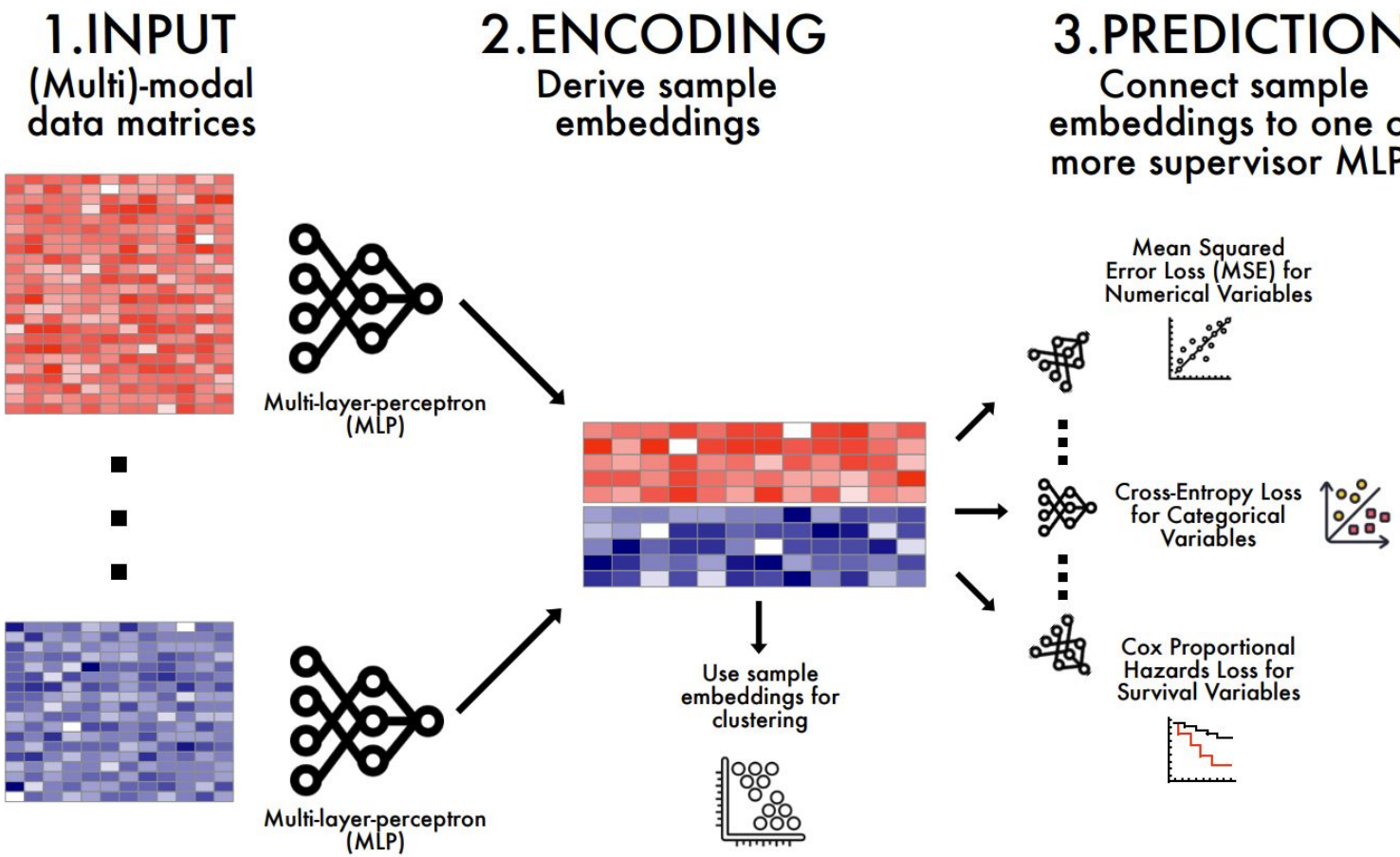
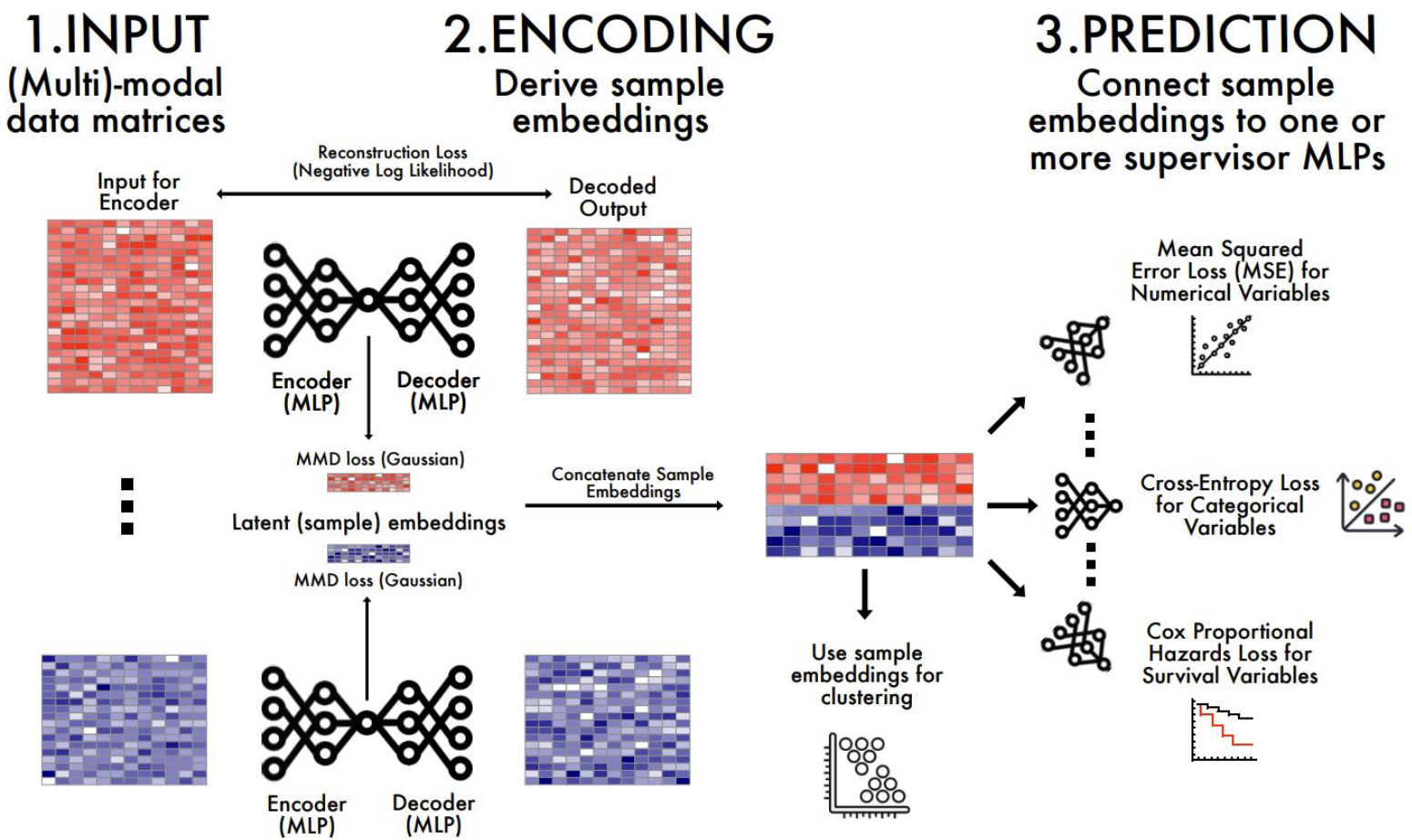
DirectPred: Standard Fully Connected Networks



