Graph Refinement based Tree Extraction using Mean-Field Networks and Graph Neural Networks

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Abstract—Graph refinement, or the task of obtaining subgraphs of interest from over-complete graphs, can have many varied applications. In this work, we extract tree structures from image data by, first deriving a graph-based representation of the volumetric data and then, posing tree extraction as a graph refinement task. We present two methods to perform graph refinement. First, we use mean-field approximation (MFA) to approximate the posterior density over the subgraphs from which the optimal subgraph of interest can be estimated. Mean field networks (MFNs) are used for inference based on the interpretation that iterations of MFA can be seen as feed-forward operations in a neural network. This allows us to learn the model parameters using gradient descent. Second, we present a supervised learning approach using graph neural networks (GNNs) which can be seen as generalisations of MFNs. Subgraphs are obtained by jointly training a GNN based encoder-decoder pair, wherein the encoder learns useful edge embeddings from which the edge probabilities are predicted using a simple decoder. We discuss connections between the two classes of methods and compare them for the task of extracting airways from 3D, low-dose, chest CT data. We show that both the MFN and GNN models show significant improvement when compared to a baseline method, that is similar to a top performing method in the EXACT’09 Challenge, in detecting more branches.

Index terms — mean-field networks, graph neural networks, tree segmentation, CT, airways

I. INTRODUCTION

Tree structures occur naturally in many places and play vital anatomical roles in the human body. Segmenting them in medical images can be of immense clinical value. Airways, vessels, and neurons are some such structures that have been studied extensively from a segmentation point of view [1]–[4].

Many widely used methods for vascular and airway tree segmentation tasks are sequential in nature i.e., they start from one location (a seed point) and segment trees by making successive local decisions [1], [3], [4]. For instance, in the EXACT’09 airway segmentation challenge [4], 10 out of the 15 competing methods used some form of region growing to make the segmentation decisions and the remainder of the methods were also sequential. The methods in [5], [6] are sequential but do not rely on local decisions; these methods utilise more global information in making the segmentation decisions. Methods that rely on sequential and/or local decisions are susceptible to local anomalies in the data due to noise and/or occlusion and can possibly miss large portions of the tree-structures.

Graph-based methods have been previously used for the extraction of vessels [7], airways [8], [9] and neurons [10], predominantly in a non-sequential setting. In [7], a pixel-level conditional random field (CRF) based model is presented, with parameterised node and pairwise potentials over local neighbourhoods for the segmentation of 2D retinal blood vessels. The parameters of the CRF are learned from training data using support vector machines. Scaling these pixel-level CRF models to 3D data and performing inference using them can be expensive; instead, using nodes with higher level information so as to sparsify the data can be an efficient approximation strategy. In [9], a tube detection filter is used to obtain candidate airway branches. These candidate branches are represented as nodes in a graph and airway trees are reconstructed using a two-step graph-based optimisation procedure. This sequential two-step optimisation introduces the possibility of missing branches or sub-trees, and a global optimisation procedure is desirable. In [10], the image data is first processed to obtain local regions of interest using a tubularity measure and maximum tubularity points are selected as nodes of the graph. Nodes within a certain neighbourhood are linked using minimal paths to obtain the graph edges. Several expressive feature descriptors for segments of these edges are computed and used as input to a path classifier which further assigns weights to these edges. Finally, subgraphs of interest are recovered using integer linear programming. The emphasis of the method in [10] is to obtain complex node and edge features, and then use of a global optimisation to reconstruct structures of interest.

In this work, we also take up a graph-based approach, to overcome some of the shortcomings of the aforementioned methods, by formulating extraction of tree structures from volumetric image data as a graph refinement task. The input image data is first processed to obtain a graph-like representation, comprising nodes with information extracted from the local image neighbourhoods. This graph based representation of image data reduces the computational expense, in contrast to the pixel-level CRFs used in [7], while also abstracting the tree segmentation task to a higher level than pixel classification. The preprocessed input graphs are initially over-connected based on simple neighbourhood criteria and then the connectivity is refined to obtain the optimal subgraphs that correspond
to the tree-structures of interest. When compared to the method in [9], the proposed model uses a single global optimisation procedure which removes the chance of missing branches or sub-trees in the intermediate optimisation step. And, when compared to the method in [10], we utilise relatively simpler node features, unweighted edges and extract the subgraphs of interest based on the global connectivity. We propose two approaches to solve graph refinement task in these settings, using: 1) Mean-Field Networks (MFNs) 2) Graph Neural Networks (GNNs).

In the first proposed method, graph refinement is posed as an approximate Bayesian inference task solved using mean-field approximation (MFA) [11], [12]. The posterior density over different subgraphs is approximated with a simpler distribution and the inference is carried out using MFA. We introduce parameterised node and pairwise potentials that capture behaviour of the optimal subgraph corresponding to the underlying tree structure and obtain MFA update equations within the variational inference framework [13]. By unrolling thus obtained MFA update iterations as layers in a feedforward network, we demonstrate the use of gradient descent to learn parameters of this model and point it out to be Mean-Field Network as was suggested in [14]. We extend the previously published conference work in Selvan et al. (2018) [15] in this paper by performing more comprehensive experiments and presenting a thorough comparison with GNNs.

