A candidate secular variation model for IGRF-13 based on geodynamo simulation and En4dVar data assimilation

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This document briefly describes how our candidate secular variation model for the next generation of International Geomagnetic Reference Field has been constructed by a combined use of a data assimilation method (Ensemble-based 4-dimendional variation method; Liu et al., 2008; Nakano et al., 2019) and geodynamo simulation (Takahashi, 2012; 2014). As for 'data', we used a series of MCM field models evaluated/provided by a French group (Ropp and Lesur, 2019). The task force chairs, therefore, are advised to refer to the associated document with the MCM models and the references therein for, e.g., what kind of data were used in the field modeling, their selection/rejection criteria and spatial coverage, the inversion schemes and their details (starting models, number of iterations etc.) and so on. Because our French colleagues kindly sent us their very latest version up to Epoch 2019.50, we think the difference between the final set of the French field model submitted to the task force and what we used is quite minor, if any.

1. SV prediction from 2019.50 to 2025.00

Data assimilation of the geomagnetic field was conducted by our En4dVar method for 10 years from 2009.50 using the provided MCM model within that time window. The ensemble size was set to 960. Further MHD dynamo runs for all the ensemble members were conducted for another 5.50 years starting from 2019.50. The best linear combinations of all ensemble members for each epoch from 2019.50 through 2025.00 yielded time-series of Gauss coefficients, $p_l^m(t)$, for each mode from $(l, m) = (1, 0)$ through (8, 8). Line fitting was applied to each time-series so as to estimate the averaged secular variation, a_l^m, during the 5.50 years;

$$p_l^m(t) = a_l^m \cdot (t - t_0) + p_l^m(t_0), \tag{1-1}$$

where the time origin, t_0, was set to the release instance of our data assimilation, i.e., 2019.50.

Whether the line fit model in Eq. (1-1) gives a good secular variation estimate over the 5.50 years or not depends on each mode. For some modes, it may be necessary to include higher order terms such as secular acceleration in order to describe the time variation in concern properly. It, therefore, is necessary to diagnose the validity of the line fit models by examining the distribution of residuals for each mode, a part of which will be described in Section 5.

2. Data assimilation theory: En4dVar

We consider the minimization of the following cost function:

$$V(\boldsymbol{x}_0) = \frac{1}{2}\sum_{k=1}^{K}[\boldsymbol{y}_k - \boldsymbol{h}_k(\boldsymbol{x}_k)]^T \mathbf{R}_k^{-1} [\boldsymbol{y}_k - \boldsymbol{h}_k(\boldsymbol{x}_k)], \tag{2-1}$$

where the vector $\boldsymbol{x}_k$ consists of all the state variables of the dynamo model at time t_k, $\boldsymbol{y}_k$ denotes the observation, $\mathbf{R}_k$ is the covariance matrix of observation noise, and $\boldsymbol{h}_k$ is a function which converts a state vector $\boldsymbol{x}_k$ at time t_k to observable variables for the comparison with $\boldsymbol{y}_k$. $\boldsymbol{x}_k$ is uniquely determined if the initial state $\boldsymbol{x}_0$ is given. Thus, we can define a function $\boldsymbol{g}_k$ satisfying $\boldsymbol{g}_k(\boldsymbol{x}_0) = \boldsymbol{h}_k(\boldsymbol{x}_k)$. Using this function, the cost function in Eq. (2-1) can be rewritten as follows:

$$V(\boldsymbol{x}_0) = \frac{1}{2}\sum_{k=1}^{K}[\boldsymbol{y}_k - \boldsymbol{g}_k(\boldsymbol{x}_0)]^T \mathbf{R}_k^{-1} [\boldsymbol{y}_k - \boldsymbol{g}_k(\boldsymbol{x}_0)], \tag{2-2}$$

The minimization of this cost function is achieved by an iterative algorithm similar to the four-dimensional ensemble-based variational (En4dVar) method (Liu et al., 2008). At m-th iteration, we approximated a cost function using an ensemble of the simulation outputs $\left\{\boldsymbol{x}_{0:K,m}^{(1)}, \ldots, \boldsymbol{x}_{0:K,m}^{(N)}\right\}$. This ensemble is generated so that the ensemble mean is equal to the m-th estimate $\bar{x}_{0,m}$. Now we define the following matrix $\breve{\mathbf{X}}_{0,m}$ and $\breve{\boldsymbol{\Gamma}}_{k,m}$ for convenience:

$$\breve{\mathbf{X}}_{0,m} = \frac{1}{\sqrt{N-1}}\left(\boldsymbol{x}_{0,m}^{(1)} - \overline{\boldsymbol{x}}_{0,m} \quad \cdots \quad \boldsymbol{x}_{0,m}^{(N)} - \overline{\boldsymbol{x}}_{0,m}\right), \tag{2-3}$$

