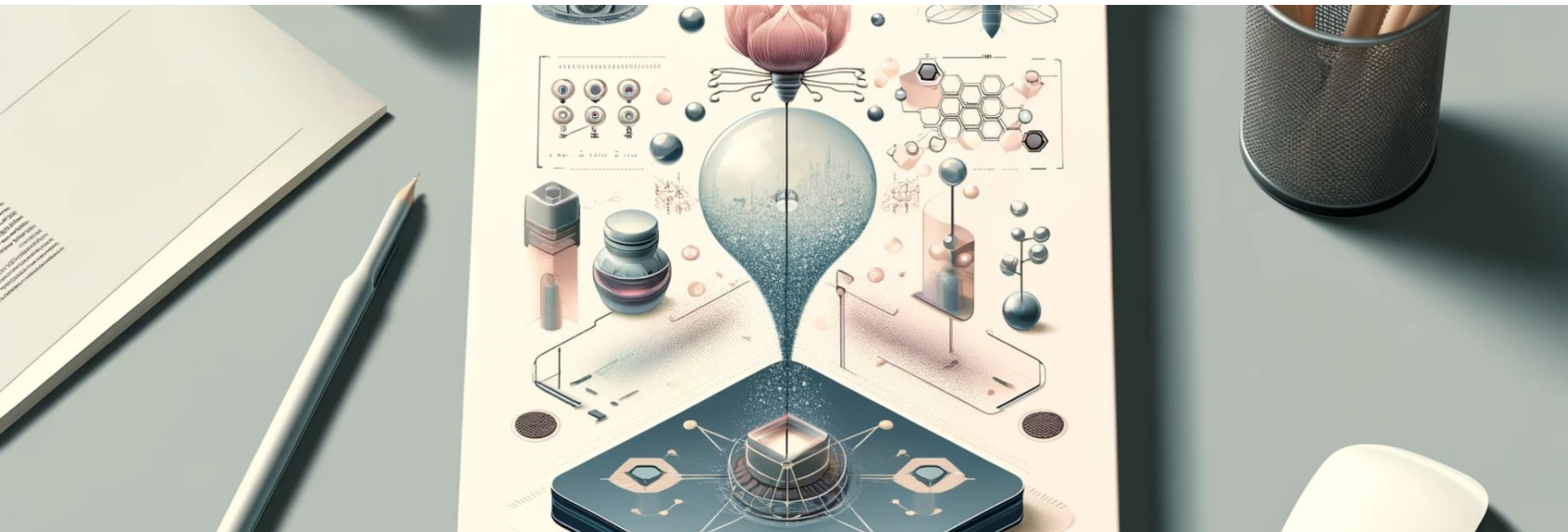


# CSE7850/CX4803 Machine Learning in Computational Biology



## Lecture 23: ML for Network Biology

Yunan Luo

# Networks (graphs)



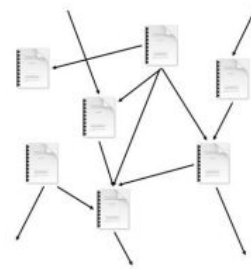
Image credit: [Medium](#)

**Social networks**



Image credit: [Missoula Current News](#)

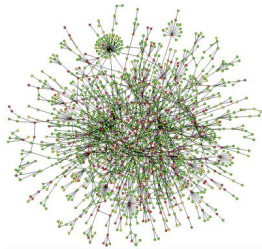
**Internet**



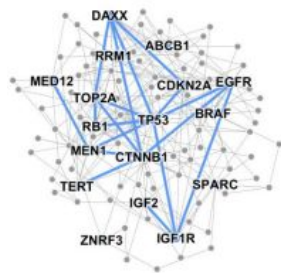
**Citation networks**



**Underground networks**



**Protein-protein interaction networks**



**Disease pathways**

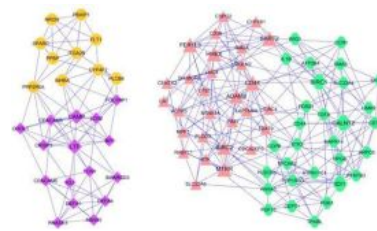


Image credit: [ese.wustl.edu](#)

**Gene regulatory networks**

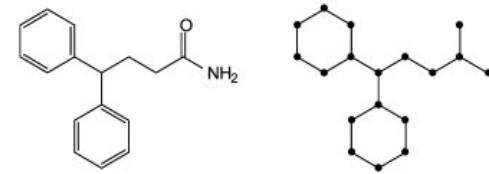


Image credit: [MDPI](#)

