Multi-modal data integration using deep learning and applications in precision oncology

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Computational Genomics Workshop

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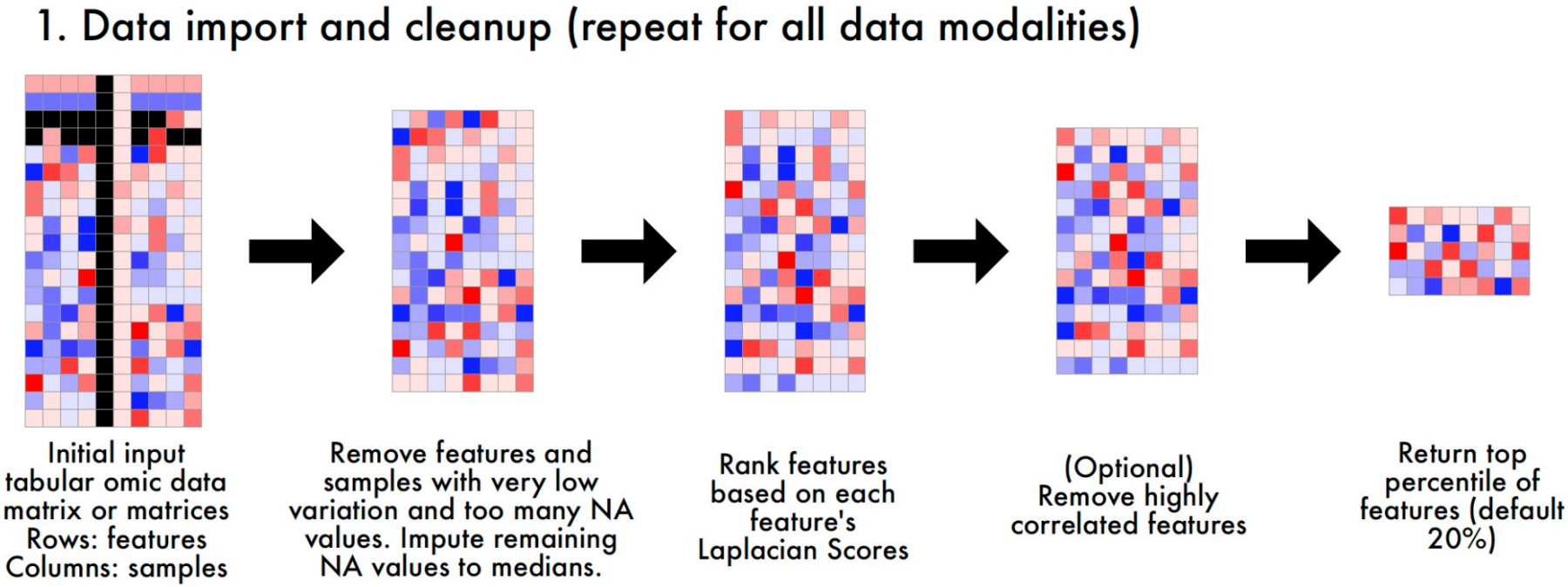
Bioinformatics & Omics Data Science Platform

