Munich Center for Machine Learning

LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

From Statistical Modeling to Deep Learning

David Rügamer, LMU Munich and MCML

Workshop @ TU Dortmund, Oct 12, 2023

Data Science Group @ LMU Munich

https://datascience-lmu.github.io/website/

My Research:

38% Statistics

- Post-Selection Inference
- Model Selection
- Functional Data Analysis
- Neural Statistical Models

30% Deep Learning

- Semi-Structured Models
- Generative Models
- Deep Probabilistic Models
- Representation Learning

18% Applications

- Biomechanics
- Medical Research
- Psychology

14% Machine Learning

- Boosting
- AutoML

More than 50% at the intersection

t1p.de/dl_handout | t1p.de/dl_notebook

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This Workshop

What’s Deep Learning (good for)?

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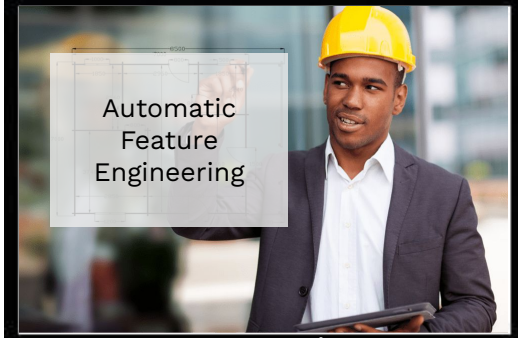
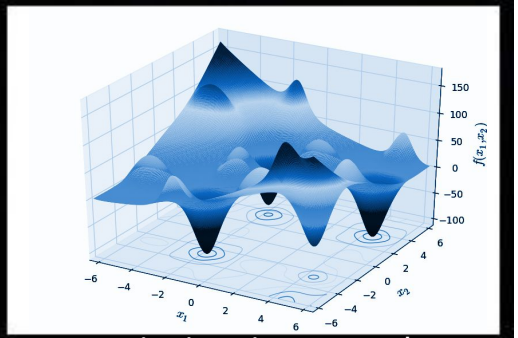
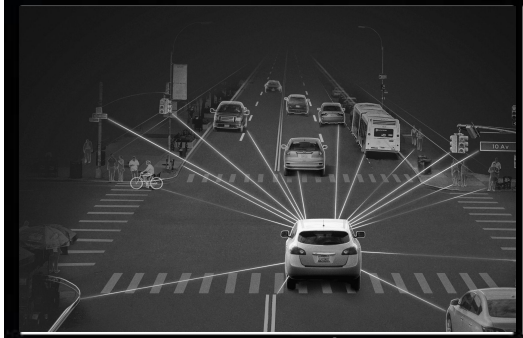


Pragmatist

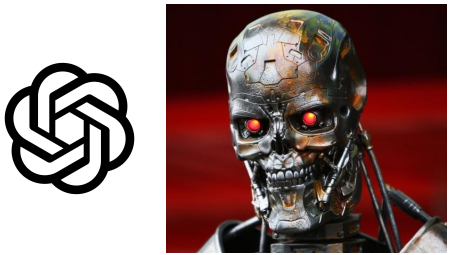
Enthusiast



Optimization Oracle



AI Researcher



General Public

?

Statistical Modeller

Prerequisites

- Linear Models
- Statistical Modeling (basics)
- Machine Learning (basics)
- R

Learning Goals

- When to use Deep Learning / Neural Networks
- Foundations of Neural Networks
- Neural Networks from a Statistical Point of View
- Semi-Structured Neural Networks
- Practical Implementation of Neural Networks

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Google Colab Link

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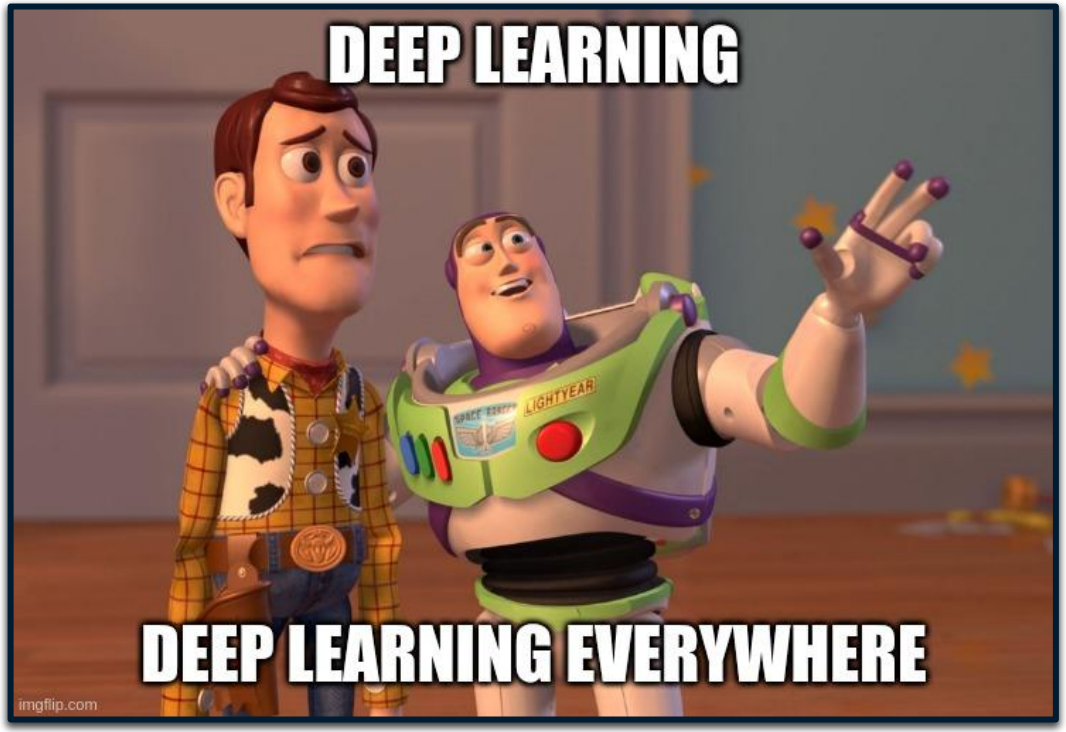
copy notebook and run
the first two chunks

Why (not) Deep Learning


DEEP LEARNING
DEEP LEARNING EVERYWHERE
LIGHTYEAR
imgflip.com

Deep Learning “Taxonomy”

Deep Learning

= Learning with neural networks that are deep

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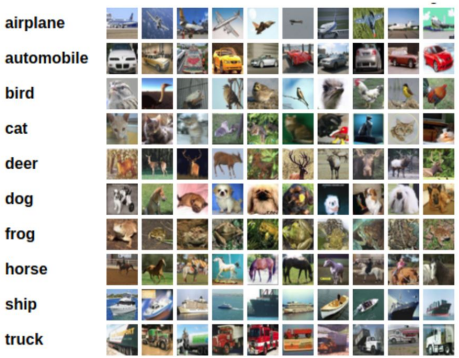
Deep Learning

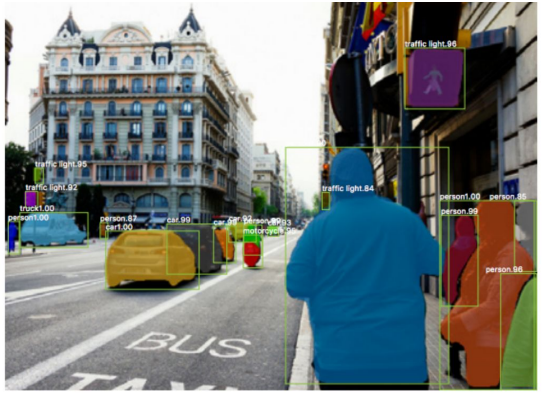
= Learning with neural networks that are deep

Deep ⇒ different definitions, most common:
… at least one hidden layer
… at least two hidden layers

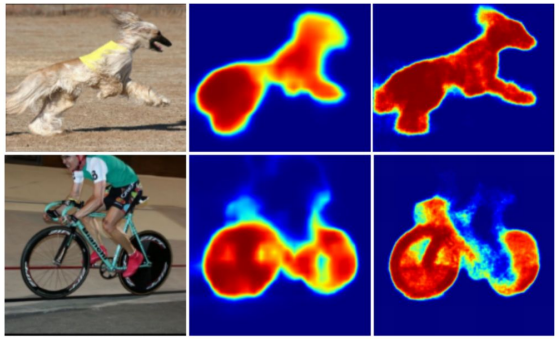
Possible Use-Cases



Credit: Alex Krizhevsky (2009)



Credit: Kaiming He (2017)



Credit: Hyeonwoo Noh (2015)

Positive

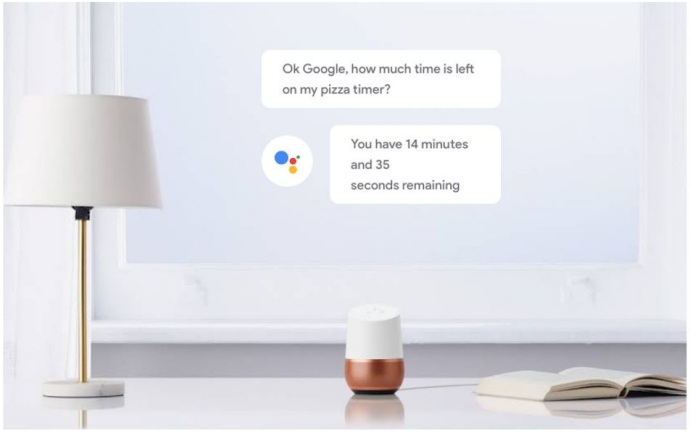
Great job! Your customer support is fantastic.

Neutral

Not bad, but it should be improved in the future.

Negative

The worst customer service I have ever seen.



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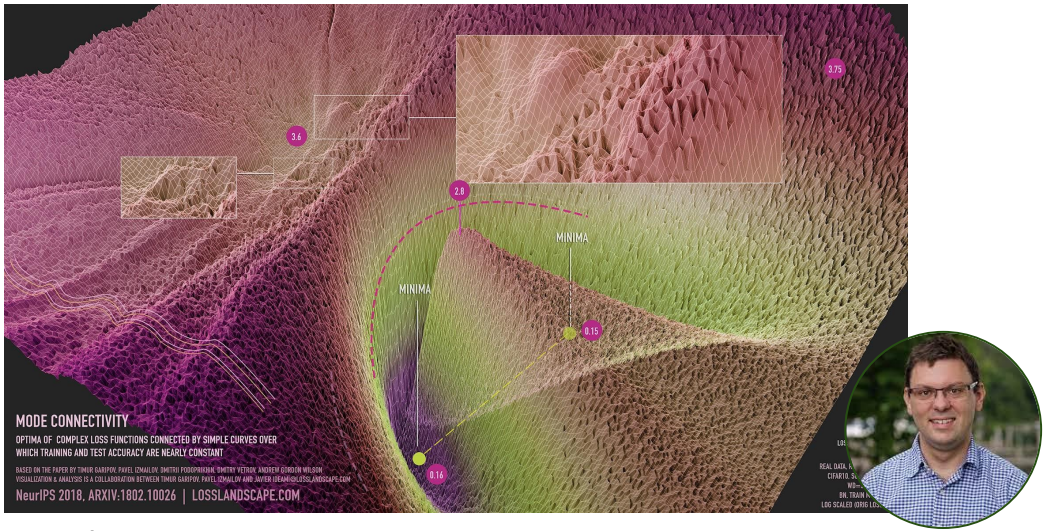

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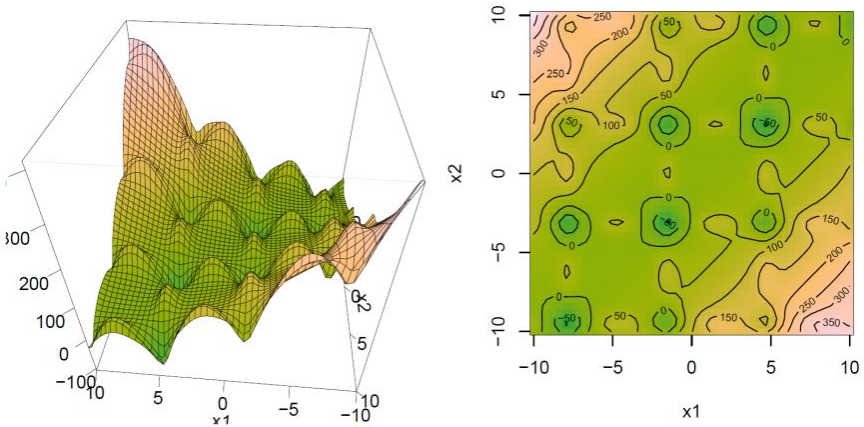
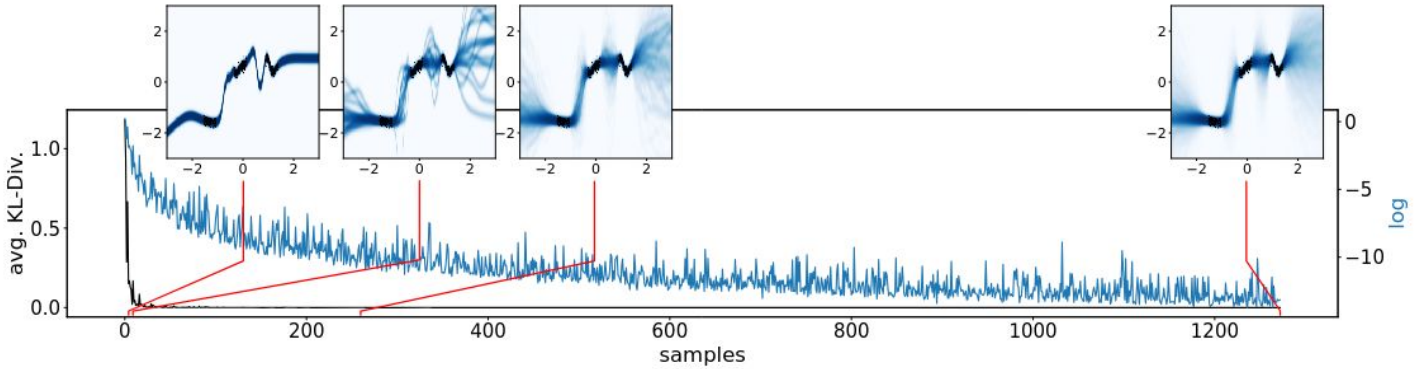


[7] **Best Paper @ ECML-PKDD 2023**



Why ~~not~~ Deep Learning

Flexibility & Automation

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Flexibility & Automation

- Data modalities (Text, Images, Audio, Video, ...)
- Modularity
- Scalability
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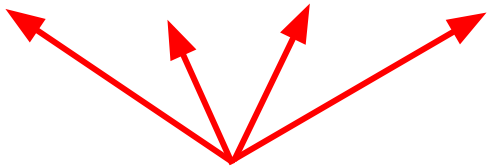

Often no way around Automation

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Generative Models?

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Generative Models?

(a) *"Large pleural effusion is in the right lower lung. A pacemaker is in the left upper chest."*

(b) *"Acute cardiomegaly."*

(c) *"Prominent left-sided atelectasis."*

(d) *"Mass filling is in the upper zone of the right lung."*

(e) *"Pneumonia is in the right lung."*

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[5]

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Generative Models?
Yes, but

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Generative Models?
Yes, but

- not the focus of today's session
- requires enormous amounts of data

Why ~~not~~ Deep Learning

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- Optimization

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- Optimization
  - ➢ Implicit Regularization ... leads to
  - ➢ ... Benign Overfitting [7]
  - ➢ ... Better test error in linear models than Lasso/Ridge

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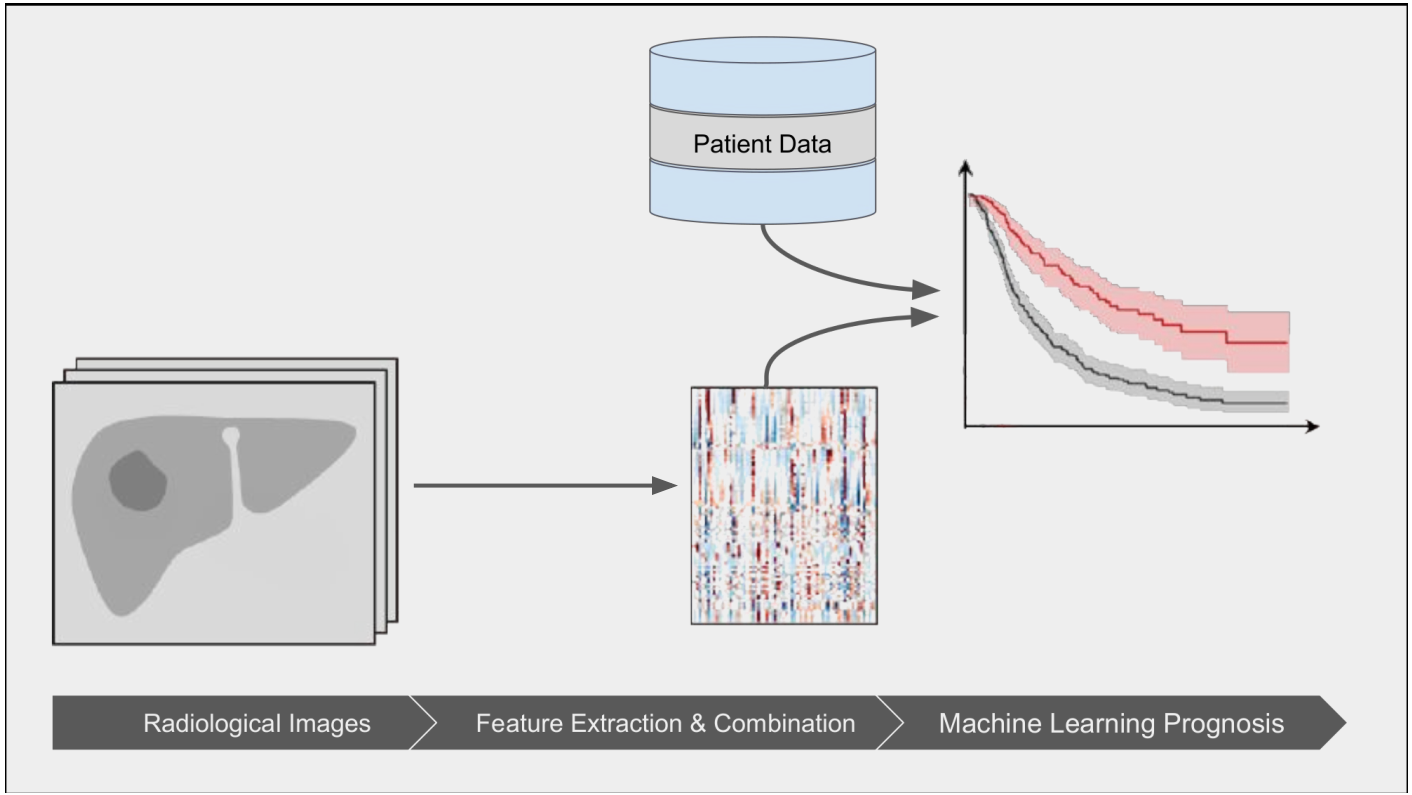
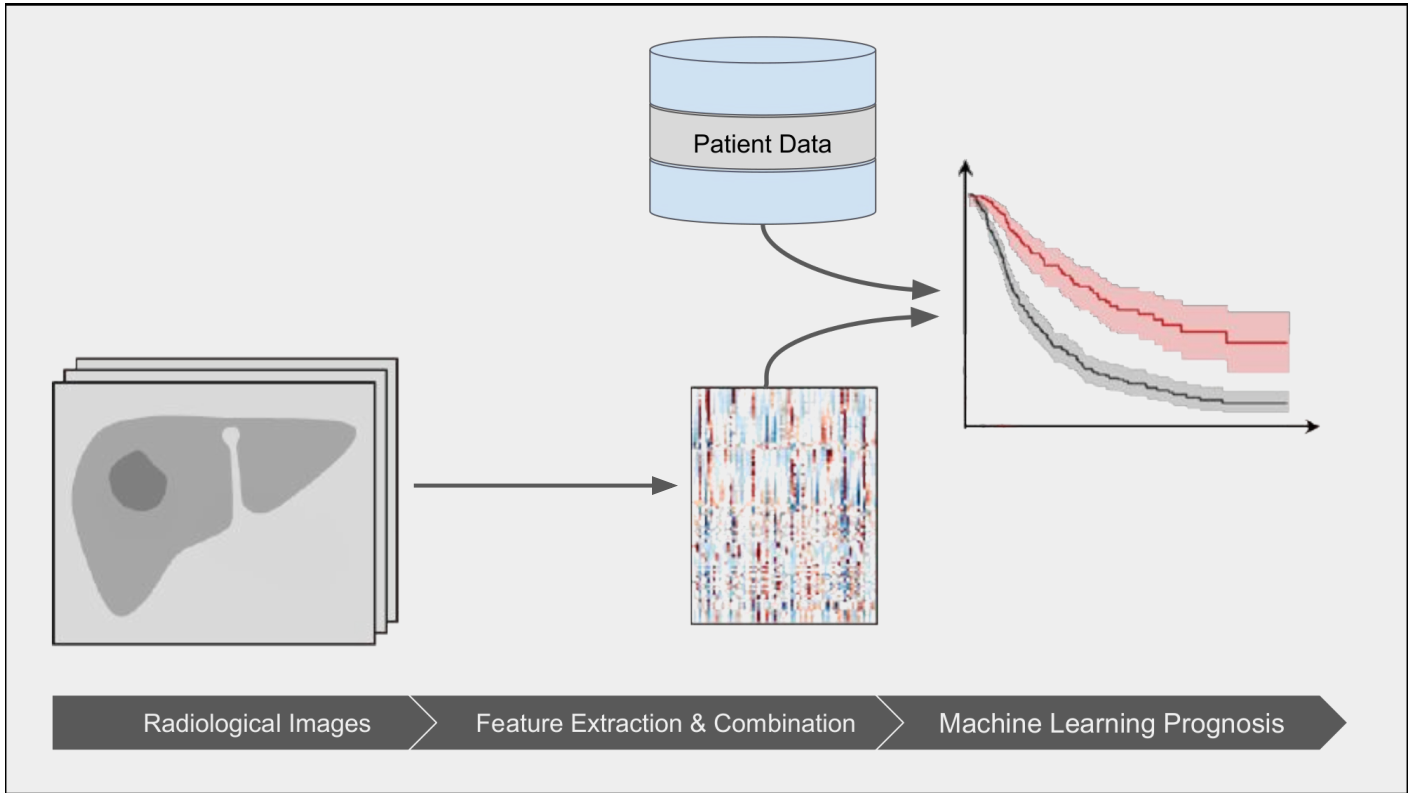
⇒ Deep Learning and Neural Networks — for Statistical Modeling

Motivating Example: Multimodal Data Sets



Prof. Ingrisch (LMU)
Clinical Data Science

Motivating Example: Multimodal Data Sets

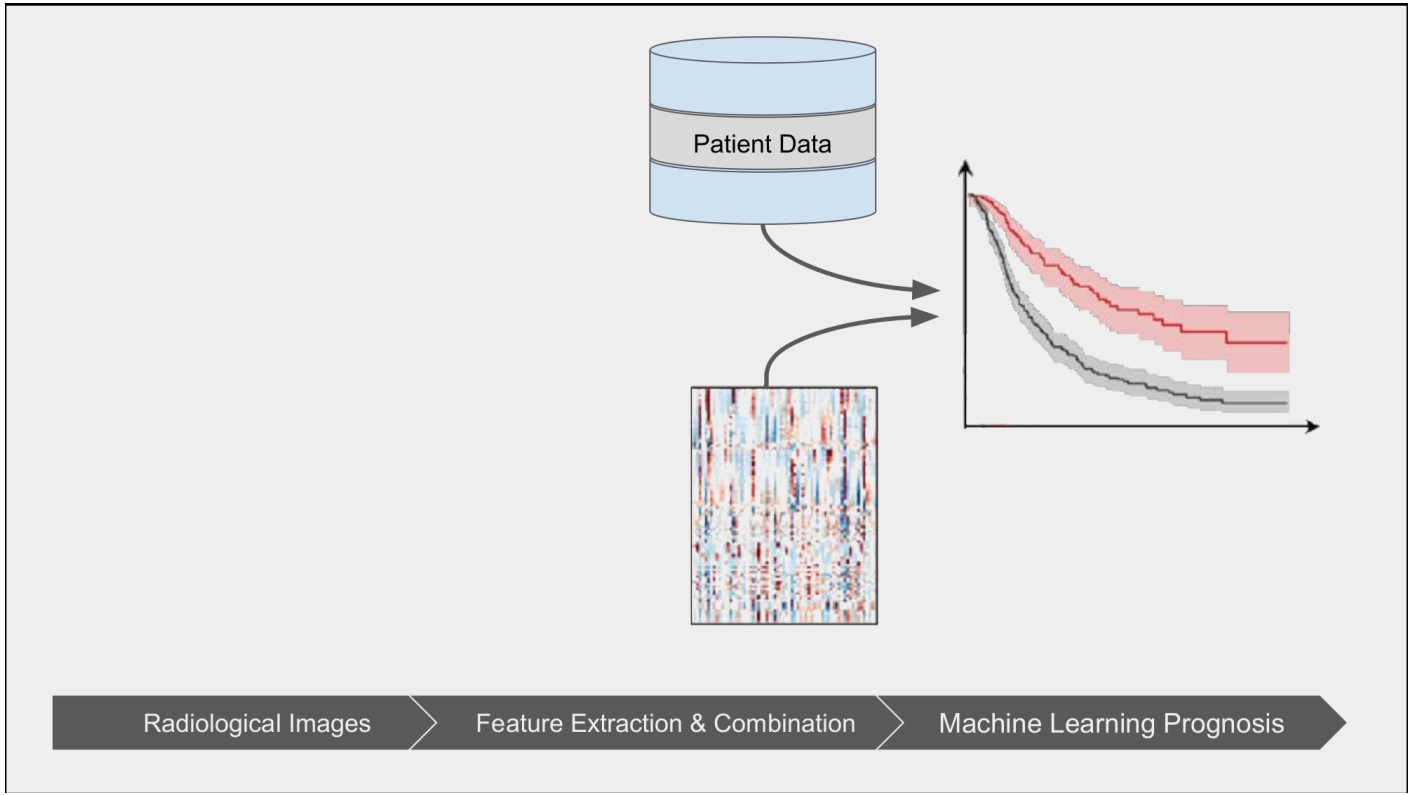


Motivating Example: Multimodal Data Sets

Radiomics

Radiological Images → Feature Extraction & Combination → Machine Learning Prognosis

