Abstract:

The distance-geometric graph representation adopts a unified scheme (distance) for representing the geometry of three-dimensional (3D) graphs. It is invariant to rotation and translation of the graph and it reflects pair-wise node interactions and their generally local nature. To facilitate the incorporation of geometry in deep learning on 3D graphs, we propose a message-passing graph convolutional network based on the distance-geometric graph representation: DG-GCN (distance-geometric graph convolution network). It utilizes continuous-filter convolutional layers, with filter-generating networks, that enable learning of filter weights from distances, thereby incorporating the geometry of 3D graphs in graph convolutions. Our results for the ESOL and FreeSolv datasets show major improvement over those of standard graph convolutions. They also show significant improvement over those of geometric graph convolutions employing edge weight / edge distance power laws. Our work demonstrates the utility and value of DG-GCN for end-to-end deep learning on 3D graphs.

1 Introduction

The geometry of three-dimensional (3D) graphs, consisting of nodes and edges, plays a crucial role in many important applications. An excellent example is molecular graphs, whose geometry influences important properties of a molecule including its reactivity and biological activity. As in [1], we focus on 3D graphs whose geometry can be fully specified in terms of edge distances ($d$), angles ($\theta$) and dihedrals ($\phi$). A key advantage of such specification is its invariance to rotation and translation of the graph.

Distance geometry [2-3] is the characterization and study of the geometry of 3D graphs based only on given values of the distances between pairs of nodes. From the perspective of distance geometry, the geometry of 3D graphs can be equivalently specified in terms of edge distances ($d$), angle distances ($d_{\theta}$) and dihedral distances ($d_{\phi}$). In addition to invariance to rotation and translation of the graph, such specification adopts a unified scheme (distance) and reflects pair-wise node interactions and their generally local nature.

To facilitate the incorporation of geometry in deep learning on 3D graphs, three types of geometric graph representations are defined in [1]: positional, angle-geometric and distance-geometric. The positional graph representation is based on node positions, i.e., Cartesian coordinates of nodes. The angle-geometric graph representation centers on edge distances ($d$), angles ($\theta$) and dihedrals ($\phi$); it is invariant to rotation and translation of the graph. The distance-geometric
graph representation is based on distances: edge distances \( (d) \), angle distances \( (d^\theta) \) and dihedral distances \( (d^\phi) \); it is invariant to rotation and translation of the graph and it reflects pair-wise node interactions and their generally local nature.

Graph convolutional networks (GCNs) [7] have been applied to deep learning on graphs. However, standard GCNs do not take spatial arrangements of the nodes and edges into account. Therefore, they can accommodate only graph constitution, but not graph geometry. To incorporate geometry in graph convolutions, geometric graph convolutions [1] use the distance-geometric graph representation and employ edge weight / edge distance power laws. The combination enables the incorporation of geometry in graph convolutions utilizing standard GCNs by (1) expanding the kinds of edges involved to include not just edges \( (e) \) with neighbor nodes, but also angle edges \( (e^\theta) \) with second-order-neighbor nodes and dihedral edges \( (e^\phi) \) with third-order-neighbor nodes, and (2) assigning different weights to different edges based on their kind and their distance.

We take the step further and propose DG-GCN (distance-geometric graph convolutional network), a message-passing graph convolutional network based on the distance-geometric graph representation. Similar to geometric graph convolutions, DG-GCN considers all edges that are important to graph geometry in graph convolutions. These include (connected) edges, angle edges and dihedral edges.

However, instead of using hand-crafted edge weight / edge distance power laws, DG-GCN utilizes continuous-filter convolutional layers [4-5], with filter-generating networks, which enable learning of filter weights from distances. This enables end-to-end deep learning on 3D graphs.

DG-GCN is implemented using PyTorch Geometric (PyG) [6]. In particular, the implementation adopts CFConv, extracted from the schnet module in PyG, as the continuous-filter convolutional layer.

Review of the related work that are referenced, but not discussed, in the main body of the paper is provided in the Appendix.

