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Left-Invariant Diffusions on the Space of Positions and Orientations and their Application to Crossing-Preserving Smoothing of HARDI images

Remco Duits · Erik Franken

Abstract HARDI (High Angular Resolution Diffusion Imaging) is a recent magnetic resonance imaging (MRI) technique for imaging water diffusion processes in fibrous tissues such as brain white matter and muscles. In this article we study left-invariant diffusion on the group of 3D rigid body movements (i.e. 3D Euclidean motion group) SE(3) and its application to crossing-preserving smoothing of HARDI images. The linear left-invariant (convection-)diffusions are forward Kolmogorov equations of Brownian motions on the space of positions and orientations in 3D embedded in SE(3) and can be solved by $\mathbb{R}^3 \times S^2$-convolution with the corresponding Green’s functions. We provide analytic approximation formulas and explicit sharp Gaussian estimates for these Green’s functions. In our design and analysis for appropriate (nonlinear) convection-diffusions on HARDI data we explain the underlying differential geometry on SE(3). We write our left-invariant diffusions in covariant derivatives on SE(3) using the Cartan connection. This Cartan connection has constant curvature and constant torsion, and so have the exponential curves which are the auto-parallels along which our left-invariant diffusion takes place. We provide experiments of our crossing-preserving Euclidean-invariant diffusions on artificial HARDI data containing crossing-fibers.

Keywords High angular resolution diffusion imaging (HARDI) · Scale spaces · Lie groups · Partial differential equations

1 Introduction

High Angular Resolution Diffusion Imaging (HARDI) is a recent magnetic resonance imaging technique for imaging water diffusion processes in fibrous tissues such as brain white matter and muscles. HARDI provides for each position in 3-space (i.e. $\mathbb{R}^3$) and for each orientation (antipodal pairs on the 2-sphere $S^2$) an MRI signal attenuation profile, which can be related to the local diffusivity of water molecules in the corresponding direction. It is generally believed that such profiles provide rich information in fibrous tissues. DTI (Diffusion Tensor Imaging) is a related technique, producing a positive symmetric rank-2 tensor field. A DTI tensor (at each position in 3-space) can also be related to a distribution on the 2-sphere, albeit with limited angular resolution. DTI is incapable of representing areas with complex multimodal diffusivity profiles, such as induced by crossing, “kissing”, or bifurcating fibres. HARDI, on the other hand, does not suffer from this problem, because it is not restricted to functions on the 2-sphere induced by a quadratic form, see Fig. 1 where we used glyph visualizations as defined in Definition 1. For the purpose of tractography (detection of biological fibers) and visualization, DTI and HARDI data should be enhanced such that fiber junctions are maintained, while reducing high frequency noise and small incoherent structures in the joined domain.
of positions and orientations. This crossing-preserving enhancement/diffusion along fibers within distributions defined on the joined space of positions and orientations (such as HARDI and DTI images) is the main objective of this article.

**Definition 1** A glyph of a distribution \( U : \mathbb{R}^3 \times S^2 \to \mathbb{R}^+ \) on positions and orientations is a surface \( S_\mu(U)(x) = \{ x + \mu U(x, n) n \mid n \in S^2 \} \subset \mathbb{R}^3 \) for some \( x \in \mathbb{R}^3 \) and \( \mu > 0 \). A glyph visualization of the distribution \( U : \mathbb{R}^3 \times S^2 \to \mathbb{R}^+ \) is a visualization of a field \( x \mapsto S_\mu(U)(x) \) of glyphs, where \( \mu > 0 \) is a suitable constant.

Promising research has been done on constructing diffusion (or similar regularization) processes on the 2-sphere defined at each spatial locus separately (Descoteaux et al. 2007; Florack and Balmachnova 2008; Florack 2008; Hess et al. 2006) as an essential pre-processing step for robust fiber tracking. In these approaches position and orientation space are decoupled, and diffusion is only performed over the angular part, disregarding spatial context. Consequently, these methods are inadequate for spatial denoising and enhancement, and tend to fail precisely at the interesting locations where fibers cross or bifurcate.

Therefore in this article we extend our recent work on enhancement of elongated structures in 2D greyscale images (van Almsick 2005; Franken and Duits 2009; Franken 2008; Duits and van Almsick 2008; Duits et al. 2007; Duits and Franken 2009; Duits and Burge th 2007; Duits and Franken 2010) to the genuinely 3D case of HARDI/DTI, since this approach has proven to be capable of handling all aforementioned problems in various feasibility studies, see Fig. 2. In contrast to the previous works on diffusion of DTI/HARDI images (Descoteaux et al. 2007; Florack and Balmachnova 2008; Florack 2008; Hess et al. 2006; Özarslan and Mareci 2003), we consider both the spatial and the orientational part to be included in the domain, so a HARDI dataset is considered as a function \( U : \mathbb{R}^3 \times S^2 \to \mathbb{R} \). Furthermore, we explicitly employ the proper underlying group structure, that naturally arises by embedding the coupled space of positions and orientations into the group \( SE(3) \) of 3D rigid motions. The relevance of group theory in DTI/HARDI imag-
played
At each spatial position \( x \) \( \in \mathbb{R}^3 \) visualized using Q-ball glyphs in the DTI tool from two different viewpoints.

The natural 3D generalizations of Mumford’s direction process on \( \mathbb{R}^2 \times S^1 \) (Mumford 1994; Duits and van Almsick 2008), which is a contour completion process in the group \( SE(2) = \mathbb{R}^2 \times S^1 \equiv \mathbb{R}^2 \times SO(2) \) of 2D-positions and orientations;

2. The natural 3D generalizations of a (horizontal) random walk on \( \mathbb{R}^2 \times S^1 \), cf. (Duits and Franken 2010), corresponding to the diffusions proposed by Citti and Sarti (2006), which is a contour enhancement process in the group \( SE(2) = \mathbb{R}^2 \times S^1 \equiv \mathbb{R}^2 \times SO(2) \) of 2D-positions and orientations;

3. Gaussian scale space (Iijima 1962; Koenderink 1984; Alvarez et al. 1993; Duits et al. 2004) over position space, i.e. spatial linear diffusion;

4. Gaussian scale space over angular space (2-sphere) (Descoteaux et al. 2007; Özarslan and Mareci 2003; Florack and Balmachnova 2008; Florack 2008; Hess et al. 2006), i.e. angular linear diffusion,

or combinations of these four types of convection-diffusions. Previous approaches of HARDI-diffusions (Descoteaux et al. 2007; Özarslan and Mareci 2003; Florack and Balmachnova 2008) fit in our framework (third and fourth item), but it is rather the first two cases that are challenging as they involve a natural coupling between position and orientation space and thereby allow appropriate treatment of crossing fibers. In Sect. 5 we will explore the underlying differential geometry of our diffusions on HARDI-orientation scores. By means of the Cartan connection on \( SE(3) \) we put a useful relation to rigid body mechanics expressed in moving frames of reference, providing geometrical intuition behind our left-invariant (convection-)diffusions on HARDI data. Furthermore, we show that our (convection-)diffusion may be expressed in covariant derivatives and we show that both convection and diffusion locally take place along the
exponential curves in \( SE(3) \), that are explicitly derived in Sect. 5.1. In Sect. 6 we will derive suitable formulas and Gaussian estimates for the Green’s functions of linear left-invariant convection-diffusions on HARDI images. These formulas are used in the subsequent section in our numerical convolution-schemes solving the left-invariant diffusions on HARDI images.

Section 7 explains the basic numerics of our left-invariant PDE- and/or convolution schemes, which we use in the subsequent experimental section. Section 8 contains preliminary results of linear left-invariant diffusion on artificial HARDI datasets over the joined coupled domain of positions and orientations (i.e. over \( \mathbb{R}^3 \times S^2 \)).

The final section of this paper provides the theory for nonlinear adaptive diffusion on HARDI images, which is a generalization of our nonlinear adaptive diffusion schemes on the 2D Euclidean motion group (Franken and Duits 2009; Duits and Franken 2010).

2 The Group Structure on the Domain of a HARDI Image: The Embedding of \( \mathbb{R}^3 \times S^2 \) into \( SE(3) \)

In order to generalize our previous work on line/contour-enhancement via left-invariant diffusions on invertible orientation scores of 2D-images we first investigate the group structure on the domain of a HARDI image. Just like orientation scores are scalar-valued functions on the space of 2D-positions and orientations, i.e. the 2D-Euclidean motion group, HARDI images are scalar-valued functions on the space of 3D-positions and orientations. This generalization involves some technicalities since the 2-sphere \( S^2 = \{ x \in \mathbb{R}^3 | ||x|| = 1 \} \) is not a Lie-group proper\(^1\) in contrast to the 1-sphere \( S^1 = \{ x \in \mathbb{R}^2 | ||x|| = 1 \} \). To overcome this problem we embed \( \mathbb{R}^3 \times S^2 \) into \( SE(3) \) which is the group of 3D-rotations and translations (i.e. the group of 3D rigid motions). As a concatenation of two rigid body movements is again a rigid body movement, the product on \( SE(3) \) is given by

\[
(x, R)(x', R') = (Rx + x, RR'),
\]

\( R, R' \in SO(3), \quad x, x' \in \mathbb{R}^3 \).

The group \( SE(3) \) is a semi-direct product of the translation group \( \mathbb{R}^3 \) and the rotation group \( SO(3) \), since it uses an isomorphism \( R \mapsto (x \mapsto Rx) \) from the rotation group onto the automorphisms on \( \mathbb{R}^3 \). Therefore we write \( \mathbb{R}^3 \rtimes SO(3) \)

\(^1\)If \( S^2 \) were a Lie-group then its left-invariant vector fields would be non-zero everywhere, contradicting Poincaré’s “hairy ball theorem” (proven by Brouwer in 1912), or more generally the Poincaré-Hopf theorem (the Euler-characteristic of an even dimensional sphere \( S^{2n} \) is 2).

rather than \( \mathbb{R}^3 \times SO(3) \) which would yield a direct product. The groups \( SE(3) \) and \( SO(3) \) are not commutative. Throughout this article we will use Euler-angle parametrization for \( SO(3) \), i.e. we write a rotation as a product of a rotation around the \( z \)-axis, a rotation around the \( y \)-axis and a rotation around the \( z \)-axis again.

\[
R = R_{x,y} R_{x,y} R_{x,a},
\]

where all rotations are counter-clockwise, where all rotations are counter-clockwise, i.e.:

\[
R_{x,y} = \begin{pmatrix} \cos y & - \sin y & 0 \\ \sin y & \cos y & 0 \\ 0 & 0 & 1 \end{pmatrix}
\]

and

\[
R_{x,a} = \begin{pmatrix} \cos a & 0 & \sin a \\ 0 & 1 & 0 \\ - \sin a & 0 & \cos a \end{pmatrix}.
\]

The advantage of the Euler angle parametrization is that it directly parameterizes \( SO(3)/SO(2) \equiv S^2 \) as well. Here we recall that \( SO(3)/SO(2) \) denotes the partition of all left cosets which are equivalence classes \( [g] = \{ h \in SO(3) | h \sim g \} = gSO(2) \) under the equivalence relation \( g_1 \sim g_2 \Leftrightarrow g_1^{-1} g_2 \in SO(2) \) where we identified \( SO(2) \) with rotations around the \( z \)-axis and we have

\[
SO(3)/SO(2) \ni [R_{x,y} R_{x,a}] = [R_{x,y} R_{x,a} | a \in [0, 2\pi)]
\]

\[
\Leftrightarrow n(\beta, \gamma) := (\cos \gamma \sin \beta, \sin \gamma \sin \beta, \cos \beta)^T = R_{x,y} R_{x,a} e_z \in S^2.
\]

Like all parameterizations of \( SO(3)/SO(2) \), the Euler angle parametrization suffers from the problem that there does not exists a global diffeomorphism from a sphere to a plane. In the Euler-angle parametrization the ambiguity arises at the north and south-pole:

\[
R_{x,y} R_{x,a} e_0 = R_{x,y} R_{x,a} e_0 = R_{x,y} R_{x,a} e_0, \quad R_{x,y} R_{x,a} e_0 = R_{x,y} R_{x,a} e_0 + \delta,
\]

for all \( \delta \in [0, 2\pi) \).

Consequently, we occasionally need a second chart to cover \( SO(3) \):

\[
R = R_{x,y} R_{x,a} e_z.
\]

which again parameterizes \( SO(3)/SO(2) \equiv S^2 \) using different spherical coordinates \( \tilde{\beta} \in [-\pi, \pi), \tilde{\gamma} \in (-\frac{\pi}{2}, \frac{\pi}{2}) \),

\[
\tilde{\mathbf{n}}(\tilde{\beta}, \tilde{\gamma}) = R_{x,y} R_{x,a} e_z
= (\sin \tilde{\beta}, - \cos \tilde{\beta} \sin \tilde{\gamma}, \cos \tilde{\beta} \cos \tilde{\gamma})^T,
\]
Fig. 4 The two charts which together appropriately parameterize the sphere $S^2 \equiv SO(3)/SO(2)$, where the rotation-parameters $\alpha$ and $\tilde{\alpha}$ are free. The first chart (left-image) is the common Euler-angle parametrization (1), the second chart is given by (4). The first chart has singularities at north and south-pole (inducing ill-defined parametrization of the left-invariant vector fields (24) at the unity element) whereas the second chart has singularities at $\pm (1,0,0)$

but which has ambiguities at the intersection of the equator with the $x$-axis

\begin{equation}
R_{e_x, \gamma} R_{e_y, \beta} R_{e_z, \alpha} = R_{e_x, \gamma - \beta} R_{e_y, \beta = \pm \frac{\pi}{2}} R_{e_z, \alpha \pm \delta},
\end{equation}

for all $\delta \in [0, 2\pi)$.

See Fig. 4. Away from the intersection of the $z$- and $x$-axis with the sphere one can accomplish conversion between the two charts by solving for either $(\tilde{\alpha}, \tilde{\beta}, \tilde{\gamma})$ or $(\alpha, \beta, \gamma')$ in $R_{e_x, \tilde{\gamma}} R_{e_y, \tilde{\beta}} R_{e_z, \tilde{\alpha}} = R_{e_x, \gamma} R_{e_y, \beta} R_{e_z, \alpha}$.

Now that we have explained the isomorphism $n = R e_x \in S^2 \leftrightarrow SO(3)/SO(2) \ni [R]$ explicitly in charts, we return to the domain of HARDI images. Considered as a set this domain equals the space of 3D-positions and orientations $\mathbb{R}^3 \times S^2$. However, in order to stress the fundamental embedding of the HARDI domain in $SE(3)$ and the thereby induced (quotient) group-structure we write $\mathbb{R}^3 \times S^2$, which equals the following Lie-group quotient:

$\mathbb{R}^3 \times S^2 := (\mathbb{R}^3 \times SO(3))/\{0\} \times SO(2))$.

Here the equivalence relation on the group of rigid-motions $SE(3) = \mathbb{R}^3 \times SO(3)$ equals

$(x, R) \sim (x', R') \Leftrightarrow x = x'$ and $R^{-1} R'$ is a rotation around the $z$-axis

and the set of equivalence classes within $SE(3)$ under this equivalence relation (i.e. left cosets) equals the space of coupled orientations and positions and is denoted by $\mathbb{R}^3 \times S^2$.

3 Tools from Group Theory

In this article we will consider convection-diffusion operators on the space of HARDI images. We shall model the space of HARDI images by the space of quadratic integrable functions on the coupled space of positions and orientations, i.e. $L_2(\mathbb{R}^3 \times S^2)$. We will first show that such operators should be left-invariant with respect to the left-action of $SE(3)$ onto the space of HARDI images. This left-action of $SE(3)$ onto $\mathbb{R}^3 \times S^2$ is given by

$g \cdot (y, n) = (Ry + x, Rn)$,

$g = (x, R) \in SE(3), \quad x, y \in \mathbb{R}^3, \quad n \in S^2, \quad R \in SO(3)$

and it induces the so-called left-regular action of the same group on the space of HARDI images similar to the left-regular action on 3D images (for example orientation-marginals of HARDI images):

**Definition 2** The left-regular actions of $SE(3)$ onto $L_2(\mathbb{R}^3 \times S^2)$ respectively $L_2(\mathbb{R}^3)$ are given by

$(\mathcal{L}_{g=(x,R)}U)(y, n) = U(g^{-1}(y, n))$

$= U(R^{-1}(y - x), R^{-1}n)$,

$x, y \in \mathbb{R}^3, \quad n \in S^2, \quad U \in L_2(\mathbb{R}^3 \times S^2),$

$(\mathcal{L}_{g=(x,R)}f)(y) = f(R^{-1}(y - x)),$

$R \in SO(3), \quad x, y \in \mathbb{R}^3, \quad f \in L_2(\mathbb{R}^3)$.

Intuitively, $\mathcal{L}_{g=(x,R)}$ represents a rigid motion operator on images, whereas $\mathcal{L}_{g=(x,R)}$ represents a rigid motion on HARDI images.

In order to explain the importance of left-invariance of processing HARDI images in general we need to define the following operator.

**Definition 3** We define the operator $\mathcal{M}$ which maps a HARDI image $U : \mathbb{R}^3 \times S^2 \to \mathbb{R}^+$ to its orientation marginal $\mathcal{M}U : \mathbb{R}^3 \to \mathbb{R}^+$ as follows (where $\sigma$ denotes the usual surface measure on $S^2$):

$(\mathcal{M}U)(y) = \int_{S^2} U(y, n) d\sigma(n)$.

If $U : \mathbb{R}^3 \times S^2 \to \mathbb{R}^+$ is a probability density on positions and orientations then $\mathcal{M}U : \mathbb{R}^3 \to \mathbb{R}^+$ denotes the corresponding probability density on position space only.

The marginal gives us an ordinary 3D image that is a “simplified” version of the HARDI image, containing less information on the orientational structure. This is analogue to taking the trace of a DTI image. The following theorem tells us that we get a Euclidean invariant operator on the marginal of HARDI images if the operator on the HARDI image is left-invariant. This motivates our restriction to left-invariant operators, akin to our framework of invertible ori-
Lemma 1 Suppose $\Phi$ is an operator on the space of HARDI images to itself. The corresponding operator $Y$ on the orientation marginals given by $Y(M(U)) = M(\Phi(U))$ is Euclidean invariant if operator $\Phi$ is left-invariant:

$$ (\Phi \circ \Omega_g) \circ \Phi = \Omega_g \circ \Phi, \text{ for all } g \in SE(3) $$

$$ \Rightarrow \quad \Omega_g \circ Y = Y \circ \Omega_g, \quad \text{for all } g \in SE(3). $$

Proof The result follows directly by the intertwining relation $\Omega_g \circ M = M \circ \Omega_g$ for all $g \in SE(3)$. Regardless of the fact if $\Phi$ is bounded or unbounded, linear or nonlinear, we have under assumption of left-invariance of $\Phi$ that

$$ Y \circ \Omega_g \circ M = Y \circ M \circ \Omega_g $$

$$ = M \circ \Phi \circ \Omega_g $$

$$ = M \circ \Omega_g \circ \Phi = \Omega_g \circ \Phi \circ M $$

$$ = \Omega_g \circ Y \circ M. $$

\( \square \)

It follows by the Dunford-Pettis Theorem (Bukhvalov and Arendt 1994, pp. 113–114) that basically every reasonable linear operator $K$ on HARDI images and we will provide an important probabilistic interpretation of these left-invariant kernel operators.