Motivating Example: Multimodal Data Sets



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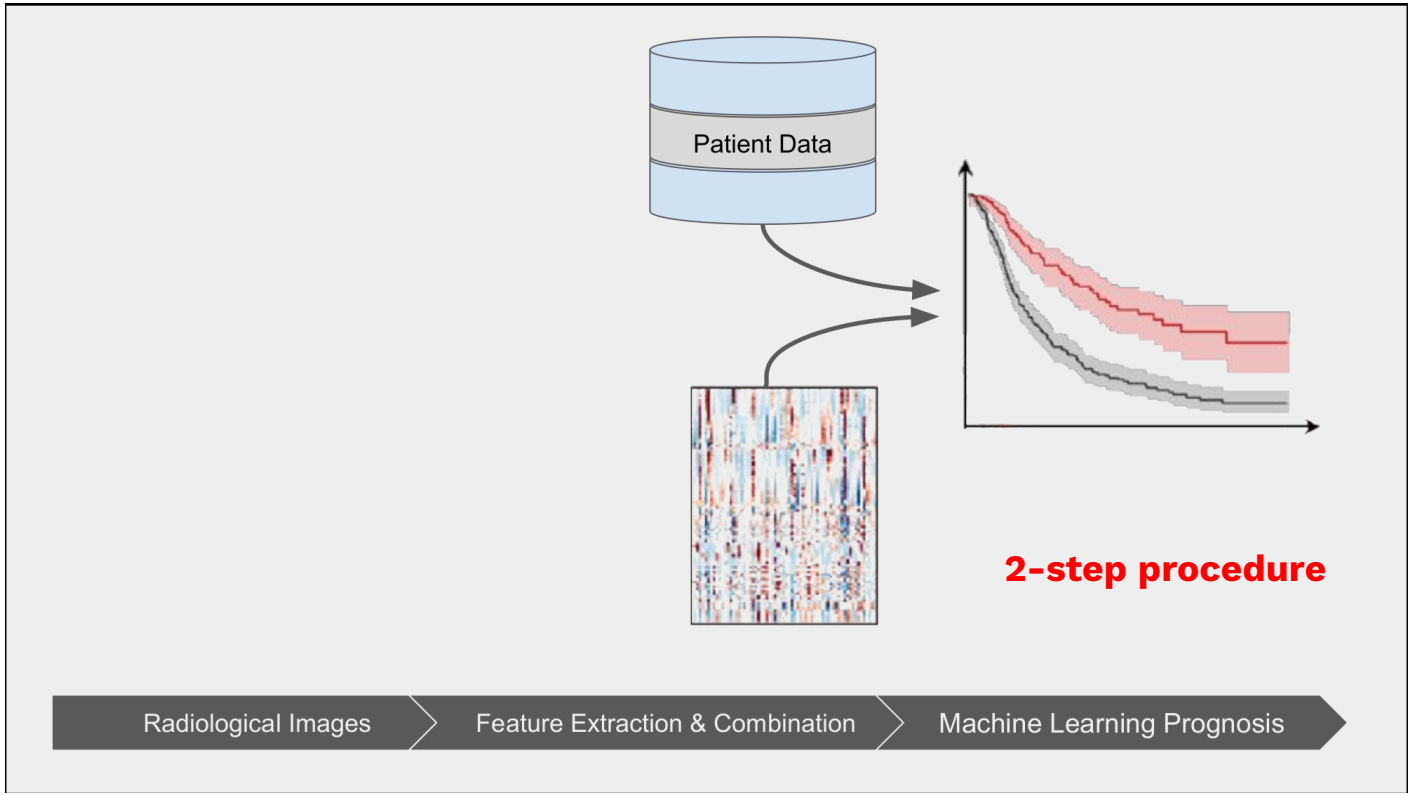

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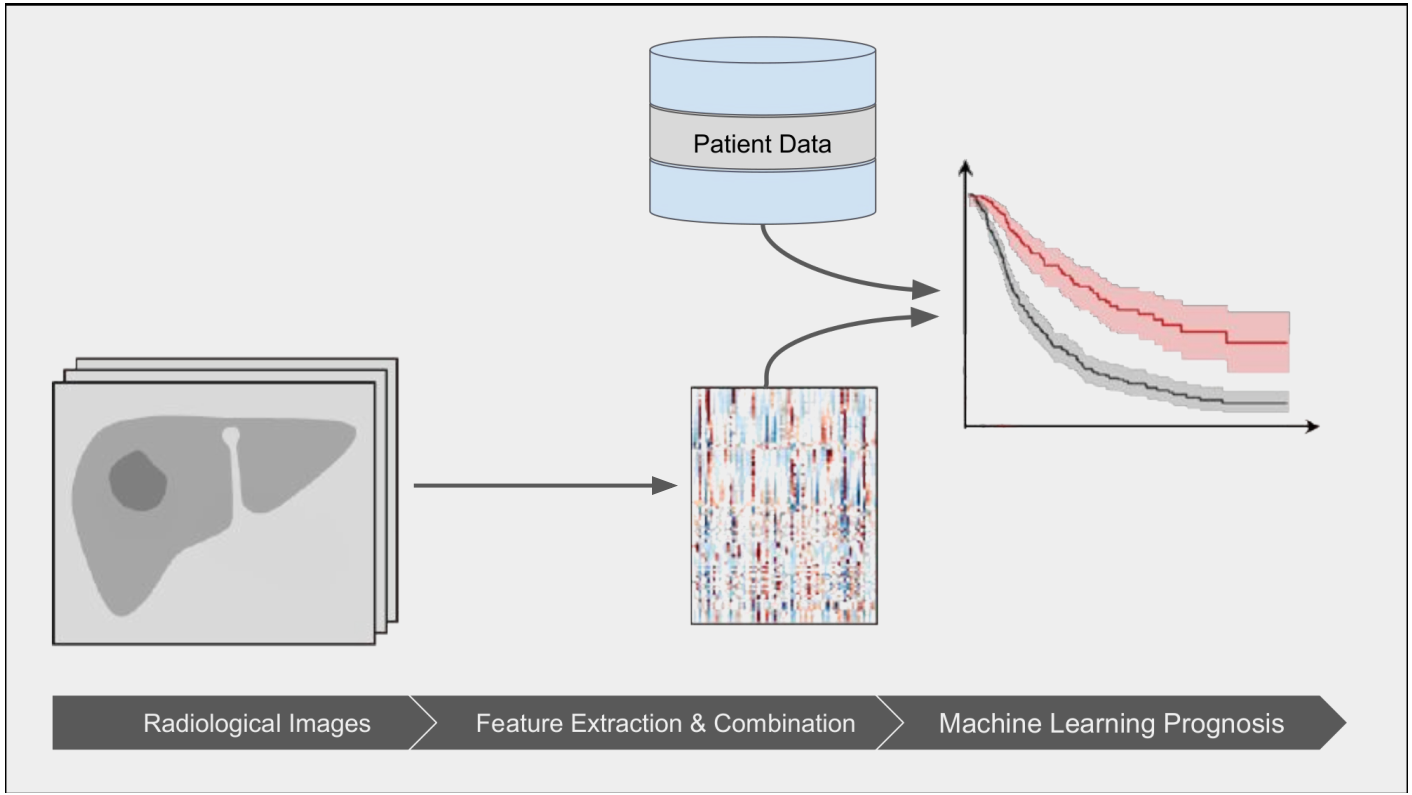

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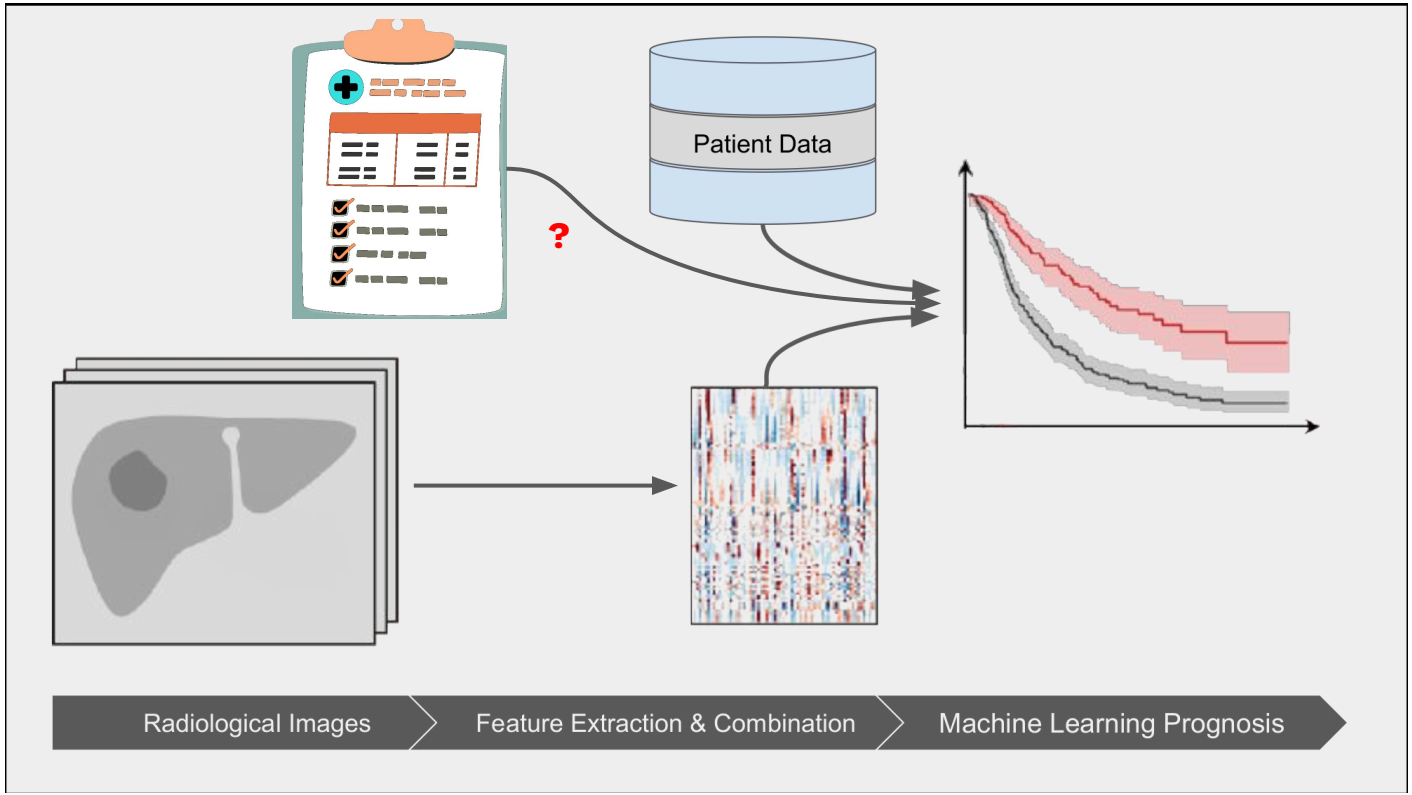

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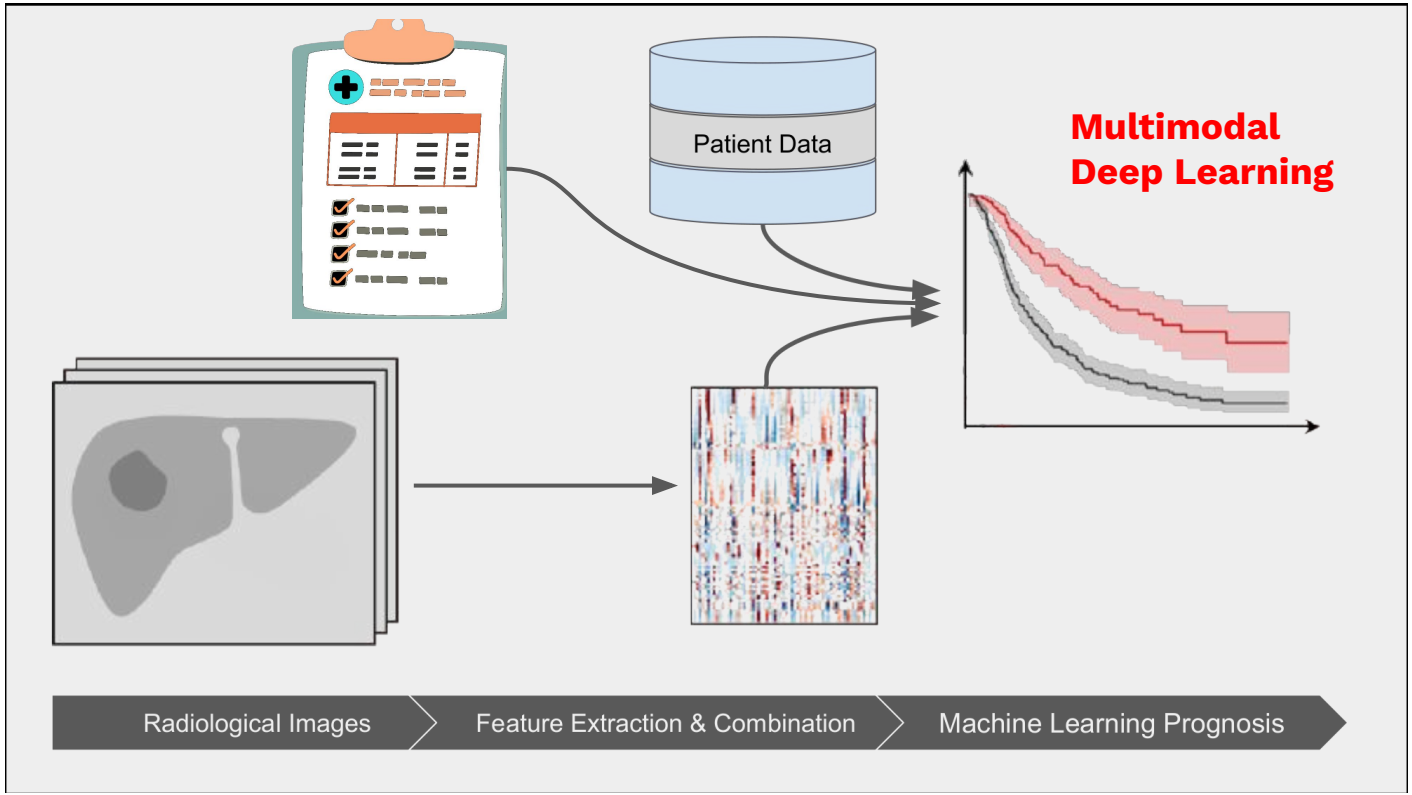

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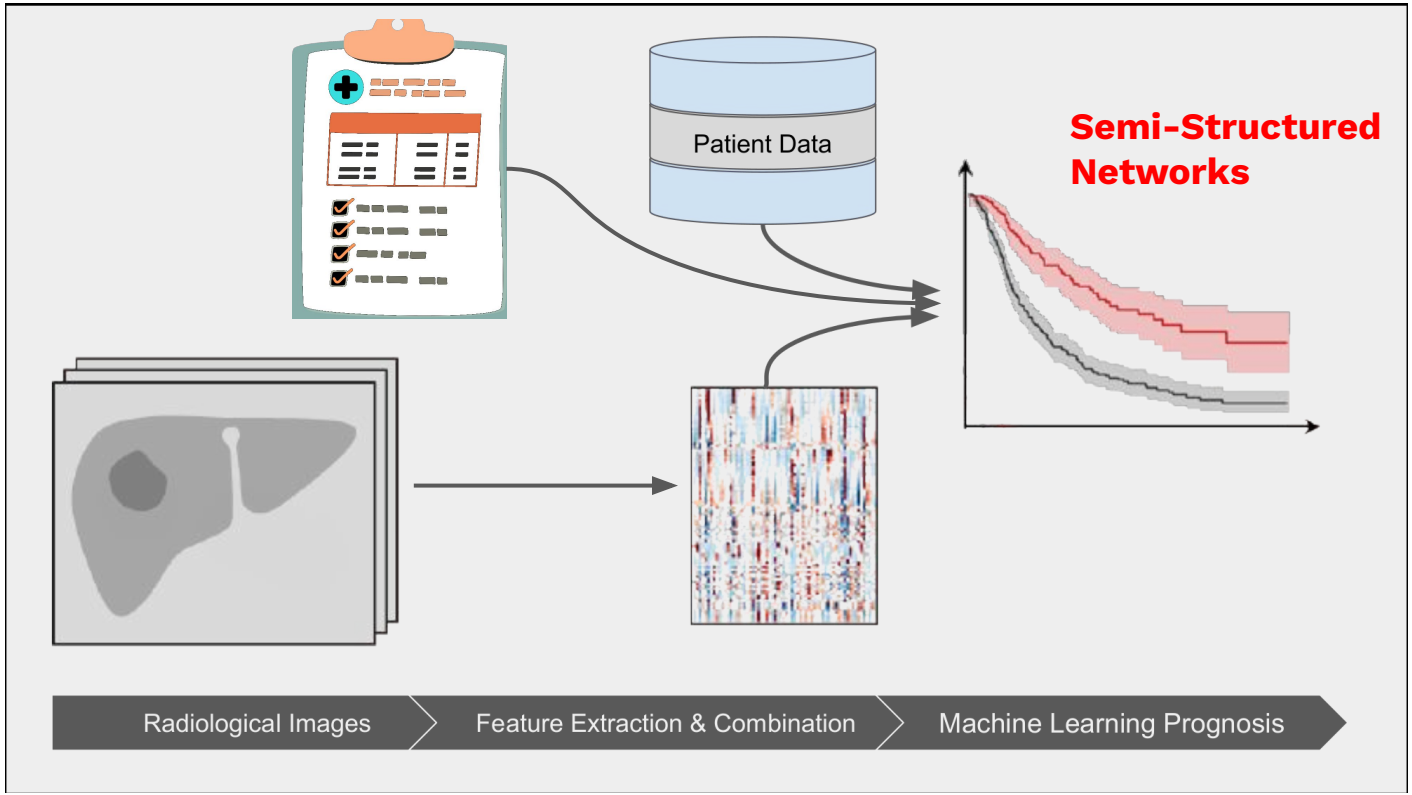

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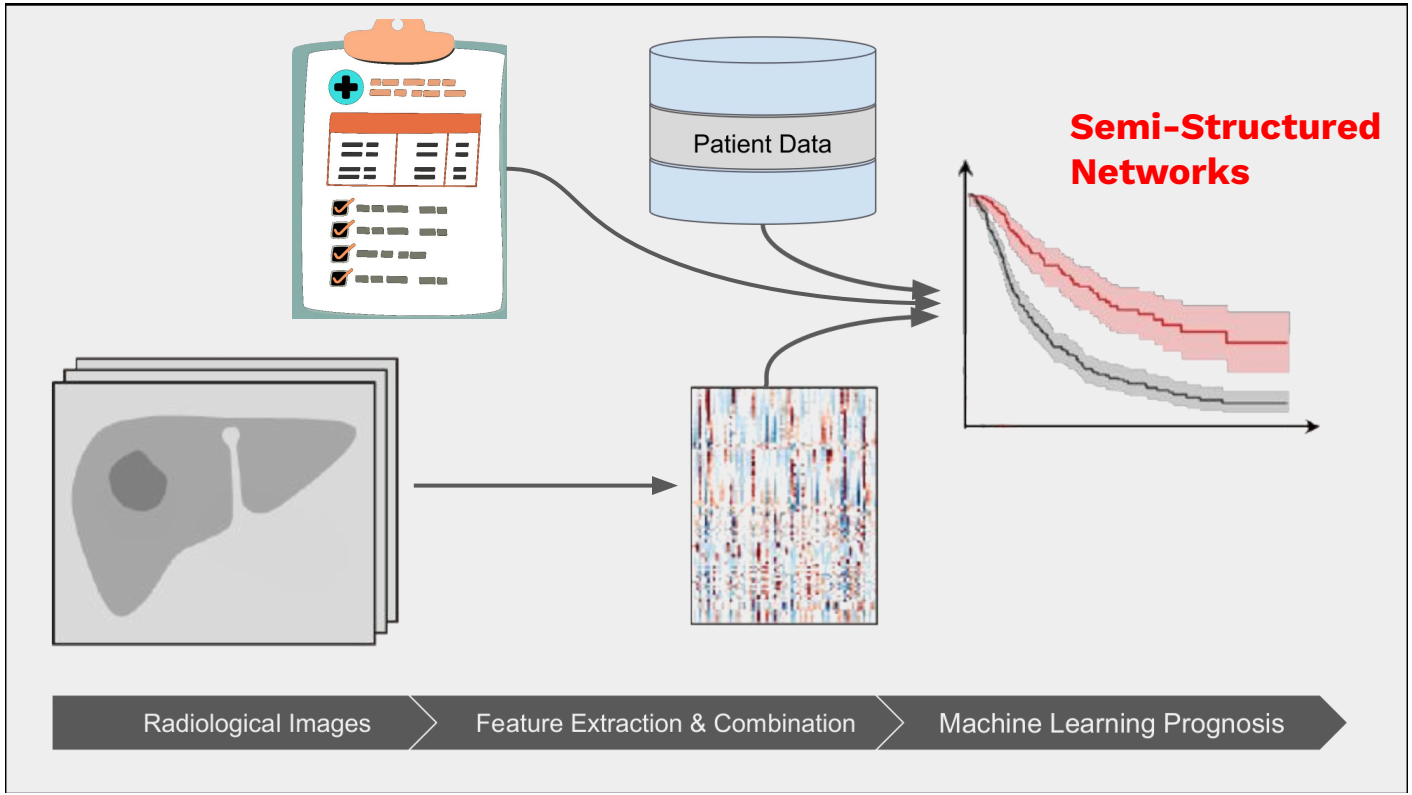

Inner Workings and Optimization of Neural Networks

Components of Neural Networks

- Architecture
- Loss
- Optimizer / Training Schedul(er)s

Components of Neural Networks

- Architecture
- Loss
- Optimizer / Training Routine

Components of Neural Networks

- Architecture
  - Often stacked in layers
  - Different layers for different purposes

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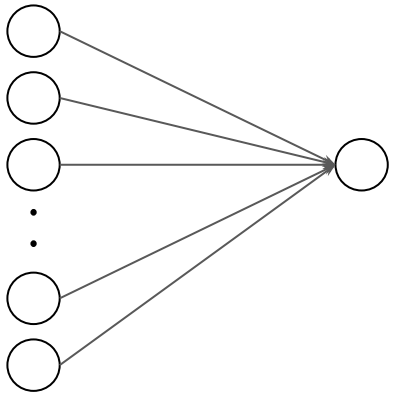

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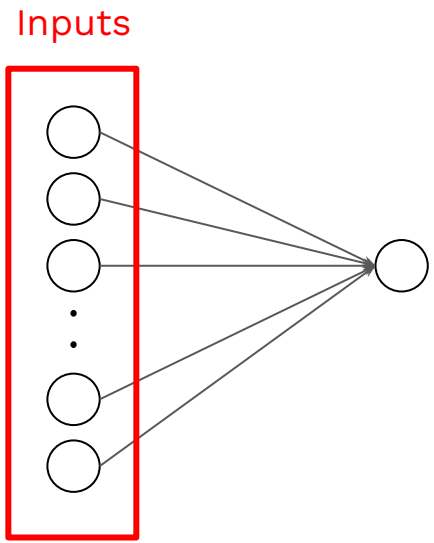

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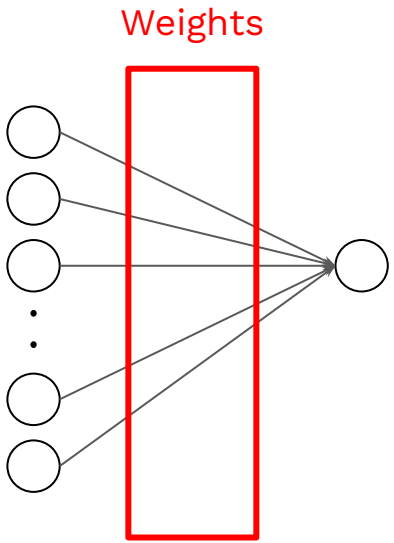

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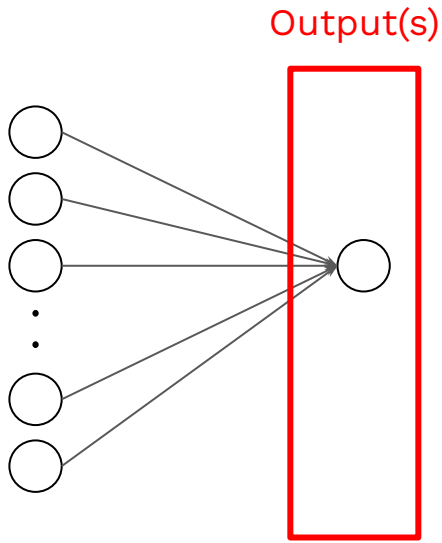

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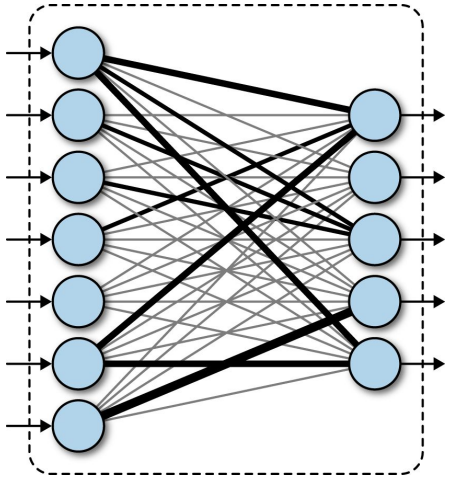

Source: oreilly.com

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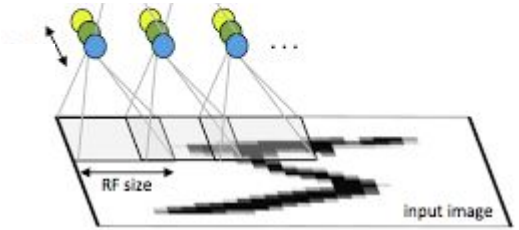

Source: stanford.edu

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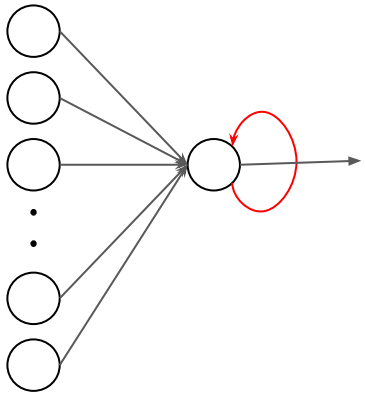

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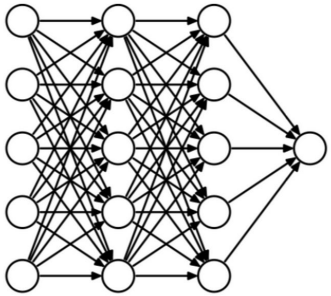

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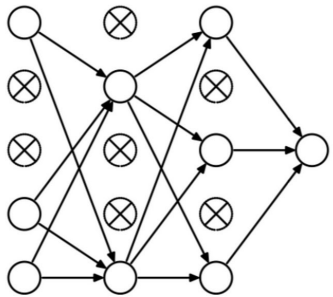

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    - ➢ “Classification” ⇒ Binary Cross Entropy / Log-loss
    - ➢ “Multiclass” ⇒ Cross Entropy

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    - ➢ DL Software works with **Auto Differentiation**
      ⇒ No need to derive anything by hand
      ⇒ Extreme flexibility

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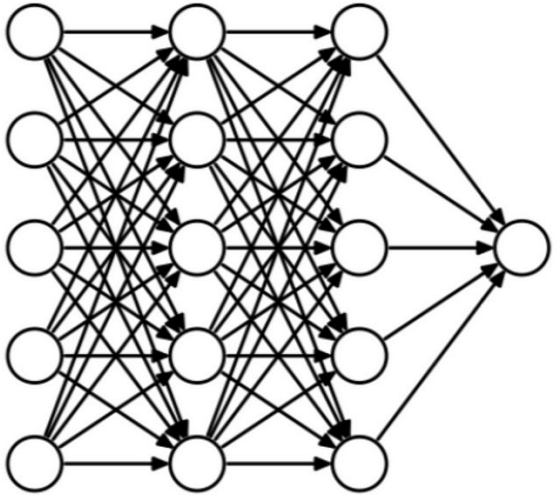

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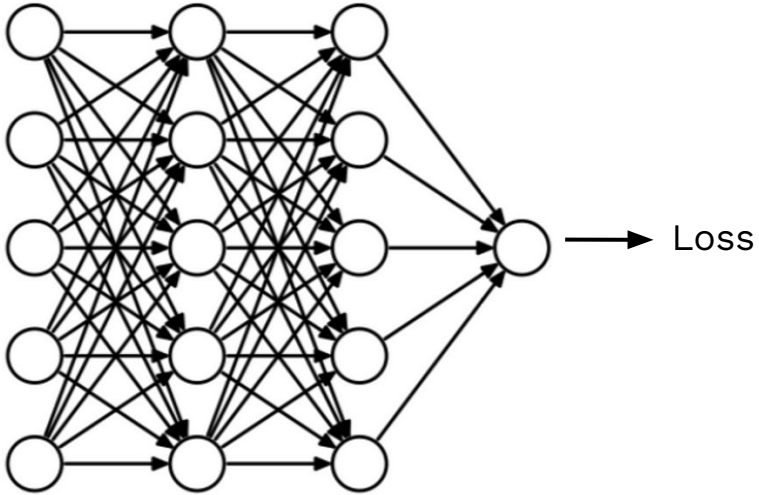