In the second method, graph refinement is performed using Graph Neural Networks. GNNs are a class of recurrent neural networks operating directly on graph-structured data [16], [17] and are now seen as an important step in generalising deep learning models to non-Euclidean domains [18]. The graph refinement task itself is solved in a supervised setting by jointly training a GNN-based encoder-decoder pair. The encoder learns edge embeddings based on the overcomplete input graph, followed by a decoder to obtain the probability of edge connections. The idea of using GNNs for graph refinement was initially proposed in our earlier work in Selvan et al. (2018) [19], where a GNN-based encoder was used to learn node embeddings and a pairwise decoder was used to predict the edge probabilities. Using node embeddings to predict edge probabilities proved to be inadequate, which we have now addressed in this work by predicting edge probabilities from learnt edge embeddings instead.

In addition to proposing MFNs and GNNs as two methods to solve graph refinement tasks, we also study connections between them. In the case of MFN model, the node and pairwise potentials are hand-crafted, incorporating useful prior knowledge. With only a handful of parameters the MFN model requires little supervision and can be seen as an intermediate between a model-based solution and the fully end-to-end training model based on GNNs. On the other hand, the GNN models can be seen as generalisation of message passing algorithms used for inference in probabilistic graphical models [12] such as MFNs. When used in a supervised setting, as we do, the GNN model can be used to learn task-specific messages to be transacted between nodes of the graph.

We investigate the usefulness of the proposed methods for segmenting tree-structures with an application to extract airway trees from CT data, comparing the MFN and GNN models to a baseline method that is similar to Lo et al. (2010) [20] that has been shown to perform well on a variety of CT datasets [4], [21], [22].

II. METHODS

In this section, we describe the task of graph refinement along with the underlying model assumptions. Based on this model, we present two approaches to performing graph refinement using MFNs and GNNs.

A. Graph Refinement Model

Consider an over-complete, undirected, input graph, $G_{in} : \{V, E_{in}\}$, with nodes $i \in V : |V| = N$ associated with $F$-dimensional features, $x_i \in \mathbb{R}^{F \times 1}$ collected into the node feature matrix, $X \in \mathbb{R}^{F \times N}$, and pairwise edges, $(i, j) \in E_{in}$, described by the input adjacency matrix, $A_{in} \in \{0, 1\}^{N \times N}$. The goal of graph refinement is to recover a subgraph, $G$, with a subset of edges, $E \subseteq E_{in}$, described by the symmetric output adjacency matrix, $A \in \{0, 1\}^{N \times N}$. This subgraph corresponds to the structure of interest, like airway trees from chest data as studied in this work. We then seek a model, $f(\cdot)$, that can recover the subgraph from the input graph, $f : G_{in} \rightarrow G$.

B. Mean-Field Networks

We next propose a probabilistic graph refinement model by introducing a random variable that captures the connectivity between any pair of nodes $i$ and $j$: $s_{ij} \in \{0, 1\}$, with the probability of the corresponding connection given as $\alpha_{ij} \in [0, 1]$. For each node $i$, the binary random variables associated with its incident connections are collected into a node connectivity variable $s_i = \{s_{ij} : j = 1 \ldots N\}$. At the graph level, all node connectivity variables are collected into a global connectivity variable, $S = [s_1 \ldots s_N]$.

The graph refinement model is described by the conditional distribution, $p(S | X, A_{in})$, where the node features, $X$, and input adjacency, $A_{in}$, are observed from the data. We use the notion of node potential, $\phi_i(s_i)$, and pairwise edge potential, $\phi_{ij}(s_i, s_j)$, to express the joint distribution $p(S | X, A_{in})$ and relate it to the conditional distribution as

$$\ln p(S | X, A_{in}) \propto \ln p(S | X, A_{in}) = \sum_{i \in V} \phi_i(s_i) + \sum_{(i,j) \in E_{in}} \phi_{ij}(s_i, s_j) - \ln Z$$

where $\ln Z$ is the normalisation constant. For ease of notation, explicit dependence on observed data in these potentials is not shown. It can be noticed this model bears similarities with the hidden Markov random field (MRF) models that have been previously used for image segmentation, where the joint distribution is approximated with unary and pairwise energy functions [7], [23]. To design suitable potentials for graph refinement we model terms that contribute positively when the nodes or the pairwise connections are likely to belong to the subgraph, and less positively or even negatively otherwise.
First, we propose a node potential that captures the importance of a given node in the underlying subgraph, \( \mathcal{G} \). For each node \( i \in \mathcal{V} \), it is given as

\[
\phi_i(s_i) = \sum_{v=0}^{D} \beta_v [\sum_j s_{ij} = v] + a^T x_i \sum_j s_{ij}, \tag{2}
\]

where \( \sum_j s_{ij} \) is the degree of node \( i \) and \([\cdot]\) is the indicator function. The parameters \( \beta_v \in \mathbb{R}, \forall v = [0, \ldots, D] \), can be seen as prior weighting on the degree per node. We explicitly model and learn this term for up to 2 edges per node and assume a uniform prior for \( D > 2 \). Nodes with \( D = 0 \) correspond to nodes that do not belong to the subgraph, \( D = 1 \) are root or terminal nodes, and \( D = 2 \) are the most common nodes in the subgraph which are connected to a parent node and a child node. For these cases we explicitly learn the parameter \( \beta_v \forall v = [0, 1, 2] \), further. In the second term, a weighted combination of individual node feature scores is computed using the parameter \( \alpha \in \mathbb{R}^{F \times 1} \) to represent the contribution of each feature to the node’s importance. A node’s importance, and hence its contribution to the node potential, is made dependent on its degree as seen in the second term in Equation (2). That is, a node with more connections is more important to the subgraph and it contributes more to the node potential.

