Directing neural networks to learn graph abstractions

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2018 Summer Internship

Directing neural networks to learn graph abstractions

1. Classical methods for image classification: limitations and our motivation

2. Directing the neural network to learn graph abstractions

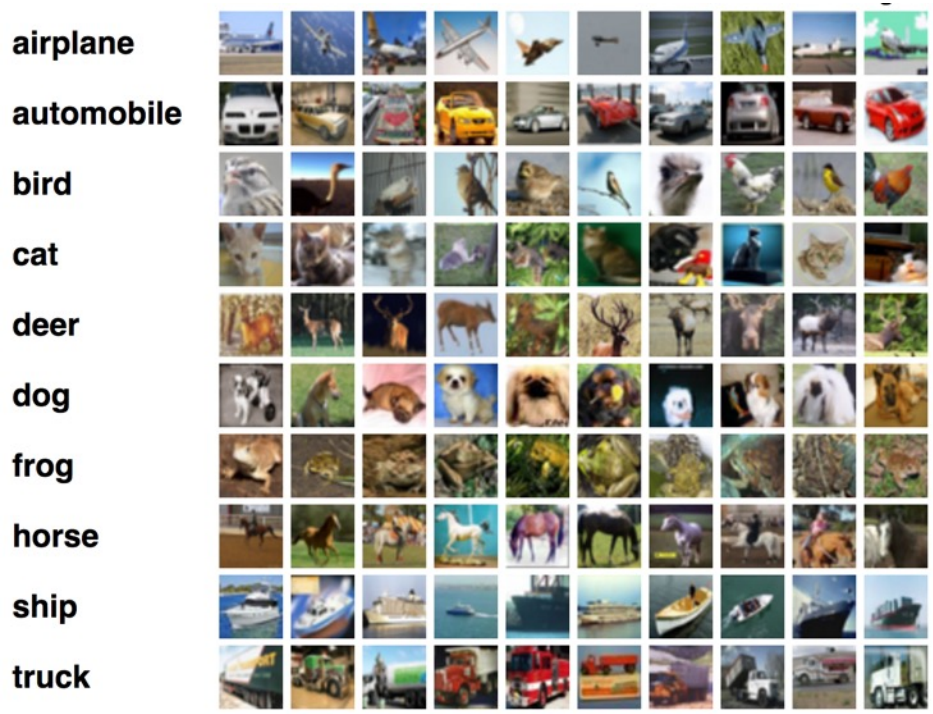
3. Two sub-problems when dealing with graphs

4. Preliminary results

Image Classification

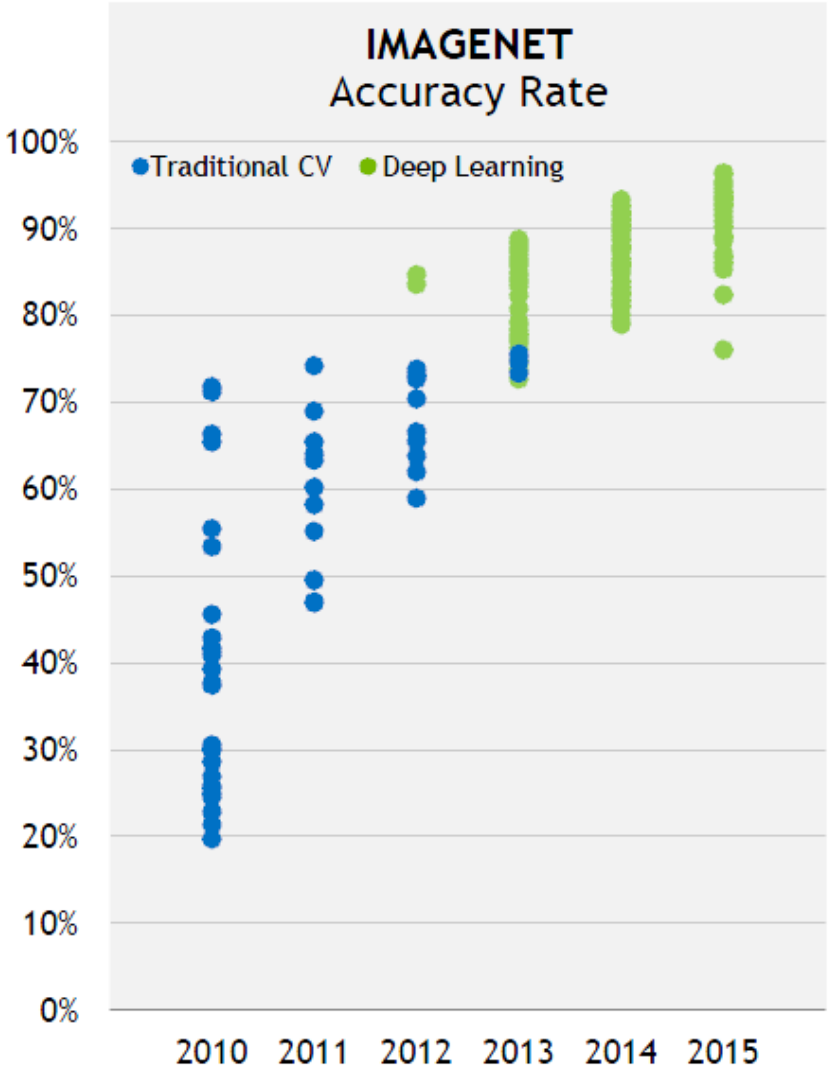
Training images

Test case



Airplane : 3 %
Automobile : 10 %
…
Truck : 85 %

Success = higher accuracy



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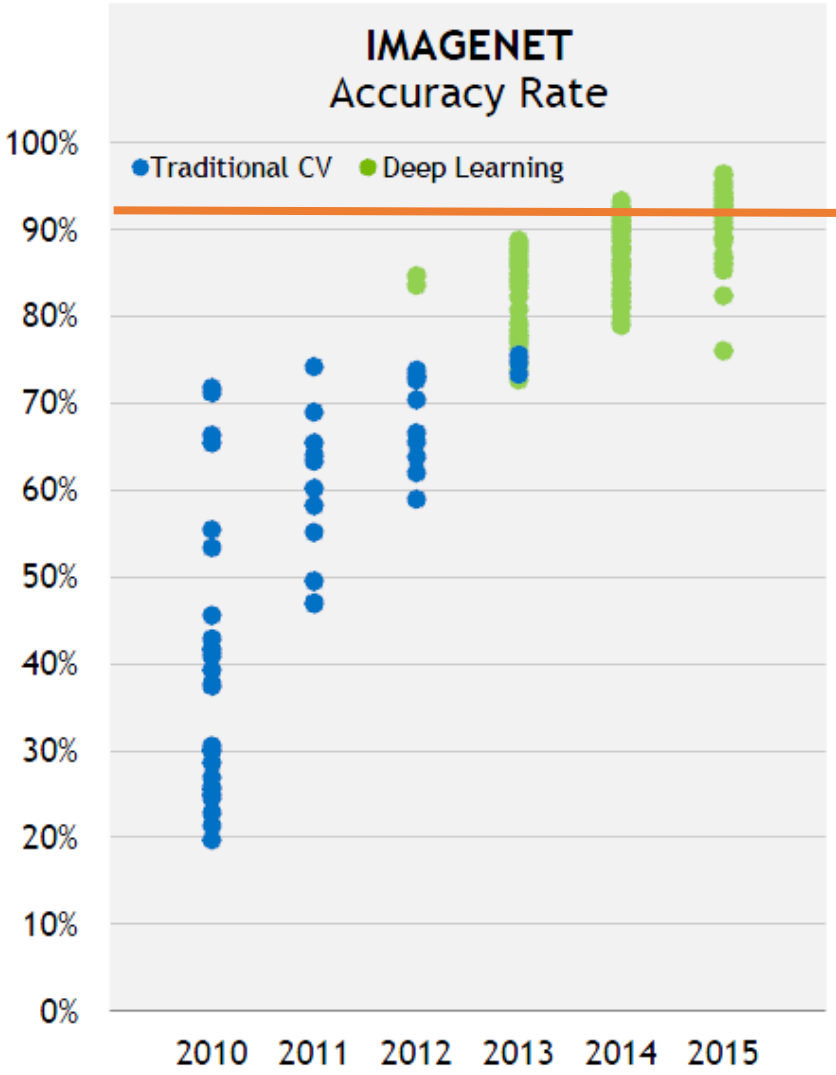


Human performance = 92.9%

Today:
Error of ~2 % and ImageNet problem is considered solved

Convolutional Neural Networks

- The key operation: Convolution

Input Image

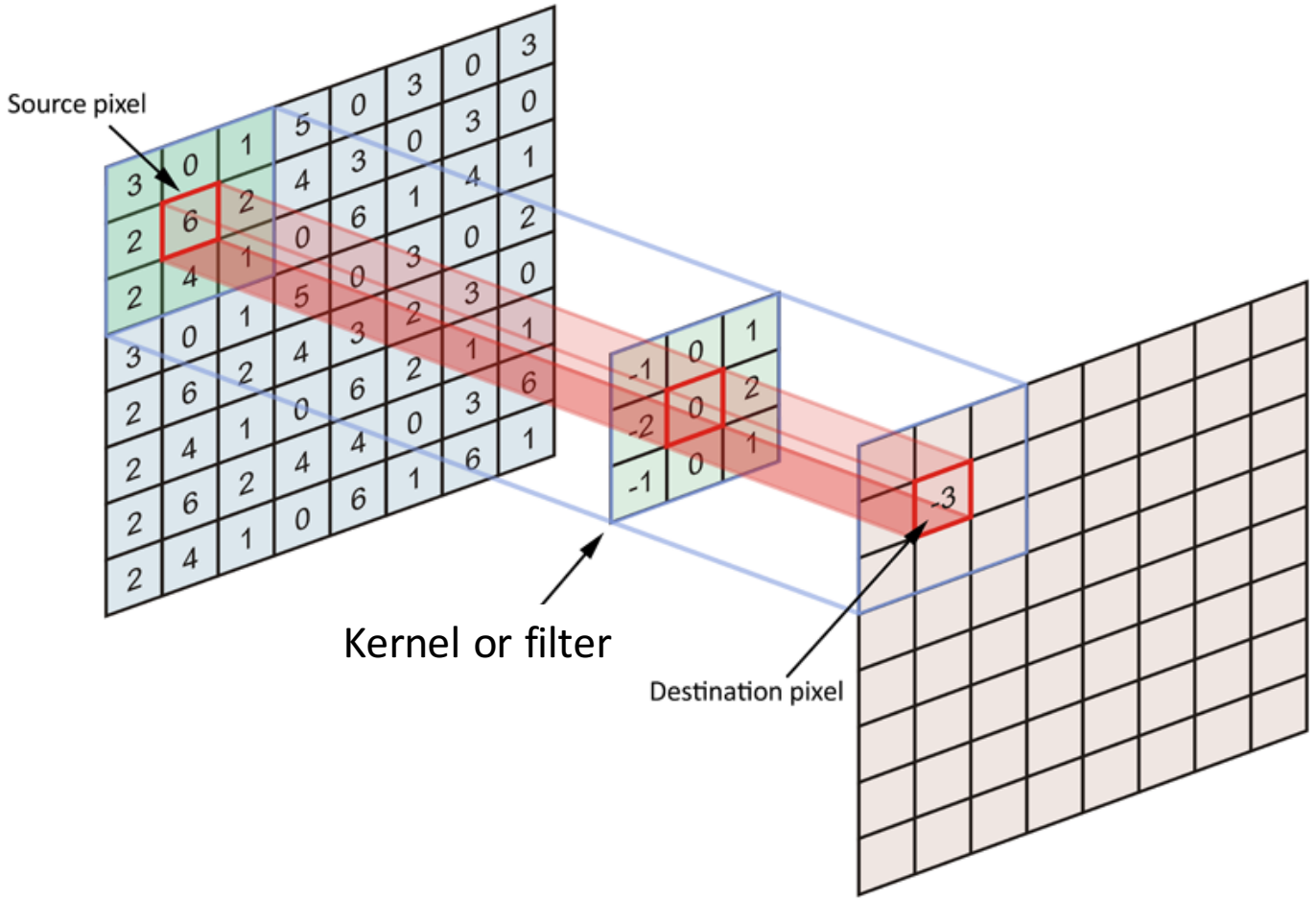
Convolution Kernel

$$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$$

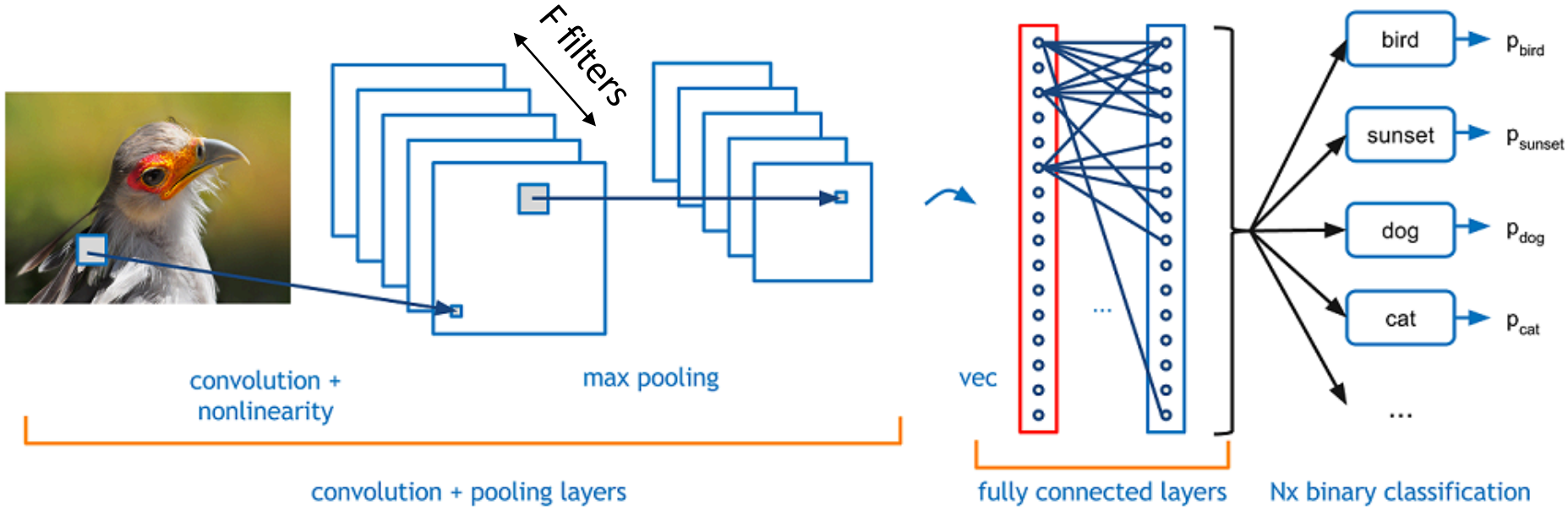
Output Image

Convolutional Neural Networks

- The numbers in the kernel are `learnt'



CNN architecture



So what does a CNN learn?