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    - ➢ “Classification” ⇒ Binary Cross
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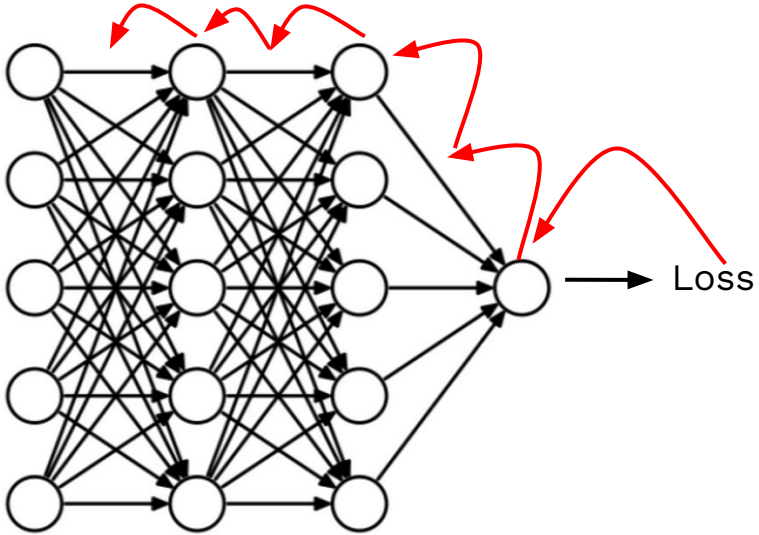

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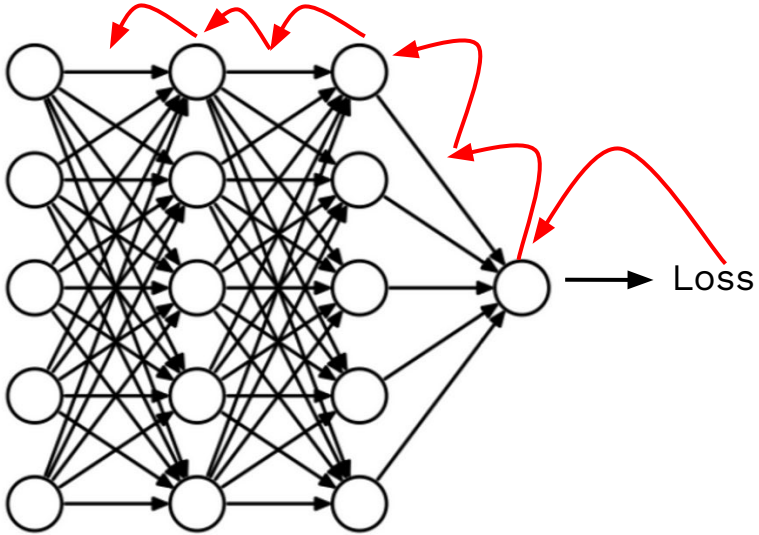

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TensorFlow, PyTorch, JAX, MXNET

Components of Neural Networks

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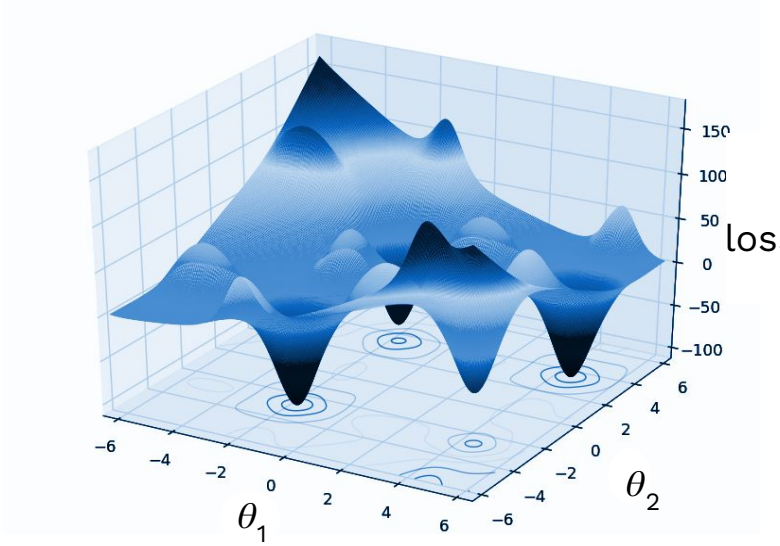

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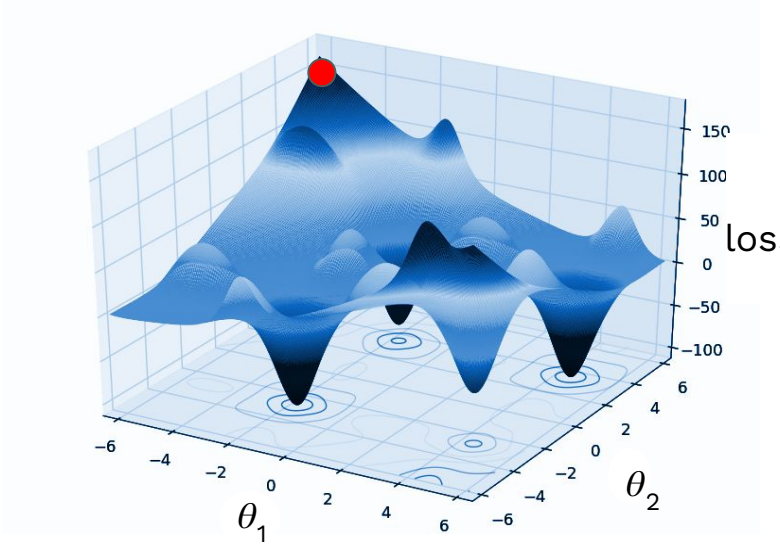

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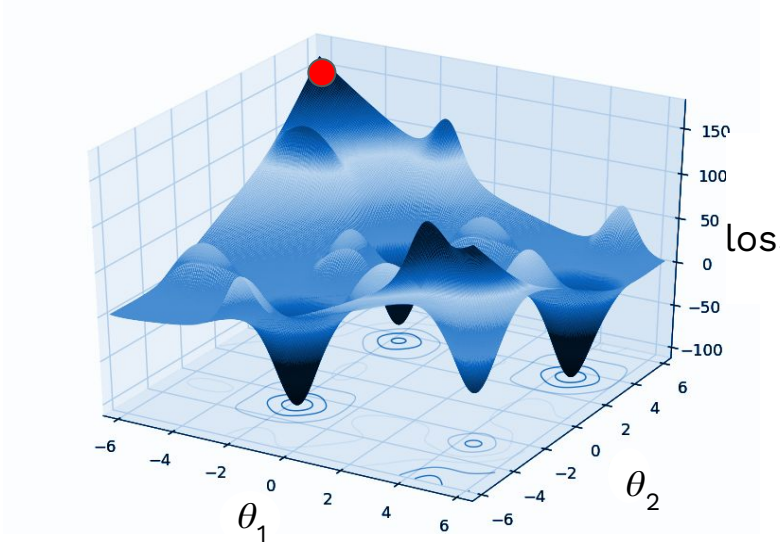

Most common variants are some form of gradient descent:

$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^{t} + \boldsymbol{\nu} \cdot \nabla_{\boldsymbol{\theta}} \text{loss}$$

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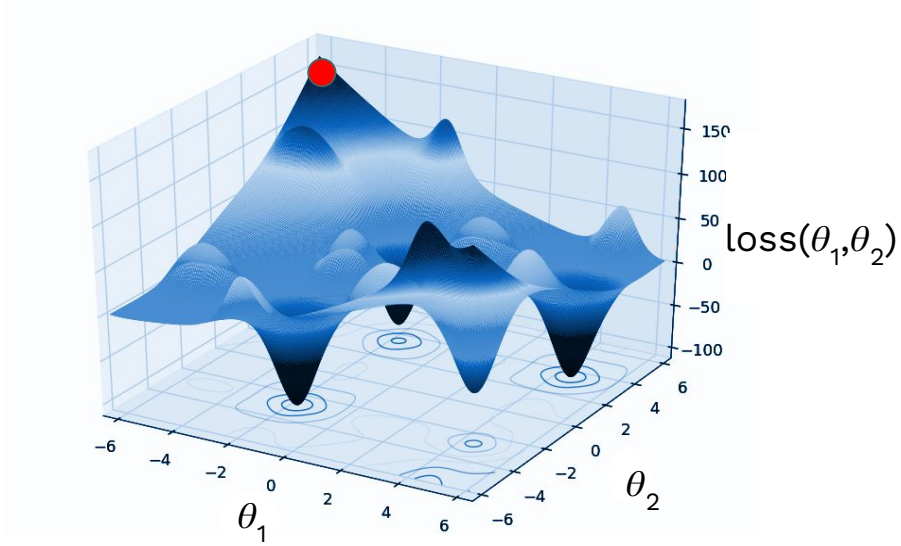

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new weights — old weights — learning rate — gradients

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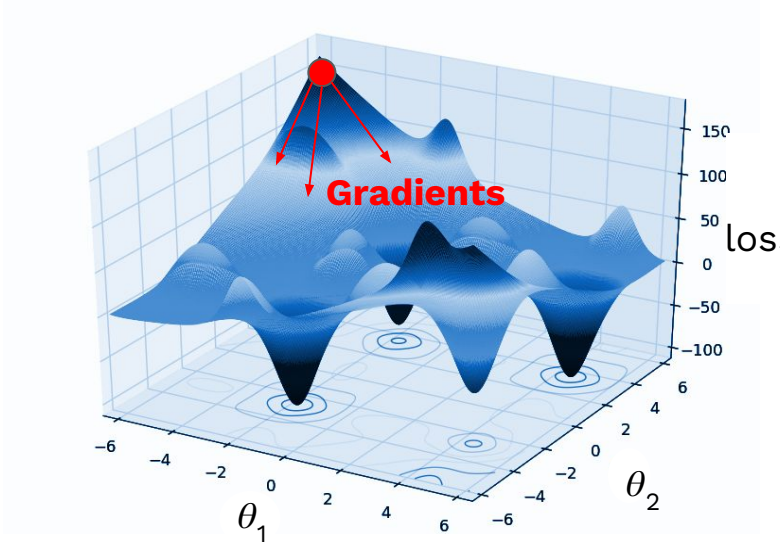

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t1p.de/dl_handout | t1p.de/dl_notebook

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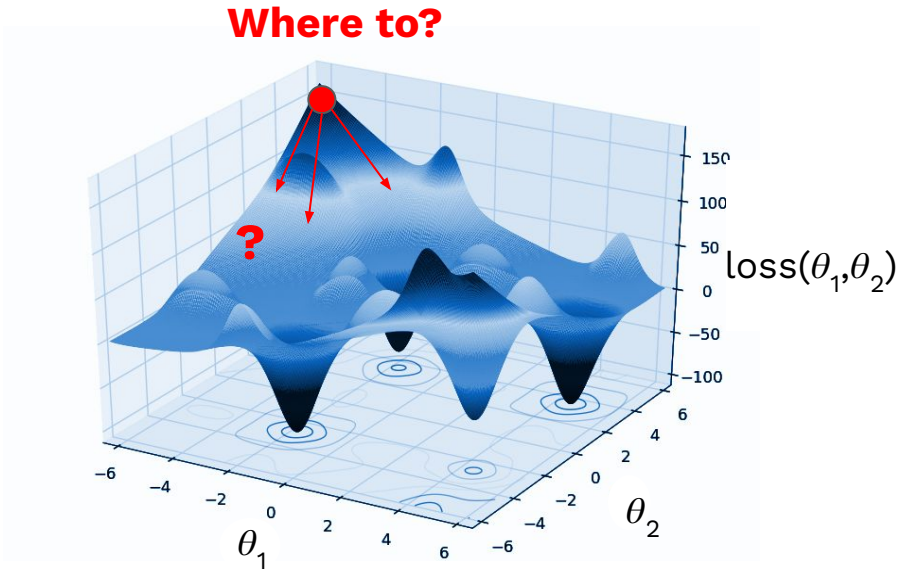

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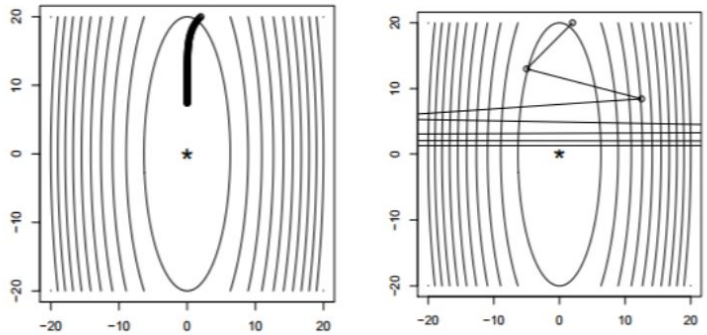
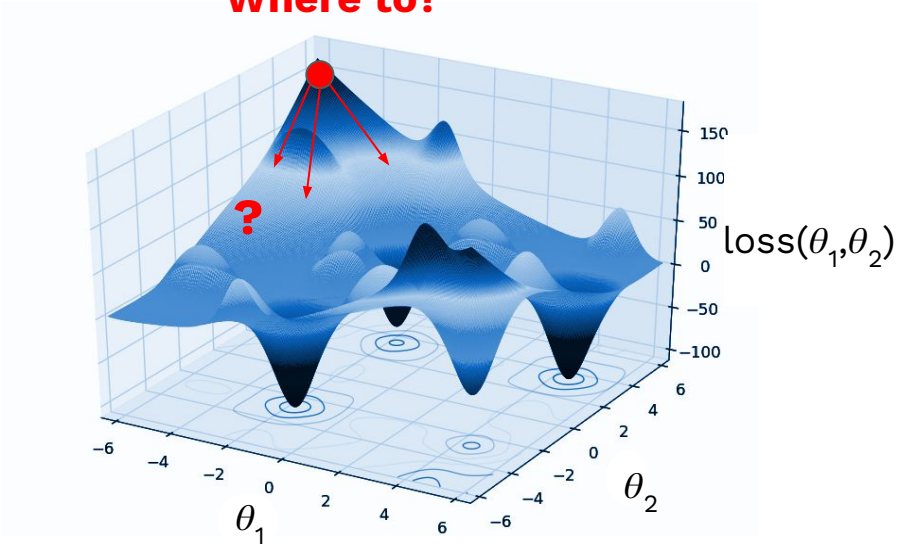
What speed?



Where to?



Components of Neural Networks

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Components of Neural Networks

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    - → The most successful ones (Adam, RMSprop, Adagrad, ...) use
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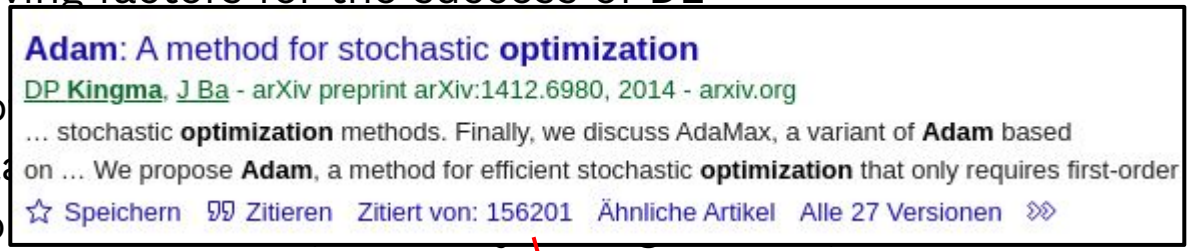

on average 48 citations per day for the last 9 years

Components of Neural Networks

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Source: Towards Data Science

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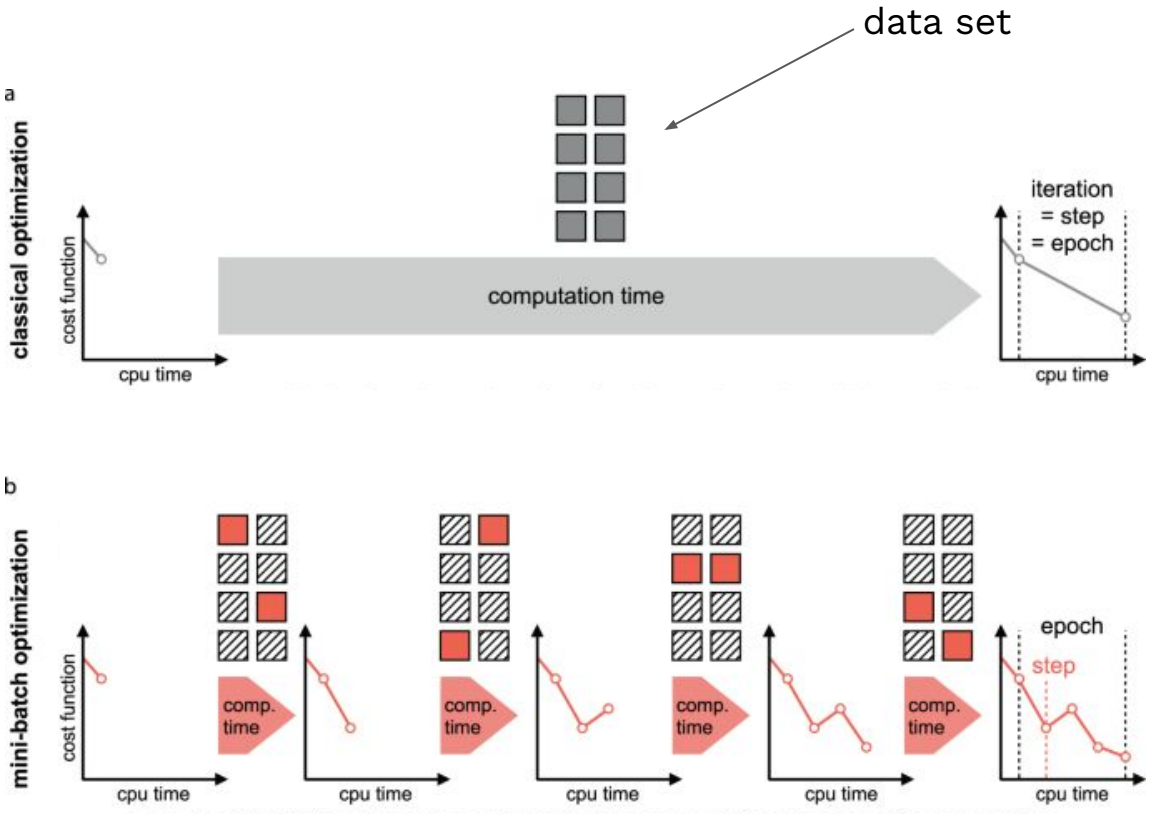
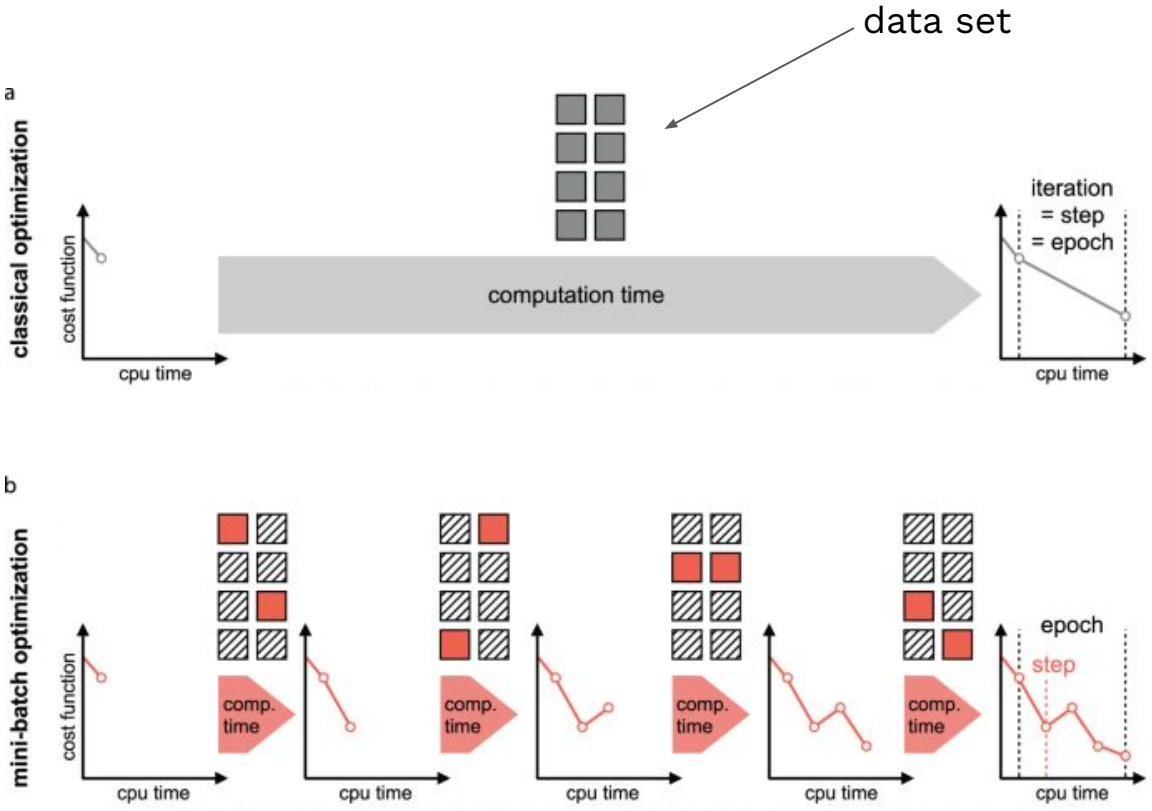
  - Optimization is usually done in Mini-batches
    - → for each iteration (called *epoch*), data is divided in *B* batches
    - → i.e. *B* optimization steps for the whole data set
    - → “Stochastic gradient descent (SGD)-optimization”

Components of Neural Networks



Source: [9]

Components of Neural Networks



Typical batch sizes:
32, 64, 128

Source: [9]

Components of Neural Networks

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Putting all together

Components of Neural Networks

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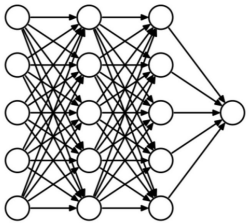

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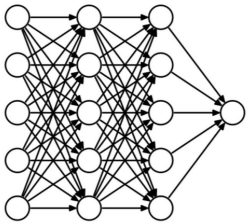

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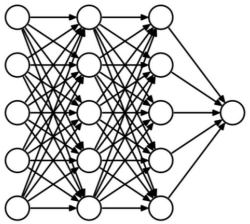

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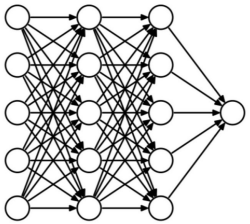

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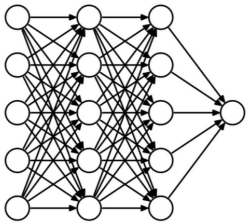

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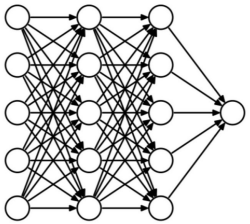

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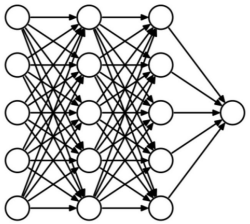

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higher-level APIs (keras, luz, lightning) will do this for you

Components of Neural Networks

- Architecture
- Loss
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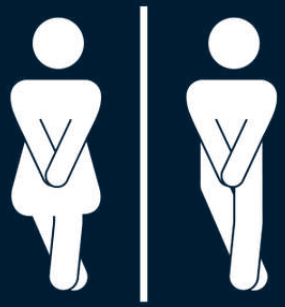
Putting all together

Munich Center for Machine Learning

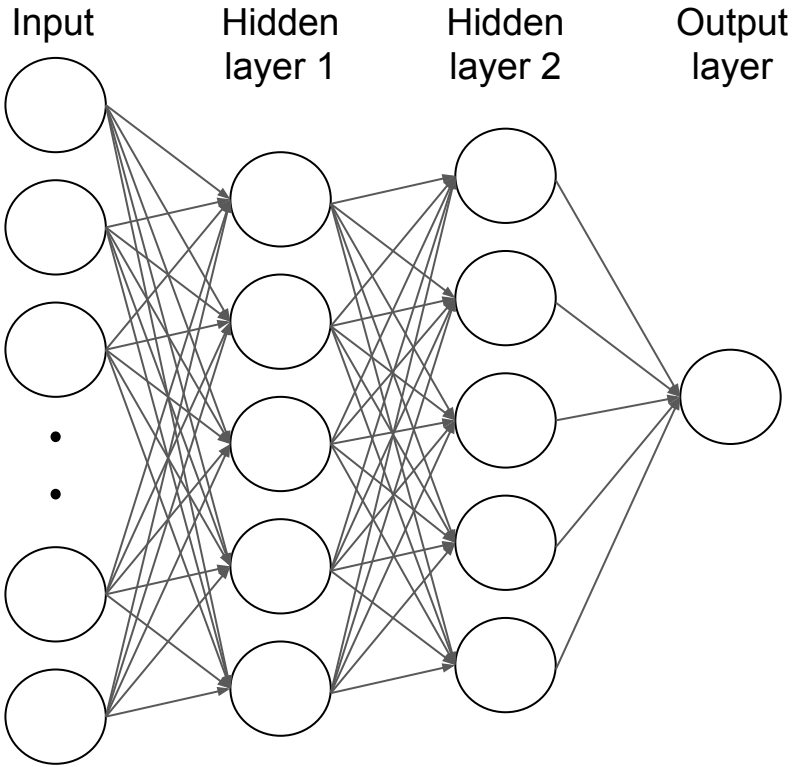
LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

Break?



