Registering Image Volumes using 3D SIFT and Discrete SP-Symmetry

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Abstract—This paper proposes to extend local image features in 3D to include invariance to discrete symmetry including inversion of spatial axes and image contrast. A binary feature sign \( s \in \{-1, +1\} \) is defined as the sign of the Laplacian operator \( \nabla^2 \), and used to obtain a descriptor that is invariant to image sign inversion \( s \rightarrow -s \) and 3D parity transforms \( (x, y, z) \rightarrow (-x, -y, -z) \), i.e. SP-invariant or SP-symmetric. SP-symmetry applies to arbitrary scalar image fields \( I : R^3 \rightarrow R^1 \) mapping 3D coordinates \( (x, y, z) \in R^3 \) to scalar intensity \( I(x, y, z) \in R^1 \), generalizing the well-known charge conjugation and parity symmetry (CP-symmetry) applying to elementary charged particles. Feature orientation is modeled as a set of discrete states corresponding to potential axis reflections, independently of image contrast inversion. Two primary axis vectors are derived from image observations and potentially subject to reflection, and a third axis is an axial vector defined by the right-hand rule. Augmenting local feature properties with sign in addition to standard (location, scale, orientation) geometry leads to descriptors that are invariant to coordinate reflections and intensity contrast inversion. Feature properties are factored in to probabilistic point-based registration as symmetric kernels, based on a model of binary feature correspondence. Experiments using the well-known coherent point drift (CPD) algorithm demonstrate that SIFT-CPD kernels achieve the most accurate and rapid registration of the human brain and CT chest, including multiple MBI modalities of differing intensity contrast, and abnormal local variations such as tumors or occlusions. SIFT-CPD image registration is invariant to global scaling, rotation and translation and image intensity inversions of the input data.

Index Terms—Local Features, 3D SIFT, Discrete Symmetry, CP-symmetry, Charge conjugation, Sign inversion, Parity transform, Contrast Inversion, Image Registration, Multiple Modalities, right-hand rule.

1 INTRODUCTION

3D structure is often described in terms of localized phenomena or features. In classical physics, fine-scale matter in the atomic model is characterized via the Schrodinger equation [1], where the symmetry of the Laplacian operator ensures that atomic properties remain invariant to changes in the viewpoint of the observer. Similarly, elementary 3D image features may be identified in generic image volumes via fundamental mathematical operators, e.g. the 3D Laplacian-of-Gaussian operator [2], [3], following from scale-space theory and the 2D scale-invariant feature transform (SIFT) [4], [5]. These are used in highly robust and efficient memory-based applications, e.g. detection [6], registration [7], [8], segmentation [9], [10], indexing [11], [12] in a manner invariant to transformations including translation, rotation and scaling, and are applicable in generic contexts with no training or calibration procedures.

Our work here seeks to advance the understanding of 3D keypoints observed in image volumes from the notion of symmetry, specifically discrete symmetry in feature orientation. A geometrical object may be said to exhibit a symmetry if its observed properties remain unaffected by (or are invariant to) a group of transforms, i.e., a symmetry group. In particle physics, discrete symmetries include axis reflections and also simultaneous charge conjugation (inversion), 3D parity transformation and time reversal (CPT-symmetry). The CPT transform models the transition of a charge-associated particle to its anti-particle, e.g. a proton to an anti-proton, and is currently a topic of high interest [13], [14] as symmetry violations have been observed in special cases including charge conjugation and parity (CP) transforms [15], [16]. Nevertheless in image analysis, discrete shape symmetries including reflections [17], [18] and image contrast inversion [19], [20], [21], [22], [23] are typically represented as separate, unrelated phenomena, typically in 2D coordinate space where 3D parity does not apply. Indeed, image processing and graphics research focuses largely on representations and challenges stemming from 2D data, including photographs, surface meshes or projections, and achieving invariance to viewpoint changes. Despite the compelling analogy between local features and the atomic model, the notion of a local feature sign, analogous to a particle charge, has not been proposed nor linked to the 3D parity transform in the context of image processing.

Our primary contribution is the first model of discrete symmetry including intensity inversion in the context of local feature processing as shown in Figure[1] We note that a CP-like transform occurs in the context of image processing, where a local feature observed in different imaging modalities may exhibit simultaneous contrast inversion and gradient reversal. We refer to this as a sign inversion and parity transform (SP-transform), which applies generally to arbitrary scalar image fields \( I : R^3 \rightarrow R^1 \) mapping 3D coordinates \( (x, y, z) \in R^3 \) to a scalar image intensity \( I(x, y, z) \in R^1 \), and we seek SP-invariance. Local features are endowed with a binary sign \( s \in \{-1, +1\} \) and a set of discrete orientation states, allowing feature descriptors and image registration to be computed in a manner invariant to...
reflections and intensity contrast inversions, thus achieving SP-invariance. Volumetric data allows physical matter and local image features to be observed in situ within isotropic 3D space and free from projective distortion, thus facilitating the analogy between local image features and atoms in terms of charge. Local feature orientation is defined by a 3D rotation matrix or coordinate reference frame, where two primary axes are estimated from dominant image gradient directions and the third vector is defined by the cross product, ensuring feature reference frames are restricted to $SO(3)$ despite potential parity transform due to contrast inversion. Four discrete orientation states are defined, corresponding to inversions of the two primary axis vectors, due to a combination of symmetric image gradient patterns and intensity contrast inversion. Gradient-based descriptors may be inverted via sign change, independently of orientation state.

Our secondary contribution is to incorporate invariant feature properties into a probabilistic point-based registration framework. The variability of feature scale, orientation and location between images is modeled via an exponential kernel function, approximating a zero-mean noise model, invariant to feature reflection and intensity contrast inversion. Experiments adapt our model to the well-known Coherent Point Drift (CPD) [24] algorithm, and demonstrate that our SIFT-CPD model of enhanced feature geometry leads to faster and more accurate inter-subject registration, in a diverse variety of image data including multiple T1 and T2 weighted MRI modalities of the human brain, tumors and CT images of the human torso. We also demonstrate that our model may be used to achieve SP-invariance independently of the method used to estimate feature orientation, e.g. via principal component analysis or maximum gradient directions.

