DeepSTAPLE: Learning to predict multimodal registration quality for unsupervised domain adaptation

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Abstract. While deep neural networks often achieve outstanding results on semantic segmentation tasks within a dataset domain, performance can drop significantly when predicting domain-shifted input data. Multi-atlas segmentation utilizes multiple available sample annotations which are deformed and propagated to the target domain via multimodal image registration and fused to a consensus label afterwards but subsequent network training with the registered data may not yield optimal results due to registration errors. In this work, we propose to extend a curriculum learning approach with additional regularization and fixed weighting to train a semantic segmentation model along with data parameters representing the atlas confidence. Using these adjustments we can show that registration quality information can be extracted out of a semantic segmentation model and further be used to create label consensi when using a straightforward weighting scheme. Comparing our results to the STAPLE method, we find that our consensi are not only a better approximation of the oracle-label regarding Dice score but also improve subsequent network training results.

Keywords: domain adaptation · multi-atlas registration · label noise · consensus · curriculum learning

1 Introduction

Deep neural networks dominate the state-of-the-art medical image segmentation [10], but their high performance is depending on the availability of large-scale labelled datasets. Such labelled data is often not available in the target domain and direct transfer learning leads to performance drops due to domain shift [28]. To overcome these issues transferring existing annotations from a labeled source to the target domain is desirable. Mutli-atlas segmentation is a popular method, which accomplishes such a label transfer in two steps: First, multiple sample annotations are transferred to target images via image registration resulting in multiple "optimal" labels [2]. Secondly label fusion can be applied to build the label consensus. Although many methods for finding a consensus label have been developed [2, 7, 19, 25, 26], the resulting fused labels are still not perfect and exhibit label noise, which complicates the training of neural networks and degrades performance.

Motivation The pixel-wise classification i.e. segmentation performance of organs and structures of interest in medical imaging has been improved significantly over the past years [10, 14, 20]. Although segmentation within an imaging domain like CT or MRI can work well, problems arise when no target label data is available and the segmentation task on target data contains a domain shift [28]. One way to overcome this problem is propagating labels from the source domain to the target domain via image registration [8, 18, 24]. A propagated label could be used directly as a solution for the target label, but in general image registration is a challenging task and a "perfect" registration is hard to obtain [27].

Related work To tackle this problem label fusion methods have been proposed, which take several registered candidates as input and output a common consesus label via a non-trivial weighted voting task [2, 7, 19, 26]. More elaborate fusion methods also use image intensities [25] however when predicting across domains source and target intensities can differ substantially complicating intensity-based fusion and would therefore require handling of the intensity gap i.e. with image-to-image translation techniques [30]. When using the resulting consensus labels from non-optimal registration and fusion for subsequent CNN training, noisy data is introduced to the network [12]. Network training can then be improved with techniques of curriculum learning to estimate label noise (i.e. difficulty) and guide the optimization process accordingly [4, 22] but the techniques have not been used in the context of noise introduced through registered pixel-wise labels [3, 4, 11, 22, 29] or employ more specialized and complex pipelines [5, 6, 15]. Other deep learning-based techniques to address ambiguous labels are probabilistic networks [13].

Contributions We propose to use data parameters to weight noisy atlas samples as a simple but effective extension of semantic segmentation models. During training the data parameters (scalar values assigned to each instance of a registered label) are able to estimate the label trustworthiness globally across all multi-atlas candidates of all images. We extend the original formulation of data parameters by additional *risk regularization* and *fixed weighting* terms to adapt to the specific characteristics of the segmentation task and show that our adaptation improves network training performance for 2D and 3D tasks in the single-atlas scenario. Furthermore, we apply our method to the multi-atlas 3D image scenario where the network scores do not improve but yield equal performance in comparison to normal cross-entropy loss training when using out-of-line backpropagation. Nonetheless, we still can achieve an improvement by deriving an optimized consensus label from the extracted weights and applying a straightforward weighted-sum on the registered label candidates.

2   Method

In this section, we will describe our data parameter adaption and introduce our proposed extensions when using it in semantic segmentation tasks, namely a special regularization and a fixed weighting scheme. Furthermore, a multi-atlas specific extension will be described, which improves training stability.