Neural Networks from a Statistical Point of View

A Multi-layer Perceptron



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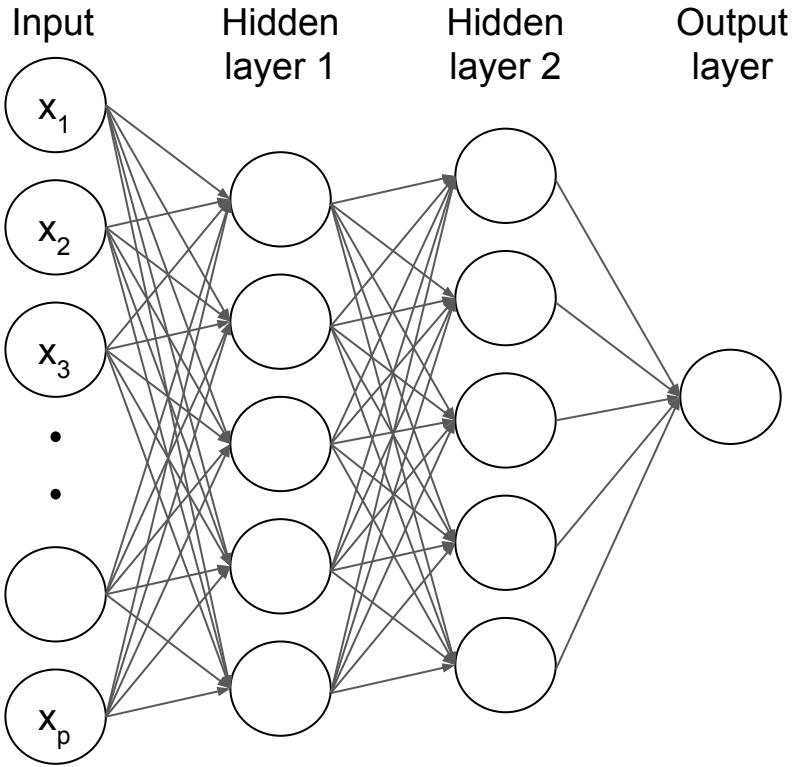

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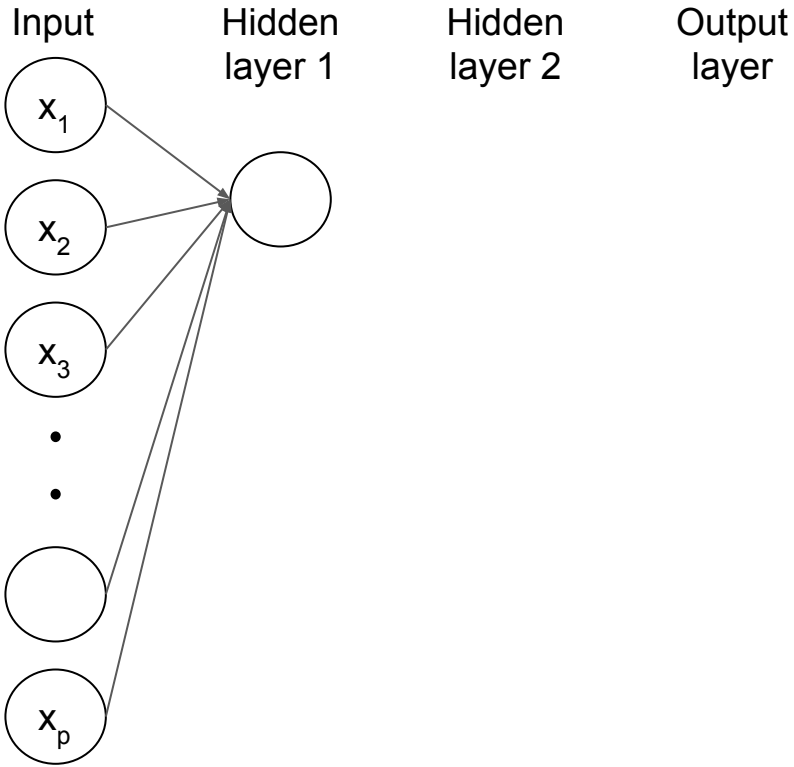

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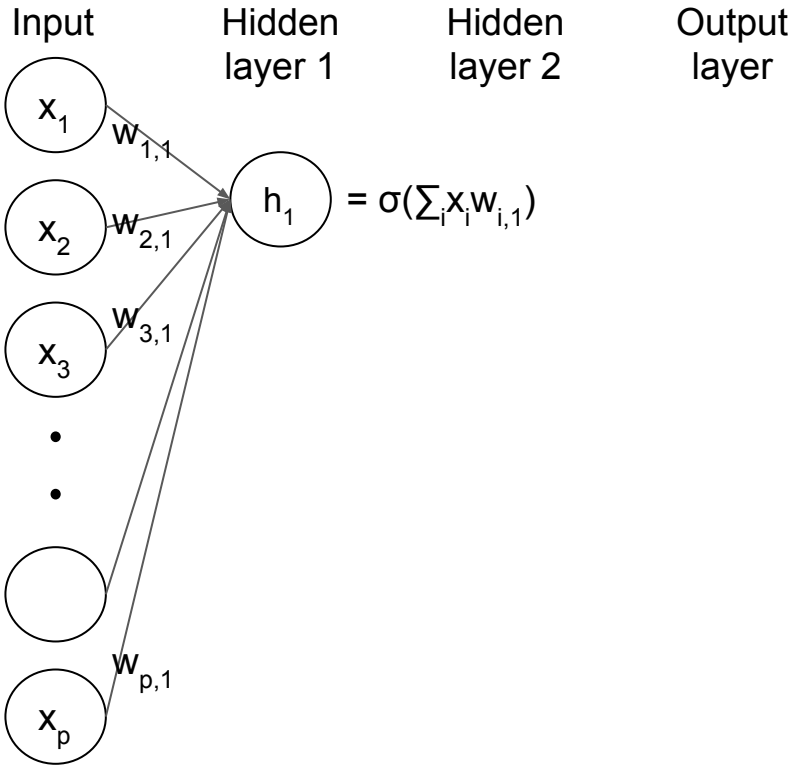

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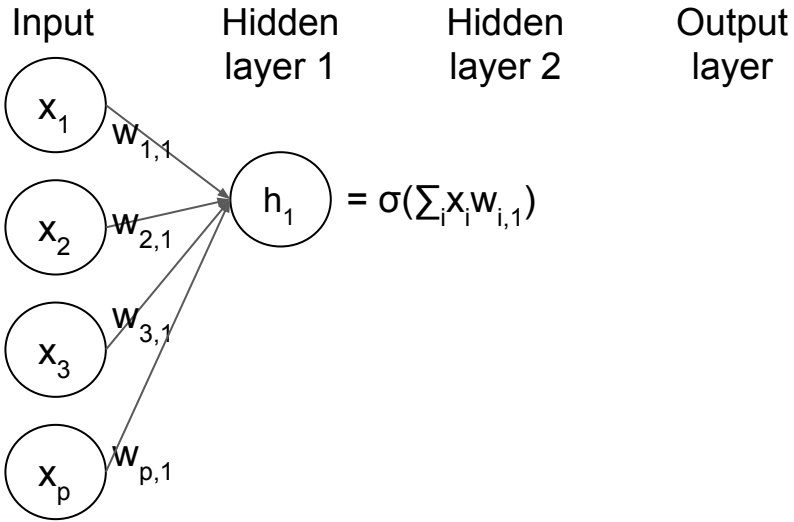

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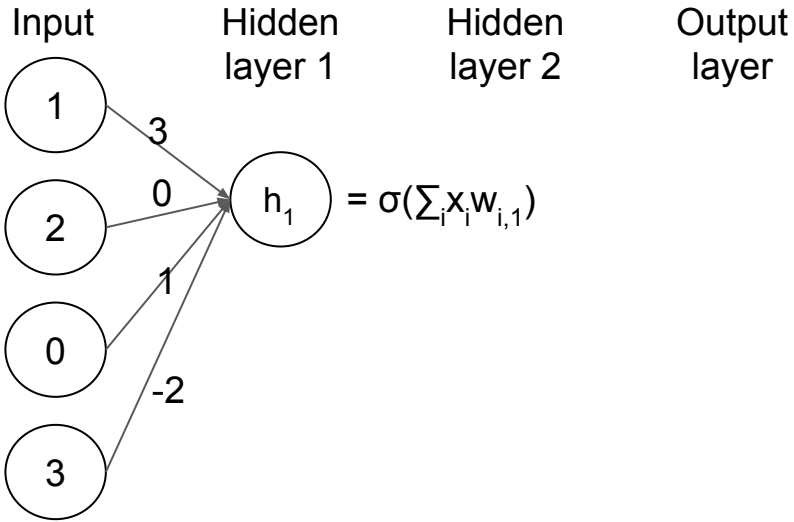

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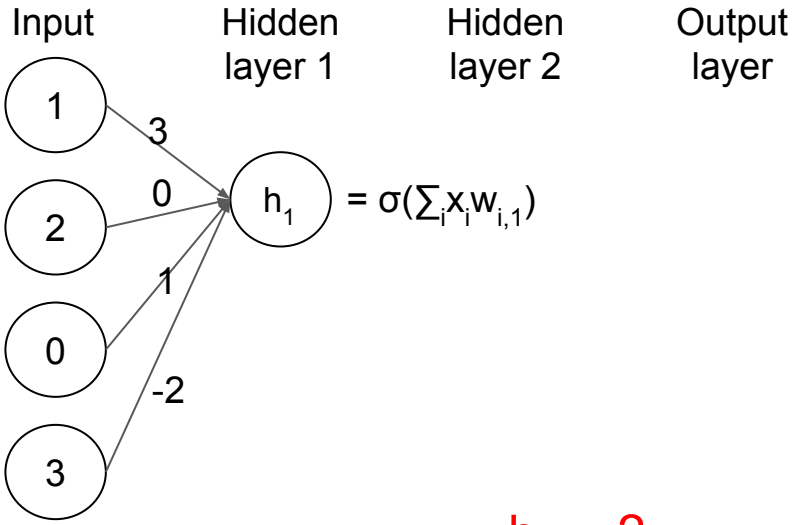

$h_1 = ?$

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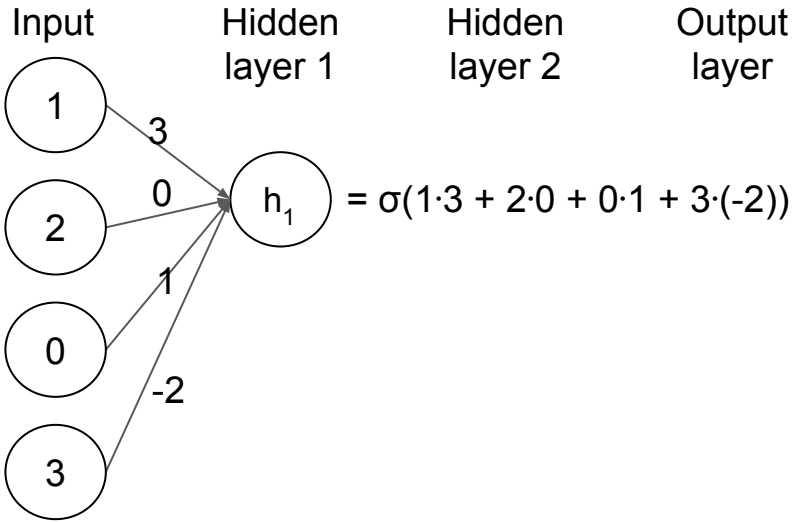

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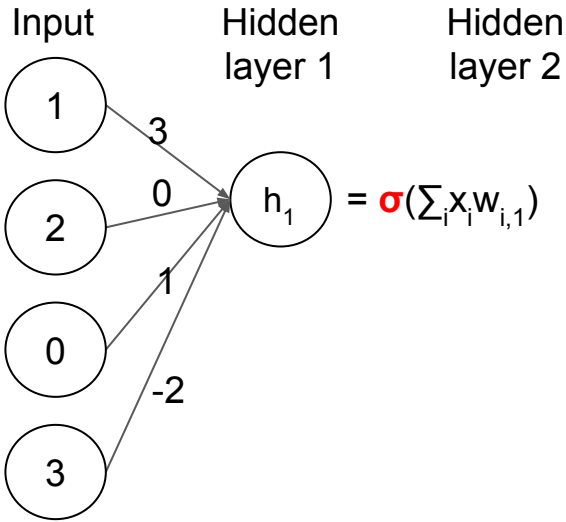
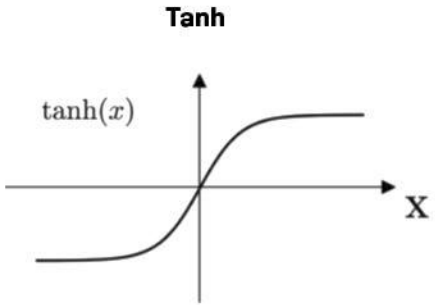
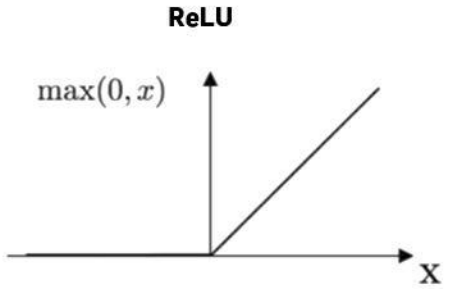
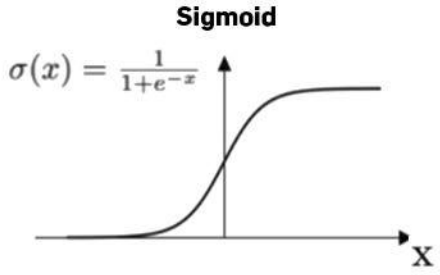
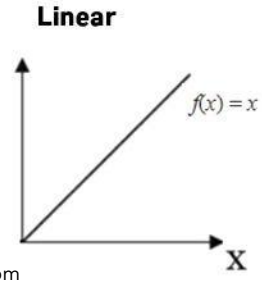


σ: Activation Function



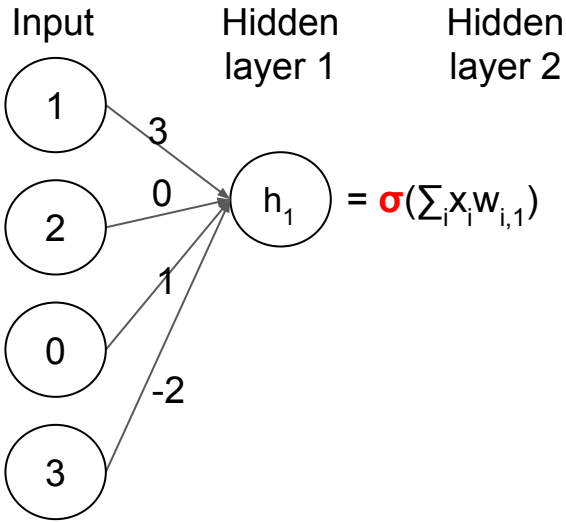




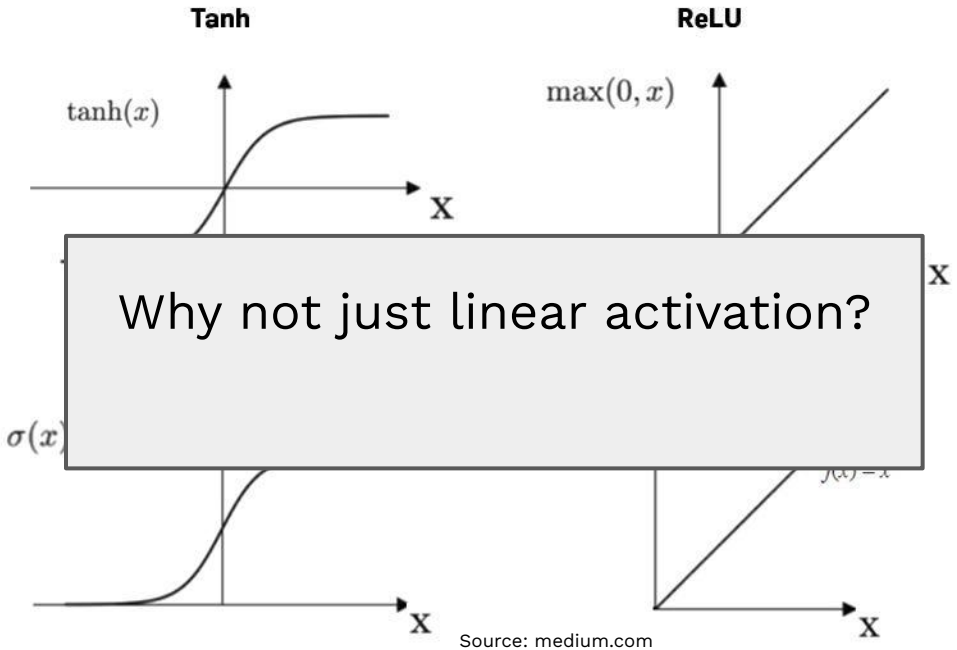


Source: medium.com

A Multi-layer Perceptron



σ: Activation Function



Why not just linear activation?

Source: medium.com

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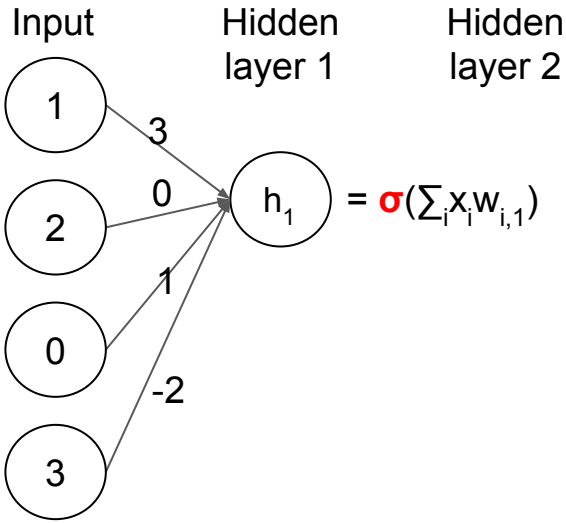

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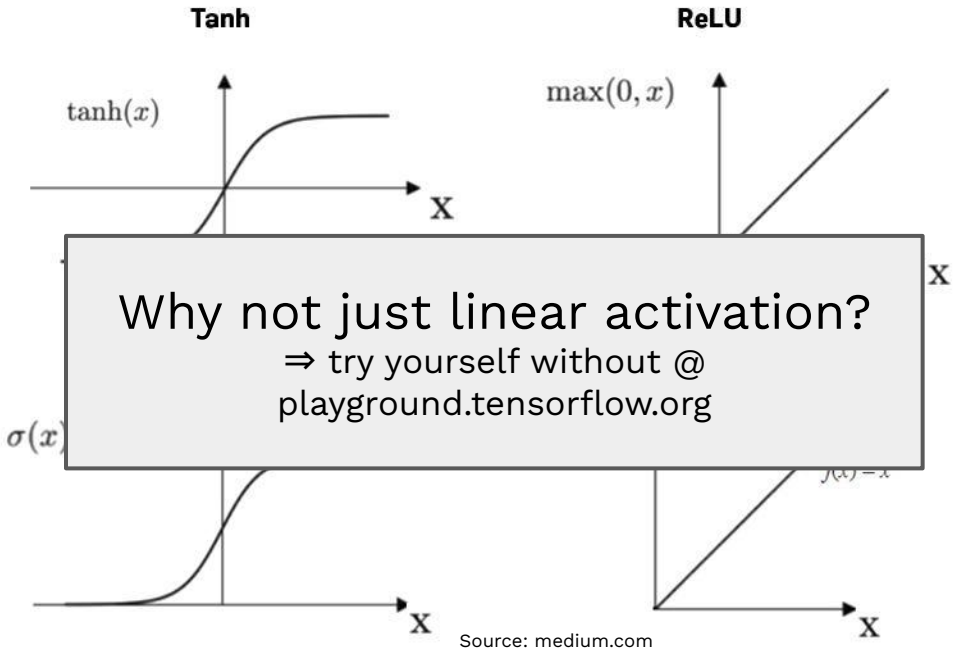

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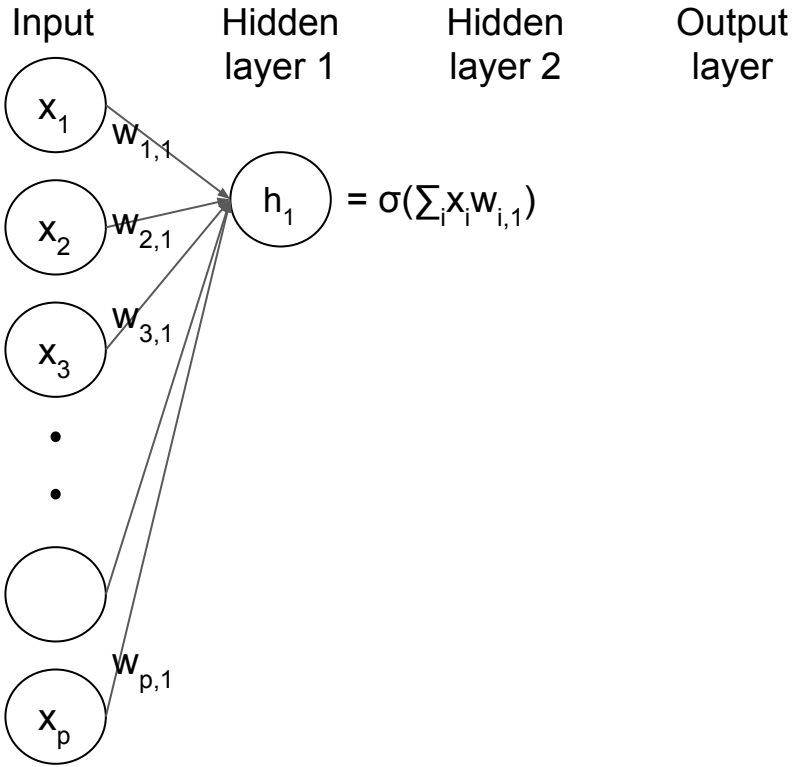
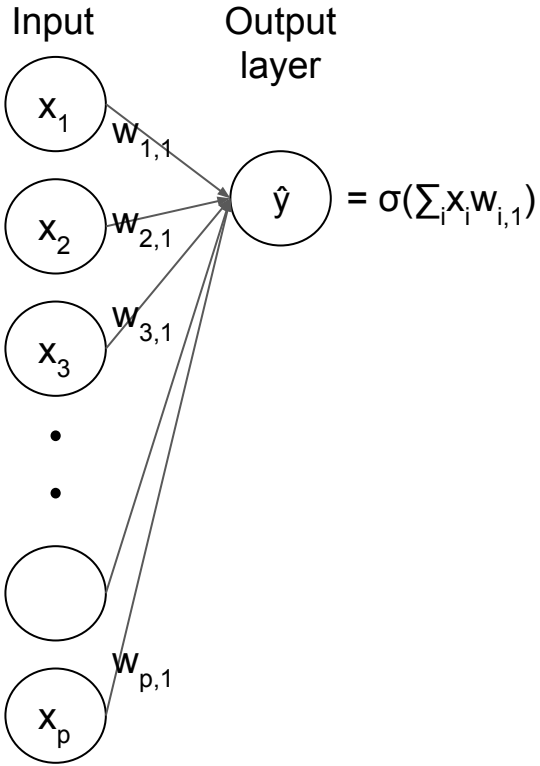
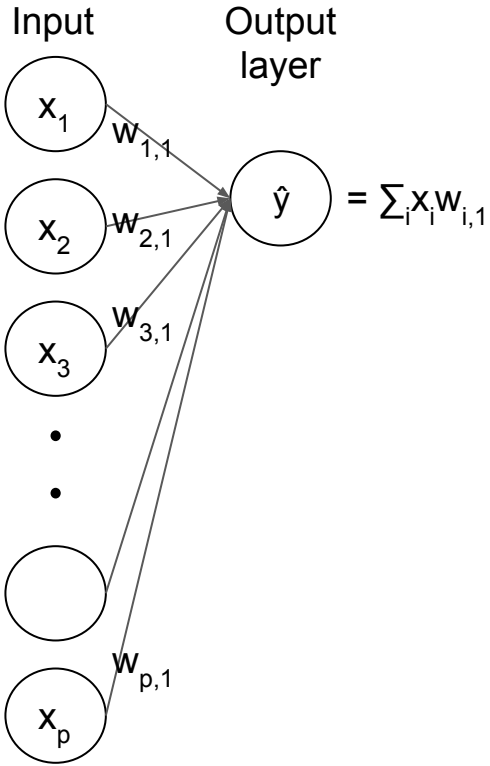


A Single-layer Perceptron

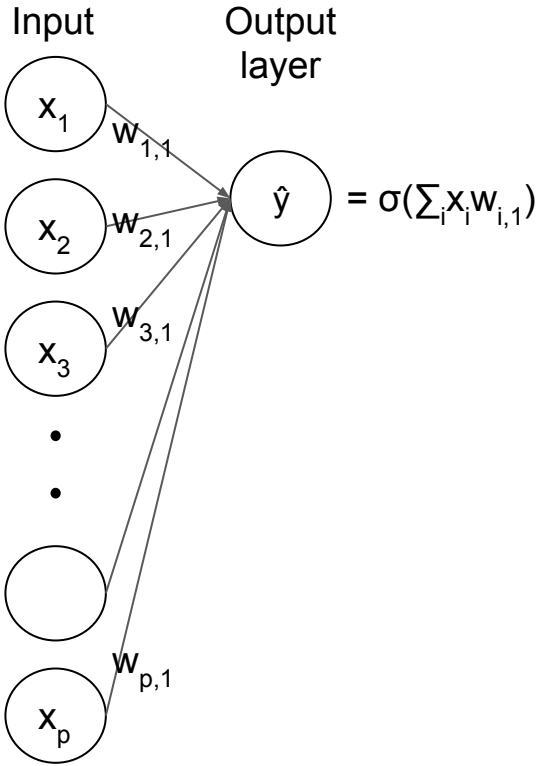


A Linear Model



with loss $(\hat{y}-y)^2$

A Generalized Linear Model



with loss = neg. log-Likelihood

and σ = …

… sigmoid for Bernoulli
… exp for Poisson

Components of Neural Networks

- Architecture
- Loss
  - The typical decision process:
    - ➢ “Regression” ⇒ L2-loss
    - ➢ “Classification” ⇒ Binary Cross Entropy / Log-loss
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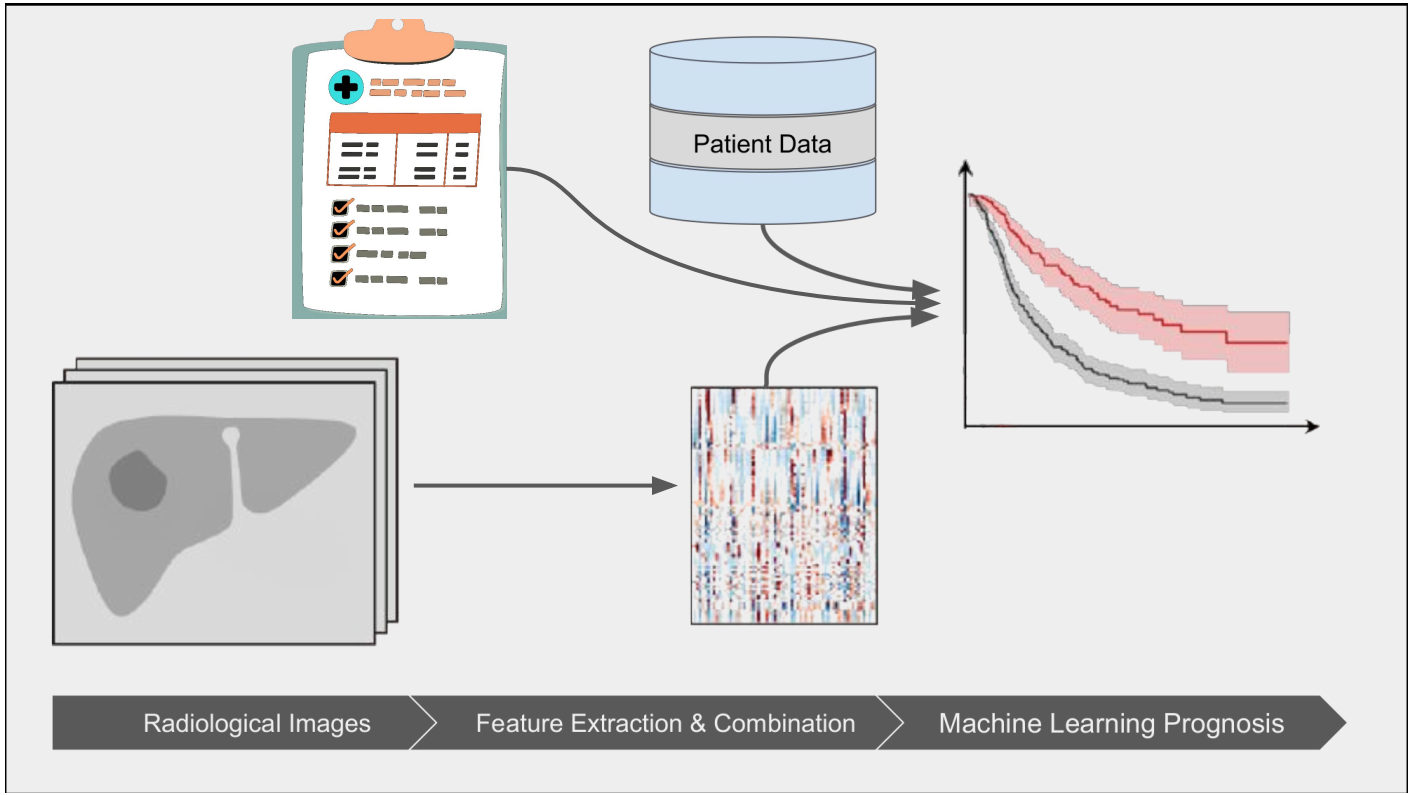
Semi-Structured Neural Networks