Lemma 1 Let $K$ be a bounded linear operator from $L_2(\mathbb{R}^2 \times S^2)$ into $L_\infty(\mathbb{R}^2 \times S^2)$ then there exists an integrable kernel $k : \mathbb{R}^2 \times S^2 \times \mathbb{R}^2 \times S^2 \rightarrow \mathbb{C}$ such that

$$ \|K\|^2 = \sup_{(y, n) \in \mathbb{R}^2 \times S^2} \int_{\mathbb{R}^2 \times S^2} |k(y, n; y', n')|^2 d\sigma(n') $$

and we have

$$ (KU)(y, n) = \int_{\mathbb{R}^2 \times S^2} k(y, n; y', n')U(y', n')d\sigma(n'), $$

for almost every $(y, n) \in \mathbb{R}^2 \times S^2$ and all $U \in L_2(\mathbb{R}^2 \times S^2)$. Now $K_k := K$ is left-invariant iff $k$ is left-invariant:

$$ \forall g \in SE(3) : \Omega_g \circ K_k = K_k \circ \Omega_g $$

$$ \Leftrightarrow \quad \forall g \in SE(3) \forall y, y' \in \mathbb{R}^2 \forall n, n' \in S^2 :$$

$$ k(g \cdot (y, n); g \cdot (y', n')) = k(y, n; y', n'). $$

Proof The first part of the lemma follows by the general Dunford-Pettis Theorem (Bukhvalov and Arendt 1994, pp. 113–114). With respect to the left-invariance we note that on the one hand we have

$$ (K_k \Omega_g U)(y, n) $$

$$ = \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} k(y, n; y'', n'') $$

$$ \times U(R^{-1}(y'' - x), R^{-1}n'') d\sigma(n'') $$

$$ = \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} k(y, n; Ry' + x, Rn')U(y', n')d\sigma(n') $$

$$ = \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} k(y, n; g \cdot (y', n'))U(y', n')d\sigma(n') $$

whereas on the other hand $(\Omega_g K U)(y, n) = \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} k(g^{-1}(y, n); y', n')U(y', n')d\sigma(n')$, for all $g \in SE(3)$, $U \in L_2(\mathbb{R}^2 \times S^2)$, $(x, n) \in \mathbb{R}^2 \times S^2$. Now $SE(3)$ acts transitively on $\mathbb{R}^3 \times S^2$ from which the result follows. \( \square \)

From the invariance property, (8), we deduce that

$$ k(y, n; y', n') $$

$$ = k((R_{e_\alpha y} R_{e_\beta})^T(y - y'), (R_{e_\alpha y} R_{e_\beta})^T n; 0, e_\epsilon), $$

$$ k(R_{e_\alpha y} R_{e_\alpha n}; 0, e_\epsilon) = k(y, n; 0, e_\epsilon), $$

and consequently we obtain the following result:

Corollary 1 By the well-known Euler-angle parametrization of $SO(3)$, we have $SO(3)/SO(2) \equiv S^2$ via isomorphism $[R_{e_\beta} R_{e_\gamma}] = [R_{e_\beta} R_{e_\gamma} R_{e_\alpha} | \alpha \in [0, 2\pi)] \leftrightarrow n(\beta, \gamma) = (\sin \beta \cos \gamma, \sin \beta \sin \gamma, \cos \beta)^T = R_{e_\beta} R_{e_\gamma} R_{e_\alpha} e_\epsilon.$

To each positive left-invariant kernel $k : \mathbb{R}^3 \times S^2 \times \mathbb{R}^3 \times S^2 \rightarrow \mathbb{R}^+$ with $\int_{\mathbb{R}^3} \int_{S^2} k(0, e_\epsilon; y, n)d\sigma(n) = 1$ we associate a unique probability density $p : \mathbb{R}^3 \times S^2 \rightarrow \mathbb{R}^+$ with the invariance property

$$ p(y, n) = p(R_{e_\alpha y} R_{e_\alpha n}), \quad \text{for all } \alpha \in [0, 2\pi), $$

such that

$$ k(y, n(\beta, \gamma); y', n(\beta', \gamma')) $$

$$ = p((R_{e_\beta} R_{e_\gamma})^T(y - y'), (R_{e_\beta} R_{e_\gamma})^T n(\beta, \gamma)) $$

with $p(y, n) = k(y, n; 0, e_\epsilon).$ We can briefly rewrite (Franken 2008, (7.59)) and (7), coordinate-independently, as

$$ K_k U(y, n) = (p *_{\mathbb{R}^3 \times S^2} U)(y, n) $$

$$ = \int_{\mathbb{R}^3} \int_{S^2} p(R_{n}^T(y - y'), R_{n}^T n)U(y', n')d\sigma(n')d\epsilon', $$

where $\sigma$ denotes the surface measure on the sphere and where $R_{n}^T$ is any rotation such that $n' = R_{n} e_\epsilon$.  

\( \square \) Springer
By the invariance property (9), the convolution (10) on $\mathbb{R}^3 \times S^2$ may be written as a (full) $SE(3)$-convolution. An $SE(3)$ convolution (Chirikjian and Kyatkin 2001) of two functions $\tilde{p} : SE(3) \to \mathbb{R}$, $U : SE(3) \to \mathbb{R}$ is given by:

$$ (\tilde{p} *_{SE(3)} U)(g) = \int_{SE(3)} \tilde{p}(h^{-1} g) U(h) d\mu_{SE(3)}(h), \quad (11) $$

where Haar-measure $d\mu_{SE(3)}(x, R) = dxd\mu_{SO(3)}(R)$ with $\mu_{SO(3)}(R_{e\gamma}, y R_{e\gamma}, \beta R_{e\gamma, \alpha}) = \sin \beta d\alpha d\beta dy$. If we now set $\tilde{p}(x, R) \equiv p(x, Re_z)$ and $U(x, R) \equiv U(x, Re_z)$, it follows by (9) that the following identity holds:

$$ (\tilde{p} *_{SE(3)} U)(x, R) = 2\pi (p *_{\mathbb{R}^3 \times S^2} U)(x, Re_z). \quad (12) $$

Later on in this article (in Sects. 4.2 and 4.3) we will relate scale spaces on HARDI data and first order Tikhonov regularization on HARDI data to Markov processes. But in order to provide a road map of how the $\mathbb{R}^3 \times S^2$-convolutions will appear in the more technical remainder of this article we provide some preliminary explanations on probabilistic interpretation of $\mathbb{R}^3 \times S^2$-convolutions.

In particular we will restrict ourselves to conditional probabilities where $p_t(y, n) = p_t(y, n)$ represents the probability density of finding an oriented random walker at position $y$ with orientation $n$ at time $t > 0$, given that it started at $(0, e_z)$ at time $t = 0$. In such a case the probabilistic interpretation of the kernel operator is as follows. The function $(y, n) \mapsto (K_k U)(y, n) = (p_t *_{\mathbb{R}^3 \times S^2} U)(y, n)$ represents the probability density of finding some oriented particle, starting from the initial distribution $U : \mathbb{R}^3 \times S^2 \to \mathbb{R}^+$ at time $t = 0$, at location $y \in \mathbb{R}^3$ with orientation $n \in S^2$ at time $t > 0$. Furthermore, in a Markov process traveling time is memoryless, so in such process traveling time is negatively exponentially distributed $P(T = t) = \lambda e^{-\lambda t}$ with expectation $E(T) = 1/\lambda$. Consequently, the probability density $p^k_t$ of finding an oriented random walker starting from $(0, e_z)$ at time $t = 0$, regardless its traveling time equals

$$ p^k_t(y, n) = \int_0^\infty p_t(y, n) P(T = t) dt = \lambda \int_0^\infty p_t(y, n) e^{-\lambda t} dt. \quad (12) $$

Summarizing, we can always apply Laplace-transform with respect to time to map transition densities $p_t(g)$ given a traveling time $t > 0$ to unconditional probability densities $p^k(g)$. The same holds for the probability density $P^k(y, n)$ of finding an oriented random walker at location $y \in \mathbb{R}^3$ with orientation $n \in S^2$ starting from initial distribution $U$ (i.e. the HARDI data) regardless the traveling time, since

$$ P^k_t(y, n) = \lambda \int_0^\infty e^{-\lambda t} (p_t *_{\mathbb{R}^3 \times S^2} U)(y, n) dt = (p_k *_{\mathbb{R}^3 \times S^2} U)(y, n). \quad (13) $$

### 3.1 Relation of the Method Proposed by Barmpoutsou et al. to $\mathbb{R}^3 \times S^2$-Convolution

In Barmpoutsou et al. (2008) the authors propose the following practical decomposition for the kernel $k$:

$$ k^l \cdot (y, n; y', n') = \frac{1}{4\pi} k^l_{\text{dist}}(\|y - y'\|) \cdot k^e_{\text{orient}}(n \cdot n'). $$

$$ k^k_{\text{fiber}} \left( \frac{1}{\|y - y'\|} \cdot n \cdot (-(y - y')) \right). \quad (14) $$

with $k^l_{\text{dist}}(\|y - y'\|) = \frac{1}{(4\pi)^{\frac{d}{2}}} e^{-\frac{(y - y')^2}{4}}$ and $k^e_{\text{orient}}(\cos \phi) = k^k_{\text{fiber}}(\cos \phi) = \frac{e^{\cos \phi}}{2\pi \sin \phi}$ with $\phi \in (-\pi, \pi]$ the angle, respectively, between the vectors $n$ and $n'$ and the angle between the vectors $n$ and $-y'$. So $k^e_{\text{orient}}(\cos \phi)$ denotes the von Mises distribution on the circle, which is indeed positive and $\int_{-\pi}^{\pi} \frac{e^{\cos \phi}}{2\pi \sin \phi} d\phi = 1$. The decomposition (14) automatically implies that the corresponding kernel operator $K_k$ is left-invariant, regardless the choice of $k^l_{\text{dist}}$, $k^e_{\text{orient}}$, $k^k_{\text{fiber}}$ since

$$ k^e_{\text{dist}}(\|R^{-1}(y - x) - R^{-1}(y' - x)\|) \cdot k^e_{\text{orient}}(R^{-1}n \cdot R^{-1}n') $$

$$ k^k_{\text{fiber}} \left( \frac{1}{\|R^{-1}(y - x) - R^{-1}(y' - x)\|} \cdot R^{-1}(y - x - (y' - x)) \right) $$

$$ = k^l_{\text{dist}}(\|y - y'\|) \cdot k^e_{\text{orient}}(n \cdot n') $$

$$ k^k_{\text{fiber}} \left( \frac{1}{\|y - y'\|} \cdot n \cdot (-(y - y')) \right) \iff k^l \cdot (g^{-1}(y, n); g^{-1}(y', n')) = k^l \cdot (y, n; y', n'), $$

for all $g = (x, R) \in SE(3)$.

The corresponding probability kernel (which does satisfy (9)) reads

$$ p_{(t, \lambda)}(y, n) = \frac{1}{4\pi} k^l_{\text{dist}}(\|y\|) k^e_{\text{orient}}(e_z \cdot n) k^k_{\text{fiber}}(-\|y\|^{-1}n \cdot y), \quad y \neq 0. \quad (15) $$

For a simple probabilistic interpretation we apply a spatial reflection and define $p^+_{(t, \lambda)}(y, n) = p_{(t, \lambda)}(y, n)$. Now $p^+_{(t, \lambda)}$ should be interpreted as a probability density of finding an oriented particle at position $y \in \mathbb{R}^3$ with orientation $n \in S^2$ given that it started at position $0$ with orientation $e_z$. The practical rationale behind the decomposition (14), is that two neighboring local orientations $(y, n) \in \mathbb{R}^3 \times S^2$.

2We used slightly different conventions as in the original paper to ensure $L_1$-normalizations in (14).

3Later on in Sect. 8.2.1 we will return to the important practical consequences of this spatial reflection in full detail.
\[n = \text{ent} \]tions to a reasonable connectivity measure between two local ori-

\[\text{finite maximum of the kernel is now obtained at } y\]

\[\text{Set } R_{238} \text{ Int J Comput Vis (2011) 92: 231–264}\]

\[n = \text{finite maximum of the kernel is now obtained at } y\]

\[\text{singularity at the origin convolution with itself will allow the}

\[k_{\text{fiber}}^k\]

\[\text{kernel is not entirely suited for iteration unless combined}

\[\text{oriented kernel operator has the right covariance properties, the}

\[\text{process (Duits and van Almsick 2008) and its approximations}

\[\text{thorner and Williams 2000; Duits and Franken 2009;}

\[\text{before we consider scale spaces on HARDI data whose}

\[\text{process (Duits and van Almsick 2008) and its approximations}

\[\text{3.2 Introductory Example: Scale Space and Tikhonov}

\[\text{the Gaussian scale space equation and corresponding resol-

\[\text{circle, } T \equiv \{e^{i\theta} \mid \theta \in [0, 2\pi]\} \equiv S^1 \text{ with group product}

\[e^{i\theta_1} e^{i\theta_2} = e^{i(\theta_1 + \theta_2)} \}

\[\left\{ \begin{array}{l}
\partial_t u(\theta, t) = D_{11} \partial^2_{\theta} u(\theta, t), \\
u(0, t) = u(2\pi, t) \text{ and } u(\theta, 0) = f(\theta) \end{array} \right. \]

\[p_{\gamma}(\theta) = \gamma(D_{11} \partial^2_{\theta} - \gamma I)^{-1} f(\theta), \]

\[\text{under the periodicity condition } p_{\gamma}(0) = p_{\gamma}(2\pi) \text{. By left-}

\[\mathcal{E}(p_{\gamma}) := \int_0^{2\pi} \gamma|p_{\gamma}(\theta) - f(\theta)|^2 + D_{11}|p_{\gamma}'(\theta)|^2 d\theta \]

\[\mathcal{E}(p_{\gamma}) := \int_0^{2\pi} \gamma|p_{\gamma}(\theta) - f(\theta)|^2 + D_{11}|p_{\gamma}'(\theta)|^2 d\theta \]

\[\text{under the periodicity condition } p_{\gamma}(0) = p_{\gamma}(2\pi) \text{. By left-}

\[\mathcal{E}(p_{\gamma}) := \int_0^{2\pi} \gamma|p_{\gamma}(\theta) - f(\theta)|^2 + D_{11}|p_{\gamma}'(\theta)|^2 d\theta \]

\[\mathcal{E}(p_{\gamma}) := \int_0^{2\pi} \gamma|p_{\gamma}(\theta) - f(\theta)|^2 + D_{11}|p_{\gamma}'(\theta)|^2 d\theta \]
with their Green’s function, say \( G^{D_{11}}_t : \mathbb{T} \to \mathbb{R}^+ \) and \( R^{D_{11}}_{\gamma} : \mathbb{T} \to \mathbb{R}^+ \). Recall that the relation between Tikhonov regularization and scale space theory is given by Laplace-transform with respect to time:

\[
u(\cdot, t) = e^{t \Delta_T} f := G_t *_{\mathbb{T}} f \quad \text{and} \quad p_{\gamma} = R^{D_{11}}_{\gamma} *_{\mathbb{T}} f,
\]

with \( R^{D_{11}}_{\gamma} = \gamma \int_0^{\infty} G_{t}^{D_{11}} e^{-t \gamma} \mathrm{d}t, \quad (18)\)

where the \( \mathbb{T} \)-convolution is given by \((f *_{\mathbb{T}} g)(e^{i\theta}) = \int_{\mathbb{T}} f(e^{i\theta-\theta'}) g(e^{i\theta'}) \mathrm{d}\theta'\). For explicit formulas of the Green’s function \( G^{D_{11}}_t \) (basically a sum of 2\(\pi\)-shifted Gaussians) and the Green’s function \( R^{D_{11}}_{\gamma} \) see Duits and Franken (2009, Chap. 3.2). Now by \( e^{s \Delta_T} e^{t \Delta_T} = e^{(s+t) \Delta_T} \) the heat-kernel on \( \mathbb{T} \) satisfies the (for iterations) important semigroup property:

\[G^{D_{11}}_s *_{\mathbb{T}} G^{D_{11}}_t = G^{D_{11}}_{s+t}, \quad \text{for all} \ s, t > 0.\]

The generator of a Gaussian scale space on the torus is given by \( D_{11} \frac{\partial^2}{\partial s^2} \). Just like the solution operator \((D_{11} \frac{\partial^2}{\partial s^2} - \lambda I)^{-1}\) of Tikhonov regularization is left-invariant on the group \( \mathbb{T} \) and thereby the solutions (18) of a Gaussian Scale Space and Tikhonov regularization are given by \( \mathbb{T} \)-convolution. In order to generalize scale space representations of functions on a torus to scale space representations of HARDI data defined on \( \mathbb{R}^3 \times S^2 \) (embedded in \( SE(3) = \mathbb{R}^3 \times SO(3) \)), we simply have to replace the left-invariant vector field \( \partial_0 \) on the group \( \mathbb{T} \) by the left-invariant vector fields on \( SE(3) \) (or rather \( \mathbb{R}^3 \times S^2 \)) in the quadratic form which generates the scale space on the group, (Duits and Burgeth 2007). This motivates the technical derivations of the left-invariant vector fields on \( SE(3) \) in the next subsection.

3.3 Left-invariant Vector Fields on \( SE(3) \) and their Dual Elements

We will use the following basis for the tangent space \( T_e(SE(3)) \) at the unity element \( e = (0, I) \in SE(3) \):

\[
A_1 = \partial_x, \quad A_2 = \partial_y, \quad A_3 = \partial_z, \\
A_4 = \partial_{\gamma}, \quad A_5 = \partial_{\theta}, \quad A_6 = \partial_{\phi}. \quad (19)
\]

where we stress that at the unity element \((0, R = I)\), we have \( \beta = 0 \) and here the tangent vectors \( \partial_{\theta} \) and \( \partial_{\phi} \) are not defined, which requires a description of the tangent vectors on the \( SO(3) \)-part by means of the second chart.

The tangent space at the unity element is a 6D Lie algebra equipped with Lie bracket

\[\{A, B\} = \lim_{t \to 0} t^{-2} (a(t)b(t)(a(t))^{-1}(b(t))^{-1} - e), \quad (20)\]

where \( t \mapsto a(t) \) resp. \( t \mapsto b(t) \) are any smooth curves in \( SE(3) \) with \( a(0) = b(0) = e \) and \( a'(0) = A \) and \( b'(0) = B \), for explanation on the formula (20) which holds for general matrix Lie groups, see Duits et al. (2009, App. G). The Lie-brackets of the basis given in (19) are given by

\[
[A_i, A_j] = \sum_{k=1}^{6} c^k_{ij} A_k, \quad (21)
\]

where the non-zero structure constants for all three isomorphic Lie-algebras are given by

\[
c^k_{ij} = \begin{cases} 
\text{sgn perm}(i - 3, j - 3, k - 3) & \text{if } i, j, k \geq 4, \ i \neq j \neq k, \\
\text{sgn perm}(i, j - 3, k) & \text{if } i, k \leq 3, \ j \geq 4, \ i \neq j \neq k.
\end{cases} \quad (22)
\]

More explicitly, we have the following table of Lie-brackets:

\[
([A_i, A_j])^{i,j=1,\ldots,6} = \begin{pmatrix}
0 & 0 & 0 & 0 & A_3 & -A_2 \\
0 & 0 & 0 & -A_3 & 0 & A_1 \\
0 & 0 & 0 & A_2 & -A_1 & 0 \\
0 & A_3 & 0 & A_1 & -A_6 & 0 \\
-A_3 & 0 & A_1 & -A_6 & 0 & A_4 \\
A_2 & -A_1 & 0 & A_5 & -A_4 & 0
\end{pmatrix},
\]

so for example \( c^4_{15} = 1, c^3_{14} = c^2_{15} = 0, c^2_{16} = -c^2_{61} = -1 \).

