Revisiting iterative highly efficient optimisation schemes in medical image registration

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Abstract. 3D registration remains one of the big challenges in medical imaging, especially when dealing with highly deformed anatomical structures such as those encountered in inter- or intra-patient registration of abdominal scans. In a recent MICCAI registration challenge (Learn2Reg) deep learning based network architectures with inference times of <2 seconds showed great success for supervised alignment tasks. However, in unsupervised settings deep learning methods have not yet outperformed their conventional algorithmic counterparts based on continuous iterative optimisation (and probably won't as they share the same objective function (image metric)). This finding has brought us to revisit conventional optimisation schemes and investigate an iterative message passing approach that enables fast runtimes (using iterative optimisation with only few displacement candidates) and high registration accuracy. We conduct experiments on three challenging abdominal datasets ((pre-aligned) inter-patient CT, intra-patient MR-CT) and carry out an in-depth evaluation with a set of selected comparison methods. Our results clearly indicate that optimisation based methods are highly competitive both in accuracy and runtime when compared to Deep Learning methods. Moreover, we show that semantic label information (when available) can be efficiently exploited by our approach (cf. weakly supervised learning). Data and code will be made publicly available to ensure reproducibility and accelerate research in the field of 3D medical registration (https://github.com/lasseha/iter_lbp).

Keywords: Registration · Discrete Optimisation · Generalisation.

1 Introduction / Motivation

While the main focus of this work is on investigating the general problem of efficient medical image registration, we here specifically deal with the clinical task of inter- and intra-patient alignment of abdominal CT/MR scans. Enabling deformable multimodal fusion (of thorax and abdomen) has numerous medical applications, e.g. for aligning pre-interventional scans for image-guided (radio)therapy and multimodal diagnostic. Inter-subject CT registration can enable statistical modelling of variations of abdominal organs for abnormality detection and to provide a canonical atlas space.

Medical image registration is often considered a task with substantial computation times that may prevent its application in clinical workflows. While fully-convolutional segmentation networks can produce contours almost instantly, a classical iterative registration algorithm may often take minutes to converge. Hence, deep learning based image registration has been proposed to improve run times, so far however often with a degradation in alignment quality. The recent comprehensive medical registration challenge Learn2Reg showed that especially for large internal motion and multimodal fusion tasks, conventional methods are more robust and accurate than learning based approaches at the cost of longer runtimes. Yet little effort has recently been devoted in designing new iterative optimisation strategies for registration. GPU-accelerated optimisation routines have been explored in the AirLab framework [19] and as instance refinement in the DL-based VoxelMorph and PDD [2,9]. Discrete optimisation may inherently reduce the number of iterations but has large memory requirements and either limited accuracy or a fixed capture range.

We hypothesis that a suitable combination of discrete and iterative schemes has been mostly overlooked in previous research but could provide new perspectives for medical registration without learning. We also note, that the limited availability of GPUs in clinical setups is often disregarded for run times - hence speeding up CPU computation bring real benefits. Since registration algorithms are often used as versatile tools to handle a variety of tasks an evaluation on complementary applications is desirable: here we consider monomodal inter-subject abdominal CT registration and multimodal intra-patient CT/MR fusion both in affine/rigid and nonlinear settings.

Related Work: Learning-based registration can be roughly subdivided in metric- and label-supervised approaches or combinations of them, where most algorithms employ a fully-convolutional multi-scale CNN architecture with (potentially multiple) spatial transformer layers [2,18]. Since, the alignment target can often not be determined alone by a limited number of manually segmented structures - e.g. fissures and lobes are not sufficient to guide intra patient lung registration - metric-supervised methods may be considered more general. In conventional image registration a generic similarity metric (possible based on hand-crafted features) is optimised together with a regulariser in a multi-scale and usually iterative fashion.