2 Geometry of 3D Graphs

The geometry of 3D graphs is the three-dimensional arrangement of the nodes and edges in a graph. It is often specified in terms of the Cartesian coordinates of nodes. However, such specification depends on the (arbitrary) choice of origin and is too general for specifying geometry.
We focus on 3D graphs whose geometry can be fully specified in terms of edge distances ($d$), angles ($\theta$) and dihedrals ($\phi$). Molecular graphs are excellent examples of such graphs. The edge distance is the distance between two nodes connected together. The angle is the angle formed between three nodes across two edges. For three edges connected in a chain, the dihedral is the angle between the plane formed by the first two edges and the plane formed by the last two edges. These are illustrated in the following diagram:

A key advantage of using edge distances, angles and dihedrals to specify geometry is its *invariance to rotation and translation* of the graph.

### 2.1 Distance Geometry of 3D Graphs

*Distance geometry* [2-3] refers to a foundation of geometry based on the concept of *distances* instead of those of points and lines or point coordinates. For 3D graphs, distance geometry is the characterization and study of their geometry based only on given values of the *distances* between pairs of nodes. From the perspective of distance geometry, the geometry of 3D graphs can be equivalently specified in terms of *edge distances* ($d$), *angle distances* ($d\theta$) and *dihedral distances* ($d\phi$). The angle distance is the distance of the *angle edge* ($e\theta$) and the dihedral distance is the distance of the *dihedral edge* ($e\phi$). The angle edge is the unconnected, end edge between the end nodes of an angle and the dihedral edge is the unconnected, end edge between the end nodes of a dihedral. (We therefore refer to both angle edges and dihedral edges as *end edges.*) These are illustrated in the following diagram (with dashed lines representing angle edges and dotted lines representing dihedral edges):
As the case of using edge distances, angles and dihedrals to specify geometry, a key advantage of specifying geometry in terms of edge distances, angle distances and dihedral distances is its invariance to rotation and translation. In addition, it adopts a unified scheme (distance) and reflects pair-wise node interactions and their generally local nature, which are additional advantages.

3 Geometric Graph Representations

To facilitate the incorporation of geometry in deep learning on 3D graphs, three types of geometric graph representations are defined in [1]: positional, angle-geometric and distance-geometric. The positional graph representation is based on node positions, i.e., Cartesian coordinates of nodes. The angle-geometric graph representation centers on edge distances \(d\), angles \(\theta\) and dihedrals \(\phi\); it is invariant to rotation and translation of the graph. The distance-geometric graph representation is based on distances: edge distances \(d\), angle distances \(d^\theta\) and dihedral distances \(d^\phi\); it is invariant to rotation and translation of the graph and it reflects pair-wise node interactions and their generally local nature.

There are recent work on deep learning on 3D graphs that use the position graph representation [9-10] and the angle-geometric graph representation [11-12]. As in [1], we focus on using the distance-geometric graph representation due to its advantages, uniformity and simplicity. For convenience of discussion, we repeat the definition of the distance-geometric graph representation in the following.

3.1 Distance-Geometric Graph Representation

From the perspective of distance geometry, a 3D graph can be represented as \(G = (X, (I, E), (D, D^\theta, D^\phi))\) where \(X \in \mathbb{R}^{N \times d}\) is the node feature matrix and \((I, E)\) is the sparse adjacency tuple. \(I \in \mathbb{N}^{M \times U}\) encodes edge indices in coordinate (COO) format.
and $E \in \mathbb{R}^{U \times U}$ is the edge feature matrix. $D \in \mathbb{R}^{U \times 1}$ is the edge distance matrix, $D^\theta \in \mathbb{R}^{U \theta \times 1}$ is the angle distance matrix, and $D^\phi \in \mathbb{R}^{U \phi \times 1}$ is the dihedral distance matrix. $U$ is the number of edges, $U^\theta$ is the number of angles, and $U^\phi$ is the number of dihedrals.