Data parameters Saxena et. al. formulate their data parameter and curriculum learning approach as a modification altering the logits input of the loss function, making integration into existing models simple. By a learnable logits-weighting improvements could be shown in different scenarios when either noisy training samples and/or classes were weighted during training. Our implementation and experiments focus on per-sample parameters DP_s determining noisy multi-atlas samples. Experiments were conducted on binary semantic tumour segmentations making per-class parameters obsolete in our selected scenario. Since weighting schemes for multi-atlas label fusion like STAPLE [26] use a confidence weight of 0.0 indicating "no confidence" and 1 indicating "maximum confidence" we slightly changed the initial formulation of data parameters for a data batch B to be the following:

$$DP_{\sigma_b} = \frac{1/(1 + e^{-DP_{s_b}})}{\frac{1}{|B|} \sum_{b=1}^{|B|} 1/(1 + e^{-DP_{s_b}})} \tag{1}$$

By applying a non-linear sigmoid scaling we limit the data parameters applied to our loss to $DP_\sigma \in (0, 1)$. As in the original implementation the parameters require a sparse implementation of the Adam optimizer to avoid diminishing momenta. During optimization the data parameters can take values from $(-\infty, +\infty)$ where $DP_s \to -\infty \leftrightarrow DP_\sigma \to 0$ indicating a down-weighted noisy sample and $DP_s \to +\infty \leftrightarrow DP_\sigma \to 1$ indicating a clean sample.

To apply the parameters to the cross-entropy loss ℓ_{CE} we calculate the loss reduced over spatial dimensions and multiply the leftover batch dimension with DP_σ:

$$\ell_{DP} = \sum_B \ell_{CE,spatial}(f_\theta, \mathbf{z}) \odot \mathbf{DP}_\sigma \tag{2}$$

Risk Regularisation Even when a foreground class is present in the image and a registered target label only contains background pixels, the network can achieve a zero-loss value by overfitting. As a consequence, upweighting the over-fitted samples will be of no harm in terms of loss reduction which leads to the upweighting of maximal noisy (empty) samples. We therefore add a so called *risk regularisation* encouraging the network to take *risk*:

$$\ell = \ell_{DP} - \sum_B \frac{\sum_{spatial} [f_\theta > 0]}{n_{spatial}} \odot \mathbf{DP}_\sigma \tag{3}$$

By multiplying the data parameters DP_σ with the positively predicted pixel-count $[f_\theta > 0]$ the network is able to reduce loss when predicting more target

Fig. 1. Left: Inline backpropagation updating (red arrow) model and data parameters together. **Right:** Out-of-line backpropagation first steps on model (gray arrow) using normal cross-entropy loss and then steps on data parameters using the model's weights of the first step.

pixels under the restriction that the sample has a high data parameter value i.e. is classified as a clean sample. This formulation is balanced because predicting more positive pixels will increase the cross-entropy term if the prediction is inaccurate.

Fixed weighting scheme By correlating the data parameter values with our target scores in preliminary experiments, we found that the parameters have a strong correlation with the ground-truth pixels present in their values. Applying a fixed compensation weighting to the data parameters DP_{σ_b} can improve the correlation of the learned parameters and our target scores:

$$DP_{\tilde{\sigma}_b} = \frac{DP_{\sigma_b}}{log\left(\left[\sum_{spatial} \mathbf{z} > 0\right] + e\right) + e} \tag{4}$$

Out-of-line backpropagation process for improved stability Due to the inter-dependency of data parameters and label noise on the one hand and initially poor segmentation predictions, the model could become susceptible to convergence issues when training *inline*, especially during earlier epochs of network training. We found that a two-step forward-backward pass, first through the main model and in the second step through the main model and the data parameters can maintain stability while still estimating label noise (see Fig. 1). First only the main model parameters will be optimized. Secondly only the data parameters will be optimized *out-of-line* leaving the main model parameters untouched. When using the *out-of-line*, two-step approach data parameter optimization becomes a hypothesis of *"what would help the model optimizing right now?"* without intervening. The data parameter optimizer momentum helps pushing the parameters to a reasonably separated state making noise estimation possible.

Consensus generation via weighted voting For weighting of label atlases and fusion numerous techniques exist like majority voting [19] or STAPLE [26]. To create a consensus we use a simple weighted-sum over all multi-atlas labels (MAL) associated to a fixed image that turned out to be effective:

$$\mathbf{C} = \left[\sum_{i}^{MAL} \mathbf{z_i} \cdot softmax(\mathbf{DP_s})_i\right] > 0.5 \tag{5}$$

3   Experiments

In this section, we will describe a set of experiments which increase in complexity up to the successful application of our method in 3D multi-atlas label noise estimation. In the following, we will refer to oracle-[1] labels as the real target labels which belong to an image and "registered/training/ground-truth"-labels when meaning training on image labels that the network used to update its weights. The experiments are structured as follows:

EXP I   2D model training, artificially disturbed ground-truth labels
EXP II   2D model training, quality-mixed registered single-atlas labels
EXP III   3D model training, registered multi-atlas labels
EXP IV   Consensus generation and subsequent network training

