Geodesic slice sampling on Riemannian manifolds

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MATHEMATICS
OF EXPERIMENT

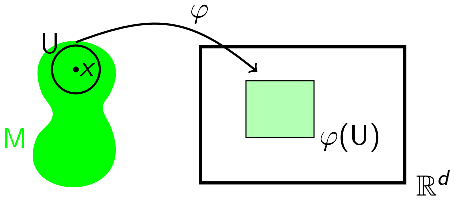
Manifolds

Definition

A d-dimensional *manifold* M is a second countable Hausdorff space such that for all $x \in \mathrm{M}$ there exists a homeomorphism

$$\varphi : \mathrm{M} \supseteq \mathrm{U} \to \mathrm{U}' \subseteq \mathbb{R}^d \qquad \text{and} \qquad x \in \mathrm{U} \text{ open.}$$

The pair (U, φ) is called a *coordinate neighbourhood* of M.



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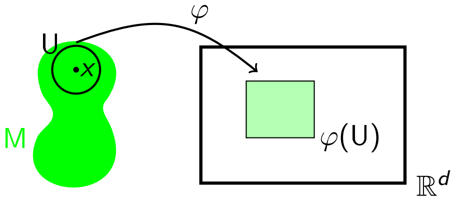

Examples: (open subsets of) $\mathbb{R}^d$, Euclidean unit sphere $\mathbb{S}^{d-1}$, Stiefel manifold $\mathrm{Stiefel}(d, k)$

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Aim: Generate samples from a distribution on a manifold.

Distributions on manifolds

We can incorporate constraints or dependencies directly into a model via manifold state spaces.

Example (Mantoux et al. 2021)

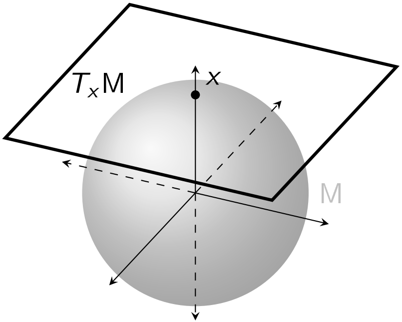
Model adjacency matrix $A \in \mathbb{R}^{d \times d}$ of an undirected graph through its eigendecomposition:

$$A = X \mathrm{diag}(a) X^\top + \text{noise}, \qquad a \in \mathbb{R}^k, X \in \mathrm{Stiefel}(d, k).$$

- Applying e.g. Bayesian inference or MCMC-SAEM requires sampling from distributions on manifolds.

Some differential geometry

- To every point $x \in \mathrm{M}$ of a smooth manifold we can attach the tangent space $T_x\mathrm{M}$, which is an $\mathbb{R}$-vector space.



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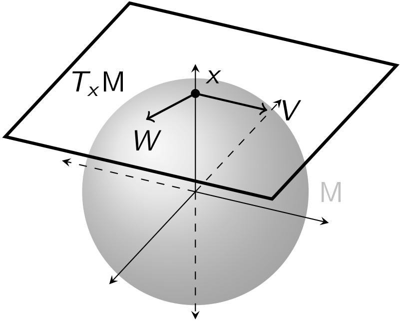
- To every point $x \in \mathrm{M}$ of a smooth manifold we can attach the tangent space $T_x\mathrm{M}$, which is an $\mathbb{R}$-vector space.
- The Riemannian metric $\mathfrak{g}$ of a Riemannian manifold M induces an inner product $\mathfrak{g}_x$ on $T_x\mathrm{M}$ for all $x \in \mathrm{M}$.



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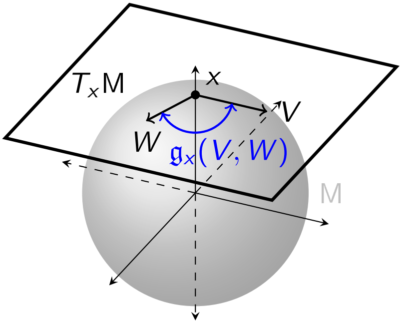

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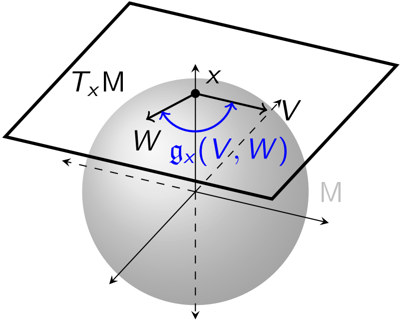
- The Riemannian metric $\mathfrak{g}$ of a Riemannian manifold M induces an inner product $\mathfrak{g}_x$ on $T_x\mathrm{M}$ for all $x \in \mathrm{M}$.
- A Riemannian manifold M can be equipped with a generalisation of the Lebesgue measure, called the Riemannian measure $\nu_{\mathfrak{g}}$.



Problem description

Let M be a Riemannian manifold with Borel-σ-algebra $\mathcal{B}(\mathrm{M})$ and Riemannian measure $\nu_{\mathfrak{g}}$.

Consider a lower semi-continuous function

$$p : \mathrm{M} \to (0, \infty) \qquad \text{with} \qquad Z := \int_{\mathrm{M}} p(x)\nu_{\mathfrak{g}}(\mathrm{d}x) \in (0, \infty).$$

Goal: Sample from

$$\pi(\mathrm{d}x) := \frac{1}{Z} p(x)\, \nu_{\mathfrak{g}}(\mathrm{d}x).$$

Approach: Simulate a Markov chain that has invariant distribution π.

Ideal Slice Sampling

Define the superlevel sets

$$L(t) := \{x \in \mathrm{M} \mid p(x) > t\}, \qquad t \geq 0.$$

The following algorithm is reversible w.r.t. π:

Input: $x \in \mathrm{M}$
1: Draw a level t from $\mathrm{Unif}(0, p(x))$.
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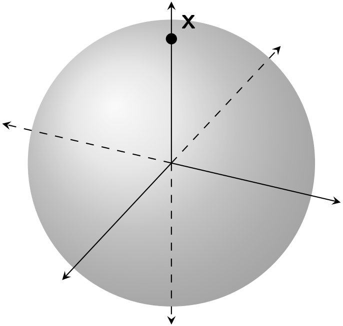

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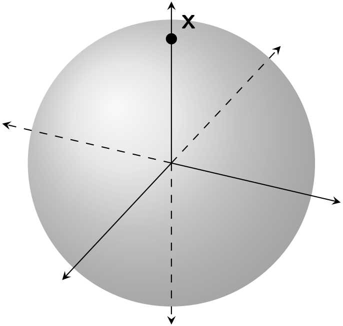

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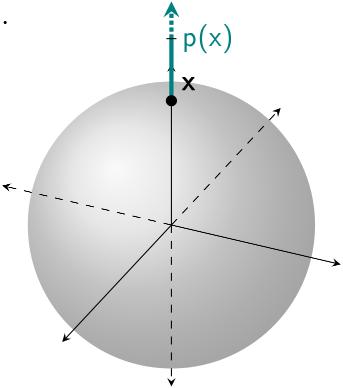

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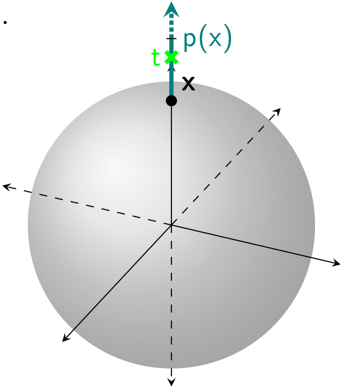

