# MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

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# Statistics of Stochastic Differential Equations on Manifolds and Stratified Spaces (hybrid meeting)

Organized by Stephan Huckemann, Göttingen Xue-Mei Li, London Yvo Pokern, London Anja Sturm, Göttingen

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ABSTRACT. Statistics for stochastic differential equations (SDEs) attempts to use SDEs as statistical models for real-world phenomena. This involves an understanding of qualitative properties of this class of stochastic processes which includes Brownian motion as well as estimation of parameters in the SDE or a nonparametric estimation of drift and diffusivity fields from observations. Observations can be in continuous time, in high frequency discrete time considering the limit of small inter-observation times or in discrete time with constant inter-observation times. Application areas of SDEs where state spaces are naturally viewed as manifolds or stratified spaces include multivariate stochastic volatility models, stochastic evolution of shapes (e.g. of biological cells), time-varying image deformations for video analysis and phylogenetic trees.

Mathematics Subject Classification (2010): 62-XX, 60-XX.

## Introduction by the Organizers

The workshop Statistics of Stochastic Differential Equations on Manifolds and Stratified Spaces organised by Stephan Huckemann (Göttingen), Xue-Mei Li (London), Yvo Pokern (London) and Anja Sturm (Göttingen) was attended by 23 participants (including 8 women) corresponding to a half-workshop size. Travel arrangements were still somewhat affected by the pandemic situation as well as the beginning of teaching at UK universities. Thus, the workshop was organized in a hybrid format with 9 participants including two of the organizers (Huckemann and Li) participating virtually.

Statistical inference and simulation for stochastic differential equations (SDEs) on Euclidean domains has been studied over several decades. This includes both parametric approaches where a small number of real-valued parameters determine simulation behaviour or are to be estimated from observations of the SDE's state and nonparametric approaches. Observations can be in continuous time, in high frequency discrete time considering the limit of small inter-observation times or in discrete time with constant inter-observation times. Statistical methodology for SDEs in the Euclidean case is an active field of research including improved methods for sampling diffusion bridges to enable dealing with constant inter-observation times (workshop contributions by M. Schauer, M. Sorensen and F. van der Meulen comment on this issue) and consistency results for nonparametric estimation (workshop contributions by V. Panaretos and E. Schmisser). Many applications drive the development of particular classes of SDEs, e.g. to capture temporal synchronization as studied in the workshop contribution by S. Ditlevsen. SDEs also play an important role as limiting objects of Markov chains arising in Markov chain Monte Carlo and the design of proposal distributions and their optimal scaling to achieve the best possible mixing of the Markov chains to reach the invariant measure (often a Bayesian posterior distribution) is of continued significant interest (workshop contribution by W. Kendall).

Stochastic analysis for SDEs whose state space is a non-trivial manifold has been studied and introductory textbooks are now available but work on statistical inference and the use of such SDEs in statistical applications is still rare. This is partly due to the considerable technical challenges applied statisticians face when considering work in the area. Application areas where state spaces are naturally viewed as manifolds or stratified spaces include multivariate stochastic volatility models (workshop contribution by M. Ngoc Bui), protein structure evolution and molecular dynamics (workshop contribution by E. García-Portugués), stochastic evolution of shapes (e.g. of biological cells) and time-varying image deformations for video analysis (workshop contribution by S. Sommer) and phylogenetic trees (workshop contribution by T. Nye). In some cases, existing algorithms can be carried over essentially unchanged (e.g. the exact algorithm to simulate SDEs on the circle rather than the real line). In other cases, the theoretical foundation is far less clear than in the Euclidean case, even though empirical observations of good behaviour are available (e.g. in the workshop contribution by M. Ngoc Bui). In other cases, it is unclear how existing methods can be translated to the manifold setting. Numerical integration schemes have been discussed by M. Mamajiwala. Aspects of curvature on convergence rates of Fréchet means have been highlighted by D. Van Tran and of diffusion means by S. Sommer. The workshop also addressed qualitative properties of Brownian motions in more general settings than the standard Euclidean space with uniformly elliptic generator as studied by T. Nye and K. Habermann in their workshop contributions and a look at statistics for stochastic partial differential equations (workshop contribution by M. Reiss) widened the horizon.

Discussions on the subtly different understanding of hypoellipticity in the applied statistics and the probability theory communities have highlighted new methodological and algorithmic research directions: sampling hypoelliptic diffusion bridges is not yet a solved problem after all! Many results in stochastic analysis on manifolds that would be desirable from a methodological point of view (e.g. convergence of Euler-like schemes, existence of time-reversed diffusions and increased generality of bounds of SDE transition densities in terms of associated Brownian motion transition densities) have been discussed. The workshop concluded with a perspective on possible future applied research directions including averaging and homogenization where the study of the generator of parametrized families of diffusion processes and their convergence properties may be amenable to translation to the manifold.

