Inverse estimation of parameters for the magnetic domain via dynamics matching using visual-perceptive similarity

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ABSTRACT
The estimation of parameters for the magnetic domain (i.e. magnetic domain parameters) based on their time evolution patterns created by magnetic spins is necessary in the development of magnetic materials. In this study, we develop a method for the inverse estimation of magnetic domain parameters that produce simulation results like those of a set of magnetic domain patterns given the time evolution patterns of magnetic domains. Further, we utilize an experimental method based on Gaussian process regression for the efficient search of magnetic domain parameters. We adopted a design of experiments based on Gaussian process regression for efficiently searching magnetic domain parameters. Portilla–Simoncelli statistics is a high-dimensional texture feature based on human visual perception, and it can quantitatively evaluate patterns in texture structure. We show that the proposed method can simultaneously and accurately inverse estimate three magnetic domain parameters.

1. Introduction
Magnetic materials are used in industrial equipment such as sensors, indicators, and transformers, as well as in large equipment such as automobiles, trains, and aircraft. The performance of magnetic devices is governed by the magnetic domain parameters (e.g. magnetic anisotropy, exchange interaction, dipole interaction) of magnetic materials; however, it is difficult to observe the magnetic domain parameters directly. Therefore, the time evolution of magnetic domain patterns formed by magnetic spins was observed in the research and development of magnetic materials [1]. The magnetic domain is a region wherein almost all spins point in the same direction. Magnetic domain patterns (i.e. texture structure) are formed by exchange and dipole interactions between magnetic spins; various patterns appear depending on the magnetic domain parameters [2,3]. Advances in measurement technology have enabled us to measure magnetic domain patterns and obtain information on the magnetic domain parameters of materials from spin dynamics. Coherent X-ray diffraction imaging and scanning microscopy based on X-ray magnetic circular dichroism are powerful methods in terms of element selectivity and high spatial resolution [4,5].
Magnetic domain pattern images dominated by magnetic domain parameters have a strong relationship with the properties of magnetic materials. For example, the spatial randomness of magnetic anisotropy is attributed to the random arrangement of impurities and defects introduced during sample preparation. Magnetic anisotropy is a factor that determines the coercive force and magnetic energy. An exchange interaction is an important magnetic parameter that can determine the strength of a magnetic force. Thus, it is important to estimate the magnetic domain parameters of magnetic materials using magnetic domain pattern images. To this end, we aim to develop a method for estimating magnetic domain parameters from magnetic domain pattern images. The evaluation methods for complex spatio-temporal patterns such as magnetic domain patterns have a wide range of applications because they are observed in various physical, chemical, and biological systems [6,7].

Various studies have focused on the mechanism of magnetic domain patterns formed in ferromagnetic thin-film single crystals. As a forward model, the numerical simulations of magnetic domain formation such as the time-dependent Ginzburg–Landau (TDGL) equation [8,9] have been established. The TDGL equation can reproduce a variety of experimentally observed phenomena such as memory effects and changes in properties attributed to swept fields. Kudo et al. used domain patterns simulated based on the TDGL equation to demonstrate the relationship between the sweeping speed of the external magnetic field and the number of magnetic domains and domain areas [10,11]. There are several methods that utilize machine learning to enhance the development of magnetic materials, such as the inverse approaches. This approach has been used for a high-throughput search for materials with desired properties [12–15], prediction of magnetic properties [16,17], and optimization of thin-film growth processes [18]. Furthermore, there are several methods for estimating magnetic domain parameters from magnetic domain patterns. For example, Buford et al. attempted to estimate fundamental parameters from magnetic domain patterns using morphological features and Fourier transforms [19,20]. In a related study, the magnetic domain patterns were analyzed using persistent homology, which is a data analysis method that focuses on the phase structure of the data. As a result, Kotsugi et al. were able to automatically visualize the pinning site as a topological defect in the original magnetic domain structure for the first time [21]. Mamada et al. proposed a method for predicting anisotropy parameters from magnetic domain patterns using convolutional neural networks and kernel regression with morphological statistics [22]. They showed that the anisotropy parameter can be estimated based on the steady-state magnetic domain pattern image. Appendix A presents the details of the framework of the conventional method.

The spatial pattern of a magnetic domain pattern image is a textured structure in image processing. Therefore, texture features are used for the magnetic domain pattern analysis. Murakami et al. focused on Portilla–Simoncelli statistics (PSS) [23–26], which is a texture feature based on visual perception, to estimate anisotropy parameters from steady-state magnetic domain patterns [27]. They demonstrated that PSS is a powerful tool for understanding magnetic domain pattern images. Furthermore, PSS could represent natural and complex structures of magnetic domain patterns well. This is highly interpretable because it comprises a combination of decomposed images obtained by a simple filtering process [28–30]. PSS can generate a variety of texture images; Portilla and Simoncelli showed that a new texture pattern visually indistinguishable from the original pattern can be generated by simply making the PSS identical [23]. In the field of physiology, Okazawa et al. showed that neurons respond to textural stimuli, which suggests textural information is beneficial to human visual perception. In this study, we use PSS to evaluate the similarity of magnetic domain patterns [24].