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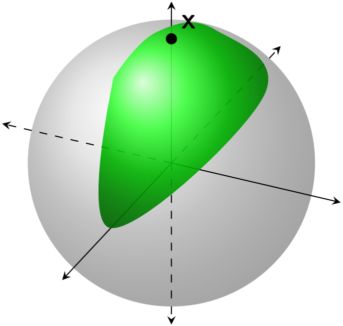

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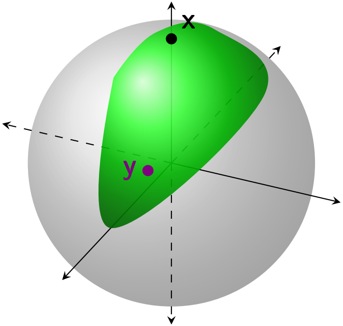

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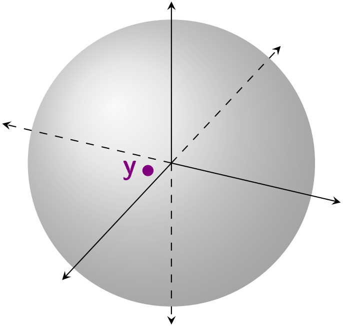

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- "Spectral gap of the slice sampler only depends on level set function $t \mapsto \nu_{\mathfrak{g}}\big(L(t)\big)$."[1]

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Hybrid slice sampling

Problem: How to sample from $\nu_{\mathfrak{g}}\big(L(t)\big)^{-1}\nu_{\mathfrak{g}}|_{L(t)}$?

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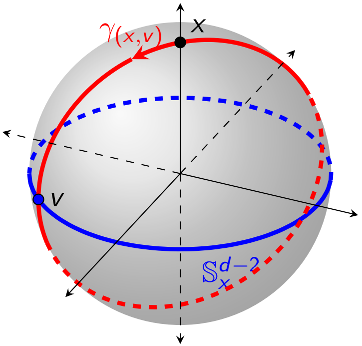
Input: $x \in \mathrm{M}$
1: Draw a level t from $\mathrm{Unif}(0, p(x))$.
2: Draw y from Markov kernel invariant w.r.t. $\nu_{\mathfrak{g}}\big(L(t)\big)^{-1}\nu_{\mathfrak{g}}|_{L(t)}$.
Output: $y \in \mathrm{M}$

Approach: Replace step 2 by Markov kernel with inv. distribution $\nu_{\mathfrak{g}}(L(t))^{-1}\nu_{\mathfrak{g}}|_{L(t)}$.

Special case: The sphere

Define $(d-2)$-dimensional great subsphere with pole $x \in \mathbb{S}^{d-1}$ as

$$\mathbb{S}_x^{d-2} := \{y \in \mathbb{S}^{d-1} \mid y^T x = 0\}.$$



For each $x \in \mathbb{S}^{d-1}$ and $v \in \mathbb{S}_x^{d-2}$ there exists a unique great circle with $\gamma_{(x,v)}(0) = x$ and velocity vector v:

$$\gamma_{(x,v)} : [0, 2\pi) \to \mathbb{S}^{d-1}, \qquad \gamma_{(x,v)}(\theta) = \cos(\theta)x + \sin(\theta)v.$$

- Apply techniques[2] from 1-dim. slice sampling to intersection of level set and great circle.

[2] Neal 2003.

Geodesic slice sampler on the sphere

(Habeck, H., Kodgirwar, and Rudolf 2023)

Input: $x \in \mathbb{S}^{d-1}$

Draw t from $\mathrm{Unif}(0, p(x))$.
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Set $\theta_{\text{min}} = \theta - 2\pi$ and $\theta_{\text{max}} = \theta$.
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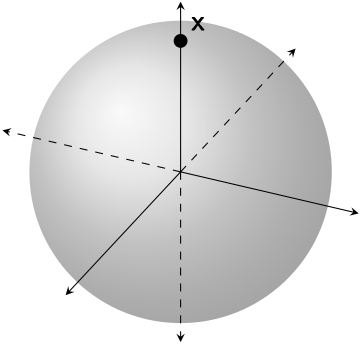

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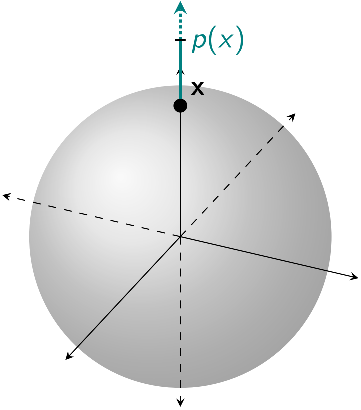

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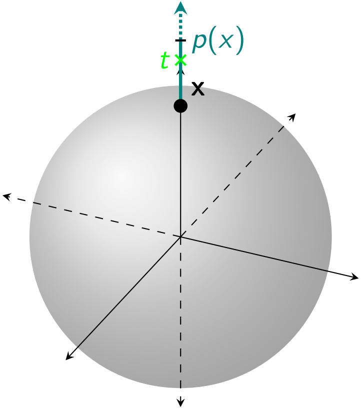

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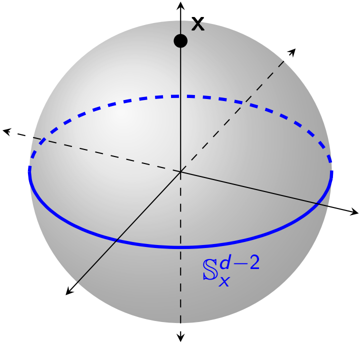

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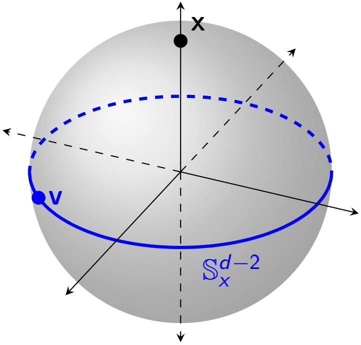

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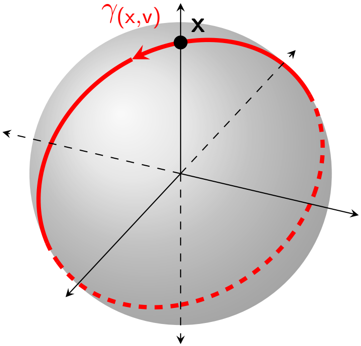

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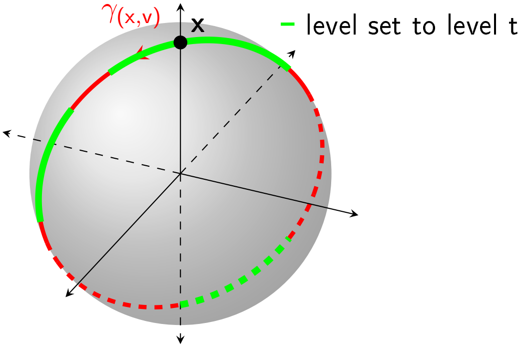

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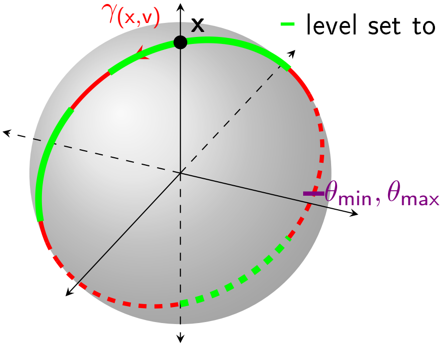

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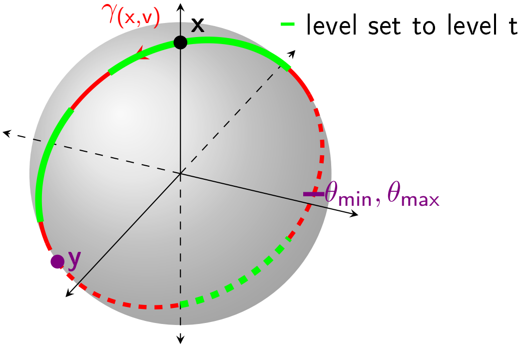