- A bunch of kernel weights

Input Image

Convolution Kernel

$$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$$

Output Image

CNN learns several such kernel matrices

A simplified picture

Image

Convolution Neural Net

Learnt parameters:

- *kernel 1*
- *kernel 2*
- *…*
- *…*
- *Fully connected layer weights*

Classification label

Airplane : 3 %
Automobile : 10 %
…
Truck : 85 %

Emerging concerns with CNNs

1. Requirement of large training datasets

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2. Not extremely interpretable

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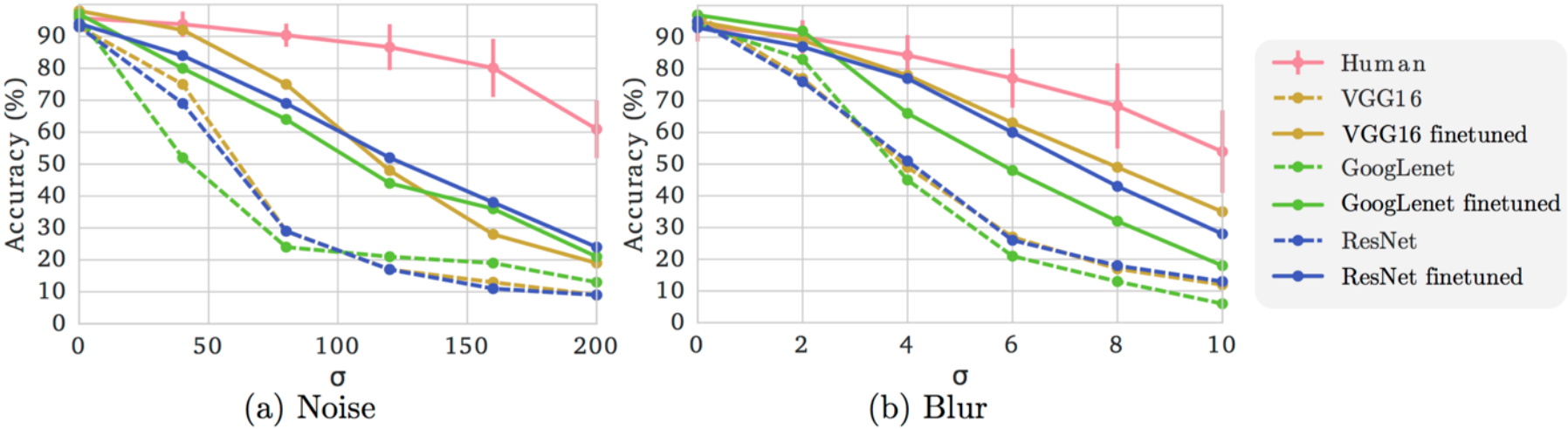
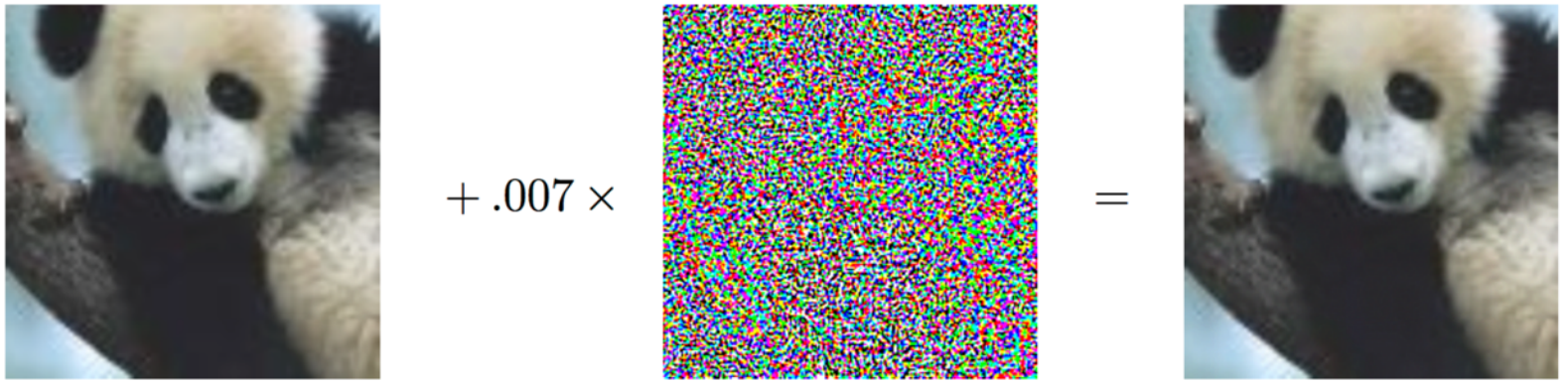
3. Robustness to perturbations



[Dodge and Karam 2017]

Emerging concerns with CNNs

1. Requirement of large training datasets
2. Not extremely interpretable
3. Robustness to perturbations



[Goodfellow et. al. 2015]

Emerging concerns with CNNs

1. Requirement of large training datasets
2. Not extremely interpretable
3. Robustness to perturbations

[Eykhlot et. al. 2018]

Key idea 1

Directing the neural network to learn an appropriate abstraction for the problem can help alleviate some of these concerns

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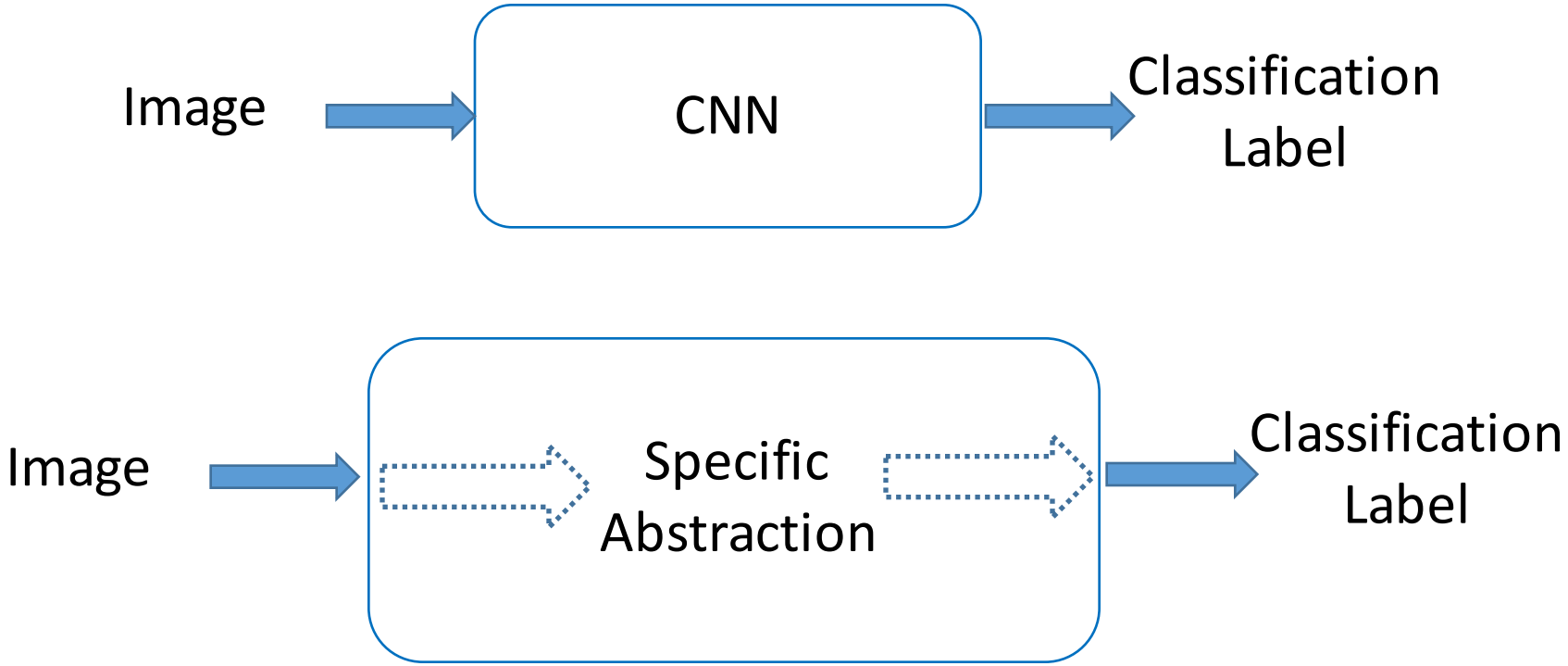
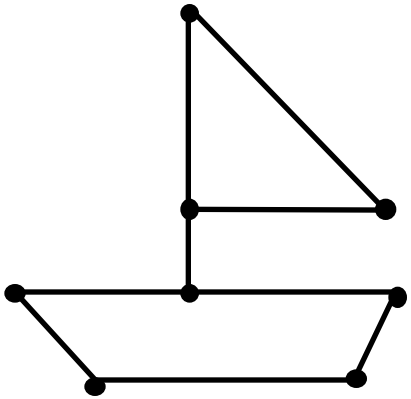
Directing the neural network to learn an appropriate abstraction for the problem can help alleviate some of these concerns



Key idea 2

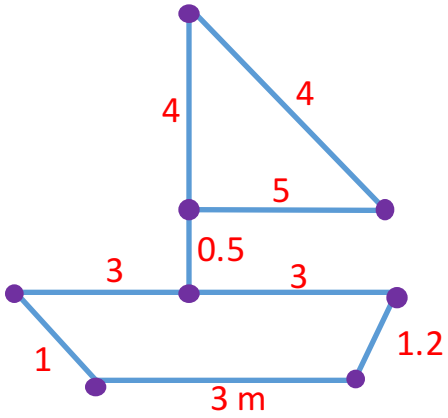
A graph is potentially a good abstraction for many classification problems



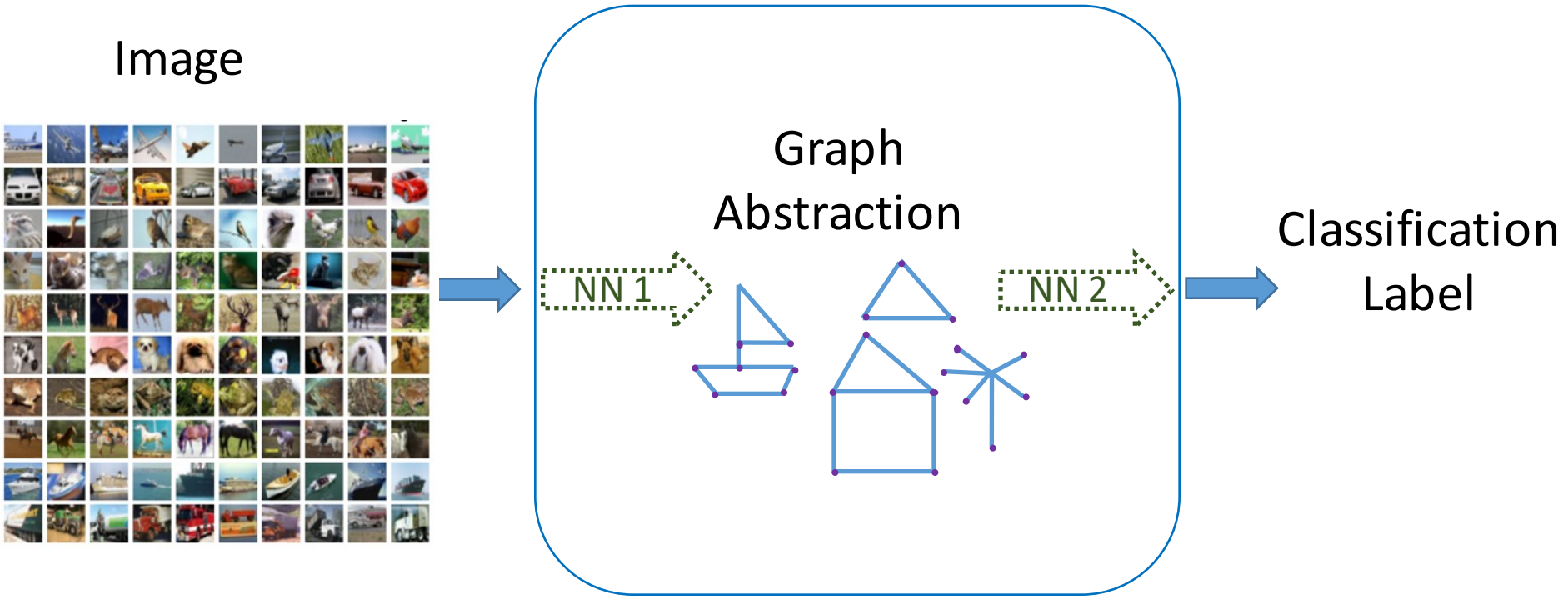
Graph as an abstraction

Can capture

- geometry (relative size) : edge weights
- Topology (shape) : edge connections
- Other features (like color) : nodal values