We proposed a new framework for estimating magnetic domain parameters; this framework is unlike the conventional methods. The proposed method has three advantages over the conventional methods:

1. It considers the time evolution of magnetic domains
2. It can estimate with a small number of simulations
3. It can estimate multiple parameters simultaneously

The proposed method simultaneously back estimates three magnetic domain parameters $M$: anisotropy $\alpha$, exchange action $\beta$, and variance of order parameter $\sigma$. The estimation of magnetic domain parameters such as $\alpha$ and $\beta$ from the time evolution pattern of magnetic domains is expected to contribute to the research and development of magnetic materials.

2. Methods

The proposed method is a framework for the inverse estimation of the magnetic domain parameters that produces simulation results similar to a set of magnetic domain patterns given the time evolution patterns of magnetic domains.
2.1. Dynamics matching using visual perceptive similarity

Figure 1 shows the overview of the proposed method. As indicated in Figure 1, the proposed method estimates the magnetic domain parameters $\mathcal{M}$ of the simulator $\{x_j(t)\}_{t=0}^T = \phi(r; \mathcal{M})$ that minimize the loss function $\mathcal{L}(\mathcal{M})$ when the measured time evolution of domain patterns $\{x_m(t)\}_{t=0}^T$ is given. Here, $\mathcal{L}(\mathcal{M})$ represents the dissimilarity of $\{x_m(t)\}_{t=0}^T$ and the simulation outputs $\{x_j(t)\}_{t=0}^T$. $\mathcal{L}(\mathcal{M})$ is defined based on the distance $D(z_m, z_j)$ in the feature $z = f(x)$. In this study, we used the TDGL equation as the simulator $\phi(r; \mathcal{M})$; we adopted Portilla–Simoncelli statistics-(PSS) as the feature $f(x)$. The loss function $\mathcal{L}(\mathcal{M})$ of a sample point $\mathcal{M}$ calculated as follows:

1. The time evolution of the magnetic domain pattern $\{x_j(t)\}_{t=0}^T$ is simulated using $\phi(r; \mathcal{M})$.
2. The feature $\{z_j(t)\}_{t=0}^T$ is calculated from $\{x_j(t)\}_{t=0}^T$ based on $z = f(x)$.
3. The dissimilarity $D(z_m, z_j)$ is calculated from $\{x_m(t)\}_{t=0}^T$ and the feature of input images $\{z_j(t)\}_{t=0}^T$.
4. $\mathcal{L}(\mathcal{M})$ is calculated from $D(z_m(t), z_j(t))$, $t \in \{0, \ldots, T\}$.

The proposed method simulates the following TDGL equation for each sample point $\mathcal{M}$. The TDGL simulation is time consuming because the magnetic domain pattern formation is observed by gradually sweeping the external magnetic field. We used the design of an experiment based on Gaussian process regression [31–33] to explore the magnetic domain parameters $\mathcal{M}$ efficiently. Thus, the magnetic domain parameters can be estimated with a smaller number of simulation trials compared to previous studies. The search procedure by using Gaussian process can optimize the parameters exhaustively and efficiently. In this study, we considered that the initial data will have a negligible impact on the estimation value. The Appendix B shows details about the Gaussian process regression.

We assumed that the TDGL equation and the calculation of the loss function were black-box. The proposed method estimated the parameters from input-output relationship of black-box using the Gaussian process regression. Therefore, the proposed method can be used for the pattern image other than the TDGL equation.

2.2. Loss function design

We designed the loss function $\mathcal{L}(\mathcal{M})$ considering the time evolution. Figure 2 shows the overview about the loss function design. As indicated in Figure 2, we calculated the distance $D(z_m(t), z_j(t))$ in the feature $z$ for each time evolution $t \in \{0, \ldots, T\}$. We defined the loss function $\mathcal{L}(\mathcal{M})$ as the weighted sum of the distance $D(z_m(t), z_j(t))$:

$$\mathcal{L}(\mathcal{M}) = \int_0^T w(t) D(z_m(t), z_j(t)) dt. \quad (1)$$

Distance $D(z_m(t), z_j(t))$ in feature $z$ was defined as:

$$D(z_m, z_j) = \frac{||z_j - z_m||^2}{|z_m|}. \quad (2)$$

Note that the distance function $D(z_m(t), z_j(t))$ used in this study is not an exact distance because it does not satisfy symmetry. The PSS has different value scales for
2.3. Time dependent Ginzburg–Landau equation – TDGL equation