$$\breve{\boldsymbol{\Gamma}}_{k,m} = \frac{1}{\sqrt{N-1}}\left(\boldsymbol{g}_k\left(\boldsymbol{x}_{0,m}^{(1)}\right) - \boldsymbol{g}_k(\overline{\boldsymbol{x}}_{0,m}) \quad \cdots \quad \boldsymbol{g}_k\left(\boldsymbol{x}_{0,m}^{(N)}\right) - \boldsymbol{g}_k(\overline{\boldsymbol{x}}_{0,m})\right). \tag{2-4}$$

We approximate $\boldsymbol{x}_0$ as a linear combination of the ensemble members. This allows us to write $\boldsymbol{x}_0 = \overline{\boldsymbol{x}}_{0,m} + \breve{\mathbf{X}}_{k,m}\boldsymbol{w}$, where w consists of weight for each ensemble member. $\overline{\boldsymbol{x}}_{0,m}$ is the prior mean of $\boldsymbol{x}_0$. The function $\boldsymbol{g}_k(\boldsymbol{x}_0)$ is then approximated based on the first-order Taylor expansion:

$$\begin{aligned} \boldsymbol{g}_k(\boldsymbol{x}_0) &\approx \boldsymbol{g}_k(\overline{\boldsymbol{x}}_{0,m}) + \boldsymbol{G}_k(\boldsymbol{x}_0 - \overline{\boldsymbol{x}}_{0,m}) \approx \boldsymbol{g}_k(\bar{\boldsymbol{x}}_{0,m}) + \boldsymbol{G}_k\breve{\mathbf{X}}_{k,m}\boldsymbol{w} \\ &\approx \boldsymbol{g}_k(\overline{\boldsymbol{x}}_{0,m}) + \breve{\boldsymbol{\Gamma}}_{k,m}\boldsymbol{w}, \end{aligned} \tag{2-5}$$

where $\boldsymbol{G}_k$ is the Jacobian of $\boldsymbol{g}_k$ at $\overline{\boldsymbol{x}}_{0,m}$. Then we have the following function

$$\begin{aligned} \hat{J}_m(\boldsymbol{w}) = &\frac{\sigma_m^2}{2}\boldsymbol{w}^T\boldsymbol{w} \\ &+ \frac{1}{2}\sum_{k=1}^{K}\left[\boldsymbol{y}_k - \boldsymbol{g}_k(\overline{\boldsymbol{x}}_{0,m}) - \breve{\boldsymbol{\Gamma}}_{k,m}\boldsymbol{w}\right]^T \mathbf{R}_k^{-1}\left[\boldsymbol{y}_k - \boldsymbol{g}_k(\overline{\boldsymbol{x}}_{0,m})\right. \\ &\left. - \breve{\boldsymbol{\Gamma}}_{k,m}\boldsymbol{w}\right], \end{aligned} \tag{2-6}$$

This cost function is minimized when

$$\widehat{\boldsymbol{w}}_m = \left(\sum_k\left[\breve{\boldsymbol{\Gamma}}_{k,m}^T\mathbf{R}_k^{-1}\breve{\boldsymbol{\Gamma}}_{k,m}\right] + \sigma_m^2\boldsymbol{I}\right)^{-1}\sum_k\left(\breve{\boldsymbol{\Gamma}}_{k,m}^T\mathbf{R}_k^{-1}[\boldsymbol{y}_k - \boldsymbol{g}_k(\boldsymbol{x}_b)]\right). \tag{2-7}$$

The $(m+1)$-th estimate $\overline{\boldsymbol{x}}_{0,m+1}$ is then obtained as

$$\overline{\boldsymbol{x}}_{0,m+1} = \overline{\boldsymbol{x}}_{0,m} + \breve{\mathbf{X}}_{0,m}\widehat{\boldsymbol{w}}_m, \tag{2-8}$$

and we proceed to the next iteration. The first term of the right-hand side in Eq. (2-6) is added to ensure the robustness. The parameter σ_m is decreased at each iteration. This iterative application of Eq. (2-7), which is similar to the algorithm of Gu and Oliver (2007), minimizes Eq. (2-2) in the subspace spanned by the ensemble members (Nakano in preparation).