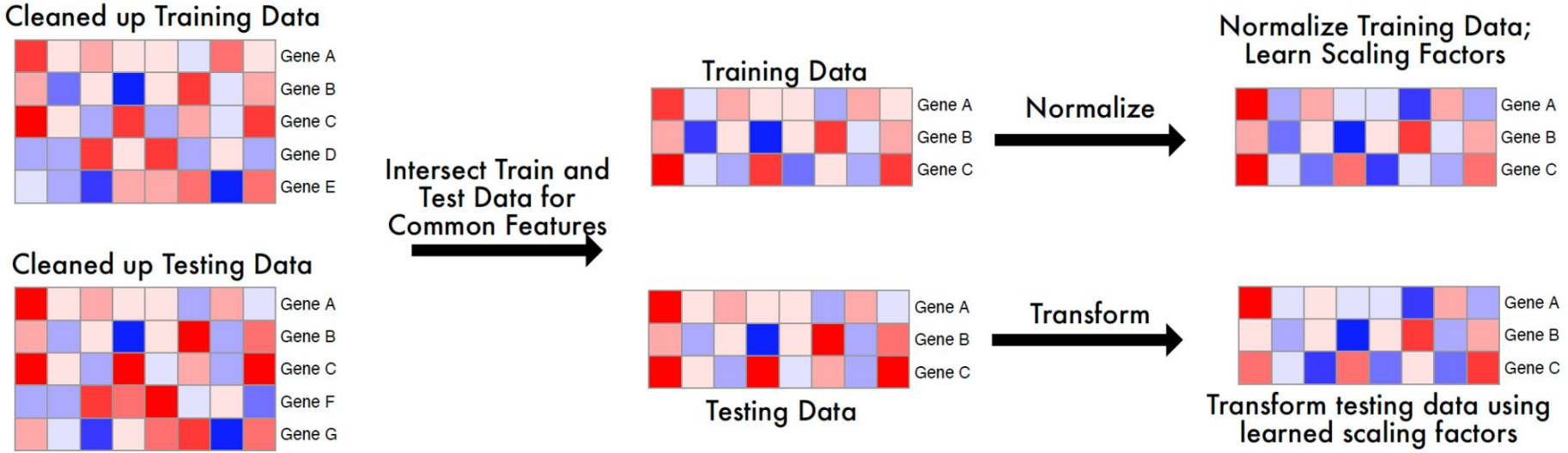
MAX DELBRÜCK CENTER

Data Import


1. Data import and cleanup (repeat for all data modalities)
Initial input tabular omic data matrix or matrices Rows: features Columns: samples
Remove features and samples with very low variation and too many NA values. Impute remaining NA values to medians.
Rank features based on each feature's Laplacian Scores
(Optional) Remove highly correlated features
Return top percentile of features (default 20%)