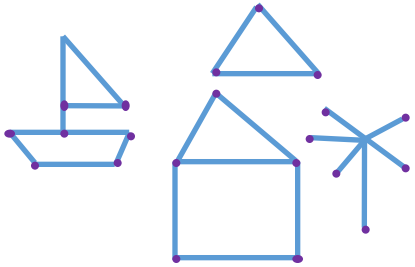
Our proposed architecture



NN1 : Image input, graph output
NN2 : Graph input, label output

The two sub-problems

Image → NN 1 → Graph Abstraction → NN 2 → Classification Label



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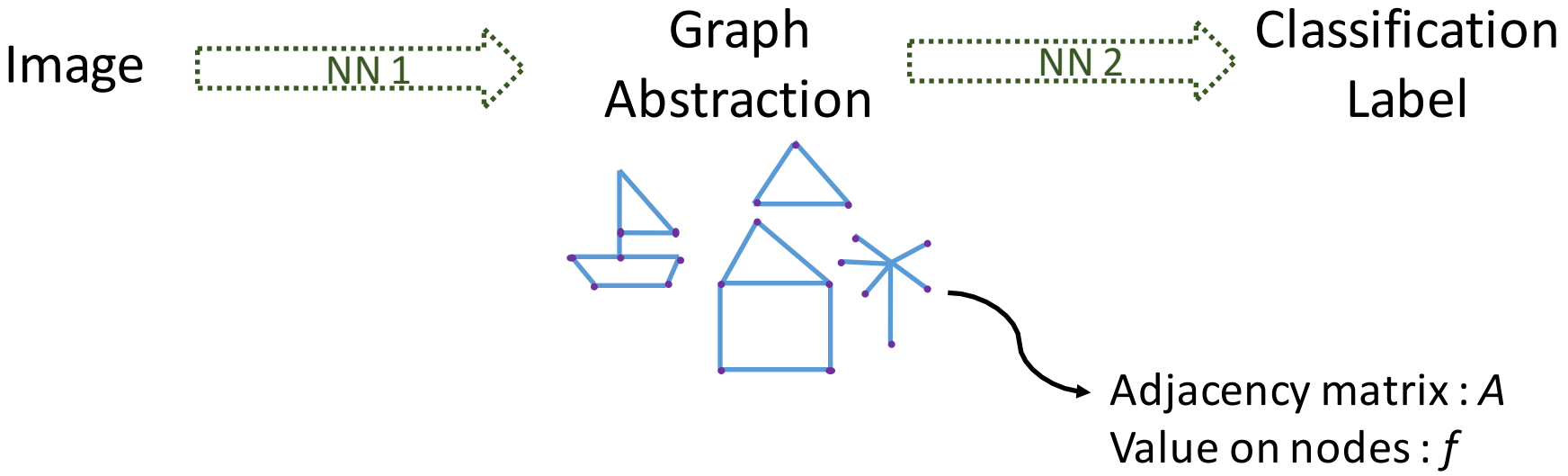

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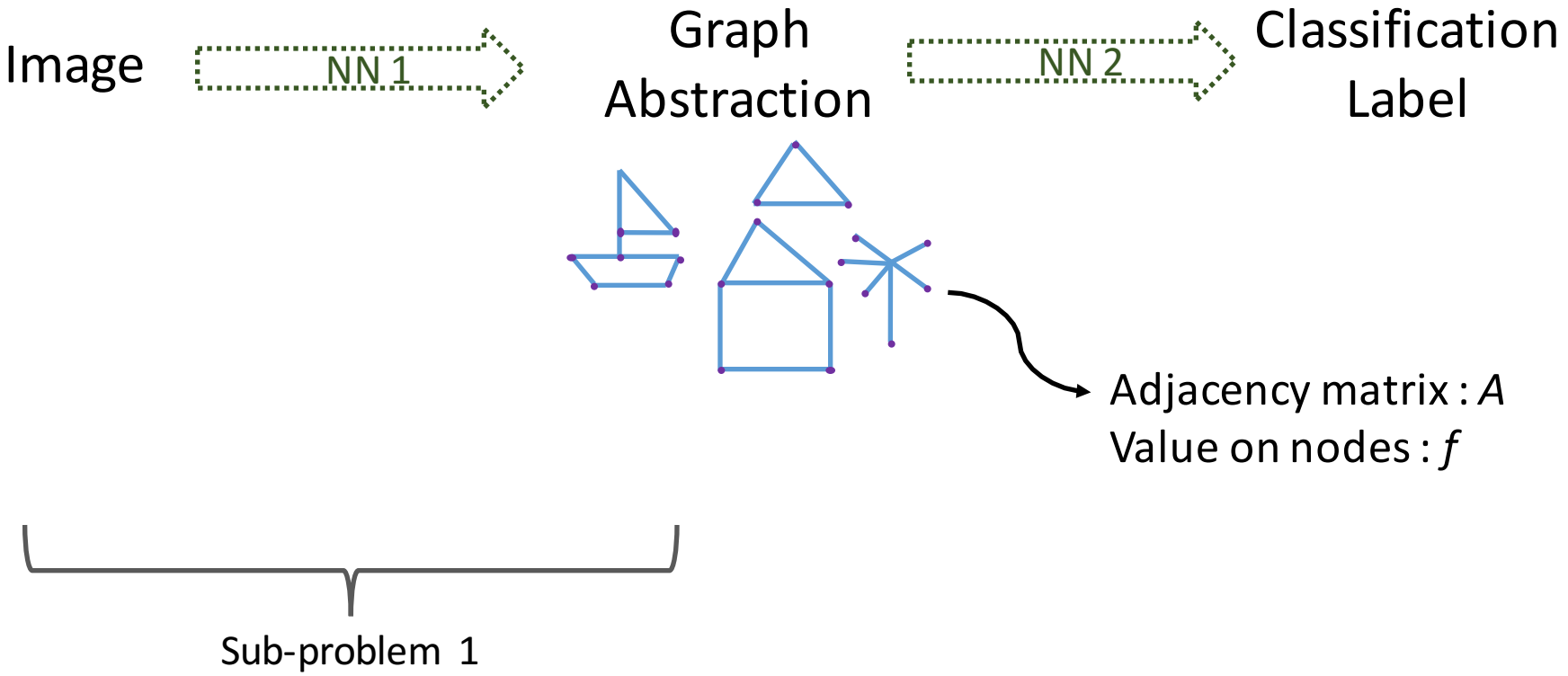
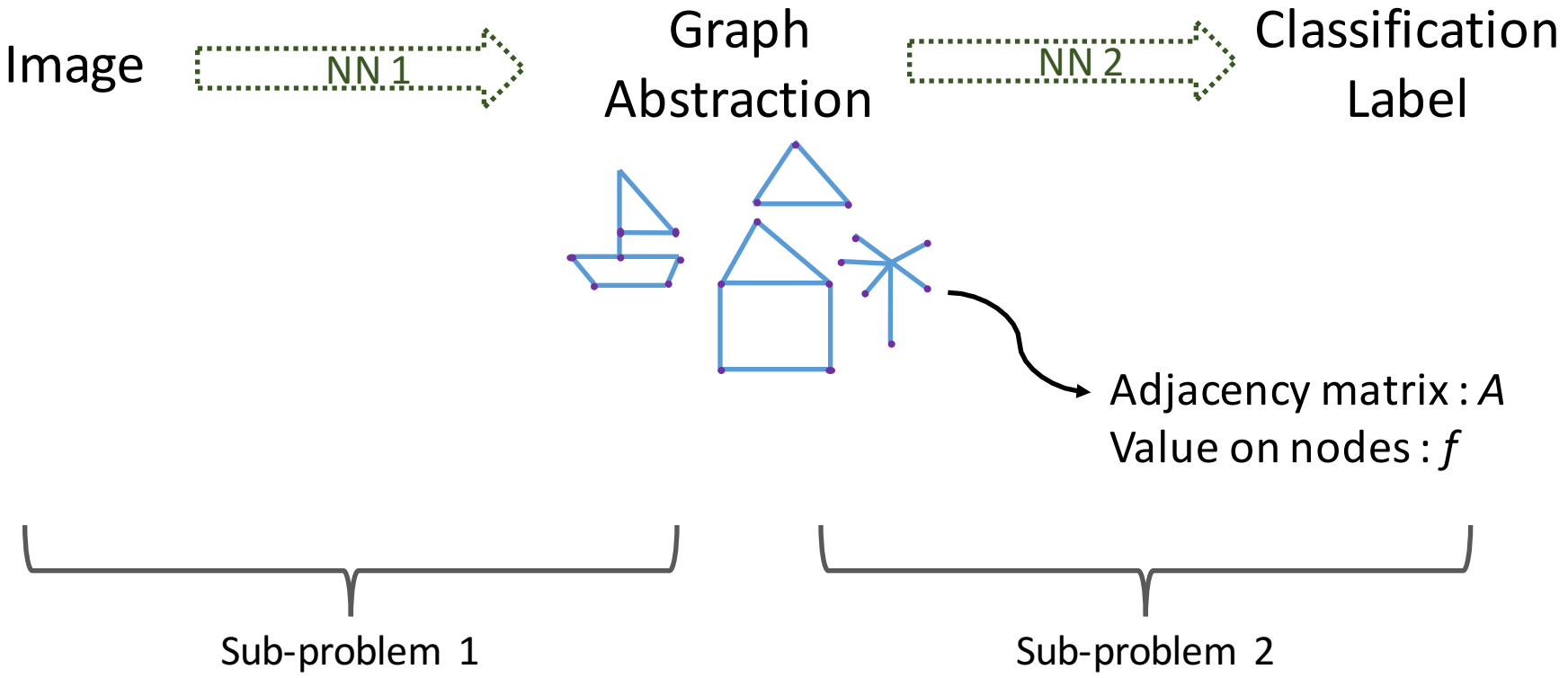


- Input : Image, Output : *image specific graph*
- No prior work

The two sub-problems

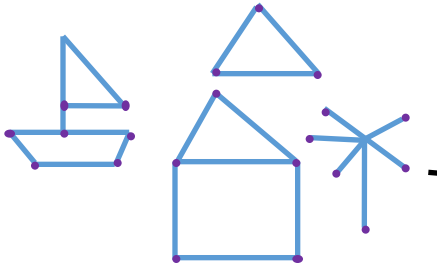


- Input : Image, Output : *image specific graph*
- No prior work

- Input: a *random* graph, Output: label
- Geometric Deep Learning

The two sub-problems

Image → NN 1 → Graph Abstraction → NN 2 → Classification Label



Adjacency matrix : A
Value on nodes : f

Sub-problem 1

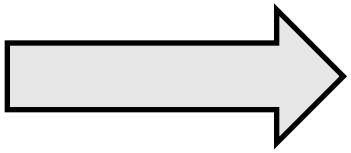
- Input : Image, Output : *image specific graph*
- No prior work