At the final (i.e., the 5-th) iteration, we also estimated the bias and trend components which correspond to model error in the dynamo model, and the following function is minimized:

$$\hat{J}_m(\boldsymbol{w}) = \frac{\sigma_m^2}{2}\boldsymbol{w}^T\boldsymbol{w} + \frac{1}{2}\boldsymbol{b}^T\mathbf{P}_b\boldsymbol{b} + \frac{1}{2}\boldsymbol{a}^T\mathbf{P}_a\boldsymbol{a}$$
$$+\frac{1}{2}\sum_{k=1}^{K}\left[\boldsymbol{y}_k - \boldsymbol{g}_k(\overline{\boldsymbol{x}}_{0,m}) - \check{\boldsymbol{\Gamma}}_{k,m}\boldsymbol{w} - \boldsymbol{b} - k\boldsymbol{a}\right]^T\mathbf{R}_k^{-1}\left[\boldsymbol{y}_k\right. \tag{2-9}$$
$$\left.- \boldsymbol{g}_k(\overline{\boldsymbol{x}}_{0,m}) - \check{\boldsymbol{\Gamma}}_{k,m}\boldsymbol{w} - \boldsymbol{b} - k\boldsymbol{a}\right],$$

where $\boldsymbol{b}$ denotes the bias component and $\boldsymbol{a}$ denotes the coefficient for the trend component. We set $\mathbf{P}_a$ and $\mathbf{P}_b$ as follows:

$$\mathbf{P}_a = \mathbf{P}_b = 10^2\mathbf{R}_k. \tag{2-10}$$

The minimization of Eq. (2-9) gives the approximate minimum of the following cost function:

$$V(\boldsymbol{x}_0) = \frac{1}{2}\sum_{k=1}^{K}[\boldsymbol{y}_k - \boldsymbol{g}_k(\boldsymbol{x}_0) - \boldsymbol{b} - k\boldsymbol{a}]^T\mathbf{R}_k^{-1}\,[\boldsymbol{y}_k - \boldsymbol{g}_k(\boldsymbol{x}_0) - \boldsymbol{b} - k\boldsymbol{a}]. \tag{2-11}$$

The final estimate and prediction are obtained by the following equation:

$$\overline{\boldsymbol{g}}_{\boldsymbol{k},\boldsymbol{M}} = \boldsymbol{g}_k(\overline{\boldsymbol{x}}_{0,M}) + \check{\Gamma}_{k,M}\widehat{\boldsymbol{w}}_m, \tag{2-12}$$

where M indicates the final step, i.e., M=5.

3. Implementation: Data vector and weighing by covariance matrix

The cost function in the data assimilation is a simple squared-misfit between the weighted sum of results from MHD ensemble members and the data vector, where no regularization is adopted. Let us rewrite Eq. (2-11) here with a specific form of $\mathbf{R}_k$;

$$V(\boldsymbol{x}_0) = \frac{1}{2}\sum_{k=1}^{K}[\boldsymbol{y}_k - \boldsymbol{g}_k(\boldsymbol{x}_0) - \boldsymbol{a}k - \boldsymbol{b}]^T\mathbf{R}_k^{-1}\,[\boldsymbol{y}_k - \boldsymbol{g}_k(\boldsymbol{x}_0) - \boldsymbol{a}k - \boldsymbol{b}], \tag{3-1}$$

$$\mathbf{R}_k = \begin{bmatrix} \alpha_S^2 \mathbf{R}_S & 0 & 0 \\ 0 & \alpha_{UW}^2 \mathbf{R}_U & 0 \\ 0 & 0 & \alpha_{UW}^2 \mathbf{R}_W \end{bmatrix}. \quad (3\text{-}2)$$

The data vector $\boldsymbol{y}_k$ consists of S_l^m, U_l^m, and W_l^m, where S_l^m is the poloidal scalar potential for the geomagnetic field at the core-mantle boundary (CMB), U_l^m and W_l^m are poloidal and toroidal scalar potentials for the core flow near the CMB, respectively. k is the time index, where k from 1 to K corresponds to the period from 2009.50 to 2019.50 with the 0.25 year interval. $\boldsymbol{x}_0$ is the initial state vector of geodynamo model of Takahashi (2012). $\boldsymbol{g}_k$ is the operator including geodynamo simulation that generates the observation vector using a given initial condition, $\boldsymbol{x}_0$. $\mathbf{R}_k$ is the observation error covariance matrix. In our assimilation scheme, we simply use $\mathbf{R}_k = \mathbf{R}$, which is independent of time, since the data field model, MCM, is a quality-controlled smooth model. Only in the final iteration, we introduced trend and bias terms, $-\boldsymbol{a}k - \boldsymbol{b}$, to help the numerical dynamo reduce the misfit, only for the magnetic field variations.