Two popular MRF-based discrete optimisation approaches, drop [7] and deeds [11] are related to our work. Drop employs Fast-PD as optimisation backend, limits the complexity by sampling discrete displacements only along the 3 principal axes (31 possible vectors in 3D) and iteratively refines the matching. It uses a B-spline transformation, in a multi-resolution setting and local cross-correlation as metric. Deeds relies on the faster MST-BP optimisation [5], and uses a dense discrete displacement search (up to 5000 vectors each). It employs a multi-scale approach with up to 5 warps, MIND features [12] for similarity and symmetry constraints. Both methods run in ≈ 1 minute on multi-thread CPUs.

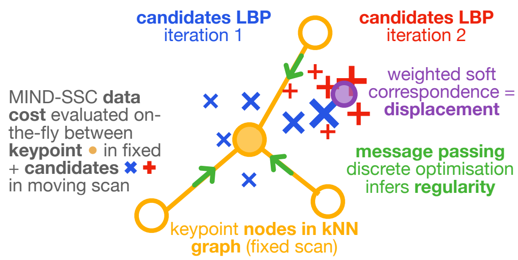
The closest work to our method in learning based registration is linearised multi-sampling [14], which was proposed as an extension for spatial transformer networks to tackle the noisy gradient estimation in differentiable trilinear interpolation. Different to other DL-registration approaches the gradient with respect to a sub-pixel displacement is not determined by differentiating the interpolation coefficients directly, but instead a hyperplane is fitted at a small number of random sampling points in the proximity of the current displacement. Using the slope of this plane as gradient estimation was shown to be more stable especially for difficult transformations.

Contribution: We propose an efficient strategy for dynamically solving a regularised cost function that is founded in graph-based optimisation and surpasses most conventional and learning-based registration algorithms in terms of accuracy and speed. Similar to multi-sampling we employ a randomised set of displacement candidates nearby the previous solution at each iteration. But instead of directly computing a metric-based displacement gradient, we perform a probabilistic discrete optimisation using a sparse variant of loopy belief propagation (LBP) [6] for the joint regularised cost function. In contrast to dense discrete optimisation, the space of considered displacements is reduced by orders of magnitudes and no fixed range of motion has to be pre-defined. The methods improves runtimes - with <1 seconds GPU or <5 seconds CPU - compared to DL registration, while matching or exceeding accuracy on three demanding tasks for inter- and intra-patient registration of CT-CT and MR-CT of the abdomen.

2 Method

Our method comprises a spatially randomly distributed sampling of control points (keypoints) and a conventional feature extraction step using hand-crafted contrast-invariant descriptors followed by the proposed iterative (dynamic) loopy belief propagation optimisation of a regularised registration cost function. The registration is performed in a small number of outer iterations in which the displacement search is dynamically changed based on the probabilistic estimate of the inner optimisation iterations for LBP. The feature descriptors can be efficiently evaluated on-line through indexing or nearest neighbour interpolation for each keypoint in the fixed image and each candidate in the moving image. Finally, either a trimmed least square or thin-plate spline fitting is employed to obtain either a linear transform or extrapolate a nonlinear displacement field.

We employ MIND with self-similarity context with 12 channels [12] as state-of-the-art descriptor and enhance the capturing of spatial context by sampling a small local patch of size 3x3x3 of these descriptors at each keypoint positions $\mathbf{p}_{f_i}$, resulting in a 324-dimensional vector. We use a symmetric k-nearest neighbour (kNN) graph on the set of keypoints in the fixed scan P_f with edges $(ij) \in E$ that connect keypoints $\mathbf{p}_{f_i}$ and $\mathbf{p}_{f_j}$. To optimise a regularised cost function that minimises the dissimilarity between feature vectors in fixed and - at a displaced position - in the moving scan we use the sum of squared difference metric and define a diffusion like regulariser. In discrete optimisation the regularisation term is considered for each pair of possible candidate displacement for each edge using $r_{ij}^{pq} = \left|(\mathbf{c}_i^p - \mathbf{p}_{f_i}) - (\mathbf{c}_j^q - \mathbf{p}_{f_j})\right|_2^2$. In contrast to most common discrete optimi-



