Lecture 10
CNNs on Graphs

CMSC 35246: Deep Learning

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Two Scenarios

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  - Scenario 1: Each data point lives in $\mathbb{R}^d$, but the dataset has an underlying graph structure

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  - Scenario 1: Each data point lives in $\mathbb{R}^d$, but the dataset has an underlying graph structure
    - Each coordinate is a value associated with a vertex of underlying graph
    - For images: The underlying graph is always a grid of fixed dimensions
  - Scenario 2: Each data point is itself a graph (Example regression task: Molecules as input, boiling points as output)
    - Each graph can be of different size
    - Sub-problem: Given a graph $\mathcal{G}$, find an embedding $\phi : \mathcal{G} \to \mathbb{R}^p$

Scenario 1

CNNs on data in irregular domains

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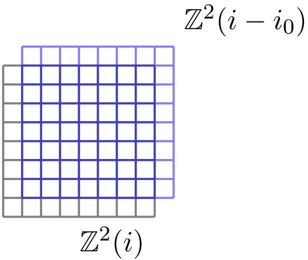
  - Translation structure (allowing use of filters)
  - Metric on the grid (allows compactly supported filters)
  - Multiscale structure of the grid (allows subsampling)

CNNs on Grids



- The translation group acts on $\mathbb{Z}^2$
- We are able to exploit this symmetry of the grid in CNNs

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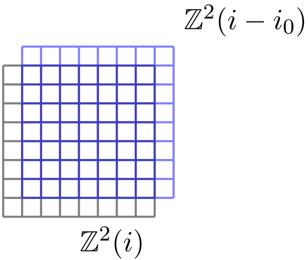

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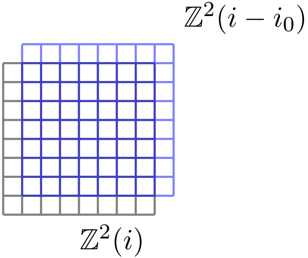

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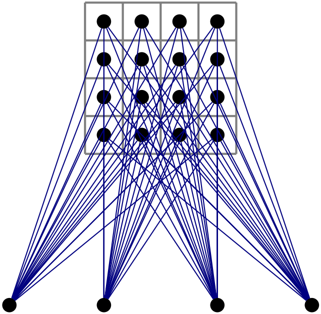

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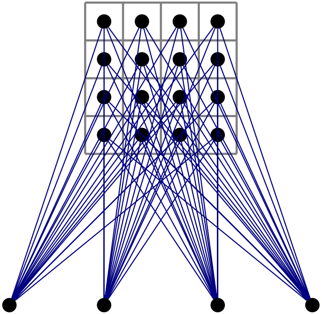

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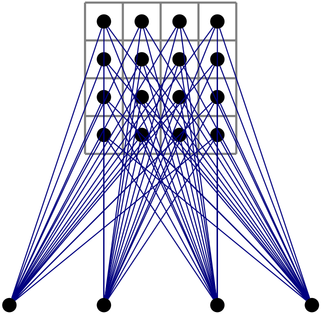

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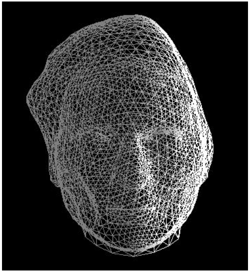
- With k filters, each with support S we have $O(kS)$ (independent of n)
- Using multiscale nature, we can pool, and reduce the number of parameters further

Data on Irregular Domains

- Often we can have *structured* data defined over coordinates that does not enjoy any of these properties



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- More: Social network data, protein interaction networks etc.

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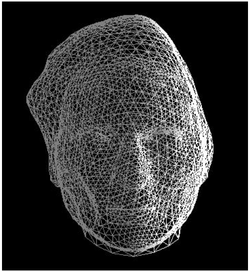
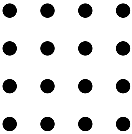


- Example: 3-D mesh data (each coordinate might be surface tension)
- More: Social network data, protein interaction networks etc.
- In each case we again have n coordinates but which don't live on a regular grid

Figure source: Eurocom Face Modeling

Functions on Graphs



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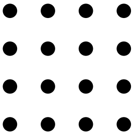

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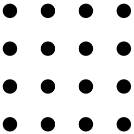

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- $\mathcal{G}$ just happens to be a grid graph with strong local structure which makes CNNs useful
- In general we can have signals defined over a general graph:

