DIFFUSIONS ON THE SIMPLEX FROM BROWNIAN MOTIONS ON HYPERSURFACES

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ABSTRACT. The (n - 1)-dimensional simplex is the collection of probability measures on a set with n points. Many applied situations result in simplexvalued data or in stochastic processes that have the simplex as their state space. In this paper we study a large class of simplex-valued diffusion processes that are constructed by first "coordinatising" the simplex with the points of a smooth hypersurface in such a way that several points on the hypersurface may correspond to a given point on the simplex, and then mapping forward the canonical Brownian motion on the hypersurface. For example, a particular instance of the Fleming-Viot process on n points arises from Brownian motion on the (n - 1)-dimensional sphere. The Brownian motion on the hypersurface has the normalised Riemannian volume as its equilibrium distribution. It is straightforward to compute the corresponding distribution on the simplex, and this provides a large class of interesting probability measures on the simplex.

1. INTRODUCTION

Many data sets come in the form of proportions that add to unity (that is, as points in a simplex with dimension one less than the number of proportions). For example, there is the breakdown of the composition of an ore sample into component minerals or the division of a family's expenditures into housing, food, clothing, leisure, *etc.* This type of data is often referred to as *compositional* and a standard reference for models and inference in this area is [Ait86].

Such data can also have a temporal component. For example, there are the proportions of the population at any time having each of the possible combinations of alleles of a given set of genes (see, for example, [Gil91]). There appears to be something of a dearth of flexible, tractable models for such stochastic processes.

Of course, stochastic processes on the simplex are an elementary instance of processes taking values in the set of probability measures on an arbitrary measurable space. However, the literature in this more general area is primarily concerned with models such as the Fleming-Viot process that arise as continuum limits of particle systems with relatively simple dynamics (see, for example, [Daw93]).

There is a substantial literature on diffusions on manifolds and particularly Brownian motion on manifolds (see, for example, [RW87, Éme89, Str00, Dri95]). The approach we follow here for building diffusions on the simplex is to first take a simplicial decomposition of some compact manifold. This gives a typically manyto-one mapping of the manifold onto the simplex. We then take Brownian motion

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on the manifold and map it forward to obtain a continuous stochastic process on the simplex. If the manifold and the associated simplicial decomposition have suitable symmetry properties, then the resulting process on the simplex will be Markovian.

The simplest example of our construction is when the manifold is the (n-1)-dimensional sphere

$$\{(x^1, x^2, \dots, x^n) : (x^1)^2 + (x^2)^2 + \dots + (x^n)^2 = 1\}.$$

We map the sphere onto the (n-1)-dimensional simplex via

$$(x^1, x^2, \dots, x^n) \mapsto ((x^1)^2, (x^2)^2, \dots, (x^n)^2).$$

If (X_t, \mathbb{P}^x) is the Brownian motion on the sphere, then the distribution of the process $X = (X^1, X^2, \ldots, X^n)$ under $\mathbb{P}^{(\pm x^1, \pm x^2, \ldots, \pm x^n)}$ is the same as the distribution of $(\pm X^1, \pm X^2, \ldots, \pm X^n)$ under \mathbb{P}^x for any x and any of the 2^n possible choices of sign. In particular, for any point $y = (y^1, y^2, \ldots, y^n)$ in the simplex the distribution of $((X^1)^2, (X^2)^2, \ldots, (X^n)^2)$ is the same under any of the measures \mathbb{P}^x for which $((x^1)^2, (x^2)^2, \ldots, (x^n)^2) = (y^1, y^2, \ldots, y^n)$. Dynkin's criterion for a function of a Markov process to be Markovian (see Theorem 13.5 of [Sha88]) then gives that $((X^1)^2, (X^2)^2, \ldots, (X^n)^2)$ is Markovian.