The corresponding left-invariant vector fields \( [A_i]_{i=1}^{6} \) are obtained by the push-forward of the left-multiplication \( L_g h = g h \) by \( A_i|_g \phi = (L_g)_* A_i \phi = A_i(\phi \circ L_g) \) for all smooth \( \phi : \Omega_g \to \mathbb{R} \) which are locally defined on some neighborhood \( \Omega_g \) of \( g \) and they can be obtained by the derivative of the right-regular representation:

\[
A_i|_g \phi = \frac{\partial R(A_i) \phi}{\partial t} \big|_{t=0} = \frac{\phi(g e^{t A_i}) - \phi(g)}{t},
\]

with \( R_g \phi(h) = \phi(h g) \). \( \quad (23) \)

Expressed in the first coordinate chart, (1), this renders for the left-invariant derivatives at position \( g = (x, y, z, R_{e, \gamma} R_{e, \beta} R_{e, \alpha}) \in SE(3) \) (see also Chirikjian and Kyatkin 2001, Sect. 9.10)

\[
A_1 = (\cos \alpha \cos \beta \cos \gamma - \sin \alpha \sin \gamma) \partial_x + (\sin \alpha \cos \gamma + \cos \alpha \cos \beta \sin \gamma) \partial_y - \cos \alpha \sin \beta \partial_z,
\]

\[
A_2 = (-\sin \alpha \cos \beta \cos \gamma - \cos \alpha \sin \gamma) \partial_x + (\cos \alpha \cos \gamma - \sin \alpha \cos \beta \sin \gamma) \partial_y + \sin \alpha \sin \beta \partial_z,
\]

\[
A_3 = \sin \beta \cos \gamma \partial_x + \sin \beta \sin \gamma \partial_y + \cos \beta \partial_z,
\]

\[
A_4 = \cos \alpha \cot \beta \partial_x + \sin \alpha \partial_y - \cos \alpha \sin \beta \partial_z,
\]

\[
A_5 = -\sin \alpha \cot \beta \partial_x + \cos \alpha \partial_y + \frac{\sin \alpha}{\sin \beta} \partial_z,
\]

\[
A_6 = \partial_z.
\]
for $\beta \neq 0$ and $\beta \neq \pi$. The explicit formulae of the left-invariant vector fields (which are well-defined in north- and south-pole) in the second chart, (4), are:

$$\begin{align*}
A_1 &= \cos \alpha \cos \beta \partial_x + (\cos \gamma \sin \alpha + \cos \alpha \sin \beta \sin \gamma) \partial_y + (\sin \alpha \sin \gamma - \cos \alpha \cos \beta \sin \gamma) \partial_z, \\
A_2 &= -\sin \alpha \cos \beta \partial_x + (\cos \alpha \cos \gamma - \sin \alpha \sin \beta \sin \gamma) \partial_y + (\sin \alpha \sin \beta \cos \gamma + \cos \alpha \sin \gamma) \partial_z, \\
A_3 &= \sin \beta \partial_x - \cos \beta \sin \gamma \partial_y + \cos \beta \cos \gamma \partial_z, \\
A_4 &= -\cos \alpha \tan \beta \partial_x + \sin \alpha \partial_y + \frac{\cos \alpha}{\cos \beta} \partial_z, \\
A_5 &= \sin \alpha \tan \beta \partial_x + \cos \alpha \partial_y - \frac{\sin \alpha}{\cos \beta} \partial_z, \\
A_6 &= \partial_x,
\end{align*}$$

for $\beta \neq \frac{\pi}{2}$ and $\beta \neq -\frac{\pi}{2}$. Note that $d\mathcal{R}$ is a Lie-algebra isomorphism, i.e.

$$[A_i, A_j] = \sum_{k=1}^{6} c_{ij}^k A_k$$

$$\iff [d\mathcal{R}(A_i), d\mathcal{R}(A_j)] = \sum_{k=1}^{6} c_{ij}^k d\mathcal{R}(A_k)$$

$$\iff [A_i, A_j] = A_i A_j - A_j A_i = \sum_{k=1}^{6} c_{ij}^k A_k.$$ 

These vector fields form a local moving coordinate frame of reference on $SE(3)$, the corresponding dual frame $\{dA_1, \ldots, dA_6\} \in (T(SE(3)))^*$ is defined by

$$\langle dA_i', A_j \rangle := dA_i'(A_j) = \delta_{ij}, \quad i, j = 1, \ldots, 6,$$

where $\delta_{ij}$ is 1 if $i = j$ and zero else. A brief computation yields the following dual frame (in both coordinate charts):

$$\begin{pmatrix}
\frac{dx}{\gamma} \\
\frac{dy}{\gamma} \\
\frac{dz}{\gamma} \\
\frac{d\alpha}{\gamma} \\
\frac{d\beta}{\gamma} \\
\frac{d\gamma}{\gamma}
\end{pmatrix} = \begin{pmatrix}
0 & \sin \alpha & -\cos \alpha \sin \beta \\
0 & \cos \alpha & \sin \alpha \sin \beta \\
1 & 0 & \cos \beta
\end{pmatrix}$$

Finally, we note that by linearity the $i$-th dual vector filters out the $i$-th component of a vector field $\sum_{j=1}^{6} v^j A_j$

$$\left( dA_i', \sum_{j=1}^{6} v^j A_j \right) = v^i, \quad \text{for all } i, j = 1, \ldots, 6.$$

### 4 Left-Invariant Diffusions on $SE(3) = \mathbb{R}^3 \ltimes SO(3)$ and $\mathbb{R}^3 \ltimes S^2$

In order to apply our general theory on diffusions on Lie groups, (Duits and Burgeth 2007), to suitable (convexion-)diffusions on HARDI images, we naturally extend all functions $U: \mathbb{R}^3 \ltimes S^2 \to \mathbb{R}^+$ to functions $\tilde{U}: \mathbb{R}^3 \ltimes SO(3) \to \mathbb{R}^+$

$$\tilde{U}(x, R) = U(x, Re_\gamma) \quad \text{or in Euler angles:}$$

$$\tilde{U}(x, R_{e_{\beta}, \gamma} R_{e_{\gamma}, \beta} R_{e_{\alpha}, \beta}) = U(x, n(\beta, \gamma)).$$

**Definition 4** We will call $\tilde{U}: \mathbb{R}^3 \ltimes SO(3) \to \mathbb{R}$, given by (27), the HARDI-orientation score corresponding to HARDI image $U: \mathbb{R}^3 \ltimes S^2 \to \mathbb{R}$.

Here we note that the function $\tilde{U}$ in general is not equal to the wavelet transform of some image $f: \mathbb{R}^d \to \mathbb{R}$, in contrast to our previous works on invertible orientations of 2D images (Franken 2008; van Almsick 2005; Duits and van Almsick 2008; Duits and Franken 2010) and invertible orientation scores of 3D images (Duits et al. 2007).

We follow our general construction of scale space representations $\tilde{W}$ of functions $\tilde{U}$ defined on Lie groups (Duits and Burgeth 2007), where we consider the special case $SE(3) = \mathbb{R}^3 \ltimes SO(3)$:

$$\begin{align*}
\partial_t \tilde{W}(g, t) &= Q^{D, a}(A_1, A_2, \ldots, A_6) \tilde{W}(g, t), \\
\lim_{t \to 0} \tilde{W}(g, t) &= \tilde{U}(g)
\end{align*}$$
which is generated by a quadratic form on the left-invariant vector fields:

\[ Q^{D_{ia}}(A_1, A_2, \ldots, A_6) = \sum_{i=1}^{6} -a_i A_i + \sum_{i,j=1}^{6} A_i D_{ij} A_j \]  

(29)

Now the Hörmander requirement, (Hormander 1968), on the symmetric \( D = [D_{ij}] \in \mathbb{R}^{6 \times 6} \), \( D \geq 0 \) and \( a \), which guarantees smooth non-singular space for \( SE(3) \), tells us that \( D \) need not be strictly positive definite. The Hörmander requirement is that all included generators together with their commutators should span the full tangent space. To this end for diagonal \( D \) one should consider the set

\[ S = \{ i \in \{1, \ldots, 6\} | D_{ii} \neq 0 \lor a_i \neq 0 \}, \]

now if for Example 1 is not in here then 3 and 5 must be in \( S \), or if 4 is not in \( S \) then 5 and 6 should be in \( S \). Following the general theory (Duits and Burgeth 2007) we note that if the Hörmander condition is satisfied the solutions of the linear diffusions (i.e. \( D, a \) are constant) are given by \( SE(3) \)-convolution with a smooth probability kernel \( p_t^{D, a} : SE(3) \rightarrow \mathbb{R}^+ \) such that

\[ \tilde{W}(g, t) = (p_t^{D, a} *_{SE(3)} \tilde{U})(g) \]

\[ = \int_{SE(3)} p_t^{D, a}((h^{-1} g)\tilde{U}(h))d\mu_{SE(3)}(h), \]

\[ \lim_{t \downarrow 0} p_t^{D, a} *_{SE(3)} \tilde{U} = \tilde{U}, \]

with \( p_t^{D, a} > 0 \) and \( \int_{SE(3)} p_t^{D, a}(g)d\mu_{SE(3)}(g) = 1, \)

where the limit is taken in \( L_2(SE(3)) \)-sense.

The left-invariant diffusions on the group \( SE(3) \) also give rise to left-invariant scale spaces on the homogeneous space \( \mathbb{R}^3 \rtimes S^2 \equiv SE(3)/(\{0\} \times SO(2)) \) within the group. There are however, two important issues to be taken into account:

1. If we apply the diffusions directly to HARDI-orientation scores we can as well delete the last direction in our diffusions because clearly \( A_6 = \partial_\alpha \) vanishes on functions which are not dependent on \( \alpha \), i.e. \( \partial_\alpha \tilde{U} = 0 \).

2. In order to naturally relate the (convection-)diffusions on HARDI-orientation scores, to (convection-)diffusions on HARDI images we have to make sure that the evolution equations are well defined on the cosets \( SO(3)/SO(2) \), meaning that they do not depend on the choice of representative in the classes.

Next we formalize the second condition on diffusions on HARDI-orientation scores more explicitly. A movement along the equivalence classes \( SO(3)/SO(2) \) is done by right multiplication with the subgroup \( \text{Stab}(e_\alpha) \equiv SO(2) \), with \( \text{Stab}(e_\alpha) = \{ A \in SO(3) | A e_\alpha = e_\alpha \} \). Therefore our diffusion operator \( \Phi_t \) which is the transform that maps the HARDI-orientation score \( \tilde{U} : \mathbb{R}^3 \times SO(3) \rightarrow \mathbb{R}^+ \) to a diffused HARDI-orientation score \( \Phi_t(\tilde{U}) = e^t Q^{D_{ia}} \tilde{U} \), with stopping time \( t > 0 \), should satisfy

\[ (\Phi_t \circ R_h)(\tilde{U}) = \Phi_t(\tilde{U}) \]

(30)

for all \( h \in \text{Stab}(e_\alpha) \equiv SO(2) \), where \( R_h \tilde{U}(g) = \tilde{U}(gh) \).

Now (30) is satisfied iff

\[ R_0 \circ R_{e_\alpha \cdot a} \circ Q^{D_{ia}}(A_1, \ldots, A_6) = Q^{D_{ia}}(A_1, \ldots, A_6). \]

(31)

Note that (30) and (31) are equivalent to

\[ (Q^{D_{ia}}(A)\tilde{W}(\cdot, \cdot, t))(g) = (Q^{D_{ia}}(A)\tilde{W}(\cdot, \cdot, t))(gh) \]

for all \( g \in SE(3) \), \( t > 0 \), \( h = (0, R_{e_\alpha \cdot a}) \) where \( A = (A_1, \ldots, A_6)^T \) and observe that \( A_{g \cdot h} \tilde{U} = Z_\alpha Z_a \tilde{U} \) with

\[ Z_\alpha = \begin{pmatrix} \cos \alpha & - \sin \alpha & 0 & 0 & 0 & 0 \\ \sin \alpha & \cos \alpha & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \cos \alpha & - \sin \alpha & 0 \\ 0 & 0 & 0 & \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \]

\[ = R_{e_\alpha \cdot a} \oplus R_{e_\alpha \cdot a}, \quad Z_a \in SO(6), \quad R_{e_\alpha \cdot a} \in SO(3). \]

(32)

Hence for constant \( D \) and \( a \) (i.e. linear diffusion on the HARDI data) the requirement (31) simply reads

\[ Q^{D_{ia}}(A) = Q^{D_{ia}}(Z_a A) = Q^{(Z_a)}(Z_a \alpha)(Z_a \alpha) (A) \]

\[ \Leftrightarrow \quad a = Z_a a \quad \text{and} \quad D = Z_a D Z_a^T, \]

(33)

which by Schur’s lemma is the case if

\[ a^1 = a^2 = a^4 = a^5 = a^6 = 0 \quad \text{and} \quad D = \text{diag}[D_{11}, D_{11}, D_{33}, D_{44}, D_{44}, D_{66} = 0]. \]

(34)

Analogously, for adaptive nonlinear diffusions, that is \( D \) and \( a \) not constant but depending on the initial condition \( \tilde{U} \), i.e. \( D(\tilde{U}) : SE(3) \rightarrow \mathbb{R}^{6 \times 6} \), with \( (D(\tilde{U}))^T = D(\tilde{U}) > 0 \) and \( a(\tilde{U}) \) the requirement (31) simply reads

\[ a(\tilde{U})(gh) = Z_a^T (a(\tilde{U}))(g) \quad \text{and} \quad D(\tilde{U})(gh) = Z_a D(\tilde{U})(g) Z_a^T. \]

(35)

for all \( g \in SE(3) \), \( h = (0, R_{e_\alpha \cdot a}) \). Summarizing all these results we conclude on HARDI data whose domain equals the homogeneous space \( \mathbb{R}^3 \times S^2 \) one has the following scale space representations:

\[ \partial_t W(y, n, t) = Q^{D(U)}(A_1, A_2, \ldots, A_5, A_6) W(y, n, t), \]

\[ W(y, n, 0) = U(y, n) \]

(36)
with $Q^{D(U),a(U)}(A_1, A_2, \ldots, A_5, A_6) = \sum_{j=1}^{5} (-a_i A_i + \sum_{j=1}^{5} A_i D_{ij}(U) A_j)$, where from now on we assume that $D(U)$ and $a(U)$ satisfy (35). In the linear case where $D(U) = D$, $a(U) = a$ this means that we shall automatically assume (34). In this case the solutions of (36) are given by the following kernel operators on $\mathbb{R}^3 \times S^2$:

$$W(y, n, t) = \left( p_t^{D,a} * \mathbb{R}^3 \times S^2 \right) U(y, n)$$

$$= \int_{0}^{\pi} \int_{0}^{2\pi} \int_{\mathbb{R}^3} p_t^{D,a} \left( (R_{e,y} \gamma R_{e,y'})^T (y - y'), \right.$$

$$\left. (R_{e,y} \gamma R_{e,y'})^T n \right) \cdot U(y', n(\beta', \gamma')) \, dy' \, \, d\sigma(n(\beta', \gamma')),$$  \tag{37}

where the surface measure on the sphere is given by $d\sigma(n(\beta', \gamma')) = \sin \beta' \, dy' \, d\beta' \equiv d\sigma(\bar{n}(\beta, \gamma)) = |\cos \beta| \, d\beta \, d\gamma$. Now in particular in the linear case, since $(\mathbb{R}^U, I)$ and $(\mathbf{0}, SO(3))$ are subgroups of $SE(3)$, we obtain the Laplace-Beltrami operators on these subgroups by means of:

$$\Delta_{S^2} = Q^{D} = diag[0, 0, 0, 0, 1], a = 0 \quad (A)$$

$$= (A_4)^2 + (A_5)^2 + (A_6)^2$$

$$= (\partial_\beta)^2 + \cot(\beta) \partial_\beta + \sin^{-2}(\beta) (\partial_\gamma)^2,$$

$$\Delta_{S^3} = Q^{D} = diag[1, 1, 1, 0, 0, 0], a = 0 \quad (A)$$

$$= (A_1)^2 + (A_2)^2 + (A_3)^2$$

$$= (\partial_x)^2 + (\partial_y)^2 + (\partial_z)^2.$$

Remark Recall that in the linear case we assumed (34) to ensure (31) so that (30) holds. It is not difficult to show, (Franken 2008, p. 170), that this implies the required symmetry (9) on the convolution kernel.

4.1 Special Cases of Linear Left-invariant Diffusion on $\mathbb{R}^3 \times S^2$

If we consider the singular case $D = diag[1, 1, 1, 0, 0, 0]$, $a = 0$ (not satisfying the Hörmander condition) we get the usual scale space in the position part only

$$W(y, n, t) = (e^{t \Delta} U(\cdot, n))(y)$$

$$= \mathcal{F}_{R^3}^{-1} \left[ \frac{e^{-|\omega|^2}}{(2\pi)^2} \mathcal{F}_{R^3} f(\omega) \right](y)$$

$$= (G_t * f)(y), \quad \text{with } G_t(y) = (4\pi t)^{-\frac{3}{2}} e^{-\frac{|y|^2}{4t}}$$

and consequently on $\mathbb{R}^3 \times S^2$ we have the singular distributional kernel $p_t^{D,a}(y, n) = G_t(y) \delta_{\mathbf{0}}(n)$, in (37).

If we consider the singular case $D = diag[0, 0, 0, 1, 1, 1]$, $a = 0$ we get the usual scale space on the sphere:

$$W(y, n(\beta, \gamma), t) = (e^{t \Delta_{S^2}} U(\cdot, \cdot))(x)$$

$$= e^{t \Delta_{S^2}} \sum_{l=-\infty}^{\infty} \sum_{m=-l}^{l} (Y_{lm}, U) Y_{lm}(\beta, \gamma)$$

$$= \sum_{l=0}^{\infty} (Y_{lm}, U) e^{t \Delta_{S^2}} Y_{lm}(\beta, \gamma)$$

where we note that the well-known spherical harmonics $(Y_{lm})_{l=0, \ldots, \infty}$ form an orthonormal basis of $L^2(S^2)$ and $\Delta_{S^2} Y_{lm} = -(l + 1) Y_{lm}$. Recall

$$Y_{lm}^m(\beta, \gamma) = \sqrt{(2l + 1)/(4\pi(1 + |m|)!)} P_l^{m}(\cos \beta) e^{im\gamma}$$

$$l \in \mathbb{N}, m = -l, \ldots, l.$$  \tag{38}

Consequently, on $\mathbb{R}^3 \times S^2$ we have the singular distributional kernel $p_t^{D,a}(y, n) = g_t(n) \delta_{\mathbf{0}}(y)$, in (37), where

$$g_t(n(\beta, \gamma)) = \sum_{l=0}^{\infty} (Y_{lm}, \beta, \gamma) Y_{lm}(\beta, \gamma) e^{-t(l+1)}$$

$$= \sum_{l=0}^{\infty} (P_l^{m}(\cos \beta))^2 \frac{(2l + 1)(l + |m|)!}{4\pi(1 + |m|)!} e^{-t(l+1)}.$$  

Note that in the two cases mentioned above diffusion takes place either only along the spatial part or only along the angular part, which is not desirable as one wants to include line-models which exploit a natural coupling between position and orientation. Such a coupling is naturally included in a smooth way as long as the Hörmander’s condition is satisfied. In the two previous examples, the Hörmander condition is violated since both the span of $\{A_1, A_2, A_3\}$ and the span of $\{A_4, A_5, A_6\}$ are closed Lie-algebras, i.e. all commutators are again contained in the same 3-dimensional subspace of the 6-dimensional tangent space. Therefore we will consider more elaborate left-invariant convection, diffusions on $SE(3)$ with natural coupling between position and orientation. To explain what we mean with natural coupling we shall need the next definitions.

**Definition 5** A curve $\gamma : \mathbb{R}^+ \rightarrow \mathbb{R}^3 \times S^2$ given by $s \mapsto \gamma(s) = (y(s), n(s))$ is called horizontal if $\|\dot{y}(s)\|^{-1} \dot{y}(s)$. A tangent vector to a horizontal curve is called a horizontal tangent vector. A vector field $A$ on
\[ \mathbb{R}^3 \times S^2 \] is horizontal if for all \((y, n) \in \mathbb{R}^3 \times S^2\) the tangent vector \(A_{(y, n)}\) is horizontal. The horizontal part \(H_x\) of each tangent space is the vector-subspace of \(T_y(SE(3))\) consisting of horizontal vector fields. Horizontal diffusion is diffusion which only takes place along horizontal curves.

It is not difficult to see that the horizontal part \(H_x\) of each tangent space \(T_y(SE(3))\) is spanned by \([A_3, A_4, A_5]\). So all horizontal left-invariant convection diffusions are given by (36) where one must set \(a_1 = a_2 = a_6 = 0, D_{j1} = D_{j2} = D_{ij} = D_{ij6} = D_{3ij} = 0\) for all \(j = 1, 2, \ldots, 6\). Now on a commutative group like \(\mathbb{R}^6\) with commutative Lie-algebra \([\delta_{s1}, \ldots, \delta_{s6}]\) omitting 3-directions (say \(\delta_{s1}, \delta_{s2}, \delta_{s3}\)) from each tangent space in the diffusion would yield no smoothing along the global \(x_1, x_2, x_6\)-axes. In \(SE(3)\) it is different since the commutators take care of indirect smoothing in the omitted directions \([A_1, A_2, A_6]\), since


Consider for example the \(SE(3)\)-analogues of the Forward-Kolmogorov (or Fokker-Planck) equations of the direction process for contour-completion and the stochastic process for contour enhancement which we considered in our previous works, (Duits and Franken 2010), on \(SE(2)\). Here we shall first provide the resulting PDEs and explain the underlying stochastic processes later in Sect. 4.2. The Fokker-Planck equation for (horizontal) \textit{contour completion} on \(SE(3)\) is given by

\[
\frac{\partial}{\partial t} W(y, n, t) = (-A_3 + D((A_4)^2 + (A_5)^2)) W(y, n, t) \]

\[
= (-A_3 + D\Delta_s^2) W(y, n, t), \quad D = \frac{1}{2}\sigma^2 > 0, \quad (39)
\]

\[
\lim_{t \downarrow 0} W(y, n, t) = U(y, n),
\]

where we note that \((A_6)^2(W(y, n(\beta, \gamma), s)) = 0\). This equation arises from (36) by setting \(D_{44} = D_{55} = D\) and \(a_3 = 1\) and all other parameters to zero. The Fokker-Planck equation for (horizontal) \textit{contour enhancement} is

\[
\frac{\partial}{\partial t} W(y, n, t) = (D_{33}(A_3)^2 + D_{44}((A_4)^2 + (A_5)^2)) W(y, n, t) \]

\[
= (D_{33}(A_3)^2 + D\Delta_s^2) W(y, n, t), \quad (40)
\]

\[
\lim_{t \downarrow 0} W(y, n, t) = U(y, n).
\]

The solutions of the left-invariant diffusions on \(\mathbb{R}^3 \times S^2\) given by (36) (with in particular (39) and (40)) are again given by convolution product (37) with a probability kernel \(p_t^{D, a}\) on \(\mathbb{R}^3 \times S^2\).

4.2 Brownian Motions on \(SE(3) = \mathbb{R}^3 \times SO(3)\) and on \(\mathbb{R}^3 \times S^2\)

Next we formulate a left-invariant discrete Brownian motion on \(SE(3)\) (expressed in the moving frame of reference). The left-invariant vector fields \([A_1, \ldots, A_6]\) form a moving frame of reference to the group. Here we note that there are two ways of considering vector fields. Either one considers them as differential operators on smooth locally defined functions, or one considers them as tangent vectors to equivalent classes of curves. These two viewpoints are equivalent, for formal proof see Aubin (2001, Prop. 2.4).