The formation of magnetic domain patterns has been studied in various fields. For example, we consider magnetic domain patterns in ferromagnetic thin films wherein the patterns are formed because of the uniaxial magnetic anisotropy and interaction between magnetic spins. We describe a two-dimensional model that captures the properties of the magnetic domain pattern formation. We use the TDGL equation to simulate the time evolution of the magnetic domain pattern. The magnetic domain pattern analysis that uses the TDGL equation was discussed in previous studies, and it is not described in detail in this paper. We consider a two-dimensional scalar field \( \phi(r; \mathcal{M}) \sim \pm 1 \). Here, the magnetic domain pattern \( \mathcal{M} \) is parametrized by \( \{ \alpha, \beta, \sigma \} \).

The TDGL equation comprises four energy terms:

\[
H_A = \alpha \lambda(r) \left( \frac{\phi(r)^2}{2} - \frac{\phi(r)^4}{4} \right), \tag{4}
\]

\[
H_J = \beta \int dr |\nabla \phi(r)|^2, \tag{5}
\]

\[
H_D = \gamma \int dr dr' \phi(r) \phi(r') G(r, r'), \tag{6}
\]

\[
H_E = -h(t) \int dr \phi(r), \tag{7}
\]

where \( r \) is the spatial position, \( H_A, H_J, H_D, \) and \( H_E \) denote the anisotropic energy, ferromagnetic exchange interactions, dipolar interactions, and interaction with external magnetic field, respectively; further, \( \alpha, \beta, \) and \( \gamma \) denote the coefficient of anisotropy, exchange interaction, and dipolar interaction, respectively. In the first term, the disordered field \( \lambda(r) = 1 + \mu(r)/4 \), where \( \mu(r) \) represents a normal distribution function with a mean 0 and variance \( \sigma \). In the third term, the Green’s function \( G(r, r') \) is defined as \( G(r, r') \sim |r - r'|^3 \). Thus, the TDGL equation can be given as:

\[
\frac{\partial \phi(r)}{\partial t} = -\frac{\delta(H_A + H_J + H_D + H_E)}{\delta \phi(r)} \tag{8}
\]

\[
= \alpha \lambda(r) \left( \phi(r) - \phi(r)^3 \right) + \beta \nabla^2 \phi(r)
- \gamma \int dr' \phi(r') G(r, r') + h(t). \tag{9}
\]
We performed the following simulations. We applied the saturated magnetic field \( h_{\text{init}} \) and reduced the magnetic field at the sweep velocity \( v \). Therefore, the magnetic field \( h(t) \) at each time \( t \) can be expressed as:

\[
h(t) = h_{\text{init}} - vt. \tag{10}
\]

The size of the simulated images was 512 × 512.

### 2.4. Portilla-Simoncelli statistics – PSS

In the proposed method, it is necessary to define a feature \( z = f(x) \) that well represents the magnetic domain pattern. We used PSS, which is an texture statistic proposed by Portilla and Simoncelli. PSS is a high-dimensional texture feature based on human visual perception, and it can represent natural texture images well. Further, the PSS is a feature for generating texture images; the texture generation algorithm can generate new visually similar texture images. We can visually confirm that the PSS can explain the time evolution of magnetic domains well using this generation algorithm.

The PSS is a set of texture features based on a steerable pyramid [28–30], which comprises images decomposed into scale and orientation using a linear filter (hereafter, decomposed images). Figure 3 shows the block diagram for calculating the PSS. As indicated in Figure 3, the steerable-pyramid decomposes the image into various scales and orientations by computing the high-pass filter \( H \), low-pass filter \( L \), and orientation filter \( B \) in a hierarchical manner. The PSS is defined based on the decomposed image obtained by the steerable-pyramid; it has the following elements.

- Spectral statistics (SS)
- The absolute mean of the input image decomposed by scale and orientation.
- Marginal statistics (MS)
- Luminance statistics of the input image (e.g., mean, variance, skewness, and kurtosis).
- Linear cross position (LCP)
- The central element of the auto-correlation matrix of a low-pass image.
- Linear cross scale (LCS)

![Figure 3](image_url)

*Figure 3.* Schematic of the steerable pyramid in the Fourier domain [34]. Rectangular blocks show the scale levels of decomposition, and the insides of the blocks show the orientation levels of decomposition. \( B_n(w) \) denotes the orientation in the filter process, where \( w \) denotes frequency. The filter to decompose the original image into multi-orientations in each block is shown. Additionally, the decomposition images are shown at the center. Indexes \( n \) and \( k \) denote the scale and orientation levels, respectively.
• The inner product of the real part of each decomposed image and the real or imaginary part of the decomposed image at one coarser scale.
• Energy cross orientation (ECO)
• The inner product of the absolute values of the decomposed images in the same scale.
• Energy cross position (ECP)
• The central element of the auto-correlation matrix of the decomposed image.
• Energy cross scale (ECS)
• The inner product of the absolute value of the decomposed image and the decomposed image at one coarser scale.