Supervised Variational Auto-Encoders



Cross-Modality Encoder Networks

1.INPUT
(Multi)-modal data matrices

Input data matrices for Encoder

2.ENCODING
Derive sample embeddings

Decoder reconstructs a different modality (Target Matrix).

Cross-Modal Reconstruction Loss

Decoded Output

Target Data Matrix

Encoder (MLP)

Decoder (MLP)

MMD loss (Gaussian)

Cross-Modal Latent Embedding Space

MMD loss (Gaussian)

Concatenate Sample Embeddings

Cross-Modal Reconstruction Loss

Decoded Output

Target Data Matrix

Encoder (MLP)

Decoder (MLP)

3.PREDICTION
Connect sample embeddings to one or more supervisor MLPs

Mean Squared Error Loss (MSE) for Numerical Variables

Cross-Entropy Loss for Categorical Variables

Cox Proportional Hazards Loss for Survival Variables

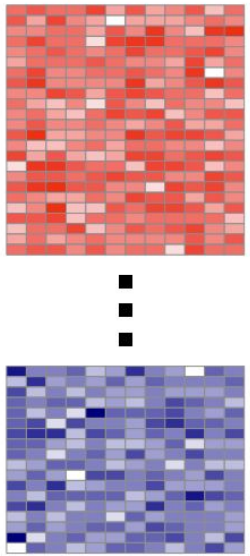
Use sample embeddings for clustering

Multi-Triplet Networks

1.INPUT

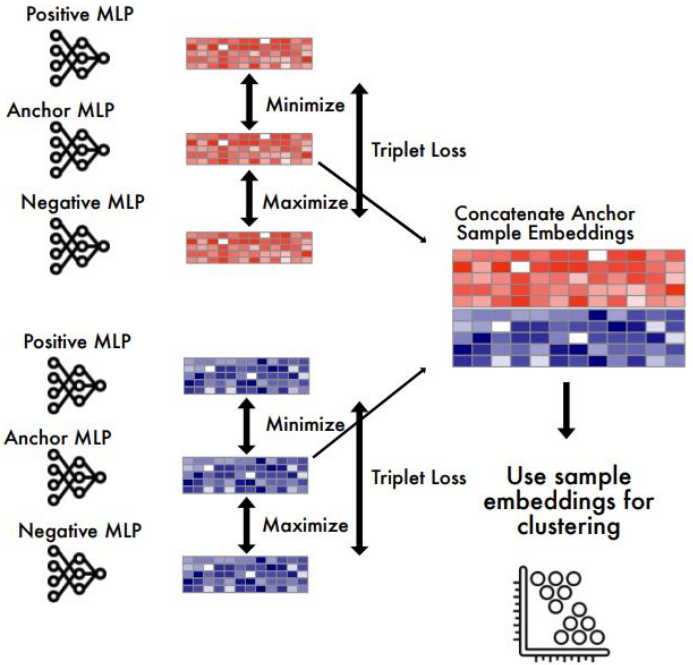
(Multi)-modal data matrices

For each "**anchor**" sample: designate one "**positive**" sample (shared class label) and a "**negative**" sample (non-shared class label). Goal is to **minimize** anchor-to-positive distance while **maximizing** anchor-to-negative distance.



