



Application of Neural Tangent Kernel in Medicine

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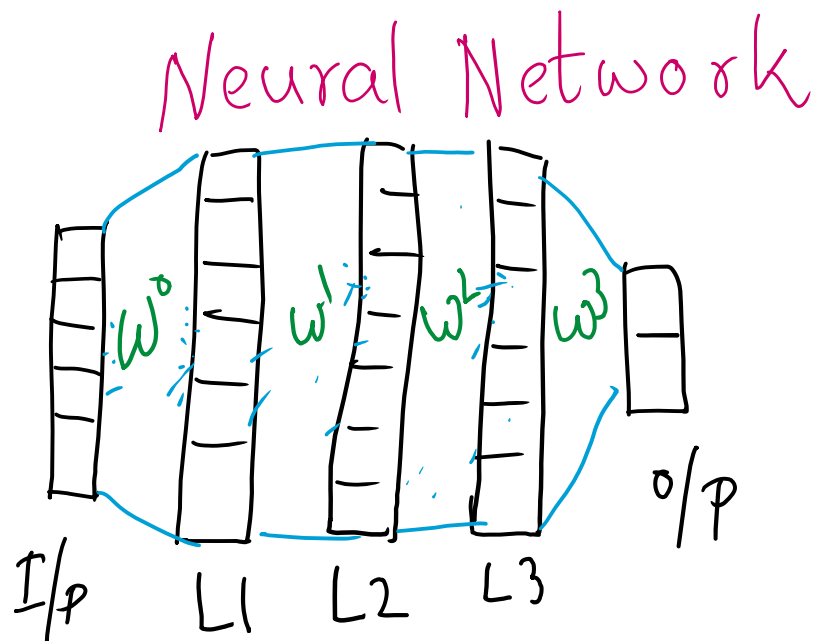
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Neural Tangent Kernel

Infinite width limit: the number of neurons in the hidden layers grow to infinity

Neural Tangent Kernel

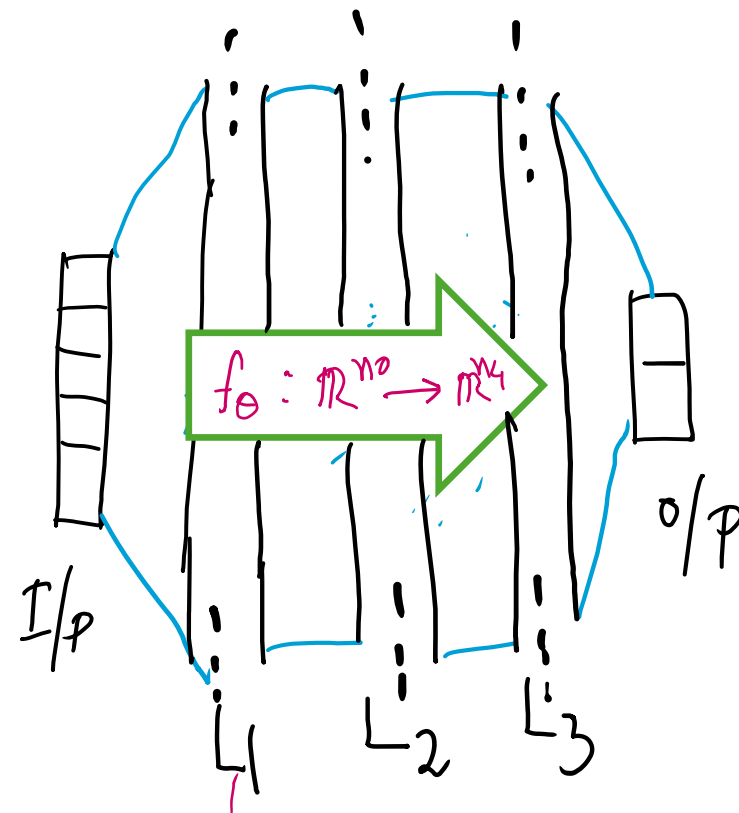
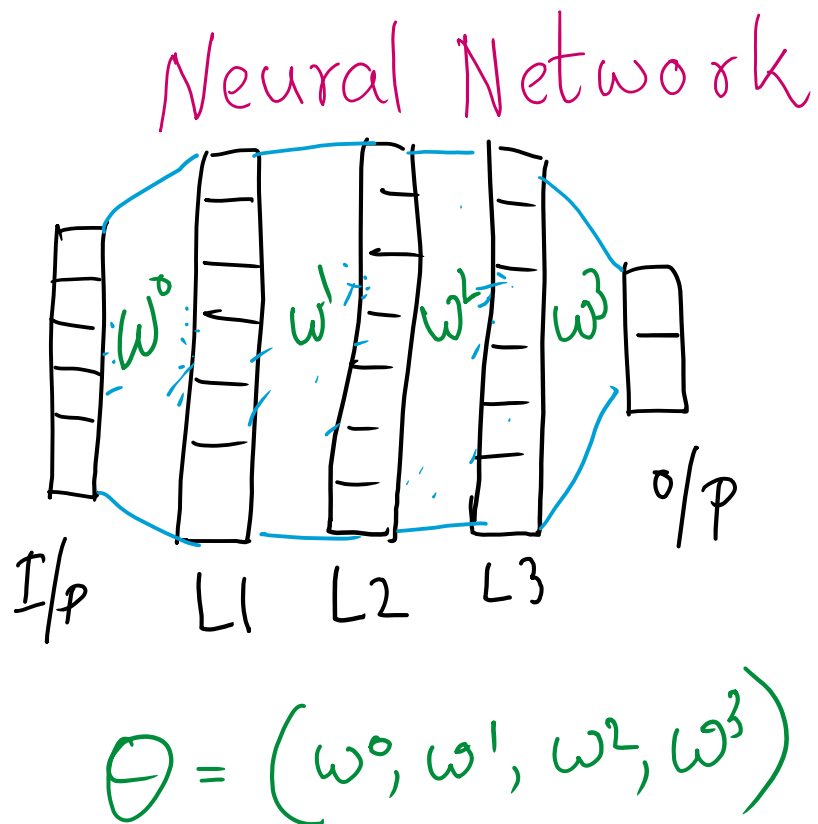
Infinite width limit: the number of neurons in the hidden layers grow to infinity in this limit