<u>Algorithmic steps for **iterative LBP registration**</u>
1) **Extract MIND** for fixed and moving scan
2) Compute sparse **keypoint graph** (symmetric kNN) on fixed scan (storing edge indices)
3) initialise with zero displacement **and iterate**
    1) **draw new displacement candidates**
    2) **compute MIND data term** (sampling)
    3) **iterate for loopy belief propagation**
        1) gather incoming messages
        2) subtract reverse messages
        3) **min-sum regularisation**
        4) scatter outgoing messages
    4) compute **soft**(max) **correspondences and update displacements**
4) **fit linear** (least squares) **or nonlinear** (thin-plate spline) **transformation** for dense displacements → **optionally** second transform

Fig. 1: Schematic overview and pseudo-code of our proposed iterative optimisation approach for keypoints based 3D medical image registration using loopy belief (LBP) message passing.

sation schemes, the set of candidates $\mathbf{c}_j^q$ is not pre-determined or even equally spaced for each keypoint but dynamically adapted throughout iterations. The actual optimisation is performed in a few inner iterations, where messages are passed in parallel that enable the exchange of information across the graph and a more accurate deformation estimation. The algorithm is described in detail in [6] and uses the following equation to compute outgoing messages $\mathbf{m}^t_{i\to j}$ from $\mathbf{p}_{f_i}$ to $\mathbf{p}_{f_j}$ at iteration t: $\mathbf{m}^t_{i\to j} = \min_{1,\dots,q,\dots,l}\left(\mathbf{d}_i + \alpha\mathbf{r}^q_{ij} - \mathbf{m}^{t-1}_{j\to i} + \sum_{(h,i)\in E}\mathbf{m}^{t-1}_{h\to i}\right)$.

Once each LBP optimisation has converged, new candidates are drawn from a local neighbourhood (uniformly spatially distributed) and the search region can gradually adapt to the true optimum. To extrapolate from the final correspondences to a dense displacement either thin-plate splines or affine least-squares fitting is employed. A visual overview of the concept with a brief pseudo-code is given in Fig. 1. The source-code is available at https://github.com/lasseha/iter_lbp.

Compared to conventional stochastic gradient descent methods our proposed optimisation scheme benefits from the discrete setting of the search that finds the combinatorial minimum of a wide range of displacements. In contrast to commonly used loopy belief propagation (which iterates only over steps of message passing) we introduce a second and important outer iteration over the capture ranges of displacements. This approach is to the best of our knowledge the first that couples a discrete belief propagation optimisation with a sparsely distributed and locally adaptive solution space of potential displacements for each control point.

3 Experiments

To demonstrate the effectiveness and robustness of our iterative optimisation approach, we perform a comprehensive evaluation on three challenging abdominal datasets covering inter- and intra-patient, multimodal (CT/MR) as well as pre- and non-pre-aligned registration tasks. The datasets are described in detail in Section 3.1. The evaluation metrics are outlined below and closely follow the evaluation design of the L2R challenge, assessing accuracy and smoothness of the displacement field as well as the runtime of the algorithm. Finally, we describe implementation and configuration details of our proposed and comparison methods. All methods and experiments (with exception of drop2) were implemented and evaluated using the latest version of PyTorch (v1.7.1).

3.1 Datasets

CT-CT (L2R 2020): For our experiments on inter-patient alignment of abdominal CT scans we use the corresponding dataset (Task 3) from the Learn2Reg (L2R) challenge [8]. It contains 30 abdominal CT scans with 13 manually labelled anatomical structures: spleen ■, right kidney ■, left kidney ■, gall bladder ■, esophagus ■, liver ■, stomach ■, aorta ■, inferior vena cava ■, portal and splenic vein ■, pancreas ■, left adrenal gland, and right adrenal gland. The image data and labels themselves stem from [20] and were pre-registered to a canonical space and resampled to same voxel resolution and spatial dimensions (192x160x256). We report evaluation results on the predefined validation set, which describes a subset of 10 CT scans and 45 registration pairs.
CT-CT: To study the effect of non-pre-aligned data and thus more complex deformations on the different registration methods we also consider the original data from [20]. The segmentation labels, resampling procedure of the CT scans and validation pairs remain the same as described above.
MR-CT: Inter-patient alignment of abdominal CT to MR is investigated on 16 selected scan pairs from different trials in The Cancer Imaging Archive (TCIA) project [3,1,17,4]. Four different sized organs (liver, spleen, left and right kidney) were manually labelled by us for each MR-CT scan pair to assess the registration accuracy. The data (with exception of a withheld test set) will be made publicly available as part of a larger dataset for abdominal registration later this year. Pre-processing comprises resampling the scan pairs to an isotropic resolution of 2 mm and cropping/padding to consistent voxel dimensions of $192 \times 160 \times 192$. We report evaluation results over all 16 MR-CT pairs.