It turns out that Brownian motion on the sphere is mapped to a particular Fleming-Viot process on the set $\{1, 2, ..., n\}$. The underlying mutation process for the Fleming-Viot process is a Markov chain that jumps at a constant rate and chooses a new state uniformly from the (n-1) possibilities. The Brownian motion on the sphere has the normalised surface area measure on the sphere as its equilibrium distribution. The corresponding process on the simplex (that is, the Fleming-Viot process) has the push-forward of this measure as its equilibrium distribution and, as is well-known, this latter probability measure is the Dirichlet distribution with parameters $(\frac{1}{2}, \frac{1}{2}, ..., \frac{1}{2})$,

The plan of the paper is the following. We construct a particular class of hypersurfaces and Brownian motions on them in Section 2. We show that the Brownian motion mapped to the simplex is Markovian in Section 3, and exhibit the semimartingale decomposition of this diffusion on the simplex in Section 4. The push-forward of the normalised Riemannian volume measure is the equilibrium distribution of the diffusion on the simplex, and an explicit formula is given for this distribution in Section 5. We illustrate the general results with the special cases where the hypersurface is an ellipsoid in \mathbb{R}^n or the unit sphere in \mathbb{R}^n equipped with the ℓ^p norm for p an even positive integer.

2. Brownian motion on a hypersurface

Fix functions $g_i : \mathbb{R} \to \mathbb{R}_+, 1 \leq i \leq n$, with the following properties:

i) g_i is C^{∞} ; ii) $g_i(0) = 0$; iii) $g_i(-u) = g_i(u)$; iv) $g'_i(u) > 0, u > 0$; v) $\{u \in \mathbb{R} : g_i(u) = 1\} \neq \emptyset$.

Define $g: \mathbb{R}^n \to \mathbb{R}^n_+$ by

$$g(x^1, x^2, \dots, x^n) := (g_1(x^1), g_2(x^2), \dots, g_n(x^n))$$

and $G: \mathbb{R}^n \to \mathbb{R}_+$ by

$$G(x^1, x^2, \dots, x^n) := \sum_{i=1}^n g_i(x^i).$$

The set $\mathcal{M} := \{x \in \mathbb{R}^n : G(x) = 1\}$ is a compact, connected, (n-1)-dimensional embedded submanifold of \mathbb{R}^n and the range of g restricted to \mathcal{M} is the simplex

$$S := \{ y \in \mathbb{R}^n : \sum_{i=1}^n y^i = 1, y_i \ge 0 \}.$$

Each $y \in \mathcal{S}$ is the image of $2^{\#\{1 \le i \le n : y^i > 0\}}$ points of \mathcal{M} .

We will construct a diffusion process $Y = (Y_t, \mathbb{Q}^y)$ or \mathcal{S} by letting $(Y_t)_{t\geq 0}$ under \mathbb{Q}^y have the law of $(g \circ X_t)_{t\geq 0}$ under \mathbb{P}^x , where $X = (X_t, \mathbb{P}^x)$ is the canonical Brownian motion on \mathcal{M} and x is any pre-image of y for g. The infinitesimal generator of X is a multiple of the Laplace-Beltrami operator on \mathcal{M} , but the most convenient way for us to describe X is as the solution of a stochastic differential equation (SDE).

 Let

$$n(x) := \frac{\operatorname{grad} G(x)}{\|\operatorname{grad} G(x)\|} \\ = \frac{(g'_1(x^1), g'_2(x^2), \dots, g'_n(x^n))}{(\sum_{i=1}^n g'_i(x^i)^2)^{\frac{1}{2}}}$$

be the unit normal to \mathcal{M} at x, and write

$$P(x) := (I - n(x)n(x)^{\top})$$

for the corresponding orthogonal projection onto the tangent plane to \mathcal{M} at x. The mean curvature at x is given by

$$\begin{aligned} c(x) &:= -\frac{1}{2} \operatorname{div} n(x) \\ &= -\frac{1}{2} \left\{ \frac{\sum_{i} g_{i}''(x^{i})}{(\sum_{i} g_{i}'(x^{i})^{2})^{\frac{1}{2}}} - \frac{\sum_{i} g_{i}'(x^{i})^{2} g_{i}''(x^{i})}{(\sum_{i} g_{i}'(x^{i})^{2})^{\frac{3}{2}}} \right\} \\ &= -\frac{1}{2} \frac{\sum_{i \neq j} g_{i}'(x^{i})^{2} g_{j}''(x^{j})}{(\sum_{i} g_{i}(x^{i})^{2})^{\frac{3}{2}}}. \end{aligned}$$

By [vdBL85], Brownian motion on \mathcal{M} starting at $x \in \mathcal{M}$ solves the SDE

$$dX_t = P(X_t) dB_t + c(X_t) n(X_t) dt$$

$$X_0 = x,$$

where B is a standard n-dimensional Brownian motion. Write \mathbb{P}^x for the distribution of the solution of this SDE.