This representation is based on distances; therefore we refer to it as the distance-geometric graph representation. As discussed in Section 2.1, it is invariant to rotation and translation of the graph. In addition, it reflects pair-wise node interactions and their generally local nature. These are very useful for graph convolutions, which are locally oriented. They are particularly useful for molecular graphs, since electrostatic, intermolecular, and other conformation-driven properties of molecules depend on the pair-wise interatomic (internodal) distances.

4 Distance-Geometric Graph Convolutional Network (DG-GCN)

Graph convolutional networks (GCNs) [7] have been applied to deep learning on graphs. However, standard GCNs do not take spatial arrangements of the nodes and edges into account. Therefore, they can accommodate only graph constitution, but not graph geometry.

To incorporate geometry in graph convolutions, geometric graph convolutions [1] use the distance-geometric graph representation and employ edge weight / edge distance power laws. The combination enables the incorporation of geometry in graph convolutions utilizing standard GCNs by (1) expanding the kinds of edges involved to include not just edges ($e$) with neighbor nodes, but also angle edges ($e^\theta$) with second-order-neighbor nodes and dihedral edges ($e^\phi$) with third-order-neighbor nodes, and (2) assigning different weights to different edges based on their kind and their distance.

We take the step further and propose DG-GCN (distance-geometric graph convolutional network), a message-passing graph convolutional network based on the distance-geometric graph representation.

4.1 Graph Convolutional Networks (GCNs)

As in [1], we start with graph neural networks (GNNs) that employ the following message passing scheme for node $i$ at layer $k$:

$$x_i^{(k)} = \gamma^{(k)}(x_i^{(k-1)}, \prod_j \lambda^{(k)}(x_i^{(k-1)}, x_j^{(k-1)}, e_{ij}))$$

where $j \in N(i)$ denotes a neighbor node of node $i$. $x_i$ is the node feature vector and $e_{ij}$ is the edge feature vector. $\gamma$ and $\lambda$ denote differentiable update and message functions, respectively, and $\prod$ denotes a differentiable aggregation function.
The standard GCN [7] implements message passing using the adjacency matrix $A$:

$$X^{(k)} = \tilde{D}^{-1/2} \tilde{A} \tilde{D}^{-1/2} X^{(k-1)} W^{(k-1)},$$

where $\tilde{A} = A + I$ denotes the adjacency matrix with inserted self-loops and $\tilde{D}_{ii} = \sum_{j} \tilde{A}_{ij}$ its diagonal degree matrix. $A_{ij}$ is one when there is an edge from node $i$ to node $j$, and zero when there is no edge. $W^{(k-1)}$ is the layer-specific weight matrix.

In the context of message-passing GNNs, the standard GCN takes the following shape: [8]

$$x_i^{(k)} = \frac{1}{c_i} (x_i^{(k-1)} + \sum_j x_j^{(k-1)}) W^{(k-1)},$$

where $c_i$ is a node-specific normalization constant.

In case the graph has edge weights, $w_{ij}$, the above equation can be expanded as:

$$x_i^{(k)} = \frac{1}{c_i} (x_i^{(k-1)} + \sum_j w_{ij} x_j^{(k-1)}) W^{(k-1)}$$

This is used by geometric graph convolutions in [1] with $w_{ij}$ determined from edge weight / edge distance power laws and $N(i)$ expanded as $N(i) = \mathcal{N}(i) + \mathcal{N}^\theta(i) + \mathcal{N}^\phi(i)$, with $\mathcal{N}(i)$ being the first-order ($1^{st}$) neighbors, $\mathcal{N}^\theta(i)$ the second-order ($2^{nd}$) neighbors and $\mathcal{N}^\phi(i)$ the third-order ($3^{rd}$) neighbors.