Throughout this article we mainly use the first way of considering vector fields, but in this section we prefer to use the second way. We will write \([e_1, e_2, e_6]\) for the left-invariant vector fields (as tangent vectors to equivalence classes of curves) rather than the differential operators \([A_1|_g, \ldots, A_6|_g]\). We obtain the tangent vector \(e_i\) from \(A_i\) by replacing

\[
\partial_x \leftrightarrow (1, 0, 0, 0, 0, 0),
\]

\[
\partial_y \leftrightarrow (0, 1, 0, 0, 0, 0),
\]

\[
\partial_z \leftrightarrow (0, 0, 1, 0, 0, 0),
\]

\[
\partial_{\partial_x} \leftrightarrow (0, 0, 0, \alpha \cos \beta \cos \gamma, \alpha \cos \beta \sin \gamma, -\alpha \sin \beta),
\]

\[
\partial_{\partial_y} \leftrightarrow (0, 0, 0, \alpha \cos \gamma, \alpha \sin \gamma, 0),
\]

\[
\partial_{\partial_z} \leftrightarrow (0, 0, 0, \cos \gamma \sin \beta, \sin \gamma \sin \beta, \cos \beta),
\]

where we identified \(SO(3)\) with a ball with radius \(2\pi\) whose outer-sphere is identified with the origin, using Euler angles \(R_{e_1, e_2, e_6} \leftrightarrow e_n\alpha(\beta, \gamma) \in B_{0, 2\pi}\). Next we formulate left-invariant discrete random walks on \(SE(3)\) expressed in the moving frame of reference \([e_i]_{i=1}^5\) given by (24) and (41):

\[
(Y_{n+1}, N_{n+1}) = (Y_n, N_n) + \Delta S \sum_{i=1}^5 a_i e_i |_{(Y_n, N_n)}
\]

\[
+ \sqrt{\Delta S} \sum_{i=1}^{5} \sum_{j=1}^{5} a_i e_j |_{(Y_n, N_n)}
\]

for all \(n = 0, \ldots, N - 1\),

\[
(Y_0, N_0) \sim U^D,
\]

with random variable \((Y_0, N_0)\) is distributed by \(U^D\), where \(U^D\) are the discretely sampled HARDI data (equidistant sampling in position and second order tessellation of the sphere) and where the random variables \((Y_n, N_n)\) are recursively determined using the independently normally distributed random variables \(\varepsilon_{i, n+1} |_{i=1, \ldots, 5}, \varepsilon_{n+1} \sim N(0, 1)\) and with stepsize \(\Delta S = \frac{\delta}{N}\) and where \(a := \sum_{i=1}^{5} a_i e_i\) denotes an a priori spatial velocity vector having constant coefficients \(a_i\) with respect to the moving frame of reference.
processes on $SE(3)$:

$$Y(t) = Y(0) + \int_0^t \left( \sum_{i=1}^3 a_i e_i \right) (Y(t), N(t)) \, dt,$$

$$N(t) = N(0) + \int_0^t \left( \sum_{j=4}^5 a_j e_j \right) (Y(t), N(t)) \, dt,$$

with $\varepsilon_i \sim \mathcal{N}(0,1)$ and $(X(0), N(0)) \sim U$ and where $\sigma = \sqrt{2D} \in \mathbb{R}^{6 \times 6}$, $\sigma > 0$. Note that $d\sqrt{\tau} = \frac{1}{2} \tau^{-\frac{1}{2}} \, dt$.

Now if we set $U = \delta_0 \varepsilon_i$ (i.e. at time zero) then suitable averaging of infinitely many random walks of this process yields the transition probability $(y, n) \mapsto p_{\lambda}^D(a)(y, n)$ which is the Green’s function of the left-invariant evolution equations (36) on $\mathbb{R}^3 \times S^2$. In general the PDEs (36) are the Forward Kolmogorov equation of the general stochastic process (42). This follows by Ito’s formula and in particular Ito’s formula for formulas on a stochastic process, see Chirikjian and Kyatkin (2001) and see van Almsick (2005, App. A) where one should consistently replace the left-invariant vector fields of $\mathbb{R}^n$ by the left-invariant vector fields on $\mathbb{R}^3 \times S^2$.

In particular we have now formulated the direction process for contour completion in $\mathbb{R}^3 \times S^2$ (i.e. non-zero parameters in (42) are $D_{44} = D_{55} > 0$, $a_3 > 0$ with Fokker-Planck equation given by (39)), and the (horizontal) Brownian motion for contour-enhancement in $\mathbb{R}^3 \times S^2$ (i.e. non-zero parameters in (42) are $D_{33} > 0$, $D_{44} = D_{55} > 0$ with Fokker-Planck equation given by (40)).

4.3 Tikhonov-Regularization of HARDI Images

In the previous subsection we have formulated the Brownian-motions (42) underlying all linear left-invariant convection-diffusion equations on HARDI data, with in particular the direction process for contour completion and (horizontal) Brownian motion for contour-enhancement. However, we only considered the time dependent stochastic processes and as mentioned before in Markov-processes traveling time is memoryless and thereby negatively exponentially distributed $T \sim \mathcal{N}E(\lambda)$, i.e. $P(T=t) = e^{-\lambda t}$ with expectation $E(T) = \frac{1}{\lambda}$, for some $\lambda > 0$. Recall our observations (12) and (13) and thereby by means of Laplace-transform with respect to time we relate the Fokker-Planck equations to their resolvent equations, as at least formally we have

$$W(y, n, t) = (e^{(Q^D_{a}A)}U)(y, n)$$

and

$$P_\gamma(y, n, t) = \lambda \int_0^\infty e^{-\lambda t}(e^{(Q^D_{a}A)}U)(y, n)dt = \lambda(\lambda I - Q^D_{aA})^{-1}U(y, n),$$

for $t, \lambda > 0$ and all $y \in \mathbb{R}^3$, $n \in S^2$, where the negative definite generator $Q^D_{a}$ is given by (29) and again with $AU = (A_1 U, \ldots, A_6 U)$. This is similar to our introductory example on the torus in Sect. 3.2. The resolvent operator $\lambda(\lambda I - Q^D_{aA})^{-1}$ occurs in a first order Tikhonov regularization as we show in the next theorem.

Theorem 2 Let $U \in L_2(\mathbb{R}^3 \times S^2)$ and $\lambda, D_{33} > 0, D_{44} = D_{55} > 0, D_{11} = D_{22} > 0$. Then the unique solution of the variational problem

$$\arg \min_{P \in \mathbb{P}(\mathbb{R}^3 \times S^2)} \int_{\mathbb{R}^3 \times S^2} \frac{\lambda}{2} (P(y, n) - U(y, n))^2$$

$$+ \sum_{k=1}^5 D_{kk} |A_k P(y, n)|^2 dy \, d\gamma(n)$$

is given by $P_\lambda^D(y, n) = (R^D_{\lambda})_* U(y, n)$, where the Green’s function $R^D_{\lambda} : \mathbb{R}^3 \times S^2 \to \mathbb{R}^+$ is the Laplace-transform of the heat-kernel with respect to time: $R^D_{\lambda}(y, n) = \lambda \int_0^\infty P_{\lambda}^D(y, n) e^{-\lambda t}dt$ with $D = \text{diag}(D_{11}, \ldots, D_{55}, 0)$. $P_\lambda^D(y, n)$ equals the probability of finding a random walker in $\mathbb{R}^3 \times S^2$ regardless its traveling time at position $y \in \mathbb{R}^3$ with orientation $n \in S^2$ starting from initial distribution $U$ at time $t = 0$.

For a proof we refer to our technical report (Duits and Franken 2009, Chap. 4.3).

5 Differential Geometry: The Underlying Cartan-Connection on $SE(3)$ and the Auto-Parallels in $SE(3)$

Now that we have constructed all left-invariant scale space representations on HARDI images, generated by means of a quadratic form (29) on the left-invariant vector fields on $SE(3)$. The question rises what is the underlying differential geometry for these evolutions?

For example, as the left-invariant vector fields clearly vary per position in the group yielding a moving frame of reference attached to luminosity particles (random walkers in $\mathbb{R}^3 \times S^2$ embedded in $SE(3)$) with both a position and an orientation, the question arises along which trajectories in
\[ \mathbb{R}^3 \times S^2 \] do these particles move? Furthermore, as the left-invariant vector fields are obtained by the push-forward of the left-multiplication on the group,

\[ A_g = (L_g)_* A_e, \quad \text{i.e.} \quad A_g \varphi = A_e (\varphi \circ L_g), \]

where \( L_g h = gh, \ g, h \in SE(3), \ \varphi : SE(3) \to \mathbb{R} \) smooth, the question arises whether this defines a connection between all tangent spaces, such that these trajectories are autoparallel with respect to this connection? Finally, we need a connection to rigid body mechanics described in a moving frame of reference, to get some physical intuition in the choice of the fundamental constants\(^{6}\) \( \{a_i\}_{i=1}^6 \) and \( \{D_{ij}\}_{i,j=1}^6 \) within our generators (29).

In order to get some first physical intuition on analysis and differential geometry along the moving frame \( \{A_1, \ldots, A_6\} \) and its dual frame \( \{dA^1, \ldots, dA^6\} \), we will make some preliminary remarks on the well-known theory of rigid body movements described in moving coordinate systems. Imagine a curve in \( \mathbb{R}^3 \) described in the moving frame of reference (embedded in the spatial part of the group \( SE(3) \)), describing a rigid body movement with constant spatial velocity \( \hat{c}^{(1)} \) and constant angular velocity \( \hat{c}^{(2)} \) and parameterized by arc-length \( s > 0 \). Suppose the curve is given by

\[ y(s) = \sum_{i=1}^3 \alpha_i(s) A_i | y(s) \] where \( \alpha_i \in C^2([0, L], \mathbb{R}) \),

such that \( \hat{c}^{(1)} = \sum_{i=1}^3 \dot{\alpha}_i(s) A_i | y(s) \) for all \( s > 0 \). Now if we differentiate twice with respect to the arc-length parameter and keep in mind that \( \frac{d}{ds} A_i | y(s) = \hat{c}^{(2)} \times A_i | y(s) \), we get

\[ \ddot{y}(s) = 0 + 2\hat{c}^{(2)} \times \hat{c}^{(1)} + \hat{c}^{(2)} \times (\hat{c}^{(2)} \times y(s)). \]

In words: The absolute acceleration equals the relative acceleration (which is zero, since \( \hat{c}^{(1)} \) is constant) plus the Coriolis acceleration \( 2\hat{c}^{(2)} \times \hat{c}^{(1)} \) and the centrifugal acceleration \( \hat{c}^{(2)} \times (\hat{c}^{(2)} \times y(s)) \). Now in case of uniform circular motion the speed is constant but the velocity is always tangent to the orbit of acceleration and the acceleration has constant magnitude and always points to the center of rotation. In this case, the total sum of Coriolis acceleration and centrifugal acceleration add up to the well-known centripetal acceleration,

\[ \ddot{y}(s) = 2\hat{c}^{(2)} \times (-\hat{c}^{(2)} \times Rr(s)) + \hat{c}^{(2)} \times (\hat{c}^{(2)} \times Rr(s)) \]

\[ = -\frac{\|\hat{c}^{(2)}\|^2}{R} Rr(s) = -\frac{\|\hat{c}^{(2)}\|^2}{R} r(s), \]

where \( R \) is the radius of the circular orbit \( y(s) = m + Rr(s), \quad \|Rr(s)\| = 1 \). The centripetal acceleration equals half the Coriolis acceleration, i.e. \( \ddot{y}(s) = \hat{c}^{(2)} \times \hat{c}^{(1)} \).

In our previous work (Duits and Franken 2010, Part II) on contour-enhancement and completion via left-invariant diffusions on invertible orientation scores (complex-valued functions on \( SE(2) \)) we put a lot of emphasis on the underlying differential geometry in \( SE(2) \). All results straightforwardly generalize to the case of HARDI images, which can be considered as functions on \( \mathbb{R}^3 \times S^2 \) embedded in \( SE(3) \). These rather technical results are summarized in Theorem 3, which answers all questions raised in the beginning of this section. Unfortunately, this theorem requires general differential geometrical concepts such as principal fiber bundles, associated vector bundles, frame-bundles and the Cartan-Ehresmann connection defined on them. These concepts are explained in full detail in Spivak (1975) (with a very nice overview on p. 386).

The reader who is not familiar with these technicalities from differential geometry can skip the first part of the theorem while accepting the formula of the covariant derivatives given in (48), where the \textit{anti-symmetric} Christoffel symbols are equal to minus the structure constants \( c^k_{ij} = -c^k_{ji} \) (recall (22)) of the Lie-algebra. Here we stress that we follow the Cartan viewpoint on differential geometry, where connections are expressed in moving coordinate frames (we use the frame of left-invariant vector fields \( \{A_1, \ldots, A_6\} \) derived in Sect. 3.3 for this purpose) and thereby we have non-vanishing torsion.\(^7\) This is different from the Levi-Civita connection for differential geometry on Riemannian manifolds, which is much more common in image analysis. The Levi-Civita connection is the unique torsion free metric compatible connection on a Riemannian manifold and because of this vanishing torsion of the Levi-Civita connection \( \nabla \) there is a 1-to-1 relation\(^8\) to the Christoffel symbols (required for covariant derivatives \( \nabla_{A^i} A^j = \partial_{A^i} A^j + \Gamma^j_{ik} A^k \)) and the derivatives of the metric tensor. In the more general Cartan connection outlined below, however, one can have non-vanishing torsion and the Christoffels are not necessarily related to a metric tensor, nor need they be symmetric.

**Theorem 3** The Maurer-Cartan form \( \omega \) on \( SE(3) \) is given by

\[ \omega_g (X_g) = \sum_{i=1}^6 \langle dA^i | g, X_g \rangle A_i, \quad X_g \in T_g (SE(3)). \]

\(^7\)The torsion tensor \( T \) of a connection \( \nabla \) is given by \( T[X, Y] = \nabla_X Y - \nabla_Y X - [X, Y] \). The torsion-tensor \( T \) of a Levi-Civita connection vanishes, whereas the torsion-tensor of our Cartan connection \( \nabla \) on \( SE(3) \) is given by \( T = \sum_{i,j=1}^3 \Gamma^3_{ij} dA^i \otimes dA^j \otimes A_j \).

\(^8\)In a Levi-Civita connection one has \( \Gamma^k_{ij} = \Gamma^k_{ji} = \frac{1}{2} \sum_m g^{km} (\delta_{mk,i} + \delta_{ml,k} - \delta_{kl,m}) \) with respect to a holonomic basis.
where the dual vectors \( \{dA^i\}_{i=1}^6 \) are given by (26) and \( A_i = A_{1i} \). It is a Cartan Ehresmann connection form on the principal fiber bundle \( P = (SE(3), e, SE(3), L(SE(3))) \), where \( \pi(g) = e, R_p u = u_g, u, g \in SE(3) \). Let \( \text{Ad} \) denote the adjoint action of \( SE(3) \) on its own Lie-algebra \( T_e(SE(3)) \), i.e. \( \text{Ad}(g) = (R_{-1}L_g)^* \), i.e. the push-forward of conjugation. Then the adjoint representation of \( SE(3) \) on the vector space \( L(SE(3)) \) of left-invariant vector fields is given by

\[
\tilde{\text{Ad}}(g) = dR \circ \text{Ad}(g) \circ \omega.
\]

(45)

This adjoint representation gives rise to the associated vector bundle \( SE(3) \times \tilde{\text{Ad}} L(SE(3)) \). The corresponding connection form on this vector bundle is given by

\[
\tilde{\omega} = \sum_{j=1}^6 \tilde{\text{ad}}(A_j) \otimes dA^j = \sum_{i,j,k=1}^6 \tilde{c}_{ij}^k \otimes dA^i \otimes dA^j.
\]

(46)

with \( \tilde{\omega} = \tilde{\text{Ad}} \omega \), i.e. \( \tilde{\text{ad}}(A_j) = \sum_{i=1}^6 [A_i, A_j] \otimes dA^i \) (Jost 2005, p. 265). Then \( \tilde{\omega} \) yields the following 6 × 6-matrix valued 1-form

\[
\tilde{\omega}^k_j(\gamma) := \tilde{\omega}(dA^k, \cdot, A_j) \quad k, j = 1, 2, \ldots, 6.
\]

(47)

on the frame bundle, (Spivak 1975, p. 353, p. 359), where the sections are moving frames (Spivak 1975, p. 354). Let \( \{\mu_k\}_{k=1}^6 \) denote the sections in the tangent bundle \( E := (SE(3), T(SE(3))) \) which coincide with the left-invariant vector fields \( \{A_i\}_{i=1}^6 \). Then the matrix-valued 1-form given by (47) yields the Cartan connection valued by the covariant derivatives

\[
D_{X|\gamma(t)}(\mu(\gamma(t))) := D \mu(\gamma(t))(X|\gamma(t))
\]

\[
= \sum_{k=1}^6 \dot{\hat{a}}^k(\gamma(t)) \mu_k(\gamma(t)) + \sum_{k=1}^6 a^k(\gamma(t)) \sum_{j=1}^6 \tilde{\omega}^j_k(\gamma(t)) \mu_j(\gamma(t))
\]

\[
= \sum_{k=1}^6 \dot{a}^k(\gamma(t)) \mu_k(\gamma(t)) + \sum_{i,j,k=1}^6 \dot{\hat{\gamma}}^i_j(\gamma(t)) a^k(\gamma(t)) \Gamma^j_{ik} \mu_j(\gamma(t))
\]

(48)

with \( \dot{\hat{a}}^k(\gamma(t)) = \sum_{i=1}^6 \dot{\hat{\gamma}}^i_j(\gamma(t)) (A_i|\gamma(t)) a^k \), for all tangent vectors \( X|\gamma(t) = \sum_{i=1}^6 \dot{\hat{\gamma}}^i_j(\gamma(t)) A_i|\gamma(t) \) along a curve \( t \mapsto \gamma(t) \in SE(2) \) and all sections \( \mu(\gamma(t)) = \sum_{k=1}^6 a^k(\gamma(t)) \mu_k(\gamma(t)) \). The Christoffel symbols in (48) are constant \( \Gamma^j_{ik} = -\epsilon^j_{ik} \), with \( \epsilon^j_{ik} \) the structure constants of Lie-algebra \( T_e(SE(3)) \). Consequently, the connection \( D \) has constant curvature and constant torsion and the left-invariant evolution equations given in (28) can be rewritten in covariant derivatives (using short notation \( \nabla_j := D A_j \)):

\[
\begin{align*}
\dot{a}_i(W,g,t) &= \sum_{i=1}^6 -a^j(W)A_i(W,g,t) + \sum_{i,j=1}^6 A_i((D_j(W))(g,t)A_j(W)(g,t)) \nabla_i(W,g,t) + \sum_{i,j=1}^6 \nabla_i((D_j(W))(g,t)) \nabla_j(W)(g,t),
\end{align*}
\]

(49)

Both convection and diffusion in the left-invariant evolution equations (28) take place along the exponential curves \( \gamma_c(s) = g \cdot e^{s \sum_{i=1}^6 c^i A_i} \) in \( SE(3) \) which are the covariantly constant curves (i.e. auto-parallel) with respect to the Cartan connection. In particular, if \( a^j(W) = c^j \) constant and if \( D_j(W) = 0 \) (connexion case) then the solutions are

\[
W(g,t) = \tilde{\hat{U}}(g \cdot e^{-\sum_{i=1}^6 c^i A_i}).
\]

(50)

The spatial projections \( P_{\mathbb{R}^3} \gamma \) of these of the auto-parallel/ exponential curves \( \gamma \) are circular spirals with constant curvature and constant torsion. The curvature magnitude equals \( \| \hat{e}^{(1)} \|^{-1} \| c^{(2)} \times \hat{e}^{(1)} \| \) and the curvature vector equals

\[
\kappa(t) = \frac{1}{\| \hat{e}^{(1)} \|} \left( \cos(t \| \hat{e}^{(2)} \|) \hat{e}^{(2)} \times \hat{e}^{(1)} + \sin(t \| \hat{e}^{(2)} \|) \hat{e}^{(2)} \times \hat{e}^{(2)} \times \hat{e}^{(1)} \right).
\]

(51)

where \( c = (c^1, c^2, c^3, c^4, c^5, c^6) = (\hat{e}^{(1)}; \hat{e}^{(2)}) \). The torsion vector equals \( \tau(t) = |\hat{e}_1 \cdot \hat{e}_2| \kappa(t) \).

Proof The proof is a straightforward generalization from our previous results (Duits and Franken 2010, Part II, Thm. 3.8 and Thm. 3.9) on the \( SE(2) \)-case to the case \( SE(3) \). The formulas of the constant torsion and curvature of the spatial part of the auto-parallel curves (which are the exponential curves) follow by the formula (54) for (the spatial part \( x(s) \) of) the exponential curves, which we will derive in Sect. 5.1. Here we stress that \( s(t) = t \sqrt{c^1 + c^2 + c^3} \) is the arc-length of the spatial part of the exponential curve and where we recall that \( \kappa(s) = \ddot{x}(s) \times \ddot{x}(s) \) and \( \tau(s) = \frac{d}{ds} (\dot{x}(s) \times \ddot{x}(s)) \). Note that both the formula (54) for the exponential curves in the next section
and the formulas for torsion and curvature are simplifications of our earlier formulas (Franken 2008, pp. 175–177). In the special case of only convection the solution (50) follows by $e^{dtR(A)} \hat{U}(g) = R_{e^{dt}A} \hat{U}(g)$, with $A = -\sum_{i=1}^{6} c^i A_i$ and $dR(A) = -\sum_{i=1}^{6} c^i \mathcal{L}_i$ with $\mathcal{L}_i = dR(A_i)$.

