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Parametric dictionary learning for modeling EAP and ODF in diffusion MRI

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Abstract. In this work, we propose an original and efficient approach to exploit the ability of Compressed Sensing (CS) to recover Diffusion MRI (dMRI) signals from a limited number of samples while efficiently recovering important diffusion features such as the Ensemble Average Propagator (EAP) and the Orientation Distribution Function (ODF). Some attempts to sparsely represent the diffusion signal have already been performed. However and contrarily to what has been presented in CS dMRI, in this work we propose and advocate the use of a well adapted learned dictionary and show that it leads to a sparser signal estimation as well as to an efficient reconstruction of very important diffusion features. We first propose to learn and design a sparse and parametric dictionary from a set of training diffusion data. Then, we propose a framework to analytically estimate in closed form two important diffusion features : the EAP and the ODF. Various experiments on synthetic, phantom and human brain data have been carried out and promising results with reduced number of atoms have been obtained on diffusion signal reconstruction, thus illustrating the added value of our method over state-of-the-art SHORE and SPF based approaches.

1 Introduction

Diffusion MRI (dMRI) modality is known to assess the integrity of brain anatomical connectivity and to be very useful for examining and quantifying white matter microstructure and organization not available with other imaging modalities. However, dMRI data acquisition is also well known to be significantly time-consuming, in particular when Diffusion Spectrum Imaging (DSI) or High Angular Resolution Diffusion Imaging (HARDI) is to be used in a clinical setting. Accelerated acquisitions, relying on a smaller number of sampling points, are thus more than welcome. Compressed Sensing (CS) [3] is a recent technique to accurately reconstruct sparse signals from few measurements. In this work, we present a CS based method for accelerating the reconstruction of the EAP and the ODF, by significantly reducing the number of measurements. Some approaches have been recently proposed in order to build dictionaries that enable sparse representations (For a summary see [1]). However, these works lead to non-parametric dictionaries, which do not enable to obtain continuous representations of the diffusion signal neither allow to get closed form for diffusion features such as EAP and ODF. For instance, in [9] and in [10], the authors

nicely proposed a dictionary for a sparse modeling in dMRI. However, their dictionary is just postulated to be the Spherical Ridgelets in [9] and the Spherical Wavelets in [10] i.e the dictionary is not learnt from a training phase as ours. In addition, their dictionary is used only for modelling diffusion signal in [9] and only the ODF in [10] i.e not the EAP and the ODF.

In this work, we propose to learn a parametric dictionary based on a framework especially designed for dMRI. This framework enables a continuous modeling of the diffusion signal and leads to analytical and closed form formulas to estimate two important diffusion features : the EAP, which represents the full 3D displacement probability function of water molecules at every voxel and the ODF, which characterizes the relative likelihood of water diffusion along any given angular direction. The article is structured as follows : we start by introducing the dMRI framework together with the proposed basis, then we focus on the parametric dictionary learning algorithm and finally we conclude with an experimental part illustrating the added-value of our approach with promising results showing how our approach allows to accurately estimate the diffusion signal with much less atoms (almost the half) than using state-of-the-art bases such as SHORE [8, 4] and SPF [2].

2 dMRI framework for recovery of EAP and ODF

In this section, we introduce the dMRI framework to model the diffusion signal and its important features: the EAP and the ODF. Due to a lack of space, we omit all the details and refer the interested reader to our research report, to be included in the final version of this article.

2.1 Basis for diffusion signal estimation :

Inspired by the basis proposed in the state-of-the-art diffusion signal estimation i.e the SHORE [8, 4], the SPF [2], we propose to express the diffusion signal as a truncated linear combination of 3D functions Ψ_{nlm} where each basis function can be decomposed in a radial part and an angular part represented by a the symmetric and real spherical harmonics (SH) $Y(\mathbf{u})$ [5].