Secondly, we propose a pairwise potential that captures the relation between pairs of nodes and reflect their affinity to be connected in the underlying subgraph, \( \mathcal{G} \). For each pair of nodes \( i, j \in \mathcal{V} \), it is given as

\[
\phi_{ij}(s_i, s_j) = \lambda (1 - 2|s_{ij} - s_{ji}|) + (2s_{ij}s_{ji} - 1) \left[ \eta^T (x_i - x_j) + \nu^T (x_i \circ x_j) \right]. \tag{3}
\]

The first term in Equation (3) multiplied by \( \lambda \) ensures symmetry in connections between nodes, i.e., for nodes \( i, j \) it encourages \( s_{ij} = s_{ji} \). As the distance between node features can be a useful indicator of existence of edges between nodes, a weighting of the absolute difference between nodes for each feature dimension, denoted as the element-wise norm \( |\cdot|_e \), is computed using the parameter \( \eta \in \mathbb{R}^{F \times 1} \). The element-wise node feature product term \( \nu^T (x_i \circ x_j) \) computes a combination of the joint pairwise node features weighted by \( \nu \in \mathbb{R}^{F \times 1} \). The second term in Equation (3) is multiplied with \( (2s_{ij}s_{ji} - 1) \) to ensure that the contribution to the pairwise potential is positive when both nodes \( i \) and \( j \) are connected to each other, otherwise, the contribution is negative.

Returning to the posterior distribution, we note that except for in trivial cases, it is intractable to estimate \( p(\mathbf{S}|\mathbf{X}, \mathbf{A}_m) \) in Equation (1) and we must resort to approximating it. We take up the variational mean field approximation (MFA) \([11]\), which is a structured approach to approximating \( p(\mathbf{S}|\mathbf{X}, \mathbf{A}_m) \) with candidates from a class of simpler distributions: \( q(\mathbf{S}) \in \mathcal{Q} \). This approximation is performed by iteratively minimizing the exclusive Kullback-Leibler divergence \([11]\), or equivalently maximising the evidence lower bound (ELBO) or the variational free energy, given as

\[
\mathcal{F}(q_\mathbf{S}) = \ln Z + \mathbb{E}_{q_\mathbf{S}} \left[ \ln p(\mathbf{S}|\mathbf{X}, \mathbf{A}_m) - \ln q(\mathbf{S}) \right], \tag{4}
\]

where \( \mathbb{E}_{q_\mathbf{S}} \) is the expectation with respect to the distribution \( q_\mathbf{S} \). In MFA, the class of approximating distributions, \( \mathcal{Q} \), are constrained such that \( q(\mathbf{S}) \) can be factored further. In our model, we assume that the existence of connection between any pair of nodes is independent of the other connections, which is enforced by the following factorisation:

\[
q(\mathbf{S}) = \prod_{i=1}^{N} \prod_{j=1}^{N} q_{ij}(s_{ij}), \tag{5}
\]

where, \( q_{ij}(s_{ij}) = \begin{cases} \alpha_{ij} & \text{if } s_{ij} = 1, \\ (1 - \alpha_{ij}) & \text{if } s_{ij} = 0 \end{cases} \tag{6} \]

with \( \alpha_{ij} \) as the probability of connection between nodes \( i \) and \( j \). Using the potentials from (2) and (3) in (4) and taking expectation with respect to \( q_\mathbf{S} \), we obtain the ELBO in terms of \( \alpha_{ij} \forall i, j = [1, \ldots, N] \). By differentiating this ELBO with respect to any individual \( \alpha_{kl} \), as elaborated in Appendix A, we obtain the following update equation for performing MFA iterations. At iteration \((t + 1)\), for each node \( k \),

\[
\alpha_{kl}^{(t+1)} = \sigma(\gamma_{kl}) = \frac{1}{1 + \exp(-\gamma_{kl})}, \quad l \in N_k, \tag{7}
\]

where \( \sigma(\cdot) \) is the sigmoid function, \( N_k \) are the \( L \) neighbours of node \( k \), and

\[
\gamma_{kl} = \sum_{j \in N_k \setminus l} \left( 1 - \alpha_{kj}^{(t)} \right) \left( \sum_{m \in N_k \setminus l} \frac{\alpha_{km}^{(t)}}{\left( 1 - \alpha_{km}^{(t)} \right)} \right) \begin{pmatrix} \beta_2 - \beta_1 \\ -\beta_2 \sum_{n \in N_k \setminus l, m} \frac{\alpha_{kn}^{(t)}}{\left( 1 - \alpha_{kn}^{(t)} \right)} \end{pmatrix} + \begin{pmatrix} x_k \\ \eta^T (x_k - x_l) + \nu^T (x_k \circ x_l) \end{pmatrix}. \tag{8}
\]

After each iteration \((t)\), the MFA procedure outputs predictions for the global connectivity variable, \( \alpha^{(t)} \), with entries \( \alpha_{kl}^{(t)} \) given in Equation (7). These MFA iterations are performed until convergence; a reasonable stopping criterion is when the increase in ELBO between successive iterations is below a small threshold.