Evaluation Metrics: The used evaluation metrics cover the three most important aspects of medical image registration: 1) registration accuracy, 2) smoothness of the displacement field and 3) runtime of the algorithm. We assess the accuracy by means of alignment of the manually labelled organ segmentations using the Dice similarity metric (F1 score). In addition, the plausibility of the deformation field is of great clinical relevance and can be estimated by the standard deviation of the (logarithmic) Jacobian determinant [16,15] (SDlogJ). Finally, we report the runtime of the registration methods, both on CPU (Apple M1) and GPU (NVIDIA RTX 2080 Ti), including all necessary computations after reading the images until predicting the final dense displacement field.

Compared Methods and hyper-parameters: We employ a number of different related state-of-the-art learning- and optimisation-based registration methods in comparison to our proposed iterative LBP approach. Hyperparameters for ours and all comparison methods were selected on a subset of training scans for CT-CT and a small number of validation scans for MR-CT. Note, that iterative registration methods are much less sensitive to manual parameter choices than deep learning approaches. First, we substantially extended and improved upon the original VoxelMorph method [2] by replacing the simplistic U-Net with a two-stream architecture and a custom MIND-based metric-loss. Despite these advancements VoxelMorph+ does not yield satisfactory results for very large misalignments (CT-CT w/o pre-align and MR-CT). Second, the overall runner-up in the Learn2Reg challenge, PDD-net [10] again with MIND loss is used with all available extensions: multiple warps and instance optimisation for CT-CT, as well as affine least squares fitting for MR-CT. Third, drop2 a recent re-implementation of [7] is used as a related baseline for discrete optimisation. We explored a wide range of settings and found that diffusion regularisation and an initial B-spline spacing of 80mm in combination with the following settings worked best: cross-correlation (weight: 0.25) and entropy correlation (weight: 0.5) for CT-CT and MR-CT respectively with three pyramid levels each: 12mm, 8mm, 4mm for CT-CT and 8mm, 6mm, 4mm for MR-CT with a doubling of the iterations for the latter.

Furthermore, we evaluate two alternatives to our proposed method, all with the same metric patch-based MIND-SSC and one (nonlinear, for CT-CT (L2R 2020)) or two warps (affine + nonlinear, for CT-CT and MR-CT): dense 3D displacement sampling with LBP and continuous Adam optimisation with diffusion regularisation. For our proposed method, we chose 20 outer and 3 inner (LBP) iterations, where 12 (CT-CT) or 16 (MR-CT) displacement candidates are drawn from a uniform distribution for each of 2048 (or 8192 for nnUNet features) keypoints using capture ranges that start from ± 15 voxels and linearly decrease to ± 3 voxels. For Adam we employed a learning rate of 0.1 and 100 iterations. For the dense variant of LBP, we considered 11^3 displacements in parallel with a range of ± 30 voxels. The regularisation is performed on a kNN graph with 10 nearest neighbours for the LBP variants and 16 neighbours for Adam. The regularisation weight (alpha) is set to 2.5 (LBP) and 0.2 (Adam), respectively. For all methods (with exception of Voxelmorph+) a coarse and convex binary mask is used to restrict registration to the region of interest (which includes approximately 50% of the original number of image voxels).