$$E(q\mathbf{u}) = \sum_{n=0}^{N} \sum_{l=0}^{L} \sum_{m=-l}^{l} c_{nlm} \Psi_{nlm}(\mathbf{a_{nlm}}, \zeta_{nlm}, q\mathbf{u}), \tag{1}$$

with $c_{nlm} = \langle E, \Psi_{nlm} \rangle$ are the transform coefficients, N the radial order, L the angular order , q the norm of the effective gradient, $\mathbf{u}$ a unitary vector. We let $j = j(n, \ell, m) = (n + 1) \times ((\ell^2 + \ell + 2)/2 + m)$ and rewrite formula 1 as $E(q\mathbf{u}) = \sum_{j=0}^{J} c_j \Psi_j(\mathbf{a_j}, \zeta_j, q\mathbf{u})$. Then, Ψ_j is given by

$$\Psi_j(\mathbf{a_j}, \zeta_j, q\mathbf{u}) = \frac{1}{\sqrt{\chi_{\mathbf{a_j}}}} \exp\left(-\frac{q^2}{2\zeta_j}\right) \left(\frac{q^2}{\zeta_j}\right)^{l/2} \sum_{i=0}^{n} \mathbf{a_j(i)} \left(\frac{q^2}{\zeta_j}\right)^{i} Y_j(\mathbf{u}), \tag{2}$$

where $\chi_{\mathbf{a_j}}$ is the normalization factor in the l_2-norm sense, $\mathbf{a_j} \in \mathbb{R}^{n+1}$ a vector of polynomial parameters associated with the scaled parameter ζ_j, and $Y_j = Y_\ell^m$ the spherical harmonic of order ℓ and degree m with ℓ, m the index related to j. $\mathbf{a_j}$ and ζ_j are the parameters we want to learn for each 3D function Ψ_j.

It's worthwhile to note that our basis Ψ_j in Eq. 2 simplifies to the SHORE basis [8, 4] by setting $\mathbf{a_j}$ as the generalized Laguerre polynomial coefficients of degree n and l.

2.2 On EAP and ODF recovery : Closed formulas

Using the basis function we proposed in the previous section, it is possible to derive important and analytical closed formulas for the two diffusion features : the EAP and the ODF.

EAP feature : The EAP, denoted $P(R\mathbf{r})$, is the inverse Fourier transform of the normalized diffusion signal, denoted $E(q\mathbf{u})$. From eq. 1, we can derive the following expression for the EAP :

$$P(\mathbf{a_j}, \zeta_j, R\mathbf{r}) = \sum_{j=0}^{J} c_j \frac{2\pi(-1)^{\frac{l}{2}}}{\sqrt{\chi_{\mathbf{a_j}}}R} Y_j(\mathbf{r}) \sum_{i=0}^{n} \frac{\mathbf{a_j(i)}}{\zeta_j^{\frac{l}{2}+i}} \frac{(2\pi R)^{l+\frac{1}{2}} \Gamma(\frac{3}{2}+l+i)}{2^{l+\frac{3}{2}}(\frac{1}{2\zeta_j})^{\frac{3}{2}+l+i} \Gamma(l+\frac{3}{2})} {}_1F_1(\frac{3}{2}+l+i; l+\frac{3}{2}; -2\zeta_j\pi^2 R^2),$$
(3)

where ${}_1F_1$ is the confluent hypergeometric function and Γ the Gamma function.

ODF feature : The ODF is given by $\Upsilon(\mathbf{r}) = \int_0^\infty P(R \cdot \mathbf{r})R^2 dR$. We can show that the following closed form can be derived for the ODF :

$$\Upsilon((\mathbf{a_j}, \zeta_j, \mathbf{r}) = \frac{1}{\sqrt{4\pi}} + \sum_{j=0}^{J} Y_j(\mathbf{r}) \left(\sum_{n=0}^{N} c_j \frac{(-1)^{\frac{l}{2}}\pi^{l+1}}{2^{\frac{3}{2}}\sqrt{\chi_{\mathbf{a_j}}}} \left(\frac{1}{2\zeta_j\pi^2}\right)^{\frac{3}{2}+\frac{l}{2}} \sum_{i=0}^{n} \frac{\mathbf{a_j(i)}}{\zeta_j^{\frac{l}{2}+i}} \frac{\Gamma(\frac{l}{2}+\frac{3}{2})\Gamma(\frac{l}{2}+i)}{\left(\frac{1}{2\zeta_j}\right)^{\frac{3}{2}+l+i} \Gamma(\frac{l}{2})} \right).$$
(4)