It can be noticed that the MFA update procedure described in Equation (7) and Equation (8) resemble the computations in a feed-forward neural network. The predictions from iteration \((t)\), \( \alpha^{(t)} \), are combined and passed through a non-linear activation function, a sigmoid in our case, to obtain predictions at iteration \((t + 1)\), \( \alpha^{(t+1)} \). This allows us to perform \( T \) iterations of MFA with a \( T \)-layered network based on the underlying graphical model. This can be seen as the mean field network (MFN) \([14]\). The parameters of our model, \( [\lambda, \beta, \alpha, \eta, \nu] \), form weights of such a network and are shared across all layers. Given this setting, parameters for the MFN can be learned by back-propagating any suitable loss, \( \mathcal{L}(\alpha, \mathbf{A}_r) \), computed between the predicted global connectivity variable at the final iteration \( \alpha = \alpha^{(T)} \) and the reference adjacency, \( \mathbf{A}_r \). We recover a symmetric adjacency matrix from the predicted global connectivity variable as \( \mathbf{A} = \mathbb{I}(\alpha > 0.5) \wedge (\alpha^T > 0.5) \), because symmetry is not enforced on the predicted global connectivity variable i.e., the equality \( \alpha_{ij} = \alpha_{ji} \) does not
always hold. This is because of the MFA factorisation in Equation (5) where we assume connections between pairs of nodes to be independent of other connections. Details of the MFN training procedure are presented in Section II-D.

C. Graph Neural Networks

With MFN in Section II-B, we presented a hand-crafted model to perform graph refinement. In this section, we investigate if the messages transacted between nodes according to Equations (7) and (8) in the MFN can be learnt in a supervised setting using Graph Neural Networks.

GNNs are neural networks that operate directly on graph-structured data by passing local messages between nodes [16]. Several closely related formulations of GNNs are prevalent in the literature [18], [23]–[26]. In this work, we focus on a model variant, termed a graph auto-encoder (GAE), first introduced in Kipf & Welling (2016) [27]. A GAE is comprised of an encoder-decoder pair that is jointly trained to learn expressive node and/or edge embeddings of the input graph. A GNN model that uses only node embeddings is referred to as the node-GNN [17], [24], [28]. In comparison, models that use explicit edge representations and learn edge embeddings are referred to as an edge-GNN [25], [26], [28]. In this work, we extend the preliminary work in Selvan et al. [19], where graph refinement was performed using an encoder that learnt node embeddings, and a pairwise decoder that predicted edge probabilities from the node embeddings. We now propose the use of an edge-GNN based encoder and a decoder that predicts edge probabilities directly from the learnt edge embeddings.

The graph refinement task, as formulated in Section II-A, provides a conducive setting to use GNN based encoder-decoder pairs to learn a model, \( f : G_m \rightarrow G \). The GNN model, in our case, is used in a supervised setting to learn edge embeddings from which the subgraphs of interest can be reconstructed. Joint training of the encoder-decoder pair yields an encoder that maps the input node features, \( X \), to node embeddings, computes the corresponding edges based on the input adjacency matrix, \( A_m \), and obtains edge embeddings. The decoder, then, uses the learnt edge embeddings to predict the global connectivity variable, \( \alpha \).

Following the notation in [26], we present a GNN based encoder with a receptive field of two, that is with two GNNs (identified by the superscripts):

Node Embedding:

\[
h^{(1)}_j = g_n(X_j) \quad (9)
\]

Node-to-Edge mapping:

\[
h^{(1)}_{(i,j)} = g_{ne}(h^{(1)}_i, h^{(1)}_j) \quad (10)
\]

Edge-to-Node mapping:

\[
h^{(2)}_j = g_{en}(\sum_{i \in N_j} h^{(1)}_{(i,j)}) \quad (11)
\]

Node-to-Edge mapping:

\[
h^{(2)}_{(i,j)} = g_{ne}(h^{(2)}_i, h^{(2)}_j) \quad (12)
\]

where each of the \( g_{\ldots}(\cdot) \) above is a 2-layered multi-layer perceptron (MLP) with rectified linear unit activations, dropout [29] between the two hidden layers, skip connections [30] and layer normalisation [31]. Equation (9) describes the node embedding corresponding to the first GNN, \( h^{(1)}_j \). The MLP, \( g_{ne}(\cdot) \), has \( F \) input channels and \( E \) output channels transforming the \( F \)-dimensional input node features into \( E \)-dimensional node embedding. The edge embedding, \( h^{(1)}_{(i,j)} \) for a pair of nodes, \((i,j)\) is obtained by simply concatenating the corresponding node features and propagating these features through the edge MLP as described in Equation (10). The edge MLPs, \( g_{ne}(\cdot) \) have \( 2E \) input channels and \( E \) output channels. Going from these edge embeddings to node representation is performed by simply summing over all the incoming edges to any given node \( j \) from its neighbourhood, \( N_j \) according to Equation (11). A new node embedding is obtained by propagating these node features through the second node MLP, \( g_{en}(\cdot) \) with \( E \) input and output channels, as described in Equation (11). The second edge MLP, \( g_{ne}(\cdot) \) also has \( 2E \) input and \( E \) output channels. Finally, the output from the encoder, \( h^{(2)}_{(i,j)} \) in Equation (12) is the \( E \)-dimensional edge embedding used to predict the edge probabilities with a simple decoder.