Dataset For our experiments, we chose a challenging multimodal segmentation task which was part of the CrossMoDa challenge [23]. The data contains contrast-enhanced T1-weighted brain tumour MRI scans and high-resolution T2-weighted images (initial resolution of $384/448 \times 348/448 \times 80$ vox @ 0.5 $mm \times 0.5$ $mm \times 1.0-1.5$ mm and $512 \times 512 \times 120$ vox @ $0.4 \times 0.4 \times 1.0-1.5$ mm). In experiment III, we use T2-weighted data as source domain and propagate labels by utilizing the Convex Adam method [24] to the T1-weighted target domain. In experiment IV, we follow the CrossMoDa challenge, use the T1-weighted data as source domain and propagate labels via deformable registration with *deeds* [8] to the T2-weighted target domain. We used the original TCIA dataset [23] to provide omitted labels of the CrossModa challenge which served as oracle-labels. Prior to training isotropic resampling to 0.5 $mm \times 0.5$ $mm \times 0.5$ mm was performed as well as cropping the data to $128 \times 128 \times 128$ vox around the tumour. We omitted the provided cochlea labels and train on binary masks of background/tumour. As the tumour is either contained on the right- or left side of the hemisphere, we flipped the left samples to provide pre-oriented training data and omit the data without tumour structures. For the 2D experiments we sliced the last data dimension.

Model and training settings For 2D segmentation, we employ a LR-ASPP MobileNetV3-Large model [9]. For our 3D experiments we use a custom 3D-MobileNet backbone similar as proposed in [21] with an adapted 3D-LR-ASPP head [1]. 2D training was performed with an AdamW [17] optimizer with a learning rate of $\lambda_{2D} = 0.0005$, $|B|_{2D} = 32$, cosine annealing [16] as scheduling method with restart after $t_0 = 500$ batch steps and multiplication factor of 2.0. For the data parameters we used the SparseAdam-optimizer implementation together with the sparse Embedding structure of PyTorch with a learning rate of $\lambda_{DP} = 0.1$, no scheduling, $\beta_1 = 0.9$ and $\beta_2 = 0.999$. 3D training was conducted with learning rate of $\lambda_{3D} = 0.01$, $|B|_{3D} = 8$ due to memory restrictions

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[1] "The word oracle [...] properly refers to the priest or priestess uttering the prediction.". "Oracle." Wikipedia, Wikimedia Foundation, 03 Feb 2022, en.wikipedia.org/wiki/Oracle

Fig. 2. Left: Sample disturbance ■ at strengths [0.1, 0.5, 1.0, 5.0]. **Middle:** Validation Dice when training with named disturbance strenghts, either with data parameters enabled (—) or disabled (- -). **Right:** Parameter distribution for combinations of risk regularization (RR) and fixed weighting (FW): RR+FW ■ | RR ■ | FW ■ | NONE ■. Saturated data points indicate higher oracle-Dice. Value of ranked Spearman-correlation r_s between data parameters and oracle-Dice given.

and exponentially decayed scheduling with factor of $d = 0.99$. As opposed to Saxena et. al. during our experiments we did not find weight-clipping, weight decay or ℓ_2-regularisation on data parameters to be necessary. Parameters DP_s were initialized with a value of 0.0. For all experiments, we used spatial affine- and b-spline-augmentation and random-noise-augmentation on image intensities. Prior to augmenting we upscaled the input images and labels to $256 \times 256\ px$ in 2D- and $192 \times 192 \times 192\ vox$ in 3D-training. For experiment IV, we trained an nnUnet-model — a more powerful but also more resource demanding segmentation model which employs various techniques in pre- and postprocessing to optimize segmentation results [10]. We split the data into 2/3 training images and 1/3 validation images during all runs and used global class weights defined as $1/n_{bins}{}^{0.35}$.

For experiment I-III we benchmark our results against the same model without data parameters and standard cross-entropy loss. For experiment IV we use randomly selected registered labels as lower and oracle-labels as upper baseline. We refer to the Dice score between a label and the oracle-label as the "oracle dice".

Experiment I: 2D model training, artificially disturbed ground-truth labels This experiment shows the general applicability of data parameters in the semantic segmentation setting when using one parameter per 2D slice. To simulate label-noise, we shifted 30% of the non-empty oracle-slices with different strengths (Fig. 2, left) to see how the network scores behave (Fig. 2, middle) and whether the data parameter distribution captures the artificially disturbed samples (Fig. 2, right). In case of runs with data parameters the optimization was enabled after 10 epochs.