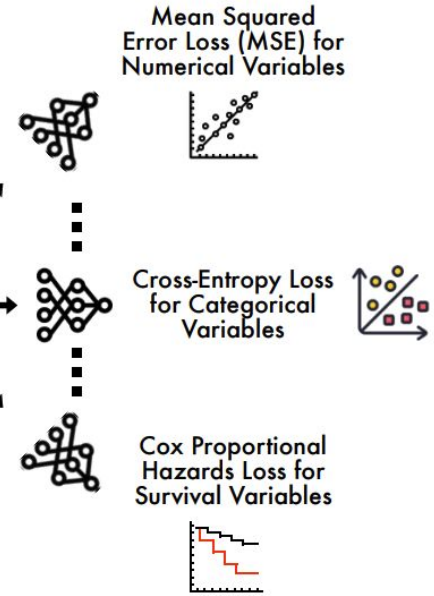
2.ENCODING

Derive sample embeddings

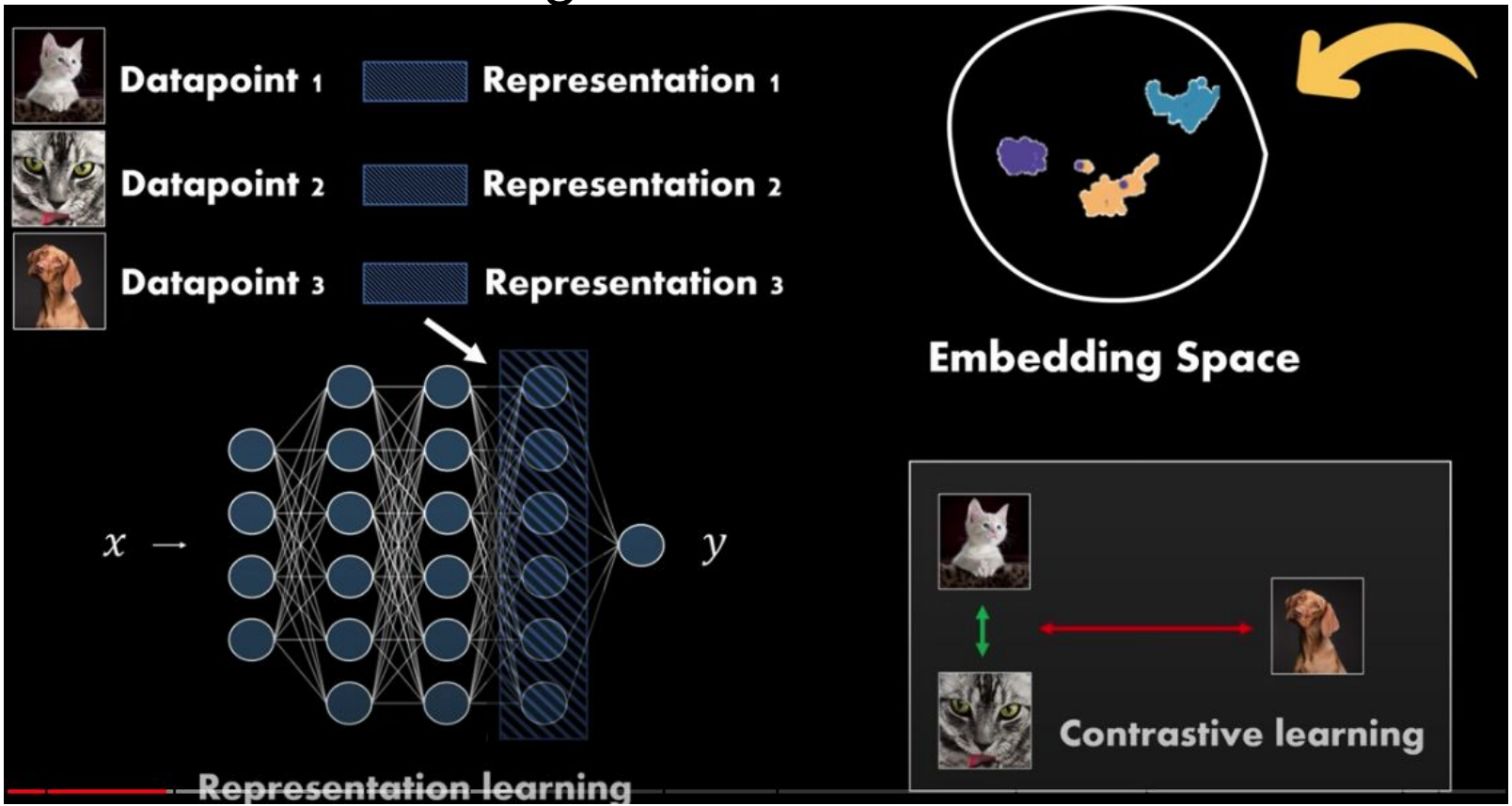


3.PREDICTION

Connect sample embeddings to one or more supervisor MLPs