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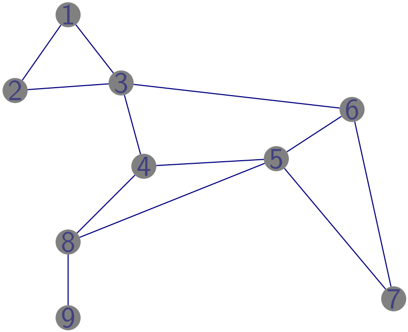

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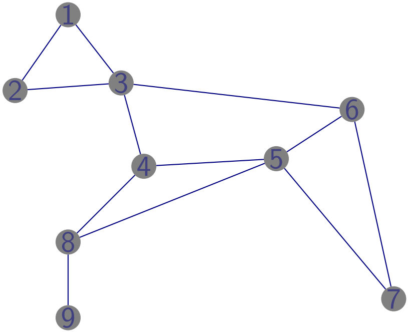

- Ω is the vertex set (input coordinates), $W_{i,j}$ the similarity between any two coordinates i and j
- Note: $W_{i,j}$ is similarity between coordinates, not datapoints

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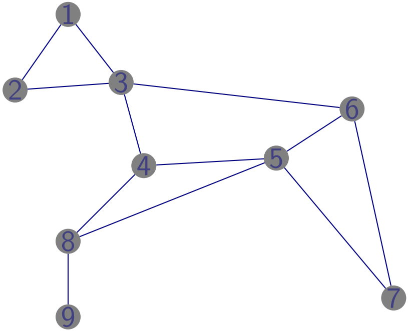

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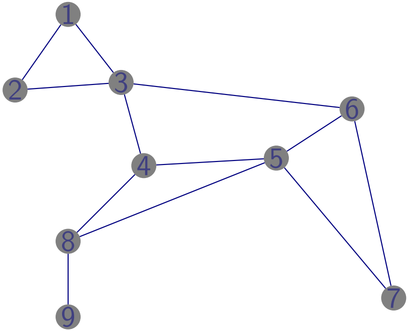

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- If unknown: Need to estimate it from training data

Spatial Construction

Locally Connected Networks

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- Number of parameters: $O(Sn)$ (S is average neighbhorhood size)

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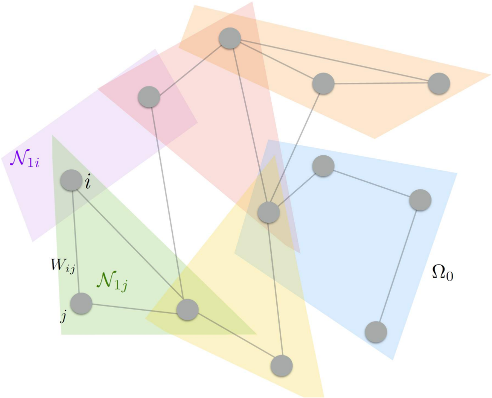
Locally Connected Networks: In Pictures



- Level 1 clustering

This and next few illustrations are by Joan Bruna

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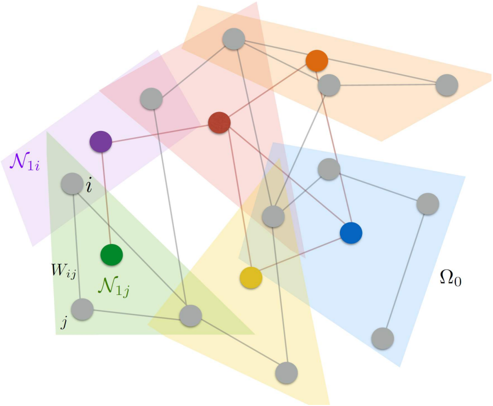

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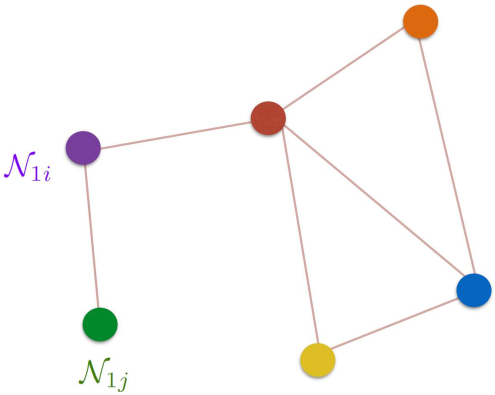