Motivating Example: Multimodal Data Sets

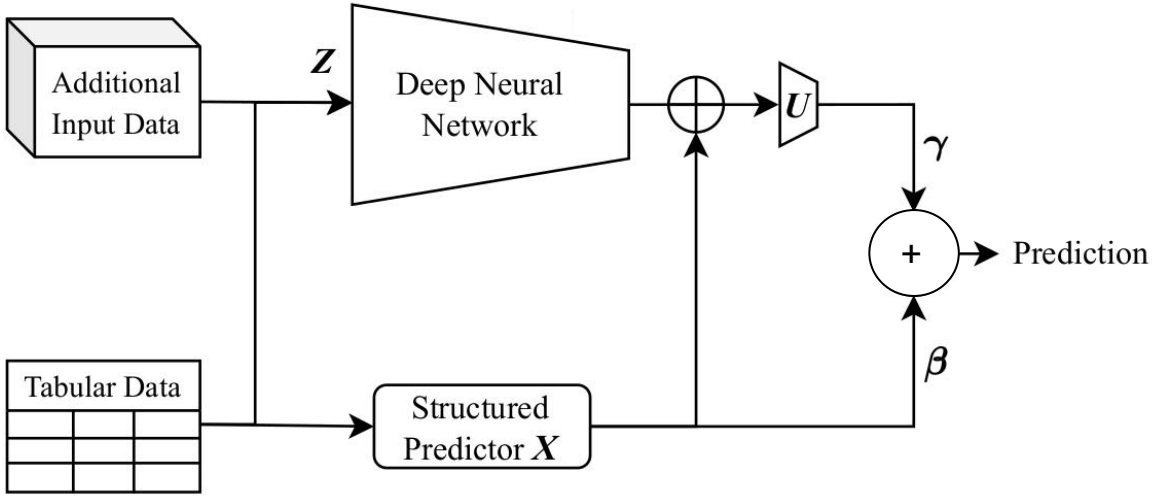


Semi-Structured Neural Networks

Idea:

- Jointly train statistical model
- and deep neural network(s)
- in one unifying large network

Semi-Structured Neural Networks



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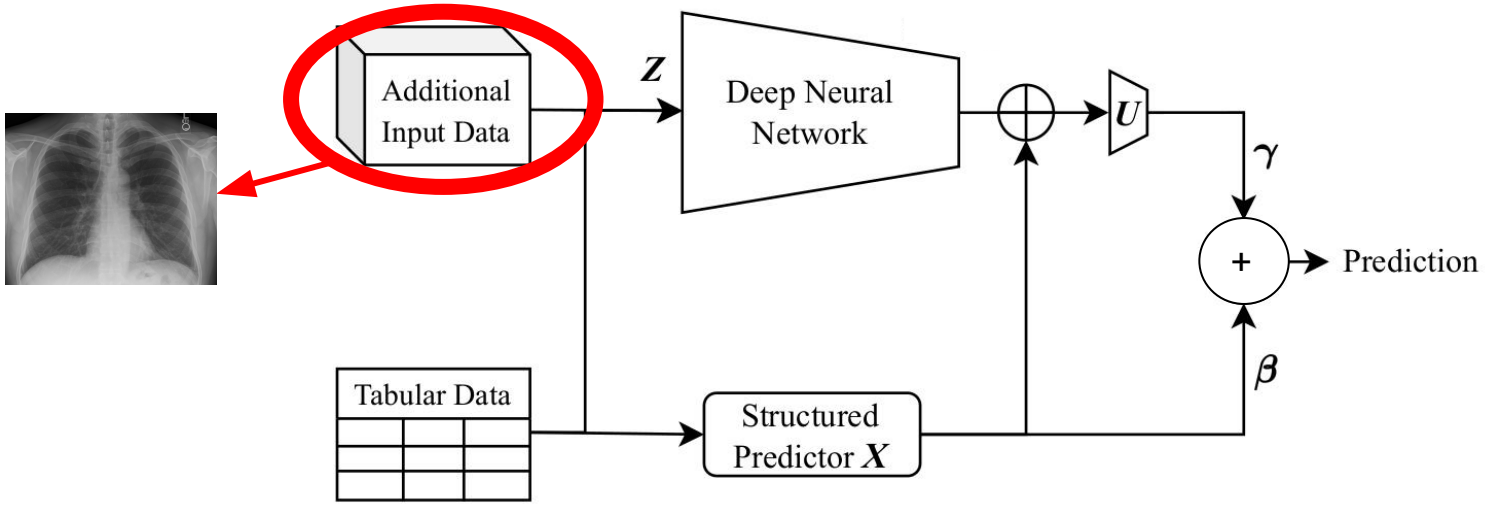

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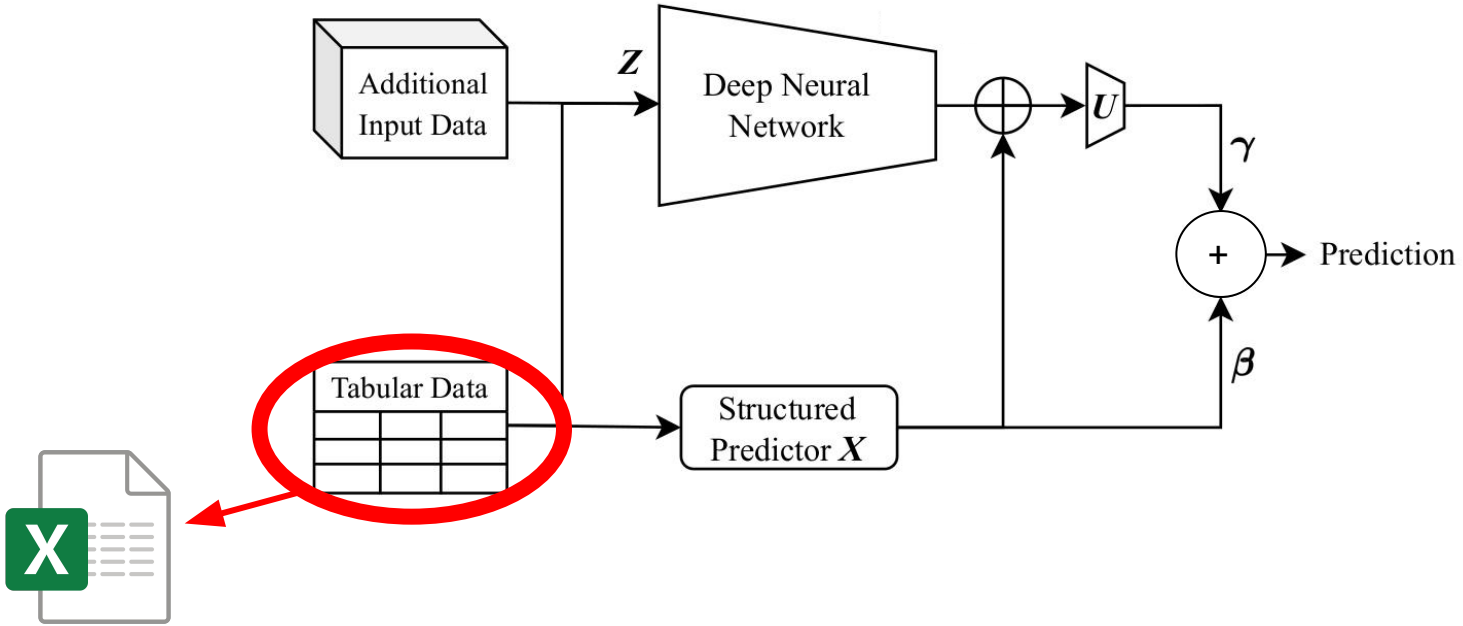

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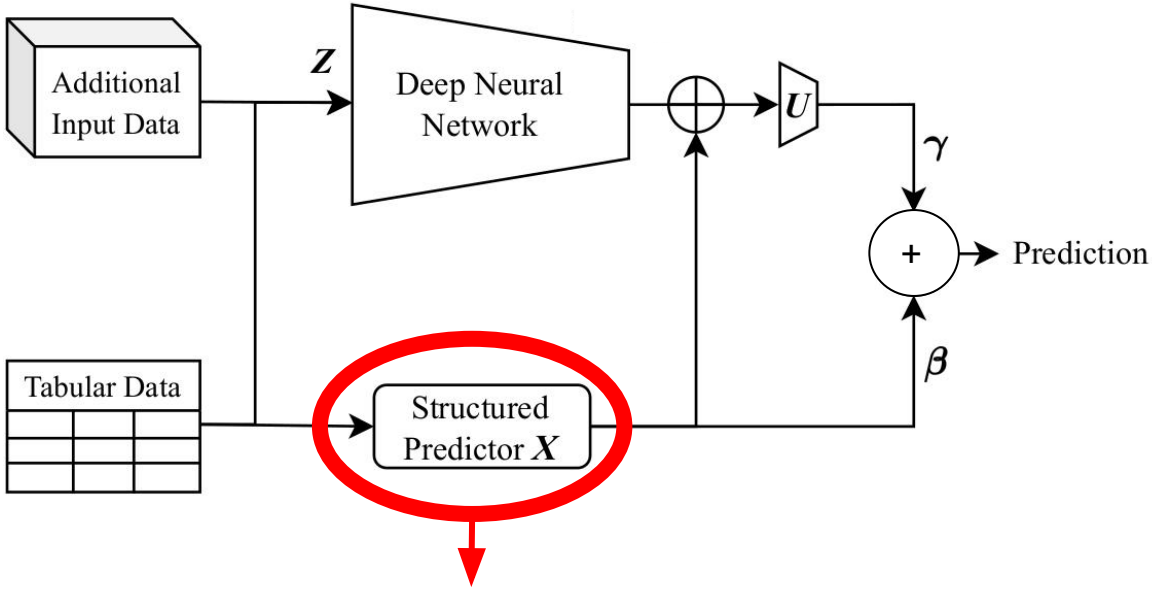
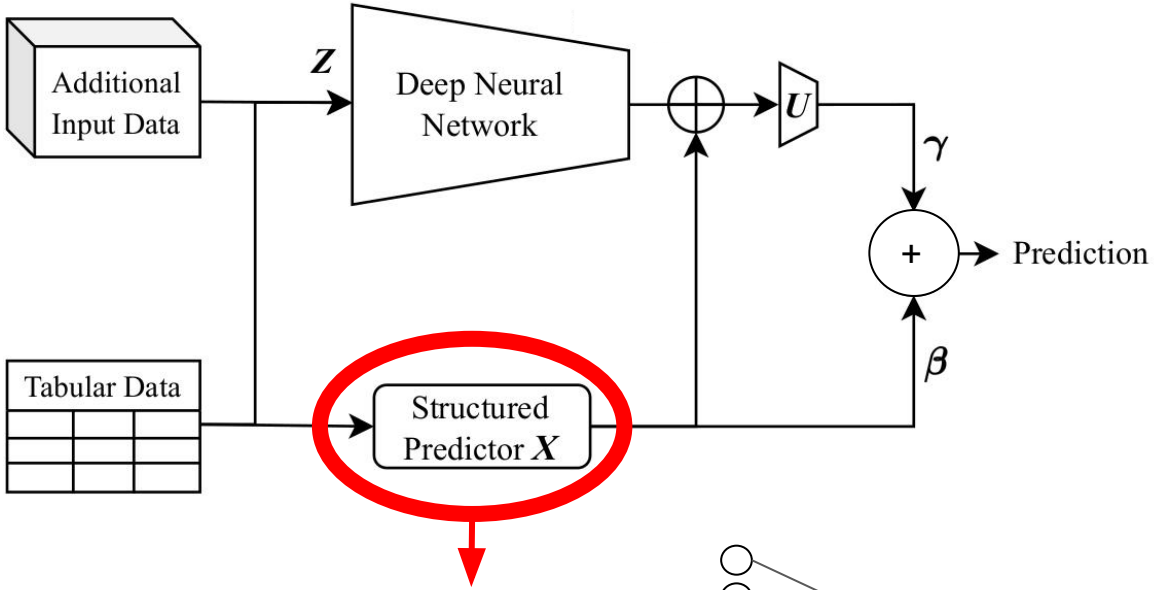


- linear effects
- splines
- tensor-product splines
- ...

Semi-Structured Neural Networks



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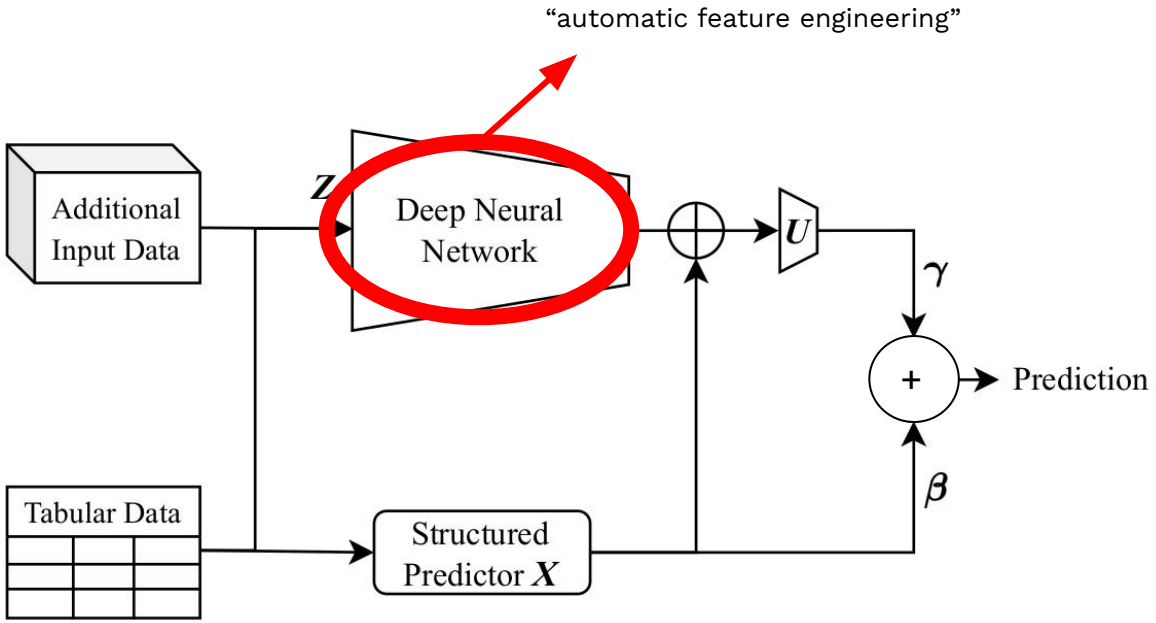

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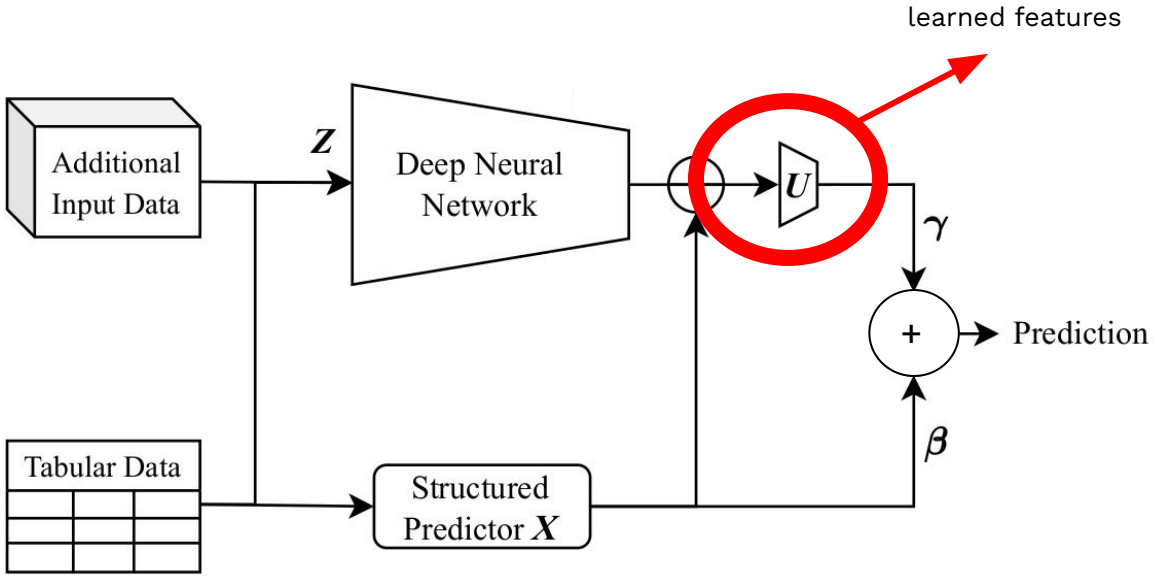

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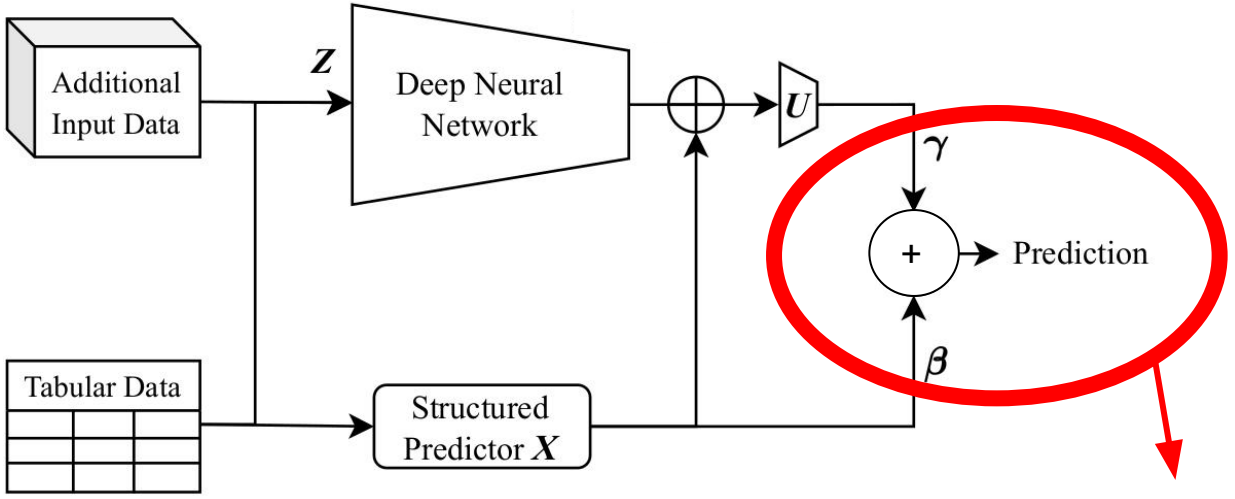

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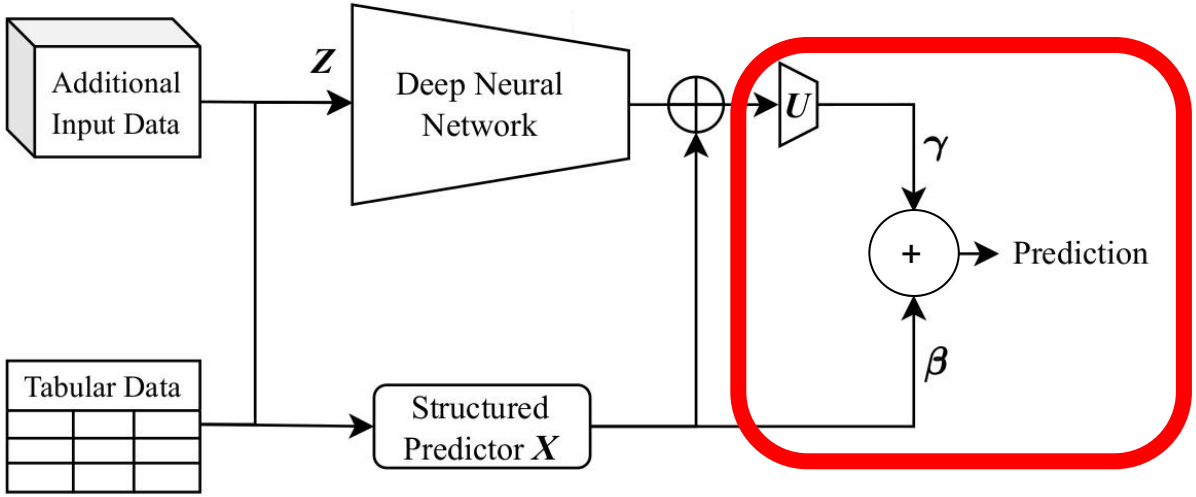
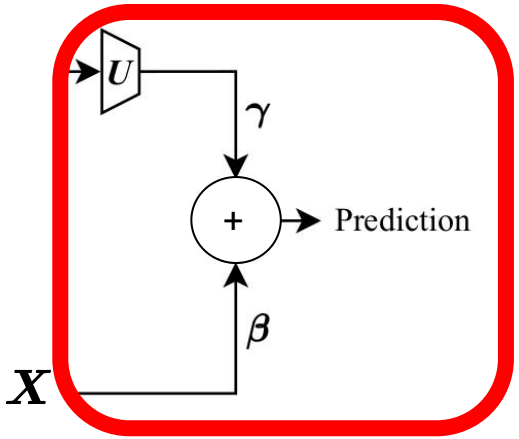


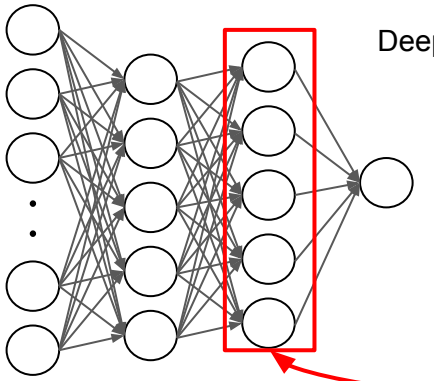
An additive model

Semi-Structured Neural Networks



$$\mathbb{E}(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{Z}) = \boldsymbol{\eta} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{U}\boldsymbol{\gamma}$$

Semi-Structured Neural Networks



Deep Neural Network

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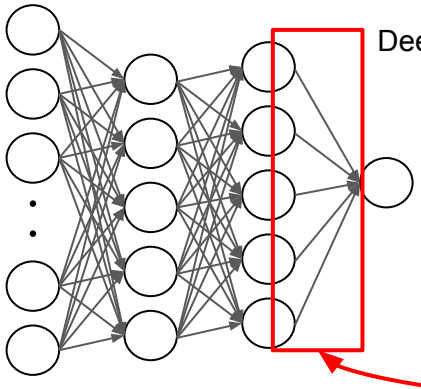

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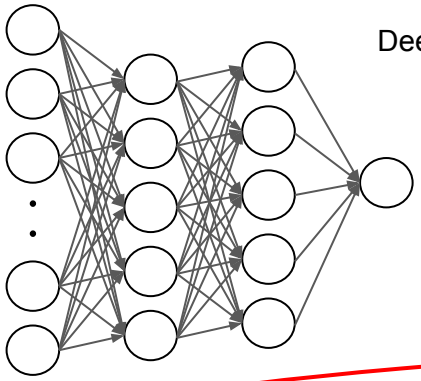

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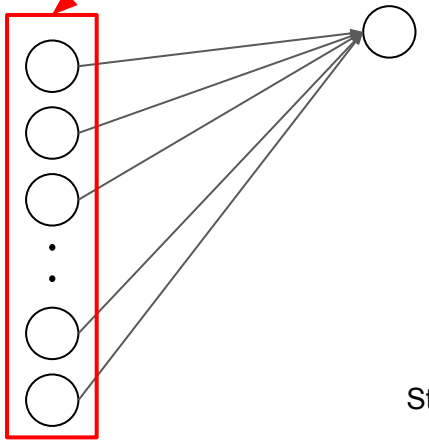
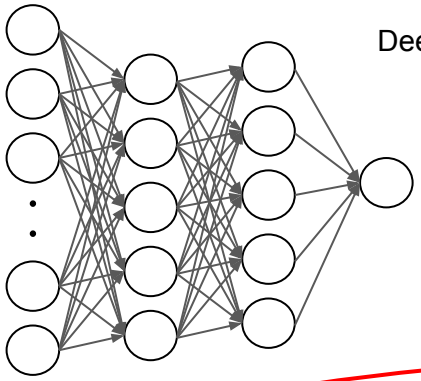


Structured Predictor

Semi-Structured Neural Networks



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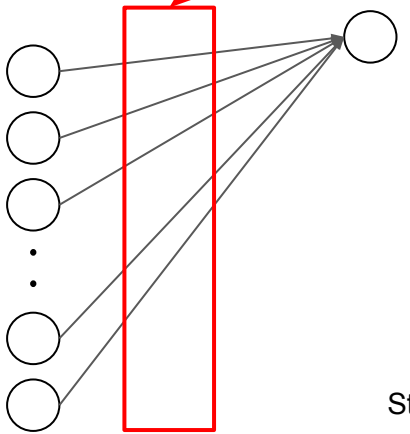

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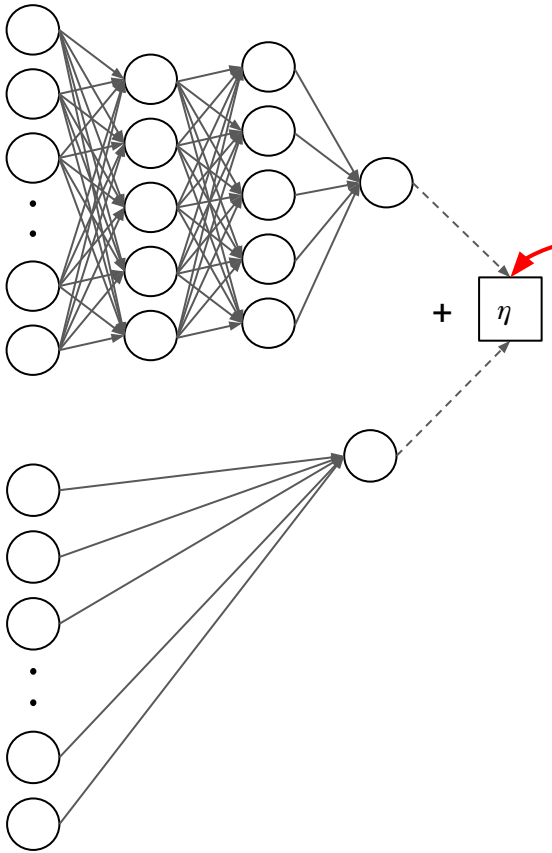

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Practical Implementation of Neural Networks

Software implementation

`deepregression` [10] (CRAN / Github)
R package combining TensorFlow/torch and mgcv

- Many different models (GLMs, GAMs, GAMLSS, etc.)
- Many different feature effects (splines, lasso, ridge, etc.)
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- Combine it with arbitrary neural networks

Example: Predicting Airbnb Prices in Munich

- Tabular information:
  - bathrooms, bedrooms, room type,
  - latitude, longitude,
  - ...
- Text description
- Image

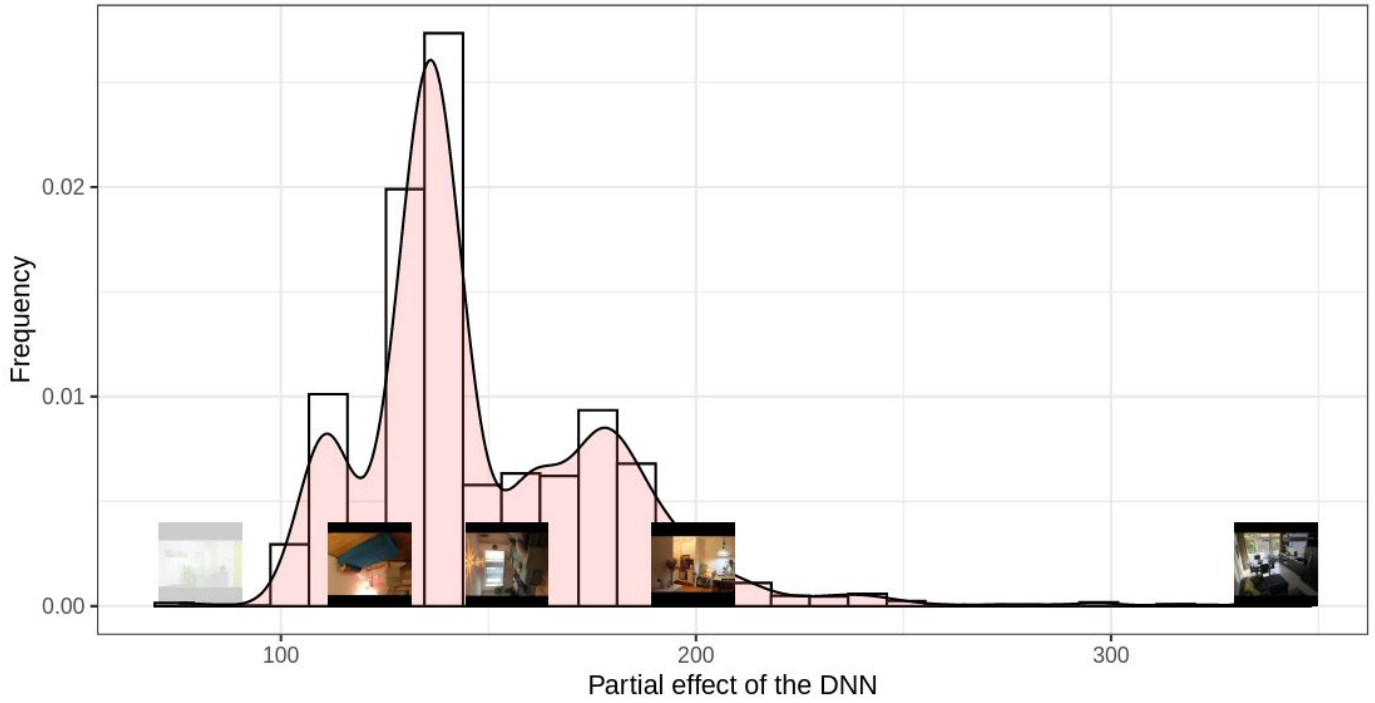
Example: Predicting Airbnb Prices in Munich

[...] Station for Metro, Bus, Tram are ony 1 minute walking.
The room is 16 square meters, Free WIFI.
We use together Bathroom and Kichen.
I prepare your Bath Towel.
you get Breakfast, cafe oder Tee, Bread..