The number of features in PSS is determined by the number of scales $N$, number of orientations $K$, and number of central elements $M$ of the auto-correlation matrix with respect to the decomposed steerable pyramid image. We use the most commonly used setting, i.e., $N = 4$, $N = 4$, and $M = 7$.

3. Results and discussion

The time evolution of magnetic domain patterns from the TDGL simulation, where the true magnetic parameter values are known, are used as pseudo-measurement data $\left\{ x_m^{(t)} \right\}_{t=0}^T$. In this experiment, we set the hyperparameter of the loss function as $\eta = 0.2$. We use the texture generation algorithm of the PSS to confirm that the PSS has the information capacity to represent the time evolution of magnetic domain patterns qualitatively.

### 3.1. Expression of magnetic domain pattern images by PSS

PSS is a feature that is well described with natural textures. To this end, we use the PSS texture generation algorithm to confirm that PSS has the information capacity required to represent the time evolution of magnetic domain patterns. Figure 4 shows the results of generating the time evolution of the magnetic domain pattern based on PSS parameters, and Figure 4 (a–d) shows the time evolution pattern of magnetic domains simulated by the TDGL equation. Figure 4 (e–h) shows the time evolution pattern of magnetic domains based on the parameters of PSS. The simulation images of (a)–(d) are the magnetic domain patterns obtained by simulation based on the TDGL equation under $\nu = 0.01$, $\alpha = 2.0$, $\beta = 2.0$, $\gamma = 2.0/\pi$, and $\sigma = 0.3$. The generated images in (e)–(h) correspond to (a)–(d), respectively; the generated images in (e)–(h) correspond to (a)–(d), respectively. This figure presents an excerpt of the magnetic domain pattern images that illustrate the significant pattern changes in time evolution. As indicated in Figure 4, the PSS parameter can well describe the time evolution of the magnetic domain pattern. Figure 4 (b) and (f) show that the sparse presence of the round and long thin regions is visually similar in both magnetic domain pattern images. As shown in Figure 4 (c) and (g), the elongation of the white magnetic domain area can be viewed in both images of the domain pattern. Therefore, it is confirmed that the PSS retains the amount of information representing the time evolution of the magnetic domain pattern.

![Figure 4](image_url)

Figure 4. Result of generating the time evolution pattern of magnetic domains based on the parameters of PSS. (a)–(d) time evolution pattern of magnetic domains simulated by the TDGL equation, (e)–(h) time evolution pattern of magnetic domains based on the parameters of PSS. The simulation images of (a)–(d) are magnetic domain pattern obtained by simulation based on the TDGL equation under $\nu = 0.01$, $\alpha = 2.0$, $\beta = 2.0$, $\gamma = 2.0/\pi$, and $\sigma = 0.3$. The generated images in (e)–(h) correspond to (a)–(d), respectively. The generated images in (e)–(h) correspond to (a)–(d), respectively. This figure shows an excerpt of the magnetic domain pattern images that show significant pattern changes in time evolution.
To qualitatively confirm that the PSS has the information content to classify the magnetic domain patterns, we performed a visualization with dimensionality reduction. Figure 5 shows the result of the nonlinear dimensionality reduction of PSS computed from steady-state magnetic domain patterns obtained using the locally linear embedding (LLE) algorithm [35]. We used magnetic domain patterns with various combinations of $\alpha$ and exchange interaction $\beta$. The combinations were determined by sampling $\alpha$ and $\beta$ from the uniform distribution in the range $[1.5, 3.5]$. Figure 5 shows that visually similar domain pattern images are located near each other, which indicates that PSS is a useful measure of domain pattern images.

![Figure 5](image)

**Figure 5.** The result of nonlinear dimensionality reduction of PSS computed from steady-state magnetic domain patterns using the locally linear embedding algorithm.

3.2. Inverse estimation of anisotropy $\alpha$

Figure 6 shows the estimation result of $\alpha$ obtained using the proposed method. We fixed $\nu = 0.01$, $\beta = 2.0$, $\gamma = 2.0/\pi$, $\sigma = 0.3$, and estimated only the $\alpha$. We set the search range for $\alpha$ to $[1.0, 4.0]$. Figure 6 shows that the proposed method efficiently samples the region around $\alpha = 2.0$. The estimation result of the proposed method is $\hat{\alpha} = 1.98$, which is very close to $\alpha = 2.00$. Thus, we confirm that the proposed method can estimate the $\alpha$ with a high accuracy.

