Learning Delaunay Triangulation using Self-attention and Domain Knowledge

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Abstract

Delaunay triangulation is a well-known geometric combinatorial optimization problem with various applications. Many algorithms can generate Delaunay triangulation given an input point set, but most are nontrivial algorithms requiring an understanding of geometry or the performance of additional geometric operations, such as the edge flip. Deep learning has been used to solve various combinatorial optimization problems; however, generating Delaunay triangulation based on deep learning remains a difficult problem, and very few research has been conducted due to its complexity. In this paper, we propose a novel deep-learning-based approach for learning Delaunay triangulation using a new attention mechanism based on self-attention and domain knowledge. The proposed model is designed such that the model efficiently learns point-to-point relationships using self-attention in the encoder. In the decoder, a new attention score function using domain knowledge is proposed to provide a high penalty when the geometric requirement is not satisfied. The strength of the proposed attention score function lies in its ability to extend its application to solving other combinatorial optimization problems involving geometry. When the proposed neural net model is well trained, it is simple and efficient because it automatically predicts the Delaunay triangulation for an input point set without requiring any additional geometric operations. We conduct experiments to demonstrate the effectiveness of the proposed model and conclude that it exhibits better performance compared with other deep-learning-based approaches.

Keywords: Delaunay Triangulation, Deep Learning, Combinatorial Optimization, Self-Attention, Transformer, Pointer Network

1. Introduction

Delaunay triangulation (DT) finds a triangulation such that no point in P is inside the circumcircle of any triangle when a point set P is given [Jiang et al. (2010)]. Moreover, DT maximizes the minimum angle of the triangles and avoids skinny triangles.
with very large or very small angles. In addition, DT has various applications in many different fields. It is often used to generate triangular meshes when solving partial differential equations using the finite element method (FEM) or finite volume method (FVM) for a given geometric domain. Further, DT generates triangles close to equilateral triangles for a given point set, which is preferred when using the FEM and FVM for solution accuracy and efficiency. Additionally, DT is used for data clustering. After connecting the data points using DT, data clustering is completed by removing the long edges of a certain length or longer and leaving only the remaining connected edges. In addition, DT is also used when generating Voronoi diagrams because DT corresponds to the dual graph of the Voronoi diagram. The circumcenter of the Delaunay triangle becomes the vertices of the Voronoi diagram, which has many applications in biology, ecology, computational fluid dynamics, and computational physics.

DT is an important combinatorial optimization problem involving geometry with various applications, but most of the existing algorithms are nontrivial algorithms, requiring the understanding of geometric requirements or performing geometric operations, such as the edge flip. The combinatorial optimization problem is a significant problem in computer science. The combinatorial optimization problem finds an optimal subset from a finite set of objects. Several examples of combinatorial optimization problems include the convex hull, traveling salesman problem (TSP), knapsack, and vehicle routing problem [Bello et al. (2016); Nazari et al. (2018); Gu & Hao (2018)]. Many combinatorial optimization problems are NP problems, and heuristic algorithms are often used to find nearly optimal solutions when solving these problems. Recently, deep-learning-based techniques have been used to solve these complex combinatorial optimization problems. Both supervised learning and reinforcement learning are used to solve these problems.

A representative supervised learning-based deep learning model for solving combinatorial optimization problems is the pointer network (Ptr-Net) [Vinyals et al. (2017)]. The conventional sequence-to-sequence (seq2seq) model computes conditional probabilities from a fixed dictionary. Therefore, it has limitations for solving combinatorial optimization problems in which the size of the output dictionary changes depending on the input size. However, Ptr-Net solves this problem. Vinyal et al. proposed and applied Ptr-Net to find (approximate) solutions to the following combinatorial optimization problems with variable-sized inputs and output dictionaries: convex hull, DT, and TSP. In addition, Ptr-Net demonstrates the possibility to solve these combinatorial optimization problems, but it has limitations for practical use, especially for solving DT and TSP. Afterward, various studies on the TSP problem using supervised and reinforcement learning were conducted, but studies on the DT problem are scarce.

Recently, a transformer model has been proposed to solve the long-term dependency problem of the recurrent neural network (RNN) model [Vaswani et al. (2017b)]. The transformer model consists of self-attention, multi-head attention, and positional encoding and has the advantage that it does not involve recurrence. The transformer model is widely used in natural language processing, voice recognition, and image recognition [Zhao et al. (2020); Devlin et al. (2018); Dong et al. (2018)]. The concept of self-attention used in the transformer model indicates that attention is carried out toward itself and can be used in encoder and decoder models. The transformer model learns by considering the relationships between all pairs in the input/output sequence.
In this paper, we propose a new neural network model to solve DT using self-attention and domain knowledge. The proposed method is based on supervised learning. It has the advantage of being simple and efficient because it automatically outputs DT for an input point set when the neural network model is sufficiently trained without requiring any additional geometric operations. The sequence order of input and output has a significant effect on the performance of the seq2seq-based models. However, the effect of applying input/output sequence ordering is not well studied. We first propose a method of ordering input and output sequences that can significantly improve the model learning performance for the DT problem. Second, we apply self-attention in the encoder to better learn the point-to-point relationship when generating DT. Our model can effectively learn the topological relationship between distant points in the encoder by applying the self-attention mechanism. Finally, we develop a new attention score function that can augment the existing attention mechanism using domain knowledge. It is a newly developed penalty-based attention score function, making the conditional probability very small if the Delaunay condition is not satisfied. Our main contributions are summarized as follows:

• We propose a novel neural network model that can learn DT based on self-attention and domain knowledge. To the best of our knowledge, the proposed model exhibits the best performance among deep-learning-based techniques.