4 Results

Quantitative and qualitative results of our experiments are shown in Table 1 and Figure 2, respectively. For the pre-aligned CT-CT dataset our proposed iterative LBP approach yields a Dice score of 40.1%, which is competitive to the best performing deep learning based comparison method, PDD-Net, with 41.5%. The sparse candidate sampling strategy of our method enables fast runtimes of <1 second on GPU and approximately 5 seconds on CPU. Making use of label information (weakly supervised learning for Voxelmorph+, using nnUNet

Table 1: Quantitative evaluation results of proposed and comparison methods on all three abdominal datasets considered. Runtimes are given for both GPU and CPU (GPU/CPU). Experiments in the first half (after the first double rule) are based on similarity metrics (MIND, NCC), while experiments in the second half (after the second double rule) make use of label information.

	CT-CT (L2R 2020)			CT-CT			MR-CT		
	Dice [%]	SDlogJ	Time [s]	Dice [%]	SDlogJ	Time [s]	Dice [%]	SDlogJ	Time [s]
Initial	25.1			11.6			26.5		
VoxelMorph+	35.4	.134	**0.2**/13						
PDD-Net	**41.5**	.129	1.4/73	35.1	.131	1.4/73	63.6	.210	**1.0**/37
drop2	37.0	.147	-/43	31.5	.132	-/43	56.2	.109	-/68
Adam	36.6	.080	1.6/27	30.9	.087	2.7/46	71.1	.074	2.7/46
dense LBP	38.6	.119	0.8/14	36.4	.098	1.3/23	71.7	.085	1.3/23
iterative LBP	40.1	.093	0.6/**5**	**37.7**	.092	**1.0/13**	**76.4**	.075	**1.0/13**
VoxelMorph+	43.9	.162	**0.2/13**						
Adam	54.6	.046	3.4/52						
dense LBP	62.1	.170	2.2/33						
iterative LBP	**65.2**	.088	1.9/22						

[13] softmax features for optimisation based approaches) consistently and significantly improves the registration results by 8.5% points (VoxelMorph+), 18% points (Adam), 22% points (dense LBP) and 25.1% (iterative LBP). The inference time of the network is included in the total runtimes of the optimisation based methods. Our methods final Dice score of 65.2% is also comparable to the reported score of 67% of the winning entry (LapIRN [18]) of the L2R challenge on the hidden test set (validation and test results are generally comparable). Results on the non-pre-aligned CT-CT data show only a moderate decrease in Dice score of 37.7% for our method (-2.4% points). Other comparison methods are less robust, e.g. drop2 or Adam, decrease by 5.5% points and 5.7% points Dice score, respectively. In this experiment, in addition to the Dice metric, we evaluate the 95th percentile of the Hausdorff Distance (HD95) to further highlight the differences between the state-of-the-art continuous optimiser (Adam) and our proposed iterative LBP approach. We find initial values of 30.14 voxels, which are reduced by Adam to 26.1 voxels. Our proposed method can substantially and statistically significantly (p ¡ 0.0002 using a Wilcoxon signed rank test) improve upon this with an error of only 17.3 voxels. For the inter-patient MR-CT dataset our iterative LBP method clearly yields the best Dice score of 76.4% with runtimes of 1.0 seconds on GPU and approximately 13 seconds on CPU.