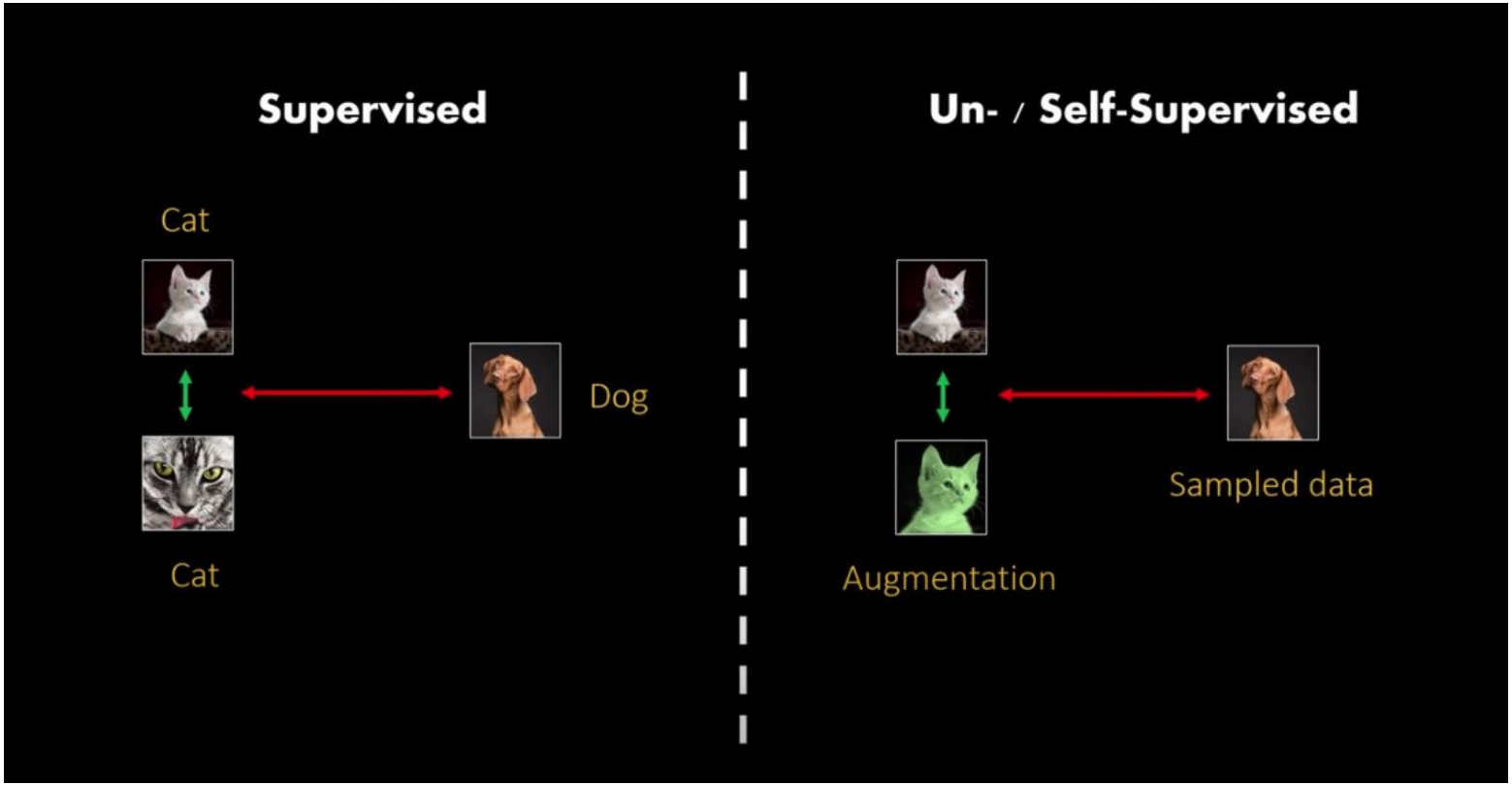


Contrastive Learning



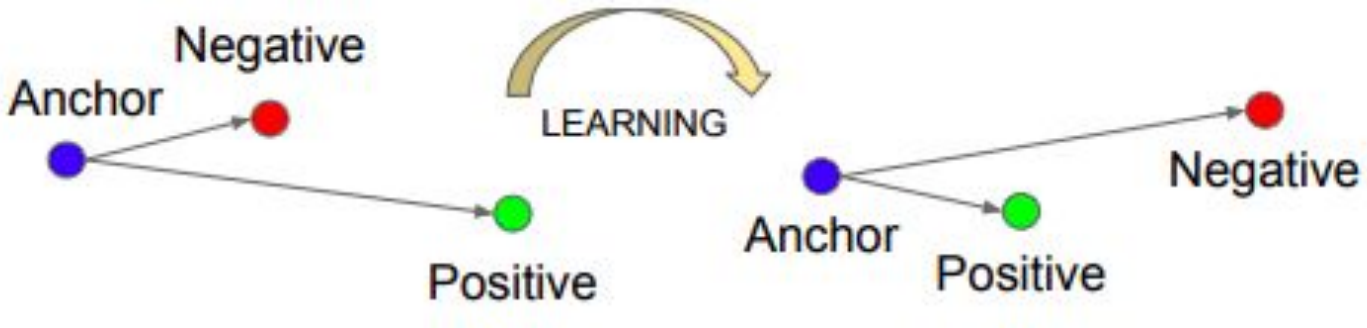
DeepFindr: [Contrastive Learning in PyTorch - Part 1: Introduction]