• The proposed model is the first that applies a self-attention mechanism for learning DT in the encoder. We also propose an efficient input/output sequence ordering method to learn the sequence more regularly and effectively.

• We propose a new type of attention score function using domain knowledge, a flexible function that can be applied to other combinatorial optimization problems involving geometry. We also develop several evaluation metrics that measure model performance.

2. Related Work

2.1. Delaunay Triangulation

Triangulation is a fundamental and essential problem in computer graphics and computational geometry. Triangulation of a set of points $P$ is a partition of the convex hull into simplices, such that the union of all these simplices equals its convex hull and that any pair of them intersects in a common face. In the plane, triangulations comprise triangles with their edges and vertices. Among various triangulations, the triangulation of particular interest is DT. Specifically, DT for a point set $P$ is a triangulation such that no point in $P$ is inside the circumcircle of any triangle Jiang et al. (2010). Figure 1 presents one example of DT with circumcircles. Further, DT maximizes the minimum angle of all angles of the triangle in the triangulation and avoids sliver triangles Jiang et al. (2010).

Many algorithms have been proposed for generating DT with the algorithm complexity of $O(n\log(n))$ or $O(n^2)$ Guibas & Stolfi (1985); Lee & Schachter (1980); Rebay (1993). One of the most popular DT algorithms is the flip algorithm, which constructs any triangulation from the points and then repeatedly flips the edges until every
triangle meets the Delaunay condition. When two triangles ABC and ABD share an edge AB, if the sum of the $\alpha$ and $\beta$ angles is less than or equal to $180^\circ$, the Delaunay condition is satisfied. Figure 2 displays two triangulations, where one triangulation (left) does not meet the Delaunay condition and the other triangulation (right) meets the Delaunay condition after performing an edge flip (swap).

There are incremental algorithms and divide conquer algorithms for generating DT [Shewchuk (2002); Blelloch et al. (2016)]. Recently, sweep-hull algorithm is also proposed [Sinclair (2016)]. However, most of the existing algorithms are non-trivial algorithms, which often require to perform repeated edge flips and often require to install extra software.

**Figure 1** Delaunay triangulation with circumcircles (dotted).

**Figure 2** Triangulation that (a) does not meet the Delaunay condition and (b) meets the Delaunay condition after performing an edge flip.

### 2.2. Delaunay Triangulation using Deep Learning

The DT problem belongs to combinatorial optimization problems involving geometry similar to the convex hull and TSP problems. The problem finds subsets of triangles that satisfy the Delaunay condition in each point set. Most of these combinatorial optimization problems are not trivial to solve and are often NP problems. Research on generating DT using deep learning has been studied minimally for several reasons. First, when the solution of DT is expressed as an input/output sequence, the input/output length varies depending on the problem size. However, conventional seq2seq-based models are not effective for this variable-length dictionary. Second, the mesh data structure is not a regular data structure, such as an image, but is an irregular data structure, making learning difficult for the model. Applying unmodified
deep learning methods, such as the convolutional neural network (CNN), is challenging Hanocka et al. (2018). Third, it is possible to predict the coordinates of a point when creating a mesh using a deep learning method, such as the RNN, but in this case, there is no limit to the feature space, which causes blurring Vinyals et al. (2017). Lastly, the elements constituting the triangular mesh consist of three points, which must be learned as a group, and it is difficult for the model to learn the relationships and dependencies between points in distant locations. In particular, as the number of points forming a point set increases, the sequence length becomes longer, making it challenging to learn the dependencies between points in distant locations in the sequence.

To the best of our knowledge, two deep learning-based approaches can generate DT from a given input point set. Both methods are based on supervised learning and use the encoder-decoder model. These methods automatically predict DT for a given point set after the model sufficiently learns DT. In Vinyals et al. (2017), the authors used the Ptr-Net for generating DT. It obtains 80.7% accuracy and 93.0% triangle coverage when the number of points \( m \) is 5. However, when \( m = 10 \), the accuracy dramatically decreases to 22.6%, and the triangle coverage decreases to 81.3%. In addition, when \( m = 50 \), it does not produce any precisely correct triangulation, and the triangle coverage is also significantly reduced to 52.8%.

