Voronoi Graph Neural Networks

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Machine Learning Overview

- Point Estimation
- Generative Models
  - Beta-Binomial
  - Dirichlet Multinomial
  - Naive Bayes
- Classifiers
  - Logistic Regression
  - Softmax Regression
- Dimensionality Reduction
  - Singular Value Decompositions
- Mixture Models
- Kernels and Sparse Vector Machines
- Hyperparameters

Voronoi Diagrams and Tesselations

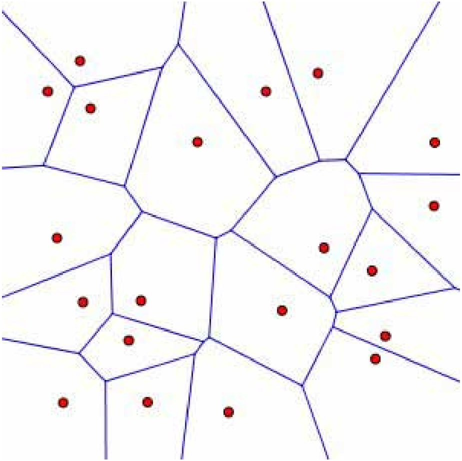

Figure: Voronoi Diagram

Neural Networks

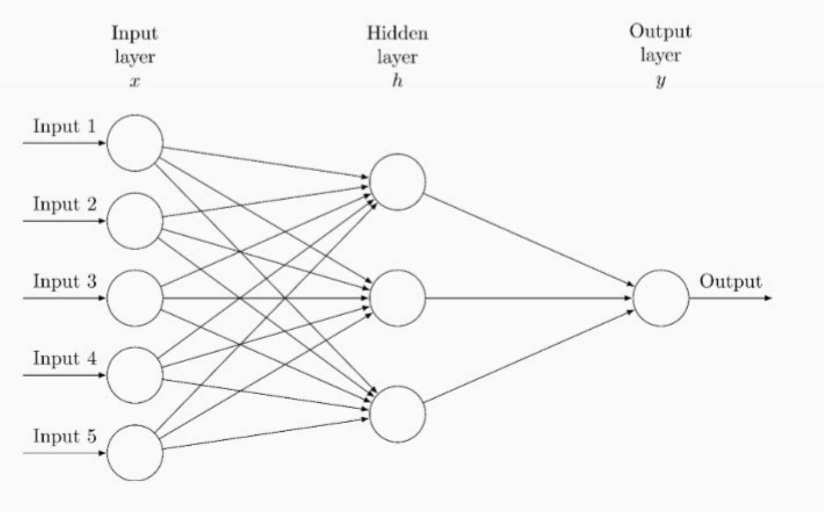

Figure: The layers in a neural network

Graph Neural Networks

- Combine graph node information with neighbouring nodes
- Aggregating the information
- Feeding it into a neural network
- Non-linear activation function

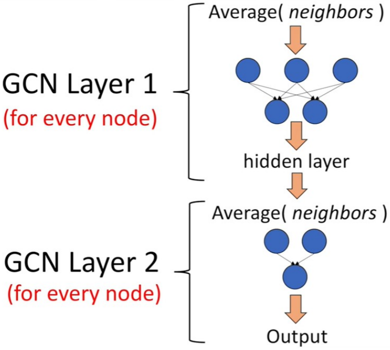

Figure: GCN Layer Outline

Voronata

From Proteins to Voronoi:

- Computing the Voronoi diagrams of given complex 3D shapes representing biological macromolecules (proteins and RNA)
- Using van der Waals radii instead of proteins or nucleic acid atoms directly

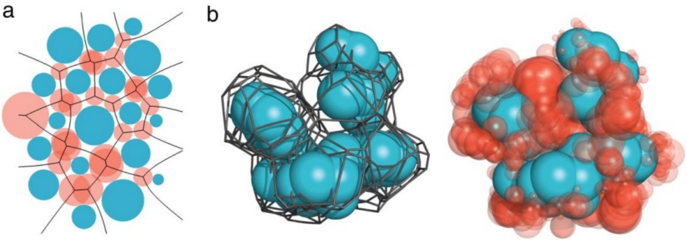

Figure: Voronoi cells and corresponding empty tangent spheres and their vertices.