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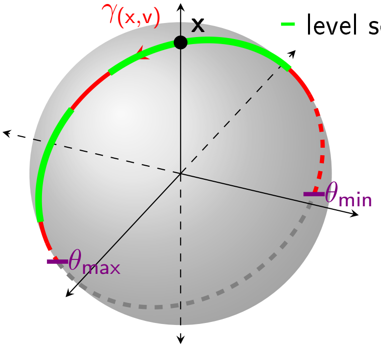

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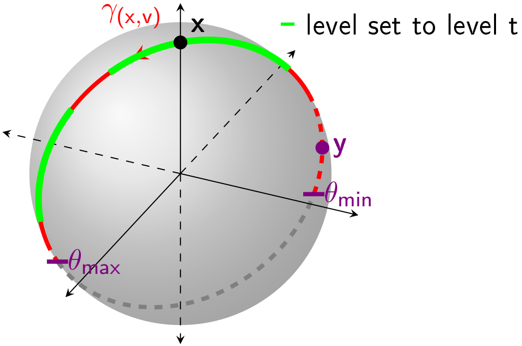
    if $\theta < 0$
        $\theta_{\min} = \theta$
    else
        $\theta_{\max} = \theta$
until $p(y) > t$

Output: $y \in \mathbb{S}^{d-1}$



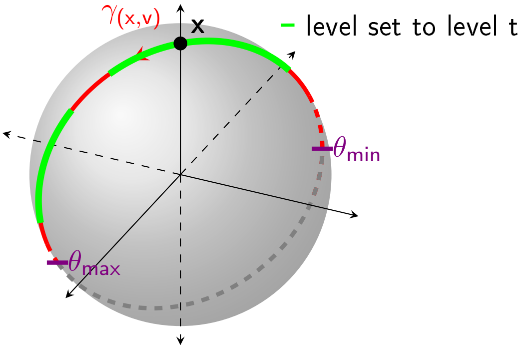
Geodesic slice sampler on the sphere

(Habeck, H., Kodgirwar, and Rudolf 2023)

Input: $x \in \mathbb{S}^{d-1}$

Draw t from $\mathrm{Unif}(0, p(x))$.
Draw v from $\mathrm{Unif}(\mathbb{S}_x^{d-2})$.
Draw θ from $\mathrm{Unif}(0, 2\pi)$.
Set $\theta_{\min} = \theta - 2\pi$ and $\theta_{\max} = \theta$.
repeat:
    Draw θ from $\mathrm{Unif}(\theta_{\min}, \theta_{\max})$.
    Set $y = \cos(\theta)x + \sin(\theta)v$.
    if $\theta < 0$
        $\theta_{\min} = \theta$
    else
        $\theta_{\max} = \theta$
until $p(y) > t$

Output: $y \in \mathbb{S}^{d-1}$



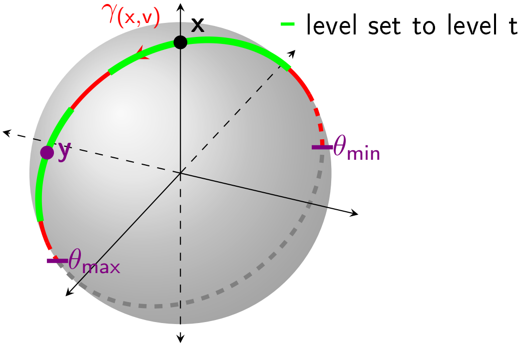
Geodesic slice sampler on the sphere

(Habeck, H., Kodgirwar, and Rudolf 2023)

Input: $x \in \mathbb{S}^{d-1}$

```
Draw t from Unif(0, p(x)).
Draw v from Unif(S_x^{d-2}).
Draw θ from Unif(0, 2π).
Set θ_min = θ − 2π and θ_max = θ.
repeat:
    Draw θ from Unif(θ_min, θ_max).
    Set y = cos(θ)x + sin(θ)v.
    if θ < 0
        θ_min = θ
    else
        θ_max = θ
until p(y) > t
```

Output: $y \in \mathbb{S}^{d-1}$



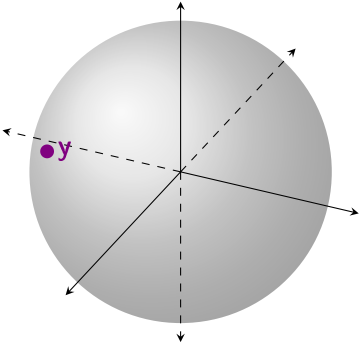
Geodesic slice sampler on the sphere

(Habeck, H., Kodgirwar, and Rudolf 2023)

Input: $x \in \mathbb{S}^{d-1}$

Draw t from $\mathrm{Unif}(0, p(x))$.
Draw v from $\mathrm{Unif}(\mathbb{S}_x^{d-2})$.
Draw θ from $\mathrm{Unif}(0, 2\pi)$.
Set $\theta_{\min} = \theta - 2\pi$ and $\theta_{\max} = \theta$.
repeat:
    Draw θ from $\mathrm{Unif}(\theta_{\min}, \theta_{\max})$.
    Set $y = \cos(\theta)x + \sin(\theta)v$.
    if $\theta < 0$
        $\theta_{\min} = \theta$
    else
        $\theta_{\max} = \theta$
until $p(y) > t$

Output: $y \in \mathbb{S}^{d-1}$



Validity of the geodesic slice sampler on the sphere

Call the resulting kernel H.

Theorem (Habeck, H., Kodgirwar, and Rudolf 2023)

The kernel H is reversible w.r.t. π. Moreover, assume

$$\alpha := \sup_{x \in \mathbb{S}^{d-1}} p(x) < \infty.$$

Then for $\rho = 1 - \frac{\beta}{2\pi}\frac{}{\alpha}\frac{\mathrm{vol}(C)}{\mathrm{vol}(\mathbb{S}^{d-2})} \in (0,1)$ *holds*

$$\sup_{x \in \mathbb{S}^{d-1}} \|H^n(x,\cdot) - \pi\|_{tv} \le \rho^n, \qquad \forall n \in \mathbb{N},$$

for some $C \in \mathcal{B}\left(\mathbb{S}^{d-1}\right)$ *with* $\mathrm{vol}(C) > 0$ *and* $\beta := \inf_{x \in C} p(x) > 0$.

Geodesics

Definition

A curve $\gamma : \mathbb{R} \supseteq \mathrm{I} \to \mathrm{M}$ is called *geodesic* if the covariant derivative of the velocity vector field is zero everywhere.

- The great circles are the geodesics of the sphere.

We call a Riemannian manifold *geodesically complete* if for all $x \in \mathrm{M}$, $v \in T_x\mathrm{M}$ there exists a unique geodesic

$$\gamma_{(x,v)} : \mathbb{R} \to \mathrm{M} \quad \text{such that} \quad \gamma_{(x,v)}(0) = x, \ \frac{\mathrm{d}\gamma_{(x,v)}}{\mathrm{d}t}|_0 = v.$$

Choosing a random geodesic

We can turn the unit tangent spheres of a Riemannian manifold $(\mathrm{M}, \mathfrak{g})$

$$U_x\mathrm{M} := \{v \in T_x\mathrm{M} \mid \mathfrak{g}_x(v, v) = 1\}$$

into Riemannian manifolds isometric to $\mathbb{S}^{d-1}$.