Contrastive Learning



DeepFindr: [Contrastive Learning in PyTorch - Part 1: Introduction]

Triplet Loss



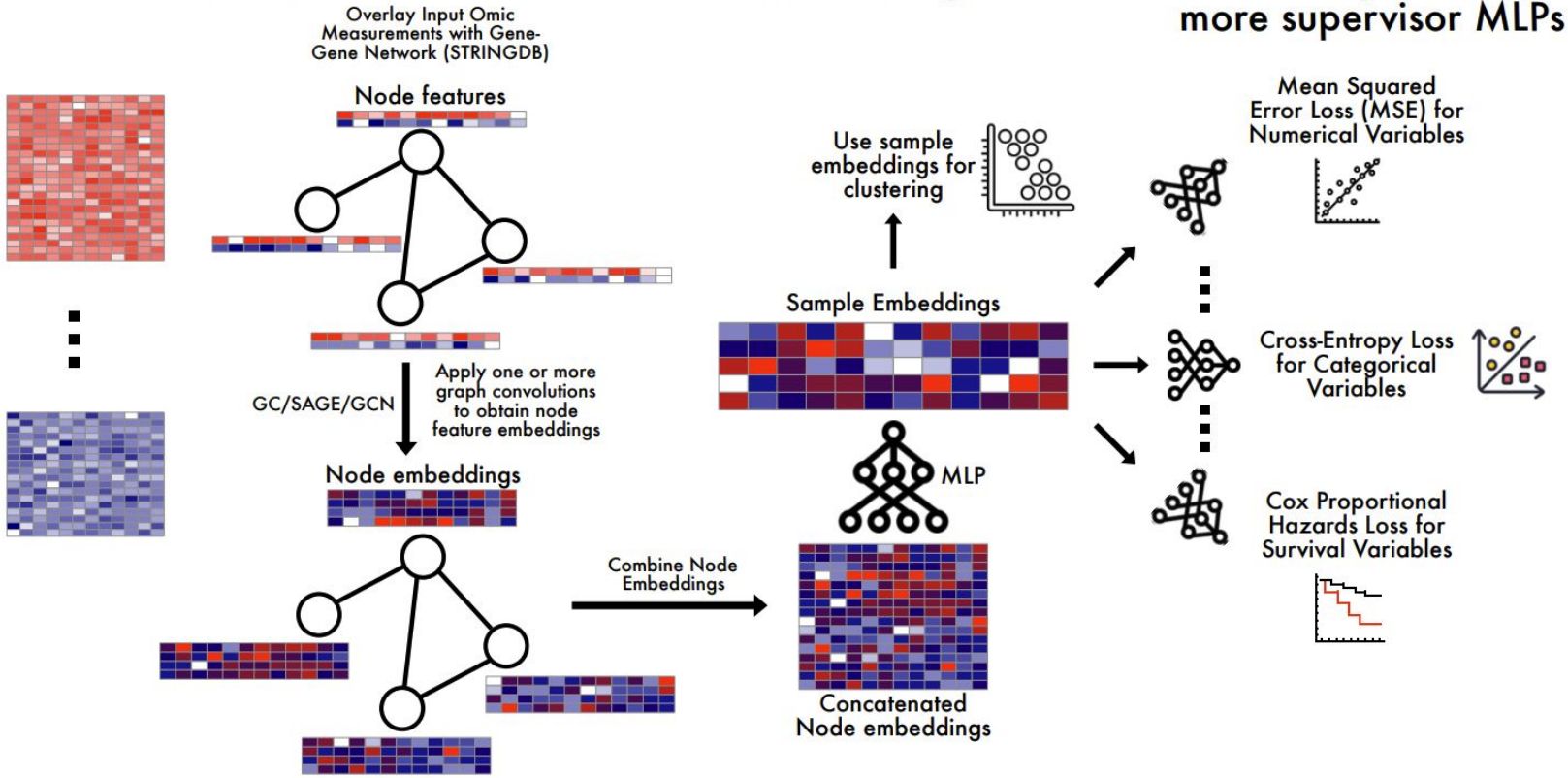
https://github.com/adambielski/siamese-triplet