The remainder of this paper describes related work, method and experiments. Throughout the paper, we aim to provide an accessible yet complete presentation of related concepts in 3D geometry, image processing and particle physics.
made use of gradients $V_I$, including gradient orientation histograms SIFT [3], binary comparisons [39] and variants such as rank ordering [40]. RootSIFT [41]. Descriptors may be learned via triplet loss and gradient analysis [43], [42]. While GPU-based deep learning is the de facto state-of-the-art for image classification [43], variants of the traditional gradient representations remain competitive with learned variants [44], [45], specifically for matching images of non-planar objects [46] and image retrieval [47].

The SIFT algorithm has been generalized to 3D volumetric images. A body of work investigates SIFT-like detectors in 3D video coordinates $(x, y, t)$ defined by 2D space $x, y$ and 1D time $t$ [48], [49]. In the context of 3D space $x, y, z$, applications include object detection [6], medical image analysis [2], [3], [50], [51], segmentation [9], [10], alignment [52], image stitching [53], large-scale indexing [12], population studies [54], [55]. Most recently, the Jaccard distance between feature sets was introduced to automatically flag errors in large public training MRI datasets [56], [57], and to identify family members from brain MRI [11], capabilities facilitated by highly efficient feature indexing. We adopt the 3D SIFT-Rank method [2] using a GPU-optimized implementation [37] first used in the context of brain MRI analysis [58].

2.2 Image Registration

Registration is a fundamental image processing task, and seeks to identify a coordinate transform $T : \Omega_1 \rightarrow \Omega_2$ between the coordinate systems $\Omega_1 \in \mathbb{R}^3$, $\Omega_2 \in \mathbb{R}^3$ of the same object or scene, often in three spatial dimensions, based on a pair of observed images $(I_1, I_2)$. Registration generally makes use of intensity and geometry information [59], our work focuses on properties of local feature geometry, specifically location, orientation, scale and sign.

Point-based registration approaches are most generally applicable to local features, where the loss function minimizes the distance between pairs of points or points and a model. Examples of point cloud registration algorithms [60] include iterative algorithms such as the Iterative Closest Point (ICP) algorithm [61] where points contribute uniformly to a solution, or the Coherent Point Drift (CPD) algorithm [24] where points contribute according to a probabilistic weighting. 3D SIFT keypoint correspondences have been used to achieve point-based registration the context of image-guided neurosurgery [5], including non-rigid image registration via thin plate splines [52], finite element methods [53] and the CPD algorithm [64], however these have made use of keypoint locations and not orientation and scale properties as we propose.

Feature-based registration methods generally consider points with properties beyond simple location. Points on a surface model may be endowed with properties such as mass [65] or charge [66], however these properties tend to be assigned algorithmically, e.g. uniformly assigned across points, and not derived from the image content itself. Local properties including orientation, scale and affine deformation may be used to enhance point-based registration [67], [68]. Smooth deformations may be computed in a manner consistent with local rigid or affine reference frames [69]. The variability of geometrical misalignment is related to feature scale $\sigma$ [56], [70], consistent with uncertainty due to Gaussian blur. The localization accuracy of SIFT correspondences has been compared to that of manual human labeling in 2D and 3D [7], [70], showing similar accuracy, where experts preferred automatic SIFT correspondences in 80% cases [7] in the case of brain imaging. Our 3D SIFT-CPD algorithm proposed in the following section accounts for feature properties of orientation and scale, in addition to point locations.

Multi-modal image registration is a major challenge, where intensities may vary locally in a non-linear manner between modalities. Training may be used to approximate an intensity mapping for a specific domains, e.g. MRI and CT [71], however this mapping may not be functional or stationary throughout the image. In the general case with no specific training domain or data, intensity-based registration must adopt statistical similarity measures such as mutual information [72]. In the case of 2D image keypoints, invariance to local contrast inversion may be achieved by transforming the image intensity into a contrast-invariant format, including phase congruency [73] or Laplacian [74] images. As contrast inversion leads to image gradient reversal, attempts have been made to reverse aspects linked to the gradient, including descriptor orientation [19], [20], [75], [76]. Combinations of multiple keypoints [21] including self-similarity [23] may be adopted. In preliminary work, we proposed to account for 3D gradient reversal [77], here we extend this to include reflections and SP-symmetry via the notion of a binary sign $s \in \{-1, +1\}$.

2.3 Discrete Symmetry

In a physical system, a symmetry refers to a property that remains unchanged under set of transforms, i.e. an invariant property. The symmetry group is the Lie group of transforms under which a geometrical object such as a particle is invariant [17]. A symmetry may be described as continuous or discrete. Continuous symmetry pertains to continuous parameters of pose and scale, e.g. translation and orientation relative to the reference frame of an image acquisition device, and are analogous to a consequence of Noether’s theorem for Lagrangian mechanical systems [73], [79]. Continuous symmetry has been investigated in the computer vision literature in terms of differential invariance [4], [80], [81]. Classical neural networks such as CNNs are generally invariant to translations but not to reflections or scale changes [82], [83]. Robustness to certain transforms may be improved via regularization [84]. Recently models of invariance or equivariance in trainable neural networks have emerged, including SO(3) [85], [86] rotations, 3D rigid transforms [87] non-linear transforms [86], probabilistic symmetries [88] and gauge theory [18]. Much of this work has been limited to 2D image modalities, i.e. surfaces or projective images, and has not considered the 3D notion of SP-symmetry including a binary sign $s \in \{-1, +1\}$.