Experiment II: 2D model training, quality-mixed registered single-atlas labels We use deformable registered data with the Convex Adam method [24] and select two registration qualities while training with 30 registered T2-weighted moving labels for each of the T1-weighted fixed images. *Best*-quality

Fig. 3. Selected samples with low- and high parameters: Oracle-label □, network prediction ■ and registered label ■

Fig. 4. Inline ■ and out-of-line ■ backpropagation. Validation Dice (—) and Spearman-corr. of params. and oracle-Dice (- -)

Fig. 5. FG: Boxplots showing STAPLE ■ and DP ■ consensus (median —, mean - -). **BG:** nnUNet training scores ■ with: randomly selected atlases, all atlases, consensi and oracle-labels

registration means the single best registration with an average of around 80% oracle-Dice across all atlas registrations. *Combined*-quality means a clipped, gaussian-blurred sum of all 30 registered atlas registrations. We then input a mix of 50%/50% randomly selected best/combined labels into training resulting in a single-atlas experiment. Validation scores were as follows (descending): best@no-data-parameters 81.1%, mix@data-parameters 74.1%, mix@no-data-parameters 69.6% and combined@no-data-parameters 61.9%.

Experiment III: 3D model training, registered multi-atlas labels We follow the CrossMoDa [23] challenge task and use T2-weighted images as fixed targets (non-labelled) and T1-weighted images and labels as moving pairs registered with the deeds-algorithm [8]. 10 registered atlases per image are fed to the training routine expanding the T2-weighted training size from 40 to 400 label-image pairs. Fig. 4 shows a run with inline and out-of-line data parameter training as described in Sec. 2.

Experiment IV: Consensus generation and subsequent network training We took the trained data parameters and applied the proposed weighted-sum method for consensus generation (see Sec. 2). Fig. 5 shows the oracle-Dice distribution of 40 consensi (10 registered @ 40 fixed T2 images) as well as the mean validation Dice of a subsequent nnUnet-model training [10] after 150 training epochs for 40 randomly selected atlas labels (RND, 48.0%), all 400 atlas labels (ALL, 56.9%), STAPLE consensi (63.6%), data parameter consensi (DP, 67.8%) and oracle-labels (84.4%).

4 Results and discussion

Fig. 2 (middle) shows an increase of validation scores when activating stepping on data parameters after 10 epochs for disturbance strengths > 0.1, indicating that our usage of data parameters is effective. Examining the ranked correlation

in Fig. 2 (right), one can see that data parameters and oracle-Dice correlate most, when using the proposed risk regularization as well as the fixed weighting-scheme which we suppose to be related to the cross-entropy mean reduction (see Sec. 2). We did not notice any score improvements when switching between configurations and therefore conclude a sorting of samples can also be learned inherently by the network. However our data parameter implementation can extract this information and make it explicitly visible increasing explainability. In experiment II we show that our approach works for registered 2D data: When comparing best, combined and 50%/50% mix of best/combined registrations, we observed that using a mixture of different registration qualities drops scores from 81.1% to 69.6% Dice. By using data parameters we can recover to a score of 74.1% meaning an improvement of 4.5%. Experiment III covers our target scenario: 3D training with registered multi-atlas labels. When using our proposed out-of-line training approach (see Sec. 2) we can see improvements in validation Dice and ranked correlation (see Fig. 4). Experiment IV shows that data parameters can be used to create a weighted-sum consensus as described in Sec. 2. We can improve mean consensus-Dice from 58.1% of STAPLE [26] to 64.3% (+6.2%, ours). When using the consensi in a subsequent nnUNet training [10], scores behave likewise leading to an increase of +4.2% Dice (see Fig. 5). Regarding training times of over an hour with our LR-ASPP MobileNetV3-Large training, one has to consider that applying the STAPLE algorithm is magnitudes faster. However network training yields the opportunity to furthermore predict segmentations on the target domain directly.

5   Conclusion and outlook

Within this work, we showed that using data parameters in a multimodal prediction setting with propagated source labels is a valid approach to improve network training scores, get insight into training data quality and use the extracted info about sample quality in subsequent steps namely to generate consensus segmentations and provide these to further steps of deep learning pipelines. Our improvements over the original data parameter approach for semantic segmentation show strong results in both 2D- and 3D-training settings. Although we could extract sample quality information in the multi-atlas setting successfully, we could not improve network training scores in this setting directly since using the data parameters inline of the training loop resulted in unstable training. Regarding that, we want to continue investigating how an inline training can directly improve training scores in the multi-atlas setting. Furthermore our empirically chosen fixed weighting needs more theoretical foundation and probably a better weighting can be found. The consensus generation could be further improved by trying more complex weighting schemes or incorporating the network predictions itself. Also we would like to compare our registration-segmentation pipeline against specialized approaches of Ding et. al. and Liu et. al. [5, 6, 15] which we consider as very interesting baselines.

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