### 4.2 DG-GCN

Similar to geometric graph convolutions, DG-GCN considers all edges that are important to graph geometry in graph convolutions. These include (connected) edges ($e$) with $1^{st}$ neighbors, angle edges ($e^\theta$) with $2^{nd}$ neighbors, and dihedral edges ($e^\phi$) with $3^{rd}$ neighbors. The following diagram [12] shows the neighborhood of a node of a molecular graph where a) includes $1^{st}$ neighbors (black), b) includes $1^{st}$ neighbors and $2^{nd}$ neighbors (blue), and c) includes $1^{st}$ neighbors, $2^{nd}$ neighbors and $3^{rd}$ neighbors (red). It can be seen that DG-GCN, i.e., case c), fully captures the local geometry (and substructures) of a node in graph convolutions.
However, instead of using hand-crafted edge weight / edge distance power laws, DG-GCN utilizes *continuous-filter convolutional layers* [4-5], with *filter-generating networks*, which enable learning of filter weights from distances. This enables end-to-end deep learning on 3D graphs.

The architecture of DG-GCN is shown below, where \{d_{ij}\} denotes the set of all distances, including edge distances (d), angle distances (d^\theta) and dihedral distances (d^\phi).
4.3 Continuous-Filter Convolutional Layer (CFConv)

The *continuous-filter convolutional layer (CFConv)* [2-3] is a generalization of the discrete convolutional layers commonly used for image or audio data. This generalization is necessary since nodes in a 3D graph are not located on a regular grid like pixels, but can be located at arbitrary positions.

The filters are modeled in a continuous fashion with a *filter-generating network (FGNet)*, to be discussed next, that maps from distances, \( d_{ij} \), to corresponding filter weights, \( W^{(k)}(d_{ij}) \), at layer \( k \). The output for the convolutional layer is then given by

\[
x^{(k)}_i = \frac{1}{c_i} (x_i^{(k-1)} + \sum_j w_{ij} x_j^{(k-1)} W^{(k-1)}(d_{ij}))
\]

where \( j \in N(i) \) denotes the set of neighbors of node \( i \). \( N(i) = N(i) + N^\theta(i) + N^\phi(i) \), with \( N(i) \) being the 1st neighbors, \( N^\theta(i) \) the 2nd neighbors and \( N^\phi(i) \) the 3rd neighbors. \( w_{ij} \) is determined from \( d_{ij} \) using

\[
w_{ij} = 0.5 \times \cos((d_{ij} / d_{\text{cutoff}}) \times \pi) + 1)
\]

where \( d_{\text{cutoff}} \) is the distance cutoff (see Section 4.4). \( w_{ij} \) varies from 1 \((d_{ij} = 0)\) to 0 \((d_{ij} = d_{\text{cutoff}})\).

The architecture of CFConv is shown below:
4.4 Filter-Generating Network (FGNet)

The filter-generating network (FGNet) [2-3] learns filter weights from distances. It is a fully-connected network and it is rotational invariant since it uses distances as input. The distance, $d_{ij}$, is first expanded in a basis of Gaussians

$$e_k(d_{ij}) = \exp(-\gamma(d_{ij} - \mu_k)^2)$$

with centers $\mu_k$ located on a uniform grid between zero and the distance cutoff. Due to this additional non-linearity, the initial filters are less correlated leading to a faster training procedure. The number of Gaussians and the hyperparameter $\gamma$ determine the resolution of the filter. For the feasibility study, we use the default values provided in SchNet [2-3] for the number of Gaussians, distance cutoff, $\mu_k$ and $\gamma$.

The architecture of FGNet is shown below. ShiftedSoftPlus is defined as $ssp(x) = \ln(0.5e^x + 0.5)$. The shifting ensures that $ssp(0) = 0$ and improves the convergence of the network while having infinite order of continuity.
5 Experiments

A number of experiments have been carried out using the ESOL and FreeSolv datasets, which are used in [9-10] for training and evaluating 3D-extended GCNs. Specifically, dataset files provided by Geo-GCN [10] are used, same as [1], which contain molecular graph data including three-dimensional node coordinates. These are small datasets with 901 / 113 / 510 / 65 / 64 training / test / validation samples, respectively. Our focus, however, is on qualitatively comparing results of DG-GCN with those of standard graph convolutions and geometric graph convolutions, reported in [1], all based on the same sample sizes. That is, our interest is on relative accuracy not absolute accuracy.