The decoder is given as:

\[
\alpha_{ij} = \sigma(g_{dec}(h^{(2)}_{(i,j)})) \quad (13)
\]

where \( g_{dec} \) is a linear layer with bias and one output unit, and \( \sigma(\cdot) \) is the sigmoid activation function. This decoding operation converts the \( E \)-dimensional edge embedding into a single scalar for each edge and the sigmoid function yields the edge probability, \( \alpha_{ij} \). These form entries of the predicted global connectivity variable, \( \alpha \), similar to the predictions using MFN in Equation (7). As with MFN, the GNN model loss is computed based on edge probability predictions, \( \alpha \), and the reference adjacency matrices, \( L(\alpha, A_r) \).

Although the GNN model described above is for individual nodes and edges, these can be vectorised for faster implementation [29]. Also, the receptive field of the encoder can be easily increased by stacking more GNNs i.e, successive repetition of pairs of Equations (11) and (12).

D. Loss Function

Both, MFN and GNN, models output predictions for the global connectivity variable, \( \alpha \), which has entries corresponding to the probability of pairwise connections. From a loss point of view, this is similar to binary classification tasks, as the reference adjacency matrix, \( A_r \), has binary entries indicating the presence of edges in the underlying subgraph. In most applications, the graphs are sparse as the edge class is in minority. To overcome challenges during training due to such class skew we use the Dice loss [32] for optimising both the models, for its inherent ability to account for class imbalance. Dice loss is given as:

\[
L(\alpha, A_r) = 1 - \frac{2 \sum_{i,j=1}^{N} \alpha_{ij} A_{ij}}{\sum_{i,j=1}^{N} \alpha_{ij}^2 + \sum_{i,j=1}^{N} A_{ij}^2}, \quad (14)
\]

where \( A_{ij} \) are the individual binary entries in the reference adjacency matrix.
Figure 1: The preprocessing to transform the input image (left) into a probability image (center) and then into graph format (right). Nodes in the graph are shown in scale (as different colours) to capture the variations in their local radius.

Figure 2: Input graph derived from a chest scan depicting the initial connectivity based on $A_0$ between nodes (left). Nodes of the input graph (grey dots) overlaid with connections derived from the reference adjacency matrix, $A_r$ (center). Binary volume segmentation obtained from the reference adjacency matrix and the corresponding node features (right).

### III. Experiments and Results

#### A. Airway Tree Extraction as Graph Refinement

Both the MFN and GNN models presented are general models that can be applied to most graph refinement tasks with slight modifications. Here we present extraction of airway tree centerlines from CT images as a graph refinement task and describe the specific features used for this application.

1) **Preprocessing:** The image data is preprocessed to convert it into a graph format. First, the 3D CT image data is converted into a probability map using a trained voxel classifier according to Lo et al. (2010) [20]. This step converts intensity per voxel into a probability of that voxel belonging to the airway lumen. These probability images are transformed to a sparse representation using a simple multi-scale blob detector. Next, we perform Bayesian smoothing, with process and measurement models that model individual branches in an airway tree, using the method of [33]. This three-step preprocessing procedure yields a graph output of the input image data, as illustrated in Figure 1. Each node in this graph is associated with a 7-dimensional Gaussian density comprising of spatial location $x_p = [x, y, z]$ in the image, local radius ($r$), and orientation $(u_x, u_y, u_z)$, such that $x_i = [x_i^0, x_i^1, x_i^2]^T$, comprising mean, $x_i^0 \in \mathbb{R}^7$, and variance for each feature, $x_i^1 \in \mathbb{R}^7, x_i^2 \in \mathbb{R}^7$. To obtain an initial connectivity, $A_{in}$, we connect nodes to their 10 nearest neighbours based on spatial distance. Thus obtained graphs, with node features $x_i \in \mathbb{R}^{14 \times 1}$, are the input graphs for both models. Figure 2 (left) visualises an over-connected input graph.

2) **Adapting the MFN model:** The node and pairwise potentials in Equations (2) and (3) are general and applicable to commonly encountered trees. Due to the nature of features extracted for the nodes in Section III-A1, one of the terms in the pairwise potential in Equation (3) requires a minor modification. The factor in Equation (3) associated with $\eta$ is the element-wise absolute difference in node features, $|x_i - x_j|_e$. We normalise the position features with the average radius of the nodes, i.e., $|x_i^0 - x_j^0|_e/r + r'$, as the relative positions of each pair of connected nodes is proportional to their radii.

3) **Reference Adjacency Matrices:** Reference adjacency matrices are obtained from the reference segmentations using the preprocessing procedure described in Section III-A1. The extracted nodes and edges that are inside the corresponding reference segmentations are connected using a minimum spanning tree algorithm to obtain a single connected tree, yielding reference adjacency matrices that are used for training both the GNN and MFN models. A sample input graph along with the connections based on the reference adjacency matrix is shown in Figure 2 (center).

#### B. Data

The experiments were performed on 3-D, low-dose CT, chest scans from the Danish lung cancer screening trial [21]. All scans have voxel resolution of approximately $0.78 \times 0.78 \times 1$ mm$^3$. We use two non-overlapping sets of 100 scans and 32 scans for training and evaluation purposes. The 32 scans in the first subset have reference segmentations that are treated as the ground truth for the purpose of evaluations, referred to as the reference dataset. These reference segmentations are obtained by combining results from two previous airway segmentation methods [2, 20] that are corrected by an expert user. First of these methods uses a trained voxel classifier to distinguish airway regions from the background to yield probability images, and airway trees are extracted with region growing on these probabilities using an additional vessel similarity measure [20]. The second method extracts airways by extending locally optimal paths on the same probability images [5]. The second set comprising 100 scans has automatic segmentations obtained using [4]. As the reference dataset is relatively small, we use the second set of 100 scans to perform pre-training and to tune hyperparameters of both the models, referred to as the pre-training dataset.