3 Dictionnary learning

Here, we introduce a parametric dictionary learning method that enables a sparse representation of any diffusion signal from continuous functions. We started by considering the K-SVD [1] algorithm as a model for our own method. However, the K-SVD technique designs non-parametric dictionaries, which presents some shortcomings among which : 1) a non-parametric method does not enable to compute a continuous version of our signal (not suitable for interpolation, neither data extrapolation) , 2) we could not get closed form for diffusion features, which would be very appreciated for EAP and ODF estimations, and 3) the K-SVD is acquisition-dependant. Although the K-SVD method appears powerful in designing sparse dictionary, these drawbacks push towards a better design via parametric dictionary learning. This algorithm consists in a sparse coding step

and a dictionary update step, where the polynomial and scale parameters $\mathbf{a_j}$, ζ_j are estimated using a non linear approach, the Levenberg-Marquardt algorithm (LMA). The section 3.1 presents our dictionary learning algorithm and the section 3.2 describes the method we use to reconstruct any diffusion signal using the dictionary previously learned.

3.1 Dictionary learning algorithm

Notation : Suppose the training set consists in M observations $\{\mathbf{s}_i\}_{i=1}^{M}$ (i.e. M voxels). For each observation s_i we have m_s samples in the q-space, i.e. $\mathbf{s}_{1..M} \in \mathcal{R}^{m_s}$. We represent $\{\mathbf{s}_i\}_{i=1}^{M}$ in matrix form $\mathbf{S} \in \mathcal{R}^{m_s \times M}$ where $\mathbf{s}_i$ is the ith column. The algorithm searches for the dictionary $\mathbf{D} \in \mathcal{R}^{m_s \times J}$, that enables the sparsest representation for every column of $\mathbf{S}$. The dictionary consists in J atoms $\{\mathbf{d}_j\}_{j=1}^{J}$ with $\mathbf{d}_j \in \mathcal{R}^{m_s}$ a column of $\mathbf{D}$. $\mathbf{d}_j$ corresponds to the 3D function Ψ_j in eq. 2. Here, we do not try to directly estimate $\mathbf{d}_j$ but the polynomial and scale parameters $\mathbf{a_j}$ and ζ_j, that characterize the atom $\mathbf{d}_j$. For each observation $\mathbf{s}_i$, we define a coefficient vector $\mathbf{c}_i \in \mathcal{R}^{n_c}$, which forms the ith column of the coefficient matrix $\mathbf{C} \in \mathcal{R}^{n_c \times M}$.

Given a training data set $\mathbf{S}$, we search for the dictionary D that gives the sparsest representation of this set. The overall problem is to find the dictionary $\mathbf{D}$ and the vectors $\mathbf{c}_i$ in $\mathbf{C}$ by solving :

$$\arg\min_{\mathbf{c}_i, \mathbf{D}} \{\|\mathbf{S} - \mathbf{DC}\|_2^2\} \quad subject \quad to \quad \forall_i \|\mathbf{c}_i\|_1 \leq \epsilon \tag{5}$$

with $\epsilon \in \mathbb{R}$. The method to solve Eq. 5 is described in the following and a summary of the algorithm is given in alg. 1. This algorithm iteratively alternates between sparse signal estimations (i.e. $\mathbf{C}$) and updates of the dictionary (i.e. $\mathbf{D}$) so to better fit the training data set (i.e. $\mathbf{S}$).

In the first step, the estimation of the column vector $\mathbf{c}_i$ is performed separately for each signal $\mathbf{s}_i$, i.e for each column of $\mathbf{S}$. Sparse estimation is achieved through a fast iterative thresholding shrinkage algorithm (FISTA) [6].

In the second step, we update the dictionary $\mathbf{D}$. For this purpose, we compute an absolute averaged coefficient vector, $\hat{\mathbf{c}} = 1/M \sum_i |\mathbf{c}_i|$, and find the atoms associated with the non zeros values of $\hat{\mathbf{c}}$. It gives a rough idea of which atoms are used for modeling the signal and enables to discard some unnecessary atoms, which enforces sparsity. Then, in this set of atoms, we update one atom at a time, while fixing all the others. This process is repeated for all the non-zero coefficients in $\hat{\mathbf{c}}$. The in-update atom is denoted $\mathbf{d}_k$. To update this atom, we begin by decomposing the error term in eq. 5 as in [1], i.e.