A discrete symmetry generally involves discrete displacements in location and/or orientation, e.g. translations, rotations, reflections, glide reflections or repetitive crystal structure. Charge conjugation and parity symmetry (CP-symmetry) [18], and generally space-time reversal in CPT-symmetry including time relating to the transition of a
particle to its anti-particle \cite{13, 14} are important aspects of discrete symmetry relating to 3D reflection of elementary physical particles. CP-symmetry is closely related to reflection symmetry, which exists in a function exhibiting one or more planes of symmetry, i.e. a reflection about a single axis \( x = 0 \) such that \( f(x) = f(-x) \), or in a 3D system, the parity coordinate transform \( f(x, y, z) = f(-x, -y, -z) \), both characterized in 3D by a rotation matrix \( R \) with determinant \( \det(R) = -1 \). The effect of the parity transform may be seen by first representing \( f(x) \) in terms of \( f(x) = f_a(x) + f_b(x) \), the sum purely symmetric and antisymmetric image components \( f_a(x) \) and \( f_b(x) \) defined by \( f_a(-x) = f_a(x) \) and \( f_b(-x) = -f_b(x) \). Symmetric or even functions \( f_a(x) \) include the Gaussian and Laplacian-of-Gaussian operators, wave functions associated with bosonic particles such as the photon, the cosine function, etc. Anti-symmetric or odd functions \( f_b(x) \) include the gradient operator \( \nabla I \), wave functions associated with fermionic particles such as electrons, and the sine function, etc. As the gradient is an anti-symmetric operator, an image contrast inversion \( -\nabla I(x) = \nabla (-x) \) is equivalent to an axis reflection. This phenomenon is analogous to charge conjugation and parity (CP) symmetry, and describes the transition of a charge-associated particle to its antiparticle, e.g. electrons and positrons. Notably, CP-symmetry was thought to be an inviolable in nature until the discovery of special cases beginning with the composite meson particle \cite{15}. In our work here, charge is equivalent to image sign or contrast, which may be inverted, and we propose SP-invariance to register images of differing modality.

Image processing methods specifically relating to our work have analyzed discrete shape symmetry (ie. reflections) \cite{17} and image contrast inversion \cite{19, 20, 21, 22, 23} as separate, unrelated phenomena. Our work is the first to consider these within the unified framework of discrete SP-symmetry, including a binary sign and discrete states of local reference frame orientation. Our method generalizes to various contexts where orientation is estimated from dominant local image gradients \( \nabla I \). For example, Toews et al. identify maxima in a 3D spherical gradient histogram \cite{2}, such that \( \hat{\theta}_1 = \arg\max_{\hat{\theta}} |\nabla I \cdot \hat{\theta}|, \hat{\theta}_2 = \arg\max_{\hat{\theta}} |\hat{\theta} \times (\nabla I \times \hat{\theta})| \), with a third axis defined by the cross product \( \hat{\theta}_3 = \hat{\theta}_1 \times \hat{\theta}_2 \), Rister et al. compute the eigenvectors of the local gradient structure tensor, ie. the \( 3 \times 3 \) gradient correlation matrix \cite{3}. We demonstrate that both such representations may be modeled in terms of discrete SP-symmetry.

3 Method

Our method provides a means of characterizing 3D image features in a manner invariant to discrete symmetry transforms, including symmetric image patterns and sign inversion and parity (SP-symmetry) transforms due to image contrast inversion. We begin by describing the properties of a single local image feature, which we augment to include a binary sign and a set of discrete axis reflections. This allows us to compute a descriptor that is invariant to reflections and changes in sign due inversion of intensity contrast. We then define a kernel function \( K(f_n, f_m) \) to quantify the similarity of a pair of features \( (f_n, f_m) \) potentially arising from the same underlying structure in two different images. Finally, this kernel is incorporated into probabilistic image registration in order to estimate a transform \( T : f_m \rightarrow f_n \) aligning the coordinate systems of two images.

3.1 Single-Feature Properties

A feature is a distinctive spherical region localized in 3D image space, as illustrated in Figure 1. An individual feature \( f = (y, a, s) \) is characterized within the image by its geometry \( g \), a descriptor of the image appearance \( a \) surrounding the feature and a binary sign \( s \). The feature geometry \( g = (\Theta, \sigma, x) \) is \( SO(3) \times R^+ \times R^3 \) is a scaled coordinate reference frame in 3D defined by 7 parameters. These include a scale \( \sigma \in R^+ \), a coordinate location \( x \in \mathbb{R}^3 \) and a reference frame \( \Theta \in SO(3) \). The reference frame may be defined as a set \( \Theta = \{\hat{\theta}_1, \hat{\theta}_2, \hat{\theta}_3\} \) of orthonormal unit vectors \( \hat{\theta}_i, i \in \{1, 2, 3\} \) where \( \hat{\theta}_i \cdot \hat{\theta}_j = 0, i \neq j \). Note equivalently 3D rotation could make use of alternative representations, eg. \( SU(2) \) Pauli matrices or unit quaternions. Feature appearance \( a \in \mathbb{R}^{M} \) is an M-dimensional descriptor of the image, resampled according to geometry \( g \). The sign \( s \in \{-1, 1\} \) is used to achieve invariance to image contrast inversion.

Let \( I : \mathbb{R}^3 \rightarrow \mathbb{R}^1 \) be a scalar image sampled over 3D coordinates where \( I(x) \) represents a voxel measurement at location \( x \). Let \( I(x, \sigma) = I(x) * G(x, \sigma) \) be a scale-space defined by convolution of the image with a Gaussian filter \( G(x, \sigma) \) of parameter \( \sigma \) \cite{4}. Features are detected as points in scale-space \( \{x_m, \sigma_m, s_m\} \) at which the magnitude of the scale-normalized Laplacian operator is maximized, similarly to the original SIFT method \cite{5}, here \( m \) is a feature index. Furthermore, they are endowed with a binary sign as follows.

\[
\{x_m, \sigma_m\} = \text{local argmax}_{x, \sigma} (\nabla^2 I(x, \sigma)),
\]

\[
s_m = \text{sign} (\nabla^2 I(x_m, \sigma_m)).
\]

Scale-space loci \( \{x_m, \sigma_m, s_m\} \) represent generic spherical regions in which the divergence of the local gradient field \( \nabla I(x, \sigma) \) is maximized. Feature sign \( s_m \) is novel to our characterization, and is defined as the sign of the Laplacian-of-Gaussian.