#### C. Evaluation

The output of graph refinement models yields connectivity information about the airway centerlines. For evaluation purposes, we convert the predicted subgraph into a binary segmentation. This is done by drawing binary voxels within a tubular region that interpolates the radii of the nodes, along edges given by $A = [\langle \alpha > 0.5 \rangle \land (\alpha^T > 0.5)]$. One such binary segmentation is visualised in Figure 2 (right).

Comparison of the graph refinement performance of the MFN and GNN models is done based on computing Dice similarity coefficient using the predicted and reference adjacency matrices

$$\text{Dice} = \frac{2|A \circ A_r|}{|A| + |A_r|}. \quad (15)$$

To evaluate the binary segmentations obtained using the procedure in Section III-C, centerline distance is used. Centerlines are extracted from the binary segmentations using a 3-D...
Each input graph, on average, has 8000 nodes which is divided into sub-images comprising 500 nodes, such that all the nodes in the input graph are taken into account to reduce memory utilisation. Batch size of 12 images (comprising all sub-images corresponding to an input graph) was used in the training procedure.

2) GNN model parameters: Based on the pre-training dataset, we designed an architecture for the GNN model comprising an encoder with a receptive field of 2 as described in Section II-C obtained from the range [1, . . ., 5]. Each of the MLPs, g(.), used in the encoder in Equations (9)–(12) has two hidden layers chosen from the range [1, 2, 3, 4] and the number of channels per layer parameter E = 8 chosen from the exponential range [4, 8, 16, . . ., 256]. A dropout rate of 0.5 was used between each layer in the MLPs, chosen from the interval [0, 0.1, . . ., 0.9]. The number of training epochs for the GNN model was set to 500. Batch size of 12 was used during training.

E. Results

We compare the performance of the MFN and GNN models to each other, and with a baseline airway extraction method that uses region growing on probability images obtained using a voxel classifier, denoted Vox+RG. The baseline method is similar to the method in Lo et al. [20], which was one of the top performing methods in EXACT’09 Challenge scoring the best FPR and was in the top five performing methods in TL measure. Further, as the input to both graph refinement methods were nodes processed using the Bayesian smoothing method in [33], we also report the results for the Bayesian smoothing method. The output of Bayesian smoothing method is a collection of branches and not a complete segmentation; we merge its predictions with results of Vox+RG as in [33], denoted BS+RG. Parameters of the region growing threshold of Vox+RG and BS+RG are tuned to optimise the average centerline distance in Equation (16) using 8-fold cross validation procedure on the reference dataset. Test set centerline predictions for two cases along with the reference segmentations for Vox+RG and the two graph refinement models are visualised in Figure 4.
Table 1: Performance comparison of four methods: Region growing on probability images (Vox+RG), Bayesian smoothing merged with Vox+RG (BS+RG), MFN and GNN models. Dice similarity, centerline distances ($d_{FP}$, $d_{FN}$, $d_{err}$), fraction of tree length detected (TL) and false positive rate (FPR) are reported based on 8–fold cross validation. Significant improvements when compared to the baseline, Vox+RG, are shown in boldface.

| Method      | Dice(%) | $d_{FP}$(mm) | $d_{FN}$(mm) | $d_{err}$ (mm) | TL(%) | FPR(%) |
|-------------|---------|--------------|--------------|----------------|-------|--------|
| Vox+RG      | –       | 3.624 ± 0.776| 5.155 ± 0.580| 4.389 ± 0.441  | 79.6 ± 7.2 | 5.0 ± 3.9 |
| BS+RG       | –       | 3.921 ± 0.612| 4.218 ± 0.334| 4.069 ± 0.476  | 82.3 ± 6.1 | 8.7 ± 3.4 |
| MFN         | 86.5 ± 2.5 | 3.599 ± 0.583| 3.491 ± 0.295| 3.595 ± 0.321  | 83.1 ± 6.7 | 8.6 ± 3.3 |
| GNN         | 84.8 ± 3.3 | 3.045 ± 0.329| 2.951 ± 0.757| 2.998 ± 0.399  | 85.3 ± 6.7 | 4.7 ± 3.3 |

To isolate the improvements due to preprocessing using Bayesian smoothing method in [33] on the graph refinement models as described in Section III-A, we report the centerline error for the predictions from BS+RG. From the centerline distance measure entries in Table I, we notice that both the graph refinement models show large and significant improvement ($p < 0.001$) when compared to BS+RG method reported in the second row. A similar improvement is observed in TL for both the graph refinement models.

When comparing the performance between the MFN and GNN models in Table I, we see a significant improvement using the GNN model in all centerline distance measures: $d_{FP}$, $d_{FN}$, $d_{err}$ ($p < 0.05$). Further, as the two graph refinement models predict the global connectivity variable, $\alpha$, this performance is quantified by computing the Dice similarity coefficient, in Equation (15), and reported in the second column in Table I. We see that the MFN model obtains a higher score when compared to the GNN model indicating that the MFN model is better at predicting pairwise node connectivity. All the reported significance values are based on paired sample $t$–tests.