In our data assimilation scheme, two types of data sets were used; S_l^m data came directly from the MCM model, U_l^m and W_l^m were calculated by a modified method of Matsushima (2015) using time series of S_l^m. In the assimilation, we assembled data vectors with coefficients up to degree 14 for both S_l^m and (U_l^m, W_l^m). We adopted a simple covariance matrix for S_l^m based on Lowes (1975). We assumed that degree dependence of the variance of Gauss coefficients is $\sigma_G^2 \propto (l+1)^{-1}$. On the other hand, the variance of Schmidt semi-normalized poloidal and toroidal scalar potential of the core surface flow was assumed to be $\sigma_{UW}^2 \propto (2l+1)/\big(l(l+1)\big)$. Weights for data sets were controlled by the factors of α_S and α_{UW} in Eq. (3-1), where $\mathbf{R}_S$, $\mathbf{R}_U$, and $\mathbf{R}_W$ are the diagonal covariance matrices with their own degree dependences based on σ_G^2 and σ_{UW}^2. Table 1 lists the adopted values of α_S and α_{UW} through the iterations.

Table 1. Weight factors for observation error covariance matrices.

Iteration #	α_S (Factor for σ_S) [*1.4*10^4]	α_{UW}(Factor for σ_U, σ_W)[*300]
1	1.0	1.0
2	0.2	0.2
3	0.1	0.2
4	0.02	0.2
5	0.001	0.2

In the final iteration of the data assimilation procedure, the adopted weights for S_l^m and

$(U_l^m,\ W_l^m)$, i.e. $\alpha_S^{-1}$and α_{UW}^{-1}, are approximately 4:1, in terms of the observation errors.

4. Fit to the data

We evaluated how our model fits the data in terms of $\sqrt{dP}$, where dP is defined as

$$dP = \sum_{l}^{14}\sum_{m}(l+1)\left[\left(g_l^m{}_{\text{model}} - g_l^m{}_{\text{data}}\right)^2 + \left(h_l^m{}_{\text{model}} - h_l^m{}_{\text{data}}\right)^2\right] \qquad (4\text{-}1)$$

in the same manner as Whaler and Beggan (2015). $g_l^m{}_{\text{model}}$ and $g_l^m{}_{\text{data}}$ are Gauss coefficients for the assimilated MHD dynamo model and data, respectively. After the five iterations, $\sqrt{dP}$ became less than 7 nT throughout the assimilation window from 2009.50 to 2019.50.

5. Error estimates of each SV coefficient

After carrying out the data assimilation, we estimated a 5-year SV candidate model by fitting a linear model of Eq. (1-1) to the prediction by the weighted sum of MHD ensemble members over the period from 2019.5 to 2025.0. We applied the same SV estimation procedure to every ensemble member and obtained 960 SV models from the ensemble with the posterior distribution. We present the standard deviation of SV values of 960 SV models as the error of our SV candidate model. Figure 1 shows two examples of the distribution of SV values estimated for all the ensemble members. The best linear combination (Fit in Fig. 1) becomes identical to the mean of 960 SV candidates (Ens Ave in Fig. 1) when the posterior distribution is adopted.

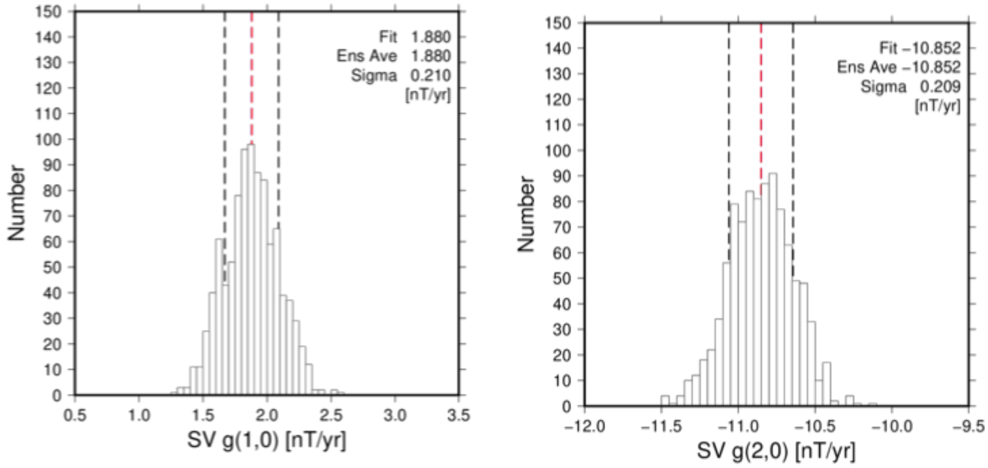

Figure 1. Histogram of a_l^m in Eq. (1-1) estimated for all the 960 ensemble members. Examples for g_1^0 (left) and g_2^0 (right).

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