Feature orientation \( \Theta \) is derived from the image gradient \( \nabla I \) surrounding the feature origin \( x \). Orientation axis vectors \( \hat{\theta}_1, \hat{\theta}_2, \hat{\theta}_3 \) may be determined according dominant gradient orientations within a window \( w(x, \sigma) \in [0, 1] \) centered upon \( x \) with spatial extent proportional to scale \( \sigma \). As \( \Theta \in SO(3) \), the determinant \( \det(\Theta) = 1 \) is positive, ie. no reflections. Axes are thus defined by two primary axis vectors \( \hat{\theta}_1 \) and \( \hat{\theta}_2 \), with the third constrained according to a handedness convention, ie. the right-hand rule via the cross product \( \hat{\theta}_3 = \hat{\theta}_1 \times \hat{\theta}_2 \). Furthermore, we assume that axis vectors may be ordered uniquely according to the gradient magnitude along their directions, i.e. \( |\nabla I \cdot \hat{\theta}_i| > |\nabla I \cdot \hat{\theta}_j| \), where \( |\nabla I \cdot \hat{\theta}_i| = \int w(x, \sigma) |\nabla I(u) \cdot \hat{\theta}_i| \ du \) is the expected value of the gradient magnitude along axis \( \hat{\theta}_i \).

Our primary contribution is a descriptor that is invariant to discrete SP-transforms, i.e. is SP-symmetric, based on binary sign \( s \). We first note that the sign of the orientation axes \( \hat{\theta}_1, \hat{\theta}_2 \) may generally be ambiguous due to a variety of
factors including bilateral symmetry of the image pattern or its local gradient distribution (e.g. an ellipsoid or rectangular box), an image contrast inversion (e.g. different imaging modalities), or the algorithm used to estimate orientation (e.g. principal component analysis has an inherent eigenvector sign ambiguity). Sign ambiguity may be represented by maintaining a discrete set of possible orientation reference frames \( \Theta \). We consider four potential reference frame states \( \{ \pm \Theta_1, \pm \Theta_2 \} \) (with \( \Theta_3 = \pm \Theta_1 \times \pm \Theta_2 \)) resulting from axis inversion, i.e. due to either intensity contrast inversion or pattern symmetry, which are equivalent to the identity in addition to rotations of \( \pi \) about each of the 3 axes. By defining the third axis vector \( \hat{\Theta}_3 \) using the cross product, we ensure feature orientation follows the right-hand rule. Figure 2 illustrates the four possible orientation states, including an initial reference frame and rotations of \( \pi \) about each of the 3 axes.

Feature sign \( s \) is used to generate a novel contrast inversion-invariant descriptor \( a_m \) for each orientation state, based on the image content surrounding location \( x_m \) at scale \( \sigma_m \) and orientation \( \Theta_m \). Note that the geometry defines a 7-parameter similarity transform from the local feature reference frame to a canonical reference frame, including rotation, translation and scaling. This thus is used to resample the image according to a characteristic reference frame \( \hat{I}(u) = I(\sigma_m \Theta_m u + x_m) \) that is invariant to global similarity transforms of the image. A variety of descriptors may be computed, e.g. spherical harmonics \( \text{[9]} \), we adopt a computationally efficient variant of the gradient orientation histogram \( \text{[2]}, \text{[3]}, \text{[5]} \). As in \( \text{[2]} \), 3D space surrounding the feature origin \( x_m \) is quantized uniformly into eight discrete octants \( r = \{ \pm 1, \pm 1, \pm 1 \} \), and the image gradient at each point \( u \) eight discrete symmetric directions \( \phi = \{ \pm 1, \pm 1, \pm 1 \} \). These are combined into an \( 8 \times 8 = 64 \)-element appearance descriptor, by accumulating the gradient magnitude into a histogram over spatial location and orientation

\[
a(r, \phi) = \sum_{u \in r} \| \nabla \hat{I}(u) \cdot \phi \| [\phi = s \phi_u],
\]

where \( \phi_u = \text{argmax}_{\phi} (\nabla \hat{I}(u) \cdot s \phi) \) is the direction of maximum gradient at image location \( u \), which is inverted in the case of \( s = -1 \) by the Iverson bracket \( [\phi = s \phi_u] \) evaluating to 1 upon equality and 0 otherwise. Thus descriptor orientation elements \( \phi \) are invariant to reversal due to sign change \( a(r, \phi) = a(r, s \phi) \), and parity transformations of orhtants \( r \rightarrow -r \) are accounted for by feature orientation states \( \{ \pm \Theta_1, \pm \Theta_2 \} \), as illustrated in Figure 2.

### 3.2 Two-Feature Observations

Image registration requires identifying pairs of features \( (f_n, f_m) \) arising from the same underlying structure in different images. To do this, we propose a kernel function \( K(f_n, f_m) \in [0, 1] \) to quantify the similarity of two features \( f_n \) and \( f_m \) potentially sampled from the same distribution. We construct \( K(f_n, f_m) \) as a product of squared exponential kernels, ensuring that it is positive, symmetric \( K(f_m, f_n) = K(f_n, f_m) \), and proportional to a Gaussian density. It may be expressed as the product of three factors

\[
K(g_n, g_m) = K_\sigma(\sigma_n, \sigma_m)K_\Theta(\Theta_n, \Theta_m)K_z(x_n, x_m),
\]

quantifying the variability in scale, orientation and location, respectively. As in the notions of linear and angular moment from classical physics, deviations of location and orientation are modeled as orthogonal and independent.

The first factor in Equation (3), \( K_\sigma(\sigma_n, \sigma_m) \), is a kernel penalizing the log scale difference:

\[
K_\sigma(\sigma_n, \sigma_m) = \exp \left( -\|\log \sigma_n - \log \sigma_m\|^2 \right),
\]

and is proportional to a log normal density about mean \( \log 1 = 0 \) with unit variance 1. The log maps multiplicative variations in feature scale on the range \( \sigma \in [0, \infty] \) to additive variations on the range \( \log \sigma \in [-\infty, \infty] \), which may be modelled as symmetric and Gaussian.