# Workshop (hybrid meeting): Statistics of Stochastic Differential Equations on Manifolds and Stratified Spaces

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# Abstracts

# Adaptive non parametric drift estimation of an integrated jump diffusion process

ÉMELINE SCHMISSER (joint work with Benedikt Funke)

We consider a two-dimensional stochastic process  $(X_t, V_t)_{t \ge 0}$  such that

$$dX_t = V_t dt, \ X_0 = 0, \quad dV_t = b(V_t)dt + \sigma(V_t)dW_t + \xi(V_{t_-})dL_t, \ V_0 \stackrel{D}{=} \eta,$$

where  $W = (W_t)_{t\geq 0}$  is a standard Brownian Motion and  $L = (L_t)_{t\geq 0}$  is a centered Lévy process with finite variance  $\mathbf{E}(L_1^2) := \int_{\mathbf{B}} y^2 \nu(dy) < \infty$  such that

$$dL_t = \int_{\mathbf{R}} z(\mu(dt, dz) - \nu(dz)dt).$$

W and L are independent and  $\eta$  is independent of both W and L. This process is observed at discrete times  $0, \Delta, \ldots, n\Delta$  where  $\Delta \to 0$  and  $n\Delta \to \infty$ . Our aim is the nonparametric estimation of the unknown drift function b exclusively based on observations of the integrated jump diffusion process  $X_t$ .

The main difficulty is that we do not observe directly  $V_t$ , but only the integrated jump diffusion  $X_t$ . We consider the random variables

$$\bar{V}_{k\Delta} := \frac{1}{\Delta} \left( X_{(k+1)\Delta} - X_{k\Delta} \right) = \frac{1}{\Delta} \int_{k\Delta}^{(k+1)\Delta} V_s ds, \ 1 \le k \le n+1.$$

and, to avoid some unnecessary dependence,

$$Y_{(k+1)\Delta} = \frac{\bar{V}_{(k+2)\Delta} - \bar{V}_{(k+1)\Delta}}{\Delta} = b(\bar{V}_{k\Delta}) + R_{k\Delta} + Z_{k\Delta}$$

where  $Z_{k\Delta}$  is centred, and  $R_{k\Delta}$  a remainder term. To construct our estimator, we choose a sequence of increasing vectorial subspaces  $S_m$  of  $L^2$ , and we minimize a contrast function  $\gamma_n(s)$  on  $S_m$  where

$$\gamma_n(t) = \frac{1}{n} \sum_{k=1}^n (Y_{(k+1)\Delta} - s(\bar{V}_{k\Delta}))^2.$$

We control the empirical risk of our estimator:

$$\mathcal{R}_{n}(\hat{b}_{m}) = \mathbf{E}\left(\frac{1}{n}\sum_{k=1}^{n}(\hat{b}_{m}(\bar{V}_{k\Delta}) - b(\bar{V}_{k\Delta}))^{2}\right) \le c \|b_{m} - b\|_{L^{2}}^{2} + C\frac{D_{m}}{n\Delta} + K\Delta$$

where  $b_m$  is the orthogonal projection of b on  $S_m$ , and  $D_m$  is the dimension of  $S_m$ . Then we introduce a penalty term to choose the "best" estimator  $\hat{b}_{\hat{m}}$ .

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# Simulation of diffusion bridges and estimation for stochastic differential equation

#### MICHAEL SØRENSEN

The complexity of statistical inference for diffusions based on discrete time samples often necessitates the use of computational techniques such as Markov chain Monte Carlo. These require sampling of diffusion bridges that are coherent with observed data, typically bridges between the observed values of the diffusion. A diffusion bridge from a to b in [0, T] is a solution X to a stochastic differential equation started at a and conditioned to have the terminal value  $X_T = b$ .

A method for simulating diffusion bridges for ergodic diffusions is presented. A main advantage is that computing time is linear in T. Approximate bridges are obtained by simulating (e.g. by the Euler scheme) two unconditional diffusions - one with starting point a and another started at b. The first is spliced to the time-reversal of the second the first time they meet. If they do not meet, a new pair is simulated. For real diffusions the two diffusions can be independent. In higher dimensions coupling methods are needed to ensure that the two diffusions have a positive probability of meeting, and the stochastic differential governing the second diffusion must be that of the time reversal of the stationary version of the diffusion. The distribution of the approximate bridge is derived and used to construct a Metropolis-Hastings algorithm where the proposals are approximate bridges and the target distribution is that of an exact bridge from a to b.

It is briefly explained how the approach can be combined with methods of exact simulation of diffusions to obtain a bridge simulation method that is both without discretization error and with computing time linear in T; for details see Jenkins, Pollock, Roberts and Sørensen (2021).

The usefulness of the approach is demonstrated by an application to estimation for stochastic differential equations with random effects, i.e. where some statistical parameters are random, while other parameters are fixed.