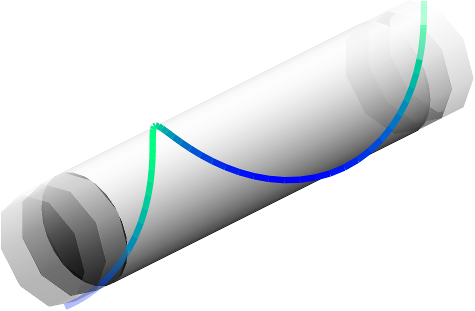
Let $\nu_{\mathfrak{g},x}$ the corresponding Riemannian measure and define the probability measure on $U_x\mathrm{M}$

$$\mu_x := \mathrm{vol}(\mathbb{S}^{d-1})^{-1}\nu_{\mathfrak{g},x}.$$

- We can sample μ_x using any isometry between the inner product spaces $(T_x\mathrm{M}, \mathfrak{g}_x)$ and $(\mathbb{R}^d, \langle\cdot,\cdot\rangle)$.

An additional complication

Problem: The geodesics of a Riemannian manifold are in general not closed.



- Determine "approximation" of the intersection of the level set and the geodesic with techniques[3] from 1-dim. slice sampling.

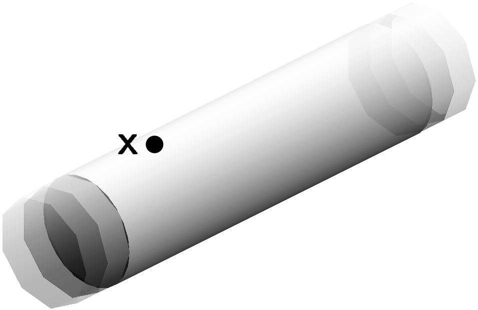
[3] Neal 2003.

Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$

Input: $x \in \mathrm{M}$

1: Draw t from $\mathrm{Unif}(0, p(x))$.
2: Draw v from μ_x.



Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$

Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$
Input: $x \in \mathrm{M}$

1: Draw t from $\mathrm{Unif}(0, p(x))$.
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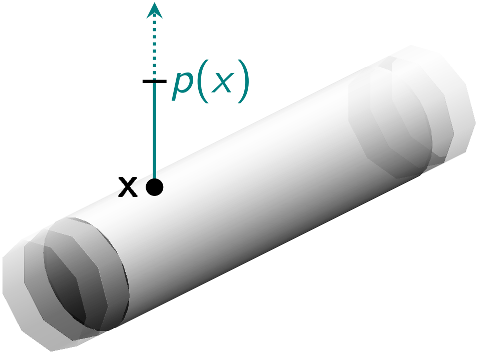


Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$

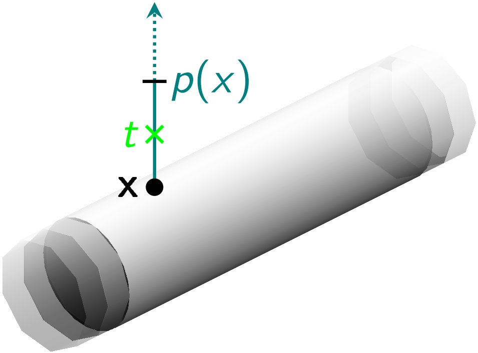
Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$

Input: $x \in \mathrm{M}$

1: Draw t from $\mathrm{Unif}(0, p(x))$.

2: Draw v from μ_x.



Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$

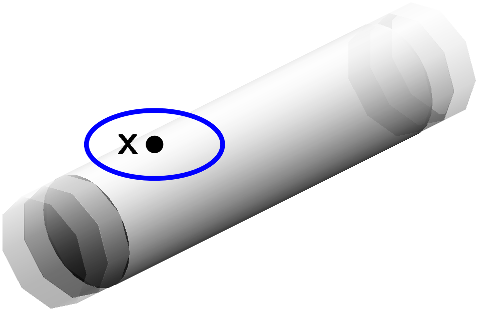
Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$

Input: $x \in \mathrm{M}$

1: Draw t from $\mathrm{Unif}(0, p(x))$.

2: Draw v from μ_x.



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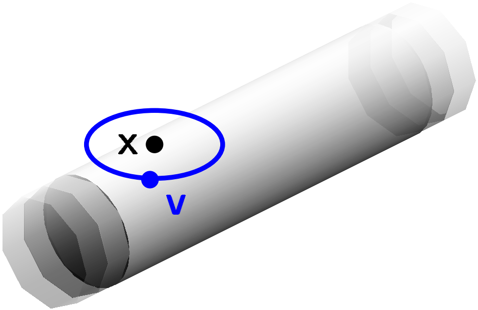
Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$

Input: $x \in \mathrm{M}$

1: Draw t from $\mathrm{Unif}(0, p(x))$.

2: Draw v from μ_x.



Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$

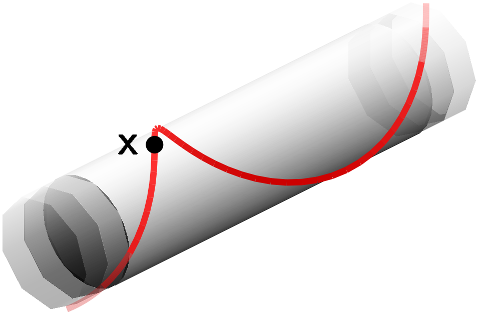
Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$

Input: $x \in \mathrm{M}$

1: Draw t from $\mathrm{Unif}(0, p(x))$.

2: Draw v from μ_x.

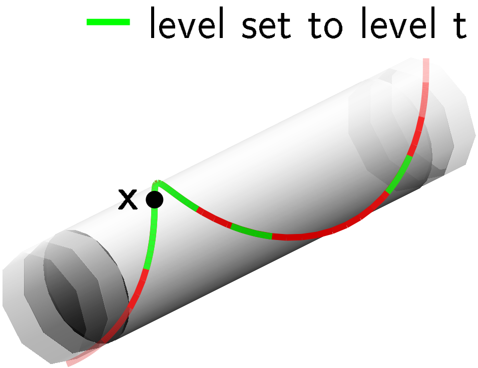


Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$

Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$
Input: $x \in \mathrm{M}$

1: Draw t from $\mathrm{Unif}(0, p(x))$.
2: Draw v from μ_x.



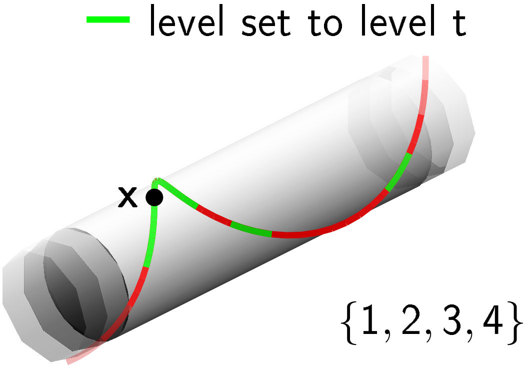
Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$

Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$

Input: $x \in \mathrm{M}$

Draw ι from $\mathrm{Unif}(\{1, \ldots, m\})$.
Draw u from $\mathrm{Unif}\big([0, w]\big)$.
Set $\ell := -u$ and $r := \ell + w$.
Set $i = 2$ and $j = 2$.
while $i \leq \iota$ and $p\left(\gamma_{(x,v)}(\ell)\right) > t$ **do**
    Set $\ell = \ell - w$.
    Update $i = i + 1$.
while $j \leq m + 1 - \iota$ and $p\left(\gamma_{(x,v)}(r)\right) > t$ **do**
    Set $r = r + w$.
    Update $j = j + 1$.



Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$

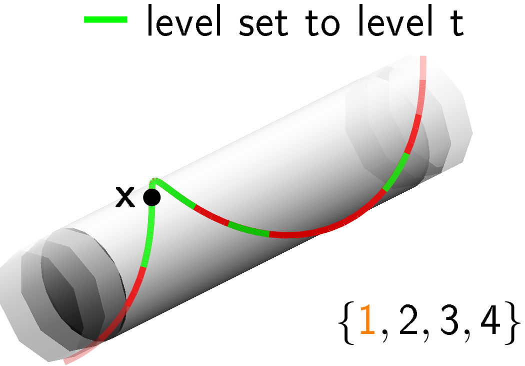
Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$

Input: $x \in \mathrm{M}$

```
Draw ι from Unif({1, …, m}).
Draw u from Unif([0, w]).
Set ℓ := −u and r := ℓ + w.
Set i = 2 and j = 2.
while i ≤ ι and p(γ_(x,v)(ℓ)) > t do
    Set ℓ = ℓ − w.
    Update i = i + 1.
while j ≤ m + 1 − ι and p(γ_(x,v)(r)) > t do
    Set r = r + w.
    Update j = j + 1.
```

Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$

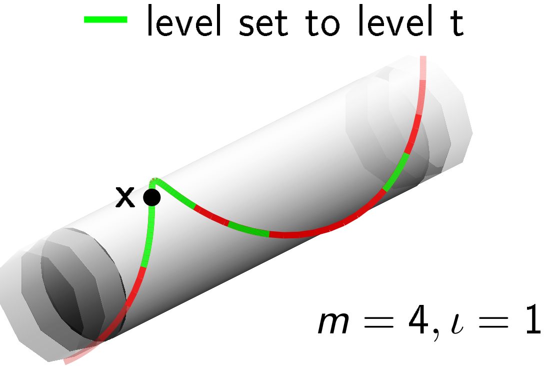


Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$
Input: $x \in \mathrm{M}$

Draw ι from $\mathrm{Unif}(\{1, \ldots, m\})$.
Draw u from $\mathrm{Unif}\big([0, w]\big)$.
Set $\ell := -u$ and $r := \ell + w$.
Set $i = 2$ and $j = 2$.
while $i \leq \iota$ and $p\left(\gamma_{(x,v)}(\ell)\right) > t$ **do**
    Set $\ell = \ell - w$.
    Update $i = i + 1$.
while $j \leq m + 1 - \iota$ and $p\left(\gamma_{(x,v)}(r)\right) > t$ **do**
    Set $r = r + w$.
    Update $j = j + 1$.

Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$



Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$

Input: $x \in \mathrm{M}$

Draw ι from $\mathrm{Unif}(\{1, \ldots, m\})$.
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Set $\ell := -u$ and $r := \ell + w$.
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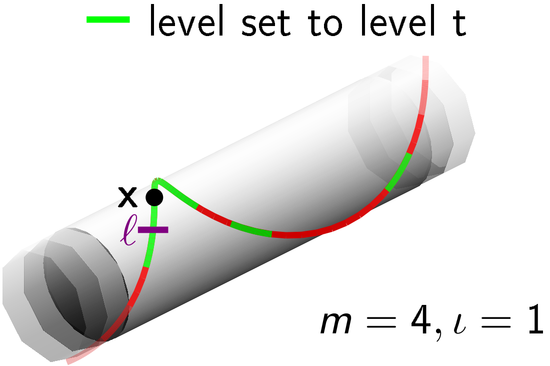
    Set $\ell = \ell - w$.
    Update $i = i + 1$.
while $j \leq m + 1 - \iota$ and $p\left(\gamma_{(x,v)}(r)\right) > t$ **do**
    Set $r = r + w$.
    Update $j = j + 1$.

Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$



Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$

Input: $x \in \mathrm{M}$

Draw ι from $\mathrm{Unif}(\{1, \ldots, m\})$.

Draw u from $\mathrm{Unif}\big([0, w]\big)$.

Set $\ell := -u$ and $r := \ell + w$.

Set $i = 2$ and $j = 2$.

while $i \leq \iota$ and $p\left(\gamma_{(x,v)}(\ell)\right) > t$ **do**

  Set $\ell = \ell - w$.

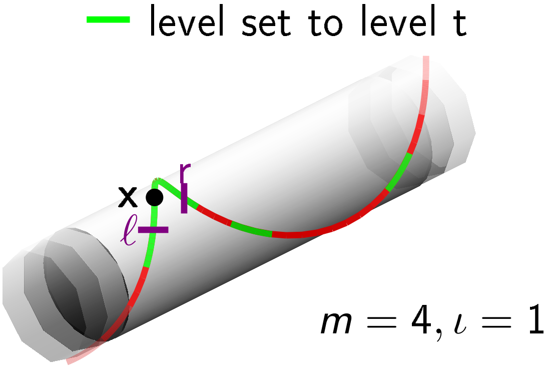
  Update $i = i + 1$.

while $j \leq m + 1 - \iota$ and $p\left(\gamma_{(x,v)}(r)\right) > t$ **do**

  Set $r = r + w$.

  Update $j = j + 1$.

Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$



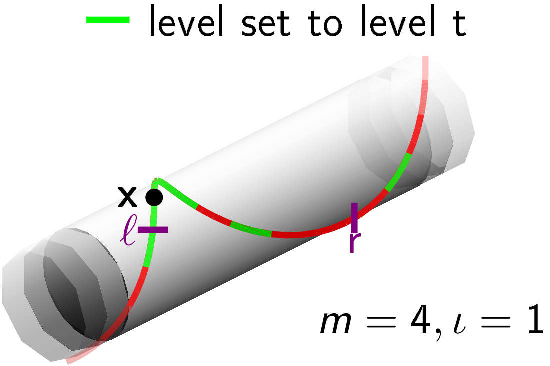
Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$

Input: $x \in \mathrm{M}$

Draw ι from $\mathrm{Unif}(\{1, \dots, m\})$.
Draw u from $\mathrm{Unif}([0, w])$.
Set $\ell := -u$ and $r := \ell + w$.
Set $i = 2$ and $j = 2$.
while $i \leq \iota$ and $p\left(\gamma_{(x,v)}(\ell)\right) > t$ **do**
  Set $\ell = \ell - w$.
  Update $i = i + 1$.
while $j \leq m + 1 - \iota$ and $p\left(\gamma_{(x,v)}(r)\right) > t$ **do**
  Set $r = r + w$.
  Update $j = j + 1$.

Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$

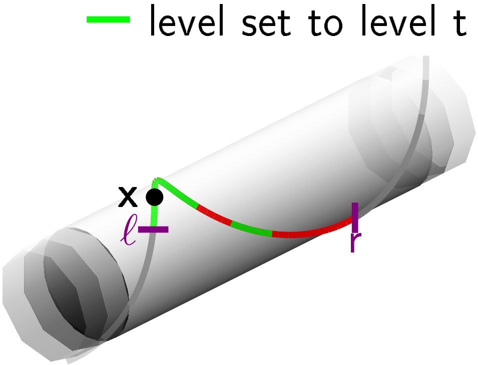


Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$
Input: $x \in \mathrm{M}$

```
Draw $\iota$ from $\mathrm{Unif}(\{1, \dots, m\})$.
Draw $u$ from $\mathrm{Unif}\big([0, w]\big)$.
Set $\ell := -u$ and $r := \ell + w$.
Set $i = 2$ and $j = 2$.
while $i \leq \iota$ and $p\left(\gamma_{(x,v)}(\ell)\right) > t$ do
    Set $\ell = \ell - w$.
    Update $i = i + 1$.
while $j \leq m + 1 - \iota$ and $p\left(\gamma_{(x,v)}(r)\right) > t$ do
    Set $r = r + w$.
    Update $j = j + 1$.
```

Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$



Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$

Input: $x \in \mathrm{M}$

Draw θ_h from $\mathrm{Unif}\big((0, r - l)\big)$.