Example: Predicting Airbnb Prices in Munich

```
mod_airbnb <- deepregression(
    y = price,
    family = "log_normal",
    list_of_formulas = list(
      location = ~1 + te(latitude, longitude) + room_type + bedrooms +
                  cnn(image) + lstm(desc),
      scale = ~1
    ),
    data = d_train
)
```

Example: Predicting Airbnb Prices in Munich



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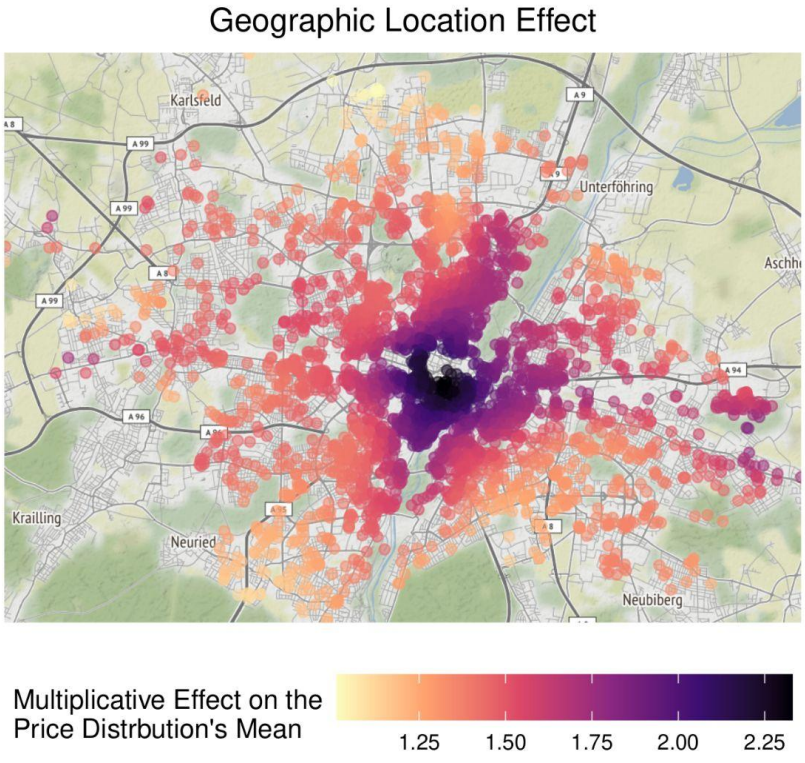

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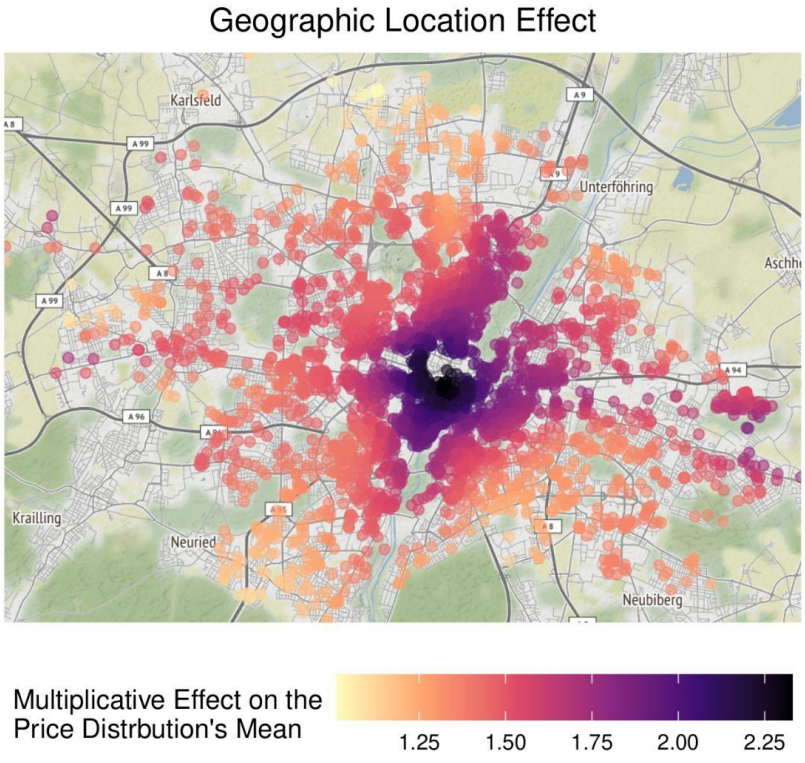

Outlook: How do different layers work?

Outlook: How do different layers work?
Convolutional Layers

... for processing Images

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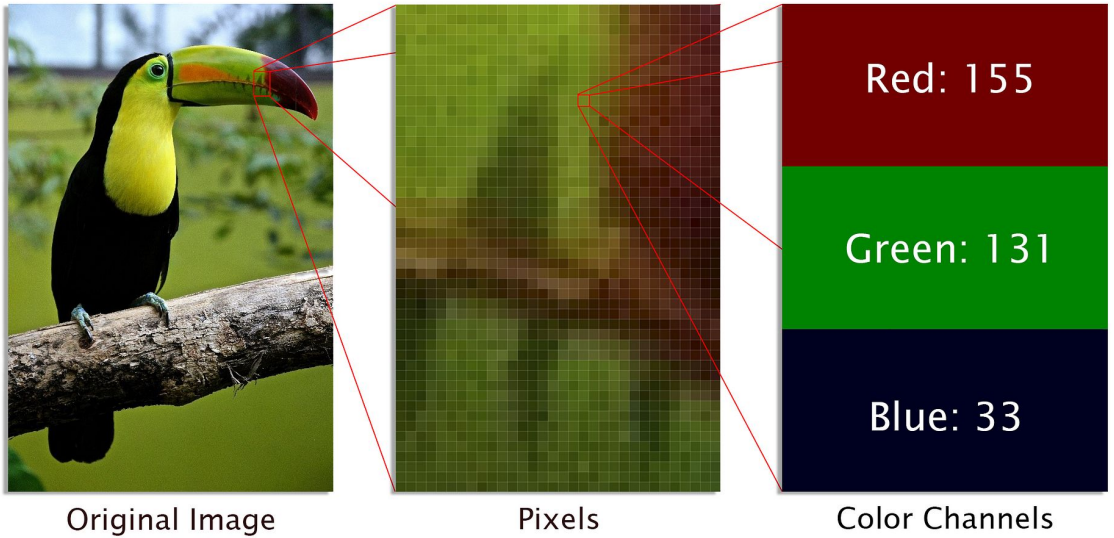

Source: medium.com

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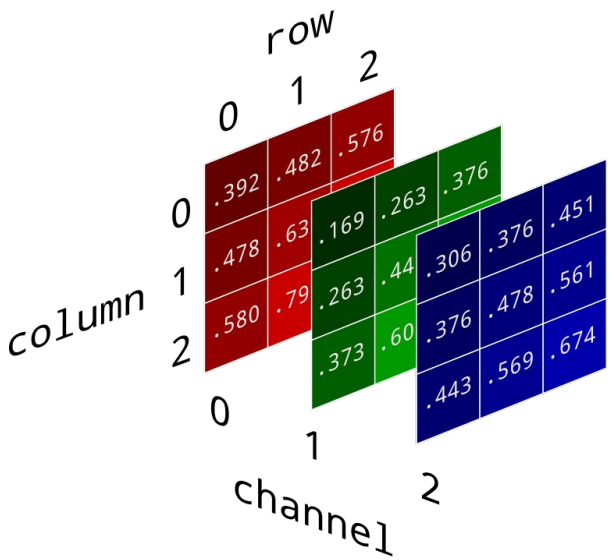
Convolutional Layers

... for processing Images



Source: e2eml.school

Outlook: How do different layers work?
Convolutional Layers

Why not fully-connected layers?

Hint: Think about the scaling for a 512x512 pixel image in RGB

Source: e2eml.school

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Hint: Think about the scaling for a 512x512 pixel image in RGB

With only one hidden layer and a moderate amount of units (say 20) ...

... we would have 512*512*3*20 ≈ 15.7 mio parameters already

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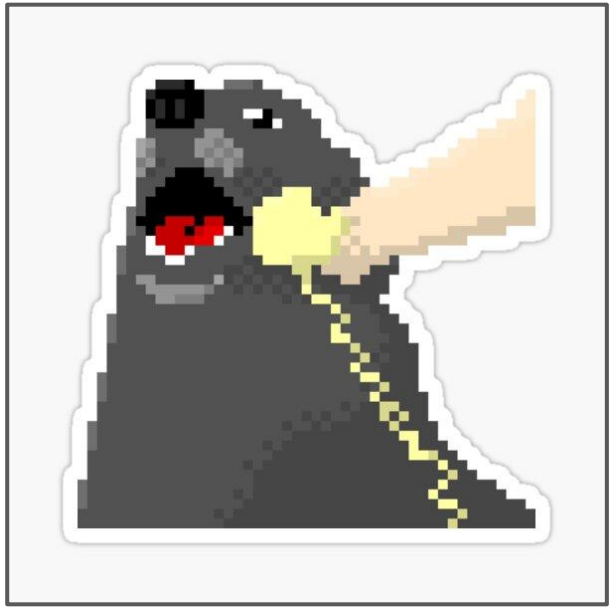
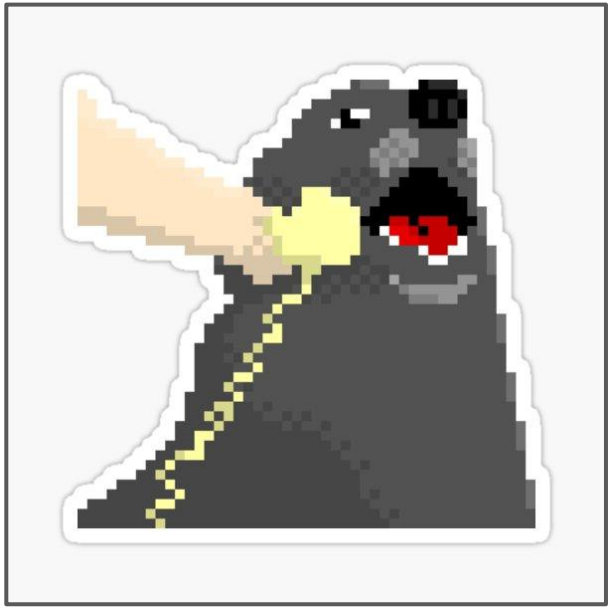
Convolutional Layers





Source: redbubble.com

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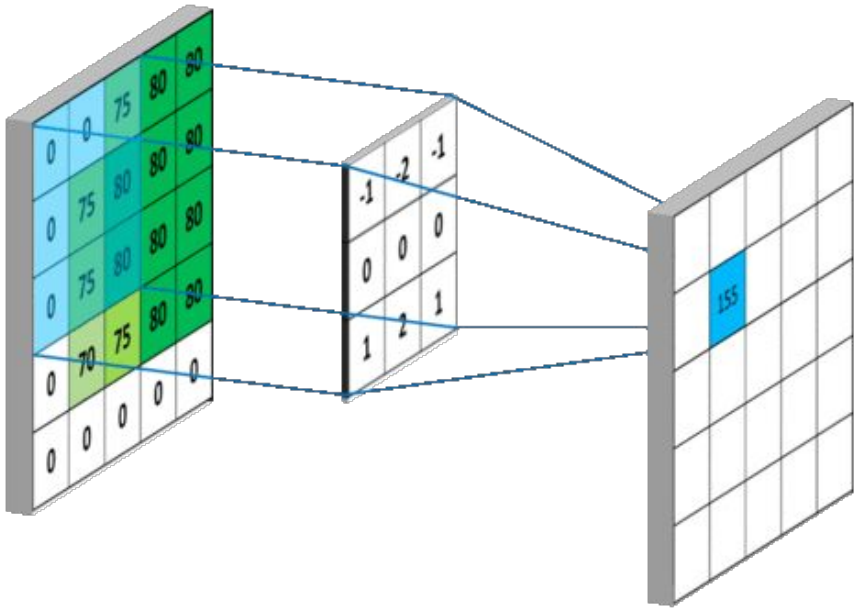

Keyword: Weight sharing

Source: medium.com

Outlook: How do different layers work?
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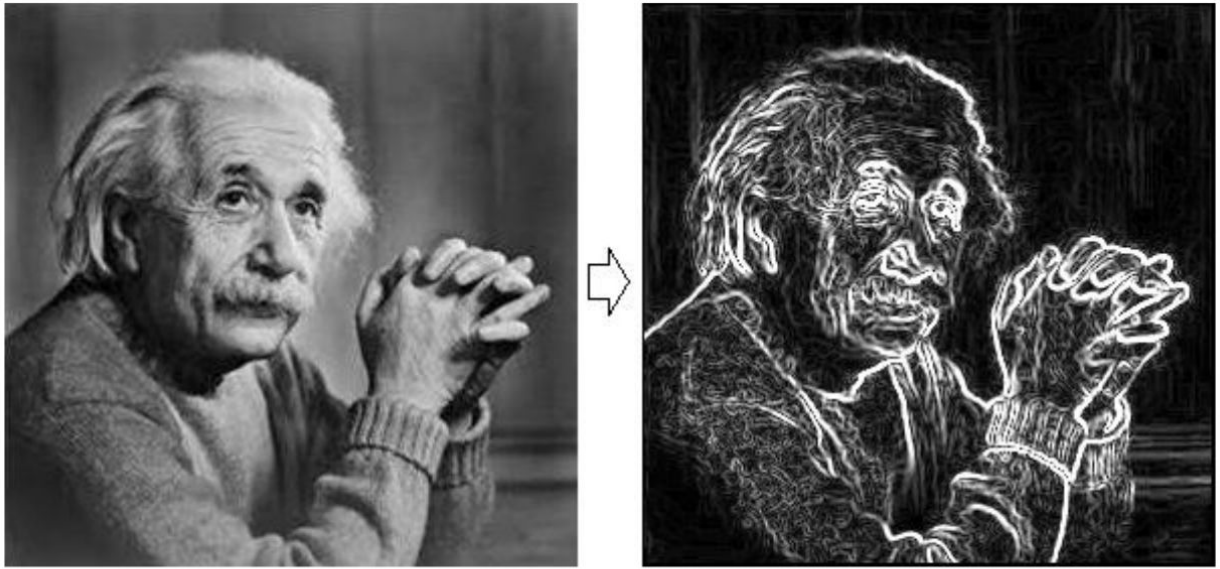
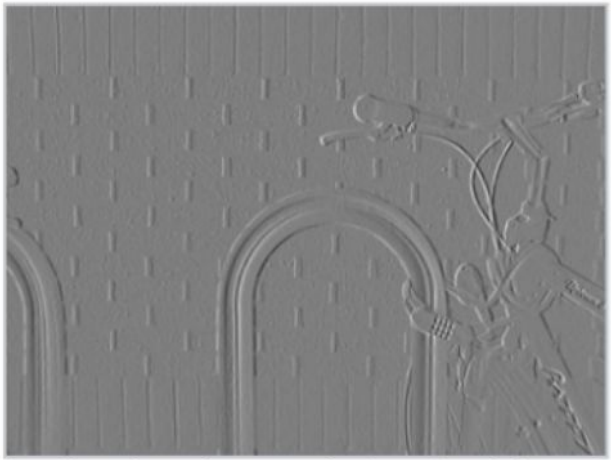


Figure: Sobel-filtered image.

Outlook: How do different layers work?
Convolutional Layers

Input



Vertical edges detected by S_x

Outlook: How do different layers work?
Convolutional Layers

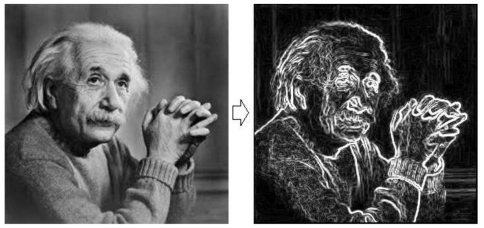
Figure: Sobel-filtered image.

Sobel showed that the gradient image $\mathbf{G}_x$ of original image $\mathbf{A}$ in x-dimension can be approximated by

$$\mathbf{G}_x = \begin{bmatrix} -1 & 0 & +1 \\ -2 & 0 & +2 \\ -1 & 0 & +1 \end{bmatrix} * \mathbf{A} = \mathbf{S}_x * \mathbf{A}$$

where $*$ indicates a mathematical operation known as a convolution, not a traditional matrix multiplication

Outlook: How do different layers work?
Convolutional Layers



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the filter

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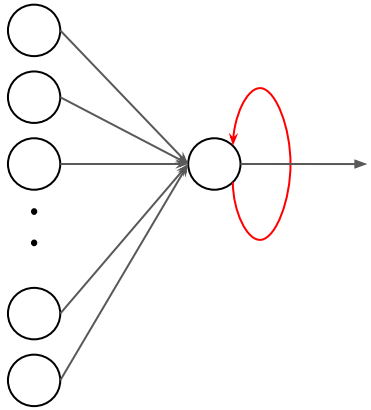
Outlook: How do different layers work?

Convolutional Layers

Source: medium.com

Outlook: How do different layers work?

Recurrent Neural Network Layers



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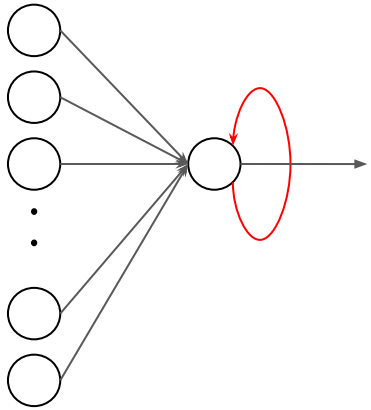
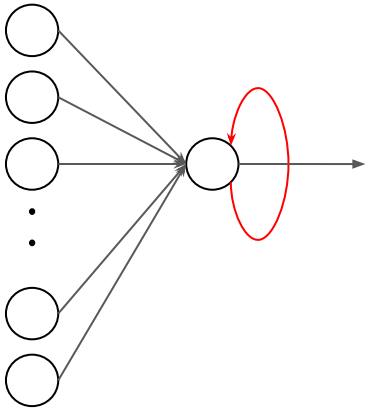
Recurrent Neural Network Layers



Usually for sequential data

Outlook: How do different layers work?
Recurrent Neural Network Layers

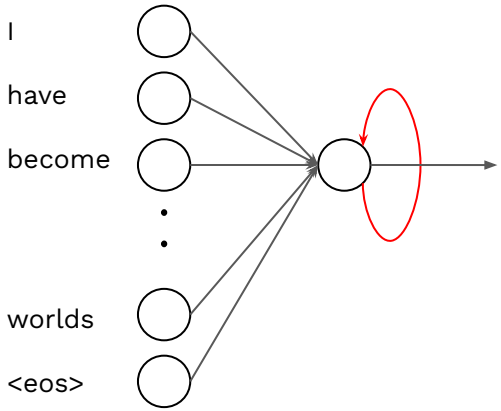


Usually for sequential data

Here: Text sentence

Outlook: How do different layers work?

Recurrent Neural Network Layers



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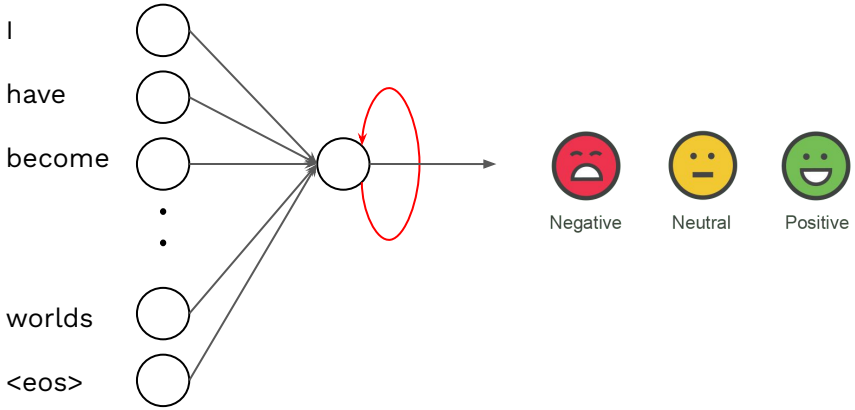
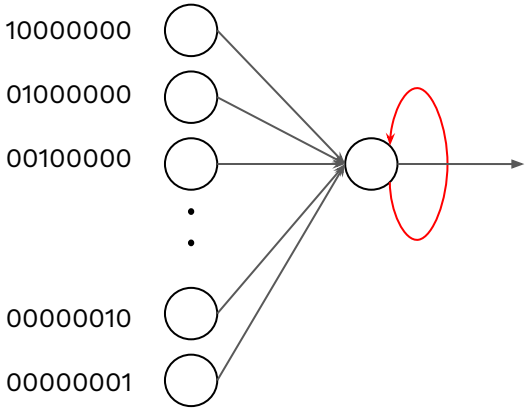
Recurrent Neural Network Layers



Outlook: How do different layers work?

Recurrent Neural Network Layers

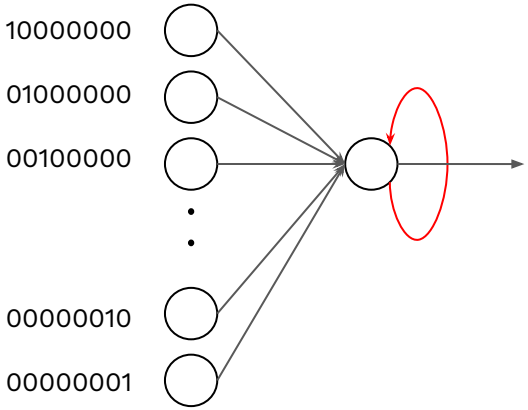


After binary text encoding*,
we can feed the text into a network

*there are better ways to encode or tokenize text

Outlook: How do different layers work?

Recurrent Neural Network Layers

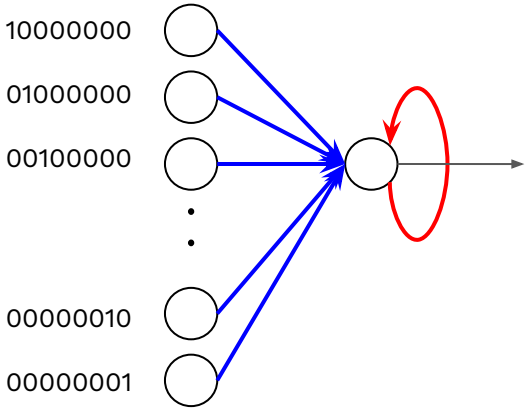


After binary text encoding*,
we can feed the text into a network

Keyword: Weight sharing

Outlook: How do different layers work?

Recurrent Neural Network Layers

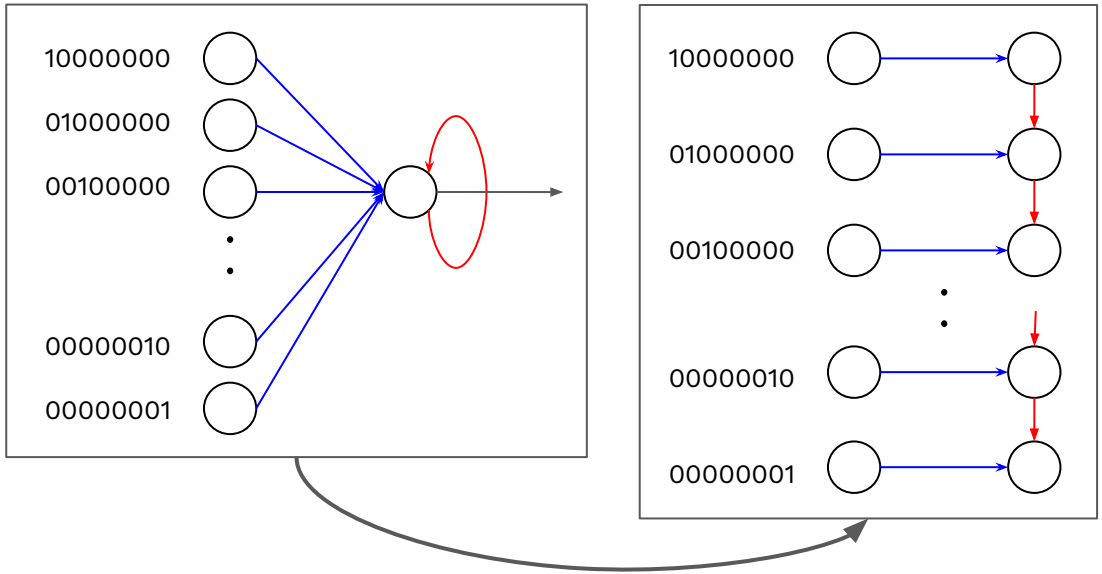


Blue connections (weights) are shared, same for red connection

Keyword: Weight sharing

Outlook: How do different layers work?