In Guo et al. (2019), the authors proposed the multi-Ptr-Net (M-Ptr-Net), a variant of the Ptr-Net, which uses multiple “pointers” to learn by combining the vertices that constitute a triangle into a group for the DT problem. It uses multiple “pointers” using the multi-label classification idea Guo et al. (2019). It fits a loss function of the multi-label classification using the sigmoid function instead of the softmax function. They reported that when \( m = 5 \), the accuracy improves by 0.45% compared to the Ptr-Net. However, two existing deep learning-based approaches for generating DT still have limitations for practical use due to the low accuracy and triangle coverage. In addition, the model does not sufficiently learn point-to-point relationships forming triangles.

2.3. Neural Combinatorial Optimization

In recent years, various efforts have been made to solve combinatorial optimization problems using state-of-the-art artificial intelligence techniques Mao et al. (2016); Kool et al. (2019); Joshi et al. (2019). Both supervised learning and reinforcement learning are used to solve combinatorial optimization problems, but their effectiveness depends on the problem. Supervised learning is effective when an optimal solution is available and sufficient data are given in the training data. However, in many cases, it is not easy to obtain such a high-quality labeled dataset. The supervised learning-based approach is complex, and scalability is poor when the problem is large or NP. In such a large or NP problem, many reinforcement learning-based methods have been proposed. Bello et al. proposed a framework to solve combinatorial optimization problems using neural networks and reinforcement learning Bello et al. (2016). The method solves the TSP and demonstrates nearly optimal results on two-dimensional Euclidean graphs for up to 100 nodes. Nazari et al. presented a framework for solving the vehicle routing problem using reinforcement learning Nazari et al. (2018). The framework provides a nearly optimal solution and outperforms the classical heuristics proposed for solving the vehicle routing problem. Recently, several attempts have been made to solve the combinatorial optimization problem using a graph CNN Bresson & Laurent (2017).
3. Background

3.1. Seq2seq Models

The RNN-based seq2seq models are efficient neural networks for the task of corresponding one sequence to another and are widely used in machine translation Sutskever et al. (2014); Cho et al. (2014). The typical seq2seq models have two RNNs called the encoder and decoder. The encoder reads the input sequence sequentially to create a context vector, and the decoder receives the context vector and sequentially outputs the output sequence.

For the input sequence \( P \) and the corresponding output sequence \( O \)

\[
O = (O_1, O_2, ..., O_n)
\]

the seq2seq model estimates the probability of sequence \( O \) using the chain rule as follows:

\[
p(O | P; \theta) = \prod_{i=1}^{n} p(O_i | O_1, ..., O_{i-1}, P; \theta),
\]

where \( \theta \) is a learnable parameter. During the inference process, in decoder step \( i \), the model predicts the sequence by selecting \( O_i \), which maximizes \( p(O_i | O_1, ..., O_{i-1}, P; \theta) \).

However, this seq2seq model contains all information in a context vector with a fixed size, resulting in the loss of information, and an attention mechanism is used to solve this problem Bahdanau et al. (2016). The basic idea of the attention mechanism is that the decoder predicts the output and attention for the entire input sequence of the encoder once again at every time step. However, even with the attention mechanism, there is still a problem that the output dictionary depends on the length of the input sequence Mottini & Acuna-Agost (2017).

3.2. Pointer Network (Ptr-Net)

In the existing seq2seq model, the model is difficult to use for problems where the size of the output dictionary changes according to the input size (e.g., combinatorial optimization problems) because the conditional probability, \( p(O_i | O_1, ..., O_{i-1}, P; \theta) \) is calculated and selected from a fixed dictionary. Similar to the seq2seq model, the Ptr-Net consists of two RNNs: an encoder and a decoder. For each time step, the encoder takes an element of the input sequence as input and outputs the embedding at that time. The decoder outputs a pointer to the input data from the embedding received from the encoder through a modified attention mechanism. The Ptr-Net calculates the probability as follows using the modified attention mechanism:

\[
u'_j = v^T \tanh(W_1 e_j + W_2 h_i), j \in \{1, ..., m\}
\]

\[
p(O_i | O_1, ..., O_{i-1}, P) = \text{softmax}(u'),
\]

where the hidden states of the encoder and decoder are \((e_1, ..., e_m)\) and \((h_1, ..., h_n)\), respectively. In addition, \( u' \) is a vector of length \( m \) representing each score of the encoder step, and \( W_1, W_2 \), and \( v \) are learnable parameters. Unlike previous attention mechanisms that create a new context vector due to \( \text{softmax} u' \), the Ptr-Net considers this to be a probability for each input element. In a dictionary of input elements, \( u' \) is a vector of “pointers” to the input elements.
3.3. Multi-Ptr-Net

For the DT problem, three points form a triangle when creating a triangulation. However, the Ptr-Net has limitations in learning the topological relationship of the points, especially when the number of input points is large. Moreover, the Ptr-Net has a limitation in learning the sequence as a pair; thus, multi-Ptr-Net (M-Ptr-Net) is proposed to improve these limitations Guo et al. (2019). The M-Ptr-Net is motivated by the multi-label classification method so that multiple embedding results in the encoder can be pointed at simultaneously in one step of the decoder. At each time step of the decoder, it calculates the probability using the following equation:

$$p(O_i|O_1, ..., O_{i-1}, P) = \text{sigmoid}(u^i).$$ (3)

The original Ptr-Net uses the softmax function for “pointing”, which is used for the multi-class classification problem. In M-Ptr-Net, the sigmoid function used in the multi-label classification problem is employed instead of the softmax function. Figure 3 depicts an example of applying M-Ptr-Net to the DT problem. The input includes five planar points, $$P_1 = (x_1, y_1), ..., P_5 = (x_5, y_5)$$ with four elements where $$(x_i, y_i)$$ are the Cartesian coordinates of the points. The output sequence represents the solution for the DT problem. Unlike the Ptr-Net, the strength of the M-Ptr-Net is that it is not affected by the order of the points forming a triangle because it learns the three points forming a triangle as a group.