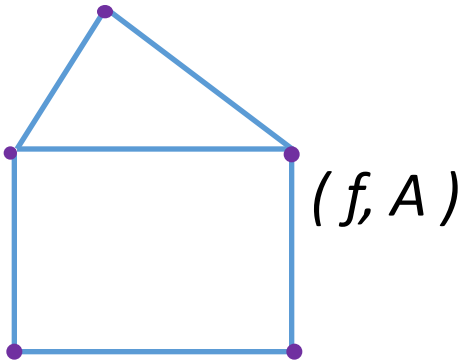
Sub-problem 2

- Input: a *random* graph, Output: label
- Geometric Deep Learning

Need to be compatible for end-to-end learning

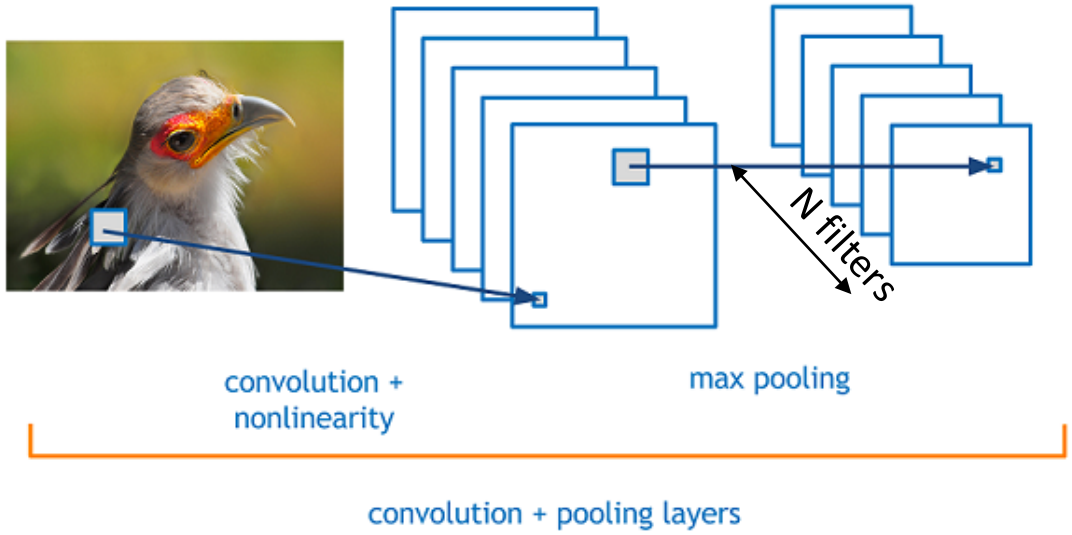
Sub-problem 1:
Image to a Graph





A possible architecture

Objective: Obtain a graph with N nodes



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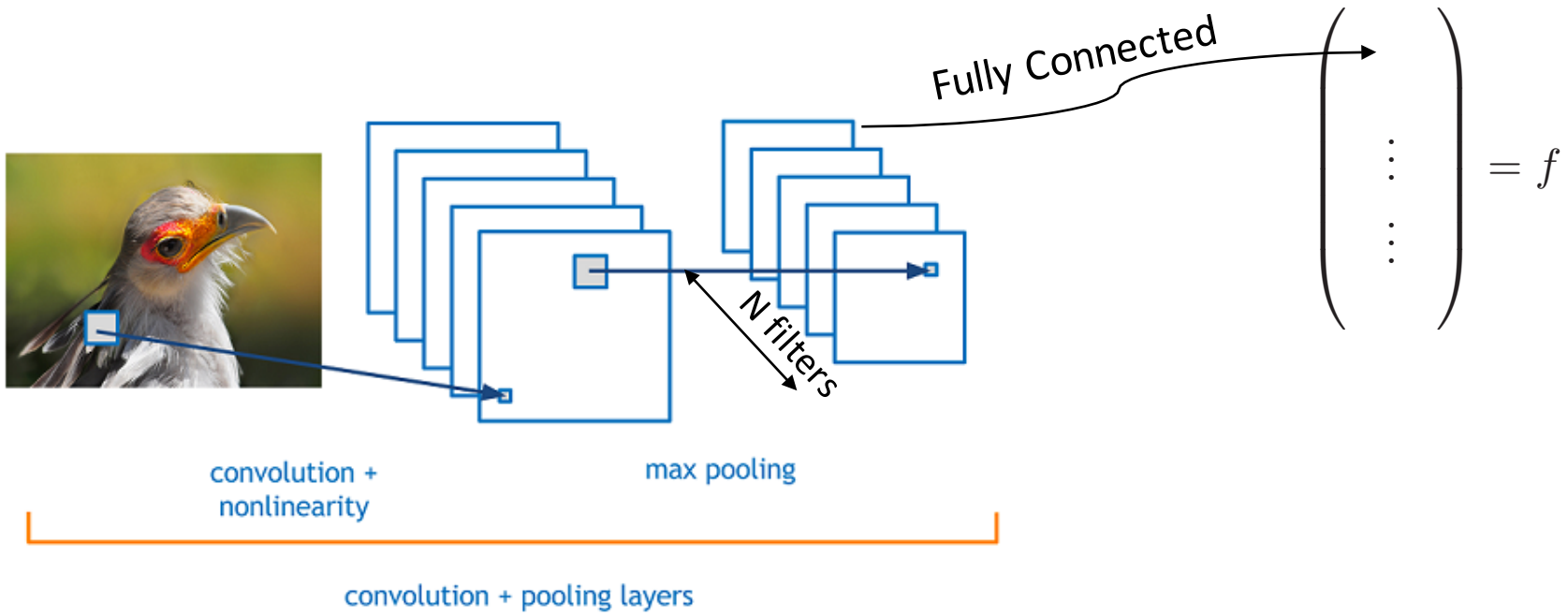

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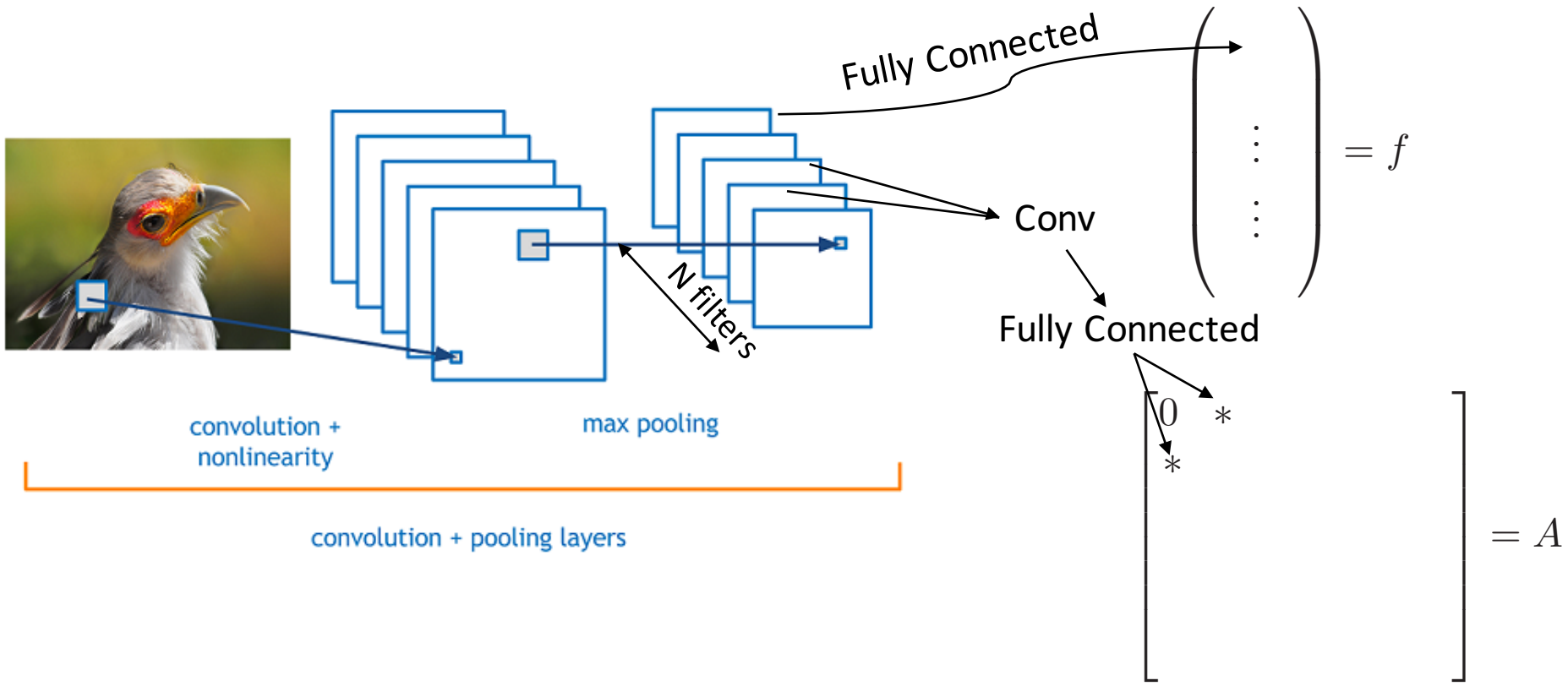
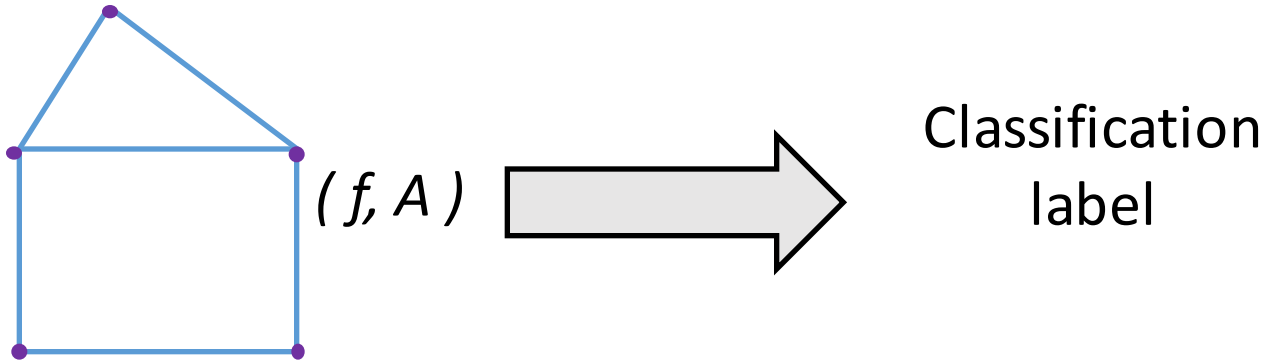
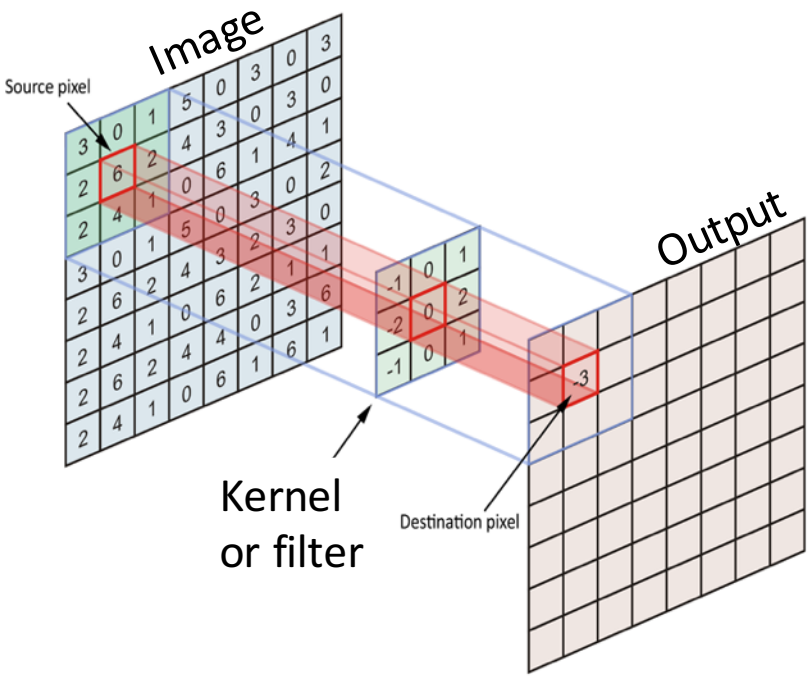


Sub-problem 2:
Graph to a classification label



Extension of CNNs to graphs!

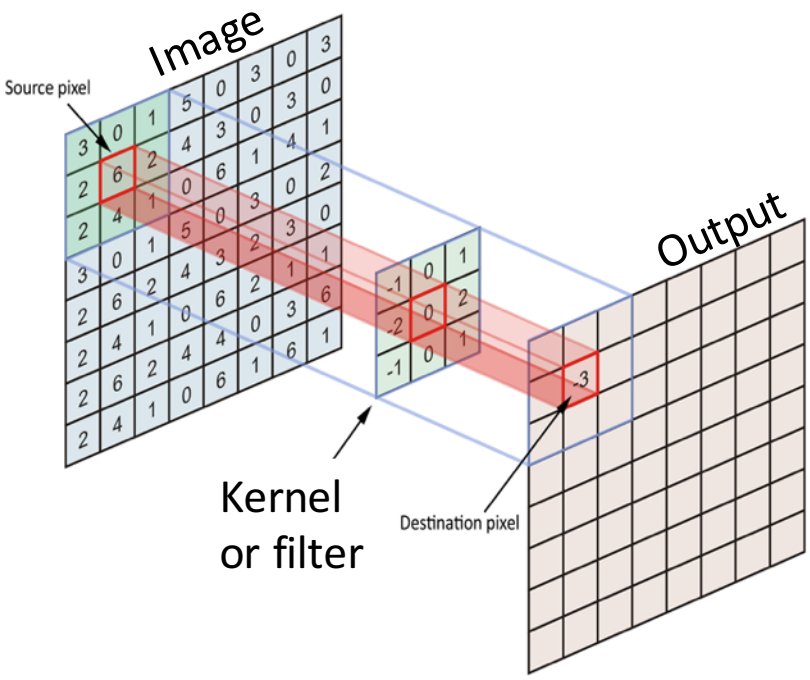
Graph convolution is non-trivial



For Images,

- kernel is fixed
- Can slide it over easily

Graph convolution is non-trivial



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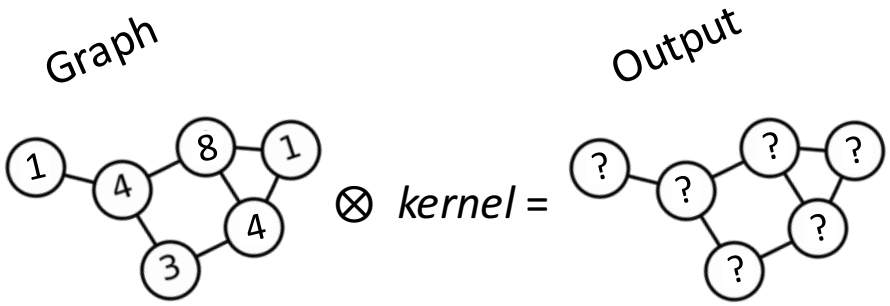
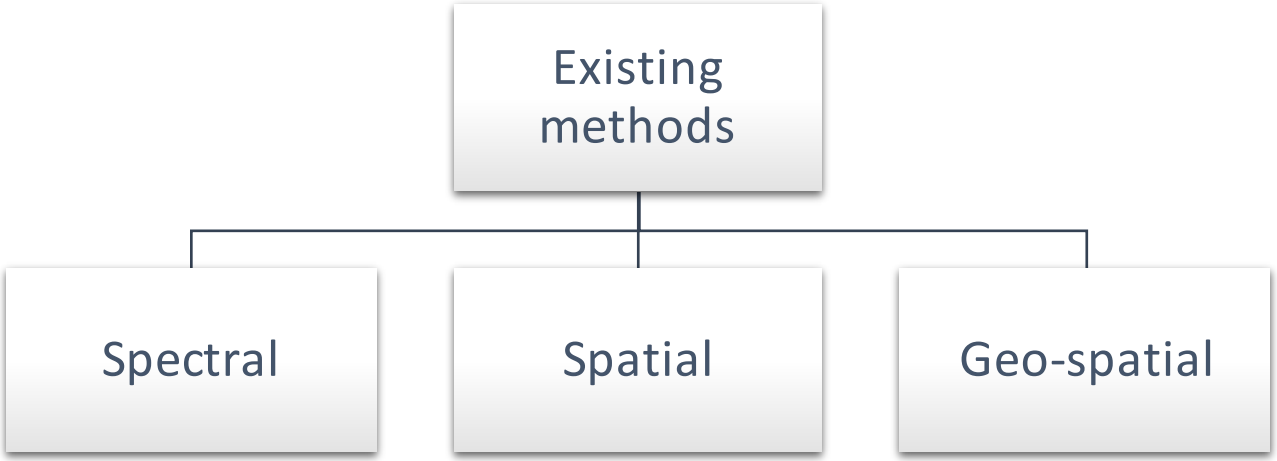