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# Brownian motion on Billera-Holmes-Vogtmann tree space. TOM NYE

Statistics on non-Euclidean spaces is characterized by the lack of an addition operation and scalar multiplication on the data space. This raises the question of how to make sense of stochastic differential equations on such spaces, particularly metric spaces which are not Riemannian manifolds. I will start by describing some simple stratified spaces and explain how to obtain analytic expressions for the transition kernel of Brownian motion. Next I will describe the Billera-Holmes-Vogtmann (BHV) tree space of phylogenetic trees, a more complex stratified data space. BHV tree space is a non-positively curved geodesic metric space, and existing statistical methods on the tree space mostly rely on least squares estimators. It is highly desirable, though challenging, to construct a family of parametric distributions on BHV tree space parametrised by a location and a dispersion parameter, akin to the family of isotropic Gaussians in Euclidean space. One way to do this is via transition kernels of Brownian motion. I will define Brownian motion on BHV tree space and describe a bridge construction which enables Bayesian inference of the model parameters when data are modelled as identical independently distributed draws from a Brownian motion kernel.

# Inference for partially observed Riemannian Ornstein–Uhlenbeck diffusions of covariance matrices

MAI NGOC BUI (joint work with Yvo Pokern, and Petros Dellaportas)

We construct a generalization of the Ornstein–Uhlenbeck processes on the cone of covariance matrices endowed with the Log-Euclidean and the Affine-Invariant metrics. Our development exploits the Riemannian geometric structure of symmetric positive definite matrices viewed as a differential manifold. We then provide Bayesian inference for discretely observed diffusion processes of covariance matrices based on an MCMC algorithm built with the help of a novel diffusion bridge sampler accounting for the geometric structure. Our proposed algorithm is illustrated with a real data financial application.

## References

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# Stochastic Dynamical Systems Developed on Riemannian Manifolds

MARIYA MAMAJIWALA (joint work with Debasish Roy)

We propose a method for developing the flows of stochastic dynamical systems, posed as Ito's stochastic differential equations, on a Riemannian manifold identified through a suitably constructed metric. The framework used for the stochastic development, viz. an orthonormal frame bundle that relates a vector on the tangent space of the manifold to its counterpart in the Euclidean space of the same dimension, is the same as that used for developing a standard Brownian motion on the manifold. Mainly drawing upon some aspects of the energetics so as to constrain the flow according to any known or prescribed conditions, we show how to expediently arrive at a suitable metric, thus briefly demonstrating the application of the method to a broad range of problems of general scientific interest. These include simulations of Brownian dynamics trapped in a potential well, a numerical integration scheme that reproduces the linear increase in the mean energy of conservative dynamical systems under additive noise and non-convex optimization. The simplicity of the method and the sharp contrast in its performance vis-á-vis the correspondent Euclidean schemes in our numerical work provide a compelling evidence to its potential.

#### References

 Mamajiwala, Mariya, and Debasish Roy, Stochastic dynamical systems developed on Riemannian manifolds, arXiv preprint arXiv:2007.11927 (2020).

# MCMC Optimal Scaling and Dirichlet forms WILFRID KENDALL (joint work with Jure Vogrinc, Giacomo Zanella and Mylene Bédard)

This talk reports work in progress on the use of Dirichlet forms to investigate optimal scaling phenomena for Markov chain Monte Carlo algorithms (specifically, Metropolis-Hastings random walk samplers) under regularity conditions which are substantially weaker than those required by the original approach (based on the use of infinitesimal generators). The Dirichlet form method has the added advantage of providing an explicit construction of the underlying infinite-dimensional context, with intriguing possibilities for useful development using infinite-dimensional stochastic analysis. In particular, this enables us directly to establish weak convergence to the relevant infinite-dimensional diffusion. We also explore the behaviour of optimal scaling when regularity does not hold, using models based on fractional Brownian motion: intriguing examples of anomalous scaling then arise.

#### References

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# Statistics for Stochastic Partial Differential Equations MARKUS REISS

In the first part we give a survey on statistical methods for stochastic partial differential equations (SPDEs). We start with the questions of singularity and equivalence of the observation laws on path space for simple stochastic differential equations. In contrast to stochastic ordinary differential equations main parameters in SPDEs give rise to singular observation laws for different diffusivity and transport parameters in a linear SPDE with second order differential operator in the drift. Statistically, this means that we can pursue inference from observing the realisation of an SPDE solution on a fixed time interval. The classical spectral method, based on observing spatial Fourier modes in time, is discussed in detail.

Then we consider the observation of spatially local measurements and see that the space resolution  $\delta$ , tending to zero, plays a similar role as the frequency in spectral methods tending to infinity. Based on the scalar local measurements in time two estimators are derived, the augmented and the proxy maximum-likelihood estimator. For the stochastic heat equation we derive that the diffusivity estimators are asymptotically normal with rate  $\delta$  and explicit bias and variance. This allows to pursue also nonparametric estimation for a space-dependent diffusivity function  $\theta(x)$ , for which the spectral method is not feasible because the eigenfunctions of the differential operator depend on the unknown function  $\theta(x)$ . The convergence rate  $\delta$  is minimax-optimal for this estimation problem and simulations show the finite sample properties of the estimators as well as their robustness with respect to nonlinear perturbations in the source term (zero order of the differential operator).

