

Generalized Fiducial Inference on Riemannian Manifolds



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How do you define a fiducial distribution on a manifold M?

Express your data y in terms of a known random quantity u and unknown parameter vector θ through a Data Generating Algorithm: $y = A(u, \theta)$.

Generalized Fiducial Distribution (GFD) [1]

$$r_{\mathbf{y}}(\theta) = \frac{f(\mathbf{y}|\theta)J(\mathbf{y},\theta)}{\int f(\mathbf{y}|\theta')J(\mathbf{y},\theta')d\theta'}$$

$$J(\mathbf{y}, \theta) = D\left(\nabla_{\theta} A\left(u, \theta\right)|_{u=A^{-1}(\mathbf{y}, \theta)}\right)$$

$$f(\mathbf{y}|\theta)$$
 the data likelihood $J(\mathbf{y},\theta)$ change of variables Jacobian

$$D(M) = (\det M'M)^{\frac{1}{2}}$$
 det based on the l2 norm

(a)

Constrained Generalized Fiducial Distribution

$$r_{\mathbf{y},\mathcal{M}}(\theta|\mathbf{y}) = \frac{f(y|\theta)D^{\star}\left(\nabla_{\theta}A(u,\theta)|_{u=A^{-1}(\mathbf{y},\theta)}P_{\theta}\right)}{\int_{\mathcal{M}}f(y|\theta^{*})D^{\star}\left(\nabla_{\theta^{*}}A(u,\theta^{*})|_{u=A^{-1}(\mathbf{y},\theta^{*})}P_{\theta^{*}}\right)d\lambda(\theta^{*})}, \quad \theta \in \mathcal{M},$$

$$P_{\theta} := I_d - (\nabla_{\theta} g)' (\nabla_{\theta} g (\nabla_{\theta} g)')^{-1} \nabla_{\theta} g,$$

$$D^{\star}(M) = (\operatorname{pdet} M'M)^{\frac{1}{2}}$$

pseudodeterminant analogue

Two Approaches

Our approach against the direct solution with a parameterization.

Assume there exists a differentiable function **g** such that $\theta \in M \leftrightarrow g(\theta) = 0$. When our parameter space is M, the gradient must be updated!

Two MCMC Algorithms

How we sample our Constrained GFD on a constrained space

Constrained GFD

Sample from $r_{\mathbf{y},\mathcal{M}}(\theta|\mathbf{y})$, calculating the projection P_{θ} at each point on the manifold.

This **only** uses the information from **g**, and does not require a parameterization of the manifold!

For this simple example, we can compare to a direct solution (below).

Constrained Hamiltonian MCMC

Simulates a Hamiltonian's movement through the system, using the RATTLE [2] algorithm to satisfy the constraints

$$0=g(heta)$$
 and $0=(
abla g(heta))rac{\partial H}{\partial p}$

For the Hamiltonian [3],

$$H(\theta,p) = \left(\frac{1}{2}p'M(\theta)^{-1}p\right) + \left(\frac{1}{2}\log|M(\theta)| - \log\pi(\theta)\right) + \lambda'g(\theta)$$
 $M(\theta)$, user-defined mass matrix, $\pi(\theta) := r_{\mathbf{y},\mathbf{\mathcal{M}}}(\theta|\mathbf{y})$