Set $\theta := \theta_h - \mathbb{1}_{\{\theta_h > r\}}(r - l)$.

Set $\theta_{\min} := \theta_h$ and $\theta_{\max} := \theta_h$.

while $\big(\gamma_{(x,v)}(\theta)\big) \le t$ **do**

  if $\theta_h \in [\theta_{\min}, r - l)$ **then**

    Set $\theta_{\min} = \theta_h$.

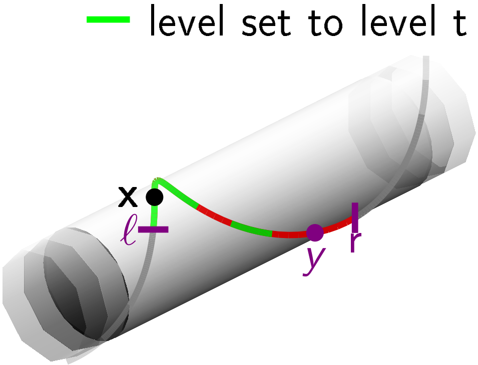
  else

    Set $\theta_{\max} = \theta_h$.

  Draw θ_h from $\mathrm{Unif}\big((0, \theta_{\max}) \cup [\theta_{\min}, r - l)\big)$.

  Set $\theta = \theta_h - \mathbb{1}_{\{\theta_h > r\}}(r - l)$.

Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$

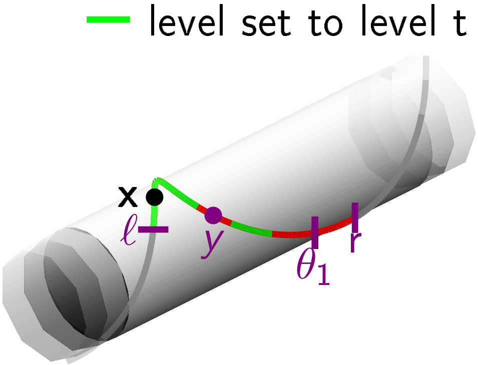


Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$
Input: $x \in \mathrm{M}$

```
Draw θ_h from Unif((0, r − l)).
Set θ := θ_h − 1_{θ_h > r}(r − l).
Set θ_min := θ_h and θ_max := θ_h.
while (γ_(x,v)(θ)) ≤ t do
    if θ_h ∈ [θ_min, r − l) then
        Set θ_min = θ_h.
    else
        Set θ_max = θ_h.
    Draw θ_h from
    Unif((0, θ_max) ∪ [θ_min, r − l)).
    Set θ = θ_h − 1_{θ_h > r}(r − l).
```

Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$



Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

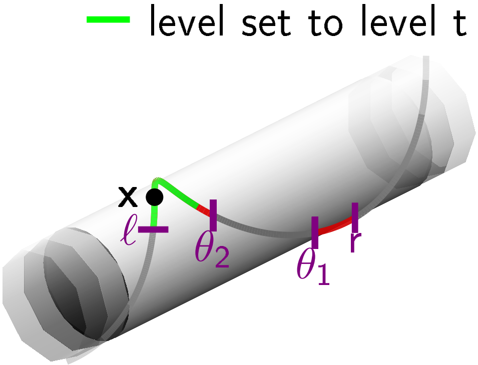
Parameters: $m \in \mathbb{N}$, $w > 0$

Input: $x \in \mathrm{M}$

```
Draw θ_h from Unif((0, r − l)).
Set θ := θ_h − 1_{θ_h > r}(r − l).
Set θ_min := θ_h and θ_max := θ_h.
while (γ_(x,v)(θ)) ≤ t do
    if θ_h ∈ [θ_min, r − l) then
        Set θ_min = θ_h.
    else
        Set θ_max = θ_h.
    Draw θ_h from
    Unif((0, θ_max) ∪ [θ_min, r − l)).
    Set θ = θ_h − 1_{θ_h > r}(r − l).
```

$$\text{Draw } \theta_h \text{ from } \mathrm{Unif}\big((0, r-l)\big).$$
$$\text{Set } \theta := \theta_h - \mathbb{1}_{\{\theta_h > r\}}(r-l).$$
$$\text{Set } \theta_{\min} := \theta_h \text{ and } \theta_{\max} := \theta_h.$$
$$\textbf{while } \big(\gamma_{(x,v)}(\theta)\big) \le t \textbf{ do}$$
$$\quad \textbf{if } \theta_h \in [\theta_{\min}, r-l) \textbf{ then}$$
$$\qquad \text{Set } \theta_{\min} = \theta_h.$$
$$\quad \textbf{else}$$
$$\qquad \text{Set } \theta_{\max} = \theta_h.$$
$$\quad \text{Draw } \theta_h \text{ from } \mathrm{Unif}\big((0, \theta_{\max}) \cup [\theta_{\min}, r-l)\big).$$
$$\quad \text{Set } \theta = \theta_h - \mathbb{1}_{\{\theta_h > r\}}(r-l).$$

Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$



Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$

Input: $x \in \mathrm{M}$

Draw θ_h from $\mathrm{Unif}\big((0, r-l)\big)$.

Set $\theta := \theta_h - \mathbb{1}_{\{\theta_h > r\}}(r - l)$.

Set $\theta_{\min} := \theta_h$ and $\theta_{\max} := \theta_h$.

while $\big(\gamma_{(x,v)}(\theta)\big) \leq t$ **do**

    if $\theta_h \in [\theta_{\min}, r - l)$ **then**

        Set $\theta_{\min} = \theta_h$.

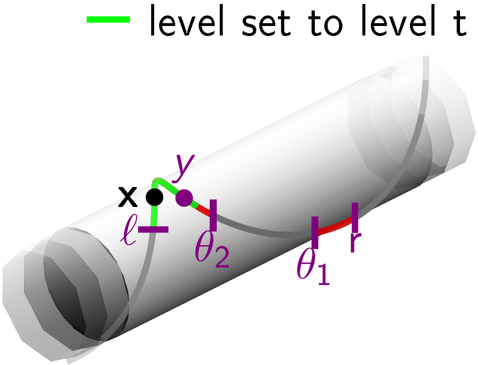
    else

        Set $\theta_{\max} = \theta_h$.

    Draw θ_h from $\mathrm{Unif}\big((0, \theta_{\max}) \cup [\theta_{\min}, r - l)\big)$.

    Set $\theta = \theta_h - \mathbb{1}_{\{\theta_h > r\}}(r - l)$.

Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$

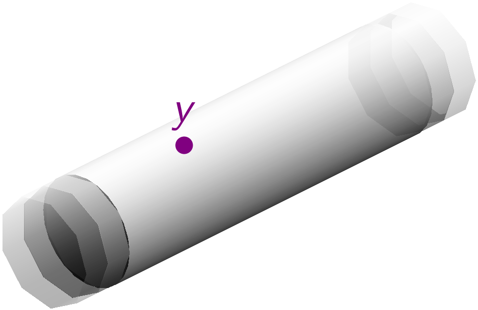


Geodesic slice sampler (Durmus, Gruffaz, H., and Rudolf 2023)

Parameters: $m \in \mathbb{N}$, $w > 0$
Input: $x \in \mathrm{M}$

Draw θ_h from $\mathrm{Unif}\big((0, r-l)\big)$.
Set $\theta := \theta_h - \mathbb{1}_{\{\theta_h > r\}}(r-l)$.
Set $\theta_{\min} := \theta_h$ and $\theta_{\max} := \theta_h$.
while $\big(\gamma_{(x,v)}(\theta)\big) \leq t$ **do**
  if $\theta_h \in [\theta_{\min}, r-l)$ **then**
    Set $\theta_{\min} = \theta_h$.
  else
    Set $\theta_{\max} = \theta_h$.
  Draw θ_h from $\mathrm{Unif}\big((0, \theta_{\max}) \cup [\theta_{\min}, r-l)\big)$.
  Set $\theta = \theta_h - \mathbb{1}_{\{\theta_h > r\}}(r-l)$.