5.1 The Exponential Curves and the Logarithmic Map

Explicitly in Euler Angles

Next we compute the exponential curves in $SE(3)$ by an isomorphism of the group $SE(3)$ to matrix group $\mathfrak{S}(3)$

$$SE(3) \ni (x, R_{\gamma, \beta, \alpha}) \mapsto \left( R_{\gamma, \beta, \alpha} x \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right) \in \mathfrak{S}(3)$$

with $R_{\gamma, \beta, \alpha} = R_{\gamma} \cdot R_{\beta} \cdot R_{\alpha}$.

This isomorphism induces the following isomorphism between the respective Lie-algebras

$$\sum_{i=1}^{6} c^i A_i \in \mathcal{L}(SE(3)) \leftrightarrow T_c(SE(3))$$

where $\{c^i\}_{i=1}^{6} \in \mathbb{R}^6$ and with matrices $\{X_i\}_{i=1}^{6} \in \mathbb{R}^{4 \times 4}$ are given by

$$X_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad X_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$X_3 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad X_4 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$X_5 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad X_6 = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (52)$$

Note that $A_i \leftrightarrow A_i \leftrightarrow X_i \Rightarrow [A_i, A_j] \leftrightarrow [A_i, A_j] \leftrightarrow [X_i, X_j]$ and indeed direct computation yields:

$$\sum_{k=1}^{6} c^i A_k = [A_i, A_j]$$

$\leftrightarrow [X_i, X_j] = \sum_{k=1}^{6} c^i X_k$ with commutator table

\[
\begin{pmatrix}
0 & 0 & 0 & 0 & -X_3 & -X_2 \\
0 & 0 & 0 & -X_3 & 0 & X_1 \\
0 & 0 & 0 & X_2 & -X_1 & 0 \\
0 & X_3 & -X_2 & 0 & X_6 & -X_5 \\
-X_3 & 0 & X_1 & -X_6 & 0 & X_4 \\
X_2 & -X_1 & 0 & X_5 & -X_4 & 0
\end{pmatrix}, \quad (53)
\]

where $i$ enumerates vertically and $j$ horizontally and $[A_i, A_j] = A_i A_j - A_j A_i$ and $[X_i, X_j] = X_i X_j - X_j X_i$. Each element in the Lie-algebra of the matrix group $\mathfrak{S}(3)$ can be written

$$A = \sum_{i=1}^{6} c^i X_i = \left( \begin{array}{cc}
\Omega & \hat{c}^{(1)} \\
0 & 0
\end{array} \right),$$

$$\Omega = \begin{pmatrix} 0 & -c^6 & c^5 \\ -c^6 & 0 & -c^4 \\ -c^5 & c^4 & 0 \end{pmatrix} \in \mathfrak{so}(3),$$

$$\hat{c}^{(2)} = (c^1, c^2, c^3) \in \mathbb{R}^3,$

with $\mathfrak{so}(3) = \{ A \in \mathbb{R}^{3 \times 3} \mid A^T = -A \}$. Note that exp($\mathfrak{so}(3)$) = $SO(3)$ and $\Omega x = \hat{c}^{(2)} \times x$ and set $\tilde{q} = \|\hat{c}^{(2)}\| = \sqrt{(c^1)^2 + (c^2)^2 + (c^3)^2}$ so that $\Omega^3 = -\tilde{q}^2 \Omega$ and therefore

$$A^k = \left( \begin{array}{cc}
\Omega^k & \Omega^{k-1} \hat{c}^{(1)} \\
0 & 0
\end{array} \right)$$

$$\Rightarrow e^{A} = \sum_{k=1}^{\infty} \frac{t^k}{k!} A^k = \left( e^{t\Omega} \quad t \int_0^1 e^{t\Omega} \tilde{q} x \Omega \frac{x}{q^3} \Omega^2 \right),$$

$$= \left( R \begin{pmatrix} x \\ 0 \\ 1 \end{pmatrix} \right) \in \mathfrak{S}(3),$$

with

$$\int_0^1 e^{t\Omega} \tilde{q} x \Omega \frac{x}{q^3} \Omega^2 = I + \frac{1}{t} \left( 1 - \frac{q}{\tilde{q}} \sin(\tilde{q} t) \right) \Omega^2,$$

and

$$R = e^{t\Omega} = I + \frac{\sin(\tilde{q} t)}{\tilde{q}} \Omega + \frac{1 - \cos(\tilde{q} t)}{q^2} \tilde{q}^2 \Omega^2$$

so that the exponential curves are given by

$$\gamma(t) = e^{t \sum_{i=1}^{6} c^i A_i} = \left( \begin{array}{cc}
(c_1 t, c_2 t, c_3 t, t) & \text{if } \hat{c}^{(2)} = 0 \\
(t \hat{c}^{(1)} + \frac{1 - \cos(\tilde{q} t)}{\tilde{q}^2} \tilde{q} \Omega \hat{c}^{(1)} + (t q^{-2} - \sin(\tilde{q} t) \tilde{q}^{-2} \tilde{q}^2 \hat{c}^{(1)}, \\
I + \frac{\sin(\tilde{q} t)}{\tilde{q}} \Omega + \frac{(1 - \cos(\tilde{q} t))}{q^2} \tilde{q}^2 \Omega^2 \end{array} \right) \text{ else.} \quad (54)$$
As the exponential map is surjective we are also interested in the logarithmic map. This means we have to solve for \( \hat{c}^{(1)} \in \mathbb{R}^3 \) and \( \Omega \in \mathfrak{so}(3) \), given a group element \( g = (x, R_{y, \beta, \alpha}) \in SE(3) \). Note that \( \Omega = -\Omega, (\Omega^2)^T = \Omega^2 \) so that \( R - R^T = 2 \sin \frac{\theta}{2} \Omega \) from which the logarithmic map \( \Omega = \log_{SE(3)} R, R = R_{y, \beta, \alpha} \) follows explicitly:

\[
\begin{align*}
    c^4 &= c_{y, \beta, \alpha}^4 := \frac{\hat{q}}{2 \sin \hat{q}} \sin \beta (\sin \alpha - \sin \gamma), \\
    c^5 &= c_{y, \beta, \alpha}^5 := \frac{\hat{q}}{2 \sin \hat{q}} \sin \beta (\cos \alpha - \cos \gamma), \\
    c^6 &= c_{y, \beta, \alpha}^6 := \frac{\hat{q}}{2 \sin \hat{q}} (2 \cos^2 \left( \frac{\beta}{2} \right) \sin (\alpha + \gamma)),
\end{align*}
\]

and thereby \( \hat{q} = \sqrt{(c^4)^2 + (c^5)^2 + (c^6)^2} = \tilde{q}_{y, \beta, \alpha} = \arcsin \sqrt{\cos^2(\frac{\theta}{2}) \sin^2 \beta + \cos^2(\frac{\theta}{2}) \sin^2(\alpha + \gamma)} \). So it remains to express \( \hat{c}^{(1)} = (c^1, c^2, c^3)^T \) in Euler angles \( (\gamma, \beta, \alpha) \). Now \( \Omega^3 = -\hat{q}^2 \Omega \) implies that

\[
\begin{align*}
    (1 + \hat{q}^{-2} (1 - \cos \hat{q}) \Omega + \hat{q}^{-3} (\tilde{q} - \sin \hat{q}) \Omega^2) \hat{c}^{(1)} &= x \\
    \Leftrightarrow \quad \tilde{c}^{(1)} &= \tilde{c}^{(1)}_{x, y, \beta, \alpha} \\
    &= (1 - \frac{1}{2} \Omega_{y, \beta, \alpha} + \frac{\tilde{q}_{y, \beta, \alpha}}{2}) \left( 1 - \frac{\tilde{q}_{y, \beta, \alpha}}{2} \right) \cdot \cot \left( \frac{\tilde{q}_{y, \beta, \alpha}}{2} \right) (\Omega_{y, \beta, \alpha}^2) x.
\end{align*}
\]

Now equality (55) and (56) provide the explicit logarithmic mapping on \( SE(3) \):

\[
\log_{SE(3)}(x, R_{y, \beta, \alpha}) = \sum_{i=1}^{3} c_{y, \beta, \alpha}^i A_i + \sum_{i=4}^{6} c_{y, \beta, \alpha}^i A_i.
\]

**Remark** It can be shown that \( \frac{d}{dt} \| \xi(t) \| = \sqrt{(c^1)^2 + (c^2)^2 + (c^3)^2} \). Consequently the arc-length parameter \( s > 0 \) is expressed in \( t \) by means of \( s(t) = t \sqrt{(c^1)^2 + (c^2)^2 + (c^3)^2} \). If we want to impose spatial arc-length parameterizations of curves in \( SE(3) \) we must rescale all \( c_i \rightarrow \frac{c_i}{\sqrt{(c^1)^2 + (c^2)^2 + (c^3)^2}} \) so that \( \| \hat{c}^{(1)} \| = \sqrt{(c^1)^2 + (c^2)^2 + (c^3)^2} = 1 \).

**Remark** The group \( SE(3) \) is isomorphic to the group of rigid motions in \( \mathbb{R}^3 \) well-known in mechanics. The vector \( \hat{c}^{(1)} \) denotes constant velocity in the moving coordinate frame \( \{ A_i \}_{i=1}^3 \) whereas \( \hat{c}^{(2)} \) denotes constant angular velocity with respect to the same moving coordinate frame attached to a particle on a moving rigid body in \( \mathbb{R}^3 \). Note that \( \kappa(0) \) equals the **centripetal acceleration** at the moving frame of reference \( \{ A_1, A_2, A_3 \} \), whereas \( \kappa(s) \) equals the **centripetal acceleration** at the moving frame of reference \( \{ A_1, A_2, A_3 \} \) about \( s \), but again expressed in the global coordinate system \( \{ A_1, A_2, A_3 \} = \{ e_1, e_2, e_3 \} \) of the spatial part \( \mathbb{R}^3 \) of the group, which is for \( s > 0 \) no longer aligned with the moving frame of reference. To re-express \( \kappa(s) \) in \( \{ A_1, A_2, A_3 \} \) one must rotate \( \kappa(0) \) over an angle of \( s \| \hat{c}^{(2)} \| \) around the angular velocity \( \hat{c}^2 \), which explains (51).

### 6 Analysis of the Convolution Kernels of Scale Spaces on HARDI Images

It is a notorious problem to find explicit formulas for the exact Green’s functions \( p^D_{t,a} : \mathbb{R}^3 \times S^2 \rightarrow \mathbb{R^+} \) of the left-invariant diffusions, (36), on \( \mathbb{R}^3 \times S^2 \). Explicit, tangible and exact formulas for heat-kernels on \( SE(3) \) do not seem to exist in literature. Nevertheless, there does exist a nice general theory overlapping the fields of functional analysis and group theory, see for example (Nagel and Ricci 1990; ter Elst and Robinson 1998), which at least provides Gaussian estimates for Green’s functions of left-invariant diffusions on Lie groups, generated by subcoercive operators. In the remainder of this section we will employ this general theory to our special case where \( \mathbb{R}^3 \times S^2 \) is embedded into \( SE(3) \) and we will derive new explicit and useful approximation formulas for these Green’s functions. Within this section we always use the second coordinate chart, (4), as it is highly preferable over the more common Euler angle parametrization, (1), since we rather avoid singularities at the unity element of \( SE(3) \). We refer to Duits and Franken (2009, App. A) for an accurate approximation to the exact Green’s functions for the direction process 39 (a contour-completion process) in \( \mathbb{R}^3 \times S^2 \), likewise (Duits and van Almsick 2008), where we managed to derive the exact Green’s functions of the direction process in \( SE(2) \). However, unlike the \( SE(2) \)-case, we do have to apply a reasonable approximation in the generator in order to get tangible approximation formulas. These approximations are valid for 4D diffusion small and are nearly exact in a sharp cone around the z-axis where the Green’s function is concentrated.

We shall first carry out the method of contraction. This method typically relates the group of positions and rotations to a (nilpotent) group positions and velocities and serves as an essential pre-requisite for our Gaussian estimates and approximation kernels later on. The reader who is not so much interested in the detailed analysis can skip this section and continue with the numerics explained in Chap. 7.

#### 6.1 Local Approximation of \( SE(3) \) by a Nilpotent Group via Contraction

The group \( SE(3) \) is not nilpotent. This makes it hard to get tangible explicit formulae for the heat-kernels. Therefore we shall generalize our Heisenberg approximations of the Green’s functions on \( SE(2) \), (Duits and van Almsick 2008;
Thornber and Williams 2000; van Almsick 2005), to the case $SE(3)$. Again we will follow the general work by ter Elst and Robinson (1998) on semigroups on Lie groups generated by weighted subcoercive operators. In their general work we consider a particular case by setting the Hilbert space $L_2(SE(3))$, the group $SE(3)$ and the right-regular representation $\mathcal{R}$. Furthermore we consider the algebraic basis $\{A_3, A_4, A_5\}$ leading to the following filtration of the Lie algebra

$$g_1 = \text{span}\{A_3, A_4, A_5\}$$

$$g_2 = \text{span}\{A_1, A_2, A_3, A_4, A_5, A_6\} = \mathcal{L}(SE(3)).$$

Now that we have this filtration we have to assign weights to the generators

$$w_3 = w_4 = w_5 = 1 \quad \text{and} \quad w_1 = w_2 = w_6 = 2.$$  (59)

For example $w_3 = 1$ since $A_3$ already occurs in $g_1$, $w_6 = 2$ since $A_6$ is within in $g_2$ and not in $g_1$. Now that we have these weights we define the following dilations on the Lie-algebra $T_e(SE(3))$ (recall $A_i = A_i|_e$):

$$\gamma_q \left( \sum_{i=1}^{6} q^{w_i} c^i A_i \right) = \sum_{i=1}^{6} q^{w_i} c^i A_i, \quad \text{for all } c^i \in \mathbb{R},$$

and for $0 < q \leq 1$ we define the Lie product $[A, B]_q = \gamma_q^{-1} \gamma_q \gamma_q^{-1} \gamma_q [A(B)]$. Now let $(SE(3))_q$ be the simply connected Lie group generated by the Lie algebra $(T_e(SE(3)), [\cdot, \cdot]|_q)$. This Lie group is isomorphic to the matrix group with group product:

$$(x, R_{\tilde{\beta}, \tilde{\alpha}}) \cdot (x', R_{\tilde{\beta}', \tilde{\alpha}'}) = (x + S_q \cdot (R_{\tilde{\beta}, \tilde{\alpha}} \cdot (x', R_{\tilde{\beta}', \tilde{\alpha}'})) = (x + S_q \cdot (R_{\tilde{\beta}, \tilde{\alpha}} \cdot (x', R_{\tilde{\beta}', \tilde{\alpha}'})),$$  (60)

where $S_q := \text{diag}(1, 1, q) \in \mathbb{R}^{3 \times 3}$ and we used short-notation $R_{\tilde{\beta}, \tilde{\alpha}} = R_{\tilde{\beta}} R_{\tilde{\alpha}} R_0$, i.e. our elements of $SO(3)$ are expressed in the second coordinate chart, (4). Now the left-invariant vector fields on the group $(SE(3))_q$ are given by $A_i = \gamma_q^{-1} \gamma_q \gamma_q^{-1} \gamma_q A_i$, $i = 1, \ldots, 6$. Straightforward (but intense) calculations yield (for each $g = (x, R_{\tilde{\beta}, \tilde{\alpha}}) \in (SE(3))_q$):

$$A_1^g = -(\sin(\tilde{\alpha} q^2) \cos(\tilde{\beta} q) \partial_x + (\cos(\tilde{\alpha} q^2) \cos(\tilde{\beta} q)) \partial_y + \cos(\tilde{\alpha} q^2) \sin(\tilde{\beta} q)) \partial_z$$

$$A_2^g = -\sin(\tilde{\alpha} q^2) \cos(\tilde{\beta} q) \partial_x + (\cos(\tilde{\alpha} q^2) \cos(\tilde{\beta} q)) \partial_y + \cos(\tilde{\alpha} q^2) \sin(\tilde{\beta} q)) \partial_z.$$  (61)

6.1.1 The Heisenberg-approximation of the Contour Completion Kernel

Recall that the generator of contour completion diffusion equals $-A_3 + D_{44}((A_4)^2 + (A_3)^2)$. So let us replace the true left-invariant vector fields $\{A_i\}_{i=3}^6$ on $SE(3) = (SE(3))_{q=1}$
by their Heisenberg-approximations \( \{ \tilde{A}^i_{\pm \pm} \}_{i=3}^5 \) that are given by (62) and compute the Green's function \( \tilde{p}_t \) on \( (SE(3))_0 \) (i.e. the convolution kernel which yields the solutions of contour completion on \( (SE(3))_0 \) by group convolution on \( (SE(3))_0 \)). For \( 0 < D_{44} \ll 1 \) this kernel is a local approximation of the true contour completion kernel \( \tilde{p}_t^{a_1, D_{44}; (SE(2))_0} \); SE(2) \( \rightarrow \mathbb{R}^+ \) for contour completion in \( SE(2) \) can be found in Duits and van Almsick (2008).

### 6.1.2 The Heisenberg-approximation of the Contour Enhancement Kernel

Recall that the generator of contour completion diffusion equals \( D_{33}(\tilde{A}_3)^2 + D_{44}(\tilde{A}_4)^2 + (\tilde{A}_5)^2 \). So let us replace the true left-invariant vector fields \( \{ \tilde{A}_i \}_{i=3}^5 \) on \( SE(3) \) by their Heisenberg-approximations \( \{ \tilde{A}^0_{i=3} \} \) given by (62) and consider the Green's function \( \tilde{p}_t^{a_1, D_{44} = D_{55}} \) on \( (SE(3))_0 \):

\[
\tilde{p}_t^{a_1, D_{44} = D_{55}} (x, y, z, \tilde{\beta}, \tilde{\gamma}) = \delta(t - z)(e^{t(\tilde{\beta} \partial_\tilde{\gamma} + D_{44}(\partial_\tilde{\gamma})^2) \delta_0^y \otimes \delta_0^\beta} - 3 \sqrt{\frac{3}{\pi}} 3 \sqrt{\frac{3}{\pi}} \frac{\tilde{\beta}}{D_{44}} e^t \frac{\tilde{\beta}}{D_{44}^{3/2}} \frac{D_{44}^{3/2} \tilde{\gamma}}{D_{44}^{3/2}} \frac{\tilde{\gamma}}{D_{44}^{3/2}},
\]

where \( \tilde{n}(\tilde{\beta}, \tilde{\gamma}) = R_{x \cdot \tilde{\gamma}} R_{x \cdot \tilde{\beta}} e_x = (\sin \tilde{\beta}, -\sin \tilde{\gamma} \cos \tilde{\beta}, \cos \tilde{\gamma} \cos \tilde{\beta})^T \). The corresponding resolvent kernel on the group \( (SE(3))_0 \) is now directly obtained by Laplace transform with respect to time

\[
\tilde{R}_k^{a_1, D_{44} = D_{55}} (x, y, z, \tilde{n}(\tilde{\beta}, \tilde{\gamma})) = \left\{ \begin{array}{ll}
\frac{3}{4(D_{44}^{3/2} \tilde{\gamma})^2} e^{-t \frac{12(1 - 2)\tilde{\gamma}^2 \tilde{\beta}^2}{D_{44}^{3/2}}} \\
\cdot \frac{12(1 - 2)\tilde{\gamma} \tilde{\beta}^2}{D_{44}^{3/2}} & \text{if } z > 0 \\
0 & \text{if } z \leq 0 \text{ and } (x, y) \neq (0, 0).
\end{array} \right.
\]

So we make a remarkable observation: The Heisenberg-approximation, (63), of the contour completion kernel in \( (SE(3))_0 \) is a direct product of two Heisenberg approximations of contour completion kernels in \( SE(2) \), (Duits and van Almsick 2008),

\[
\tilde{p}_t^{a_1, D_{44} = D_{55}; (SE(3))_0} (x, y, z, \tilde{n}(\tilde{\beta}, \tilde{\gamma})) = \tilde{p}_t^{a_1, D_{44}; (SE(2))_0} (z, x, \tilde{\beta}) \cdot \tilde{p}_t^{a_1, D_{44}; (SE(2))_0} (z, -y, \tilde{\gamma}).
\]

Now since the Heisenberg approximation kernel \( \tilde{p}_t^{D_{33}, D_{44}; (SE(2))_0} \) is for reasonable parameter settings (that is \( 0 < D_{44} \ll 1 \)) close to the exact kernel \( \tilde{p}_t^{D_{33}, D_{44}; (SE(2))_0} \) we heuristically propose for these reasonable parameter settings the same direct-product approximation for the exact contour-enhancement kernels on \( \mathbb{R}^3 \times S^2 \):

\[
\tilde{p}_t^{a_1, D_{44} = D_{55}; \mathbb{R}^3 \times S^2} (x, y, z, \tilde{n}(\tilde{\beta}, \tilde{\gamma})) \approx \tilde{p}_t^{a_1, D_{44}; (SE(2))_0} (z, x, \tilde{\beta}) \cdot \tilde{p}_t^{a_1, D_{44}; (SE(2))_0} (z, -y, \tilde{\gamma}).
\]

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\[\tilde{p}_t^{D_{33},D_{44}}(x,y,\theta) \approx \frac{1}{32\pi t^2 c^4 D_{44} D_{33}} e^{-\frac{1}{4ct \sqrt{\frac{D_{33}}{D_{44}} + \frac{D_{33}}{D_{44}} + \frac{1}{4t^2 \gamma}}} \cdot p_t^{D_{33},D_{44};(SE(2))}(x,y,\theta).\] (68)

So similar to the contour-completion kernel on \(\mathbb{R}^3 \times S^2\) derived in the previous section, recall (65), the Heisenberg-approximation kernel on \(\mathbb{R}^3 \times S^2\) is a direct product of two Heisenberg-approximation kernels on \((SE(2))_0\).