**Molecules**

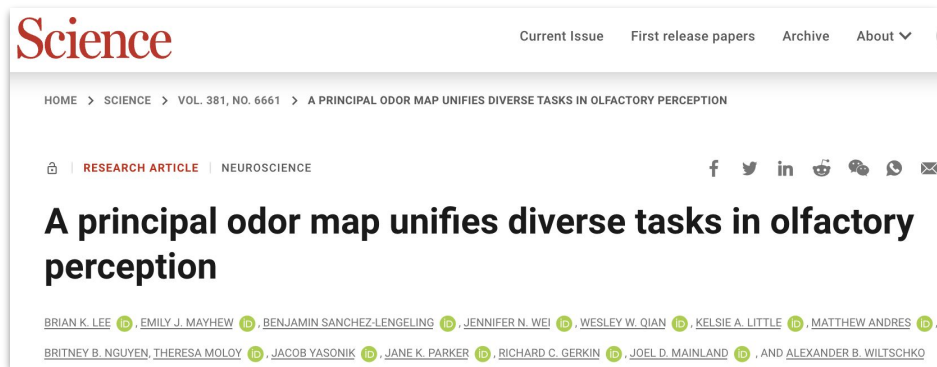
# Today's papers

- Paper #1: Representation learning on protein networks

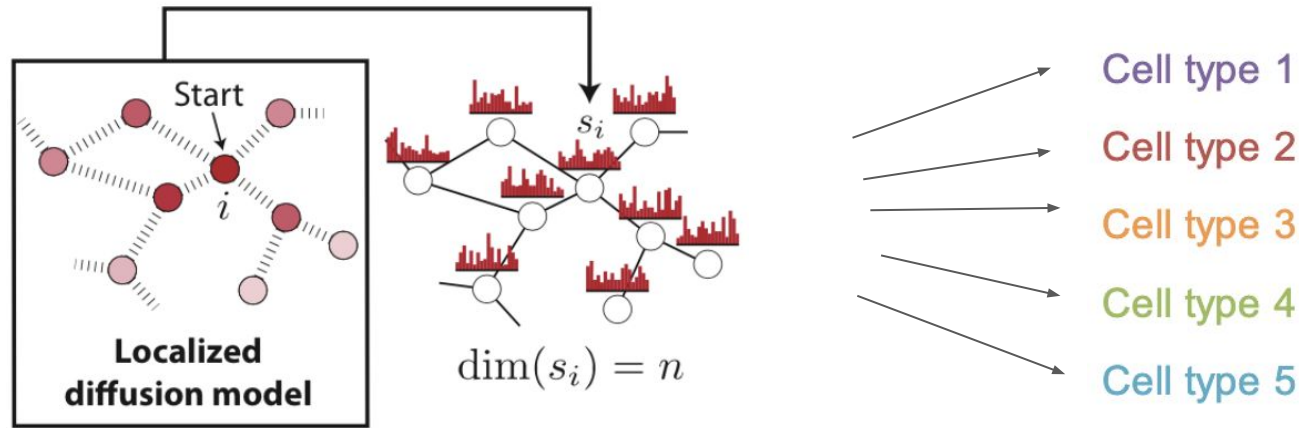
## Contextualizing protein representations using deep learning on protein networks and single-cell data

Michelle M. Li<sup>1</sup>, Yepeng Huang<sup>1</sup>, Marissa Sumathipala<sup>1</sup>, Man Qing Liang<sup>1</sup>, Alberto Valdeolivas<sup>2</sup>, Ashwin N. Ananthakrishnan<sup>1,3</sup>, Katherine Liao<sup>1,4</sup>, Daniel Marbach<sup>2</sup>, and Marinka Zitnik<sup>1,5,6,7†</sup>

- Paper #2: Deciphering odors of molecules using graph ML



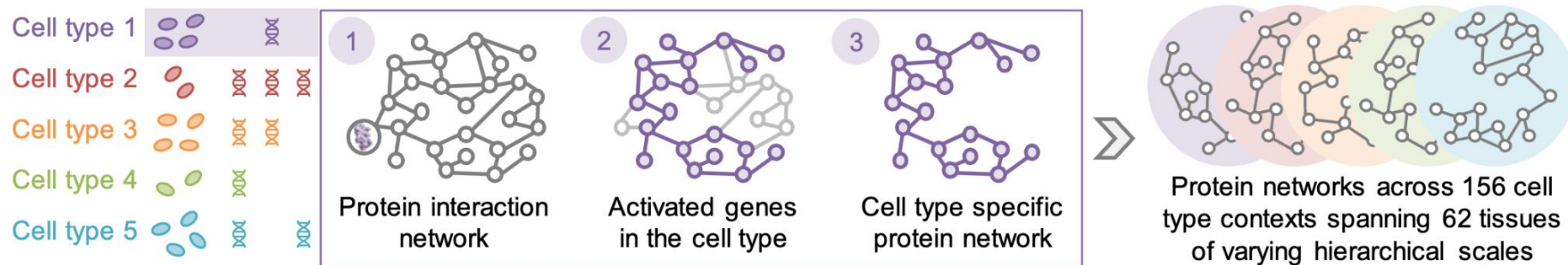
# Paper #1: Representation learning on protein networks