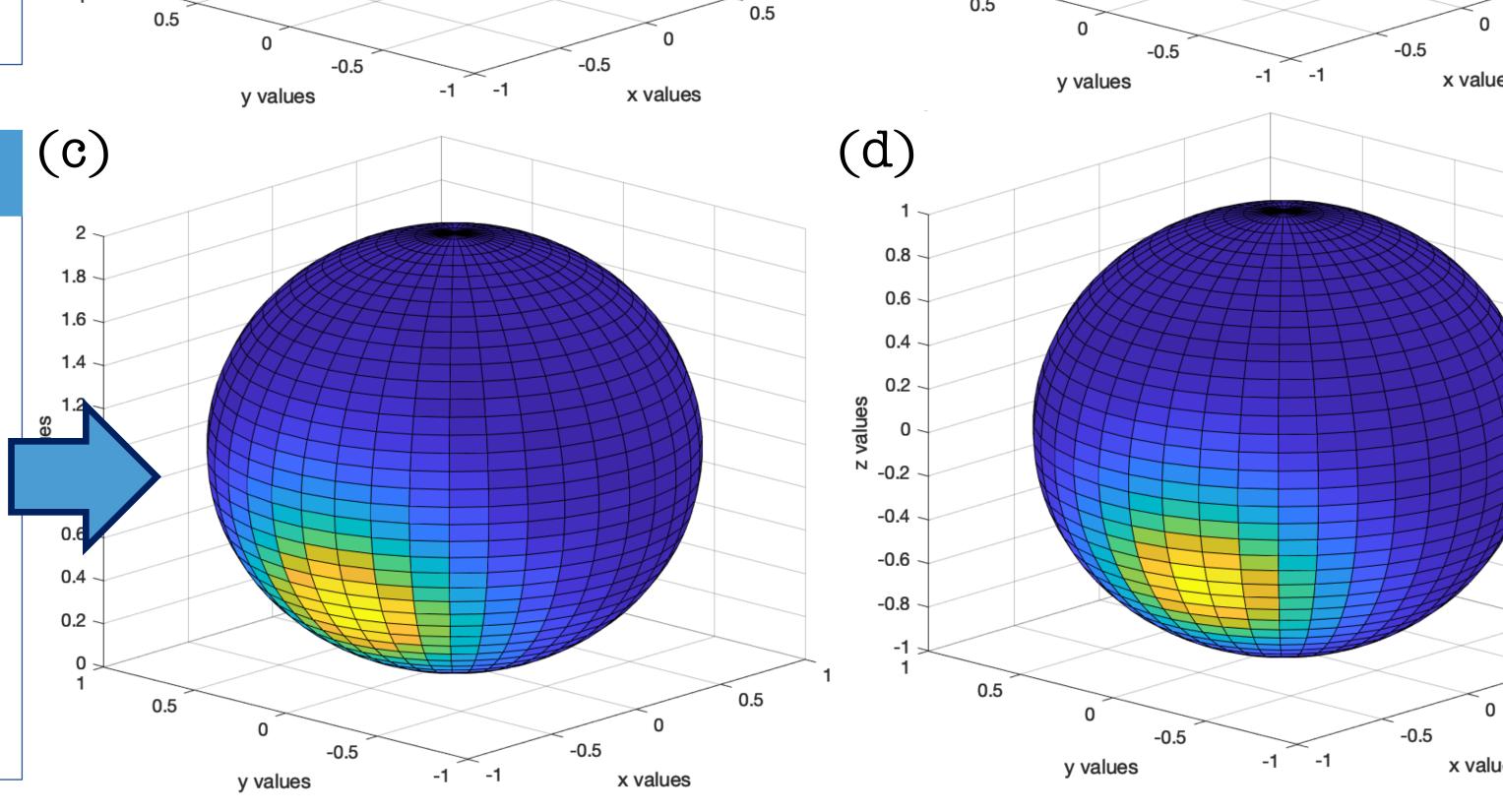
GFD with Parameterization

Sample from the usual GFD on the parameterized space. By the chain rule,

$$r_{\mathbf{y}} \propto f(\Psi(\varphi,\zeta)|\mathbf{y})D(\nabla_{\theta}A(\mathbf{y},\theta)\nabla_{\varphi,\zeta}\Psi(\varphi,\zeta))$$
 where

$$\Psi(\varphi,\zeta) = \left(\cos\varphi\sin\zeta \quad \sin\varphi\sin\zeta \quad \cos\zeta\right)'$$
 for $0 \le \varphi \le 2\pi, \ 0 \le \zeta \le \pi$

This is *not* new theory.



Constrained Metropolis-Hastings

New samples are drawn using a lowerdimensional Gaussian on the tangent plane, then projected downwards onto the manifold.

The lower-dimensional Gaussian density is used for the sampling distribution in a Metropolis ratio

Tangent vectors are calculated from a SVD of $P_{ heta}$

Two Theorems

The two approaches above are equivalent

Two Further Examples

Linear logsplines and the AR(1) Model

Equivalent Distributions

The Constrained GFD and the GFD with Parameterization lead to the same distribution locally, and is invariant to the choice of g.

We can piece this local result to the whole space using a partition of unity.

Local Asymptotic Normality

In terms of the local parameter the Constrained GFD will approach a Gaussian density on the manifold, whenever it does so in the ambient space.