As a concrete application in biophysics we consider stochastic models for cell motility. A two-dimensional system of stochastic-reaction equations models cell repolarisation, generalising the classical deterministic Meinhard model. Qualitative implications of the dynamical noise on the repolarisation time are exhibited and the performance of the diffusivity estimation for synthetic and experimental data are shown. The talk is mainly based on the two references given below.

#### References

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# Backward Filtering Forward Guiding for Markov processes

FRANK VAN DER MEULEN (joint work with Moritz Schauer, and Marcin Mider)

Consider a Markovian process that evolves on a prescribed tree-structure. The transition on each inner edge is obtained by running a continuous-time Markov process for a fixed time interval. At each vertex leaves can be attached; the values at these leaves represent observations. An example is given in Figure 1. Suppose

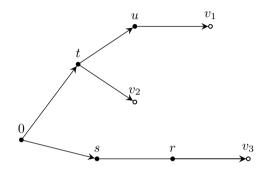


FIGURE 1. Example of a tree with leaf-vertices  $v_1$ ,  $v_2$  and  $v_3$ . The inner vertices and root vertex are depicted by solid dots. At vertex t the process splits (branches) independently, conditional on the value at t (similar branching occurs at the root vertex).

the forward dynamics, i.e. the Markov process over the edges, is parametrised by an unknown parameter  $\theta.$ 

As an example, on the branch (t, u) a diffusion process evolves for a time span [t', u'] according to the stochastic differential equation (sde)

(1) 
$$dX_t = b_\theta(t, X_t) dt + \sigma_\theta(t, X_t) dW_t, \qquad X_{t'} = x_t.$$

Branches leading to leaf-vertices correspond to a particular observations scheme, e.g. the branch  $[u, v_1]$  may correspond to assuming that  $X_{v_1} \mid X_u = x \sim N(Lx, \Sigma)$  for matrices L and  $\Sigma$ .

Interest lies in (i) sampling the process X conditional on its values at the leafvertices and (ii) inferring the distribution of  $\theta$  conditional on the leaf-vertices. Here, I implicitly assume a Bayesian framework where the parameter  $\theta$  is endowed with a prior distribution. The task can be accomplished by an algorithm called *Backward Filtering Forward Guiding* (BFFG). Here, one first computes the Backward Information Filter (BIF) to a simplified version of the forward dynamics, to ensure that the computations involved are tractable. In the SDE case, rather than backward filtering (1) one would backward filter the linear SDE  $d\tilde{X}_t = (B\tilde{X}_t + \beta(t)) dt + \tilde{\sigma}(t) dW_t$ . The BIF then boils down to (backward) Kalman-filtering on a tree. The output of the BIF can subsequently be used to adjust the dynamics of the forward process such that it ends up in the observations at the leaf-vertices. This adjustment is in fact an approximation to Doob's h-transform. We call the adjusted forward process a *guided process*, as it guides the process to the observations. One can deduce closed-form expressions for the likelihood ratio between the true conditioned process and the guided process. This in turn can be used for Bayesian inference.

The BFFG-algorithm for diffusions is discussed in the paper [1], while generalisations to graphical models and other stochastic processes is treated in [2].

This concerns joint work with Moritz Schauer (Chalmers University of Technology - University of Gothenburg) and Marcin Mider (Trium Analysis Online GmbH).

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## Langevin diffusions on the torus

Eduardo García-Portugués

Motivated by their use in modeling the evolution of proteins' structures, we introduced stochastic processes for continuous-time evolution of angles and developed their estimation. The state space of such stochastic processes is the *p*-dimensional torus  $\mathbb{T}^p = \mathbb{R}^p/(2\pi\mathbb{Z})$ , diffusions  $\{\Theta_t\}$  on it being defined as the "wrapping" by the modulus operator (·) mod  $2\pi$  of (time-homogeneous) diffusions on  $\mathbb{R}^p$  given by

$$\mathrm{d}\mathbf{X}_t = b(\mathbf{X}_t)\mathrm{d}t + \sigma(\mathbf{X}_t)\mathrm{d}\mathbf{W}_t,$$

where  $b(\cdot)$  and  $\sigma(\cdot)$  are  $2\pi$ -periodic functions, this requirement being key for ensuring the Markovianity of the resulting process  $\{\Theta_t\}$ . The important class of Langevin diffusions can be exported to  $\mathbb{T}^p$ ; it was seen that this class characterizes ergodic time-reversible diffusions on  $\mathbb{T}^p$ . Two specific Langevin diffusions were exploited to define Ornstein–Uhlenbeck (OU) analogues on the torus, guided by the characterization of the OU process on  $\mathbb{R}^p$  as the unique ergodic time-reversible diffusion with Gaussian stationary density and constant volatility. These two diffusions are the multivariate von Mises and Wrapped Normal (WN) diffusions, the last one given by