Figure 7(a,b) show simulated images of the time evolution of the magnetic domain patterns for the true $\alpha = 2.00$ and the estimated $\hat{\alpha} = 1.98$. Figure 7 shows a selection of images with significant pattern changes. Figure 7(a,b) show that the time evolution of the magnetic domain patterns is visually similar in both cases. Furthermore, as shown in Figure 7, we suggest that the proposed method can estimate $\alpha$, which yields simulation results similar to the input images.

![Figure 6](image)

**Figure 6.** The estimation result of anisotropy parameter $\alpha$ by the proposed method. The vertical axis shows the loss function $\mathcal{L}(\alpha)$, The dot lines show the true anisotropy $\alpha = 2.00$. The shading map shows the predictive distribution from the Gaussian process regression.

Figure 8 shows the number of image data (number of simulation trials) used by the conventional [22,27] proposed methods for estimating $\alpha$. Figure 8 shows that the proposed method accurately estimated $\alpha$ in 21 simulation trials. We did an experiment using a random search to evaluate the proposed method as the baseline. As a result, it shows that an average of about 75 trials was required to achieve the same level of accuracy as the proposed method. The proposed method can search for magnetic domain parameters more efficiently than random search.

As shown in Figure 8, the proposed method successfully reduced the number of required simulations by 95% compared to that using the conventional method [22]. Further, the estimation accuracies of the conventional and proposed methods are listed in Table 1. The proposed method has the same estimation accuracy as the conventional method. The proposed and conventional methods cannot be compared directly because they have completely different frameworks.

Although the conventional method [22,27] that builds a predictor in advance can perform the inference process faster than the proposed method, it requires a large number of simulation data with consistent magnetic domain parameters other than $\alpha$ when magnetic domain parameters other than $\alpha$ are different and used to reconstruct the predictor.

3.3. Inverse estimation of anisotropy $\alpha$ and exchange interaction $\beta$

The characteristic wavenumber of a magnetic domain pattern is determined by the ratio of $\beta$ to $\gamma$. In this experiment, we fixed $\gamma$ and estimated $\beta$ as the parameter. Figure 9 shows the results of the simultaneous estimation $\alpha$ and $\beta$ using the proposed
We fixed $\nu = 0.01$, $\gamma = 2.0/\pi$, $\sigma = 0.3$, and only estimated $\alpha$ and $\beta$. We set the search ranges for $\alpha$ and $\beta$ to $[1.0, 4.0]$ and $[1.0, 3.0]$, respectively. As shown in Figure 9, the proposed method efficiently samples around the true $\alpha = 2.00$ and the true exchange interaction $\beta = 2.00$. The sample points in Figure 9 indicate that anisotropy and exchange interaction are negatively correlated with the PSS feature. As shown in Figure 9, we did not see that the multiple local minima of the loss function appears in these search spaces.

Table 2 lists the estimated values of $\alpha$ and $\beta$ obtained using the proposed method. We performed 10 estimation experiments, and Table 2 shows their means and standard deviations. As shown in Table 2, the estimated values obtained using the proposed

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**Figure 7.** Simulated images of the time evolution of magnetic domain patterns. [(a) True images $\alpha = 2.00$. (b) estimated anisotropy parameter $\alpha = 1.98$.] The time evolution of the magnetic domain pattern is shown from left to right.

**Figure 8.** The number of image data used by the conventional [22,27] and proposed methods to estimate the anisotropy $\alpha$ (the number of simulation trials).

**Figure 9.** Results of simultaneous estimation of anisotropy $\alpha$ and exchange interaction $\beta$ by the proposed method. The color scale represents the logarithmic loss function $\log(\mathcal{L}(\alpha, \beta))$. The dot lines show the true anisotropy $\alpha = 2.00$ and the true exchange interaction $\beta = 2.00$. The contours show the predicted distribution from the Gaussian process regression.

**Table 1.** Estimation accuracy of anisotropy parameter $\alpha$ by conventional and proposed methods.

| Method           | Absolute error |
|------------------|----------------|
| Murakami [27]    | 0.028          |
| Mamada [22]      | 0.018          |
| Proposed method  | 0.020          |

**Table 2.** True and estimated values of anisotropy parameter $\alpha$ and exchange interaction parameter $\beta$. We performed 10 estimation experiments, and the table shows their means and standard deviations.

|                       | Anisotropy $\alpha$ | Interaction $\beta$ |
|-----------------------|----------------------|---------------------|
| True values           | 2.00                 | 2.00                |
| Estimated values      | 2.02 $\pm$ 0.04      | 2.03 $\pm$ 0.06     |
method are very close to the true values. Therefore, these results confirm that the proposed method can accurately estimate $\alpha$ and $\beta$ simultaneously.