$$\Theta = (w^0, w^1, w^2, w^3)$$

Neural Tangent Kernel

Infinite width limit: the number of neurons in the hidden layers grow to infinity in this limit



Advantage of Neural Tangent Kernel (NTK)

- **Exact description:** It provides an exact description of the evolution of neural network parameters during training in the infinite-width limit (more interpretable than traditional NN).
- **Stability and theoretical insight:** It exhibits improved stability during training (small changes in the training data or parameters are less likely to cause significant fluctuations or disruptions in the training process). The stability offered by NTK analysis provides insights into convergence property, generalization behaviour and optimization algorithm.

Use of Neural Tangent Kernel (NTK)

Dr. Adityanarayanan Radhakrishnan (Thesis: “Foundations of Machine Learning: over-parameterization and Feature Learning) used NTK for **Matrix completion problem**.

Radhakrishnan A, Stefanakis G, Belkin M, Uhler C. Simple, fast, and flexible framework for matrix completion with infinite width neural networks. Proceedings of the National Academy of Sciences (PNAS). 2022 Apr 19;119(16):e2115064119.

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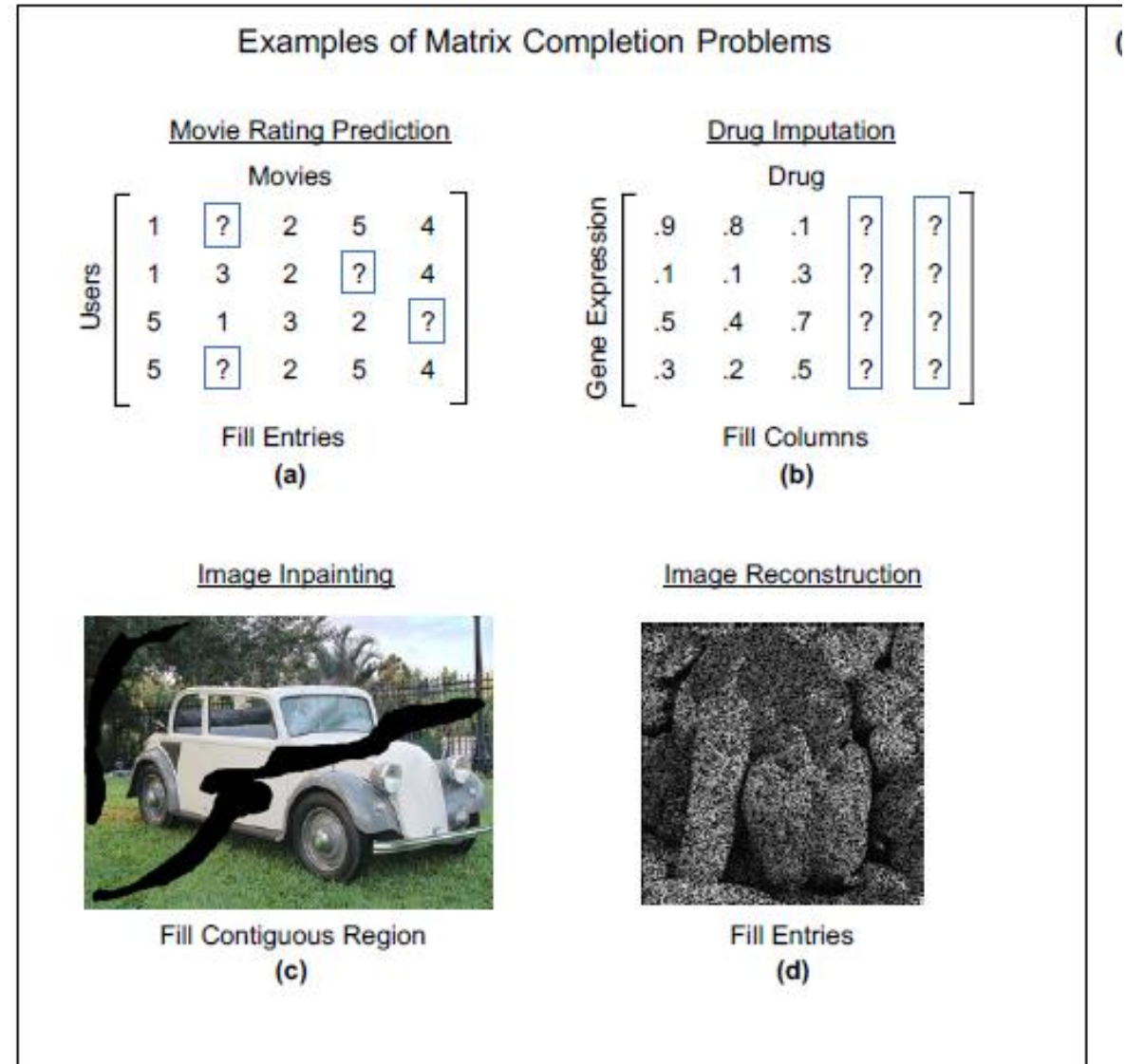
The concept of the Neural Tangent Kernel (NTK) was introduced in a paper titled “Neural Tangent Kernel: Convergence and Generalization in Neural Networks” by Arthur Jacot, Frank Gabriel, Clement Hongler in 2018 (arxiv)

Matrix completion problem

Matrix completion refers to the task of **filling in missing entries or reconstructing** a partially observed matrix from available data.

Matrix completion techniques typically involve optimization algorithms that minimize a loss function to reconstruct the missing entries in the matrix.

Dr. Radhakrishnan A's thesis



Matrix completion problem in Medicine

In medicine, matrix completion problems arise in various scenarios where incomplete data needs to be reconstructed or inferred to support diagnosis, treatment planning and healthcare research.

**Precision
medicine**