For graphs,

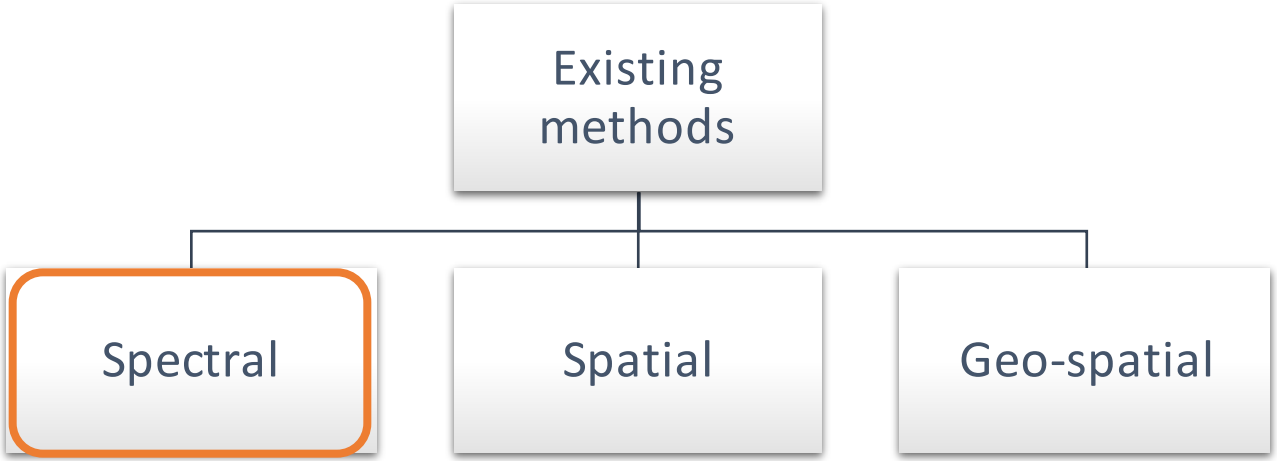
- kernel cant be a fixed template
- Diff num. of edges for each node
- No sense of orientation

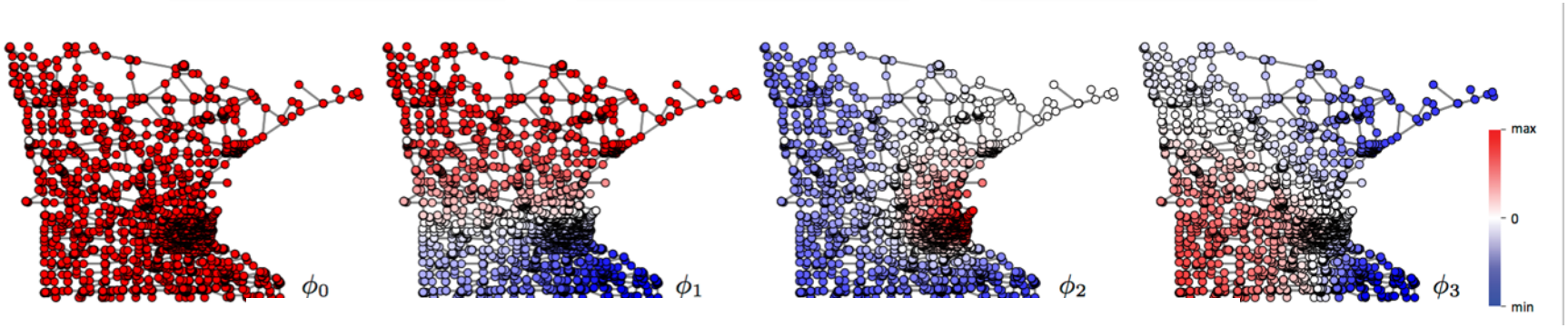
Geometric Deep Learning

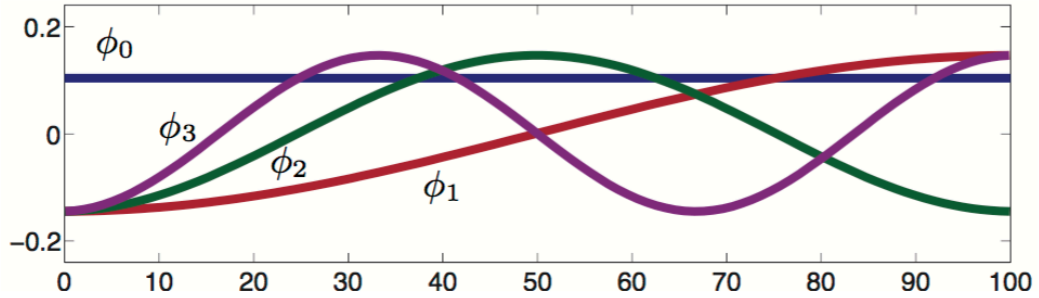
- Maps a graph signal to a classification label
- Different approaches to enable convolution on graphs



Geometric Deep Learning

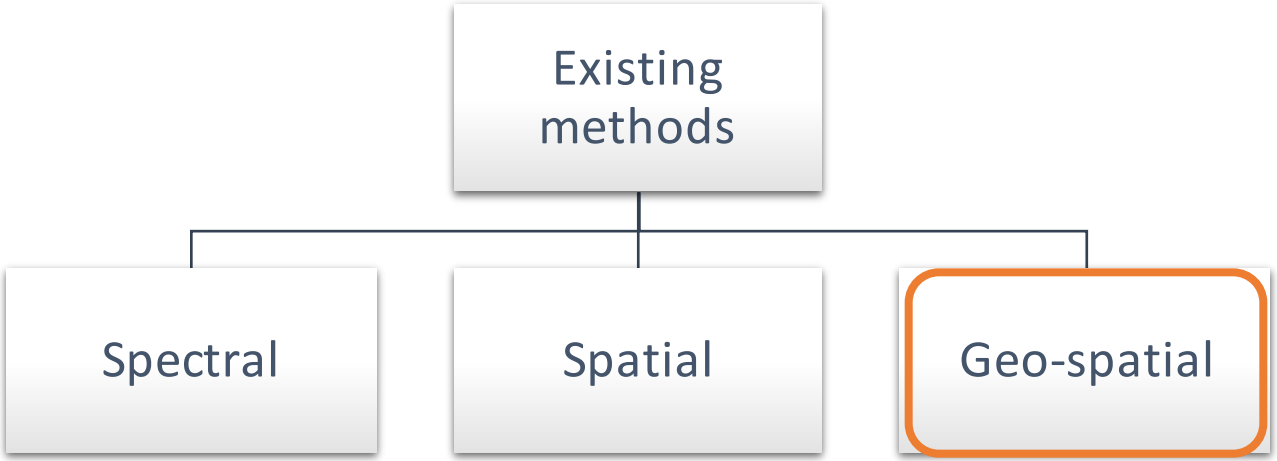


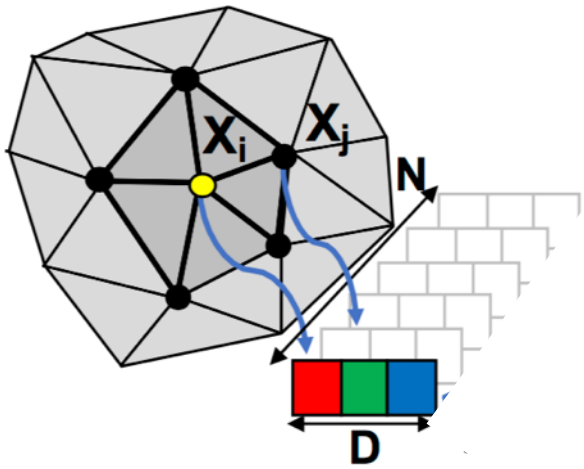




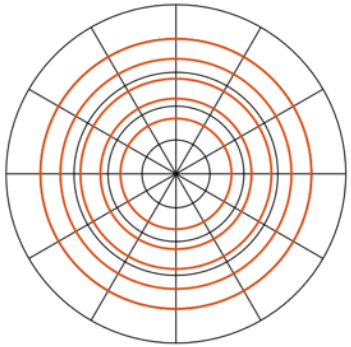
[Bronstein et. al. 2017]

Geometric Deep Learning





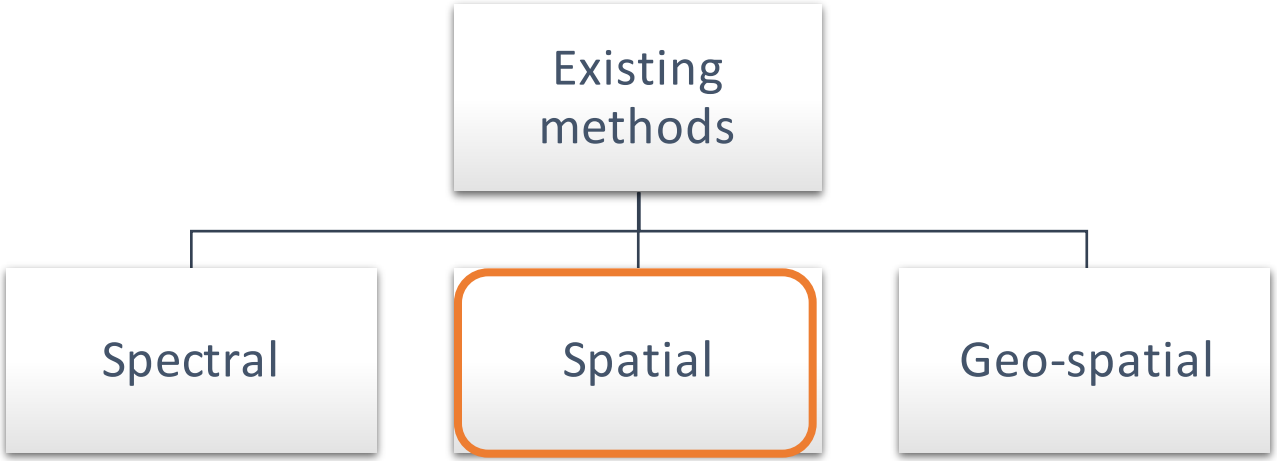
Interpolate function, create a field



Learn and apply a simple kernel at every node

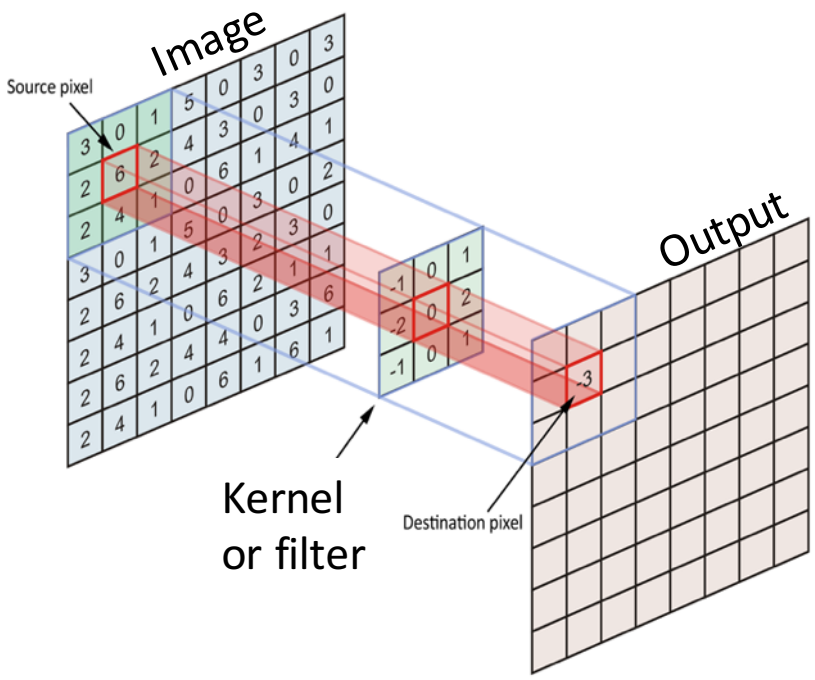
[Verma et. al. 2018, Monti et. al. 2017]