Graph-convolutional Neural Networks

1.INPUT
(Multi)-modal data matrices

2.ENCODING
Derive sample embeddings

3.PREDICTION
Connect sample embeddings to one or more supervisor MLPs

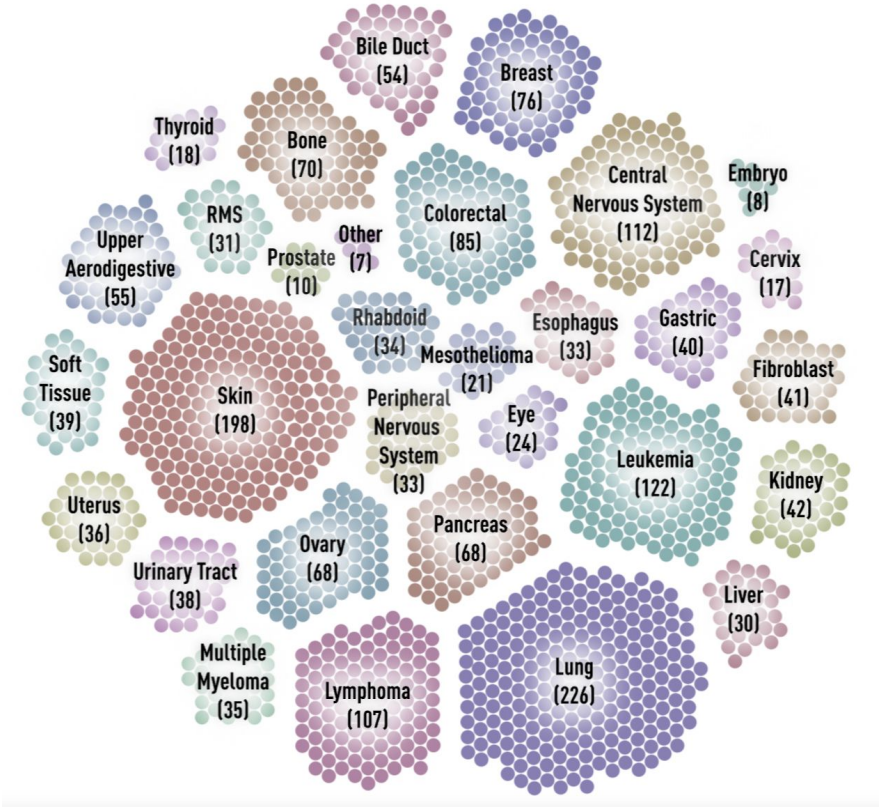


Flexynesis Command-Line Demo

Homework

https://github.com/BIMSBbioinfo/compgen_course_2025_module3/tree/main/homeworks/hw3

CCLE Cancer Cell Line Encyclopedia



GDSC²

989 cancer cell lines

453 cancer drugs (licensed and experimental)

10 years of experiment and analysis

494,973 genomic associations

386,293 drug dose response curves

Genomics of Drug Sensitivity in Cancer database in numbers