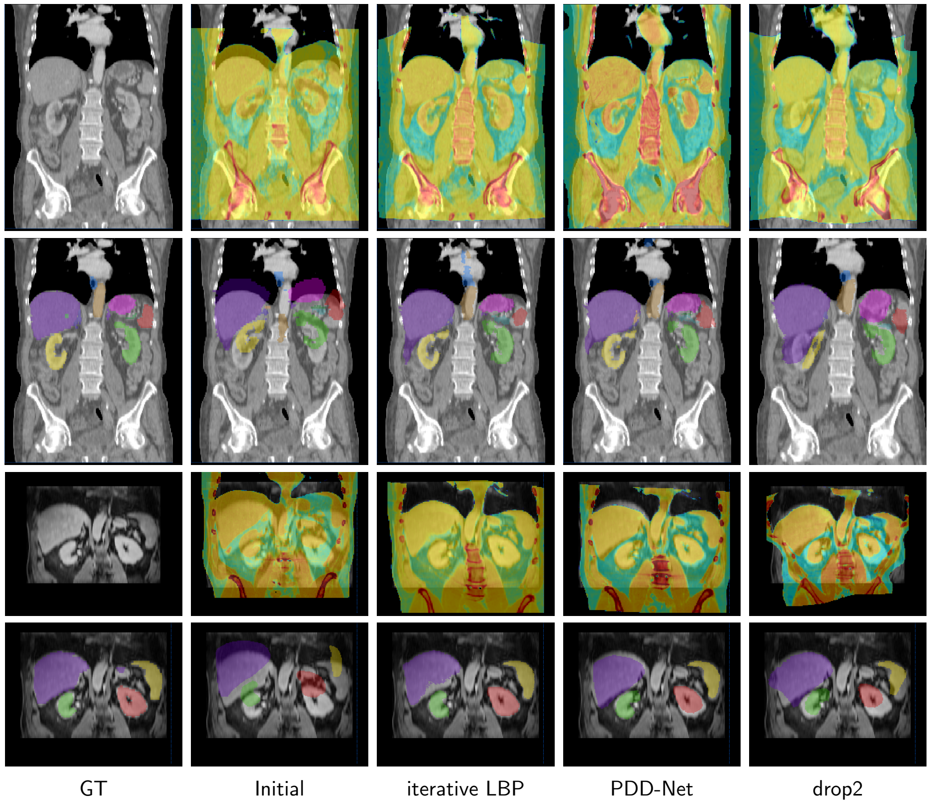


Fig. 2: Qualitative results of selected methods (coronal view). Row 1-2: Overlayed warped moving CT scan and warped segmentation labels for inter-patient CT-CT (L2R 2020). Row 3-4: intra-patient MR-CT. PDD and our proposed iterative LBP achieve more regular transformations than drop2 and are both very close to the ground truth for inter-subject alignment. Our method yields the highest accuracy for multimodal fusion especially at organ boundaries (lungs, kidneys).

Differences to drop2 the iterative MRF registration technique proposed in [7]: while the general idea of solving registration as iterative discrete optimisation is similar our method differs in a number of important design choices that greatly improve accuracy and runtime. First, our model uses a sparse keypoint graph and computes the similarity cost of displacements separately for each node, while [7] uses a grid-based model. We employ a feature-based metric and found that spatially sampling one high-dimensional vector per keypoint sufficiently captures similarity and no spline interpolant has to be evaluated. Loopy belief propagation is used as discrete optimisation backend, which has a simpler implementation, provides probabilistic estimates and lends itself to parallelism. Finally, our displacement sampling injects more randomness by avoiding an axis parallel selection of motion vectors and thus converges faster.

5 Discussion and Conclusion

We have developed an efficient discrete optimisation framework for versatile medical image registration that contrary to recent trends does not rely on learned convolutions and improves both runtime and accuracy compared to deep learning registration. This avoids lengthy preparations for supervised training and makes our method generally applicable. In addition, separating label prediction and optimisation-based registration offers improved explainability for clinicians compared to end-to-end learning methods (black box approach). The extensive experimental validation on three different abdominal registration tasks demonstrate substantial advantages over both unsupervised learning based and previous (iterative) discrete optimisers. We believe this is due to the following reasons: 1) our method avoids regular grids and dynamically adapts the shape of the solution space, finding an optimal balance between coverage and accuracy. 2) the combination of locally discriminative image features and globally regular graph optimisation can more efficiently address the computational demands on medical image registration than convolutional network architectures. A further surprising outcome is the competitiveness of Adam optimisation using regularisation across keypoints and MIND as loss term. This shows that iterative optimisation for registration should always be considered as a strong baseline when discussing new learning-based approaches. Future work could further reduce the complexity of supervised nnUNet feature extraction through quantisation and pruning.

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