Geometric Deep Learning



Spatial method: An example

CNN on images



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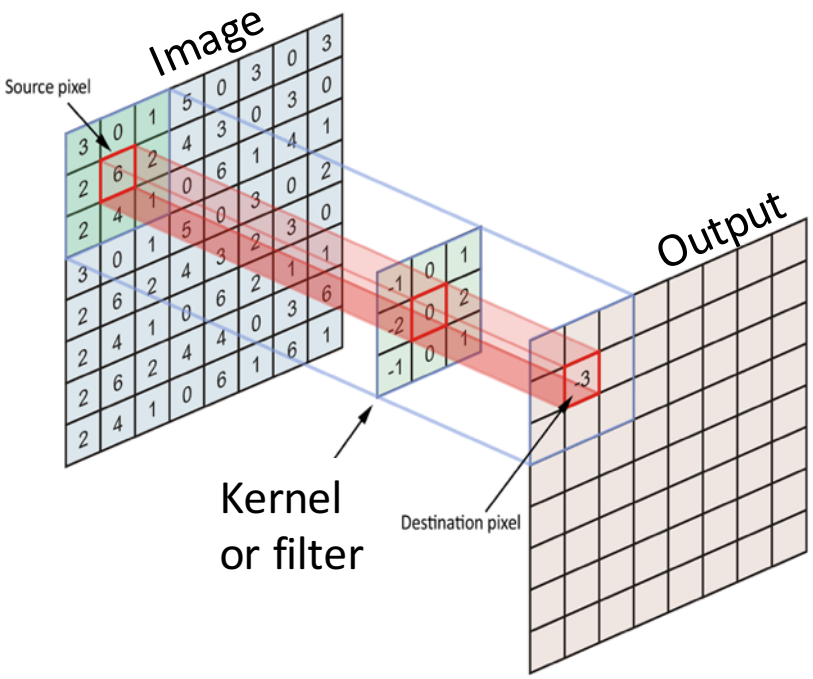
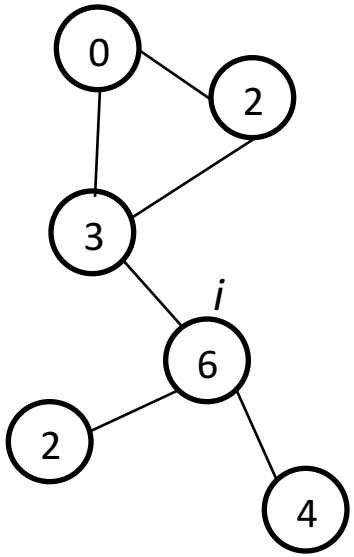
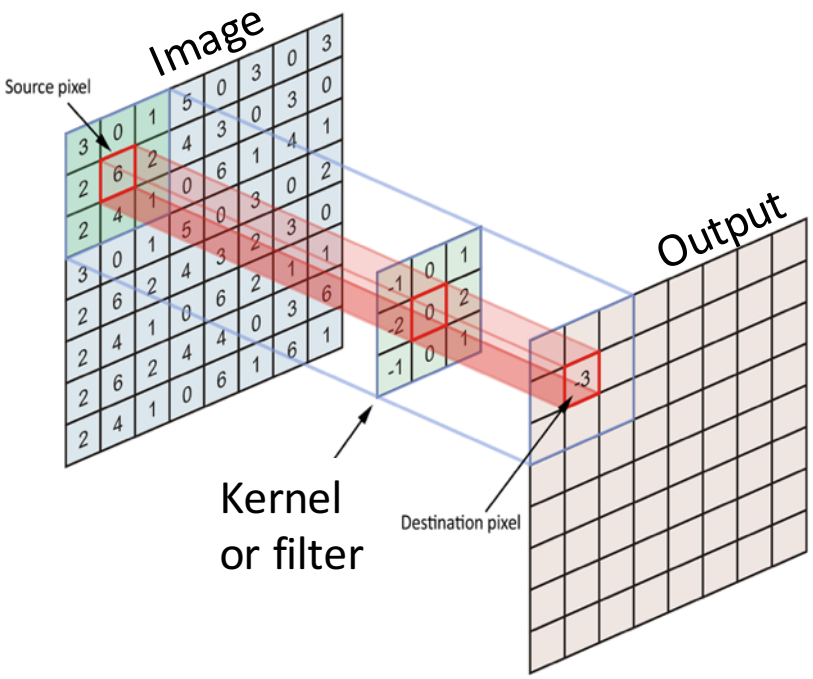


Graph CNN [Such et. al. 2017]

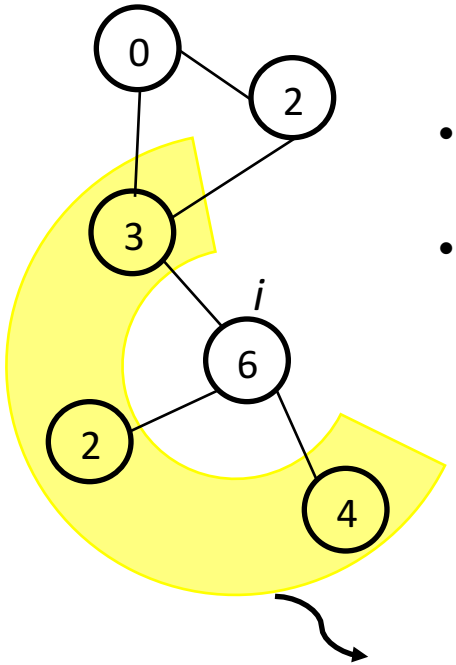


Spatial method: An example

CNN on images

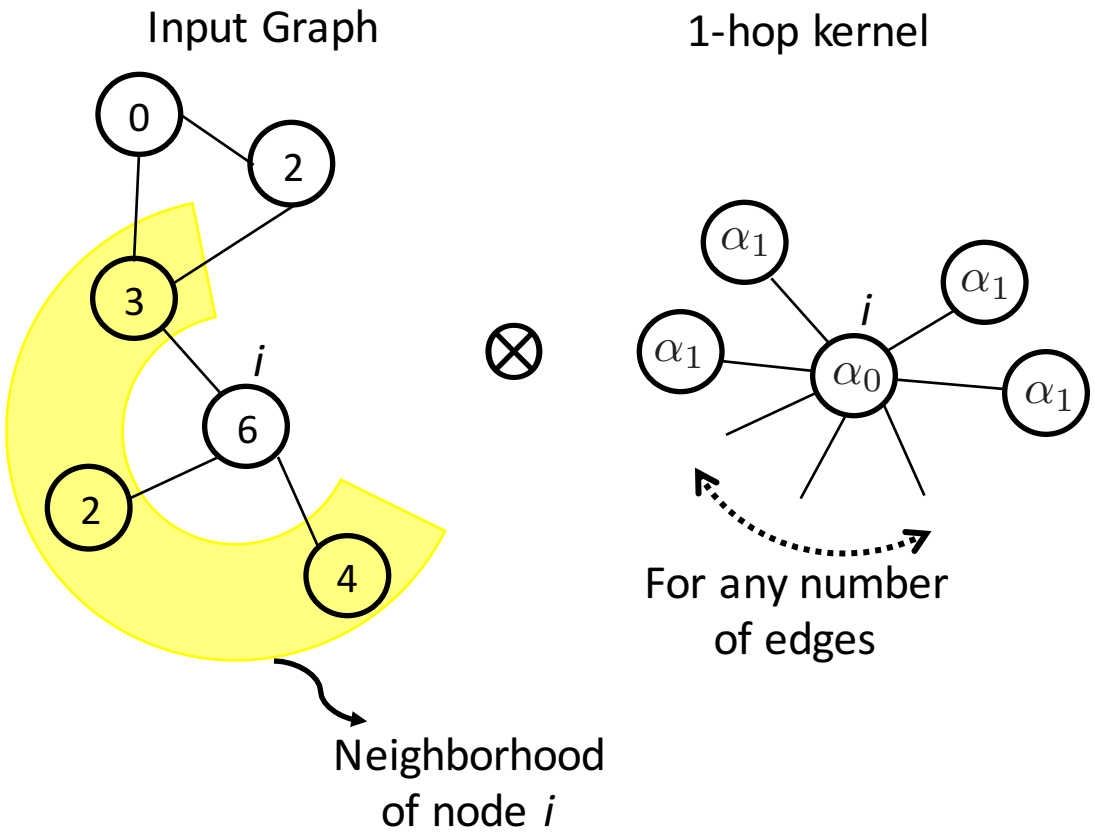


Graph CNN [Such et. al. 2017]



- Want a fixed kernel (template)
- It must 'morph' based on the neighborhood of a node *i*

Example: Graph CNN



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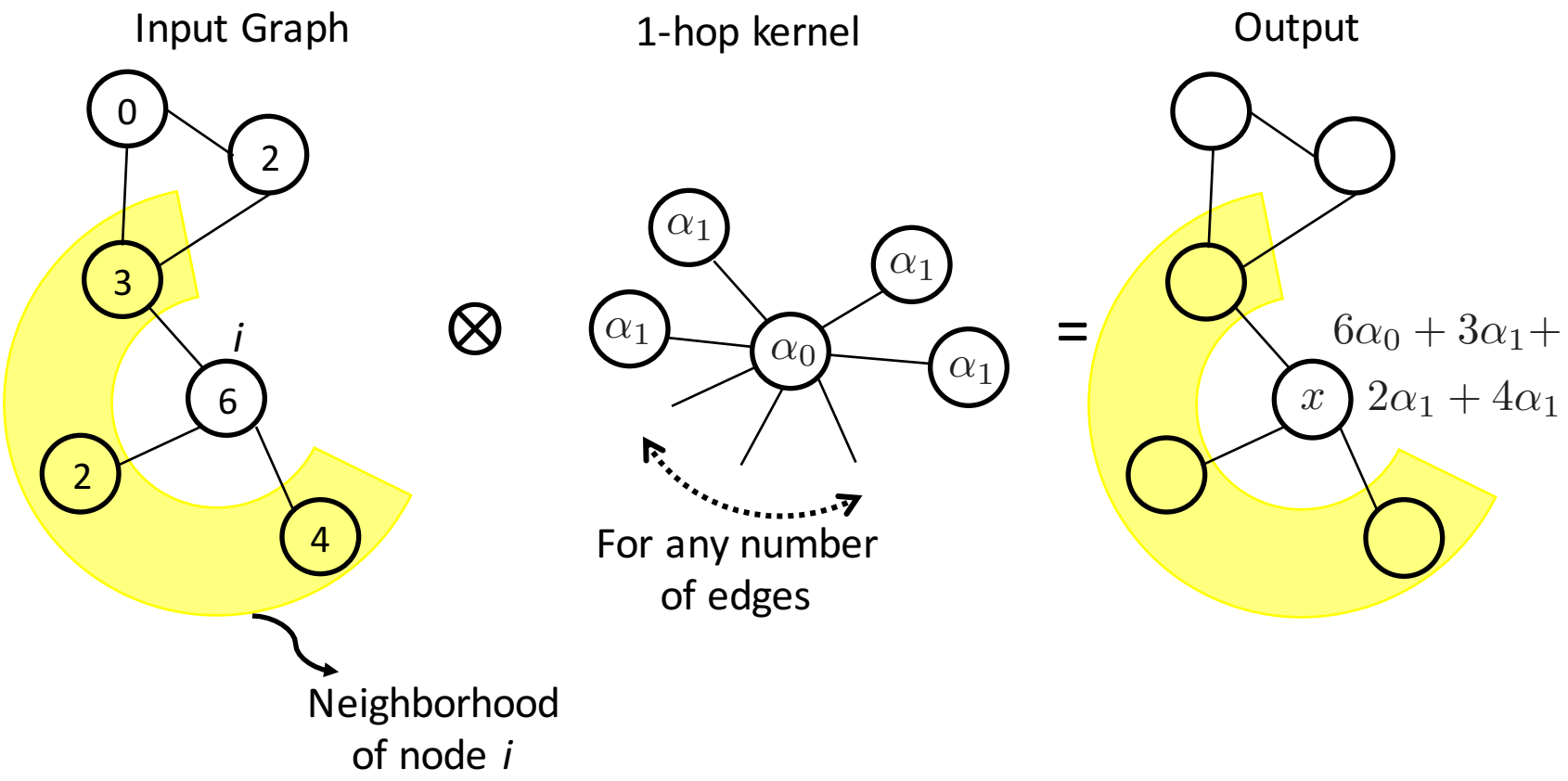
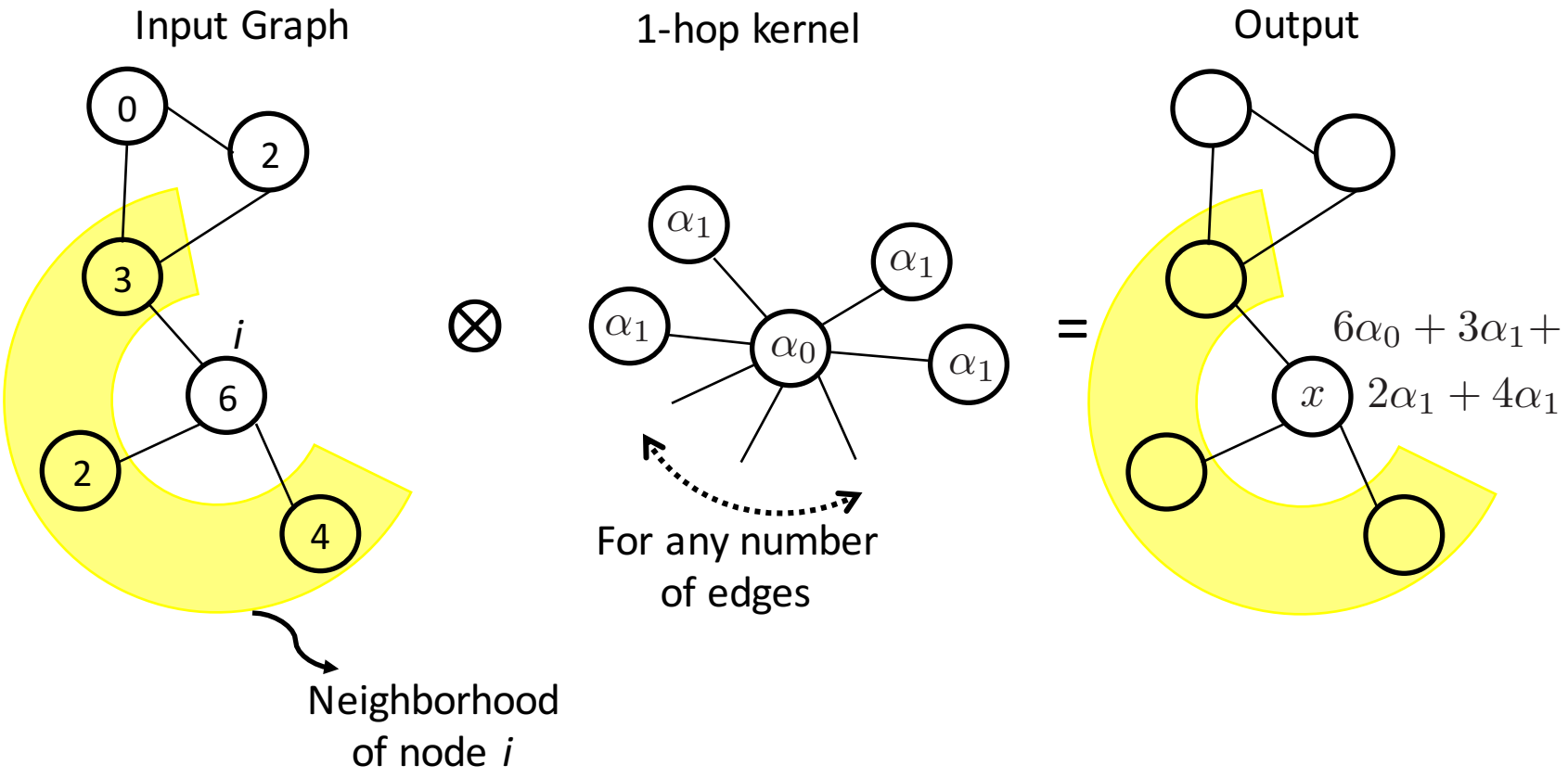
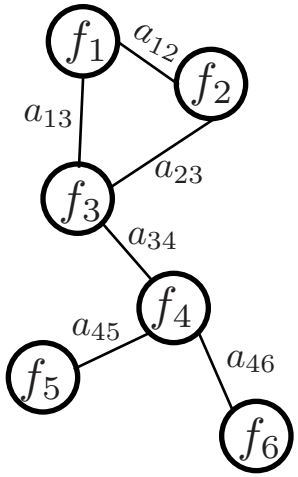