IV. DISCUSSION AND CONCLUSIONS

Detecting small branches and overcoming occlusions due to pathology and/or noise in data, during extraction of airways from CT data is challenging. By posing tree extraction as a graph refinement task we presented an exploratory approach that, to a large extent, overcomes these challenges. Two models for graph refinement based on mean-field networks and graph neural networks were presented, evaluated on chest CT data and compared to a baseline method that is similar to Lo et al. (2010) [20]. The method in Lo et al. (2010) [20] was one of the top performing methods in EXACT’09 airway extraction challenge [4] and forms a useful baseline for comparison.

Some existing airway segmentation methods also have taken up an exploratory approach. The most recent and relevant work in this regard is [9], where candidate airway branches are obtained using a tube detection filter and tree reconstruction is performed as a two-step graph-based optimisation. Candidate airway branches form nodes of this graph and plausible edges between these nodes are worked out in the first step of the optimisation. In the second step of the optimisation, subtrees below a certain score are pruned away. In comparison to [9], the proposed graph refinement setting operates on nodes that are local regions of interest and reconstructs branches and connections between branches simultaneously from these nodes. This graph refinement framework takes up a more...
global approach to tree reconstruction, as it does not rely on thresholding local sub-trees.

A. MFN model

The main contribution within the presented MFN framework is the novel formulation of airway extraction in a graph refinement setting and the formulation of the node and pairwise potentials in (2) and (3). By designing the potentials to reflect the nature of tasks we are interested in, the MFN model can be applied to diverse applications. For instance, it has been shown that information from pulmonary vessels can be used to improve airway segmentation in Lo et al. [20]. Modeling potential functions that take this information into account and encode the relation between vessel and airway branches could be done with MFN. Also, semantic segmentation tasks that predict voxel-level labels can also be modelled in the MFN setting, bearing similarities with the models used in Orlando et al. [7].

The MFN model can be seen as an intermediate between an entirely model-based solution and an end-to-end learning approach. It can be interpreted as a structured neural network where the interactions between layers are based on the underlying graphical model, while the parameters of the model are learnt from data. This, we believe, presents an interesting link between probabilistic graphical models and neural network-based learning.

B. GNN model

In Selvan et al. [19], we introduced the GNN model for graph refinement tasks. In that work, however, the GNN model was used to learn node embeddings using node GNNs. A pairwise decoder was then used to predict edge probabilities from the learnt node embeddings. With our experiments we found the model to be performing inadequately. With the model presented here, in Section II-C, we introduced edge GNNs in the encoder to explicitly represent the edges, in order to learn edge embeddings. By jointly training the encoder-decoder pair now, we use the learnt edge embeddings to predict the probability of edges, showing clear improvements compared to the node GNN model in Selvan et al. [19].

The graph encoder used in this work consists of two GNN layers, meaning that nodes of the GNN have access to messages from first and second order neighbourhoods. The choice of this receptive field was based on initial experiments done using the pre-training dataset. This receptive field can be further increased by adding GNN layers. A sufficiently deep GNN-based encoder should allow each node to receive messages from all other nodes with increasing computational expense. For the graph refinement task considered here, we observed a receptive field of two to be sufficient.

C. Comparison between MFN and GNN models

The MFN model update Equations (7) and (8) reveal the message passing nature of the underlying inference procedure (12). The state of each node i.e., the edge update message from node $k$ to node $l$ is dependent on their corresponding data terms and all neighbours of node $k$ except node $l$. These messages transacted in a $T-$layered MFN are hand-crafted based on the model in Equations (2) and (3) and deriving an analytical solution that guarantees an increase in ELBO. However, deriving such analytical solutions might not be feasible for all scenarios.

As GNNs can be seen as generalisation of message passing based inference methods [25], [28], with a capability of learning complex task-specific messages, an interesting connection with the MFN model can be made. Given sufficient training data, in principle, the GNN model should be able to learn messages to approximate the same posterior density as the MFN model. This connection is confirmed based on the centerline error measures reported in Table I wherein we see the two graph refinement models perform at least equally well for the same task.

The mean-field factorisation, according to Equation (5) that resulted in the MFN model, means the connections between nodes are independent of each other, which is a strong assumption resulting in asymmetric predicted adjacency matrices. And, as the GNN model is trained in a supervised setting using symmetric adjacency matrices, the model predicts symmetric adjacency matrices in most cases.

The GNN model is able to detect more missing branches than the MFN model as seen in Table I. There is a reduction in $d_{FP}$ for the GNN model; this is due to several spurious and disconnected branches predicted by the MFN model. The GNN model predicts fewer disconnected edges, indicating that, perhaps, the model is able to learn that stand-alone, disconnected edges are unlikely in an airway tree. This is clearly captured in the visualisations in Figure 4.

From a graph refinement perspective, we see the MFN model scores higher in dice similarity (second column of Table I). This is contrary to the centerline distance performance but can be explained by noticing that each edge in the dice accuracy in Equation (15) has the same importance. That is, edges between nodes in branches of large and small radii have the same importance. However, a missing edge in a branch of large radius can contribute more to the centerline distance than a missing edge in a branch of smaller radius.