### 3.4. Inverse estimation of anisotropy $\alpha$ and variance $\sigma$

Both $\alpha$ and $\sigma$ are magnetic domain parameters involved in the anisotropic Hamiltonian $H_A$. The parameter $\sigma$ represents the variance of the disordered field $\lambda(\mathbf{r})$. Figure 11 shows the time evolution pattern of the magnetic domain when only $\sigma$ is changed. The simulation conditions are $\alpha = 2.0$, $\nu = 0.01$, $\beta = 2.0$, and $y = 2.0/\pi$.

Figure 10 shows the result of the simultaneous estimation of $\alpha$ and $\sigma$ using the proposed method. We fixed $\nu = 0.01$, $\beta = 2.0$, $y = 2.0/\pi$, and we estimated only $\alpha$ and $\sigma$. We set the search ranges for $\alpha$ and $\sigma$ to $[1.0, 4.0]$ and $[0.1, 0.5]$, respectively. As shown in Figure 10, the proposed method efficiently samples the true $\alpha = 2.00$ and the true $\sigma = 0.30$. Further, as per the sampling points and contours illustrated in Figure 10, the spread of the distribution of $\sigma$ is larger than that of $\alpha$. As shown in Figure 10, we did not see the multiple local minima of the loss function appear in these search spaces.

Table 3 summarizes the estimated values of $\alpha$ and $\sigma$ using the proposed method. We performed 10 estimation experiments and Table 3 shows their means and standard deviations. As shown in Table 3, the estimated values obtained using the proposed method

![Figure 10](image_url)

Figure 10. The result of simultaneous estimation of anisotropy $\alpha$ and variance $\sigma$ by the proposed method. The color scale represents the logarithmic loss function $\log(L(\alpha, \beta))$. The dot lines show the true anisotropy $\alpha = 2.00$ and the true variance $\sigma = 0.30$. The contours show the predicted distribution from the Gaussian process regression.

![Figure 11](image_url)

Figure 11. Time evolution pattern of magnetic domains obtained by simulations following the TDGL equation when only the variance $\sigma$ of disorder parameter is varied. [(a)-(f) $\sigma = 0.3$, (g)-(l) $\sigma = 0.5$]. The simulation conditions are $\nu = 0.01$, $\alpha = 2.0$, $\beta = 2.0$, and $y = 2.0/\pi$.

![Figure 12](image_url)

Figure 12. Results of simultaneous search for anisotropy $\alpha$ and variance $\sigma$ when loss functions are designed from steady-state magnetic domain patterns. The color scale represents the logarithmic loss function $\log(L(\alpha, \beta))$. The dot lines show the true anisotropy $\alpha = 2.00$ and the true variance $\sigma = 0.30$. The contours show the predicted distribution from the Gaussian process regression.
are very close to the true values. The proposed method can estimate $\alpha$ and $\sigma$ simultaneously with high accuracy. It was confirmed that $\alpha$ and $\sigma$ involved in the anisotropic Hamiltonian $H_k$, which are highly relational parameters, can be estimated simultaneously and accurately.

Figure 11 (a)–(f) and (g)–(l) depict the time evolution of the magnetic domain when $\sigma = 0.3$ and $\sigma = 0.5$, respectively. As shown in Figure 11 (a)–(c) and (g)–(i), the velocity at which the magnetic domain pattern is formed differs depending on the dispersion $\sigma$. As shown in Figure 11(f)(l), the steady-state magnetic domain patterns are visually similar even for the time development with different $\sigma$. Therefore, it is difficult for $\sigma$ to estimate the steady-state magnetic domain pattern, and it is important that there is similarity in the time evolution of the magnetic domains.

Figure 12 shows the results of the simultaneous estimation for $\alpha$ and $\sigma$ when the loss functions are designed from steady-state magnetic domain patterns. This loss function is equivalent to the loss function of the proposed method $L(M) = \int_0^T w(t) D(z^{(t)}_{\text{true}}, z^{(t)}_{\text{est}}) dt$ with the weight factor $w(t) = \delta(t-T)$, where $\delta(t)$ denotes the delta function. As shown in Figure 12, the value of the loss function becomes smaller and independent of $\sigma$. The estimated $\alpha$ and $\sigma$ are $\hat{\alpha} = 2.23$ and $\hat{\sigma} = 0.16$, respectively. The estimated value of $\alpha$ is relatively close to the true value; however, the estimated value of $\sigma$ is far from the true value. Thus, it is necessary to consider the time evolution pattern of magnetic domains when estimating $\sigma$.