Algorithm

- Two balls are considered to be neighbours if their Voronoi cells intersect.
- The intersection of four cells is a Voronoi vertex

Procedures

- Find valid quadruples of spheres
- 4 balls with at least one tangent non-intersecting sphere
- Gift-wrapping algorithm
- Find a valid neighbour of a triple in a halfspace
- Select group centers in a bounding spheres hierarchy
- Algorithm takes advantage of macromolecular structures; majority of valid atom triples have two tangent planes

VoroCNN

- Using Voronata
- Represent interatomic interactions as a Voronoi tessellation of protein atoms
  - Voronoi cell = atom
  - Voronoi cell face = interatomic contact
- Weighted unordered multi-graph representation
- Key: implicitly retains spatial relationship of atoms
- 3D tessellation can be reduced to a graph without significant information loss
- Interaction graphs used to construct a trainable neural network

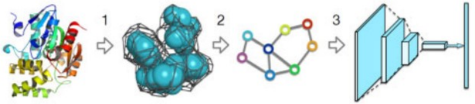

Figure: VoroCNN methods using Voronata

Nodes:

- Represent atoms in protein structure
- Each node has a vector of features describing the atom using one-hot encoding

Edges

- Contact Edges
  - Represent spatial relationship b/w atoms
  - Two atoms are in contact if their Voronoi cells have non-zero contact surface
- Covalent Edges
  - Correspond to covalent bonds between atoms in contact
- Weighted matrices equal to the respective contact surface of atoms if there is a contact/covalent edge, and 0 otherwise

- Convolutional layer contains trainable tensors
- Transformed feature matrix combining neighboring graph node information
- Non-linear activation function, ELU
- Downsampling operations
  - Reduce data representation and extract hierarchical features
  - VoroCNN uses prior topology and structure information for downsampling
  - Atoms are grouped into residues; primitive covalent edges representing the peptide chain of the protein

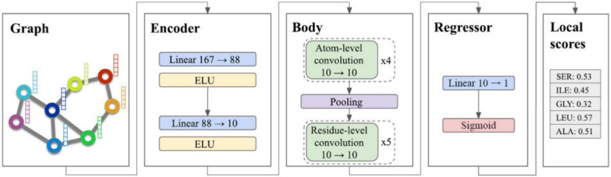

Figure: Architecture of the VoroCNN network

Neural Network Architecture:

- Encoder
  - Two linear layers with ELU activation function
  - Reduces the size of the feature vectors
- Body
  - Contains aforementioned convolutional layers and graph downsampling
- Regressor
  - Predicts local CAD scores, using MSE loss function, Adam optimizer and L2 regularization

Tag-VGNN

- Tactile Voronoi Graph Neural Network to achieve tactile pose estimation
- GNN used to model distribution between shear motions of tactile markers
- Voronoi diagram adds contact depth-related features
- 28% increase in pose estimation compared to vanilla GNN

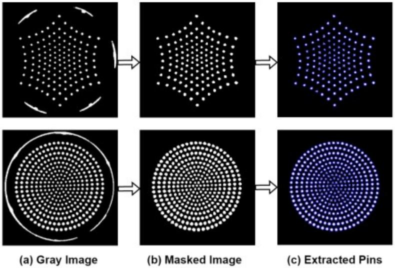

Figure: Tactile data preprocessing

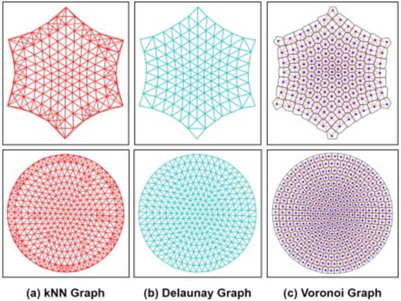

Figure: Different graph representations

Conclusion

Key Takeaways:

- Voronoi diagrams and tessellations must be constructed in a manner that maintains the structure and information of the data
- Voronoi diagram constructions are heavily dependent on the context of the data and the constrictions that exist

Next steps:

- Identifying dataset for initial testing of performance
- Deciding Voronoi computation method
- Applications and use cases
- Expected results