3. Diffusion on the simplex

Set $Y := g \circ X$. That is, $Y_t = g(X_t) \in S$. We claim that Y is Markovian. As with the example on the sphere in the Introduction, this will follow from Dynkin's criterion for a function of a Markov process to be Markovian if we can show that the law of Y is the same under $\mathbb{P}^{x'}$ and $\mathbb{P}^{x''}$ for any two points $x', x'' \in \mathcal{M}$ such that g(x') = g(x'') (see Theorem 13.5 of [Sha88]). For any $x \in \mathcal{M}$, let $X^{(x)}$ denote the solution of the SDE

$$dX_t^{(x)} = P\left(X_t^{(x)}\right) dB_t + c\left(X_t^{(x)}\right) n\left(X_t^{(x)}\right) dt$$
$$X_0^{(x)} = x.$$

Fix $\epsilon \in \{\pm 1\}^n$ and write E for the diagonal matrix diag $(\epsilon_1, \epsilon_2, \ldots, \epsilon_n)$ so that for $z \in \mathbb{R}^n$, $Ez = (\epsilon_1 z^1, \epsilon_2 z^2, \ldots, \epsilon_n z^n)$. Note that if $x', x'' \in \mathcal{M}$ are such that g(x') = g(x''), then x'' = Ex' for some such E. Observe by our assumptions on the g_i that

$$g'_i(-u) = -g'_i(u),$$

 $g''_i(-u) = g''_i(u),$

and so

$$n(Ex) = En(x),$$

$$P(Ex) = EP(x)E,$$

$$c(Ex) = c(x).$$

Thus,

$$d\left[EX_{t}^{(x)}\right] = EP\left(X_{t}^{(x)}\right) dB_{t} + c\left(X_{t}^{(x)}\right) En\left(X_{t}^{(x)}\right) dt$$
$$= EP\left(X_{t}^{(x)}\right) Ed[EB_{t}] + c\left(X_{t}^{(x)}\right) En\left(X_{t}^{(x)}\right) dt$$
$$= P\left(EX_{t}^{(x)}\right) d\tilde{B}_{t} + c\left(EX_{t}^{(x)}\right) n\left(EX_{t}^{(x)}\right) dt,$$

where $\tilde{B} = EB$ is a standard *n*-dimensional Brownian motion. Moreover,

$$EX_0^{(x)} = Ex$$

and so we conclude that $EX^{(x)}$ has the same distribution as $X^{(Ex)}$. That is, the law of EX under \mathbb{P}^x is the same as that of X under \mathbb{P}^{Ex} , and Dynkin's criterion holds. Write \mathbb{Q}^y for the distribution of Y starting at $y \in \mathcal{S}$. Because X is a Feller process and g is continuous, it follows that Y is also a Feller process.

4. Semimartingale description

By Itô's formula we have

$$dY_{t}^{i} = g_{i}'(X_{t}^{i})dX_{t}^{i} + \frac{1}{2}g_{i}''(X_{t}^{i})d\langle X^{i}\rangle_{t}$$

$$= g_{i}'(X_{t}^{i})\sum_{j}P_{ij}(X_{t})dB_{t}^{j}$$

$$+g_{i}'(X_{t}^{i})c(X_{t})n^{i}(X_{t})dt + \frac{1}{2}g_{i}''(X_{t}^{i})\sum_{j}P_{ij}(X_{t})^{2}dt.$$

By our assumptions on g_i , for $0 \le v \le 1$ there exists a unique $u \ge 0$ such that $g_i(u) = v$. Write $u = h_i(v)$. Observe that $g_i(-h_i(v)) = v$, $g'_i(-h_i(v)) = -g'_i(h_i(v))$, and $g''_i(-h_i(v)) = g''_i(h_i(v))$. Put

$$\begin{aligned} \alpha_i(y) &:= g'_i(h_i(y^i))^2 = \frac{1}{h'_i(y_i)^2}, \\ \bar{\alpha}_i(y) &:= \frac{\alpha_i(y)}{\sum_j \alpha_j(y)}, \end{aligned}$$

 and

$$\beta_i(y) := g''_i(h_i(y^i)) = -\frac{h''_i(y^i)}{h'_i(y^i)^3}.$$

Note that because P(x) is a projection matrix,

$$\sum_{j} P_{ij}(x)^{2} = \sum_{j} P_{ij}(x) P_{ji}(x)$$

= $P_{ii}(x)$
= $1 - n^{i}(x)^{2}$.