### 3.5. Inverse estimation of parameters for magnetic domain $M$

| Table 4. True and estimated values of magnetic domain parameters $M = \{\alpha, \sigma, \gamma\}$. We performed 10 estimation experiments, and the table shows their means and standard deviations. |
|-------------------------------|-----------------|-----------------|-----------------|
| True values                   | interaction $\beta$ | variance $\sigma$ |
| $\alpha$                      | $\gamma$         | $\sigma$        |
| $\hat{\alpha}$                | $\hat{\gamma}$   | $\hat{\sigma}$  |
| Estimated values              | $\hat{\alpha} \pm .08$ | $\hat{\beta} \pm 2.00$ | $\hat{\sigma} \pm 0.30$ |

Table 4 shows the estimated values of the magnetic domain parameters $M = \{\alpha, \beta, \sigma\}$ obtained using the proposed method. We fixed $\nu = 0.01$, $\gamma = 2.00/\pi$ and we estimated $\alpha$, $\beta$, and $\sigma$. We set the search range for $\alpha$, $\beta$, and $\sigma$ to $[1.0, 4.0]$, $[1.0, 3.0]$ and $[0.1, 0.5]$, respectively. We performed 10 estimation experiments and Table 4 shows their means and standard deviations. As shown in Table 4, the estimated values obtained using the proposed method are very close to the true values. The proposed method can estimate the magnetic domain parameters $M = \{\alpha, \beta, \sigma\}$ simultaneously with high accuracy. Appendix C shows the results of estimating the magnetic domain parameters using the proposed method with a set of true values different from those in the main section. Appendix D shows the learning curve that is the relationship between loss function and sample data size.

### 4. Conclusion

In this study, we developed a method for the inverse estimation of magnetic domain parameters that can produce simulation results similar to those of a set of magnetic domain patterns given the time evolution patterns of the magnetic domains. A design of experiments based on the Gaussian process regression is employed in the proposed method to search for magnetic domain parameters efficiently. We focused on the similarity of the features describing the texture structure (PSS) proposed by Portilla and Simoncelli because of the similarity between the time evolution patterns of the magnetic domains.

We showed that the proposed method can infer to the three magnetic domain parameters simultaneously and with high accuracy. In addition, we show that the proposed method can estimate the magnetic domain parameters with a smaller number of simulation trials compared to that with the conventional method.

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Appendix A. Framework of conventional methods

Mamada et al. proposed a method for predicting anisotropy parameters from magnetic domain patterns using kernel regression with convolutional neural networks and morphological statistics. We previously proposed a method to predict anisotropy parameters from magnetic domain patterns using PSS, wherein the texture features are based on visual perception. We showed that the anisotropy parameter can be estimated from the magnetic domain pattern using these conventional methods. Figure A1 shows a schematic of these conventional methods. As indicated in Figure A1, the conventional method first prepares a number of steady-state magnetic domain pattern images simulated with various anisotropy parameters. Then, a prediction model is trained using the image features of the magnetic domain pattern images as explanatory variables, and the anisotropy parameter is used as the objective variable to predict the anisotropy parameter.

![Figure A1. Overview of the conventional method. The conventional method consists of three components: simulation based on the TDGL equation, feature extraction, and training of the predictor.](image)

Appendix B. Gaussian process regression

We model the loss function $y_i = \mathcal{L}(\mathcal{M}_i)$ in the magnetic parameter $\mathcal{M}_i$ as:

$$ y_i = \mu + g(\mathcal{M}_i). $$

where $\mu$ represents the mean, and $g(\mathcal{M}_i)$ denotes the Gaussian process. We denote:

$$ \mathbb{E}[g(\mathcal{M}_i)] = 0, $$

$$ \text{Cov}(g(\mathcal{M}_i), g(\mathcal{M}_j)) = K_{ij}. $$

In a Gaussian process, $\mathcal{L}(\mathcal{M}_i)$ is assumed to follow a multivariate Gaussian distribution $\mathcal{N}(\mathbf{1}_n, \mu, \mathbf{K})$. Here, $\mathbf{1}_n$ represents a vector with 1 element and $n \times 1$ elements, respectively, and $\mathbf{K}$ represents a co-variance matrix with $K_{ij}$ as an element. We use as the correlation structure $k(\cdot, \cdot)$ as the radial basis function defined as $k(\cdot, \cdot)$:

$$ K_{ij} = k(\mathcal{M}_i, \mathcal{M}_j), $$

$$ = \theta_1 \exp\left(-\frac{|\mathcal{M}_i - \mathcal{M}_j|^2}{\theta_2}\right). $$

where $\theta_1, \theta_2 \in \mathbb{R}$ represents the hyperparameter that determines the properties of the radial basis functions. The radial basis function is a function whose value decays exponentially like a Gaussian distribution, based on the distance between $\mathcal{M}_i$ and $\mathcal{M}_j$.