Now since the Heisenberg approximation kernel \(\tilde{p}_t^{D_{33},D_{44};(SE(2))_0}\) is for reasonable parameter settings (that is \(0 < \frac{D_{33}}{D_{44}} \ll 1\)) close to the exact kernel \(\tilde{p}_t^{D_{33},D_{44};(SE(2))}\) we heuristically propose for these reasonable parameter settings the same direct-product approximation for the exact contour-enhancement kernels on \(\mathbb{R}^3 \times S^2\):

\[\tilde{p}_t^{D_{33},D_{44}}(x,y,\theta) \approx N(D_{33},D_{44},\theta) \cdot p_t^{D_{33},D_{44};(SE(2))_0}(x,\cdot,\cdot,\cdot) \cdot p_t^{D_{33},D_{44};(SE(2))}(\cdot,\cdot,\cdot),\] (69)

where \(N(D_{33},D_{44},\theta) \approx \frac{g}{\sqrt{\pi t \sqrt{D_{33}} \sqrt{D_{33} D_{44}}}}\) takes care of \(\text{L}_{1}(\mathbb{R}^3 \times S^2)\)-normalization. In Duits and Franken (2010), Citti and Sarti (2006) one can find the exact solutions of the Green’s function \(\tilde{p}_t^{D_{33},D_{44};(SE(2))_0}\) related to the Green’s function (Gaveau 1977) on \((H)\) by means of a coordinate transform, but these exact formulae are not as tangible as the following asymptotical formulas:

\[\tilde{p}_t^{D_{33},D_{44};(SE(2))}(x,y,\theta) = \frac{1}{32\pi t^2 c^4 D_{44} D_{33}} e^{-\frac{1}{4ct \sqrt{\frac{D_{33}}{D_{44}} + \frac{D_{33}}{D_{44}} + \frac{1}{4t^2 \gamma}}} \cdot p_t^{D_{33},D_{44};(SE(2))}(x,y,\theta).\] (70)

For the purpose of numerical computation, we simplify \(EN(x,y,\theta)\) to

\[\begin{align*}
EN(x,y,\theta) &= \left(\frac{\theta^2}{D_{44}} + \frac{\theta^2(y - (-x \sin \theta + y \cos \theta))^2}{4(1 - \cos(\theta))^2 D_{33}}\right)^2 \\
&+ \left(\frac{1}{D_{44} D_{33}} \frac{\theta((x \cos \theta + y \sin \theta) - x)^2}{2(1 - \cos(\theta))}\right)^2
\end{align*}
\]

and which for \(\theta = 0\) equals

\[\begin{align*}
EN(x,y,0) &= \left(\frac{x^2}{D_{33}}\right)^2 + \left|\frac{y^2}{D_{44} D_{33}}\right|^2
\end{align*}
\]

The estimates (70) are globally sharp, with \(\frac{1}{2} \leq c \leq \sqrt{2}\), for details see Duits and Franken (2010, Chap. 5.4).

According to the general theory (ter Elst and Robinson 1998) the heat-kernels \(p_t^{SE(3);q}:D = \text{diag}(0,0,D_{33},D_{44},D_{44},0): SE(3)_q \to \mathbb{R}^+\) (i.e. kernels for contour enhancement whose convolutions yield horizontal\(^9\) diffusion on \((SE(3))_q\) on the parameterized class of groups \((SE(3))_q\), \(q \in [0,1]\) in between \((SE(3))\) and its nilpotent Heisenberg approximation \((SE(3))_0\) satisfy the following Gaussian estimates (for \(D\) isomorphic to the \(3 \times 3\) identity matrix \(I_3\), \(D = \text{diag}(0,0,1,1,1,0)\))

\[C_1 e^{-\frac{c_2 \|q\|^2}{4q}} \leq p_t^{SE(3);q}:D = I_3 (g) \leq C_3 e^{-\frac{c_4 \|q\|^2}{4q}},\]

with \(0 < C_1 < C_3\) and \(0 < C_4 < C_2\), where the norm \(\|\cdot\|_q: (SE(3))_q \to \mathbb{R}^+\) is given by

\[\|g\|_q = |\log_t((SE(3))_q) (g)\|_q,\]

where \(\log_t((SE(3))_q) : (SE(3))_q \to T_e((SE(3))_q)\) is the logarithmic mapping on \((SE(3))_q\) (which we computed explicitly for \((SE(3))_q=1 = SE(3)\) in Sect. 5.1 and which we will compute for \(q = 0\) as well) and where the weighted modulus, (ter Elst and Robinson 1998), in our special case of interest is given by

\[\sum_{q=1}^{6} |c_q| A_i |q| = \sqrt{|c_1|^2 + |c_2|^2 + |c_3|^2 + |c_4|^2 + |c_5|^2 + |c_6|^2},\]

where \(c_q \in \mathbb{R}\) and where we recall our weighting given in (59). However, similar to our work (Duits and Franken 2010, Chap. 5.4) on estimating heat-kernels on \((SE(2))_0\), we estimate the weighted modulus by an equivalent differentiable modulus:

\[\begin{align*}
\sum_{i=1}^{6} |c_q A_i |q| &= \frac{\sqrt{|c_1|^2 + |c_2|^2 + |c_3|^2 + |c_4|^2 + |c_5|^2 + |c_6|^2}}{2(1 - \cos(\theta/2))}\]
\]

\(^9\)Horizontal diffusion in \((SE(3))_q\) is diffusion which takes place along horizontal curves in \(\mathbb{R}^3 \times S^2 \leftrightarrow SE(3)\). Recall Definition 5.
where we note that \( \sqrt{6}|g|^q \geq |g|^q \) for all \( g \in (SE(3))_q, q \in [0, 1] \).

Now suppose \((c^1_q, \ldots, c^6_q) = (c^1_q(g), \ldots, c^6_q(g)) := \log_{(SE(3))_q}(g)\), then there exist constants \( 0 < \tilde{C}_1 < \tilde{C}_3 \) and \( 0 < \tilde{C}_4 < \tilde{C}_2 \) such that the following Gaussian estimates hold:

\[
\tilde{C}_1 e^{-\frac{c_2 \sqrt{\|a_1\|^2 + \|a_3\|^2 + \|a_5\|^2 + \|a_2\|^2 + \|a_4\|^2 + \|a_6\|^2}}{4u}} \\
\leq p_{1}(SE(3)_q, D=I_3, \tilde{q})(g) \\
\leq \tilde{C}_3 e^{-\frac{c_4 \sqrt{\|a_1\|^2 + \|a_3\|^2 + \|a_5\|^2 + \|a_2\|^2 + \|a_4\|^2 + \|a_6\|^2}}{4u}},
\]

(71)

where we again use short notation \( c^i_q = c^i_q(g), i = 1, \ldots, 6 \).

Now, from the applied point of view \( D = \text{diag}(0, 0, 1, 1, 1, 0) \) is an unrealistic situation and only for \( q = 0 \) there exist dilations on the group \((SE(3))_q\) so that we can easily generalize the estimates to the diagonal case \( D = \text{diag}(0, 0, D_{33}, D_{44}, D_{55}, 0) \).

Since \((SE(3))_0\) is a nilpotent Lie-group isomorphic to the matrix group given by (60) (where we take the limit \( q \downarrow 0 \)) it is not difficult (this is much easier than the case \( q = 1 \), recall Sect. 5.1) to compute the exponent (recall (61)):

\[
\begin{pmatrix}
0 & -a_6 & c^5_0 & c^1_0 \\
0 & 0 & -a_4 & c^2_0 \\
0 & 0 & 0 & c^3_0 \\
0 & 0 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
1 & -a_6 & c^5_0 & c^1_0 \\
0 & 1 & -a_4 & c^2_0 \\
0 & 0 & 1 & c^3_0 \\
0 & 0 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
x \\
y \\
z \\
1
\end{pmatrix}
\]

and inverting these relations we find the simple formulas for the functions \( c^i_0 \) that we use in our estimates (73)

\[
c^1_0(g) = x - \frac{1}{2} y \tilde{a} \tilde{\beta} - \frac{1}{2} z \tilde{\gamma} \tilde{\beta} + \frac{1}{3} z \tilde{a} \tilde{\gamma}, \\
c^2_0(g) = y + \frac{1}{2} y \tilde{a} \tilde{\gamma}, \\
c^3_0(g) = z, \\
c^4_0(g) = \tilde{\beta}
\]

defined for all \( g = \begin{pmatrix} x, y, z, 1 \end{pmatrix} \in (SE(3))_0 \). By our embedding \( \mathbb{R}^3 \times S^2 \) into \( SE(3) \), we must set \( c^5_0 = \tilde{a} = 0 \).

Consequently, for the Heisenberg approximations of the diffusion kernels we have

\[
\tilde{C}_1 e^{-\frac{c_2 \sqrt{\|y\|^2 + \|\tilde{x}\|^2 \tilde{a} + \|\tilde{\gamma}\|^2 + \|\tilde{\beta}\|^2 \|\tilde{\gamma}\|^2}}{4u}} \\
\leq \tilde{p}_{1}(x, y, z, \tilde{\beta}, \tilde{\gamma}) \\
\leq \tilde{C}_3 e^{-\frac{c_4 \sqrt{\|y\|^2 + \|\tilde{x}\|^2 \tilde{a} + \|\tilde{\gamma}\|^2 + \|\tilde{\beta}\|^2 \|\tilde{\gamma}\|^2}}{4u}}.
\]

(73)

where we used short notation \( \tilde{p}_{1} = \tilde{p}_{1}(SE(3))_0, D=I_3 : \mathbb{R}^3 \times S^2 \rightarrow \mathbb{R}^+ \) for the Heisenberg approximation \( q = 0 \) of the contour enhancement kernel with \( D_{33} = D_{44} = D_{55} = 1 \). Now by application of the following dilation:

\[
z' = \frac{z}{\sqrt{D_{33}}}, \quad x' = \frac{x}{\sqrt{D_{33}D_{44}}}, \\
\tilde{\beta}' = \frac{\tilde{\beta}}{\sqrt{D_{44}}}, \quad \tilde{y}' = \frac{y}{\sqrt{D_{33}D_{44}}}, \quad \tilde{\gamma}' = \frac{\tilde{\gamma}}{\sqrt{D_{44}}}
\]

the generator of the corresponding diffusion on \( \mathbb{R}^3 \times S^2 \) for the general case where \( D = \text{diag}(0, 0, D_{33}, D_{44}, D_{55}, 0) \) relates to the diffusion generator for the case \( D = \text{diag}(0, 0, 1, 1, 1, 0) \), recall (62):

\[
\sum_{i=3}^{5} D_{ii}(A^i_0)^2 = D_{33}(\tilde{\beta} \tilde{a} \tilde{\gamma} - \tilde{y} \tilde{\beta} + \tilde{\gamma} \tilde{x})^2 \\
+ D_{44}(\tilde{\beta} \tilde{y})^2 + D_{44}(\tilde{\beta} \tilde{y})^2 \\
\left( \begin{array}{c}
\tilde{y}' \tilde{x}' - \tilde{\gamma}' \tilde{x}' + \tilde{\beta}' \tilde{\gamma}' + (\tilde{\beta}')^2 + (\tilde{\gamma}')^2,
\end{array} \right)
\]

consequently, we find the following estimates for the general Heisenberg approximation kernels

\[
\tilde{C}_1 e^{-\frac{c_2 \sqrt{\|y\|^2 + \|\tilde{x}\|^2 \tilde{a} + \|\tilde{\gamma}\|^2 + \|\tilde{\beta}\|^2 \|\tilde{\gamma}\|^2}}{4u}} \\
\leq \tilde{p}_{1}(x, y, z, \tilde{\beta}, \tilde{\gamma}) \\
\leq \tilde{C}_3 e^{-\frac{c_4 \sqrt{\|y\|^2 + \|\tilde{x}\|^2 \tilde{a} + \|\tilde{\gamma}\|^2 + \|\tilde{\beta}\|^2 \|\tilde{\gamma}\|^2}}{4u}}.
\]

(74)

where we used short notation \( c^k_0 = c^k_0(x, R_{\tilde{\beta}}, \tilde{\gamma}, 0), k = 1, \ldots, 5 \), \( x = (x, y, z)^T \in \mathbb{R}^3 \), recall (72).

In fact in Duits and Franken (2009, Chap. 6.2) it is shown that the constants \( \tilde{C}_3, \tilde{C}_4 \) are very close and that a reasonably sharp approximation and upperbound of the horizontal diffusion kernel on \( \mathbb{R}^3 \times S^2 \) is given by

\[
\tilde{p}_{1}(x, y, z, \tilde{\beta}, \tilde{\gamma}) \\
\approx \frac{1}{(4\pi t^2D_{33}D_{44})^2} e^{-\frac{\|y\|^2 + \|\tilde{x}\|^2 \tilde{a} + \|\tilde{\gamma}\|^2 + \|\tilde{\beta}\|^2 \|\tilde{\gamma}\|^2}{4u}} \\
\]

(75)

where we again use short notation \( c^k := c^k(x, R_{\tilde{\beta}}, \tilde{\gamma}, 0), k = 1, \ldots, 6 \). Recall from Sect. 5.1 that these constants
are computed by the logarithm, (57), on SE(3) or more explicitly by (55) and (56). The latter two equalities are analogously expressed in the second coordinate chart yielding formulas for the functions $c^k$ in (75):

$$q = \arcsin \sqrt{\cos^2(\tilde{\psi}/2) \sin^2(\tilde{\beta}) + \cos^2(\tilde{\beta}/2) \sin^2(\tilde{\psi})},$$

$$e^{(2)} = (e^4, e^5, e^6)^T$$

$$= \frac{q}{\sin(q)} \left( \sin \tilde{\psi} \cos^2(\frac{\tilde{\beta}}{2}), \sin \tilde{\beta} \cos^2(\frac{\tilde{\psi}}{2}) \right),$$

$$e^{(1)} = (e^1, e^2, e^3)^T$$

$$= x - \frac{1}{2} e^{(2)} \times x$$

$$+ \tilde{q}^{-2} \left( 1 - \left( \frac{\tilde{q}}{q} \right) \cot \left( \frac{\tilde{q}}{q} \right) \right) e^{(2)} \times x.$$

These functions $c^k$ (the case $q = 1$) are indeed consistent with the functions $c^k_0$ (the case $q = 0$) in the sense that $\lim_{q \to 0} c^{\mu} \cdot c_0 = c^{\mu}(x, y, z, \tilde{\beta}, \tilde{\psi})$, where we recall (59) for $k = 1, 2, \ldots, 5$.

### 7 Implementation of the Left-Invariant Derivatives and $\mathbb{R}^3 \times S^2$-Diffusion

In our implementations we do not use the two charts (among which the Euler-angles parametrization) of $S^2$ because this would involve cumbersome and expensive bookkeeping of mapping the coordinates from one chart to the other (which becomes necessary each time the singularities (3) and (6) are reached). Instead we recall that the left-invariant vector fields on HARDI-orientation scores $\tilde{U} : SE(3) \rightarrow \mathbb{R}$, which by definition (recall Definition 4) automatically satisfy

$$\tilde{U}(y, R R_e_{e_\alpha}) = \tilde{U}(y, R), \text{ for all } y \in \mathbb{R}^3,$$  

(77)

are constructed by the derivative of the right-regular representation

$$A_j \tilde{U}(g) = (d\mathcal{R}(A_j) \tilde{U})(g)$$

$$= \lim_{t \to 0} \frac{\tilde{U}(g e^{A_j} t) - \tilde{U}(g)}{t},$$

$$= \lim_{t \to 0} \frac{\tilde{U}(g e^{A_j}) - \tilde{U}(g e^{-t A_j})}{2t},$$

where in the numerics we can take finite step-sizes in the right-hand side. Now in order to avoid a redundant computation we can also avoid taking the de-tour via HARDI-orientation scores and actually work with the left-invariant vector fields on the HARDI data itself. To this end we need the consistent right-action $\mathcal{R}$ of $SE(3)$ acting on the space of HARDI images $L_2(\mathbb{R}^3 \times S^2)$. Let $H$ denote the space of HARDI-orientation scores, i.e. $H$ is the space of quadratic integrable functions on the group $SE(3)$ which satisfy (77). To construct this consistent right-action on $H$ we first define $S : L_2(\mathbb{R}^3 \times S^2) \rightarrow H$, by

$$(SU)(x, R) = \tilde{U}(x, R) = U(x, R e_z).$$

This mapping is injective and its left-inverse is given by $(S^{-1} U)(x, R) = \tilde{U}(x, R_n)$, where again $R_n$ is $SO(3)$ is some rotation such that $R_n e_z = n$. Now the consistent right-action $\mathcal{R} : SE(3) \rightarrow B(L_2(\mathbb{R}^3 \times S^2))$, where $B(L_2(\mathbb{R}^3 \times S^2))$ stands for all bounded linear operators on the space of HARDI images, is given by

$$(\mathcal{R}_{(x, R)} U)(y, n) = (S^{-1} \circ \mathcal{R}_{(x, R)} \circ SU)(y, n)$$

$$= U(R_n y + y, R_n R e_z).$$

This yields the left-invariant vector fields (directly) on sufficiently smooth HARDI images:

$$A_j U(y, n) = (d\mathcal{R}(A_j) U)(y, n)$$

$$= \lim_{h \to 0} \frac{(\mathcal{R}_{e_{A_j}} U)(y, n) - U(y, n)}{h}$$

$$= \lim_{h \to 0} \frac{(\mathcal{R}_{e_{-A_j}} U)(y, n) - (\mathcal{R}_{e_{-A_j}} U)(y, n)}{2h}.$$

Now in our algorithms we take finite step-sizes and elementary computations (using the exponent given by (54)) yield the following simple expressions for the (horizontal) left-invariant vector fields:

$$A_1 U(y, n) \approx U(y + h R_n e_z, n) - U(y - h R_n e_z, n),$$

$$A_2 U(y, n) \approx U(y + h R_n e_z, n) - U(y - h R_n e_y, n),$$

$$A_3 U(y, n) \approx U(y + h R_n e_z, n) - U(y - h R_n e_z, n),$$

$$A_4 U(y, n) \approx U(y, R_n R_{e_h} e_z) - U(y, R_n R_{e_{-h}} e_z),$$

$$A_5 U(y, n) \approx U(y, R_n R_{e_h} e_z) - U(y, R_n R_{e_{-h}} e_z).$$

(78)

The left-invariant vector fields $\{A_1, A_2, A_4, A_5\}$ clearly depend on the choice of $R_n \in SO(3)$ which maps $R_n e_z = n$. Now functions in the space $H$ are $\alpha$-right invariant, so thereby we may assume that $R$ can be written as $R = R_{e_t} R_{e_\gamma} \tilde{R}_{e_\beta}$, now if we choose $R_n$ again such that $R_n = R_{\tilde{R}_{e_\beta} e_\gamma} = R_{e_\gamma} \tilde{R}_{e_\beta} R_{e_{\tilde{R}_{e_\beta}} e_\gamma} = e_{\gamma_0 \alpha_0}$ then we take consistent sections in $SO(3) \subset SO(2)$ and we get full invertibility $S^{-1} : S \rightarrow S^{-1} = I$. 

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In our diffusion schemes, however, the choice of representant \( R_n \) is irrelevant, because we impose \( \alpha \)-right invariance (31) on the diffusion generator (which in the linear case boils down to (34)) and as a result we have \( D_{\alpha \alpha} = D_{SS}, \; D_{11} = D_{22}. \) The thereby obtained operators \( (A_4)^2 + (A_5)^2 = \Delta S^2 |_H \) and \( A_1^2 + A_2^2 = \Delta_{\mathbb{R}^3} - A_3^2 \) are invariant under transformations of the type \( \mathcal{A} \mapsto Z_{\alpha_0} \mathcal{A} \) for all \( \alpha_0 \in [0, 2\pi] \), recall (32).