The results are listed in the following table. Standard GC (graph convolutions) [1] utilizes the default GCNConv with all edges having a weight of one and serves as the baseline for comparison. Geometric GC [1] utilizes the GCNConv with edge weights calculated from edge distances using power laws. In particular, Geometric GC (Ref) denotes the reference geometric GC which uses fixed $R_0 = 1.39$ and $N = 4.55$ for the power law parameters.

As in [1], we consider three cases of geometric graph convolutions for Geometric GC and DG-GC: edges (1st Nbrs) which include 1st neighbor nodes, edges + angle edges (2nd Nbrs) which include 1st and 2nd neighbor nodes, and edges + angle edges + dihedral edges (3rd Nbrs) which include 1st, 2nd and 3rd neighbor nodes. We include the 1st Nbrs and 2nd Nbrs cases to verify and show the consistency of DG-GCN results. The (full) DG-GCN results are represented by the 3rd Nbrs cases.

| Dataset     | Model                      | RMSE  |
|-------------|----------------------------|-------|
| ESOL        | Standard GC                | 0.4573|
|             | Geometric GC (Ref) – 3rd Nbrs | 0.4273|
|             | DG-GCN – 1st Nbrs          | 0.3623|
|             | DG-GCN – 2nd Nbrs          | 0.3216|
|             | DG-GCN – 3rd Nbrs          | 0.3379|
| FreeSolv    | Standard GC                | 0.4183|
|             | Geometric GC (Ref) – 3rd Nbrs | 0.3710|
|             | DG-GCN – 1st Nbrs          | 0.3608|
|             | DG-GCN – 2nd Nbrs          | 0.3468|
|             | DG-GCN – 3rd Nbrs          | 0.3405|
It can be seen from the table, for both the ESOL and FreeSolv datasets, the results of DG-GCN show major improvement over those of Standard GC. They also show significant improvement over Geometric GC. This demonstrates the utility and value of DG-GCN for end-to-end deep learning on 3D graphs.

6 Summary and Conclusion

To facilitate the incorporation of geometry in deep learning on 3D graphs, we propose a message-passing graph convolutional network based on the distance-geometric graph representation: DG-GCN (distance-geometric graph convolution network). It utilizes continuous-filter convolutional layers, with filter-generating networks, that enable learning of filter weights from distances, thereby incorporating the geometry of 3D graphs in graph convolutions.

Our results for the ESOL and FreeSolv datasets show major improvement over those of standard graph convolutions. They also show significant improvement over those of geometric graph convolutions employing edge weight / edge distance power laws.

Our work demonstrates the utility and value of DG-GCN for end-to-end deep learning on 3D graphs.