The second factor \( K_\Theta(\Theta_n, \Theta_m) \) quantifies the variability of feature orientations based on the angular displacement of the axes:

\[
K_\Theta(\Theta_n, \Theta_m) = \exp \left( -3 + \sum_{i=1,2,3} \hat{\Theta}_{in} \cdot \hat{\Theta}_{im} \right).
\]

In Equation (5), the scalar product \( \hat{\Theta}_{in} \cdot \hat{\Theta}_{im} = \cos(\hat{\Theta}_{in} - \hat{\Theta}_{im}) \) quantifies the angular separation between axis unit vectors \( \hat{\Theta}_{in} \) and \( \hat{\Theta}_{im} \) on the range \([-1, 1]\). This is equivalent to modeling the angular difference between features independently in each axis \( i \) as proportional to a von Mises density over the unit circle.

The third factor \( K_z(x_n, x_m) \) is a kernel that quantifies the similarity of feature locations based on their squared displacement:

\[
K_z(x_n, x_m) = \exp \left( -\frac{\|x_n - x_m\|^2}{k \sigma_n \sigma_m + \sigma_T^2} \right),
\]

where the denominator normalizes the spatial displacement \( \|x_n - x_m\| \) via a linear function of the product of feature scales \( \sigma_n \sigma_m \). The first term \( k \sigma_n \sigma_m \) embodies intrinsic variance due to the scale of the observed feature, where \( \sigma_n \sigma_m \) represents the square of the geometric mean of feature scales and \( k \) is a positive proportionality constant. This allows quantifying the variability in location in a manner invariant to keypoint scale. The second term \( \sigma_T^2 \) represents the minimum achievable variance in mapping \( T \) given the particular imaging context, which dominates in the case of small-scaled features, i.e. \( k \sigma_n \sigma_m < \sigma_T^2 \). Note that in previous work \( \text{[1]} k = 1 \) and \( \sigma_T = 0 \), here we use \( k \) and \( \sigma_T \) to estimate a more accurate linear relationship between scale and observed variability. These are empirically set to provide a generally useful weighting, e.g. here we use \( k = 12, \sigma_T^2 = 200 \).

### 3.3 Multi-Feature Registration

Registration seeks a transform \( T \) mapping the coordinate system of a fixed image \( f_n \) to that of a moving image \( f_m \), here from sets of features extracted in the fixed \( F = \{ f_n \} \) and moving \( M = \{ f_m \} \) images. The transform maps the properties of features from one coordinate space to the next \( T : x_m \rightarrow x_n \), and here is taken to be a global similarity transform, followed by independent zero-mean deviations
for individual features. Note that the similarity transform is a 7-parameter representation $T = (d\theta, dx, dy, da) \in SO(3) \times R^+ \times R^3$ equivalent that of an individual feature.

Let $g_m$ represent the geometry of feature $f_m$ as transformed by $T$, i.e. $g_m = T \circ g_m$, note that $T$ may act on location, scale and orientation parameters in a consistent manner. We propose using our kernel function $\mathcal{K}(g_n, g_m')$ to account for feature properties including scale and orientation in a standard point-based registration framework. Our kernel lends itself naturally to a probabilistic algorithm such as Coherent Point Drift (CPD) in Algorithm 1, which seeks a maximum likelihood solution based on the Expectation-Maximization (EM) algorithm [2]. The expectation step (E) intend estimates the log-likelihood based on the current parameters, while the maximization step (M) maximizes the log-likelihood over the parameters using the result of the E step. CPD registration is based on a probability map $p_{mn}$ between each pair of points $\{f_n, f_m\}$, and takes the form of a softmax function. We propose to bias this probability map based on a kernel function $\mathcal{K}(g_n, g_m')$ as follows:

$$p_{mn} = \frac{\exp\left(-\frac{||x_n-x_m'||^2}{2\lambda^2}\right) \mathcal{K}(g_n, g_m')}{\sum_{k=1}^M \exp\left(-\frac{||x_n-x_k'^|^2}{2\lambda^2}\right) \mathcal{K}(g_n, g_k') + \eta},$$

where $\eta = (2\pi \lambda^2)^{D/2} w \frac{M}{1-\sigma^2}$ is a constant ensuring the denominator $p_{mn}$ is non-zero, where $w$ is parameter accounting for the relative probability of a uniform background density not associated with any specific feature. In Equation (7), the exponential expression with parameter $\lambda$ is a variance parameter that is reduced iteratively to converge to a solution, and a constant kernel function $\mathcal{K}(g_n, g_m') = 1$ is identical to the original CPD algorithm [24]. Thus in our proposed SIFT-CPD, two exponential factors operate on point coordinates $x$ including Equation [5].

Iterative algorithms such as EM must be initialized within a neighborhood of the solution in order to converge correctly. We initialize registration via a global 3D Hough transform between feature sets $F$ and $M$ in 3D [4] analogously to the classic 2D SIFT algorithm [9], where all features vote independently as to the predicted transform, after which a most likely transform is identified. Here, each feature $f_n \in F$ votes for a transform $T_{nm} : g_n \rightarrow g_m$, mapping the geometry of feature $f_n$ to that of feature $f_m$, where $f_m = \arg\max_T |\{a_n-a\}|$ is the nearest neighbor of $f_n$ in terms of the Euclidean distance between appearance descriptors. Matches are identified between all features and discrete orientation states $\{\pm \hat{\theta}_1, \pm \hat{\theta}_2\}$ including parity transforms, and in a manner invariant to intensity contrast inversions due to the binary sign $s \in \{-1, +1\}$ in Equation (8). A dominant transform $T^* \in \{T_{nm}\}$ is then identified such that it is consistent with the largest number of matches, i.e. inlier correspondences. A pair of features $(f_n, f_m)$ represents an inlier of the transform $T^*$ if their transform $T_{nm} : g_n \rightarrow g_m$ differs by less than a threshold $\|T_{nm} - T^*\| < \text{Thres}$ as follows:

$$T^* = \arg\max_T |\{T : \|T_{nm} - T\| < \text{Thres}\}|.$$  (8)