$$\mathrm{d}\boldsymbol{\Theta}_{t} = \left[\mathbf{A}\sum_{\mathbf{k}\in\mathbb{Z}^{p}}\left(\boldsymbol{\mu}-\boldsymbol{\Theta}_{t}-2\mathbf{k}\boldsymbol{\pi}\right)w_{\mathbf{k}}(\boldsymbol{\Theta}_{t})\right]\mathrm{d}t + \boldsymbol{\Sigma}^{1/2}\mathrm{d}\mathbf{W}_{t}$$

for certain non-linear weights  $w_{\mathbf{k}}(\cdot)$ . Unlike in the OU case, the likelihood functions of both diffusions involve a transition probability density (tpd) with no analytical solution. To bypass this issue, we explored three alternatives: (*i*) solving the Fokker–Planck equation numerically through tailored discretization schemes; (*ii*) toroidal adaptations of the Euler and Shoji–Ozaki pseudo-likelihoods; (*iii*) a specific approximation of the tpd of the WN process via the conditional density of a wrapped OU process. A simulation study for p = 1, 2 compared the fidelity of the approximate tpds to the exact ones, and investigated the estimation performance of the approximate likelihoods. The specific approximate tpd for the WN process was shown to be superior to the rest of tpd approximations for performing estimation in this process, while numerically solving the Fokker–Planck equation was seen to be a sensible estimation approach for p = 1. Finally, two diffusions, on  $\mathbb{T}^1$  and  $\mathbb{T}^2$ , were used to model the evolution of the backbone angles of the protein 1GB1 in a molecular dynamics simulation. Empirical evidence of the performance of the diffusive processes within a larger model of protein evolution was also provided. The R package **sdetorus** implements the estimation methods and applications presented.

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## FDA of SDE?

#### VICTOR PANARETOS

(joint work with N. Mohammadi and L. Santoro)

We consider the problem of nonparametric estimation of the drift and diffusion coefficients of a Stochastic Differential Equation (SDE), based on n independent replicates  $\{X_1(t), ..., X_n(t)\}$ , observed sparsely and irregularly on the unit interval, and subject to additive noise corruption. By *sparse* we intend to mean that the number of measurements per path can be arbitrary (as small as two), and remain constant with respect to n. We focus on time-inhomogeneous SDE of the form  $dX_t = \mu(t)X_t^{\alpha}dt + \sigma(t)X_t^{\beta}dW_t$ , where  $\alpha \in \{0,1\}$  and  $\beta \in \{0,1/2,1\}$ , which includes prominent examples such as Brownian motion, Ornstein-Uhlenbeck process, geometric Brownian motion, and Brownian bridge. Our estimators are constructed by relating the local (drift/diffusion) parameters of the diffusion to their global parameters (mean/covariance, and their derivatives) by means of an apparently novel PDE. This allows us to use methods inspired by functional data analysis, and pool information across the sparsely measured paths. The methodology we develop is fully non-parametric and avoids any functional form specification on the time-dependency of either the drift function or the diffusion function. We establish almost sure uniform asymptotic convergence rates of the proposed estimators as the number of observed curves n grows to infinity. Our rates are non-asymptotic in the number of measurements per path, explicitly reflecting how different sampling frequency might affect the speed of convergence. Our framework suggests possible further fruitful interactions between FDA and SDE methods in problems with replication.

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## A polynomial expansion for Brownian motion and the associated fluctuation process

## KAREN HABERMANN

Let  $(B_t)_{t\in[0,1]}$  be a Brownian motion in  $\mathbb{R}$ , which we assume is realised as the coordinate process on the path space  $\{w \in C([0,1],\mathbb{R}): w_0 = 0\}$  under Wiener measure  $\mathbb{P}$ . We start by studying  $(B_t)_{t\in[0,1]}$  conditioned to have vanishing iterated time integrals up to order  $N \in \mathbb{N}$ . Set

$$\boldsymbol{B}_{1}^{N} = \left(B_{1}, \int_{0}^{1} B_{s_{1}} \, \mathrm{d}s_{1}, \dots, \int_{0}^{1} \int_{0}^{s_{N-1}} \cdots \int_{0}^{s_{2}} B_{s_{1}} \, \mathrm{d}s_{1} \dots \, \mathrm{d}s_{N-1}\right)$$

and let  $Q_n$  be the shifted Legendre polynomial of degree  $n \in \mathbb{N}_0$  on [0, 1]. As derived in [1], the stochastic process  $(L_t^N)_{t \in [0,1]}$  in  $\mathbb{R}$  defined by

$$L_t^N = B_t - \sum_{n=0}^{N-1} (2n+1) \int_0^t Q_n(r) \,\mathrm{d}r \int_0^1 Q_n(r) \,\mathrm{d}B_r$$

has the same law as  $(B_t)_{t \in [0,1]}$  conditioned on  $B_1^N = 0$ . Adapting the usual proof of Mercer's theorem shows that as  $N \to \infty$  the sequence of covariances  $C_N$  given by, for  $s, t \in [0, 1]$ ,

$$C_N(s,t) = \min(s,t) - \sum_{n=0}^{N-1} (2n+1) \int_0^s Q_n(r) \,\mathrm{d}r \int_0^t Q_n(r) \,\mathrm{d}r$$

converges uniformly on  $[0,1] \times [0,1]$  to the zero function. It follows that the laws of  $(L_t^N)_{t \in [0,1]}$  converge weakly on  $\Omega^{0,0} = \{w \in C([0,1],\mathbb{R}) : w_0 = w_1 = 0\}$  as  $N \to \infty$  to the unit mass  $\delta_0$  at the zero path, which establishes that Brownian motion  $(B_t)_{t \in [0,1]}$  admits the polynomial decomposition, for  $t \in [0,1]$ ,

$$B_t = \sum_{n=0}^{\infty} (2n+1) \int_0^t Q_n(r) \,\mathrm{d}r \int_0^1 Q_n(r) \,\mathrm{d}B_r \;.$$