$$\|\mathbf{S} - \mathbf{DC}\|_{\ell 2}^2 = \left\|\mathbf{S} - \sum_{j=1}^{M} \mathbf{d}_j \mathbf{c}_j^r\right\|_{\ell 2}^2 = \left\|\left(S - \sum_{j \neq k} \mathbf{d}_j \mathbf{c}_j^r\right) - \mathbf{d}_k \mathbf{c}_k^r\right\|_{\ell 2}^2 = \|\mathbf{E}_k - \mathbf{d}_k \mathbf{c}_k^r\|_{\ell 2}^2, \tag{6}$$

where $\mathbf{c}_j^r$ is the jth row of C. We could use the LMA in order to fit the atom $\mathbf{d}_k$ to the error matrix $\mathbf{E}_k$. However, because we take into account all the coefficients

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Algorithm 1 Semi-parametric dictionary learning

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1. Initialize the dictionary by fixing the polynomial and scale parameters $\mathbf{a_j}$, ζ_j.

2. Sparse estimation of the observations $\{\mathbf{s}_i\}_{i=1}^M$. We use the FISTA algorithm to solve for $\mathbf{c_i}$ associated to each observation : $\arg\min_{\mathbf{c}_i}\{\|\mathbf{s}_i - \mathbf{Dc}_i\|_2^2\}$ $subject$ to $\forall_i \|\mathbf{c}_i\|_1 \leq \epsilon$ (Eq. 5bis).

3. Updating the dictionary. Compute the absolute averaged coefficients vector $\hat{\mathbf{c}} = 1/M \sum_i |\mathbf{c}_i|$. Repeat until all the atoms of the dictionary , with non zeros value in $\hat{\mathbf{c}}$, have been scanned :
   – Let note the current atom, the kth.
   – Define the group of observation that use this atom : $w_k = \{i, 1 \leq i \leq M, c_k(i) \neq 0\}$.
   – Compute the error matrix $\mathbf{E}_{w_k} \in \mathcal{R}^{m \times card(w_k)}$.
   – Apply Levenberg - Marquardt algorithm to estimate the polynomials and scale parameters $a_{k,1..n}$, ζ_k, which enable $\mathbf{d}_k$ to best fit $\mathbf{E}_{w_k}$
   – Update the atoms according to $a_{k,1..n}$, ζ_k.

4. Go back to the step 2 unless the overall error does not vary anymore

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and atoms, this dictionary update doesn't enforce sparsity. Hence, we need to reduce the number of atoms used for modeling the signal. For this purpose, we define the group of observations that use the atom $\mathbf{d}_k$, i.e $w_k = \{i, 1 \leq i \leq M, c_i(k) \neq 0\}$. In other words, they are the observations whose the coefficients, associated with the atom $\mathbf{d}_k$ are non zeros. This forces the atom $\mathbf{d}_k$ to fit only a subset of observations and not the entire data set and, thus, enforces sparsity. Then, we compute the error matrix $\mathbf{E}_{w_k} \in \mathcal{R}^{m_s \times \mathrm{card}(w_k)}$. It corresponds to the estimation error between the observation vector $\{\mathbf{s}_i\}_{i \in w_k}$ that forms the columns of $\mathbf{S}_{w_k} \in \mathcal{R}^{m \times \mathrm{card}(w_k)}$ and the signal estimated for the group of observation w_k without taking into account the kth atom, i.e $\tilde{\mathbf{S}}_{w_k} = \sum_{j \neq k} \mathbf{d}_j \mathbf{c}_j^T(i), i \in w_k$. Finally, we use a non linear approach (the LMA) to estimate the polynomials and scale parameters $a_{k,1..n}$, ζ_k , which enable $\mathbf{d}_k$ to fit the error matrix $\mathbf{E}_{w_k}$. The method, as a whole, is given in Alg. 1.

Convergence : The sparse coding step (Eq. 5bis in Alg. 1) is well known to be convex and FISTA allows to converge to the unique solution specific to the current dictionary D. The dictionary update step, where $\mathbf{a_j}$, ζ_j are estimated using the Levenberg-Marquardt algorithm (LMA), could converge to local minima, depending on the initial solutions. In our experiments, a good convergence has been reached after few iterations with the polynomials parameters initialized as Laguerre polynomials coefficients of order n and l and a fixed $\zeta = 700$ [4].