Data Import

2. Harmonize training and testing datasets (repeat for all data modalities)



Important Terms

Neurons/Nodes

Layers: input layer, hidden layers, output layer

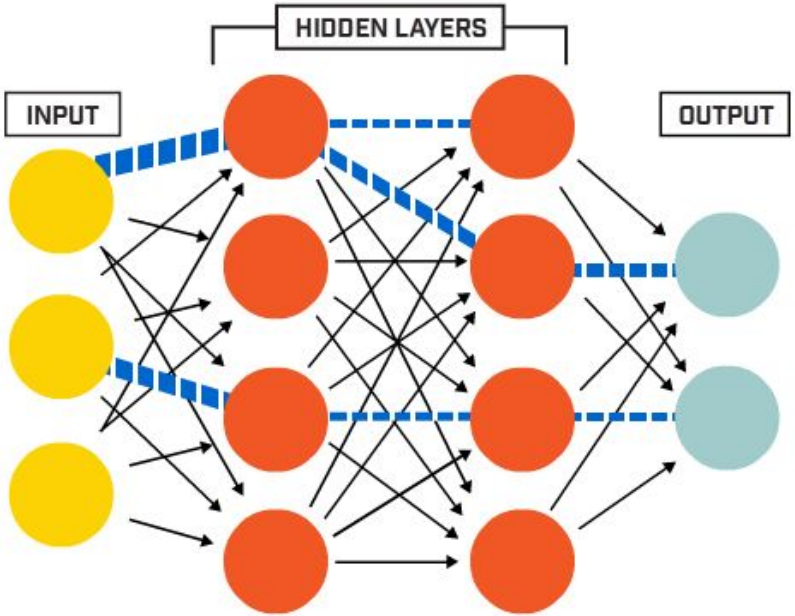
Loss functions

Learning rate

Batch size, batch iterations, epochs

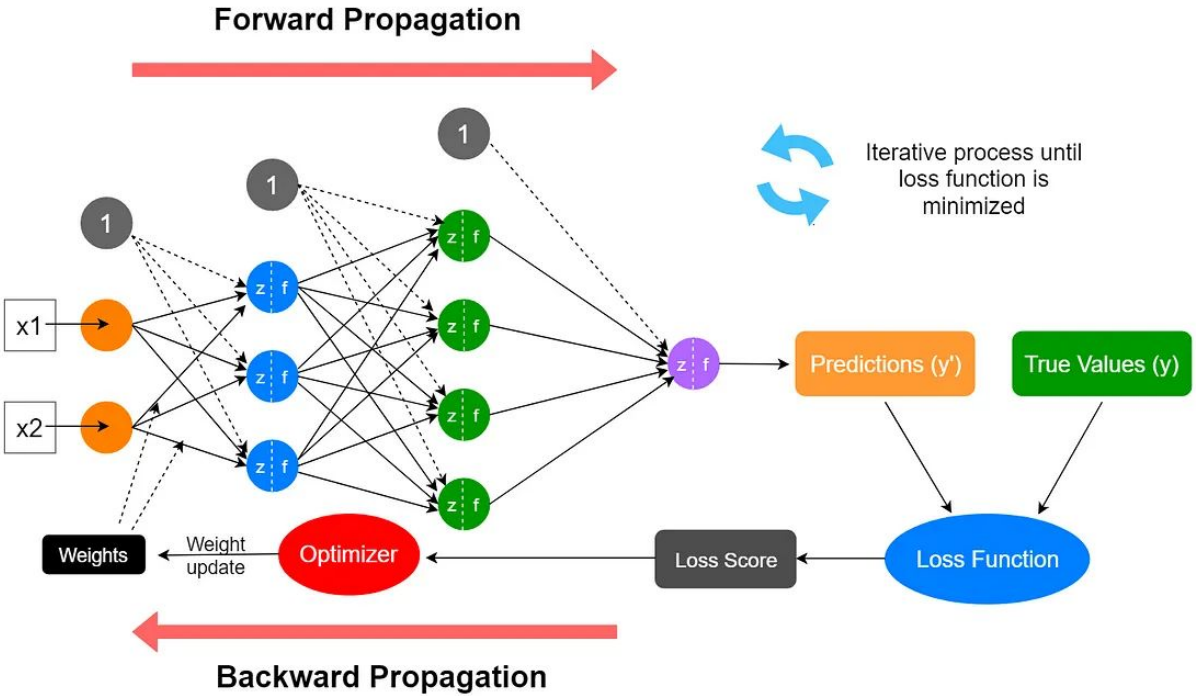
Hyperparameter optimization

Components of a neural network



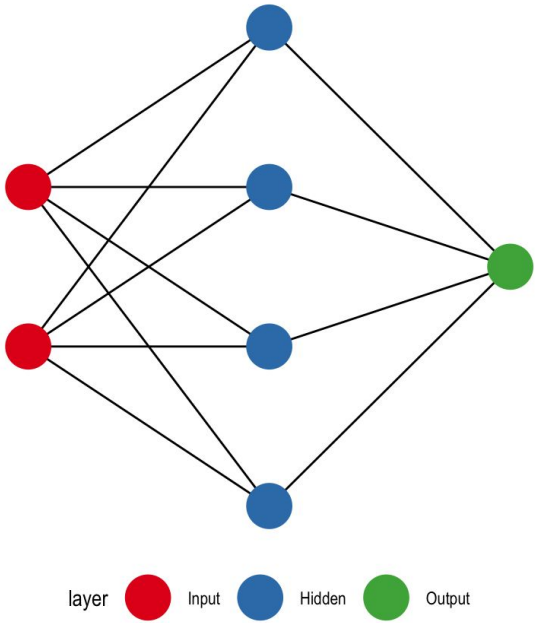
[Introduction to Neural Networks and Their Key Elements (Part-C) — Activation Functions & Layers | Towards AI]

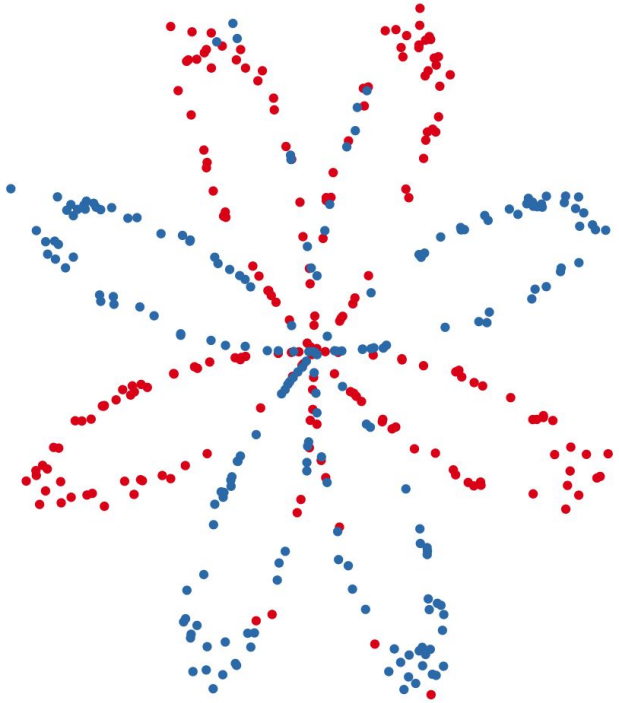
Training Process



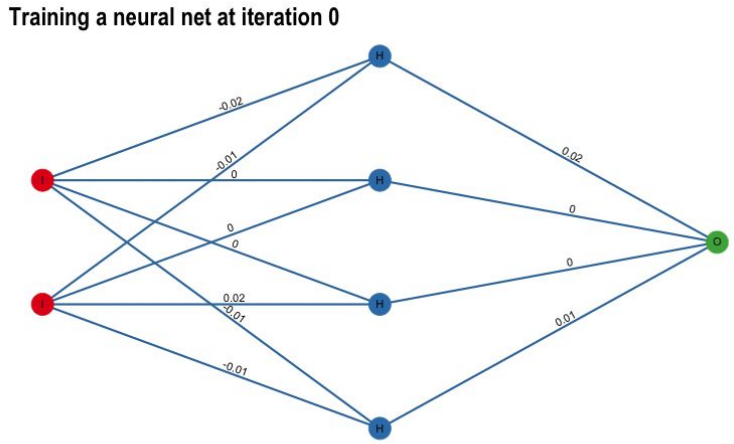
[Decoding Backpropagation and Its Role in Neural Network Learning | ml-articles – Weights & Biases]