The decomposition was obtained independently by Foster, Lyons and Oberhauser in [2] who use this representation to generate approximate sample paths of Brownian motion which respect integration of polynomials up to a fixed degree. The resulting approximation of Brownian motion was implemented by Trefethen as a Chebfun Example into MATLAB, see [5].

In [1], it is further proven that the fluctuation processes  $(F_t^N)_{t \in [0,1]}$  defined by  $F_t^N = \sqrt{N}L_t^N$  converge in finite dimensional distributions as  $N \to \infty$  to the collection  $(F_t)_{t \in [0,1]}$  of independent zero-mean Gaussian random variables whose variances are given by, for  $t \in [0, 1]$ ,

$$\mathbb{E}\left[\left(F_t\right)^2\right] = \frac{1}{\pi}\sqrt{t(1-t)} \ .$$

This is linked in [4] to the asymptotic convergence rate of the approximation for the Lévy area of Brownian motion based on the polynomial expansion of the associated Brownian bridge. The fluctuation result follows from the pointwise convergence that, for  $s, t \in [0, 1]$ ,

$$\lim_{N \to \infty} NC_N(s,t) = \begin{cases} \frac{1}{\pi} \sqrt{t(1-t)} & \text{if } s = t \\ 0 & \text{if } s \neq t \end{cases}$$

The pointwise convergence above characterises the asymptotic error in the eigenfunction expansion for the Green's function of a particular Sturm-Liouville problem, which is analysed more generally in [3]. For a complete orthonormal set  $\{\phi_n : n \in \mathbb{N}_0\}$  of eigenfunctions for the Sturm-Liouville problem

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}\phi(x)}{\mathrm{d}x}\right) - q(x)\phi(x) = -\lambda w(x)\phi(x)$$

with the corresponding eigenvalues  $\{\lambda_n : n \in \mathbb{N}_0\}$  forming a strictly increasing sequence, it is shown that, for regular Sturm–Liouville problems and for the singular Sturm–Liouville problems associated with the Hermite polynomials, the associated Laguerre polynomials and the Jacobi polynomials,

$$\lim_{N \to \infty} N^{\gamma} \sum_{n=N+1}^{\infty} \frac{(\phi_n(x))^2}{\lambda_n} = \frac{C}{\sqrt{p(x)w(x)}}$$

where the constant C of proportionality is explicitly known, and  $\gamma = \frac{1}{2}$  for the Hermite polynomials and the associated Laguerre polynomials, whereas  $\gamma = 1$  for regular Sturm-Liouville problems and the Jacobi polynomials.

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Statistical theory for Fréchet mean on non-Euclidean spaces has been intensively studied and developed in the recent years with the emerge non-Euclidean data in various applications. Initial steps can be traced back to the strong law of large numbers (LLN) for Fréchet mean on metric spaces by Ziezold, [5]. The next mile stone is the central limit theorem (CLT) for Fréchet mean on Riemannian manifolds in [3] by Bhattacharya and Patrangenaru. Since then, subsequent developments of the CLT for Fréchet mean on Riemannian manifolds and metric spaces with local manifold structure near the mean has been made, see, for example [1, 2, 4]. A common assumption in deriving CLT for Fréchet mean on manifolds is that the population measure is sufficiently concentrated in a ball at the mean. The concentration of the population distribution is to ensure the strict convexity of the Fréchet function around the mean. A more general form of the CLT for Fréchet mean is given in [4] where the authors pointed out that the CLT can be smeary, that is, the empirical Fréchet mean limiting rates that are slower than the classical  $n^{-1/2}$ , where n denotes sample size, when the Hessian of the Fréchet mean vanishes.

While smeary distributions seems rather exceptional, results in [6, 8] it was discovered that these exceptional distributions affect the asymptotics of a large class of distributions, for instance all Fisher-von-Mises distributions on the circle: the rates are smaller than  $n^{-1/2}$  until rather high sample sizes and eventually an asymptotic variance can be reached that is higher than that of tangent space data. The phenomenon is called finite sample smeariness (FSS). In theoretical side, smeary distributions show connections with positiveness of the sectional curvature of the space, c.f. [9, 7]. However, existence of smeary measures are only shown on symmetric spaces which contain a sphere, c.f. [8]. Thus, two natural questions arise: can smeariness occurs on any manifold with positive sectional curvature and is smeariness, and to some extend FSS, as exceptional as it seems.