The thresholding operation in Equation (8) may be defined as the logical conjunction of thresholds independently applied in rotation, scaling and squared displacement

$$\|T_{nm} - T\| < \text{Thres}$$  (9)

using thresholds $(\epsilon_{\cos \theta}, \epsilon_{\log \sigma}, \epsilon_{x/\sigma})$. These may be set generously to apply in a wide variety contexts, here we use $(\epsilon_{\cos \theta}, \epsilon_{\log \sigma}, \epsilon_{x/\sigma}) = (0.7, \log 1.5, 0.25)$. The Hough transform process may be implemented efficiently using hash tables and the mean-shift clustering algorithm [92]. Our modified CPD algorithm is provided in Algorithm 1, and the solve functions for similarity transforms is found in

1. The Hough transform method was originally proposed to track particles in bubble chamber photographs [91].

![Fig. 2. Illustrating an appearance descriptor $a(r, \phi)$ and four discrete orientation states given principal axes $\hat{\theta}_1, \hat{\theta}_2$ (left to right) and feature sign $s$ (upper and lower). The descriptor content is shown for an example octant $(r,+,+)$ and gradient orientation $(\phi,+,+)$. Axis orientation is defined independently of sign (left to right), and negative sign $s = -1$ inverts the descriptor gradient (lower row) achieving invariance to contrast inversion.](image)
Algorithm 1: Probabilistic SIFT-CPD registration algorithm, adapted from \[24\] to include kernel \(K(g_n, g_m)\).

**Inputs:**
- \(\mathcal{F} = \{f_n\}\): Fixed Features
- \(\mathcal{M} = \{f_m\}\): Moving Features

**Outputs:**
- \(\mathcal{T} : \mathcal{M} \rightarrow \mathcal{F}\): Transform

**Initialization:**
- \(\lambda^2 = \frac{1}{\lambda N M} \sum_{n=1}^{N} \sum_{m=1}^{M} ||x_n - x_m||^2\)
- \(\mathcal{T} \leftarrow \mathcal{F} \approx \mathcal{M}\)

**EM Optimization:** repeat until convergence:

**E-Step:** Compute matrix \(P\):
- \(p_{mn} = \frac{\exp{-\frac{1}{\sigma^2} ||x_n - x_m||^2} K(g_n, g_m)}{\sum_{k=1}^{M} \exp{-\frac{1}{\sigma^2} ||x_n - x_m||^2} K(g_n, g_k) + \eta}\)

**M-Step:** Solve for optimal transformation \(\mathcal{T}\):
- \(\{\mathcal{T}, \lambda^2\} = \text{solve}(\mathcal{F}, \mathcal{M}, P)\)
- The aligned point set is \(\mathcal{T}(\mathcal{M})\)
- The correspondence probability is \(P\).

4 EXPERIMENTS

We hypothesize that our kernel function \(K(g_n, g_m)\) incorporating feature scale and orientation will improve the accuracy of registration beyond point information alone, and that feature orientation state and binary sign will provide invariance to intensity contrast inversion and reflections, independently of the method used to identify feature orientation \(\Theta\). Experiments validate these hypotheses in the context of 3D medical imaging data, which provide the opportunity to investigate features arising from realistic, diverse anatomical structure observed across subjects and 3D imaging modalities.

Three sets of experiments are performed. The first is based on synthetic similarity transforms, and establishes baseline accuracy of methods in the case of known ground truth. The second consists of inter-subject image registration trials, first between brain MRI and then between chest CT volumes of different people, with confounds including brain tumors and contrast variations due to multiple T1 and T2-weighted MRI modalities, demonstrating superior algorithm performance in a diverse set of contexts. Variability is estimated by repeating trials following synthetic transforms of images and multiple subjects. The third investigates orientation state changes in registration trials for different feature orientation estimation methods, i.e., principal components [3] or maximum orientation directions [2].

Note that the true mapping \(T\) between the anatomies of different subjects is generally non-linear and may not exist throughout the image, due to aspects of anatomy specific to individuals or in the case of occlusion or missing structure. As mentioned, features are assumed to follow a transform \(T\) that is globally linear followed by random feature-specific deviations as specified by our kernel \(K(g_n, g_m)\). For inter-subject registration, ground truth is established from inlier correspondences identified via the Hough transform, which are visually validated for correctness and rejected or manually adjusted if necessary. This follows the work of [7], [70], where automatic and manually labeled correspondences exhibit the same error range. The average Point Registration Error (PRE) measure is used to quantify registration performance, based on the sum of 3D point differences between the registration solution and ground truth.

In all experiments, feature sets are extracted using a GPU implementation of the SIFT-Rank algorithm for computational efficiency [57], and registered using five point-cloud registration methods: ICP with 20 and 100 iterations (respectively ICP20 and ICP100), the original CPD algorithm using feature centers \(x\), SIFT-CPD using full feature geometry and our kernel \(K(g_n, g_m)\), and SIFT-CPD* using only inlier features from the Hough transform. All algorithms are initialized to the Hough transform solution prior to iterative registration in order to ensure a fair comparison.

4.1 Synthetic Image Registration

A preliminary experiment was first performed establish the baseline performances of algorithms against known ground truth, here synthetic similarity transformations of a single image. A T1w brain image from the Human Connectome Project (HCP) [93] dataset was selected (see Table 2 for more details), and 100 different synthetic transforms were applied, where each was generated by a random rotation about each axis on an angle range of \(\rho \in \pm [0^\circ, 30^\circ]\) followed by a translation \(\delta \in \pm [0 \text{ mm}, 10 \text{ mm}]\). The registration error in rotation and translation was evaluated relative to the known transform applied, and the results are presented in Table 1. As expected, the lowest error is achieved for SIFT-CPD (inliers alone), validating this method as a baseline error. SIFT-CPD and CPD perform similarly, with slightly less error for SIFT-CPD. ICP results are generally poor, failing to converge in 8 and 21 cases for 20 and 100 iterations.