Example: Graph CNN



- Kernel is symmetric, so orientation is not an issue
- Easy way to algebraically deal with variable number of edges

Example: Graph CNN

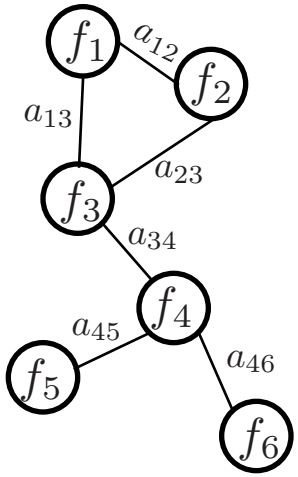


- Signal vector : *f*
- Adjacency matrix : *A*
- The convolution operation :

$$f^{out} = \xi(\alpha_0 I + \alpha_1 A) f$$

- The alphas are learnt

Example: Graph CNN



- Signal vector : *f*
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$$f^{out} = \xi(\alpha_0 I + \alpha_1 A) f$$

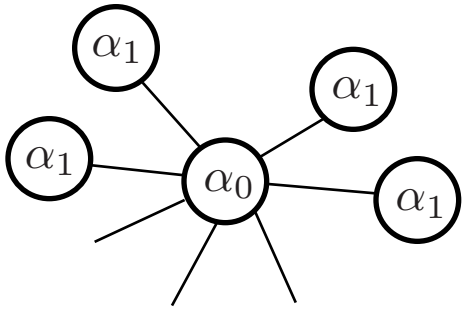
- The alphas are learnt

- In general, this kernel is less expressive than the one for images!

Image kernel

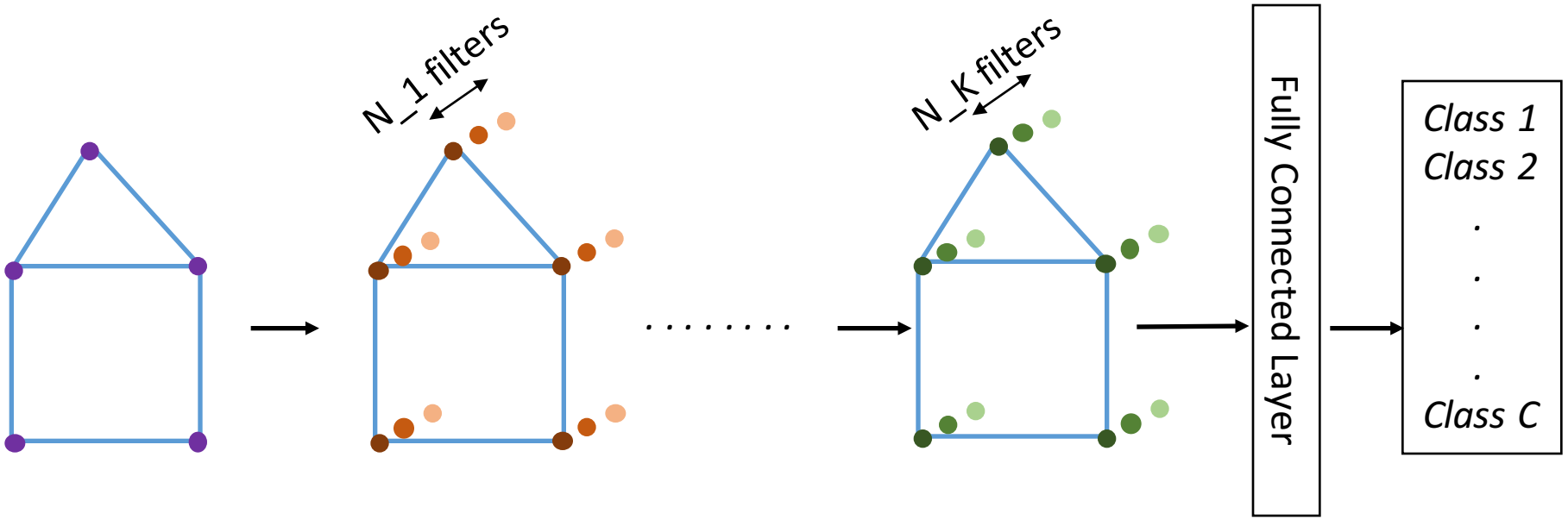
w_{11}	w_{12}	w_{13}
w_{21}	w_{22}	w_{23}
w_{31}	w_{32}	w_{33}

vs

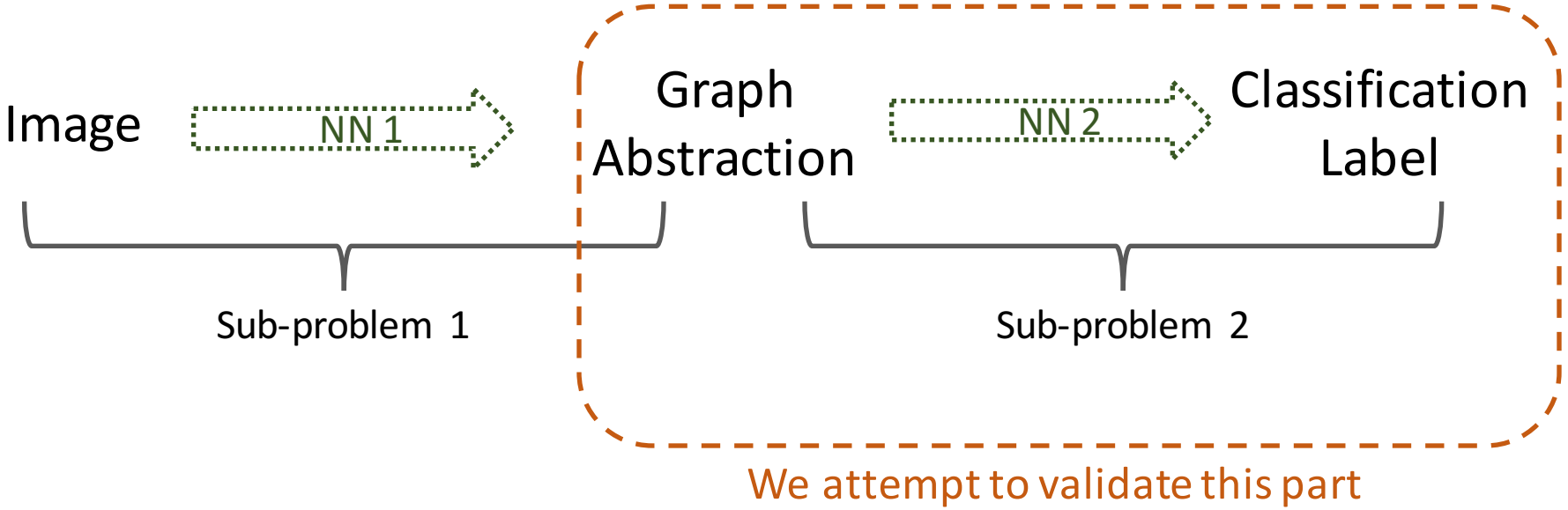


Graphs kernel

Architecture for sub-problem 2



Preliminary results



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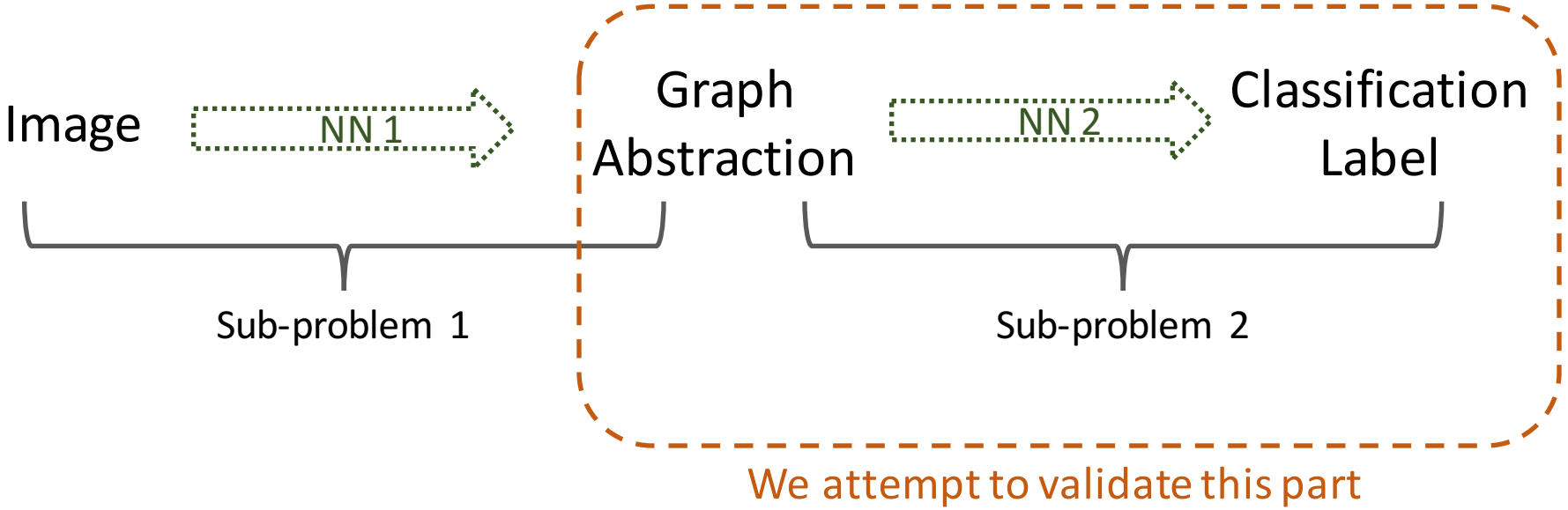
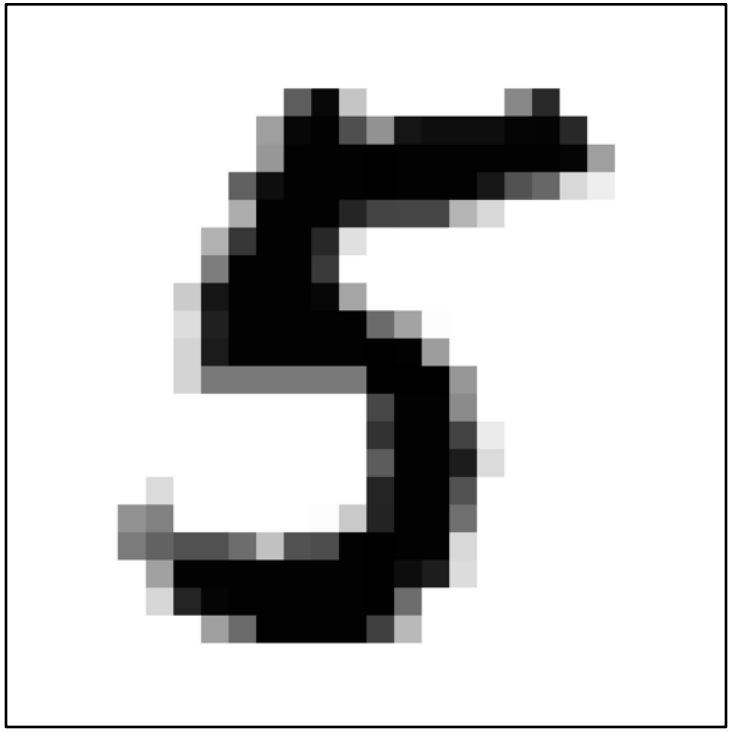