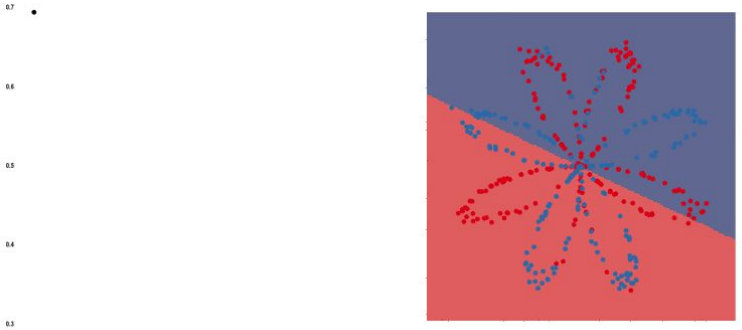
Network architecture and the problem





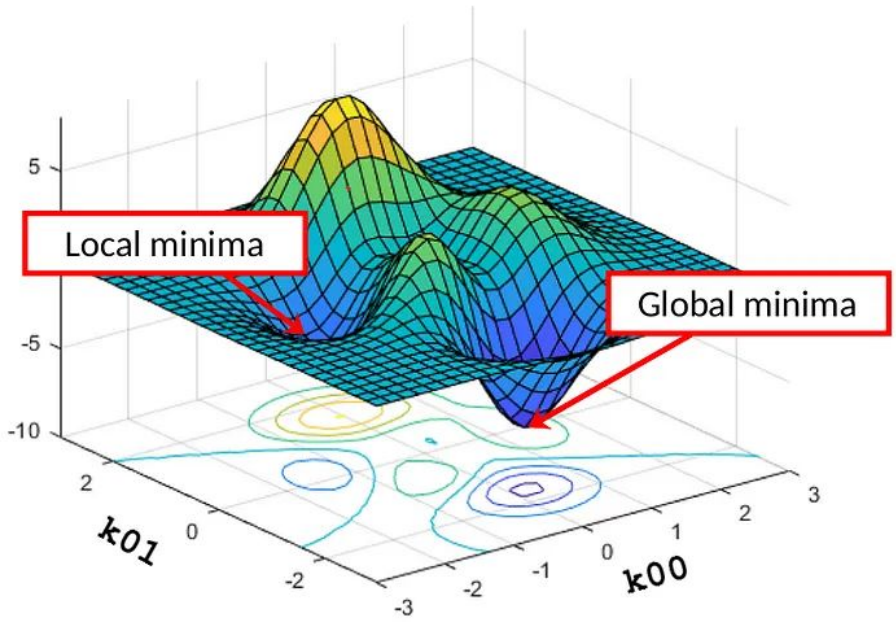
[An animated neuRal net implementation]