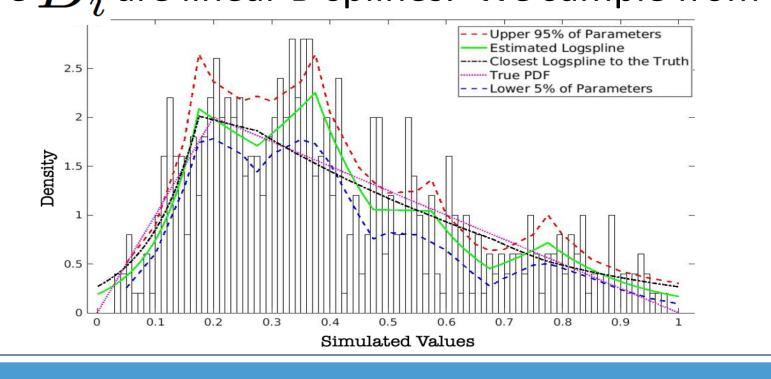
$$\int_{\mathcal{M}} \left| r_{\mathcal{M}}(\theta|\mathbf{y}) - \frac{\phi_{\hat{\theta}_{n},nI(\theta_{0})}(\theta) \left(\det \left| \nabla_{t}^{2} ||g \circ \eta||^{2} \right| \right)^{-1/2}}{\int_{\mathcal{M}} \phi_{0,nI(\theta_{0})}(s) \left(\det \left| \nabla_{t}^{2} ||g \circ \eta||^{2} \right| \right)^{-1/2} d\lambda(\theta)} \right| d\lambda(\theta) \stackrel{P_{\theta_{0}}}{\to} 0$$

Local asymptotic normality is "inherited" when a GFD is constrained to a manifold!

Density Estimation

Consider the linear logsplines model $f(y|\boldsymbol{\theta}) = \exp \left\{ \theta_1 B_1(y) + \dots + \theta_d B_d(y) \right\}$ Subject to the constraint that it is a probability density: $g(\boldsymbol{\theta}) = \log \left(\int \exp \left\{ \theta_1 B_1(y) + \dots + \theta_d B_d(y) \right\} dy \right) = 0,$

where B_i are linear B-splines. We sample from θ :



AR(1) Model

The MVN representation of an AR(1) model has cov matrix:

$$\Sigma = \frac{\sigma^2}{1 - \rho^2} \begin{pmatrix} 1 & \rho & \rho^2 & \dots & \rho^{n-1} \\ \rho & 1 & \rho & \dots & \rho^{n-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho^{n-1} & \rho^{n-2} & \rho^{n-3} & 1 \end{pmatrix}$$

which is a general cov matrix subject to the constraints $g(\Sigma) = (\mathfrak{S}_{1,1}^1 \dots \mathfrak{S}_{n-1,n-1}^1 \mathfrak{S}_1^2 \dots \mathfrak{S}_{n-2}^2)' = \mathbf{0},$

$$\mathfrak{S}_{i,j}^1 = \Sigma_{i,j} - \Sigma_{i+1,j+1}$$

$$\mathfrak{S}_k^2 = \frac{\Sigma_{1,i+1}}{\Sigma_{1,i}} - \frac{\Sigma_{1,i+2}}{\Sigma_{1,i+1}}$$

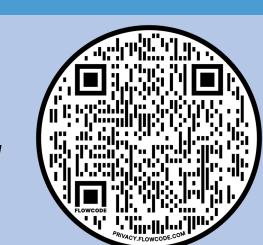
$$1 \leqslant i \leqslant j \leqslant n-1$$

 $1 \leqslant k \leqslant n - 2$. Acknowledgements

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Paper [projected to be on arXiv by BFF 2022]

References

[1] Hannig, J., Iyer, H., Lai, R. C. S. and Lee, T. C. M. (2016) Generalized fiducial inference: A review and new results. Journal of the American Statistical Association, 111, 1346–1361. [2] H. C. Andersen. Rattle: A "velocity" version of the shake algorithm for molecular dynamics calculations. Journal of Computational Physics, 52 (1):24 – 34, 1983. ISSN 0021-9991. [3] Brubaker, M. A., Salzmann, M. and Urtasun, R. (2012) A Family of MCMC Methods on Implicitly Defined Manifolds. In Proc. of the 15th Intern. Conf. on AI and Statistics, vol. 22, 161–172. [4] Zappa, E., Holmes-Cerfon, M. and Goodman, J. (2018) Monte carlo on manifolds: Sampling densities and integrating functions. Communications on Pure and Applied Mathematics, 71, 2609–2647.

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