4.2 Inter-subject Registration

Four sets of experiments quantified the accuracy of inter-subject registration, i.e. registration of images of different individuals. The goal was to evaluate the accuracy and speed of registration in a diverse set of contexts, including different aspects of anatomy (brain, chest), abnormalities (tumor) and modalities (T1w and T2w MRI, CT). Information regarding datasets is provided in Table 2. Note that minimum registration error is generally non-zero due to differences in anatomy, and the goal is to identify a robust transform minimizing the PRE for sets of inlier correspondences.

4.2.1 T1w Brain Images

The following experiment quantified inter-subject registration accuracy between brain images of a pair of different subjects. As in the previous experiment, one image was fixed, while the other was subjected to a random transform from the previously mentioned ranges \(\rho\) and \(\delta\). A pair of monozygotic twin subjects was selected, which generally share more inlier correspondences in comparison to unrelated subjects due to higher neuroanatomical similarity [57]. The results for 100 random transforms are shown in Figure 3; these are generally consistent across all registration experiments. ICP variants which weight all points uniformly do not correctly converge (red and orange). CPD and SIFT-CPD (green and light blue) both converge consistently to
acceptable results in term of PRE, both lower than that the initial robust Hough transform (purple). SIFT-CPD is consistently lower in terms of error and computation time in comparison to CPD, demonstrating that geometrical properties improve estimation, in the case where the majority of features may be outliers with no valid correspondence between images. Overall, the SIFT-CPD* (dark blue) leads to the lowest error and computation time, as it refines the original set of Hough transform inliers.

### 4.2.2 CT Chest Images

In order to show that our method is not tied to specific contexts or imaging modalities, we performed inter-subject registration of CT chest images from the Chronic Obstructive Pulmonary Disorder Genetiscs (COPDGenec) dataset [94]. Two different subject images in expiration breathing state were randomly selected (see Table 2 for more details). As in the previous experiment, we generated 100 random points on each subject and transformed with the same ρ and δ parameters, applied the transform to one image, and registered it using different registration approaches. The PRE for each registration is shown on Figure 4. Although the computational complexity of SIFT-CPD is comparable to the complexity of CPD in Figure 4, SIFT-CPD* is significantly faster, closer to the ICP20 performances.

### 4.2.3 Abnormal Variations and Occlusion

Practical image analysis requires robustly coping with occlusions, including a lack of one-to-one correspondence due to inter-subject variations including pathological tumor structure. Our method is based on local feature properties, and is thus particularly robust to occlusion and missing structure. We used 10 T1w MRI images of different subjects with tumors from the BraTS dataset [95] in order to evaluate registration in the presence of occlusion (see Table 2 for more details). Nine subject images are randomly selected, and

### Table 1

Comparison of five registration algorithms based on 100 synthetic transforms of a single T1w MRI brain volume. Error is listed in terms of individual rotation and translation axes, overall point registration error (PRE), and the sum of squared intensity differences (SSD) following registration.

| Algorithm   | X-Axis   | Y-Axis   | Z-Axis   | X-Axis   | Y-Axis   | Z-Axis   | Mean ± Std.Dev. | Mean ± Std.Dev. |
|-------------|----------|----------|----------|----------|----------|----------|-----------------|-----------------|
| ICP20       | 25.7 ± 22.0 | 16.8 ± 14.8 | 24.8 ± 17.2 | 14.2 ± 19.6 | 12.8 ± 29.1 | 17.4 ± 29.0 | 16.37 ± 8.41   | 7.62 ± 1.03     |
| ICP100      | 8.1 ± 18.9 | 6.3 ± 18.8 | 8.5 ± 18.5 | 9.0 ± 24.0 | 9.2 ± 32.8 | 8.5 ± 23.2 | 8.16 ± 17.15   | 4.89 ± 2.31     |
| CPD         | 0.06 ± 0.03 | 0.06 ± 0.03 | 0.06 ± 0.03 | 0.8 ± 0.6 | 1.3 ± 1.1 | 0.7 ± 0.5 | 1.81 ± 0.88   | 1.38 ± 0.39     |
| SIFT-CPD    | 0.02 ± 0.01 | 0.01 ± 0.01 | 0.02 ± 0.01 | 0.9 ± 0.5 | 0.8 ± 0.6 | 0.5 ± 0.4 | 1.05 ± 0.32   | 1.43 ± 0.33     |
| SIFT-CPD*   | 0.02 ± 0.01 | 0.01 ± 0.01 | 0.02 ± 0.01 | 0.9 ± 0.4 | 0.9 ± 0.4 | 0.4 ± 0.3 | 0.68 ± 0.15   | 0.96 ± 0.39     |

### Table 2

Inter-subject registration experimental data.

| Dataset | Anatomy | Modality | Resolution | Voxel Size (mm) | Features | Inliers |
|---------|---------|----------|------------|-----------------|----------|---------|
| 93      | Brain   | T1w MRI  | 260 × 260 × 311 | 0.7 × 0.7 × 0.7 | 6000 | 350     |
| 94      | Chest   | CT       | 280 × 280 × 235 | 1.2 × 1.2 × 1.2 | 3000 | 70      |
| 95      | Brain Tumor | T1w MRI  | 240 × 240 × 155 | 1.0 × 1.0 × 1.0 | 1200 | 70      |
| 93      | Brain   | T1w-12w MRI | 260 × 260 × 311 | 0.7 × 0.7 × 0.7 | 5000 | 115     |

Fig. 3. Inter-subject registration performance for healthy brain T1w MRI.

Fig. 4. Inter-subject registration performance for chest CT images.
transformed 5 times each, and registered to the remaining subject image. Results are presented in Figure 5.