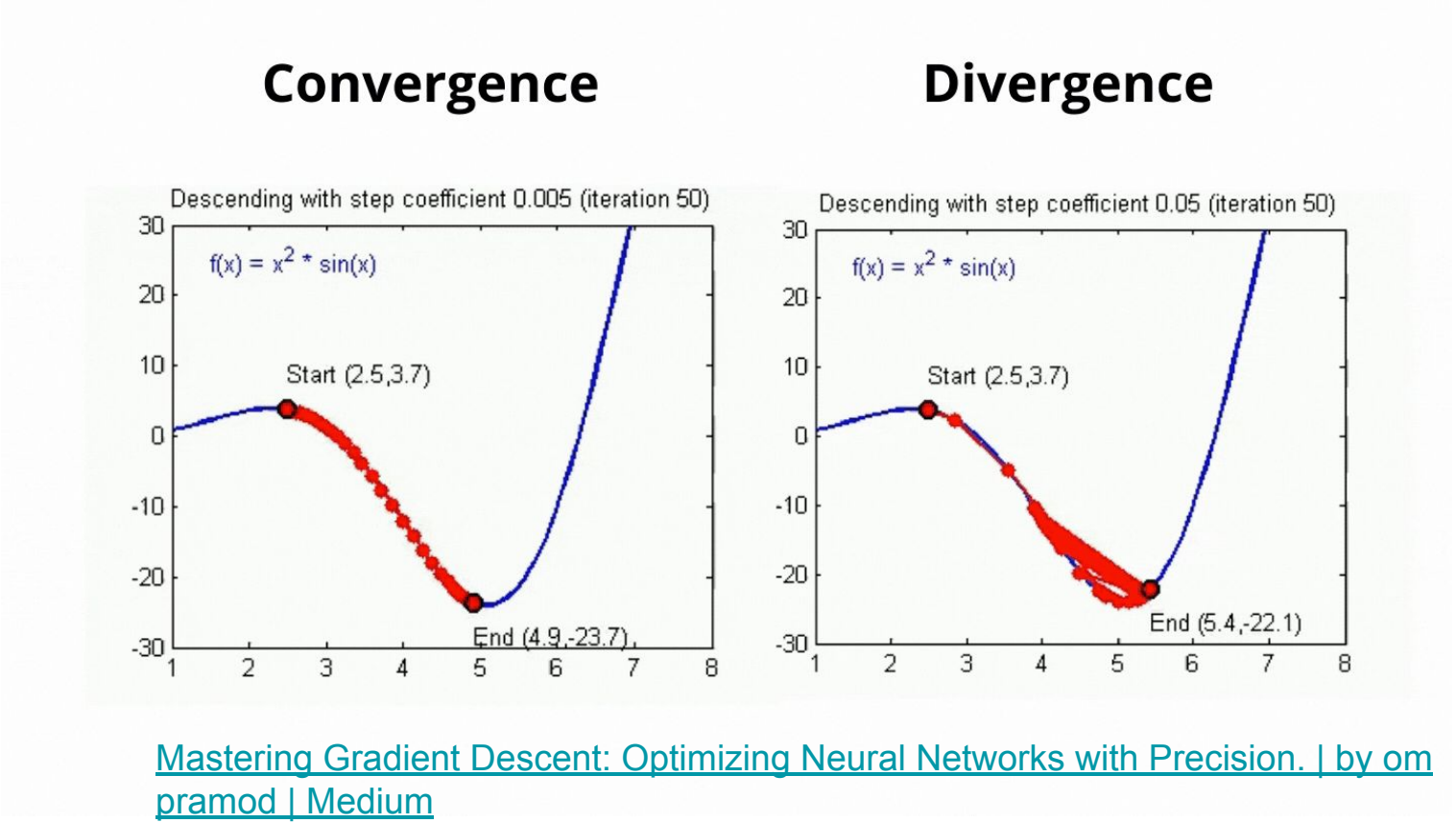
[An animated neuRal net implementation]