3.2 Reconstruction

The purpose of section 3.1 was to learn the dictionary $\mathbf{D}$. Now, using the estimated $\mathbf{D}$, we are able to model any diffusion signal s , i.e. not in the training data set used to learn D, by solving for c and with FISTA [6], the convex problem $\arg\min_{\mathbf{c}}\{\|\mathbf{s} - \mathbf{Dc}\|_2^2\}$ subject to $\|\mathbf{c}\|_1 \leq \epsilon$, where ϵ is a small number.

4 Results

Synthetic data from a multi-tensor model: The attenuation signal is described, by F fibres, as $E(q\mathbf{u}) = \sum_{f=1}^F p_f \exp(-4\pi^2 \tau q^2 \mathbf{u}^T D_f \mathbf{u})$ where a fibre f is

defined by a tensor matrix D_f and weight p_f. q denotes the norm of the effective gradient and $\mathbf{u}$ is a unitary vector in Cartesian coordinate.

Firstly, we learn our dictionary with a training data composed of $M = 5000$ synthetic signals, evaluated on $ms = 1000$ q-space samples spread between $b_{min} = 0$ and $b_{max} = 10000$ s/mm^2. For each diffusion signal generated we randomly vary the number of fibers (between 1 and 2 fibers), the fractional anisotropy related to a fiber (between 0.75 and 0.90) and the crossing angle between these fibers (between 30° and 90°). The maximal angular and radial order of the dictionary are respectively set to $L = 8$ and $N = 5$, which gives 270 atoms. The algorithm 1 converges in 9 iterations in about 20 minutes with Python and a CPU at 2.8 GHz.

Secondly, we proceed to the signal reconstruction (see sec. 3.2) using our previous learned dictionary. To evaluate the reconstruction, we compute the normalized mean square error (NMSE $=\|E - \tilde{E}\|_2^2/\|E\|_2^2$) between the original observation signal E and the estimated signal $\tilde{E}$. We consider three cases : one fiber, two fibers crossing at 90° and two fibers crossing at 60°, and generate them using the multi-tensor model. We take 50 samples, a clinically acceptable number of acquisitions, spread on three shells of b-values 500, 1500, 2500 s/mm^2 along a spherical uniform distribution, and add Rician noise with $SNR = 10, 20, 30$. We compare our results while replacing the learned dictionary by the SPF and SHORE bases [2, 8] in the reconstruction , because these bases are known to sparsely represent the diffusion signal. We average the results on 1000 trials. To perform a fair comparison, for each trial we try several regularization parameters in the reconstruction (ϵ in sec. 3.2) and keep the lowest NMSE. The averaged NMSEs are shown in table 1. We also add the averaged number of non zero coefficients after reconstruction. It indicates the sparsity of the dictionary/basis used in the reconstruction.

		SNR=10		SNR=20		SNR=30	
		NMSE	atoms number	NMSE	atoms number	NMSE	atoms number
	one fiber	0.019421	11.50	0.007712	16.18	0.004757	18.32
LD	60°- cross. fib.	0.017969	9.12	0.007079	14.04	0.004072	16.16
	90°- cross. fib.	0.015642	6.45	0.006061	9.49	0.003629	12.07
	one fiber	0.026667	16.21	0.009804	22.05	0.005246	25.90
SHORE	60°- cross. fib.	0.023187	13.31	0.009119	19.13	0.004920	24.88
	90°- cross. fib.	0.021361	12.45	0.008370	18.03	0.004569	20.64
	one fiber	0.032988	19.43	0.013062	23.62	0.005901	31.53
SPF	60°- cross. fib.	0.031719	18.79	0.012131	21.34	0.005629	28.69
	90°- cross. fib.	0.026818	14.05	0.011317	16.72	0.005273	24.19

Table 1. NMSE between the estimated signal and the ground truth signal for three different SNR. The reconstruction is based on the Learned Dictionary (top, LD), the SHORE basis (second line) and the SPF basis (third line)