Figure 3 Example using M-Ptr-Net for the DT problem. Input $$P = \{P_1, ..., P_5\}$$ and the output=$$(\Rightarrow, \{1, 2, 3\}, \{1, 2, 4\}, \{2, 3, 5\}, \{2, 4, 5\}, \Leftarrow)$$. The tokens $$\Rightarrow$$ and $$\Leftarrow$$ are beginning and end of sequence, respectively.

3.4. Transformer and Self-attention

The conventional encoder-decoder models using the attention mechanism have problems in that the amount of learning increases rapidly as the number of steps increases. Moreover, it is challenging to learn the dependence between words in distant locations. To improve these problems, the transformer model is a neural network model that avoids recurrence and relies entirely on the attention mechanism to derive
the global dependence of the input and output. The transformer model also uses the encoder-decoder model and includes multi-head attention, self-attention, and positional encoding [Vaswani et al. (2017a), Wu et al. (2019)].

Three types of attention exist in the original transformer model. The first is the attention from the encoder to the encoder, the second is the attention from the decoder to the decoder, and finally, the third is the attention from the decoder to the encoder. Among them, the first two inner attentions are called self-attention, and they occur inside the encoder or decoder. Self-attention is a process of generating a new expression of a corresponding word in consideration of the relative positional relationship of words in a sentence and differs from the recurrence layer and convolutional layer. First, the total computational complexity per layer and the minimum number of sequential operations are both small. Second, it is possible to learn a wide range of dependencies in a short path. Finally, each head presents a model that can be interpreted.

The transformer interprets the attention as receiving a query and a key-value pair and outputs an output vector that synthesizes the value vector corresponding to the query vector. Single-head attention used in the transformer can be expressed by the following formula [Vaswani et al. (2017a), Wu et al. (2019)]:

$$\text{Head} = \text{Attention} (QW^Q, KW^K, VW^V) = \text{softmax} \left( \frac{QW^Q (KW^K)^T}{\sqrt{d_k}} \right) VW^V, \quad (4)$$

where $Q$ is a $(q, d_{\text{model}})$ matrix consisting of $q$ query vectors, $K$ is a $(k, d_{\text{model}})$. Moreover, $W^Q$ and $W^K$ are learnable parameters with dimension $(d_{\text{model}}, d_k)$. $W^V$ is a learnable parameter with dimensions $(d_{\text{model}}, d_v)$. Self-attention is the case where $Q$, $K$, and $V$ are the same. The result of reinterpreting each embedding is the output considering the relationship between the input embeddings.

4. Proposed Model

The proposed neural network model consists of an encoder and decoder, and each consists of a long short-term memory (LSTM) cell [Hochreiter & Schmidhuber (1997)]. The input sequence in the training data is the point set, $P = (P_1, ..., P_m)$, where $P_i$ is the Cartesian coordinates of $m$ planar points. The outputs, $O^P = (O_1, ..., O_n)$ are sequences representing the solution to the corresponding DT problem. Each $O_i$ refers to the index of $P$ having an integer value between 1 and $m$, and three consecutive $O_i$ are combined to represent a triangle.

4.1. Sequence Ordering

For the seq2seq-based neural network models, the data order has a significant influence on learning performance in the input and output sequences [Vinyals et al. (2017, 2016)]. Sequence ordering is simple and effective in that it only requires changing the sequence order but can significantly improve learning performance. Vinyal et al. found that restricting the equivalence class as much as possible for the output is always better [Vinyals et al. (2017)]. The authors proposed a method to perform sequence ordering only for the output sequence. In Vinyals et al. (2016), the authors insisted that both
the input and output sequence orders are important, but they do not suggest a specific sequence ordering method for the DT problem. The proposed sequence ordering is motivated by the work in Vinyals et al. (2017, 2016).

We propose a new input/output sequence ordering method to improve model performance. If the sequence is ordered properly and meaningful rules are set, the rules are created in the data, making the model easier to learn. The proposed method consists of three steps. First, we sorted the input sequence in lexicographic order when putting the input sequence into the encoder. The lexicographic order in the input sequence refers to a method of sorting $P$ in the order of small $x$-axis coordinates with respect to $P$ and sorting in the order of small $y$-axis coordinates if the $x$-axis coordinates are the same.