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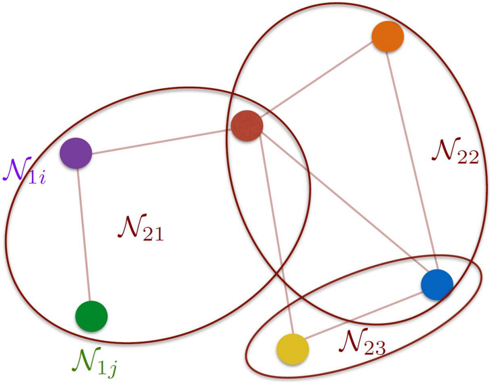

- Level 2 clustering

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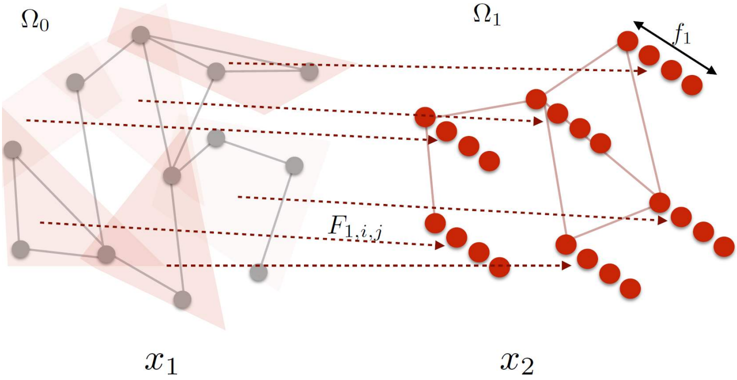

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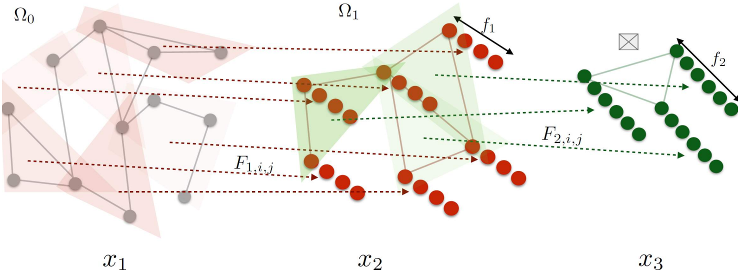

- Multiple Feature maps: Level 2

Spectral Construction

Spectral Networks

Quick Digression: The Graph Laplacian

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- Let $U = [u_1, \ldots, u_d]$ be the eigenvectors of L

Graph Convolution in Frequency Domain

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- Learning filters on a graph $\implies$ learning spectral weights:

$$x *_{\mathcal{G}} g = U^T(diag(w_g)Ux) \text{with } w_g = (w_1, \dots, w_d)$$

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- Notice that g has support over all vertices
- But we want filters that are local
- Observation: Smoothness in frequency domain $\implies$ spatial decay
- Solution: Consider a smoothing kernel $\mathcal{K} \in \mathbb{R}^{d \times d_0}$ and search for multipliers:

$$w_g = \mathcal{K} \tilde{w}_g$$

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What if Graph Structure is unknown?

- Estimate it from data:
- Method 1: **Unsupervised**
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  - Then compute $W_{i,j} = \exp^{-\frac{d(i,j)}{\sigma^2}}$

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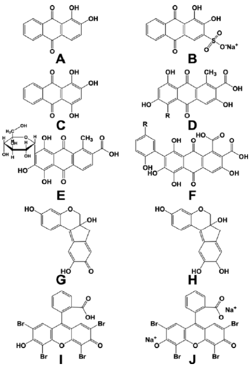
  - Use Gaussian kernel as before to get $W_{i,j}$

Scenario 2

Learning Embeddings of Graphs

Example Task: Regression



- Input: Organic Compounds (graphs)
- Output: Boiling point

Graph Embedding: Simple Algorithm

Algorithm 1 Generation of embedding

Require: $G = (V, E)$, radius δ, Hidden Weights: $H_1^1, \ldots, H_l^\delta$, Output Weights: $W_1, \ldots, W_\delta$

Initialize: Embedding $\phi \leftarrow 0$ **Initialize:** For every vertex $\mathbf{r}_v \leftarrow \Psi(v)$ (local vertex features)

```
for all L = 1 to δ (for every layer) do
    for each vertex v in graph do
        r_1, ..., r_N = neighbors(v)
        v ← r_v + Σ_{i=1}^{N} r_i
        r_v ← σ(v H_L^N)
        i ← softmax(r_v W_L)
        Update: φ ← φ + i
    end for
end for
Output embedding φ
```