Recurrent Neural Network Layers

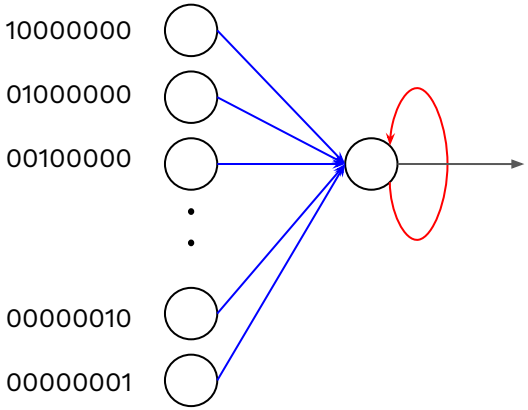


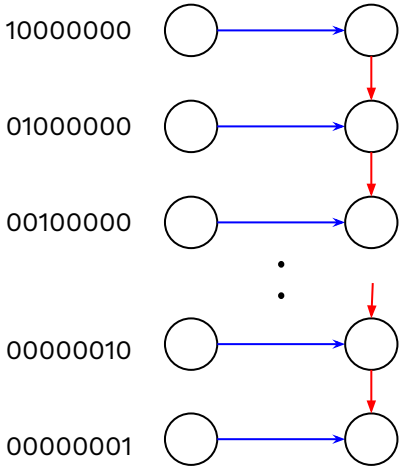
unroll network

Keyword: Weight sharing

Outlook: How do different layers work?

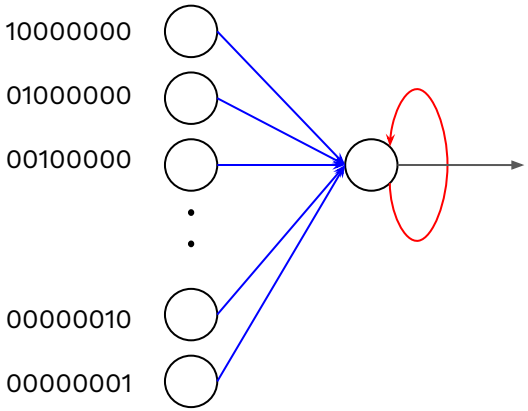
Recurrent Neural Network Layers

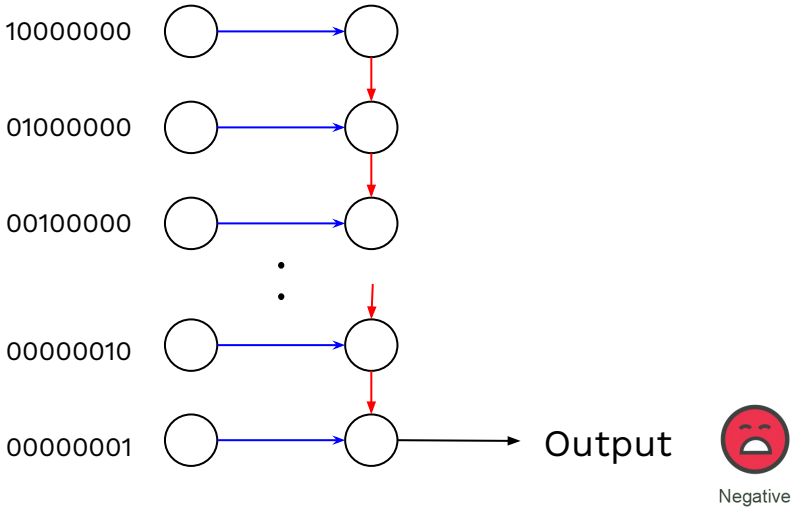




Outlook: How do different layers work?

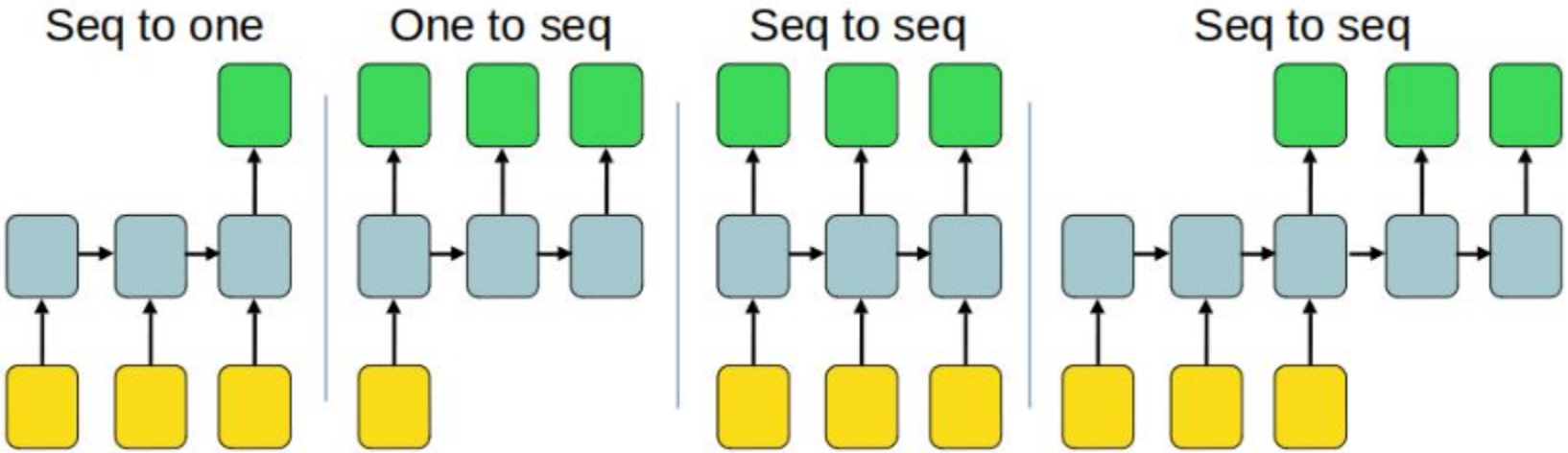
Recurrent Neural Network Layers





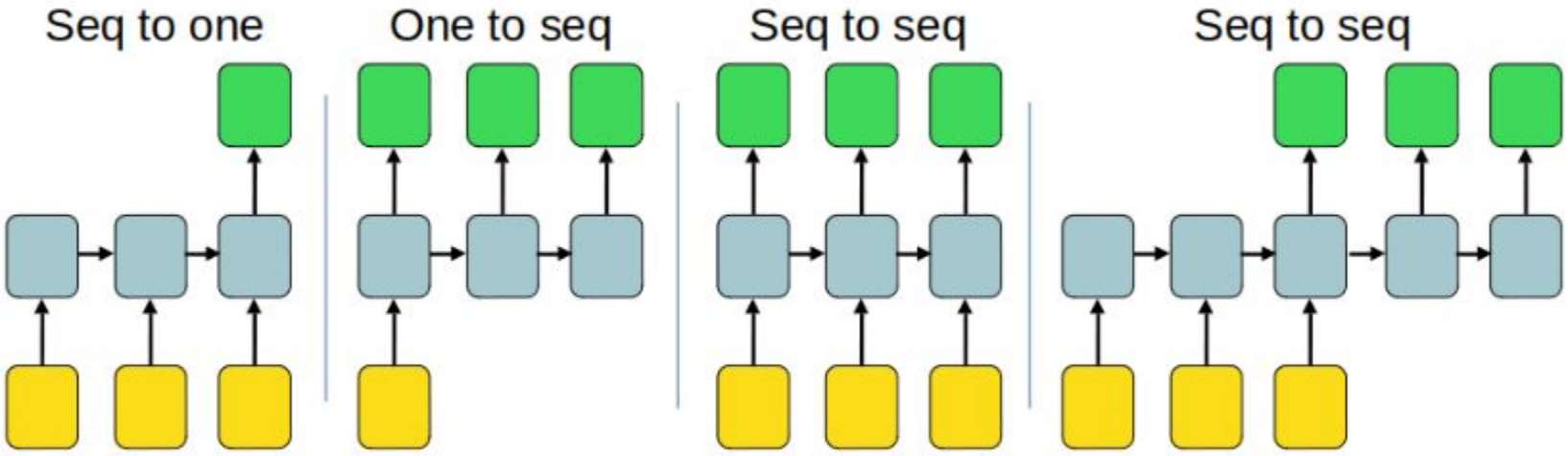
Outlook: How do different layers work?

Recurrent Neural Network Layers



Outlook: How do different layers work?

Recurrent Neural Network Layers



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Thank you for your attention.

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Next steps:

- Learn about theory ⇒ Deep Learning Book
- Learn software ⇒ Dive into Deep Learning (Python only)
- deepregression ⇒ Tutorial Paper

References

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[9] Mini-batch optimization enables training of ODE models on large-scale datasets https://www.nature.com/articles/s41467-021-27374-6

[10] deepregression: A Flexible Neural Network Framework for Semi-Structured Deep Distributional Regression https://www.jstatsoft.org/article/view/v105i02

[11] Smoothing the Edges: A General Framework for Smooth Optimization in Sparse Regularization using Hadamard Overparametrization https://arxiv.org/abs/2307.03571

[12] Semi-Structured Distributional Regression https://www.tandfonline.com/doi/abs/10.1080/00031305.2022.2164054

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Backup

Distributional Regression in Neural Networks

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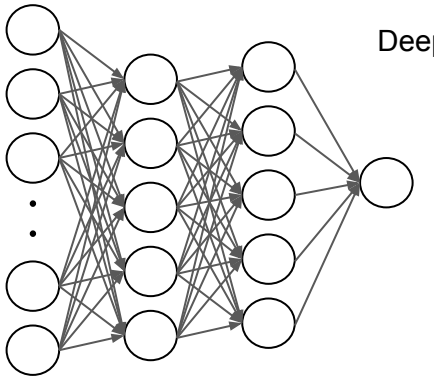
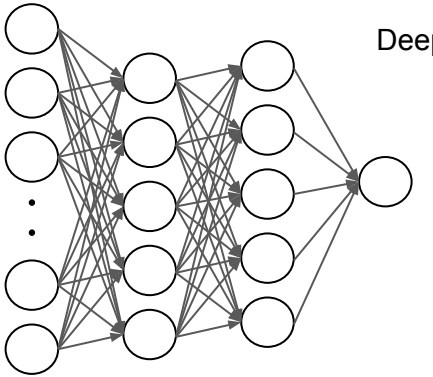
MCML

Semi-Structured Neural Networks

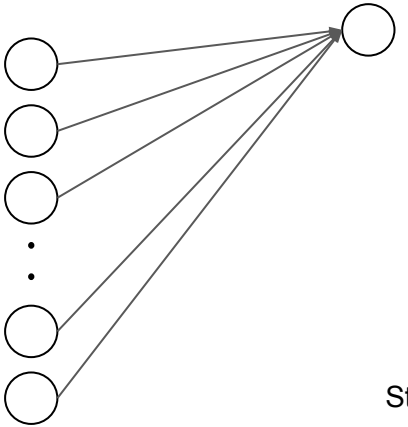


Deep Neural Network

Semi-Structured Neural Networks

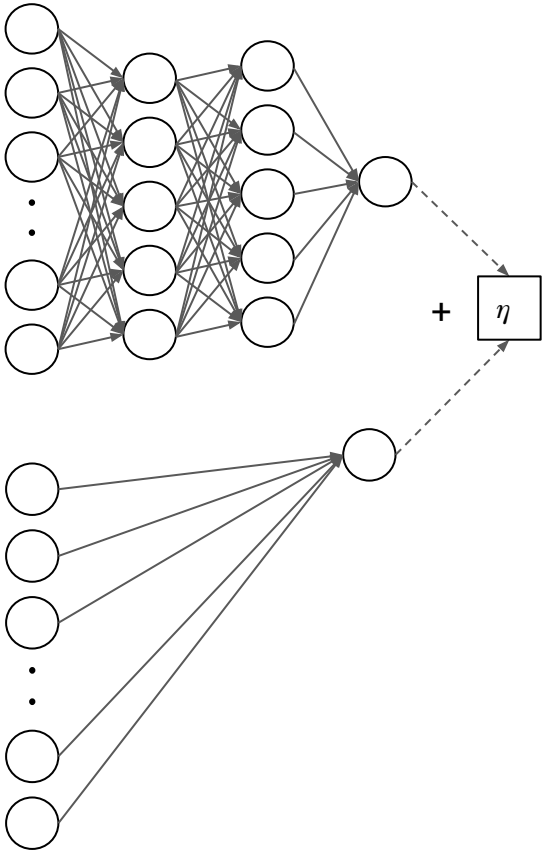


Deep Neural Network



Structured Predictor

Semi-Structured Neural Networks



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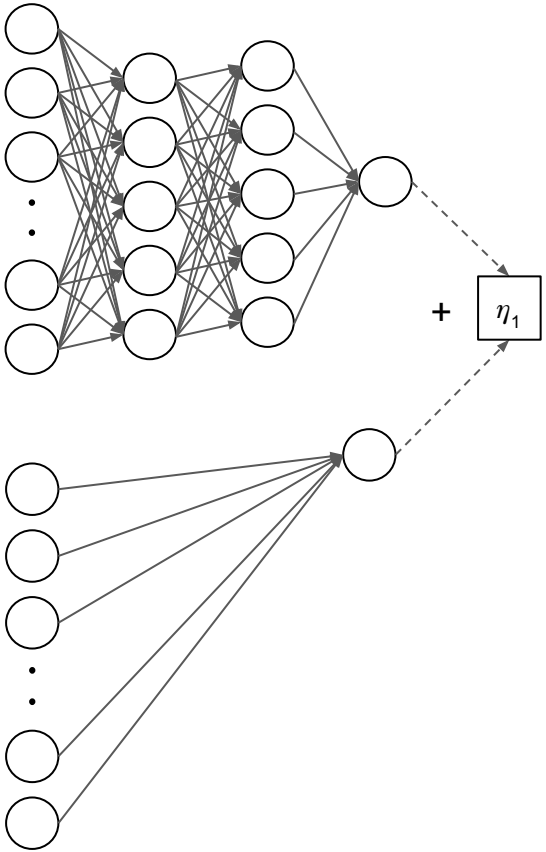

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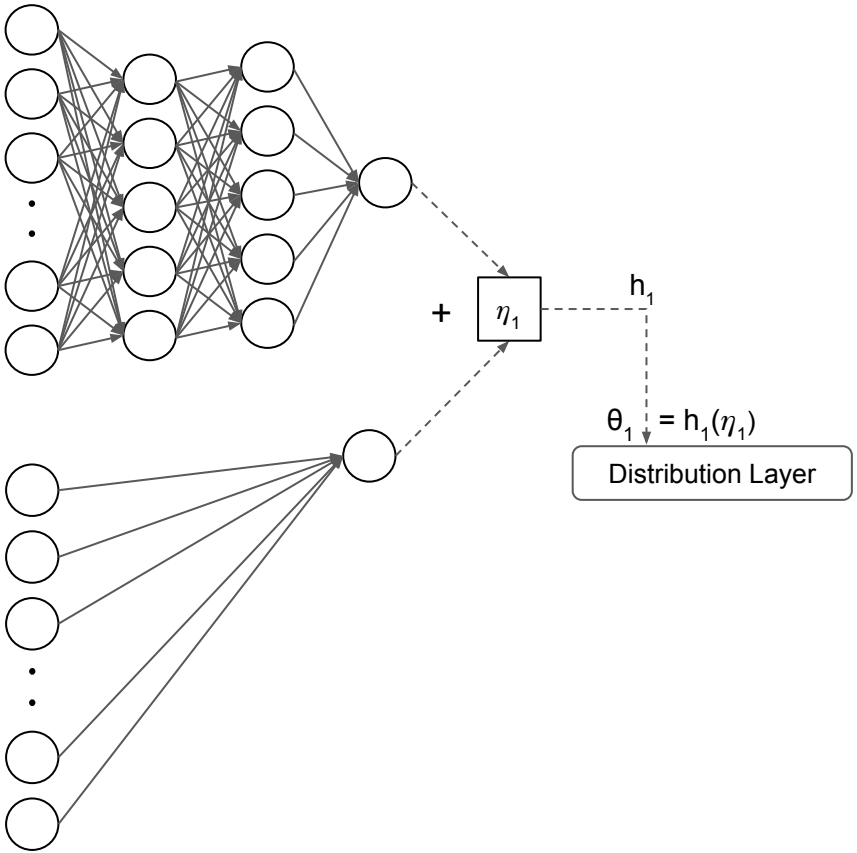

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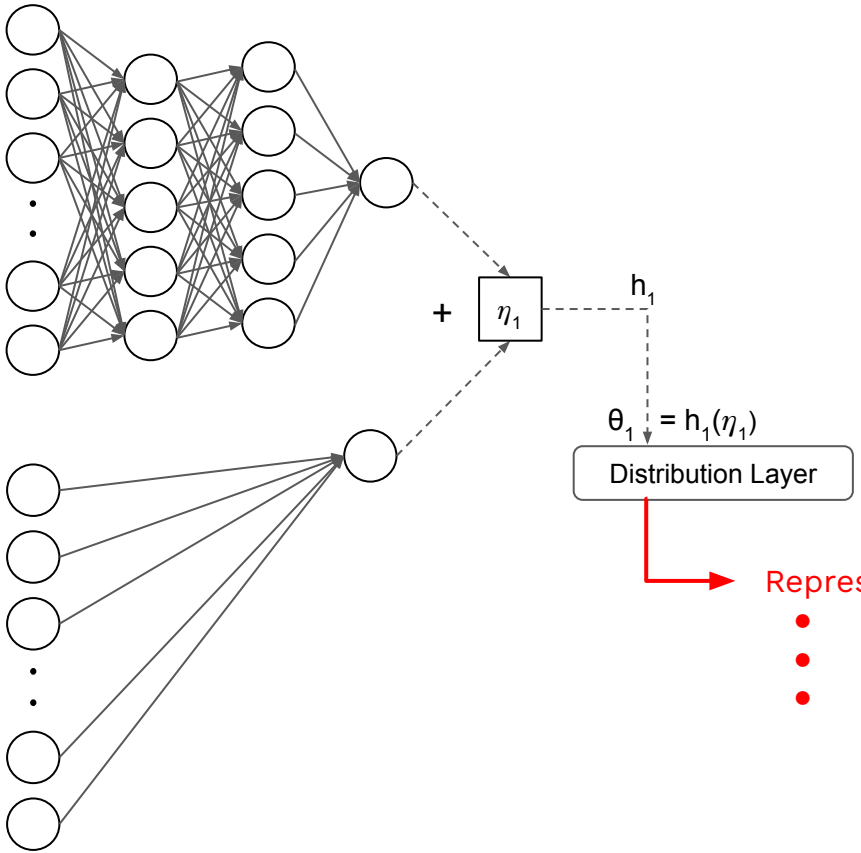
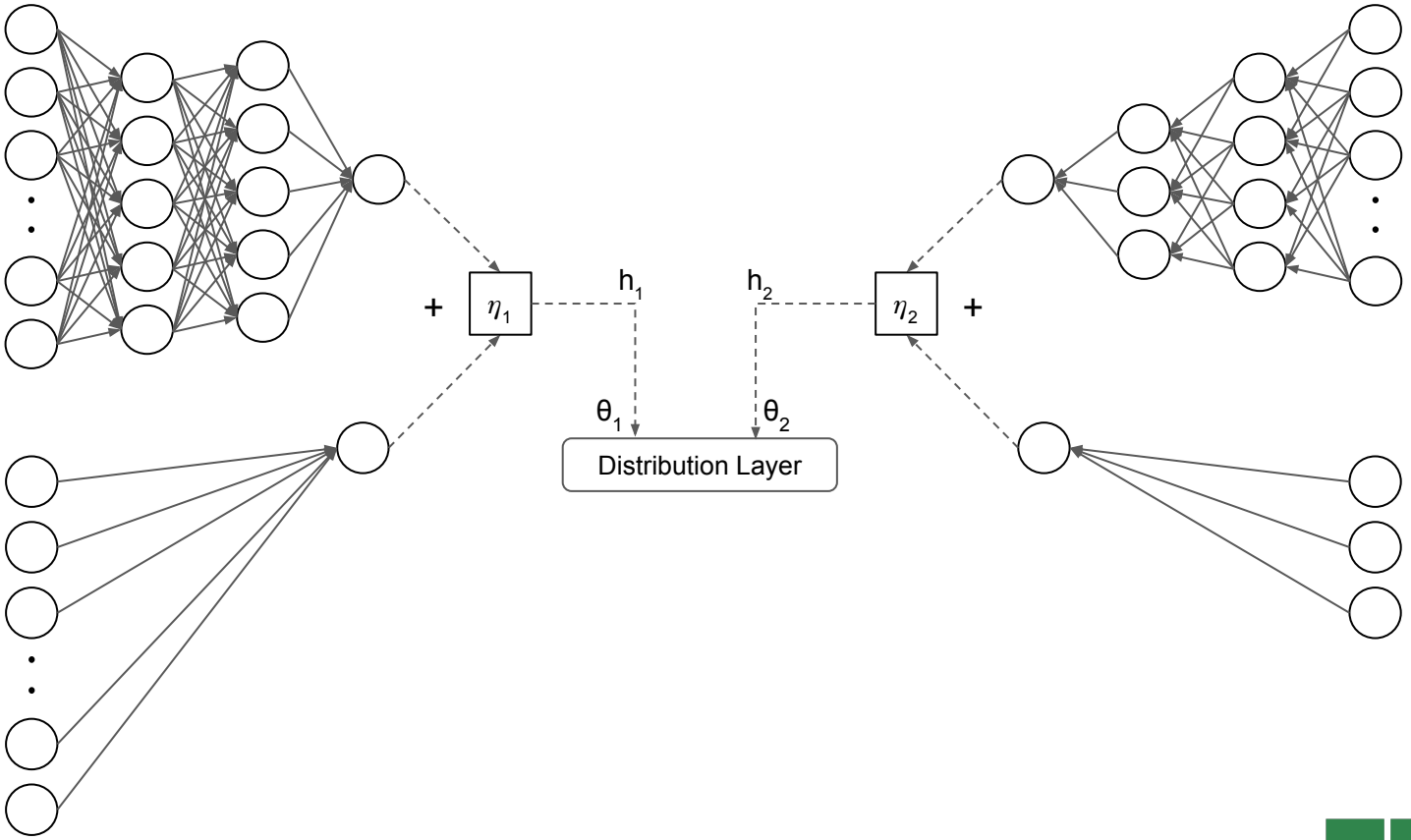


Representation of a pre-defined distribution

- Compute quantiles
- Sample
- Compute density

Semi-Structured Neural Networks



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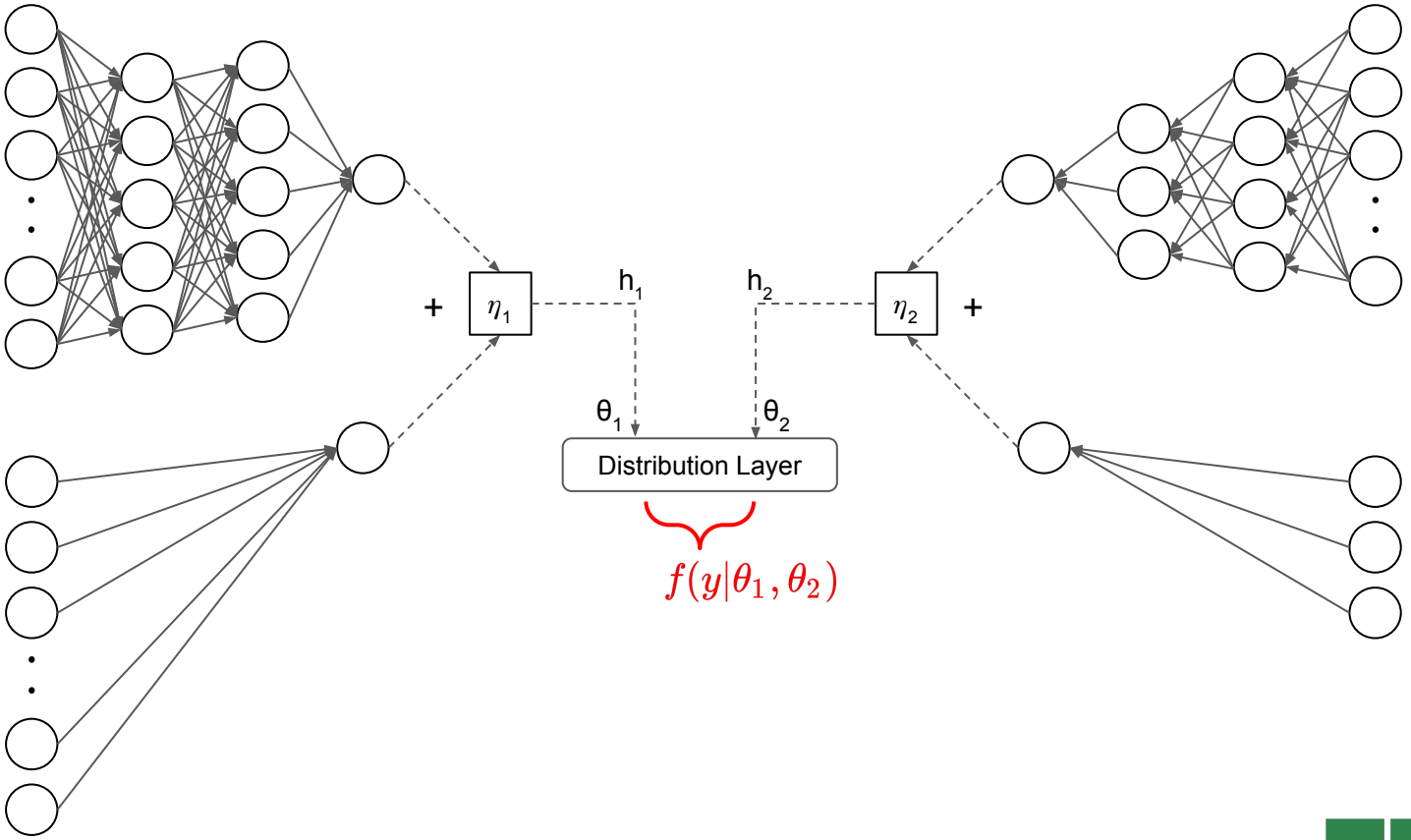