The two orders in the output sequence are the ordering between triangles and the ordering for the indices of the points that form each triangle. Second, we sorted the index of the points forming a triangle by increasing the triangle representation. For example, we used $(1, 2, 3)$ instead of $(2, 3, 1)$ to represent a triangle. Finally, we sorted each triangle by its incenter coordinates. We computed the incenter coordinates of each triangle and sort them in the order of the small $x$-axis coordinates. If the incenter coordinates of the $x$-axis were the same, we sorted them in the order of the small $y$-axis.

We also tested the other sequence ordering method for sorting input/output sequences, such as sorting the sequence by angle, but our preliminary results indicate that the proposed ordering method exhibits better performance than other sequence ordering methods. Better input/output sequence ordering of the proposed model will be explored in future work.

4.2. Attention Mechanism

4.2.1. Self-attention

Self-attention outputs a new embedding reinterpreted in consideration of the relationship between input embeddings as described earlier. Figure 4 presents the proposed neural network model based on self-attention. In the proposed model, we apply self-attention to the embeddings for each point output of the encoder. We expected that the model can learn about the relationship and dependence among points better than in the absence of self-attention. We also expected that the model would output a well-analyzed embedding by considering the relationship between points with far distances in the step in the encoder.

In the decoder, self-attention can be used like the transformer model, but we did not use the self-attention mechanism in the decoder for the following two reasons. First, in the encoder, it is difficult to include the relationship between points with far distances. However, in the decoder, the state of the surrounding step is considered more important than the step with a far distance. Second, because the decoder has a step length of up to 5 to 6 times that of the encoder, the cost of self-attention with a complexity of $O(n^2)$ becomes higher. Additional performance improvement can be achieved if the decoder also uses self-attention, but by using self-attention only in the encoder, the proposed model improves performance within a reasonable computational cost.

Similar to the transformer model Vaswani et al. (2017a); Wu et al. (2019), the proposed model also uses the residual connection, but it uses a single head. This is
**Figure 4** Proposed neural net model.

because even a single head creates enough complexity to improve performance greatly. Figure 5 displays the model to which the proposed self-attention is applied for DT. Both input/output sequences were sorted using the proposed sequence ordering method. In this example, \( P = (P_1, \ldots, P_5) \) and \( O^P = (\Rightarrow, (1, 2, 3), (1, 2, 4), (2, 3, 5), (2, 4, 5), \Leftarrow) \).

4.2.2. Attention score function

The conventional attention mechanism does not consider domain knowledge and is thus difficult to apply to geometric combinatorial optimization problems, such as DT. In this paper, we propose a novel attention score function that augments the existing attention mechanism. This function is a new type of attention score function that forcibly sets the conditional probability to zero when the desired geometric requirements are not satisfied in each step in the decoder.

The proposed attention score function is described in Algorithm 1. First it uses the definition of a triangle: each triangle consists of three points. Therefore, it makes the model generate triangles by forcing the length of the output sequence to be a multiple of three. In addition, at every third step of forming a triangle in the decoder, the function checks whether the Delaunay condition is satisfied for each (candidate) point of \( P \). If any candidate point of \( P \) violates the Delaunay condition, it adds \( \gamma \) to the attention score in Eq. (2) such that the models cannot “point” to that candidate point. For this case, the new attention score function is computed as:

\[
\bar{u}_{ji} = u_{ij} + \gamma,
\]

where \( \gamma \) (e.g., \(-\infty\)) is a user-defined parameter. Otherwise, \( \bar{u}_{ji} = u_{ij} \). The proposed attention score function is motivated by the definition of DT, and the geometric requirement is determined regarding whether it satisfies the Delaunay condition described in Section 2. However, the proposed attention score function is a flexible method that can be extended to other geometric problems.

4.2.3. Beam search decoding

Beam search is a method of improving efficiency by limiting the number of nodes to remember using the best-first search (BFS) method \cite{Bahdanau et al., 2016}. At every
Figure 5 Example of input and output sequence representation for the DT using the proposed model. Input \( P = (P_1, ..., P_5) \) and output \( \mathcal{O}^P = (\Rightarrow, (1,2,3), (1,2,4), (2,3,5), (2,4,5), \Leftarrow) \). The tokens \( \Rightarrow \) and \( \Leftarrow \) are beginning and end of sequence, respectively.

Time step, the method keeps the most likely sequence elements corresponding to the beam size Szucs & Huszti (2019). Finally, the decoder selects the sequence with the highest joint probability among the beam subsets. This can be expressed as follows:

\[
\arg\max_{\mathcal{O}^w \subseteq \mathcal{O}^B} \prod_{i=1}^w P(O_i | P, O_1, ..., O_{i-1}),
\]

where \( \mathcal{O}^w_B \) is a set of beam candidate sequences at time step \( w \).

5. Experiments

List of Experiments. We conducted experiments to investigate the performance of our model. We ran our tests by increasing the number of points \( m \) in the input point set as \( m = 5, 10, 15, \) and \( 20 \). All methods use the same hyper-parameters for all experiments.