- Generate graph inputs from images with known ground truths
  - Nodes
  - Edges

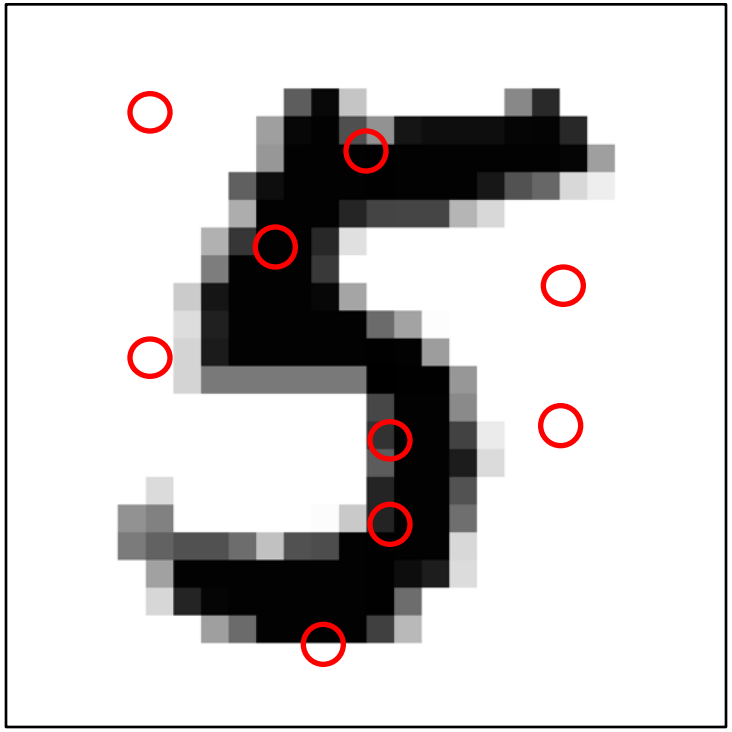
- We use MNIST dataset: images of handwritten digits (0,1,…,9)

Experiment setup to generate graphs



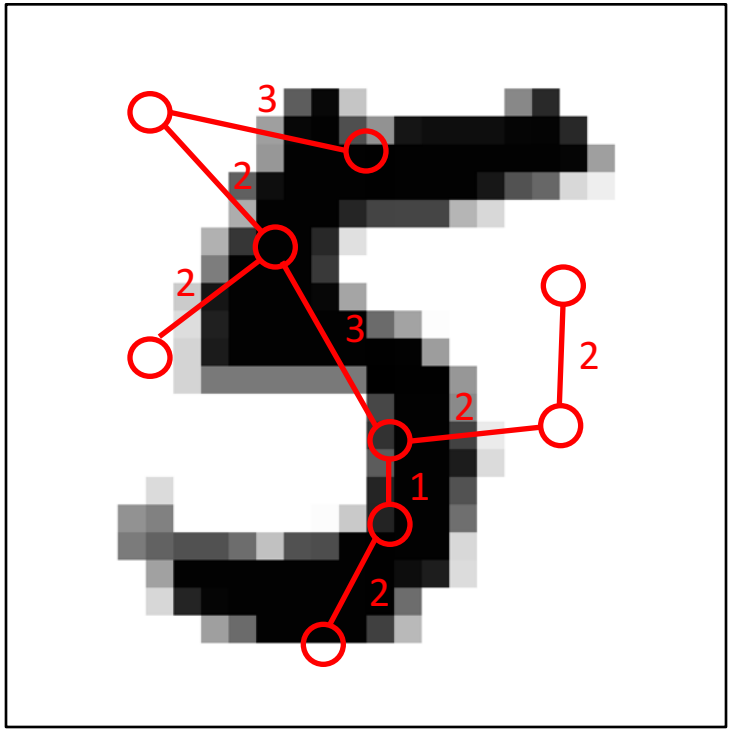
1. Take an image

Experiment setup to generate graphs



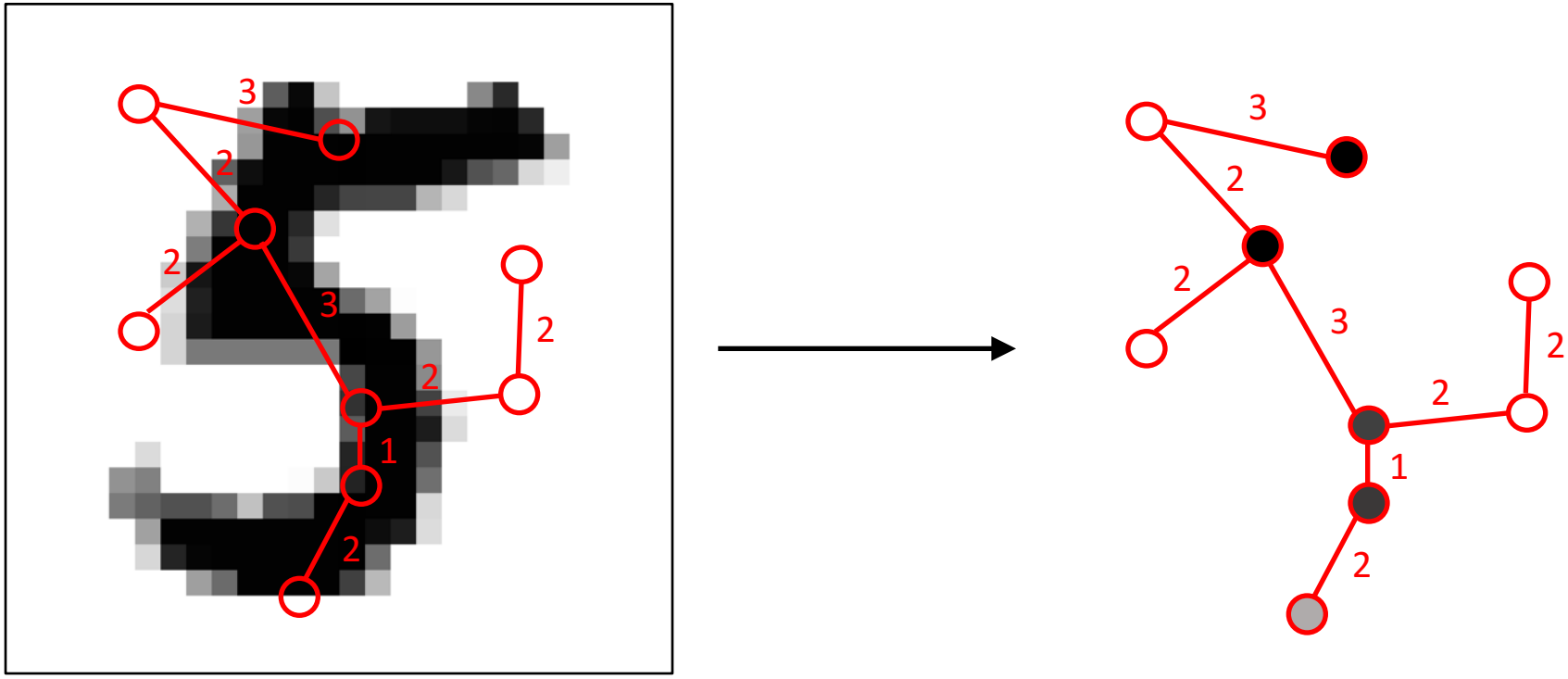
1. Take an image
2. Select N points at random

Experiment setup to generate graphs



1. Take an image
2. Select N points at random
3. Connect ever node to k-nearest neighbors (based on distance)
4. Extract the graph and color at the nodes

Experiment setup to generate graphs



Obtain f, A from the image

Preliminary results

1. As the number of nodes used to create the graph increases, accuracy increases

   With a fixed graph, 50 nodes : 84%

   200 nodes : 91%

Preliminary results

1. As the number of nodes used to create the graph increases, accuracy increases

   With a fixed graph, 50 nodes : 84%

   200 nodes : 91%

2. The technique also works for varying graphs (*A* changes)

   Classification of digits 0 and 1 : 92%

   digits 1 and 7 : 69%

   } 50 nodes

Summary

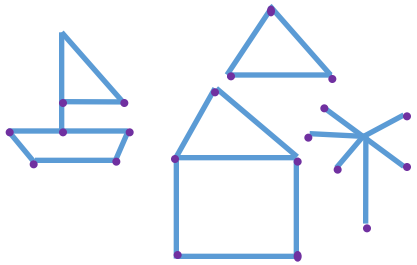
Image

Classical CNN

Classification label

Airplane : 3 %
Automobile : 10 %
…
Truck : 85 %

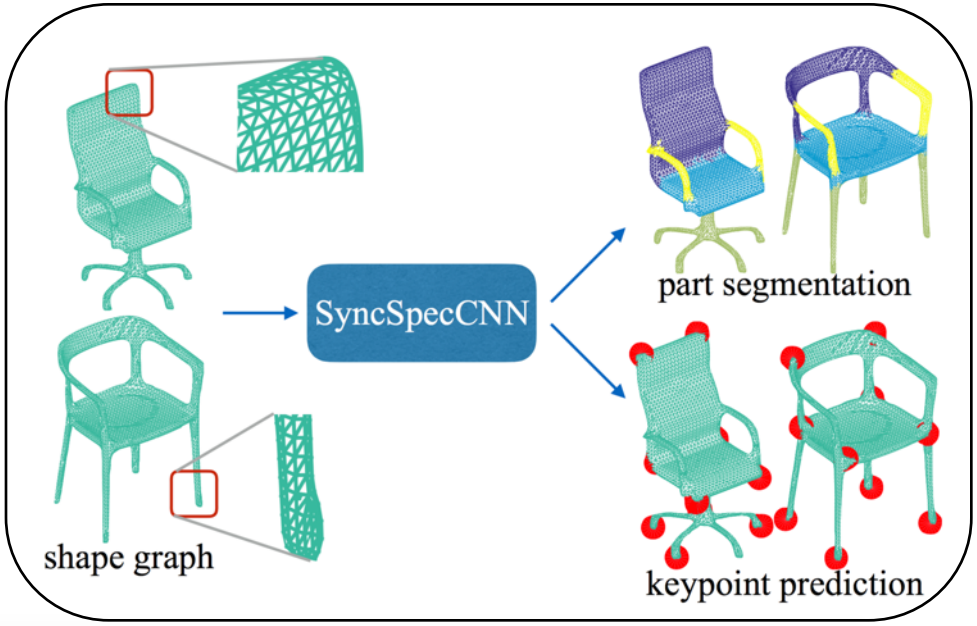
Graph abstraction



Other Applications of Geometric Deep Learning

- Analyzing meshes/ point cloud data (from Lidar)
  - Convert to graph and use Geometric Deep Learning techniques

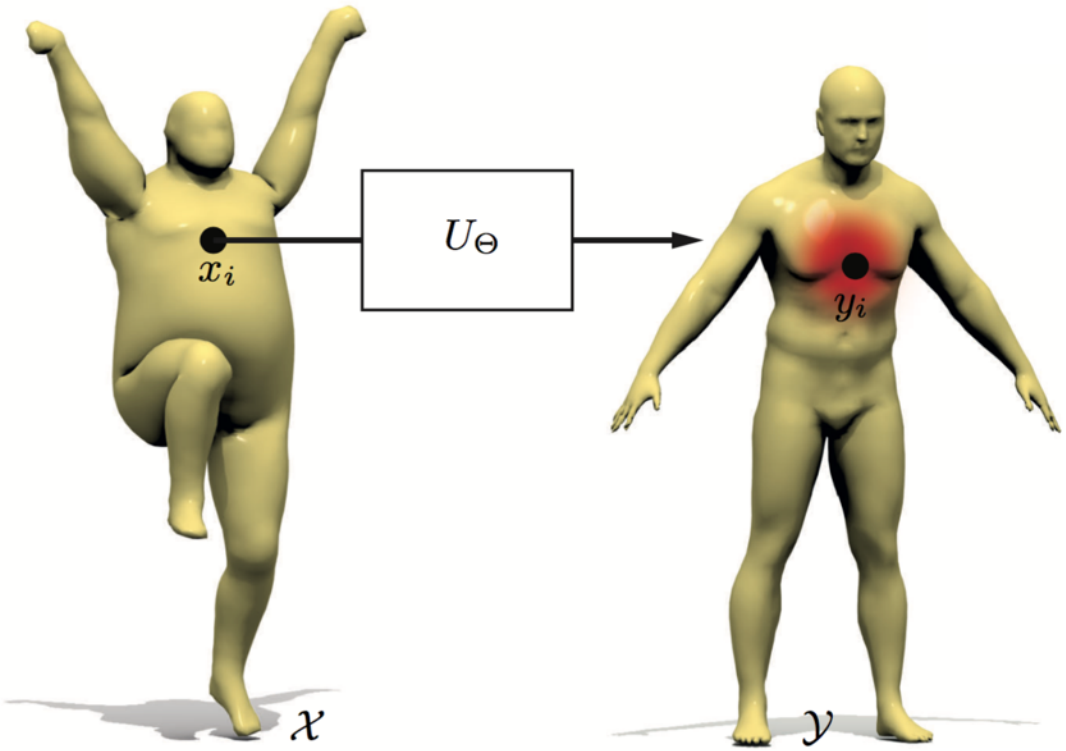
[Verma et. al. 2018]



[Yi et. al. 2017]

Other Applications of Geometric Deep Learning

- Shape correspondence for deformable objects



[Bronstein et. al. 2017]