We consider the loss function $y' = \mathcal{L}(\mathcal{M}')$ at an unknown observation point $\mathcal{M}'$. Let the observation point $y$ include the new $y'$ as $y = (y_1, \ldots, y_n, y')$, $\mathcal{M} = (\mathcal{M}_1, \ldots, \mathcal{M}_n)$, and $\mathcal{M}'$, and we let $K'$ be the co-variance matrix of $(n + 1) \times (n + 1)$ and $\mu'$ be the mean. Since the whole of these also follow a Gaussian distribution, $y'$ is represented as:

$$ y' \sim \mathcal{N}(1_{n+1}\mu', K') $$

Here, we denote:
\[ k_s = (k(M^*, M_1), k(M^*, M_2), \ldots, k(M^*, M_n))^T, \]

\[ k_{ss} = k(M^*, M^*). \]

These are the vectors of similarities between the unknown observation point \( M^* \) and the observation point \( M \), and the similarity of the unknown observation point \( M^* \) to itself.

The predictive distribution of the Gaussian process regression is expressed as:

\[ p(y^*|M^*, y, M) = \mathcal{N}(\hat{\mu}, \hat{\xi}). \]

\[ \hat{\mu} = k_s^T K^{-1} y, \]

\[ \hat{\xi} = k_{ss} - k_s^T K^{-1} k_s. \]

Multiple predictions can be calculated in the same manner.

Gaussian process regression is applied to the design of experiments because it allows probabilistic predictions to be made based on a small number of sample points and minimal assumptions. This application estimates the parameter set \( \mathcal{M} \) such that the unknown objective function \( \mathcal{L}(M) \) takes the minimum value.

In the design of experiments using Gaussian process regression, the next search point represents the point where the acquisition function \( a(\cdot) \) calculated based on the predictive distribution is minimized. The acquisition function is designed to balance the search around points with a high expected value and around points with a large uncertainty. In this study, we use the lower confidence bound (LCB) function, which is defined as:

\[ a_{LCB}(\mu, \xi, n) = \mu - \xi \sqrt{\frac{\log(n)}{n}}. \]

The system prefers to search around locations with low search density by defining an acquisition function that adds a margin of size proportional to the standard deviation \( \xi \) to the estimated mean \( \mu \).

**Appendix C. Results under different conditions**

Figure C1 shows the results for the estimation of \( a \) and \( \beta \) when the true value is set to [3.0, 2.5], respectively. In addition, Figure C2 shows the results for the estimation of \( a \) and \( \sigma \) when the true value is set to [2.5, 0.2].

Tables C1 and C2 show true and estimated values by the proposed method. We performed 10 estimation experiments and Tables C1 and C2 show their mean and standard deviations. As shown in Tables C1 and C2, the values estimated by the proposed method are very close to the true values.

**Figure C1.** Results of simultaneous estimation of anisotropy \( a \) and exchange interaction \( \beta \) by the proposed method. The color scale represents the logarithmic loss function \( \log(\mathcal{L}(a, \beta)) \). The dot lines show the true anisotropy \( a = 3.00 \) and the true exchange interaction \( \beta = 2.50 \). The contours show the predicted distribution from the Gaussian process regression.

**Appendix D. Learning curve of proposed method**

Figure D1 shows the learning curve that is the relationship between the loss function and the size of the sample data. Figure D1 (a)-(c) show the learning curve when \( \{a, \beta\}, \{a, \sigma\}, \) and \( \{a, \beta, \sigma\} \) were estimated using the proposed method, respectively. As shown in Figure D1, it can be seen that estimating \( \sigma \) requires a large number of data samples.
Figure C2. Results of simultaneous search for anisotropy \( \alpha \) and variance \( \sigma \) when loss functions are designed from steady-state magnetic domain patterns. The color scale represents the logarithmic loss function \( \log(\mathcal{L}(\alpha, \beta)) \). The dot lines show the true anisotropy \( \alpha = 2.50 \) and the true variance \( \sigma = 0.20 \). The contours show the predicted distribution from the Gaussian process regression.

Table C1. True and estimated values of anisotropy parameter \( \alpha \) and exchange interaction parameter \( \beta \). We performed 10 estimation experiments, and the table shows their means and standard deviations.

|                | anisotropy \( \alpha \) | interaction \( \beta \) |
|----------------|-------------------------|-------------------------|
| True values    | 3.00                    | 2.50                     |
| Estimated values | 2.96 ± .07              | 2.45 ± .06              |

Table C2. True and estimated values of anisotropy parameter \( \alpha \) and variance on disorder \( \sigma \). We performed 10 estimation experiments, and the table shows their means and standard deviations.

|                | anisotropy \( \alpha \) | variance \( \sigma \) |
|----------------|-------------------------|-----------------------|
| True values    | 2.50                    | 0.20                  |
| Estimated values | 2.47 ± .06              | 0.22 ± .08            |

Figure D1. Relationship between loss function and sample data size. (a)-(c) show the learning curve when \( \{\alpha, \beta\} \), \( \{\alpha, \sigma\} \) and \( \{\alpha, \beta, \sigma\} \) were estimated by the proposed method, respectively.