The first experiment determines the effect of input/output sequence ordering on model performance. For the proposed neural network model, random ordering and the proposed ordering method described in Section 4 are compared. Second, we compared the proposed model with other existing deep-learning-based DT generation methods. We compared our model to the Ptr-Net Vinyals et al. (2017) and M-Ptr-Net Guo et al. (2019) models. The method for multi-label classification was not explicitly mentioned when using M-Ptr-Net. For implementation, the cross-entropy loss was added after the sigmoid function, and then the top three were chosen from the output. There was no mention of input/output sequence ordering for the M-Ptr-Net. Therefore, the same output sequence ordering method mentioned in Vinyals et al. (2017) was used for the M-Ptr-Net.
Algorithm 1 Attention Score Function

Input: Step $i$, input sequence $P$, predicted output sequence $O^i = (O_1, ..., O_{i-1})$, attention score vector $u^i$, parameter $\gamma$
Output: New attention score $\bar{u}^i_j$

1: if $i \mod 3 \neq 1$ then
2: add $\gamma$ to a score of the end of sequence token
3: end if
4: if $i \mod 3 = 0$ then
5: for $j = 1, ..., m$ do
6: triangle $T = (P_{O_{i-2}}, P_{O_{i-1}}, P_O)$
7: if any point of $P$ is inside the circumcircle of $T$ then
8: $\bar{u}^i_j = u^i_j + \gamma$
9: else
10: $\bar{u}^i_j = u^i_j$
11: end if
12: end for
13: end if

In the experiment, we used two different decoders: greedy and beam search (BS). The greedy decoder selects the vertex with the highest probability at every decoding step [Nazari et al. 2018]. The BS decoder selects a sequence with the highest joint probability among a subset of beams within a beam width size. Our first two experiments employed greedy decoders, and a BS decoder was used for the third experiment. When using BS, a beam width of four was used in all tasks.

The fourth experiment indicates the solution time (prediction time) of the proposed model as $m$ increases. We investigated whether the proposed model can be practically used in terms of the solution time. All models were implemented using the Tensorflow 2.0 library, and experiments were conducted using a single Intel Xeon Gold 6152 CPU 2.10 GHz and a single Nvidia Titan V100 PCIe 32 GB GPU. The runtime can vary due to hardware and implementations.

Architecture and Hyper-parameters. We used virtually the same architecture throughout all experiments and datasets. Tanh was used as an activation function for the encoder and decoder of the models, and a single layer LSTM with 256 hidden units was used. The decoder attention mechanism also has 256 hidden units. The Adam optimizer was used [Kingma & Ba 2015] with a learning rate of 0.002, $\beta_1$ of 0.9, and $\beta_2$ of 0.999, and the Xavier method was employed for parameter initialization [Glorot & Bengio 2010]. Training was performed until the training loss converges. In Eq. (5), the $\gamma$ value was set to $-\infty$. We did not tune all hyper-parameters to reach the best performance.

Datasets. We generated 1M training example samples (point sets) of each task. Of the total sample data, 90% of the data were used as the training dataset, and the rest were used for testing. In all cases, we sampled from a uniform distribution in $[0, 1] \times [0, 1]$. 
For a given point set, the ground truth data of DT were obtained using MATLAB. We released all datasets at https://github.com/hunni10/DelaunayDataset.

**Performance Measure.** We evaluated the performance of the proposed neural network model using four different metrics. The first metric is the triangle coverage (TC), which is defined as the ratio of triangles that the model predicts correctly. For two triangular elements consisting of three vertices, even if the permutation of the vertices is different, it is considered as the same triangle. For example, \((1, 2, 3)\) and \((2, 3, 1)\) represent the same triangle. Additionally, any permutation of the triangles in the output sequence represents the same triangulation. We assumed that the total number of (testing) samples is \(S\). We let \(\hat{O}_i\) and \(O_i\) be the output sequence of the \(i\)th sample of the predictions and the ground truth, respectively. The second metric is accuracy (ACC), which is defined as follows:

\[
\text{ACC} = \frac{\sum_{i=1}^{S} S_i}{S},
\]

where \(S_i = 1\) if \(\hat{O}_i\) and \(O_i\) represent the same triangulation. Otherwise, \(S_i = 0\). For example, we assume two testing samples each consist of five triangles and that ground truth also has five triangles. For one testing sample, if the model predicts the same triangulation as the ground truth, and for another testing sample, if only four out of five triangles are correctly predicted, then the TC is 0.9, and ACC is 0.5, respectively.

It is also essential to determine whether the number of triangles in the triangulation predicted by the model matches the actual number of triangles in the ground truth. The third metric measures the similarity of the number of triangles predicted by the model to the actual number of triangles in the ground truth. We let \(\hat{t}_i\) and \(t_i\) be the number of triangles of the predictions and the ground truth of the \(i\)th sample, respectively. The third metric, the triangle count accuracy (TCA), is defined as follows:

\[
\text{TCA} = \frac{\sum_{i=1}^{S} T_i}{S},
\]

where \(T_i = 1\) if \(t_i\) and \(\hat{t}_i\). Otherwise it is zero. In practice, even the length of the output sequence predicted by the model may not be a multiple of three. If the length of the output sequence \(\hat{O}_i\) is not a multiple of three, the output exceeding a multiple of three is excluded when calculating \(\hat{t}_i\) because it cannot form triangles during triangulation. For example, if \(\hat{O}_i = (O_1, O_2, O_3, O_4, O_5)\), then \(O_4\) and \(O_5\) are excluded.