The GNN model used here is more complex, with 3150 tunable weights, than the MFN model, which has a small set of tunable parameters $[\lambda, \alpha, \beta, \eta, \nu]$ and in all 46 tunable weights. Each training epoch containing 28 training images for the MFN model takes about 2s and 1s for the GNN model. The implementation of the GNN model takes advantage of sparse matrix operations, for $O(\|e_m\|)$ computational complexity. A similar sparse implementation can further reduce the computation time for the MFN model.

D. Limitations and Future Work

The preprocessing performed in Section III-A1 is one possible way of obtaining graphs from image data as demonstrated in this work. A natural next step is to use more powerful local feature extractors based on CNNs and learn the initial graph extraction. Initial work involving sequential training of feature extraction using CNNs and GNNs for learning global connectivity has been proposed in Shin et al. [16] for 2-D vessel...
segmentation tasks. A joint end-to-end training procedure that dynamically extracts graphs from image data and performs graph refinement is challenging, but an interesting direction. Such models, where CNNs would be used as local feature extractors and GNNs operating on sparse graphs to model the global connectivity could be useful also to reduce the massive memory footprints of CNN models in 3D volumes.

In the MFN model, we currently only use a linear data term in the node potential, \( a^T x_i \) in (2), and a pairwise potential, \( \nu^T (x_i \circ x_j) \) in (3). There are possibilities of using more complex data terms to learn more expressive features. For example, the use of higher order potentials that take more than two nodes jointly into account help reduce the single-edge spurious branches detected in Figure 4.

While the output of the GNN has very few disconnected branches, the output in all cases is not a fully connected tree. Incorporating tree enforcing constraints, either in the loss function or, in the GNN model could be beneficial.

E. Conclusion

In this work, we presented exploratory methods for the extraction of tree-structures from volumetric data, with a focus on airway extraction, formulated as graph refinement tasks. We proposed two novel methods to perform graph refinement based on MFNs and GNNs.

We evaluated the two methods in their ability to extract airway trees from CT data and compared them to a baseline method. With our experiments, we have shown that both the MFN and GNN models perform significantly better than the baseline method on the average centerline distance measure. Between the MFN and GNN models, the GNN model is able to detect more branches with fewer false positives as shown with the fraction of tree length and false positive rate measures. We have also presented connections between the MFN and GNN models. GNNs are more complex models which can be seen as generalisation of MFN models, while the MFN models with the fraction of tree length and false positive rate measures.

We have also presented connections between the MFN and GNN models. GNNs are more complex models which can be seen as generalisation of MFN models, while the MFN models are simpler and can be viewed as structured GNNs based on underlying graphical models.

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pruning that
plugging in (19) and (20) in (21), we obtain the following:

\[ E_q(S) \left[ \beta_1 \sum_j s_{ij} = 1 \right] = \beta_1 \prod_{j \in \mathcal{N}_i} \frac{\alpha_{im}}{1 - \alpha_{nm}} \]

Similarly,

\[ E_q(S) \left[ \beta_2 \sum_j s_{ij} = 2 \right] = \beta_2 \prod_{j \in \mathcal{N}_i} \frac{\alpha_{im}}{1 - \alpha_{nm}} \frac{\alpha_{in}}{1 - \alpha_{im}}. \]

Next, we focus on the pairwise symmetry term:

\[ E_q(S) \left[ \lambda(1 - 2(s_{ij} - s_{ji})) \right] = \lambda(1 - 2(\alpha_{ij} + \alpha_{ji}) + 4\alpha_{ij}\alpha_{ji}) \]

Using these simplified terms, and taking the expectation over the remaining terms, we obtain the ELBO as,

\[ F(q(S)) = \ln Z + \sum_{i \in V} \left( 1 - \alpha_{ij} \right) \left( \beta_1 + \beta_2 \sum_{n \in \mathcal{N}_i \setminus m} \frac{\alpha_{in}}{1 - \alpha_{nm}} \right) - \frac{\alpha_{kl}}{1 - \alpha_{kl}} - 2\lambda \sum_{n \in \mathcal{N}_i \setminus m} \alpha_{kn} \left( 1 - \alpha_{nm} \right) - \ln \frac{\alpha_{kl}}{1 - \alpha_{kl}}. \]

From this we obtain the MFA update equation for iteration \((t + 1)\) based on the states from \((t)\),

\[ \alpha_{kl}^{(t+1)} = \sigma(\gamma_{kl}) = \frac{1}{1 + \exp(-\gamma_{kl})} \quad \forall k = \{1, \ldots, N\}, \quad l \in \mathcal{N}_k \]

where \(\sigma(\cdot)\) is the sigmoid activation function, \(\mathcal{N}_k\) are the \(L\) nearest neighbours of node \(k\) based of positional Euclidean distance, and

\[ \gamma_{kl} = \prod_{j \in \mathcal{N}_k \setminus l} \left( 1 - \alpha_{kj}^{(t)} \right) \left( \sum_{m \in \mathcal{N}_k \setminus \{l, k\} \cup \{m\}} \frac{\alpha_{km}^{(t)}}{1 - \alpha_{km}^{(t)}} \left( \beta_2 - \beta_1 \right) - \beta_2 \sum_{n \in \mathcal{N}_k \setminus m} \frac{\alpha_{kn}^{(t)}}{1 - \alpha_{nm}^{(t)}} + \alpha_l T x_k + 2\alpha_{lk}(\eta^T x_k - d|_e + \nu^T (x_k \circ x)) \right). \]