In the computation of (78) one would have liked to work with discrete subgroups of \( SO(3) \) acting on \( S^2 \) in order to avoid interpolations, but unfortunately the platonic solid with the largest amount of vertices (only 20) is the dodecahedron and the platonic solid with the largest amount of faces (again only 20) is the icosahedron. Nevertheless, we would like to sample the 2-sphere such that the distance between sampling points should be as equal as possible and simultaneously the area around each sample point should be as equal as possible. Therefore we follow the common approach by regular triangulations (i.e. each triangle should be as equal as possible. Therefore we follow the common approach by regular triangulations (i.e. each triangle should be as equal as possible. Therefore we follow the common approach by regular triangulations (i.e. each triangle should be as equal as possible. Therefore we follow the common approach by regular triangulations (i.e. each triangle should be as equal as possible)

\[ D_{\alpha \alpha} = D_{SS}, \; D_{11} = D_{22}. \]

\[ (A_4)^2 + (A_5)^2 = \Delta S^2 |_H, \quad A_1^2 + A_2^2 = \Delta_{\mathbb{R}^3} - A_3^2 \]

are invariant under transformations of the type \( \mathcal{A} \mapsto Z_{\alpha_0} \mathcal{A} \) for all \( \alpha_0 \in [0, 2\pi] \), recall (32).

\[ \Delta S^2 = (A_4)^2 + (A_5)^2 |_H. \]

\[ 20 \] vertices. We typically considered \( o = 1, 2, 3 \), for further details on uniform spherical sampling, see Franken (2008, Chap. 7.8.1).

For the required interpolations to compute (78) within our spherical sampling there are two simple options. Either one uses a triangular interpolation of using the three closest sampling points, or one uses a discrete spherical harmonic interpolation. The disadvantage of the first and simplest approach is that it introduces additional blurring, whereas the second approach can lead to overshots and undershots. In the latter approach a \( \pi \)-symmetric function on the sphere only requires even values for \( l \in \{0, 2, 4, \ldots \} \) in which case the total amount of spherical harmonics is \( n_{SH} = \frac{1}{2} (L + 1)(L + 2). \) Although, there exist more efficient and accurate algorithms for discrete harmonic transforms (DSHT), (Driscoll and Healy 1994; Kunis and Potts 2003), we next give a brief explanation of the basic algorithm we used. To this end we first recall that the continuous spherical harmonic transform is given by

\[ \langle SHT(f)(l, m), Y^l_m(\beta, \gamma) \rangle = \int_0^{2\pi} \int_0^\pi Y^l_m(\beta, \gamma) f(\theta, \phi) \sin \theta \, d\theta \, d\phi. \]

(79)

The spherical harmonics (38) form a complete orthonormal basis in \( L_2(S^2) \), so the inverse is given by

\[ f(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \langle SHT(f)(l, m), Y^l_m(\beta, \gamma) \rangle Y^l_m(\beta, \gamma). \]

(80)

for almost every \( \beta \in [0, \pi) \) and almost every \( \gamma \in [0, 2\pi). \) As mentioned before (in Sect. 4.1) the function \( f \) becomes a regular smooth function (which is defined everywhere) if we apply a slight diffusion on the 2-sphere:

\[ e^{-t_{reg} \Delta_{S^2}} f(\theta, \phi) \]

(81)

\[ = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} e^{-t_{reg} (l+1)^2} \langle SHT(f)(l, m), Y^l_m(\beta, \gamma) \rangle \]

with \( 0 < t_{reg} \ll 1. \) Next we explain two basic discrete versions of the SHT-transform. Both can be used in a finite difference scheme requiring discretization of for example \( \Delta S^2 = (A_4)^2 + (A_5)^2 |_H. \)

7.1 DSHT and DISHT

There exist two basic approaches to discretize the continuous spherical harmonic transform. Either one considers (79) as a starting point and approximates the integral by a Riemann sum taking care of the surface measure, yielding the DSHT-transform and its pseudo-inverse. Or one considers (80) as a starting point yielding the DISHT-transform and its pseudo-inverse. The first approach is exact on the grid if the number of spherical harmonics is larger than the number of samples \( n_{SH} \geq N_o, \) whereas the second approach is exact on the grid if \( n_{SH} \leq N_o. \)

The pseudo-inverse \( Q^+ \) of a matrix \( Q \in \mathbb{R}^{m \times n} \) is defined by \( Q^+ x = \lim_{\epsilon \to 0} (Q^T Q + \delta I)^{-1} Q^T x, \) with \( Q^T = Q^T. \)

If the columns of \( Q \) are linearly independent, then \( Q^+ = (Q^T Q)^{-1} Q^T \) and \( Q^+ Q = I. \)

Consider a “uniform” spherical sampling \( \{ n_k \}_{k=1}^{N_o} \subset S^2 \) such that the associated a \( n_{SH} \times N_o \)-matrix

\[ M = [M^l_j] = \left[ \frac{1}{\sqrt{C}} Y^l_m(j)(n_k) \right], \]

with \( l(j) = \left\lfloor \sqrt{j} - 1 \right\rfloor \) and \( m(j) = j - (l(j))^2 - l(j) - 1 \)

and \( C = \sum_{j=1}^{n_{SH}} Y^l_m(j)(0, 0)^2. \) (chosen to ensure that \( M^T M \) has 1 on the diagonal), has linearly independent columns (so \( N_o \leq n_{SH} \)). Then the DSHT and its pseudo-inverse are given by

\[ DSHT[f] = \mathbf{M} \mathbf{A} f, \]

\[ DSHT^+[s] = ((\mathbf{M})^T \mathbf{A})^{-1} (\mathbf{M})^T s, \]

\[ n_{SH} \geq N_o, \quad \text{ (82) } \]

where the matrix \( \mathbf{A} = \text{diag} \{ \delta S^2(n_1), \ldots, \delta S^2(n_{N_o}) \} \) contains discrete surface measures \( \delta S^2(n_k) \) given by

\[ \delta S^2(n_k) = \frac{1}{6} \sum_{i \neq k, j \neq k, i \neq j, i \sim j \sim k} A(n_i, n_j, n_k), \quad \text{ (83) } \]

where \( i \sim j \) means that \( n_i, n_j \) are part of a locally smallest triangle in say the second order tessellation of an icosahedron.
hedron and where the surface measure of the spherical projection of such a triangle is given by

$$A(n_i, n_j, n_k) = 4 \arctan \left\{ \tan \left( \frac{s_{ijk}}{2} \right) / \tan \left( \frac{s_{ij} - s_{jk}}{2} \right) \right\}^{1/2},$$

with $s_{ijk} = \frac{1}{2} (s_{ij} + s_{jk} + s_{jk})$ and $s_{ij} = \arccos (n_i \cdot n_j)$. The DISHT (which follows by sampling of (80)) and its pseudo-inverse DISHT$^+$ are given by

$$\text{DISHT}[s] = M^T s$$

$$\text{DISHT}^+[f] = (\overline{M}M^T)^{-1}(\overline{M})f, \quad n_{SH} \leq N_o.$$  \hspace{1cm} (84)

The pseudo-inverse DISHT$^+$ is commonly used in HARDI-DTI imaging (on separate glyphs) as initiated by Descoteaux et al. (2007) where the authors include a Tikhonov-type of regularization $(\overline{M}M^T + \gamma^2 \text{diag}(l(j)(l(j) + 1)))^{-1}(\overline{M})f$, $\gamma > 0$, within the transform DISHT$^+$. This destroys (wellposed) invertibility on the grid but clearly it stabilizes the acquisition of low order spherical harmonic coefficients from in practice often incomplete spherical samplings. However, in our framework we would like to return from the spherical harmonic coefficients to the spherical sampling on say a 2nd order tessellation of an icosahedron. Moreover, we would like to include the weighting factors $\delta_{S^2}(n_k)$ (which satisfy $\sum_{k=1}^{N_o} \delta_{S^2}(n_k) = 4\pi$) that compensate for differences in the surrounding of the sampling points. So we have two options for computing the left-invariant Laplacian on $S^2$:

$$\Delta_{S^2} W(y, n_k, t)$$

$$= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (SHT(f))(l,m)Y_{l,m}(n_k)$$

$$\approx [\text{DISHT}^+[j \mapsto l(j)(l(j) + 1)e^{-t_{reg}(l(j) + 1)}l(j)]$$

$$\cdot \text{DISHT}[k' \mapsto W(y, n_k', t)](j)](k)$$

$$\approx \frac{1}{\delta_{S^2}(n_k)} [\text{DISHT}[j \mapsto l(j)(l(j) + 1)e^{-t_{reg}(l(j) + 1)}l(j)]$$

$$\cdot \text{DISHT}[k' \mapsto W(y, n_k', t)](j)](k),$$  \hspace{1cm} (85)

with regularizing parameter $0 < t_{reg} \ll 1$. In order to stay close to the continuous setting we have applied the second option in our discrete experiments, although the second option would act entirely in the discrete setting (where DSHT$^+ \circ$ DISHT $= I$ if $n_{SH} \geq N_o$). The two methods converge to each other if $n_{SH} \to \infty$, since

$$(M^T M \to I \text{ as } n_{SH} \to \infty)$$

$$\Rightarrow (\text{DISHT}^+ \to \Lambda^{-1} M^T = \Lambda^{-1} \text{DISHT as } n_{SH} \to \infty).$$

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig6.png}
\caption{Effect of increasing spherical harmonic bandwidth $L$ on the net operator matrix $M^T M$ for the case $N_o = 32$ (1st order tessellation of dodecahedron). If one takes higher order spherical harmonics than strictly required, reconstruction of the sampled function on the sphere improves. Note that $M^T M \to I$ as $n_{SH} \to \infty$}
\end{figure}

See Fig. 6. In practice one must be careful since if $n_{SH}$ becomes too large aliasing artifacts arise and a potential decrease of numerical instability arises. Therefore we included a regularization parameter $t_{reg}$ to guarantee stability. Typically $t_{reg} > 0$ should be chosen very small, but not too small as the function $j \mapsto l(j)(l(j) + 1)e^{-t_{reg}(l(j) + 1)}l(j) \times DSHT[k' \mapsto W(y, n_k', t)](j)$ should nearly vanish at $j \geq N_o$ to avoid aliasing.

7.2 Finite Difference Scheme for Linear $\mathbb{R}^3 \times S^2$ Diffusion

The linear diffusion system on $\mathbb{R}^3 \times S^2$ can be rewritten as

$$\partial_t W(y, n, t) = (D_{11}(A_1^2) + (A_2)^2)$$

$$+ D_{33}(A_3)^2 + D_{44}A_{S^2} W(y, n, t)$$

$$W(y, n, 0) = U(y, n).$$  \hspace{1cm} (86)

This system is the Fokker-Planck equation of horizontal Brownian motion on $\mathbb{R}^3 \times S^2$ if $D_{11} = 0$. Spatially, we take second order centered finite differences for $(A_1^2)^2$, $(A_2)^2$ and $(A_3)^2$, i.e. we applied the discrete operators in the right-hand side of (78) twice (where we replaced $2h \mapsto h$ to ensure direct-neighbors interaction), e.g. we have

$$(A_3)^2 W(y, n, t)$$

$$\approx W(y + hR_u e_z, n, t) - 2W(y, n, t) + W(y - hR_u e_z, n, t)$$

$$h^2,$$  \hspace{1cm} (87)

where one can either apply the earlier mentioned interpolation methods (2nd order B-spline or (81)) or (as we did in our experiments) one first computes all second order finite differences on the cubic spatial grid and rotates them back to the spatial part of the moving frame of reference, (24), attached to $(y, n)$. The spherical Laplacian $\Delta_{LB}$ is computed by means of (85) (second approximation). For efficiency, the chain of operators, DSHT-diag $[l(l + 1)e^{-t_{reg}(l + 1)}]$-DISHT, is stored in a single $N_o \times N_o$-matrix, so that calculation of $\Delta_{S^2}$ consists of a simple matrix-vector multiplication. In our algorithm we apply a first order approximation in time.
where we choose $\Delta t$ small enough such that the algorithm is stable. As we have shown in Duits and Franken (2009, Chap. 7.2, App. B) sharp upper bounds on $\Delta t$ is stable. As we have shown in Duits and Franken (2009) where we choose $\Delta t$ small enough such that the algorithm is stable. As we have shown in Duits and Franken (2009, Chap. 7.2, App. B) sharp upper bounds on $\Delta t$ which guarantee stability are given by

$$
\Delta t \leq \frac{h^2}{4D_{11} + 2D_{33} + D_{44}h^2\frac{L(L+1)}{2\pi\text{reg}(L+1)}},
$$

if $\text{reg} \cdot L(L + 1) \leq 1$,

$$
\Delta t \leq \frac{h^2}{4D_{11} + 2D_{33} + D_{44}h^2\frac{1}{2\pi\text{reg}}},
$$

if $\text{reg} \cdot L(L + 1) > 1$

where $h$ denotes spatial step size and $L = \lceil \sqrt{n_{SH}} - 1 \rceil$. The estimate (89) is due to the wellknown Gerschgorin circle theorem, cf. Gerschgorin (1931). An increase of spatial diffusivity and angular diffusivity yields a decrease in the maximum time step, whereas an increase of the regularity parameter $\text{reg}$ allows a larger time step. We also recognize a turning point if $\text{reg} \cdot (L(L+1))=1$. The multiplier $l(j)(j + 1)e^{-\text{reg}l(j)(j + 1)}$ attains its maximum at $j < n_{SH}$ if $\text{reg} > (L(L + 1))^{-1}$. This is desirable since the multiplier is supposed to vanish at $j = n_{SH} \approx N_p$. In the experiment of Fig. 10, we have set $h = 10^{-1}$, $n_p = 162$, $L = 18$ (restricting $l$ to even order), $\text{reg} = 0.01$, $D_{33} = 1$, $D_{11} = 10^{-2}$, $D_{44} = 10^{-4}$ and $\Delta t = 0.005$.

7.3 Convolution Schemes for Linear $\mathbb{R}^3 \times S^2$-Diffusion

Instead of a finite difference scheme one can use the theoretical fact that the solutions of the linear diffusions, (36), are given by $\mathbb{R}^3 \times S^2$-convolution, (37), with the corresponding Green’s function $\rho_t^{D,a}$ that we derived analytically in Sect. 6. The convolution scheme is a relatively straightforward discretization of $W(y,n,t) = (p_t^{\mathbb{R}^3} \ast_{S^2} U)(y,n,t)$ given by (10), where the integrals are usually replaced by sums using the midpoint rule (unless one has to deal with the singularity at the origin of the contour-completion kernel). We will consider specific practical implementation issues later in Sect. 8.2. In this subsection we restrict ourselves to an overview of options for the computation of the Green’s functions.

We propose the following options to evaluate the Green’s function for contour enhancement (i.e. non-zero parameters are $D_{33} > 0$, $D_{44} = D_{55} > 0$ and $D_{11} = D_{22} \geq 0$) in (37):

1. Use the finite difference scheme to numerically approximate the Green’s function. Disadvantage: This requires interpolation. For small time steps $\Delta t \ll 1$ this numeric approximation is very accurate.

2. if $D_{11} = D_{22} = 0$ we can use the analytic approximation formulae for the contour enhancement kernel. Here one can either use (75) where the functions $(x,n) \mapsto e^{L}(x,n)$ are computed by means of the algorithm (76), or one may use the simpler but less accurate formula (69) using the asymptotical formula (70). In case $D_{44}/D_{33} \ll 1$ one may want to use the fast Heisenberg approximation kernel, (68), together with (70).

For the contour-completion case where the non-zero parameters are $a_3 = 1$, $D_{44} = D_{55} > 0$ generalizations of the finite difference scheme of the previous section are questionable due to the trade-off between accuracy of convection and stability of diffusion. Alternation of convection and diffusion with very small time steps (like described in Zweck (2004) for the $SE(2)$-case) is probably preferable here. To avoid these technical issues we propose kernel-implementations for the contour completion case, where we distinguish between the following options:

1. For the resolvent of the contour-completion process use analytic formula (64) (accurate if $4\pi D_{44} \ll 1$).

2. For the time-dependent contour completion process use analytic formula (65) (accurate if $4\pi D_{44} \ll 1$).

Figure 7 shows HARDI glyph visualizations of several contour enhancement kernels and Fig. 8 shows HARDI glyph visualizations of a contour completion kernel.

8 Experiments of Linear Crossing-preserving Diffusion on $\mathbb{R}^3 \times S^2$

In the previous section we have discussed two different kinds of implementations of crossing-preserving diffusion on HARDI images, namely left-invariance finite difference schemes and left-invariant convolution schemes. In this section we will show some experiments of these approaches and furthermore we discuss some practical issues that come along with these approaches.

Before we will consider the different practical properties of the two approaches, we briefly comment on their analogies. Firstly, each step in the finite difference schemes is a linear kernel operator and thereby in principle (due to Corollary 1) a $\mathbb{R}^3 \times S^2$-convolution with a small kernel which is non-zero on the discretization stencil). Secondly, the computational order of the algorithms is comparable. The $\mathbb{R}^3 \times S^2$-convolutions are of order $O(N_p N_o K_s K_o)$ and the finite difference schemes are of order $O(N_p N_o N_i N_{it})$, where $N_p$, $N_o$ respectively stand for the total number of spatial and orientation samples of the HARDI image, $K_s$, $K_o$ respectively stand for the number of spatial samples and average number of orientation samples of the convolution kernel and $N_{it}$ stands for number of iteration with a discretization stencil of length $N_{it}$. Thirdly, both approaches are very well suited for parallel implementation.
Fig. 7 Glyph visualization of the analytic approximations (for $0 < \frac{D_{44}}{D_{33}} \ll 1$), (69), using asymptotical formula (70) of the Green’s function $p_{D_{33},D_{44}}$ for contour enhancement, satisfying the semigroup property: $p_{D_{33},D_{44}}$ for contour completion. We normalized stretching parameter $D_{33} = 1$ and the values of $D_{44}$ and $t$ are depicted on top. The size of the kernel is controlled by $t > 0$ and $D_{44}$ controls the bending of the kernel and consequently there are no artefacts (such as in Fig. 5) in the iterative diffusion. We normalized stretching parameter $D_{33} = 1$ and the values of $D_{44}$ and $t$ are depicted on top. The size of the kernel is controlled by $t > 0$ and $D_{44}$ controls the bending of the kernel.

Fig. 8 Left: Glyph visualization of the analytic approximations (accurate for $0 < 4\lambda D_{44} \ll 1$) given by (64) of the Green’s function $p^{D_{33},D_{44}}$ for contour completion. Top right: HARDI glyphs at $(0,0,z)$ with from left to right $z = 0, 0.1, 0.5, 1, 1.5$. The contour completion kernel is single-sided (i.e. $p^{D_{33},D_{44}}(x,y,z,n) = 0$ for $z < 0$), in contrast to the contour enhancement kernel depicted in Fig. 7. The positive probability density kernel $p^{D_{33},D_{44}}$ is $L_1$-normalized but has a singularity at the origin, akin to its 2D-equivalent (Duits and van Almsick 2008; Mumford 1994).

8.1 Experiments Finite Difference Scheme

We implemented linear, left-invariant diffusion on HARDI data with diagonal diffusion matrix $D = \text{diag}(D_{ii})$ with $D_{11} = D_{22}, D_{44} = D_{55}$ (and $D_{66} = 0$) using an explicit numerical scheme as explained in Sect. 7.2. Figures 9 and 10 show results of the linear diffusion process. In these examples an artificial three-dimensional HARDI dataset is created, to which Rician noise is added, meaning that we applied the transformation.
Fig. 9 Result of \( \mathbb{R}^3 \rtimes S^2 \)-diffusion (computed by the finite difference scheme, Sect. 7.2) on an artificial HARDI dataset of two crossing straight lines, with and without added Rician noise (90) with \( \sigma = 0.17 \) (signal amplitude 1). Image size: 10 × 10 × 10 spatial and 162 orientations. Parameters of the isotropic diffusion process: \( D_{11} = D_{22} = D_{33} = 1 \), \( D_{44} = D_{55} = 0.01 \). Parameters of the anisotropic diffusion process: \( D_{11} = D_{22} = 0.01 \), \( D_{33} = 1 \), \( D_{44} = D_{55} = 10^{-4} \). In both cases we have set \( t_{reg} = 0.01 \) in (81).

\[
((\mathbf{y}, \mathbf{n}) \mapsto U(\mathbf{y}, \mathbf{n})) 
\mapsto

((\mathbf{y}, \mathbf{n}) \mapsto \sqrt{(U(\mathbf{y}, \mathbf{n}) \cos(\eta_1) + \eta_2)^2 + (U(\mathbf{y}, \mathbf{n}) \sin(\eta_1) + \eta_3)^2})
\]

(90)

where \( \eta_2, \eta_3 \sim \mathcal{N}(0, \sigma) \) normally distributed and \( \eta_1 \) uniformly distributed over \([0, 2\pi)\).