We address these two questions in this talk. We confirm that any Riemannian manifold that contain a section with positive curvature features directional smeariness. Furthermore, we show that in those Riemannian manifolds with maximal injectivity radius, by adding infinitesimal perturbations near the cut locus of the mean, one can construct a directional smeary measures converging to a given non-smeary one. On manifolds with positive sectional curvature and maximal injectivity radius, there exists a sequence of full smeary measures converging to a given non-smeary one. In particular, these results show that a small perturbation near the cut locus of the mean can change the CLT and thus the out come of a sampling process of Fréchet mean drastically.

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#### Stochastic flows and shape bridges

## STEFAN SOMMER

(joint work with Moritz Schauer, and Frank van der Meulen)

For applications in shape analysis, we are interested in stochastic flows of shapes and stochastic shape flows conditioned on fixed values in time and space, i.e. shape bridges. With shapes being subsets (sometimes submanifolds) of a domain  $D \in \mathbb{R}^d$ , we take the large deformation approach (LDDMM, see e.g. [11]) and consider stochastic flows of diffeomorphisms [8] acting on shapes to give stochastic shape flows [1]. Shape bridges have previously been studied in the finite dimensional setting [9, 2]. In this extended abstract, we outline steps to extend this to infinite dimensional shape bridges. We start with the simplest case of a Brownian flow without drift and with fixed covariance in the Eulerian frame of reference.

#### 1. FINITE DIMENSIONAL EULERIAN STOCHASTICS

Let  $(\Omega, \mathcal{F}, \mathbb{P})$  denote a probability space, let  $D \subseteq \mathbb{R}^d$  be a shape domain, and let  $x = (x_1, \ldots, x_n)$  be a set of n landmarks in D. With landmarks indexed by i and components in  $\mathbb{R}^d$  indexed by  $\alpha$ , the stochastic model from [1] without momentum (only x-variable dynamics) is

(1) 
$$dx_{i,t} = \sigma_j(x_{i,t}) \circ dW_t^j$$

Here W denotes an  $\mathbb{R}^J$ -valued Wiener process, and  $\sigma_1, \ldots, \sigma_J$  denote J vector fields on D, i.e.  $\sigma_j : D \to \mathbb{R}^d$ . We let  $\mathfrak{X}(D)$  denote the space of vector fields on D. The Stratonovich SDE has the corresponding Itô formulation

(2) 
$$dx_{i,t} = \frac{1}{2} \frac{\partial \sigma_k(x_{i,t})}{\partial x_{i,t}^{\alpha}} \sigma_k^{\alpha}(x_{i,t}) dt + \sigma_j(x_{i,t}) dW^j$$

where indices  $j, k, \alpha$  are implicitly summed over by the Einstein summation convention.

# 1.1. Lift of standard Eulerian model. We now lift this to the stochastic flow

(3) 
$$dX_t = \sigma_j(X_t) \circ dW_t^j$$

of diffeomorphisms  $X_t \in \text{Diff}(D)$  where  $\sigma_j(X_t)(x) = \sigma_j(X_t(x))$ . Solutions  $X = \{X_t\}_{t \in [0,T]}$  are examples of Brownian flows [8].

For  $X_t \in \text{Diff}(D)$ , let  $\sigma(X_t)$  be the linear map  $\mathbb{R}^J \to \mathfrak{X}(D)$ ,  $w \mapsto \sigma_j(X_t)w^j$ that to a vector w connects a vector field on D by multiplying on the noise fields  $\sigma_1, \ldots, \sigma_J$ . For time subdivisions  $0 = t_0 < t_1 < \cdots < t_k = T$ , we have

(4) 
$$\int_0^t \sigma(X_s) dW_s = \lim_{k \to \infty} \sum_{m=0}^{k-1} \sigma(X_{t_m \wedge t}) (\Delta W_{m,t}) , \ \Delta W_{m,t} = W_{t_{m+1} \wedge t} - W_{t_m \wedge t} .$$

The conditional covariance of  $X_{t_{m+1}}$  given  $X_{t_m}$ , evaluated at points  $x_1, x_2 \in D$  with finite k, a time subdivision  $0 = t_0 < t_1 < \cdots < t_k = T$ , using the sum on the lhs of (4) to define  $X_t$ , and with m < k,

(5)  

$$\begin{aligned}
\cos\left(\sigma(X_{t_m})(\Delta W_{m,t_{m+1}})(x_1),\sigma(X_{t_m})(\Delta W_{m,t_{m+1}})(x_2) \mid X_{t_m}\right) \\
&= \sigma_{j_1}(X_{t_m}(x_1))\sigma_{j_2}(X_{t_m}(x_2))^T \mathbb{E}[\Delta W^{j_1}_{m,t_{m+1}}(\Delta W^{j_2T}_{m,t_{m+1}})^T] \\
&= \sum_{j=0}^J \sigma_j(X_{t_m}(x_1))\sigma_j(X_{t_m}(x_2))^T(t_{m+1}-t_m) .
\end{aligned}$$