Output: $\gamma_{(x,v)}(\theta) \in \mathrm{M}$



Stepping-out and shrinkage procedure

- Denote by $L(x, v, t) := \{\theta \in \mathbb{R} \mid p(\gamma_{(x,v)}(\theta)) > t\}$ intersection of $L(t)$ and $\gamma_{(x,v)}$.

[4] H., Natarovskii, and Rudolf 2023.

Stepping-out and shrinkage procedure

- Denote by $L(x,v,t) := \{\theta \in \mathbb{R} \mid p(\gamma_{(x,v)}(\theta)) > t\}$ intersection of $L(t)$ and $\gamma_{(x,v)}$.
- Define random variables

$$\Upsilon \sim \mathrm{Unif}(0,w) \qquad L_i := -\Upsilon - w(i-1) \qquad R_j := -\Upsilon + jw, \qquad i,j \in \mathbb{N},$$

stopping times, where $J \sim \mathrm{Unif}(\{1,\dots,m\})$,

$$\tau_{L(x,v,t)} := \min\{i \in \mathbb{N} \mid L_i \notin L(x,v,t)\} \wedge J,$$
$$\mathfrak{T}_{L(x,v,t)} := \min\{j \in \mathbb{N} \mid R_j \notin L(x,v,t)\} \wedge (m+1-J),$$

distribution on $\mathbb{R}^2$ of the stepping-out procedure approximating $L(x,v,t)$

$$\xi_{L(x,v,t)} := \mathrm{Law}\left(L_{\tau_{L(x,v,t)}}, R_{\mathfrak{T}_{L(x,v,t)}}\right).$$

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- Let $Q^{\ell,r}_{L(x,v,t)}$ the distribution[4] of the shrinkage procedure drawing from $L(x,v,t) \cap (\ell, r)$.

[4] H., Natarovskii, and Rudolf 2023.

Validity of the geodesic slice sampler

Kernel of the geodesic slice sampler for $x \in \mathrm{M}$, $A \in \mathcal{B}(\mathrm{M})$:

$$K(x, \mathrm{A}) = \frac{1}{p(x)} \int_0^{p(x)} \int_{U_x \mathrm{M}} \int_{\mathbb{R}^2} \int_{L(x,v,t) \cap (\ell, r)} \mathbb{1}_{\mathrm{A}} \left(\gamma_{(x,v)}(\theta)\right)$$

$$Q^{\ell,r}_{L(x,v,t)}(\mathrm{d}\theta)\, \xi_{L(x,v,t)}(\mathrm{d}(\ell, r))\, \mu_x(\mathrm{d}v)\, \mathrm{d}t$$

Theorem (Durmus, Gruffaz, H., and Rudolf 2023)

The kernel K is reversible with respect to π.

Numerical experiments: von Mises-Fisher distribution

Stiefel manifold:

$$\mathrm{Stiefel}(d,k) := \{\Gamma \in \mathbb{R}^{d\times k} \mid \Gamma^\top \Gamma = \mathrm{Id}_k\}$$

Unnormalised density of the von Mises-Fisher distribution with parameter $F \in \mathbb{R}^{d\times k}$

$$p_{\mathrm{vMF}}(\Gamma) = \exp\left(\mathrm{Tr}(F^\top \Gamma)\right), \qquad \Gamma \in \mathrm{Stiefel}(d,k)$$

Choose

$$d = 30,\ k = 2, \qquad \text{and} \qquad F = \begin{pmatrix} 1 & 0 \\ 0 & \lambda \\ 0 & 0 \\ \vdots & \vdots \end{pmatrix}, \quad \lambda \in \{1, 10, 100\}.$$

Numerical experiments: von Mises-Fisher distribution

Effective sample size of $\ln(p_{\mathrm{vMF}})$ averaged over 10 repetitions:

λ	1	10	100
GSS $w = 5, m = 1$	$[28375, 34262, 37405]$	[**4901, 5283, 5477**]	[**1153, 1328, 1453**]
RMH	[**50772**, 54243, 59906]	$[1492, 2314, 3214]$	$[669, 878, 998]$
GeoRMH	[49007, **57195, 68948**]	$[1978, 2336, 3217]$	$[682, 870, 1075]$

Numerical experiments: Functional connectivity network of the brain

(Mantoux et al. 2021)

Model functional connectivity network of the brain:

$$A_j = X_j \mathrm{diag}(a_j) X_j^\top + \varepsilon_j, \qquad j \in \{1, \dots, N\}$$

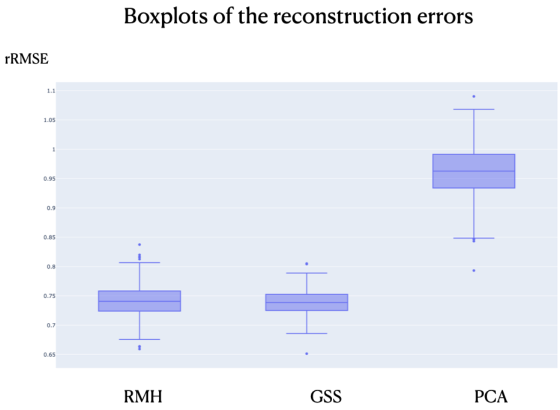
where

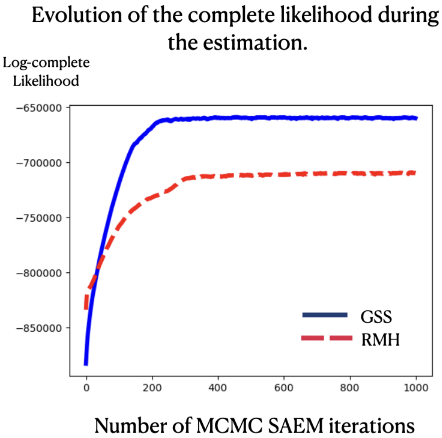
$$X_j \overset{iid}{\sim} \mathrm{vMF}(F), \quad a_j \overset{iid}{\sim} \mathcal{N}(\mu, \sigma_a^2 \mathrm{Id}_k), \quad \varepsilon_j \overset{iid}{\sim} \mathcal{N}(0, \sigma_\varepsilon^2 \mathrm{Id}_{(d+1)/2}).$$

- Use data from 812 subjects from Human Connectome Project[5].
- Estimate the parameters $F, \mu, \sigma_a, \sigma_\varepsilon$ with 1000 MCMC-SAEM.
- Use either 20 geodesic slice sampling or 80 RMH iterations within MCMC-SAEM.

[5] https://www.humanconnectome.org/study/hcp-young-adult/document/extensively-processed-fmri-data-documentation

Numerical experiments: von Mises-Fisher distribution





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Distributions on manifolds

We can incorporate constraints or dependencies directly into a model via manifold state spaces.

Example (Mantoux et al. 2021)

Model adjacency matrix $A \in \mathbb{R}^{d \times d}$ of an undirected graph through its eigendecomposition:

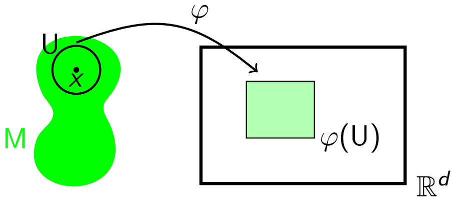
$$A = X \mathrm{diag}(a) X^\top + \text{noise}, \qquad a \in \mathbb{R}^k, X \in \mathrm{Stiefel}(d, k).$$

- Applying e.g. Bayesian inference or MCMC-SAEM requires sampling from distributions on manifolds.