Thus for y = g(x) we have

$$g_{i}'(x^{i})c(x)n^{i}(x) + \frac{1}{2}g_{i}''(x^{i})\sum_{j}P_{ij}(x)^{2}$$

$$= -\frac{1}{2}\alpha_{i}(y)\left\{\frac{\sum_{j}\beta_{j}(y)}{\left(\sum_{j}\alpha_{j}(y)\right)^{\frac{1}{2}}} - \frac{\sum_{j}\alpha_{j}(y)\beta_{j}(y)}{\left(\sum_{j}\alpha_{j}(y)\right)^{\frac{3}{2}}}\right\}\frac{1}{\left(\sum_{j}\alpha_{j}(y)\right)^{\frac{1}{2}}}$$

$$+ \frac{1}{2}\beta_{i}(y)\left\{1 - \frac{\alpha_{i}(y)}{\sum_{j}\alpha_{j}(y)}\right\}$$

$$= \frac{1}{2}\left[\beta_{i}(y)\{1 - \bar{\alpha}_{i}(y)\} - \bar{\alpha}_{i}(y)\sum_{j}\beta_{j}(y)\{1 - \bar{\alpha}_{j}(y)\}\right].$$

Note also that

$$\sum_{k} g'_{i}(x^{i}) P_{ik}(x) g'_{j}(x^{j}) P_{jk}(x) = g'_{i}(x^{i}) P_{ij}(x) g'_{j}(x^{j})$$
$$= \alpha_{i}(y) \{ \delta_{ij} - \bar{\alpha}_{j}(y) \}.$$

Putting this all together,

$$dY_t^i = dM_t^i + \frac{1}{2} \left[\beta_i(Y_t) \{ 1 - \bar{\alpha}_i(Y_t) \} - \bar{\alpha}_i(Y_t) \sum_j \beta_j(Y_t) \{ 1 - \bar{\alpha}_j(Y_t) \} \right] dt$$

where $M_t = (M_t^1, \dots, M_t^n)$ is a continuous martingale with

$$d\langle M^{i}, M^{j}\rangle_{t} = \alpha_{i}(Y_{t})\{\delta_{ij} - \bar{\alpha}_{j}(Y_{t})\}dt$$

Example 4.1. Suppose that $g_i(u) = c_i u^2$ for constants $c_i > 0, 1 \le i \le n$, so that \mathcal{M} is the ellipsoid $\{(x^1, x^2, ..., x^n) : c_1(x^1)^2 + c_2(x^2)^2 + \cdots + c_n(x^n)^2 = 1\}$. Then

$$\begin{aligned} \alpha_i(y) &= 4c_i y_i \\ \beta_i(y) &= 2c_i, \end{aligned}$$

and hence

$$dY_t^i = dM_t^i + \left[c_i \left\{1 - \frac{c_i Y_t^i}{\sum_j c_j Y_t^j}\right\} - \frac{c_i Y_t^i}{\sum_j c_j Y_t^j} \sum_j c_j \left\{1 - \frac{c_j Y_t^j}{\sum_k c_k Y_t^k}\right\}\right] dt,$$

where M is a continuous martingale with

$$d\langle M^i, M^j \rangle_t = 4c_i Y_t^i \left\{ \delta_{ij} - \frac{c_j Y_t^j}{\sum_k c_k Y_t^k} \right\} dt.$$

When $c_1 = c_2 = \cdots = c_n = c$ (so that \mathcal{M} is the sphere with radius $\frac{1}{\sqrt{c}}$), we have

$$dY_t^i = dM_t^i + c \left[1 - Y_t^i - Y_t^i \sum_j \{1 - Y_t^j\} \right] dt$$

= $dM_t^i + c[1 - nY_t^i] dt$
= $dM_t^i + cn \sum_j \left\{ \frac{1}{n} - \delta_{ij} \right\} Y_t^j dt,$

where M is a continuous martingale with

$$d\langle M^i, M^j \rangle_t = 4cY_t^i \{\delta_{ij} - Y_t^j\} dt.$$

If we associate Y_t with the probability measure on $\{1, 2, \ldots, n\}$ that assigns mass Y_t^i to *i*, then (Y_t, \mathbb{Q}^y) is a particular case of a Fleming-Viot process (see [Daw93]) in which the underlying mutation process jumps from each state at rate c(n-1)and chooses a new state uniformly from the (n-1) possibilities.