4.2.4 Multi-Modal Images

To evaluate the registration performance of our approach on multi-modal images, a random pair of brain images was selected from HCP dataset, one with a T1w image and the other one with a T2w (see Table 2 for more details). T1w and T2w images are acquired with different MRI parameters and highlight different tissue properties, where T2w imaging involves longer repetition time (TR) and time-to-echo (TE) parameters. The T2w image was randomly transformed and registered as in previous experiments, with 100 trials. Results are presented in Figure 6. An example of corresponding features identified in different modalities is shown in Figure 7 and are investigated in greater detail in the following experiment section.

4.3 Feature Sign and Orientation State

Here we investigated the binary sign $s$ and orientation state $(\theta_1, \theta_2)$ of local features in registration experiments, using two different methods for estimating feature orientation $\Theta$: eigenvectors of the local gradient structure tensor matrix $\mathbf{G}$ or maximum orthogonal gradient directions $\mathbf{g}$. Both methods have been demonstrated to achieve effective local feature correspondences between images of the same modality, but not different modalities where discrete orientation state changes may occur.

Figures 8 show distributions of orientation state transitions of inlier correspondences between images. For same modality registration (a, b, c) there are relatively few state changes (main diagonal), however in the case of multi-modal registration (d) noticeable differences exist. In the case of orientation determined via principal component analysis (PCA) of gradients $\mathbf{G}$, approximately 40% of all correspondences exhibit single-axis reflections (Figure 8 d) rather than SP transforms, this is due to eigenvector sign ambiguity, which is accounted for in our algorithm. In the case of orientation determined by maximum gradient directions, correspondences generally exhibit full SP-transforms, i.e. sign inversion and parity (Figure 8 d). Figure 9 shows examples of corresponding features and state transitions in the case of sign inversion, including identity (0-0), single axis reflections of major (0-1) and minor axes (0-2), and parity transforms (0-3).

5 DISCUSSION

This paper proposed to extend local feature methods to account for SP-symmetry and to achieved 3D multi-modal image registration. We introduced the notion of discrete SP-symmetry in the of case features extracted from a scalar intensity image $I(x) \in \mathbb{R}^3$ over $x \in \mathbb{R}^3$ space. We proposed
to model the geometrical properties of 3D image features in a manner invariant to SP-transforms observed in multimodal image registration. We proposed to include a feature sign \( s \in \{-1, +1\} \) is indicated by the white-black or black-white transitions.

![Fig. 9. Examples of feature orientation state changes observed between T1w and T2w modalities. Red and blue arrows indicate the primary \( \theta_1 \) and secondary \( \theta_2 \) orientation axes projected onto an image slice plane. Circles indicate the feature location and scale in a slice plane, sign \( s \in \{-1, +1\} \) is indicated by the white-black or black-white transitions.](image)

We integrated feature properties into a well-known probabilistic point-based image registration framework, the CPD algorithm [4], via a kernel function \( K(f_n, f_m) \), leading to a highly robust and stable SIFT-CPD registration algorithm. Image registration experiments are performed using a range of volumetric image modalities of the human brain and chest, showing that additional properties consistently improve the accuracy of registration in comparison to point locations alone. Registration error and computation time is consistently lower for our proposed SIFT-CPD vs. standard point-based CPD frameworks, indicating that feature scale and orientation improve the estimation of image-to-image transforms. An optimized version of SIFT-CPD functioning solely on sparse inlier feature correspondences exhibits the lowest error, refining the solution achieved via a robust but coarse initial Hough transform. Experiments also demonstrated how SP-symmetry may be applied despite the method used to estimate feature orientation estimation, here principal gradient orientations [3] and maximum gradient orientations [2]. Invariant feature appearance descriptors are used to identify inliers and to initialize registration, there were not explicitly incorporated into the SIFT-CPD kernel function based solely on geometrical properties here, however this possibility is left for future work.

We note that the theory of SP-symmetry we present applies generally to individual channels of convolutional neural networks, and could be used within the general neural network learning framework to achieve SP-invariance, in addition to continuous invariance [18, 84, 85, 86]. Here, 3D invariant features have been identified via unbiased, symmetric operators with no explicit training procedure, which could be used as is in general imaging contexts, or to train or validate domain-specific detectors via neural networks [85, 86].

All code required to reproduce our results may be obtained at [https://github.com/3dsift-rank/SIFT-CPD](https://github.com/3dsift-rank/SIFT-CPD)

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APPENDIX A
PROBABILISTIC REGISTRATION DETAILS

The probabilistic CPD algorithm is based on a solve function defined for rigid and affine transforms. The solve_rigid algorithm used in this work is presented in Algorithm 2, while the solve_affine can be found in Algorithm ??, from [24]. The solve_rigid() function takes as inputs a fixed and a moving point sets $\mathcal{F}$ and $\mathcal{M}$ along with their corresponding probability map $P = \{p_{ij}\}$, and outputs the covariance $\lambda^2$, and a scaled rigid transform with parameters rotation matrix $R$, translation vector $t$, and magnification $b$. The solve_affine() function returns an affine transform including invertible affine matrix $B$ and translation vector $t$.

Algorithm 2: Solve for rigid transform.

```python
def solve_rigid(F, M, P):
    Np = 1^T P 1, \mu_F = 1/Np \cdot F^T P T 1, \mu_M =
    1/Np \cdot M^T P 1,
    \hat{F} = F - 1/\mu_F, \hat{M} = M - 1/\mu_M,
    A = \hat{F}^T P T \hat{M}, \text{compute SVD of } A \text{ such as }
    A = USV^T,
    R = UCV^T, \text{ where } C = d(1, ..., 1, \det(UV^T)),
    b = tr(A^T R) / tr(M^T P 1 M),
    t = \mu_F - bR\mu_M,
    \lambda^2 = 1/Np \cdot (tr(\hat{F}^T d(P^T 1) \hat{F}) - b tr(A^T R)).
    return {b, R, t}, \lambda^2
```