Overall, we obtain a higher sparsity (lower number of atoms) and a higher accuracy (lower NMSE) using the LD. Moreover, for $SNR = 10$ the SPF basis is clearly not appropriate in an ℓ_1 minimization reconstruction. The correspond-

ing NMSE, between the reconstruction using the learned dictionary and the SPF/SHORE basis, gets closer while increasing the SNR. However the number of atoms still remains higher with the SPF and SHORE bases. These results are not surprising while taking synthetic signals as training data set. In the next section, we prove the effectiveness of our method on a phantom data set.
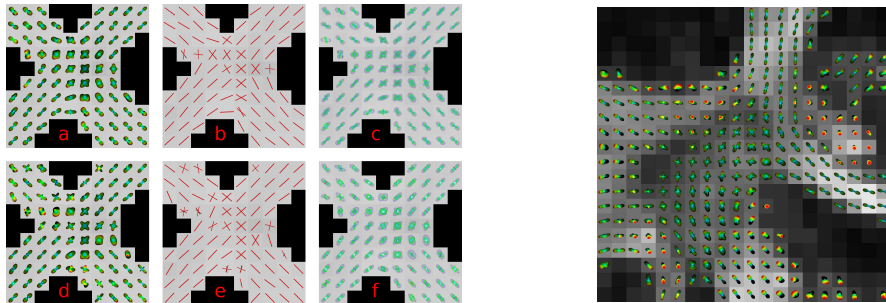

Fig. 1. Left : a, d : ODF estimations. b,e : ODF maxima. c, f : EAP estimations at radii 5 μm (red), 10 μm (green) and 15 μm (blue). Top : Our method. Bottom : SHORE estimation. **Right** : ODF from a coronal slice of a human brain.

Phantom data We perform our experiments on a phantom data used in a fiber cup contest in MICCAI 2009 [7]. The data were acquired for three different b-values b=650/1500/2000 s/mm^2, 64 orientations at each b-value, and an imaging matrix of 64x64x3. We use two slices as training data set. The test data set is the third slice. The angular and radial order of the dictionary are respectively $L = 8$ and $N = 5$.

For the reconstruction we take 50 samples following an uniform spherical law. From the estimated signals, we first present in Fig. 4 (left) : a) the ODFs computed via Eq. 4 and d) the ODF computed via the SHORE framework [8]. However, because it is quite difficult to directly give an appreciation on these figures, we compute the local maxima of the ODFs (see Fig. 4.b and e) (left)). The maxima show that the ODFs, based on our method, catch significant angular information, whereas the ODFs based on the SHORE framework do not model the angular information as precisely.

Furthermore, we present in Fig. 4.c and f (left) the EAP computed at three different radii 5 μm (red), 10 μm (green) and 15 μm (blue) respectively using the closed form at Eq. 3 and the SHORE framework [8]. It adds a new dimension to the ODF feature because both radial and angular information are caught. Again the SHORE estimation appears more noisy than the EAP estimated with our method. The EAP fully describes the diffusion process. However, few applications using this feature exist because of the large number of measurements usually required. With our method, we are able to get a continuous approximation of the EAP and ODF with a clinically acceptable number of measurements (50 samples). It is worthwhile to note that since our method requires less atoms to estimate than SHORE and SPF, we could also reconstruct the EAP and ODF with much less samples while being less sensitive to noise than SHORE and SPF.

Real data We validate our method on a real data from a human brain. The data were acquired for three different b-values b=500/1000/2000 s/mm^2, 60 orientations at each b-value,and an imaging matrix of 93x116x93. We add a part of the data set in learning process and reconstruct the signal from a coronal slice with 50 samples following an uniform spherical law. Fig. 4 (right) shows the ODF estimated via our closed form in eq. 4. These ODFs correctly show the represented crossing region.

5 Conclusions

In this work, we proposed an original and efficient approach to exploit the ability of Compressed Sensing (CS) to recover dMRI signals from limited number of samples. Our approach allows to learn a parametric dictionary characterized by a set of polynomial and scale parameters well adapted to sparsely and continuously model the diffusion signal as well as to reconstruct in closed form two of its important features : the EAP and the ODF. We showed that our framework outperforms the SPF and SHORE framework in both ODF and EAP estimations. Other diffusion features such as the probability to return to zero, the mean square displacement, and high order moments features can also be easily derived from our framework.

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