When n = 2, the process $Z := Y^1$ is a one-dimensional diffusion that solves the SDE

$$dZ_t = \mu(Z_t) dt + \sigma(Z_t) dB_t,$$

where

$$\mu(z) := c_1 \left\{ 1 - \frac{c_1 z}{c_1 z + c_2 (1 - z)} \right\}$$

$$- \frac{c_1 z}{c_1 z + c_2 (1 - z)} \left[c_1 \left\{ 1 - \frac{c_1 z}{c_1 z + c_2 (1 - z)} \right\} + c_2 \left\{ 1 - \frac{c_2 (1 - z)}{c_1 z + c_2 (1 - z)} \right\} \right]$$
and

$$\sigma^{2}(z) := 4c_{1}z \left\{ 1 - \frac{c_{1}z}{c_{1}z + c_{2}(1-z)} \right\}.$$

An interesting feature of these coefficients is that the unique zero of μ and the unique maximum of σ^2 both occur at the point $z = \sqrt{c_2}/(\sqrt{c_1} + \sqrt{c_2})$. The infinitesimal drift μ is graphed in Figures 4.1 and 4.2 for the parameter values $(c_1, c_2) = (1, 1)$ and $(c_1, c_2) = (4, 1)$, respectively. The infinitesimal variance σ^2 is graphed in Figures 4.3 and 4.4 for the parameter values $(c_1, c_2) = (1, 1)$ and $(c_1, c_2) = (4, 1)$, respectively.

Remark 4.2. If we formally send $n \to \infty$ in the martingale problem for Y, then the resulting martingale problem on the infinite simplex $\{(y^1, y^2, \ldots) : \sum_i y^i = 1, y^i \ge 1\}$ 0} makes sense when

$$\sum_{i} \sup_{0 \le v \le 1} \left| \frac{h_i''(v)}{h_i'(v)^3} \right| < \infty$$

(in Example 4.1 this is condition becomes $\sum_i c_i < \infty$). It would be interesting to know if this infinite-dimensional martingale problem is well-posed.

5. Equilibrium distribution

The Brownian motion X is reversible with respect to the normalised Riemannian volume measure on \mathcal{M} and X_t converges in distribution to this measure as $t \to \infty$ under any \mathbb{P}^x . Therefore, if we let π denote the push-forward of the normalised Riemannian volume measure by q, then the diffusion Y is reversible with respect to π and Y_t converges in distribution to π as $t \to \infty$ under any \mathbb{Q}^y .









We can calculate the Riemannian volume measure as follows. The set

$$\{(x^1, x^2, \dots, x^n) \in \mathcal{M} : x^n \neq 0\}$$

is the union of the two open sets

$$\left\{ \left(x^1, x^2, \dots, x^{n-1}, \pm h_n \left(1 - \sum_{i=1}^{n-1} g_i(x^i) \right) \right) : \sum_{i=1}^{n-1} g_i(x^i) < 1 \right\}$$

and $(x^1, x^2, \ldots, x^{n-1})$ can be used as local coordinates for \mathcal{M} in these two patches. The Riemannian metric in each patch is given by the matrix $I + J(x)J(x)^{\top}$, where







Figure 4.4

J(x) is the (n-1)-dimensional column vector

$$\left(\frac{\partial}{\partial x^i}h_n\left(1-\sum_{j=1}^{n-1}g_j(x^j)\right)\right)_{i=1}^{n-1}.$$