Learning representations on the global protein/gene network

The representations are used to make predictions in different contexts, e.g., a cell type (defined by a group of expressed genes)

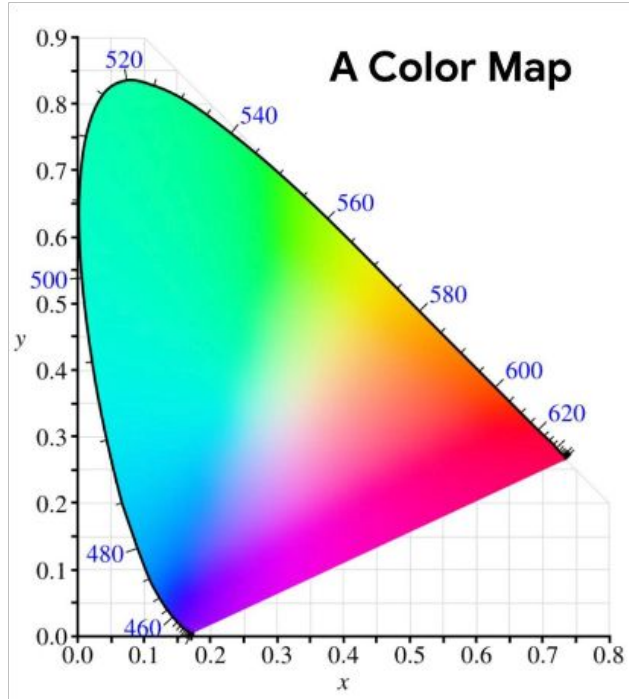
# Paper #1: Representation learning on protein networks



Extract subnetwork defined by each cell type and learn contextualized representations



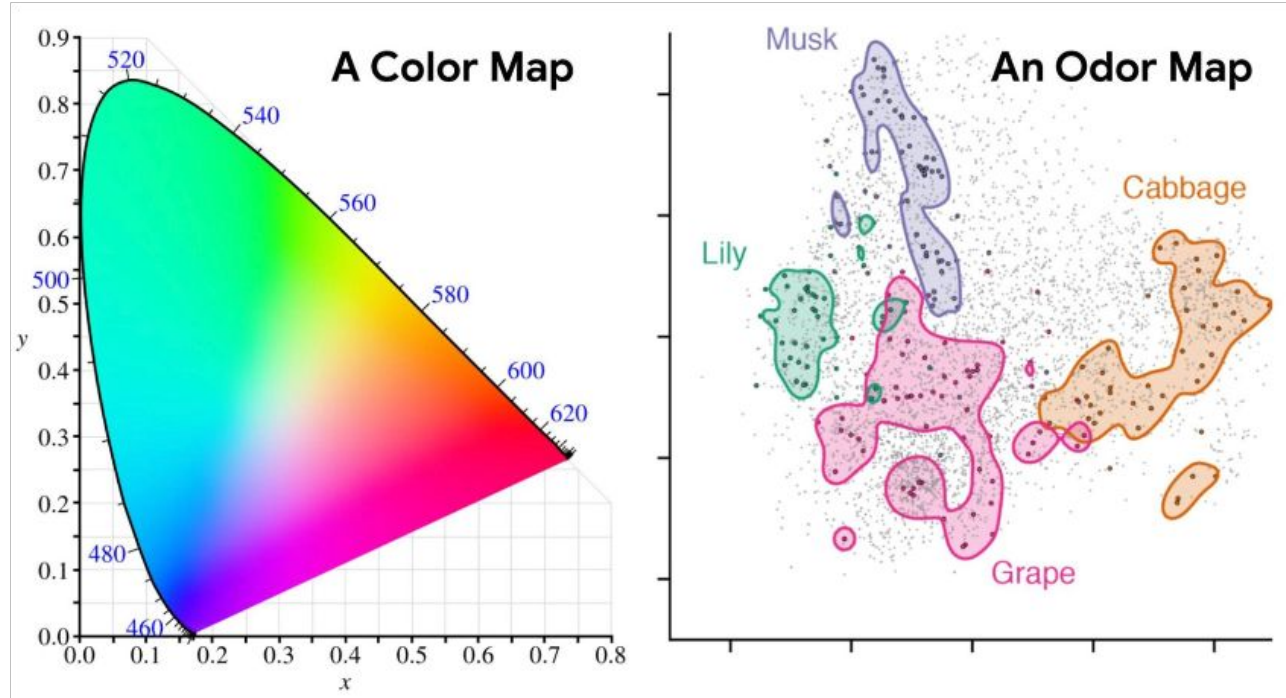
# Paper #2: Digitizing and deciphering odors



