physics*, 21(6), pp.1087-1092.
[5] Riel, N., Kaus, B. J. P., Green, E. C. R., Berlie, N. 2022. *Geochemistry, Geophysics, Geosystems*, 23, e2022GC010427.