In pharmacogenomics and personalized medicine, it's crucial to know how people **react to drugs to make treatments better and reduce side effects.**

Gene

Drug

	G1	G2	Gn
D1	resp	resp	resp	resp	resp
D2	resp	resp	?	resp	resp
..	resp	resp	resp	resp	resp
..	resp	resp	?	resp	resp
Dn	resp	resp	resp	resp	resp

Matrix completion problem in Medicine

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**Precision
medicine**

Medical Image

Imaging data might have **some missing or damaged parts** because of movements during scans, limitations in equipment, or scans that weren't finished

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**Precision
medicine**

Medical Image

**Clinical trials
Design & Analysis**

Incomplete data or patient dropouts in clinical trials can undermine the reliability and statistical power of the results, even though these trials collect diverse information about patients' backgrounds, medical histories, treatments, and outcomes to evaluate new therapies.

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Medical Image

**Clinical trials
Design & Analysis**

**Electronics Health
Records**

Matrix completion techniques can **fill in missing values in electronic health records**, allowing for a more thorough analysis of **patient health profiles and treatment outcomes**, despite the data often being incomplete due to errors, incomplete documentation, or privacy concerns.

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**Precision
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Medical Image

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**Bio-medical Data
Integration**

Biomedical research generates **diverse datasets** from **genomics, proteomics, metabolomics, and other -omics technologies**, as well as **clinical data, environmental factors, and lifestyle** information. Integrating these **heterogeneous data sources** into comprehensive models for disease risk prediction, biomarker discovery, and treatment optimization requires **addressing data sparsity and incompleteness**

Drug-Gene Response Matrix Completion Using NTK Python Code