The final metric is the DT rate (DTR), which measures how well each triangle predicted by the model satisfies the Delaunay condition. It is the ratio of triangles that satisfy the Delaunay condition among the triangles predicted by the model.

All four metrics have values between 0% and 100%, and the values closer to 100% indicate better results. In terms of solution quality, both TC and ACC are the most critical metrics for evaluating the performance of the model and should be considered together. This is because the accuracy metric is extremely strict (especially for large \(m\)) in that the accuracy is zero for one sample if even one triangle among the triangles predicted by the model is different from the ground truth.
6. Results

6.1. Experiment 1: Effect of Sequence Ordering

Figure 6 illustrates the comparison results of the proposed input/output sequence ordering and random ordering. Both methods use the same proposed model, and the only difference is whether the dataset is sorted or not. The performance is much better in all metrics when the sequence was sorted using the proposed ordering method for all \( m \) values. This is consistent with the results of previous work in which the sequence order dramatically influences the performance of the Ptr-Net-based models [2, 13]. Sequence ordering must be performed because performance is greatly improved by simply changing the sequence order of the dataset without making any changes to the model.

As the \( m \) value increases, the sorted and random ordering performance gap is much more significant in both TC and ACC metrics. For \( m = 5 \), the TC and ACC of the sorted ordering are 99.30% and 96.46%, respectively, whereas the TC and ACC of the random ordering are 97.10% and 87.79%. When the sequences are not sorted in the case of \( m = 20 \), TC is 76.61%, and ACC is 0.06%. If the sequences are sorted, TC and ACC are 97.69% and 55.16%, respectively.

Interestingly, sorting the input/output sequence also has a significant effect on the TCA. In sorting the input/output sequence for all \( m \) values, the number of triangles predicted by the model is more consistent with the actual number of triangles of the ground truth. No significant difference exists between the DTR ratio for all \( m \) values, whether the sequences were sorted or not.

Figure 6 Performance of the proposed input/output sequence ordering compared to random ordering using four metrics: triangle coverage (TC), accuracy (ACC), triangle count accuracy (TCA), and Delaunay triangle rate (DTR).
6.2. Experiment 2: Comparison with Previous Work

Figure 7 depicts the results of the proposed model compared with the existing deep learning-based DT generation methods according to \( m \) values. We observe that the performance of the proposed model outperforms other methods for all \( m \) values in the TC, ACC, and DTR. This performance is primarily for two reasons. First, the model can learn the point-to-point relationship through self-attention in the encoder. Second, the attention score function in the decoder provides a high penalty function to candidates who do not satisfy the Delaunay condition. In particular, the performance gap between the proposed model and other methods increases as the value of \( m \) increases. Specifically, the proposed model achieves TC = 98.54\% and ACC = 82.15\% when \( m \) is 10, whereas Ptr-Net achieves TC = 94.15\% and ACC = 62.71\%, and M-Ptr-Net achieves TC = 86.98\% and ACC = 38.14\%. When the value of \( m \) is 20, the proposed model achieves TC = 97.69\% and ACC = 55.16\%, whereas Ptr-Net achieves TC = 92.42\% and ACC = 24.36\%, and M-Ptr-Net achieves TC = 67.44\% and ACC = 0.39\%.

We observe that especially for large \( m \) values, the length of the output sequence predicted by the Ptr-Net is slightly longer than that of the ground truth in many cases. In these cases, the TCA may appear to be high because it excludes outputs exceeding a multiple of three from the output sequence. Even if the predicted sequence length is not exactly correct, only the length of the valid sequence, which corresponds to the number of valid triangles, is only considered.

Among the compared models, the M-Ptr-Net has the worst performance for all metrics. In particular, the ACC becomes zero when \( m = 20 \). Unlike the Ptr-Net, the M-Ptr-Net chooses three points simultaneously, so the model does not sufficiently learn the relationship among the three points to be selected. Figure 8 displays one example of the predicted triangulation of each model and the ground truth when \( m = 15 \). The blue elements represent elements in the ground truth, and red elements represent elements not in the ground truth. In this example, only the proposed model exhibits the same triangulation as the ground truth, but other models fail to predict the ground truth. We only demonstrate one example, but the proposed model performance is superior to other existing models in most testing samples.