- There are three color basis: R, G, B
- We can mix R,G,B to create other colors



# Paper #2: Digitizing and deciphering odors

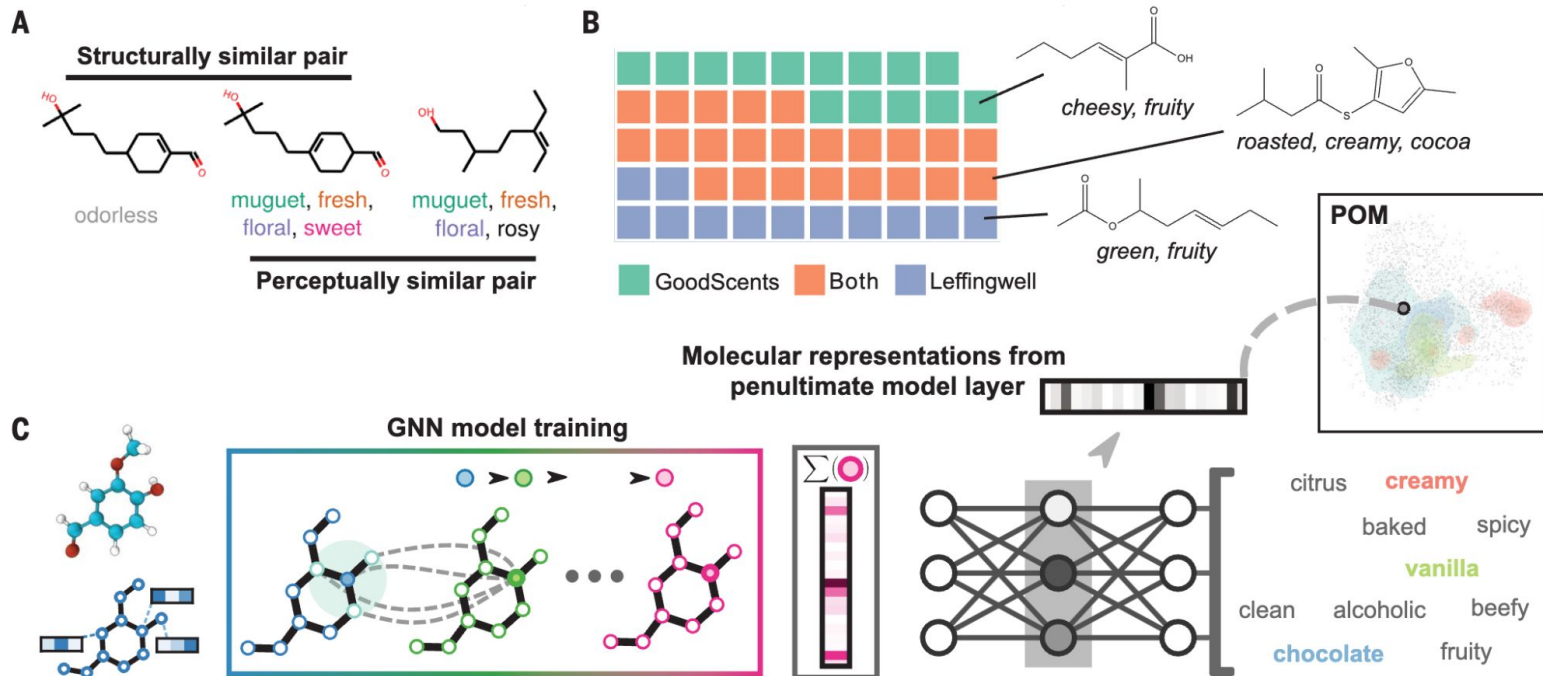


- There are three color basis: R, G, B
- We can mix R,G,B to create other colors

- Do we have such basis in the smell (odor) space?
- If so, we could create new smells by mixing the basis



# Paper #2: Digitizing and deciphering odors



# Teleporting Scent

A sensor “analyzes” a given scent and decomposes it



A “scent print” at another place synthesizes the scent using the basis scents