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References

[1] Daniel T. Chang, “Geometric Graph Representations and Geometric Graph Convolutions for Deep Learning on Three-Dimensional (3D) Graphs,” arXiv preprint arXiv:2006.01785 (2020).
[2] Leo Liberti, “Distance Geometry and Data Science,” arXiv preprint arXiv:1909.08544 (2019).
[3] T. F. Havel, “Distance Geometry: Theory, Algorithms, and Chemical Applications,” in Encyclopedia of Computational Chemistry. American Cancer Society, 2002.
[4] K. Schütt, P.-J. Kindermans, H. E. S. Felix, S. Chmiela, A. Tkatchenko, and K.-R. Müller, “Schnet: A Continuous-Filter Convolutional Neural Network for Modeling Quantum Interactions,” in Advances in Neural Information Processing Systems, pp. 992–1002, 2017.
[5] K. T. Schütt, H. E. Sauceda, P.-J. Kindermans, A. Tkatchenko, and K.-R. Müller, “Schnet – A Deep Learning Architecture for Molecules and Materials,” in J. Chem. Phys. 148, 241722 (2018).
[6] Matthias Fey and Jan E. Lenssen, “Fast Graph Representation Learning with PyTorch Geometric,” in ICLR Workshop on Representation Learning on Graphs and Manifolds, 2019.
[7] T. N. Kipf and M. Welling, “Semi-supervised Classification with Graph Convolutional Networks,” in ICLR 2017.
[8] Floris Hermsen, Peter Bloem, Fabian Jansen, and Wolf Vos, “End-to-End Learning from Complex Multigraphs with Latent Graph Convolutional Networks,” arXiv preprint arXiv: 1908.05365 (2019).
[9] H. Cho and I. S. Choi, “Three-Dimensionally Embedded Graph Convolutional Network (3DGCN) for Molecule Interpretation,” arXiv preprint arXiv:1811.09794 (2018).
[10] P. Spurek, T. Danel, J. Tabor, M. Śmieja, Ł. Struski, A Slowik, and Ł. Maziarka, “Geometric Graph Convolutional Neural Networks,” arXiv preprint arXiv:1909.05310 (2019).
[11] Johannes Klicpera, Janek Groß, and Stephan Günnemann, “Directional Message Passing for Molecular Graphs,” in International Conference on Learning Representations, 2020.
Appendix - Related Work

**L-GCN** [8] provides a learning mechanism that transforms edge attributes into latent representations, which can then serve as input to a GCN-like architecture for further propagation in the form of an adjacency tensor. Edges are represented by a vector $w_{ij}$ containing multiple weights across different edge attributes. L-GCN turns the edge weights into trainable parameters in an end-to-end fashion, using the output of the learning mechanism which operates on either a vector describing multiple edge attributes or a sequence of such vectors (multi-edges). In contrast, DG-GCN provides a learning mechanism, through FGNet as part of CFConv, that transforms (edge) distances into filter weights in an end-to-end fashion.

**3DGCN** [9] builds a three-dimensional (3D) graph convolutional network by augmenting the standard GCN layer with the relative (node) position matrix, which contains the full spatial topology of a 3D graph. Specifically, it incorporates node-level vector features, as well as conventional scalar features, and brings them together by using the interconverting operations based on the relative position matrix for 3D graph convolutions. The relative position matrix ensures translational invariance. 3DGCN is based on the positional graph representation, though using relative positions; in contrast, DG-GCN is based on the distance-geometric graph representation.

**GeoGCN** [10] uses geometric features (spatial coordinates) in GCNs and is a proper generalization of GCNs and CNNs (convolutional neural networks). The relative positions in the neighborhood of a node are transformed using a linear operation combined with non-linear ReLU function. This scalar is used to weigh the feature vectors in a neighborhood. GeoGCN is based on the positional graph representation, though using relative positions; in contrast, DG-GCN is based on the distance-geometric graph representation.

**DimeNet** [11] embeds the messages passed between nodes such that each message is associated with a direction in coordinate space and are rotationally equivariant since the associated directions rotate with the graph. The message passing scheme transforms messages based on the angle between nodes in order to encode direction. This is done by using spherical Bessel functions and spherical harmonics to construct theoretically well-founded, orthogonal representations. DimeNet is based on the angle-geometric graph representation, though considering only angles but not dihedrals; in contrast, DG-GCN is based on the distance-geometric graph representation.
Path GCN [12] generalizes GNNs to pass messages and aggregate across higher order paths. This allows for information to propagate over various levels and substructures of the graph. Specifically, Path GCN learns representations over larger node neighborhoods within each propagation layer by simply augmenting the message function to aggregate over additional neighbors. By summing over additional neighbors it enables the use of path features such as angles for paths of length two and dihedrals for paths of length three. Path GCN is inspired by the angle-geometric graph representation and includes neighbors up to path length $l$ in graph convolutions; in contrast, DG-GCN is based on the distance-geometric graph representation and includes all, but only, neighbors germane to the graph geometry: 1st neighbors, 2nd neighbors and 3rd neighbors.