1.2. Infinite dimensional noise. We now follow [4, 4.1.3] and [6]. To avoid the direct specification of the noise fields  $\sigma_j$  in (3), we let W be a cylindrical Wiener process on the Hilbert space  $H = L^2(D, \mathbb{R}^d)$ , and let Q denote a Hilbert-Schmidt operator on H. We then look at solutions to the SDE

(6) 
$$dX_t = Q^{1/2}(X_t) \circ dW_t$$

with  $Q^{1/2}$  being a square root of Q and  $Q^{1/2}(X_t)(w) = Q^{1/2}(w \circ X_t)$ . This is again a Brownian flow, and  $X_t$  takes values in Diff(D) or some subspace thereof depending on the regularity of Q, particularly the local characteristic  $k^Q$  defined below.

Since  $Q^{1/2}$  is Hilbert-Schmidt on  $H = L^2(D, \mathbb{R}^d)$ , it is an integral operator of the form

(7) 
$$Q^{1/2}v(x) = \int_D k^{Q^{1/2}}(x,y)v(y)dy$$

for some kernel  $k^{Q^{1/2}}: D \times D \to \mathbb{R}^{d \times d}$  and

(8) 
$$Qv(x) = \int_D k^Q(x, y)v(y)dy$$

with

(9) 
$$k^{Q}(x,y) = \int_{D} k^{Q^{1/2}}(x,z) k^{Q^{1/2}}(z,y)^{T} dz.$$

One can show that

(10) 
$$k^{Q}(x,y) = \frac{1}{t} \mathbb{E}[Q^{1/2}W_{t}(x)Q^{1/2}W_{t}(y)^{T}]$$

generalizing (5). The integrals in (7) and (8) substitute the sums over the J fields  $\sigma_j$ .

#### 2. Bridges of flows

Consider again the Brownian flow (6) with  $Q^{1/2}$  given by (7). We now wish to define a conditioned process, also known as a bridge process.

The flow X is a random variable with values in C([0,T], H). Let  $\mathcal{A}$  be the Borel  $\sigma$ -algebra on C([0,T], H) and let  $\mathcal{L}_X$  denote the law of X. Let  $v \in H$ . Existence of the law, as a measure on C([0,T], H), of X conditioned on  $X_T = v$  follows from disintegration or the existence of regular conditional probability measures, see e.g. [3, 10] and references therein. In the present case, the spaces C([0,T], H) and H are Polish. We let  $\eta_: C([0,T], H) \to H$  be the mapping  $X \mapsto X_T$ , i.e. the evaluation of the process X at t = T. Then there exists a disintegration  $q : \mathcal{A} \times H \to [0,1]$ ,  $q_y := q(\cdot, y)$  such that q is a transition probability and, particularly, with the marginal law  $\mu_T = (\eta_T)_* \mathcal{L}_X$ 

(11) 
$$\mathcal{L}_X(A) = \int_H q(A, y) d\mu_T(y) \; .$$

This establishes, for each v in the image of  $\eta$ , the existence of the measure of the bridge process, i.e.  $\mathcal{L}_{X|X_T=v}$ .

2.1. Bridge SDE. Finding candidates for the bridge SDE can be approached with the classical Doob's h-transform, here applied to Hilbert space valued processes [5]. A natural assumption is  $P(X_T \in \cdot | X_t = y) \ll \mu_T, t < T - \epsilon, \epsilon > 0$ , [7]. For  $v \in H$  one then defines the *h*-function

(12) 
$$h_t(Y) = \log Z_t^{(v)}(Y)$$

where

$$Z_T^{(v)}(Y) = \left. \frac{P(X_T \in dv \mid X_t = Y)}{d\mu_T} \right|_{\mathcal{A}}$$

is the Radon-Nikodym derivative with respect to the marginal distribution  $\mu_T$  in  $v \in H$ . If the derivative  $\nabla_Y \log h_t(Y)$  exists, it is expected that X conditioned on  $X_T = v$  satisfies an SDE (13)

$$dX_t = Q^{1/2}(X_t)(Q^{1/2}(X_t))^* \nabla_Y \log h_t(Y)|_{Y=X_t} + Q^{1/2}(X_t) \circ dW_t, \quad t \in [0, T-\epsilon] .$$

2.2. Shape bridges. In the LDDMM setting, shapes are objects s on which diffeomorphisms  $X \in \text{Diff}(D)$  act. For example, a curve  $s : \mathbb{S}^1 \to D$  is acted upon by composition  $X_t \cdot s = X_t \circ s$ . We now wish to condition the process X on  $X_T \cdot s = v$  for some target shape v. Denoting the action  $\pi$ , i.e.  $\pi(X_t) = X_t \cdot s$ , this corresponds to conditioning on the fiber  $\pi^{-1}(v)$ . Disintegration provides existence of the conditional law directly. Future work will investigate under which conditions Doob's h-transform can be used to derive equivalents of (13) for shape bridges.

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