The corresponding Riemannian volume measure is

$$\left[\det(I+J(x)J(x)^{\top})\right]^{\frac{1}{2}}dx^{1}dx^{2}\cdots dx^{n-1} = \left[1+J(x)^{\top}J(x)\right]^{\frac{1}{2}}dx^{1}dx^{2}\cdots dx^{n-1},$$

where we have used the familiar matrix fact that

$$\det(A + bb^{\top}) = \det(A)(1 + b^{\top}A^{-1}b).$$

The Jacobian matrix for the transformation

$$(x^1, x^2, \dots, x^{n-1}) \mapsto (g_1(x^1), g^2(x^2), \dots, g_{n-1}(x^{n-1}))$$

is the diagonal matrix

diag
$$(g'_1(x^1), g'_2(x^2), \dots, g'_{n-1}(x^{n-1})).$$

Therefore, if we coordinatise S with $\{(y^1, y^2, \ldots, y^{n-1}) : \sum_{i=1}^{n-1} y_i \leq 1, y_i \geq 0\}$, then π is the measure

$$C\left[1+\sum_{i=1}^{n-1}\left\{h'_{n}\left(1-\sum_{j=1}^{n-1}y^{j}\right)g'_{i}(h_{i}(y^{i}))\right\}^{2}\right]^{\frac{1}{2}}\prod_{i=1}^{n-1}g'_{i}(h_{i}(y^{i}))^{-1} dy^{1}dy^{2}\dots dy^{n-1}$$
$$=C\left[\sum_{i=1}^{n}g'_{i}(h_{i}(y^{i}))^{2}\right]^{\frac{1}{2}}\prod_{i=1}^{n}g'_{i}(h_{i}(y^{i}))^{-1} dy^{1}dy^{2}\dots dy^{n-1},$$

for a suitable normalisation constant C.

Example 5.1. Suppose that $g_i(u) = c_i u^2$ for constants $c_i > 0, 1 \le i \le n$. Then

$$g'_i(h_i(u)) = 2c_i^{\frac{1}{2}}u^{\frac{1}{2}}$$

so that π is

$$C\left[\sum_{i=1}^{n} c_{i} y^{i}\right]^{\frac{1}{2}} \prod_{i=1}^{n} (y^{i})^{-\frac{1}{2}} dy^{1} dy^{2} \cdots dy^{n-1}$$

for a suitable constant C. In particular, if $c_1 = c_2 = \cdots = c_n$, then π is the Dirichlet distribution with parameters $(\frac{1}{2}, \frac{1}{2}, \dots, \frac{1}{2})$. For n = 2, the equilbrium density is graphed in Figures 5.1 and 5.2 for $(c_1, c_2) =$

For n = 2, the equilbrium density is graphed in Figures 5.1 and 5.2 for $(c_1, c_2) = (1, 1)$ and $(c_1, c_2) = (4, 1)$, respectively. The equilibrium density has its unique minimum at $\sqrt{c_2}/(\sqrt{c_1} + \sqrt{c_2})$. Recall from Example 4.1 that the infinitesimal drift coefficient vanishes and the infinitesimal variance coefficient has its maximum at this same point.

6. Another example

Suppose that $g_i(u) = u^p$, $1 \le i \le n$, where p is an even positive integer. Then

$$\alpha_i(y) = p^2 (y^i)^{2\left(1 - \frac{1}{p}\right)}$$

 and

$$\beta_i(y) = p^2 (p-1) (y^i)^{(1-\frac{2}{p})}.$$

Hence, setting $r = 2\left(1 - \frac{1}{p}\right)$ and $s = \left(1 - \frac{2}{p}\right)$,

$$\begin{split} dY_t^i &= dM_t^i + \frac{p^2(p-1)}{2} \left[(Y_t^i)^s \left\{ 1 - \frac{(Y_t^i)^r}{\sum_k (Y_t^k)^r} \right\} \\ &- \frac{(Y_t^i)^r}{\sum_k (Y_t^k)^r} \sum_j (Y_t^j)^s \left\{ 1 - \frac{(Y_t^j)^r}{\sum_k (Y_t^k)^r} \right\} \right], \end{split}$$

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FIGURE 5.2

where M is a continuous martingale with

$$d\langle M^i, M^j \rangle_t = p^2 (Y^i_t)^r \left\{ \delta_{ij} - \frac{(Y^j_t)^r}{\sum_k (Y^k_t)^r} \right\} dt.$$

The equilibrium measure π is

$$C\left[\sum_{i=1}^{n} (y^{i})^{r}\right]^{\frac{1}{2}} \prod_{i=1}^{n} (y^{i})^{-\frac{r}{2}} dy^{1} dy^{2} \cdots dy^{n-1}$$

for some constant C.

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