Some differential geometry

Definition

We call coordinate neighbourhoods (U, φ), (V, ψ) *C^∞-compatible* if $\psi \circ \varphi^{-1}$ and $\varphi \circ \psi^{-1}$ are infinitely often differentiable.
A manifold M with a maximal collection of C^∞-compatible coordinate neighbourhoods that cover M is called *smooth*.



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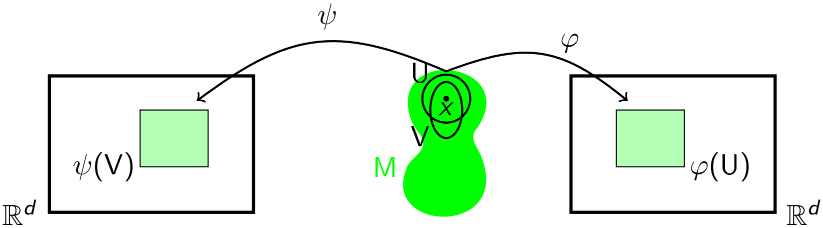

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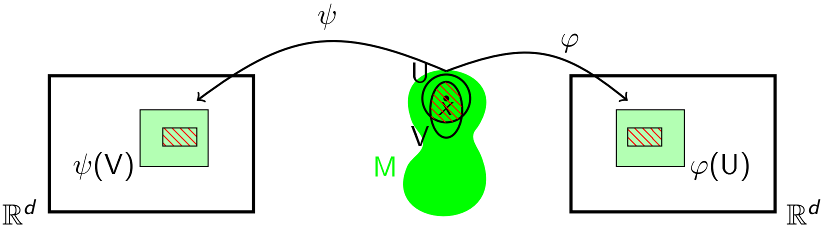

Some differential geometry

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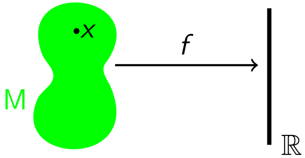
A function $f : \mathrm{A} \to \mathbb{R}$ on an open set $\mathrm{A} \subseteq \mathrm{M}$ is called *C^∞-function* if $f \circ \varphi^{-1}$ is infinitely often differentiable for all coordinate neighbourhoods (U, φ).
Set $C^\infty_{\mathrm{M}}(x) := \{f : \mathrm{A} \to \mathbb{R} C^\infty\text{-function} \mid x \in \mathrm{A}\}$.



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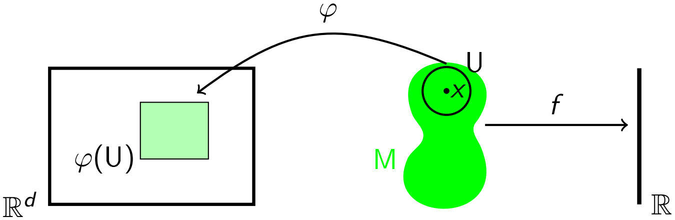


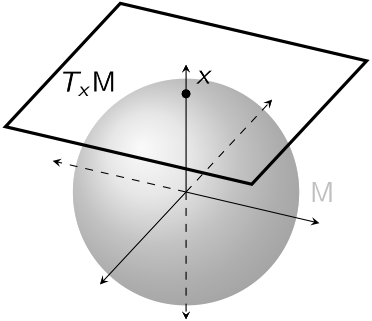
Some differential geometry

Definition

An operator $X : C^\infty_{\mathrm{M}}(x) \to \mathbb{R}$ is called *tangent vector* to M at $x \in \mathrm{M}$ if

$$X(\alpha f + \beta g) = \alpha X(f) + \beta X(g),$$
$$X(fg) = X(f)g(x) + f(x)X(g)$$

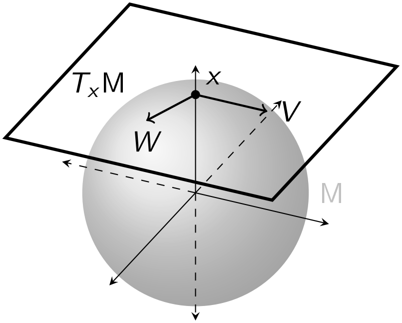
for all $\alpha, \beta \in \mathbb{R}$, $f, g \in C^\infty_{\mathrm{M}}(x)$.
The $\mathbb{R}$-vector space $T_x\mathrm{M} := \{X \text{ tangent vector to M at } x\}$ is called *tangent space*.



Some differential geometry

Definition

A mapping $\mathfrak{g} : \mathrm{M} \ni x \mapsto \mathfrak{g}_x$ is called *Riemannian metric* if $\mathfrak{g}_x$ is an inner product on $T_x\mathrm{M}$ for all $x \in \mathrm{M}$ and some smoothness condition is satisfied.
A smooth manifold M with a Riemannian metric is called *Riemannian*.



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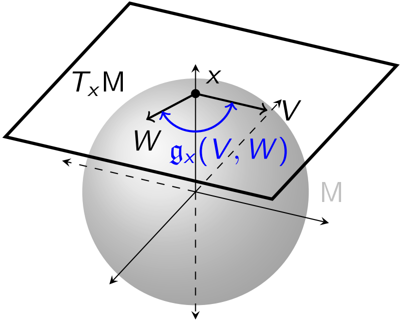

Some differential geometry

Let M be a Riemannian manifold with Borel-σ-algebra $\mathcal{B}(\mathsf{M})$, and

- (U, φ) coordinate neighbourhood,
- $\sqrt{\det(\mathfrak{g}, \varphi)}(x)$ square root of determinant of Gram matrix of coordinate frames associated to (U, φ) with respect to $\mathfrak{g}_x$.

Define the *Riemannian measure* as

$$\nu_{\mathfrak{g}}(\mathsf{A}) := \int_{\varphi(\mathsf{U})} \left(\mathbb{1}_{\mathsf{A}} \cdot \sqrt{\det(\mathfrak{g}, \varphi)} \right) \circ \varphi^{-1}(z) \, \mathrm{d}z, \qquad \mathsf{A} \subseteq \mathsf{U}, \mathsf{A} \in \mathcal{B}(\mathsf{M}).$$

Some differential geometry

Let M be a Riemannian manifold with Borel-σ-algebra $\mathcal{B}(\mathsf{M})$, and

- $\{(\mathsf{U}_i, \varphi_i)\}_{i\in\mathbb{N}}$ countable atlas of M,
- $\sqrt{\det(\mathfrak{g}, \varphi_i)}(x)$ square root of determinant of Gram matrix of coordinate frames associated to $(\mathsf{U}_i, \varphi_i)$ with respect to $\mathfrak{g}_x$,
- $\{\rho_i\}_{i\in\mathbb{N}}$ partition of unity subordinate to $\{\mathsf{U}_i\}_{i\in\mathbb{N}}$, (i.a. $\mathrm{supp}\rho_i \subseteq U_i$, $\sum_{i\in\mathbb{N}} \rho_i \equiv 1$).

Define the *Riemannian measure* as

$$\nu_{\mathfrak{g}}(\mathsf{A}) := \sum_{i\in\mathbb{N}} \int_{\varphi_i(\mathsf{U}_i)} \left(\rho_i \cdot \mathbb{1}_{\mathsf{A}} \cdot \sqrt{\det(\mathfrak{g}, \varphi_i)}\right) \circ {\varphi_i}^{-1}(z)\, \mathrm{d}z, \qquad \mathsf{A} \in \mathcal{B}(\mathsf{M}).$$