6.3. Experiment 3: Effect of Beam Search Decoder

Figure 9 shows the proposed model results when the BS decoder (BS = 4) is used instead of the greedy decoder. In the previous two experiments, the greedy decoder was used. We observe that the BS decoder significantly improves the performance compared to the greedy decoder in all four metrics. In particular, the effect of using the BS decoder increases as the \( m \) value increases. For example, the performance gap between the greedy and BS decoder is only 0.03\% for the TC metric when \( m = 5 \), and it increases to 0.59\% when \( m = 20 \). For the ACC metric, the performance gap is 0.12\% when \( m = 5 \), but it becomes 6.07\% when \( m = 20 \). If the BS decoder is used, the performance can be improved by continuously tracking the most probable candidate points at the expense of prediction time. If the BS decoder is used together with the proposed attention score function, the number of candidates of the first two steps (points) increases. Therefore, using the proposed attention score function is more effective because it offers more chances to determine the correct triangulation in the
Figure 7 Performance of the proposed model compared to the previous work using four metrics: triangle coverage (TC), accuracy (ACC), triangle count accuracy (TCA), and Delaunay triangle rate (DTR).

Figure 10 presents one example of predictions of each model with the BS decoder and the ground truth when \( m = 20 \). Only the proposed model can predict the triangulation of the ground truth correctly.

6.4. Experiment 4: Solution Time

Figure 11 presents the average solution (prediction) time for the model to predict one testing sample. Employing the BS decoder is a trade-off in terms of performance and computational time. When the BS decoder is used, the performance improves compared to the greedy decoder, but the solution time increases. Our results indicate that the performance improves significantly with only a slight increase in solution time. The solution time for both the greedy and BS decoders increases almost linearly as \( m \) increases. When \( m = 20 \), the solution time is 1 s for greedy and 2 s for BS decoders. Among the compared methods, the M-Ptr-Net has the worst performance, but the solution time is the fastest because it uses multiple pointers. The number of steps in the M-Ptr-Net decoder is fewer than other models because it predicts three points simultaneously in one step in the output sequence. The proposed model with the BS decoder is the slowest, but the difference is not large.

7. Discussion

The proposed model is based on supervised learning and therefore has the limitations of supervised learning. It requires numerous high-quality labeled data for learning, and the performance of the model depends on such labeled data. We plan to apply
Figure 8 Predictions examples for each model with the greedy decoder and the ground truth when \( m = 15 \). Blue elements represent elements in the ground truth, and red elements represent elements not in the ground truth. Only the proposed model predicts the ground truth.

reinforcement learning as a future work for the DT generation problem. The proposed model outperforms other existing deep-learning-based approaches, but it still fails in some cases especially for large \( m \) values. We present several cases of failure of the predictions of the proposed model. First, the edge consisting of the first two predicted points is an edge that is not in the ground truth. For this case, the proposed attention score function cannot exclude these points from the candidates because it evaluates the candidate points every three steps. We observe that these failure cases often occur when the testing sample points have similar or identical values in the \( x \)-axis. For these cases, the model learning performance can deteriorate because the input sequence is lexicographically ordered. The model also fails to predict the ground truth when it predicts the same triangles multiple times, especially for large \( m \) values. In addition, the number of triangles predicted by the model is sometimes more or less than the number of triangles in the ground truth.

Figure 12 depicts two cases in which the model prediction fails. In the first case, the first edge (red) predicted by the model is not in the ground truth, as described earlier. It creates an initial triangle that is not in the ground truth. In the second case, the model predicts the same triangles (hatched element) twice, but not the triangle in the ground truth (white element). Future work will also study how to solve these cases in the decoder.

8. Conclusions

We propose a novel approach for learning DT using new attention mechanisms based on self-attention and domain knowledge. The experimental results reveal that the proposed model exhibits better performance in all metrics than the existing deep-learning-based DT generation methods and presents the possibility of using a deep-learning-based approach for DT generation. Specifically, when \( m = 10 \), the proposed model achieves 98.79% triangle coverage and 84.10% accuracy. In terms of the solution time, the computational time used in practice is not long. Our experimental results reveal that the performance improvement is significant when the input/output sequence is sorted using the proposed method. We also observe that the model learns
the topological relationship between points much better using self-attention in the encoder. Significantly, the effect of using self-attention is more critical when the input sequence length becomes longer. A significant performance improvement is obtained in the decoder using the proposed penalty-based attention score function, which excludes candidate points that do not satisfy the Delaunay condition.

The proposed penalty-based attention score function is robust in that it can be applied to other geometric-based combinatorial optimization problems. As future work, we plan to apply the proposed attention score function to other geometry-based combinatorial optimization problems, such as convex hull and TSP problems. We also plan to apply the multi-head attention technique used in the transformer model to the DT generation problem.

**CRediT authorship contribution statement**

**Jaeseung Lee:** Software, Methodology, Investigation, **Woojin Choi:** Software, Investigation, **Jibum Kim:** Writing - Methodology, Supervision, Review & Editing

**Declaration of Competing Interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.
**Figure 10** Example of predictions of each model using the greedy and beam search (BS) decoders when \(m = 20\). Blue elements represent elements in the ground truth, and red elements represent elements not in the ground truth. The dotted element is a replicated element. Only the proposed model (BS) predicts the ground truth.

**Figure 11** Solution time (sec) with respect to the number of points (\(m\)).

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Figure 12 Two examples of when the model prediction fails. (a) the first edge predicted by the model is not included in the ground truth. (b) The duplicated triangle (dotted) is predicted by the model.

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