Next, we applied two different \( \mathbb{R}^3 \rtimes S^2 \)-diffusions on both the noise-free and the noisy dataset. To visualize our results we used the DTI tool (see http://www.bmia.bmt.tue.nl/software/dtitool/) which can visualize HARDI glyphs using the Q-ball visualization method (Descoteaux et al. 2007). In the results, all glyphs are scaled equivalently. The isotropic diffusion (\( D_{33} = D_{22} = D_{11} \)) does not preserve the anisotropy of the glyphs well; especially in the noisy case we observe that we get almost isotropic glyphs. With anisotropic diffusion, the anisotropy of the HARDI glyphs is preserved much better and in the noisy case the noise is clearly reduced. See Figures 9 and 10. The resulting glyphs are, however, less directed than in the noise-free input image. This would improve when using nonlinear diffusion. The basic theoretical PDE-framework for nonlinear diffusions, is the subject of the last section. As an alternative to nonlinear adaptive diffusion, we are currently investigating the inclusion of “sharpening” steps by means of left-invariant erosions (solutions of left-invariant Hamilton-Jacobi PDEs on HARDI data). Practical properties of the left-invariant finite difference schemes are:

+ + It is relatively easy to adapt and generalize to nonlinear (adaptive) diffusion schemes.

- - The explicit finite difference scheme is only stable for sufficiently small time steps.
In Sect. 7.3 we have provided an overview of options for computing the Green’s functions of contour enhancement and contour completion. Now suppose we have chosen an analytic approximation formula \( p(y, n) \) for the Green’s function \( p: \mathbb{R}^3 \times S^2 \rightarrow \mathbb{R}^+ \), then we can rewrite (37) in \( L^2 \)-inner product form

\[
(p * \mathbb{R}^3 \times S^2 U)(y, n) = (\mathcal{L}(y, R_n)^\dagger \hat{p}, U)_{L^2(\mathbb{R}^3 \times S^2)},
\]

where we recall Definition 2 of \( \mathcal{L} \) and where we define \( \hat{p}(y', n') = p(-R_n^T y', R_n^T e_i) \). Note that

\[
\hat{p}(y', n') = k(0, e_i; y', n') \quad \text{and} \quad p(y, n) = k(y, n; 0, e_i), \quad \text{for all} \quad (y, n), (y', n') \in \mathbb{R}^3 \times S^2.
\]

Now \( p(y, n) \) denotes the probability density of finding a random walker at \( (y, n) \) given that it started at \( (0, e_i) \), so that \( \hat{p}(y, n) = p(-R_n^T y, R_n^T e_i) \) denotes the probability density of finding a random walker at \( (-R_n^T y, R_n^T e_i) \) given that it started at \( (0, e_i) \), which is by left-invariance of the stochastic process the same as the probability density of finding a random walker at \( (0, e_i) \) given that it started at \( (y, n) \).

The main advantage of formula (91) is that in practice we can pre-compute/sample all rotated versions and translated versions \( \{ \mathcal{L}(y, R_n)^\dagger \hat{p} \mid y \in \mathbb{R}^3, n \in S^2 \} \) of the check-kernel \( \hat{p} \), so that the remainder of the algorithm just consists of computing \( L^2 \)-inner products which can be done in parallel. In contrast to the finite difference schemes, the convolution schemes are unconditionally stable. In fact, we even have

\[
\| p * \mathbb{R}^3 \times S^2 U \|_{L^1(\mathbb{R}^3 \times S^2)} = \| p \|_{L^1(\mathbb{R}^3 \times S^2)} \| U \|_{L^1(\mathbb{R}^3 \times S^2)} = 1 \cdot \| U \|_{L^1(\mathbb{R}^3 \times S^2)},
\]

\[
\| p * \mathbb{R}^3 \times S^2 U \|_{L^\infty(\mathbb{R}^3 \times S^2)} = \sup_{(y, n)} \| p * \mathbb{R}^3 \times S^2 U(y, n) \|,
\]

\[
\leq \| \mathcal{L}(y, R_n)^\dagger \hat{p} \|_{L^2(\mathbb{R}^3 \times S^2)} \| U \|_{L^2(\mathbb{R}^3 \times S^2)} \leq \| p \|_{L^2(\mathbb{R}^3 \times S^2)} \| U \|_{L^2(\mathbb{R}^3 \times S^2)}
\]

i.e. preservation of mass (which also holds on the discrete grid if the discretely sampled versions of \( \mathcal{L}(y, R_n)^\dagger \hat{p} \) are...
\[ R = \{ \text{Right} \} \]

\begin{align*}
\ell_1 &\text{-normalized on the grid and a small } L_2\text{-perturbation on the input yields a small } L_{-\infty}\text{-perturbation on the output.}
\end{align*}

Finally, formula (91) provides the following fast discrete approximation/truncation:

\[
(p \ast_{R^3 \times S^2} U)(y, n) 
\approx \sum_{y' \in R^3} K(y', y, n) \sum_{k=1}^{N_0} (2y, R_n \tilde{p})(y', n_k') 
\cdot U(y', n_k') \Delta y \delta_{S^2}(n_k'),
\tag{92}
\]

with spatial step size \( \Delta y = (\Delta y_1', \Delta y_2', \Delta y_3') \) and where we truncated the spatial integration to a cube \( \|y' - y\|_{\infty} = \sup_{i=1,2,3} |y_i' - y_i| \leq R, \quad R > 0 \), where we recall (83) and where \( [n_k']_{k=1}^{N_0} := [n_k'](y', y, n)_{k=1}^{N_0} \), forms an a priori defined lookup table by sorting the points \( [n_k']_{k=1}^{N_0} \) such that

\[
2y, R_n \tilde{p}(y', n_k') < 2y, R_n \tilde{p}(y', n_k)
\]

and where \( K(y', y, n) = \max\{k \in \{1, \ldots, N_0\} | 2y, R_n \tilde{p}(y', n_k) \leq \epsilon \} \), with tolerance \( \epsilon > 0 \). We usually set \( R \in \{1, 2, 3, 4\} \) (see for example Fig. 11 where we even set \( R = 1 \)) for the spatial truncation and \( \epsilon = 10^{-5} \) for angular truncation. The gain in speed mostly lies in the angular truncation, as the convolution kernels are for reasonable parameter settings of \( D_{33}, D_{44}, \iota, \lambda \) rather orientation-selective, recall Fig. 7 and Fig. 8.

Summarizing we have the following practical properties of the left-invariant convolution schemes:

+ The convolution kernels can be pre-computed and truncated.
+ The algorithm does not suffer from the typical numerical blur of finite difference schemes.
++ The algorithm is unconditionally stable.

For single sided kernels (completion) one can include reflections, as we will see in Sect. 8.2.1.

++ The algorithm is easily extended to left-invariant dilations/erosions on HARDI images by replacing the \((+, \cdot)\)-algebra by the \((\max, +)\)-algebra in the convolution, akin to previous work on regular images (Burgeth and Weickert 2003; Burgeth et al. 2008).

--- Generalization to nonlinear adaptive diffusions: Adapting the kernel to the data locally is no longer a convolution and the relation to left-invariant PDEs is no longer clear.

For further experiments of convolution schemes solving diffusion (combined with basic grey-value transformations, such as squaring \( U(y, n) \mapsto (U(y, n))^2 \)) on medical HARDI and DTI datasets, see the recent works (Rodrigues et al. 2010; Prčkovska et al. 2010), where the first author of this article collaborated with P. Rodrigues, V. Prčkovska et al.

### 8.2.1 Spherical Reflection Symmetries: Preservation of Reflection Symmetry in Contour Enhancement and including Glyph-attraction in Contour Completion

The big difference between the stochastic processes for contour completion and contour enhancement is that contour completion kernels are single-sided, whereas contour enhancement kernels are double-sided. Compare Fig. 7 to Fig. 8. This change in reflection symmetry has two consequences:

1. The initial HARDI data are usually invariant under spherical reflections, i.e. \( U(y, n) = (r_{g2} U)(y, n) := U(y, -n) \).

In contrast to contour completion, contour enhancement preserves this symmetry during the evolution, as can be seen in Fig. 9 and Fig. 10. This directly follows by the fact that the generator of contour completion \( -A_3 + \Delta_{g2} \)
and the generator of contour enhancement \((A_3)^2 + \Delta s^2\) satisfy
\[
(-A_3 + \Delta s^2) \circ r_{s^2} = r_{s^2} \circ (+A_3 + \Delta s^2),
\]
\[
((A_3)^2 + \Delta s^2) \circ r_{s^2} = r_{s^2} \circ ((A_3)^2 + \Delta s^2).
\]

2. It allows a relevant extension of our contour completion processes, where we replace the \(R^3 \times SO(2)\)-convolutions by \((R^3 \times O(3))/((0) \times SO(2))\) convolutions as we will explain next. Here \(O(3) = \{M \in R^{3 \times 3} | M^T = M^{-1}\}\) denotes the group of orthogonal matrices on \(R^3\) which includes both rotations \(d\text{et}M = +1\) and reflections \(d\text{et}M = -1\). The practical advantage of these \((R^3 \times O(3))/((0) \times SO(2))\)-convolutions is that it allows us to include attraction of glyphs, rather than continuations of contours. See Fig. 11 and compare the two images in the middle. To achieve this extension we need a different kind of reflections, namely spatial reflections given by \(r_{\mathbb{R}^2}\). These spatial reflections \(r_{\mathbb{R}^2}\) intertwine the contour enhancement and completion generators in the same way as the angular reflections \(r_{s^2}\):
\[
(-A_3 + \Delta s^2) \circ r_{\mathbb{R}^2} = r_{\mathbb{R}^2} \circ (+A_3 + \Delta s^2),
\]
\[
((A_3)^2 + \Delta s^2) \circ r_{\mathbb{R}^2} = r_{\mathbb{R}^2} \circ ((A_3)^2 + \Delta s^2).
\]
Now indeed (94) is analogous to (93) but the crucial difference between these two types of reflections is:
\[
\begin{align*}
\tau_{\mathbb{R}^3} \delta e &= \delta e \quad \text{and} \quad \tau_{s^2} \delta e \neq \delta e \quad \text{and} \\
\tau_{\mathbb{R}^3} U &\neq U \\
\tau_{s^2} U &= U.
\end{align*}
\]
Now (95) and (94) directly imply the spatial reflection symmetry of the contour enhancement kernel as can be seen in Fig. 7. Clearly the contour completion kernel does not admit such a symmetry and we arrive at the following three possible choices of \((R^3 \times O(3))/((0) \times SO(2))\)-convolutions:
\[
\begin{align*}
(p^{3-D_{33}} \ast &\{R^3 \times O(3)\}/((0) \times SO(2)) \ast U)(y, n) \\
&= \sum_{\epsilon' \in \{-1, 1\}} q_{ab}(\epsilon') \int_{S^2} \int_{R^3} p^{3-D_{33}}(\epsilon' R^T_\mu(y - y'), R^T_\mu n') \\
& \cdot U(y', n') d\mu(dy') d\sigma(n') \\
& \text{with } q_{ab}(\epsilon') = \frac{1}{2}(a \delta_{\epsilon'1} + b \delta_{-\epsilon'1}), \\
a, b \in \{0, 1\}, ab \neq 0.
\end{align*}
\]

These two issues are illustrated in Fig. 11 for a simple example of a HARDI image induced by a DTI image, i.e. \(U(y, n) = n^T D(y) n\). In Fig. 11 we have set rotation matrices \(S(y)\) such that \(D(y) = (S(y))^{-1} \text{diag}(0.1, 0.1, 1) S(y)\). Furthermore, we applied Rician noise on the HARDI data, recall (90). The particular case \(a = b = 1\) in (96) yields results that are similar to convolution with contour enhancement kernels (recall Fig. 7) for suitable choice of \(D_3\) and \(D_4\). The difference in practice is that the sum of two spatially reflected contour completion kernels yields a double sided kernel that is typically sharper kernel at the center than a contour enhancement kernel.

9 Nonlinear, Adaptive, Left-Invariant Diffusions on HARDI Images

So far we have considered linear left-invariant diffusions, whose solutions are given by convolution with a fixed Green’s function reflecting an a priori probability model for fiber-extension. In many applications however, it is important to adapt the fiber-extension model to the data, where we can include adaptive curvature and adaptive torsion. Now by Theorem 3, it follows that in order to include adaptive torsion and curvature we must re-align the left-invariant local coordinate frame \(\{A_1, \ldots, A_5\}\) by means of a locally optimally fitting exponential curve, where we recall (51).

Our first aim is to determine the exponential curve, recall (54), that optimally fits the distribution \((y, n) \mapsto U(y, n) \in R^+\) at each position \((y, n) \in R^3 \times S^2\). Recall that such a distribution gives rise to a probability distribution \((x, R) \mapsto \tilde{U}(x, R)\) on \(SE(3)\) by means of (27). To achieve our goal, we follow the same approach as in our previous works on nonlinear diffusions on invertible orientation scores (of 2D-images) defined on \(SE(2)\) (Franken et al. 2008, pp. 118–120), (Duits and Franken 2010, Part II, Chap. 3.4), (Franken and Duits 2009, Chap. 5.2).

We again formulate the minimization problem that minimizes over the “iso-contours” of the left-invariant gradient vector at \((y, n) \in R^3 \times S^2\), yielding optimal tangent vector \(c_s(y, n) = (c_s^1(y, n), \ldots, c_s^5(y, n), 0)^T\):
\[
c_s(y, n) = \arg \min_{c(y, n)} \left\{ \left\| \frac{d}{dr}(\nabla \tilde{U}(g e^{\tau c(y, n)})\right\|_{\tau=0}^2 \right\},
\]
where the left-invariant gradient
\[
d\tilde{U}(g) = \sum_{i=1}^5 (A_i(\tilde{U}))(g) dA_i|_{g=\tilde{g}}, \quad g \in SE(3),
\]
a co-vector field, is represented by a row-vector given by \(\nabla \tilde{U}(g) = (A_1 \tilde{U}(g), \ldots, A_5 \tilde{U}(g), 0)\) and where \(\| \cdot \|_\mu\) denotes both the norm on a vector in tangent space \(T_\mu(SE(3))\) and the dual norm on a covector in the dual tangent space \(T_\mu^*(SE(3))\). We represent tangent vectors \(c(y, n) = \sum_{i=1}^5 c_i(y, n) A_i|_{g=\tilde{g}=y, R_n}\) as column-vector companions.
(c_1^s(y, n), \ldots, c_5^s(y, n), 0)^T and their norm is defined by \|c\|_\mu := \sqrt{\langle c, c \rangle_\mu}, where the inner product \(\langle c, c \rangle_\mu := \mu^2(\sum_{j=1}^3 c_j c_j) + \sum_{j=4}^6 c_j c_j\), parameter \(\mu\) ensures that all components of the inner product are dimensionless. The value of the parameter determines how the distance in the spatial dimensions relates to distance in the orientation dimension. Implicitly, this also defines the norm on covectors by \(\|\hat{c}\|_\mu = \sqrt{\langle \hat{c}, \hat{c} \rangle_\mu}\), \(\hat{c} \bar{=} \langle \hat{c}, G^{-1} \hat{c} \rangle = \mu^{-2}(\sum_{j=1}^3 c_j c_j) + \sum_{j=4}^6 c_j c_j\). By means of the calculus of variations it follows that the minimizer \(c_s(y, n)\) satisfies

\[
(M_{\mu}\mathcal{H}(g) M_{\mu})^T (M_{\mu}\mathcal{H}(g) M_{\mu}) \hat{c}_s(y, n) = \lambda \hat{c}_s(y, n),
\]

(98)

with \(M_{\mu} := \text{diag}(1/\mu, 1/\mu, 1/\mu, 1, 1, 1)\), \(\hat{c}_s = M_{\mu}^{-1} c_s\), and where the \(6 \times 6\) Hessian of \(\mathcal{U}\) on \(\mathbb{R}^3 \times S^2\) equals

\[
\mathcal{H}(g) = [A_j A_i U(g)]_{ij}^{\text{row-index}} [A_j A_i U(g)]_{ij}^{\text{column-index}},
\]

g = (y, R) \in SE(3),

where the last row contains of zeros only. This amounts to eigensystem analysis of the symmetric \(6 \times 6\) matrix-valued function \(g \mapsto (M_{\mu}\mathcal{H}(g) M_{\mu})^T (M_{\mu}\mathcal{H}(g) M_{\mu})\), where one of the three eigenvectors gives \(c_s(y, n)\). The eigenvector with the smallest corresponding eigenvalue is selected as tangent vector \(\hat{c}_s(y, n)\), and the desired tangent vector \(c_s(y, n)\) is then given by \(c_s(y, n) = M_{\mu} \hat{c}_s(y, n)\).

Now that we have computed the optimal tangent vector \(c_s(y, n)\) at \((y, n) \mapsto U(y, n)\) (and thereby the best fitting exponential curve \(t \mapsto g e^{\sum_{j=1}^3 c_j A_j} \) in \(\mathbb{R}^3 \times S^2\)) we construct the nonlinear adaptive diffusion function:

\[
D(U)(y, n) = c_s(y, n) c(y, n)^T \frac{\mu^2(1 - D_u(U)(y, n))}{\|c(y, n)\|^*_\mu} + D_u(U)(y, n) \begin{pmatrix} I_3 & 0 \\ 0 & \mu^2 I_3 \end{pmatrix},
\]

where \(D_u(U)(y, n)\) is a locally adaptive anisotropy factor. Finally, we note that the conditions (35) are satisfied so our final well-defined nonlinear diffusion system on the HARDI data are:

\[
\begin{aligned}
\partial_t W(y, n, t) &= \sum_{i,j=1}^6 (A_j [D(U)(y, n)]_{ij} A_i W)(y, n, t), \\
\lim_{t \to 0} W(y, n, t) &= U(y, n).
\end{aligned}
\]

10 Conclusion

For the purpose of tractography (detection of biological fibers) and visualization, DTI and HARDI data should be enhanced such that fiber junctions are maintained, while reducing high frequency noise in the joined domain \(\mathbb{R}^3 \times S^2\) of positions and orientations. Therefore we have considered diffusions on HARDI and DTI induced by fundamental stochastic processes on \(\mathbb{R}^3 \times S^2\) embedded in the group manifold \(SE(3)\) of 3D rigid body motions.

We have shown that the processing must be left-invariant and we have classified all linear left-invariant diffusions on HARDI images. We presented two novel diffusion approaches which take place simultaneously over both positions and orientations. These two approaches do allow enhancement of fibres while preserving crossings and/or bifurcations. These two diffusions are Fokker-Planck equations of stochastic processes (random walks) for respectively contour enhancement and contour completion. In a contour completion process a random walker always proceeds forward in space along its prescribed random direction, whereas in a contour enhancement process the random walker randomly moves forward and backward in its prescribed random orientation. As a result the contour completion process is generated by \(-A_3 + D_{44} \Delta_{S^2}\) whereas the contour enhancement process is generated by the sub-Laplaceian \(+D_{33}(A_3)^2 + D_{44} \Delta_{S^2}\), with \(D_{33}, D_{44} > 0\) and \(\Delta_{S^2} |_{H} = A_4^2 + A_5^2\) the Laplace-Beltrami operator on the sphere and where \(A_i\) denotes the \(i\)-th left-invariant vector field on \(\mathbb{R}^3 \times S^2\). Consequently, the contour enhancement process preserves the angular reflection symmetry of HARDI data, whereas the contour completion process allows a choice between attraction or continuation of glyphs.

As the solutions of linear left-invariant diffusion equations are given by \(\mathbb{R}^3 \times S^2\)-convolution with their Green’s functions, we arrive at two types of implementations: Convolution schemes and finite difference schemes. Practical advantages of convolution schemes over finite difference schemes for linear diffusions are: they are unconditionally stable and do not involve the typical numerical blurring of a finite difference scheme. However, the finite difference schemes with sufficiently small time steps do provide cross-preserving diffusion as well, and they are preferable for our extensions to nonlinear adaptive diffusions proposed in Sect. 9.

The crucial theoretical observations in our framework lie in the fact that the left-invariant evolution equations are expressed by a quadratic form in the left-invariant vector fields \(\{A_i\}_{i=1}^6\) on \(\mathbb{R}^3 \times S^2\) embedded in \(SE(3)\), which form a moving frame of reference consisting of a spatial velocity part \(\{A_1, A_2, A_3\}\) and an angular velocity part \(\{A_4, A_5, A_6\}\). This moving frame of reference requires the Cartan connec-
tion viewpoint on the underlying differential geometry and by expressing the left-invariant diffusions in covariant derivatives we see that even the adaptive nonlinear left-invariant evolutions locally take place along the covariantly constant curves, which coincide with the exponential curves in $SE(3)$. The spatial part of the exponential curves are circular spirals, i.e. curves in $R^3$ with constant curvature and constant torsion. As a result our nonlinear adaptive diffusion schemes allow local adaptation for curvature and torsion, which we will further investigate and implement in future work.

Furthermore, in future work, we will apply our techniques to medical DTI-data sets and investigate whether we can create suitable orientation density distributions (to avoid expensive HARDI acquisitions) at crossings by means of $R^3 \times S^2$-diffusion. Finally, we will consider natural extensions of our scale spaces on $R^3 \times S^2$, such as the combination of left-invariant diffusion and left-invariant Hamilton-Jacobi equations (erosions, Burgeth and Weickert 2003) in a single evolution on $R^3 \times S^2$.

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