Gradient Descent

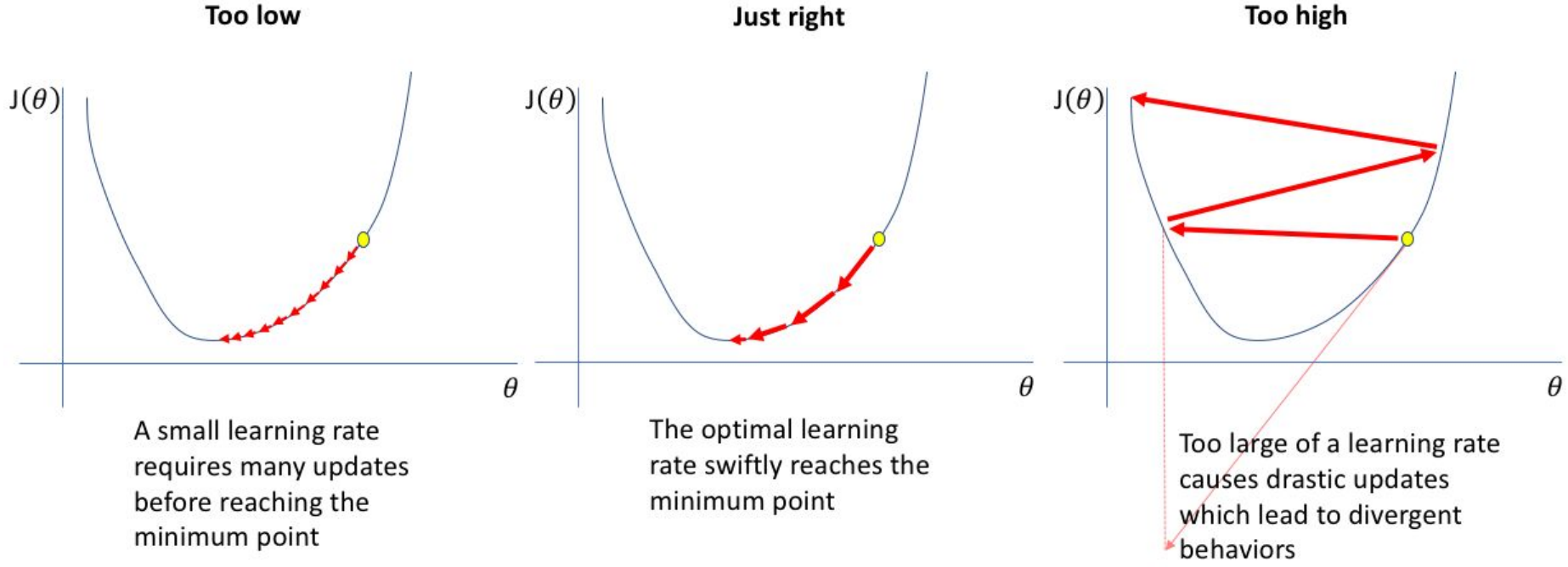


[Deep Learning from Scratch in Modern C++: Gradient Descent | by Luiz doleron | Towards AI]

Impact of the learning rate

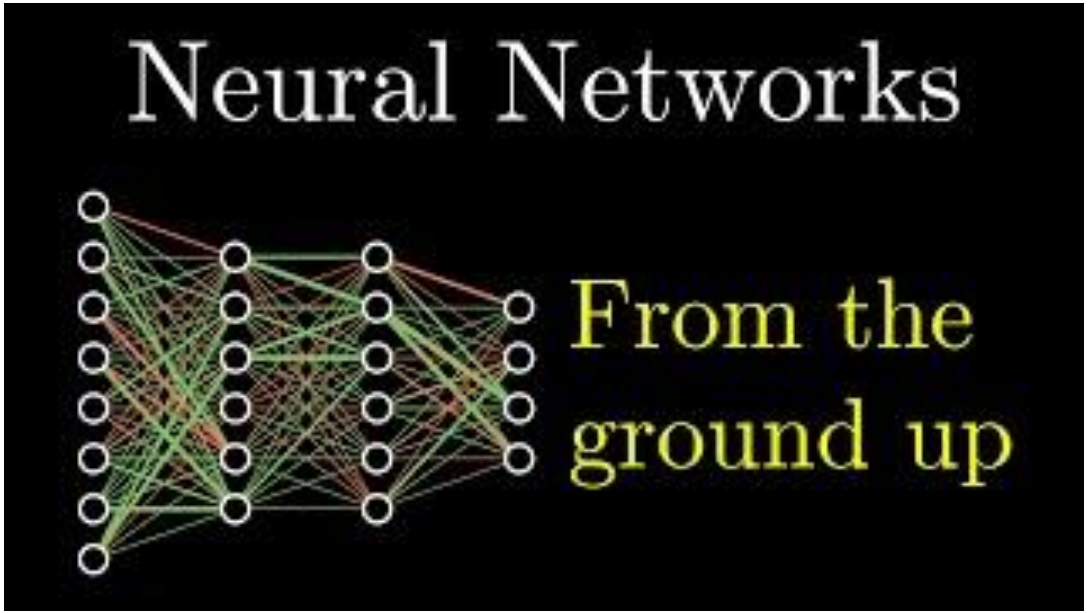


[Mastering Gradient Descent: Optimizing Neural Networks with Precision. | by om pramod | Medium]

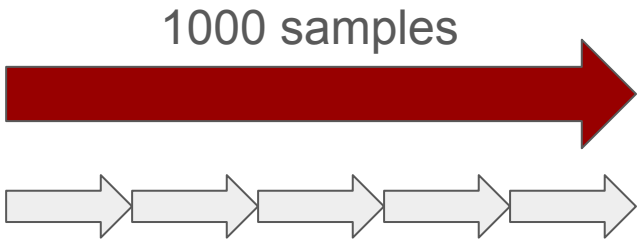


[Setting the learning rate of your neural network.]

Recommended:



Batch iterations, epochs, HPO iterations



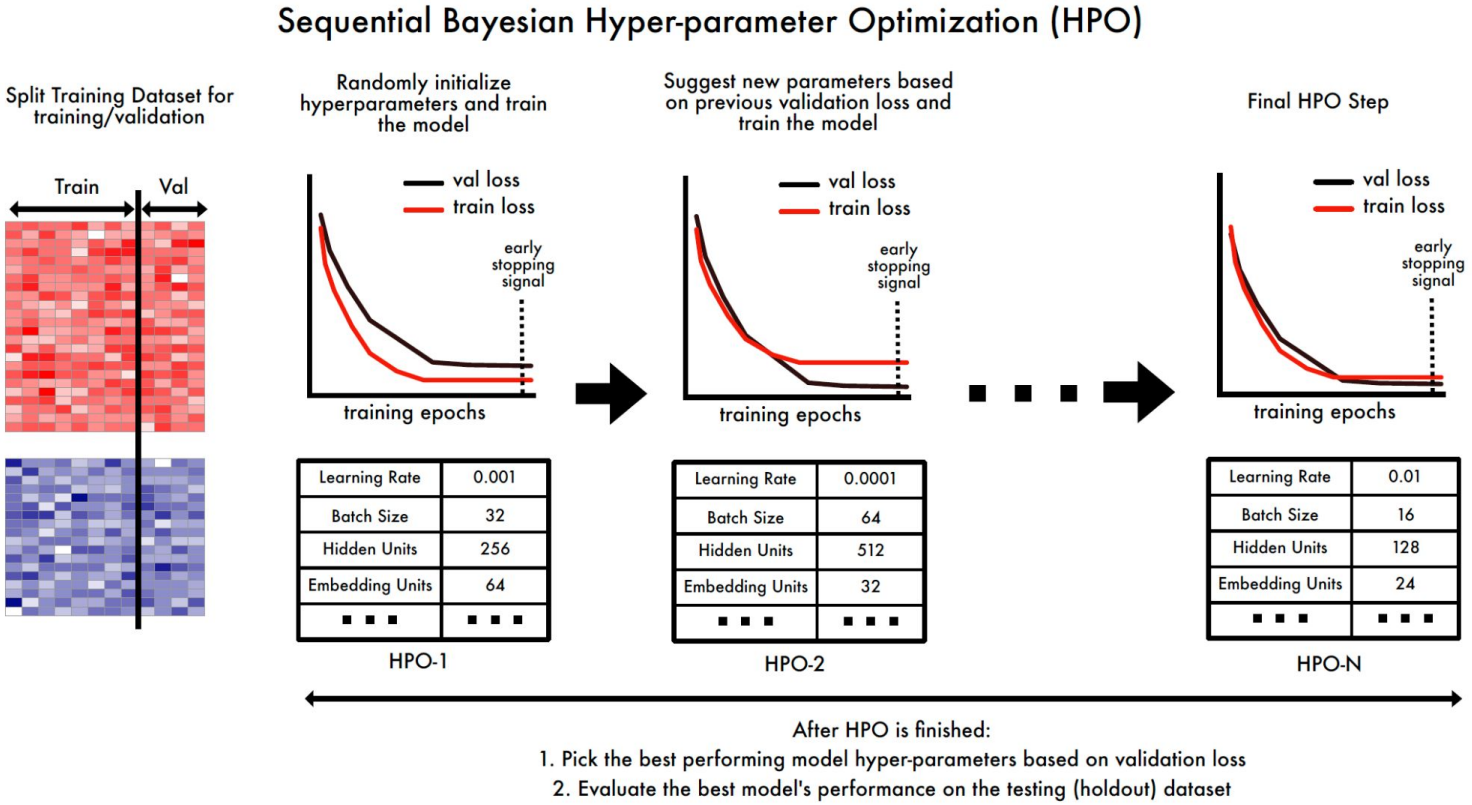
batch size: 200

5 batch iterations = 1 Epoch

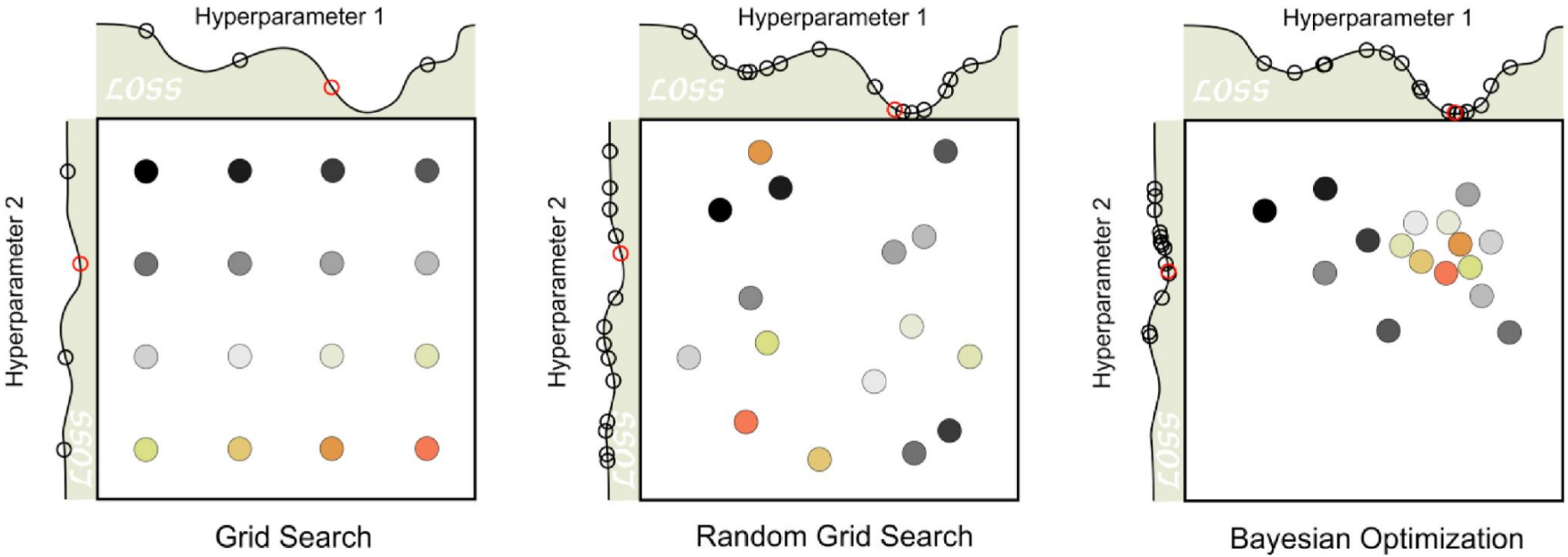
Batch iteration < Epoch < HPO iteration

[Epochs, Batch Size, Iterations - How are They Important to Training AI and Deep Learning Models]

Hyperparameter Tuning

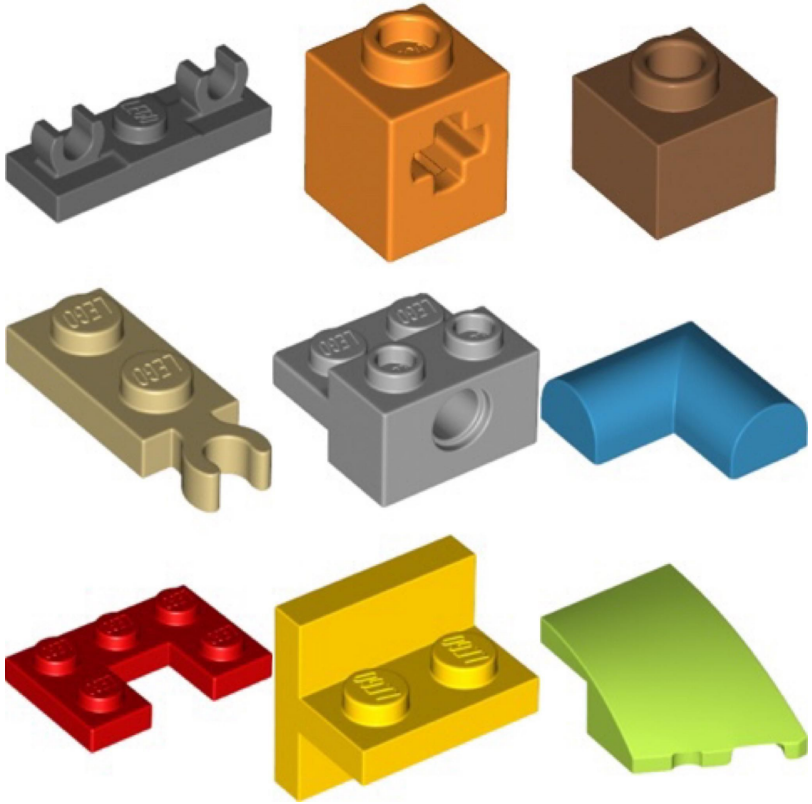


Hyperparameter tuning



[A tutorial on automatic hyperparameter tuning of deep spectral modelling for regression and classification tasks - ScienceDirect]

Neural Network Layers can be combined like Lego pieces

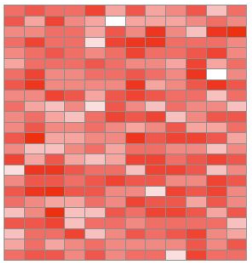


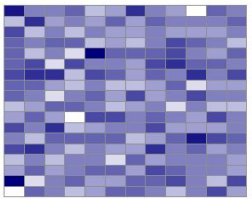
DirectPred: Standard Fully Connected Networks

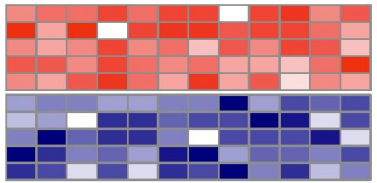
1.INPUT
(Multi)-modal data matrices

2.ENCODING
Derive sample embeddings

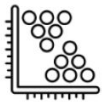
3.PREDICTION
Connect sample embeddings to one or more supervisor MLPs







Use sample embeddings for clustering



Mean Squared Error Loss (MSE) for Numerical Variables

Cross-Entropy Loss for Categorical Variables

Cox Proportional Hazards Loss for Survival Variables

Homework

https://github.com/BIMSBbioinfo/compgen_course_2025_module3/tree/main/homeworks/hw2