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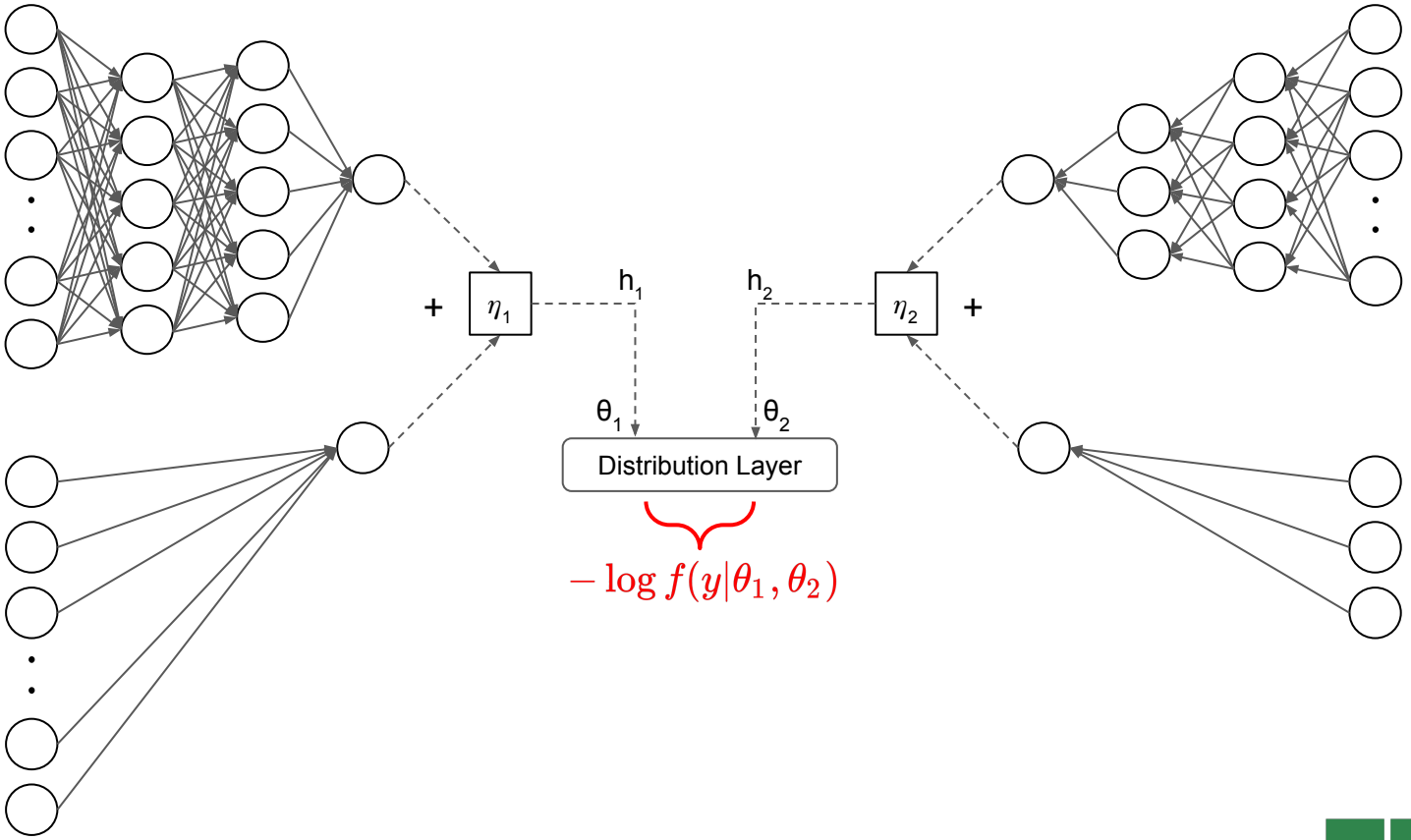

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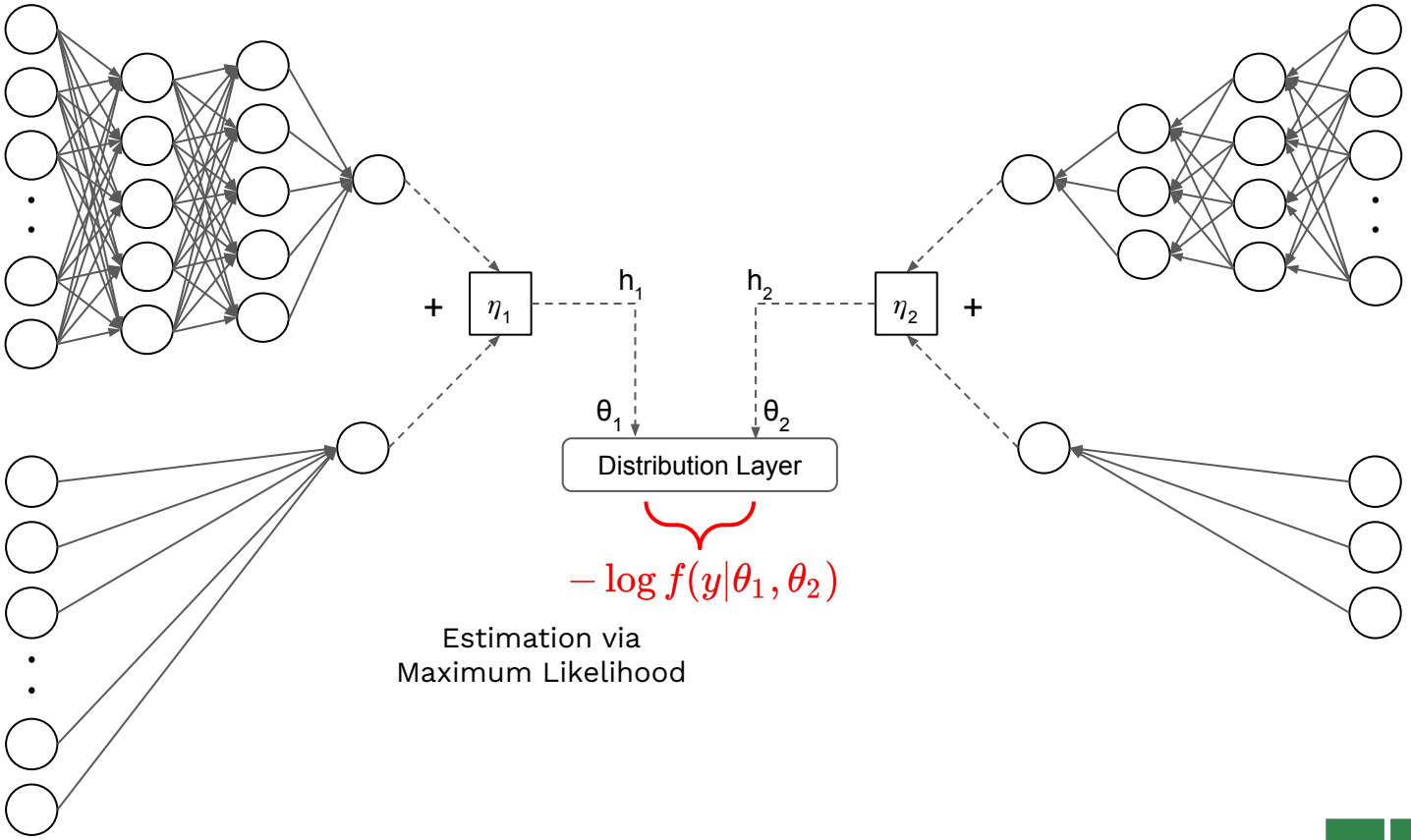

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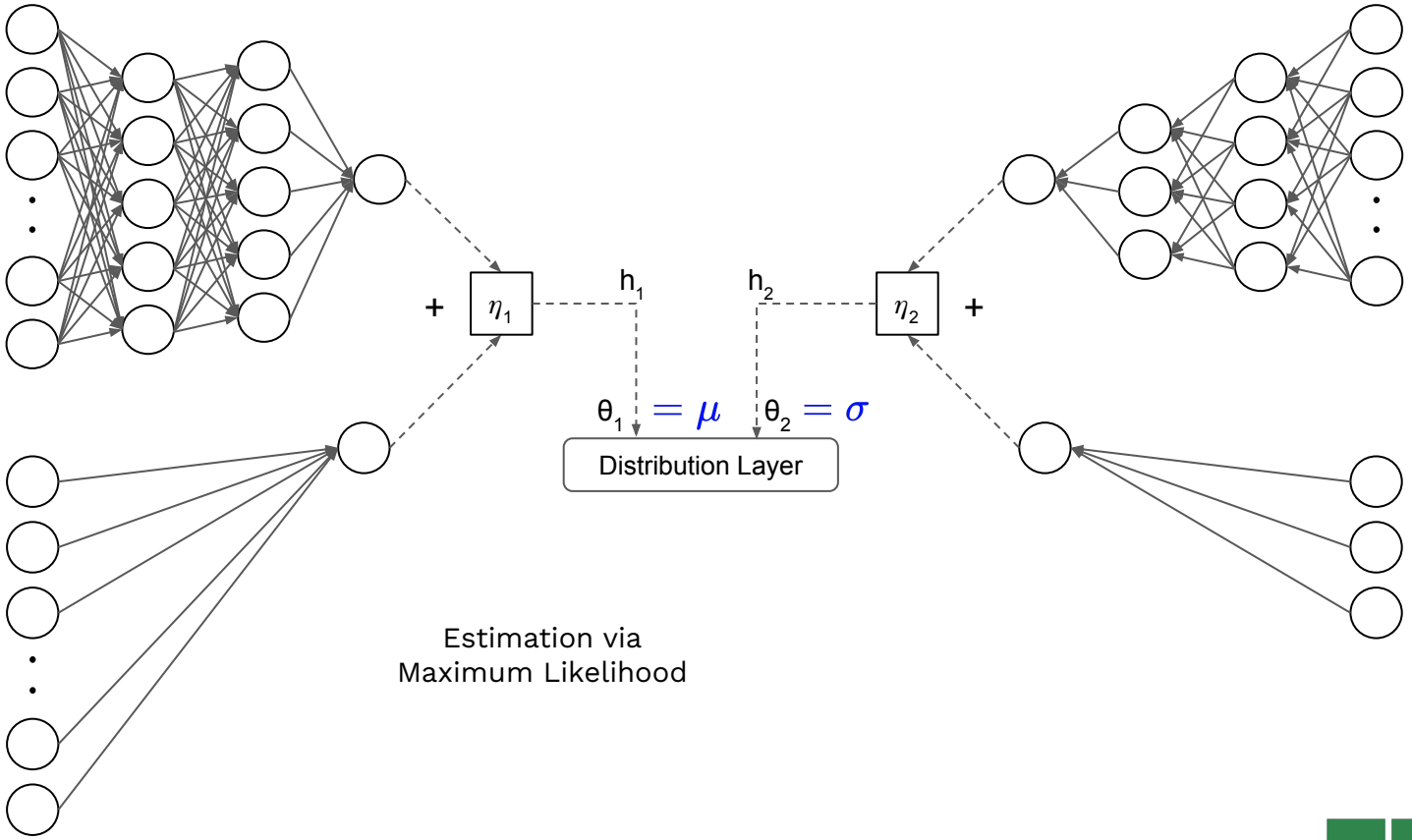

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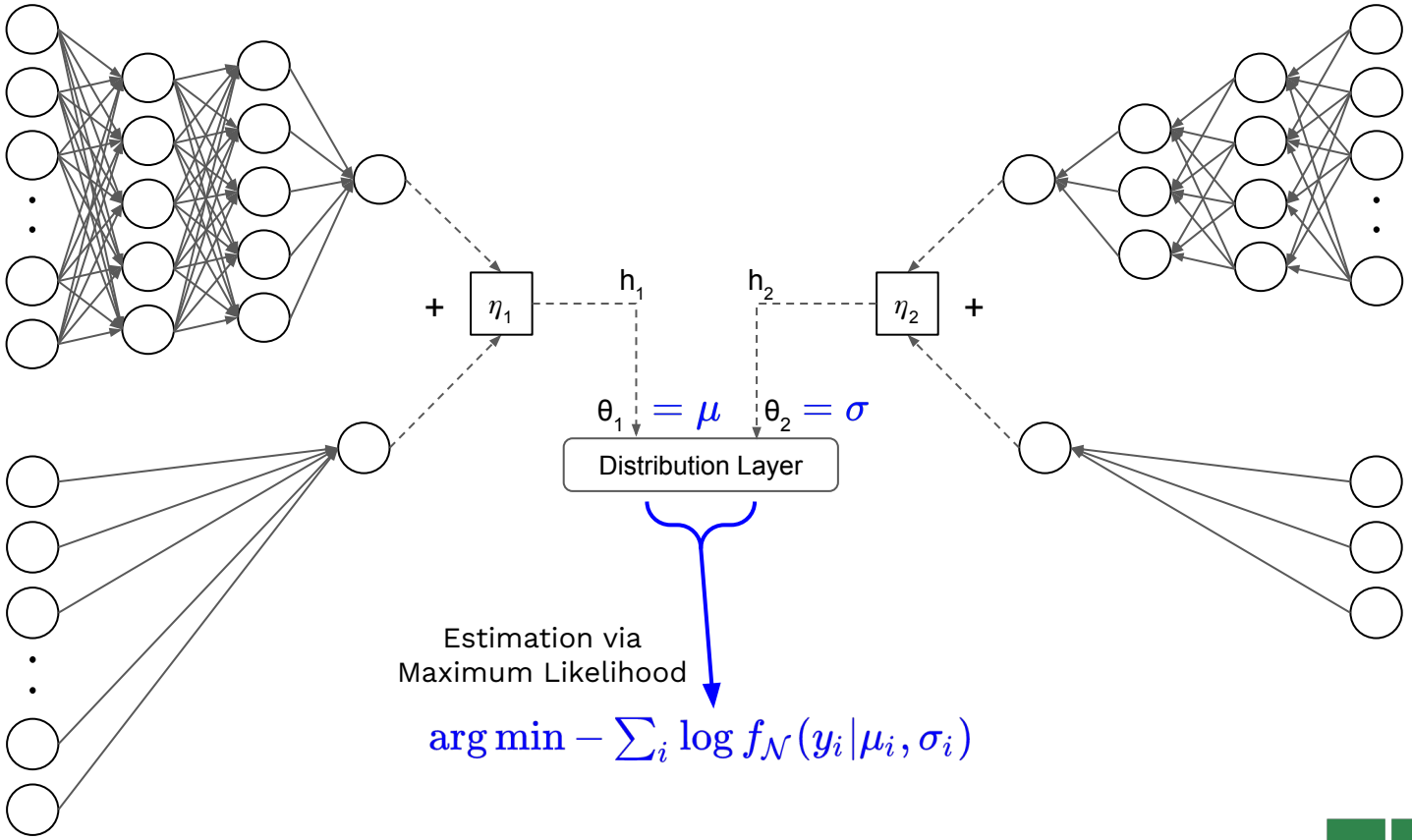

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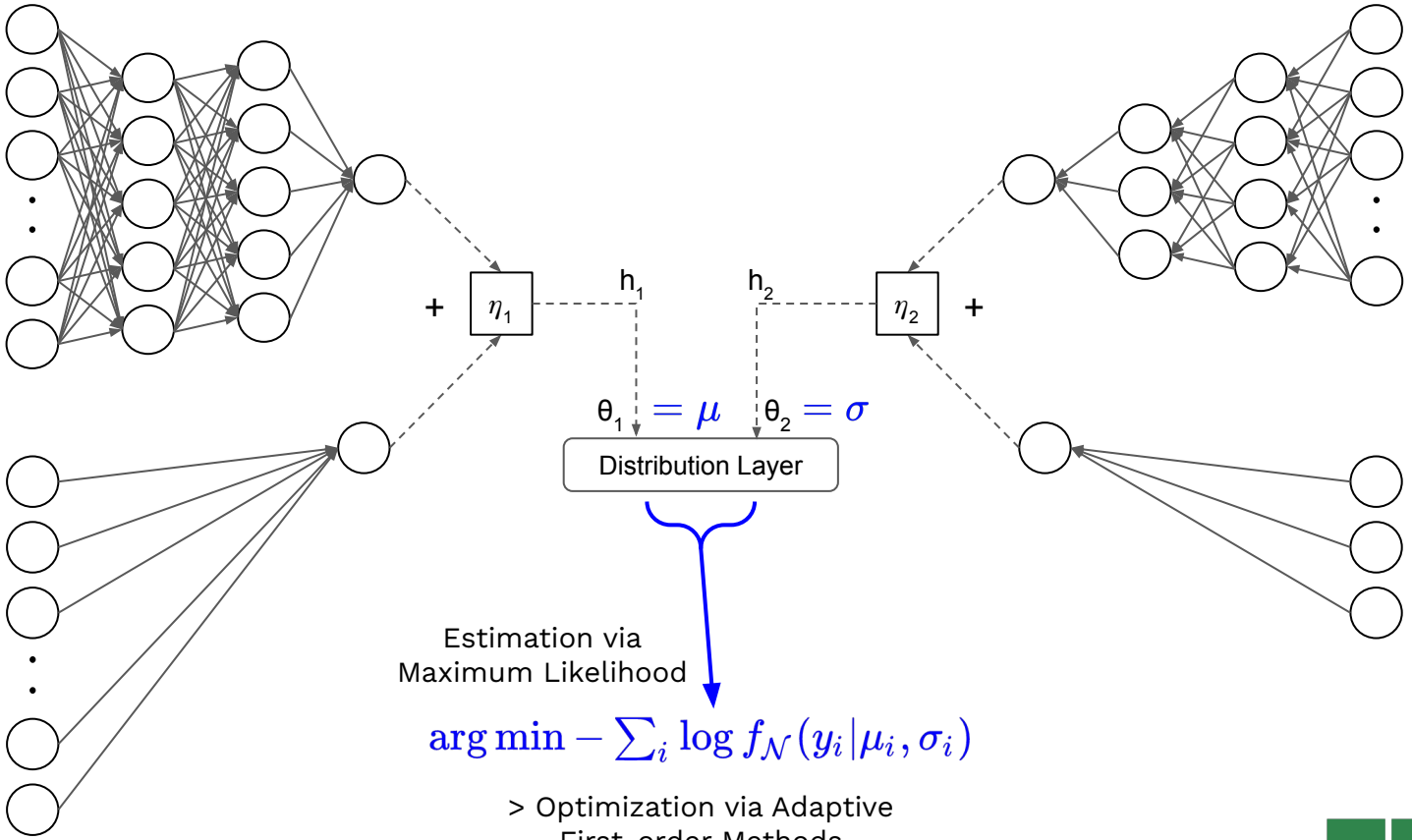
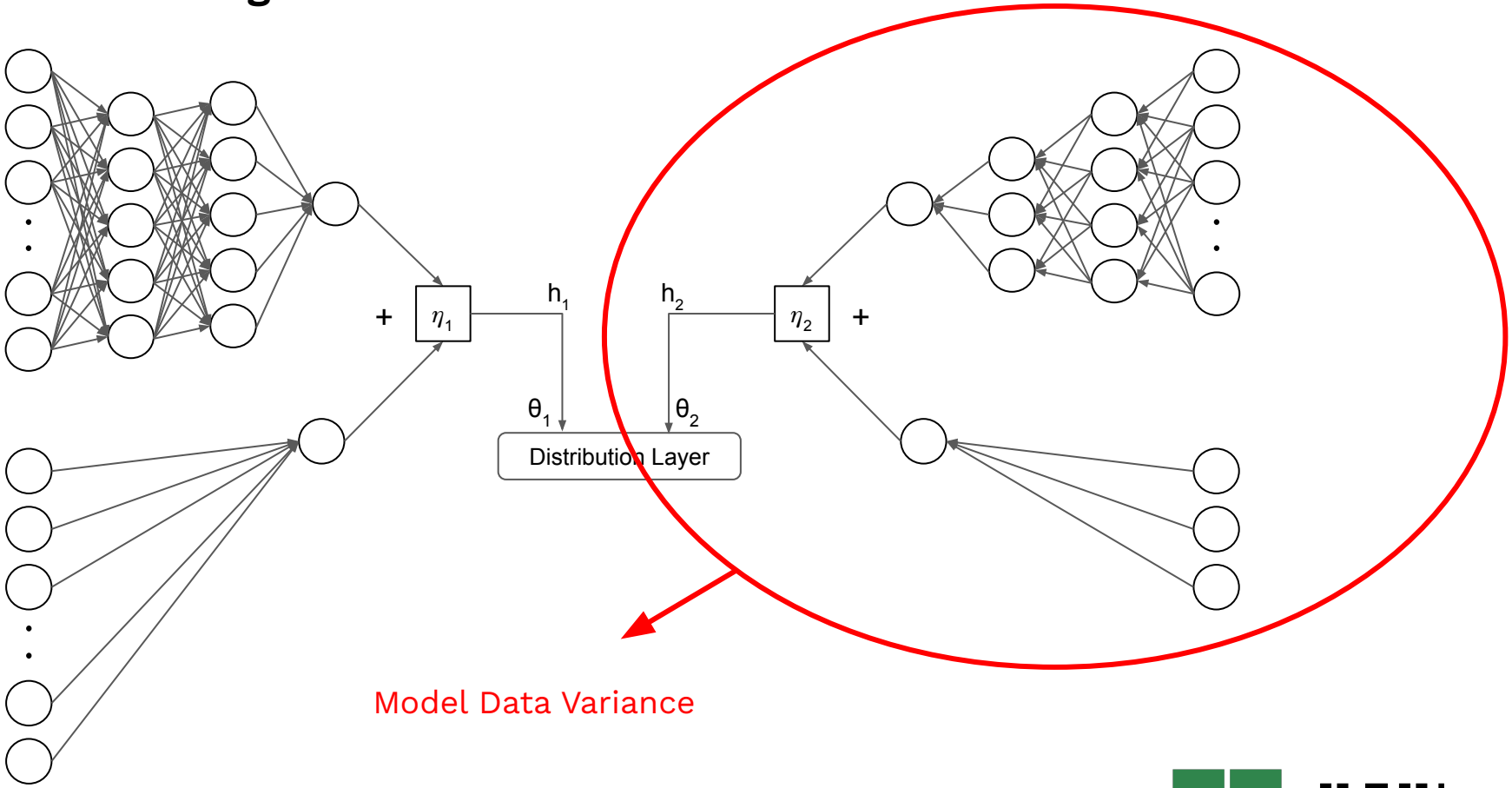


Distributional Regression – Model the Variance



Example: Predicting Airbnb Prices in Munich

```
mod_airbnb <- deepregression(
    y = price,
    family = "log_normal",
    list_of_formulas = list(
      location = ~1 + te(latitude, longitude) + room_type + bedrooms +
                  cnn(image) + lstm(desc),
      scale = ~1
    ),
    data = d_train
)
```

Example: Predicting Airbnb Prices in Munich

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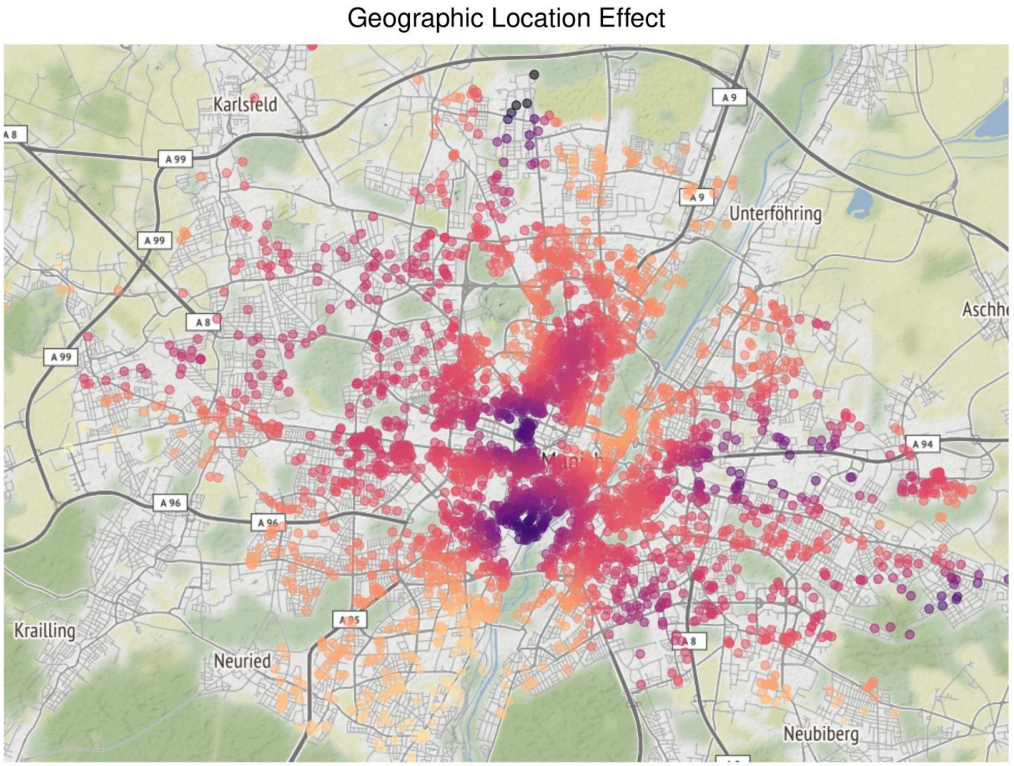
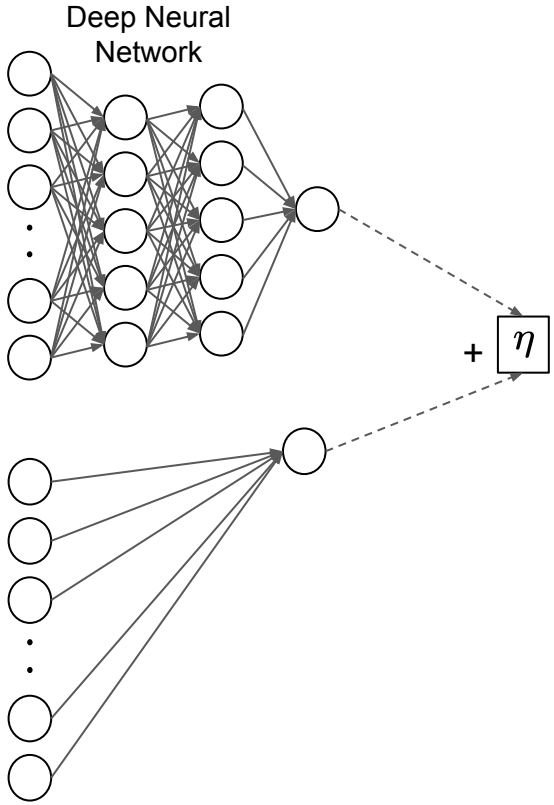


Identifiability

Non-Identifiability <-> Interpretability



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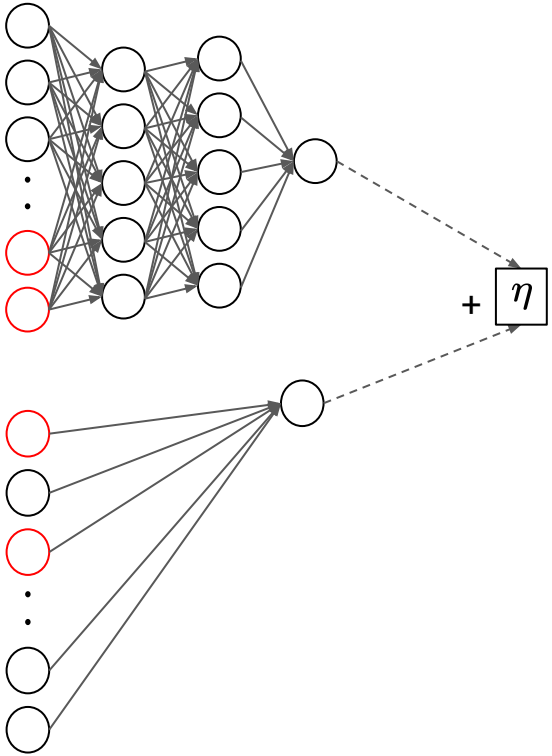

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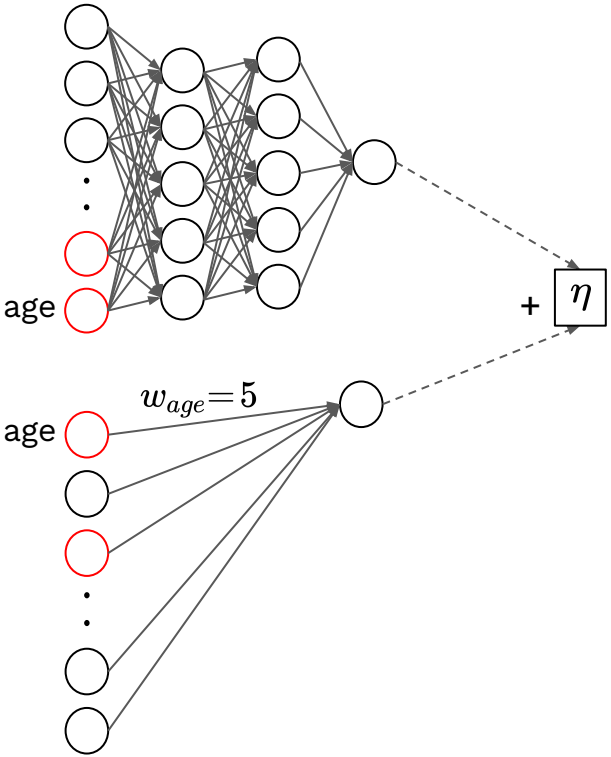

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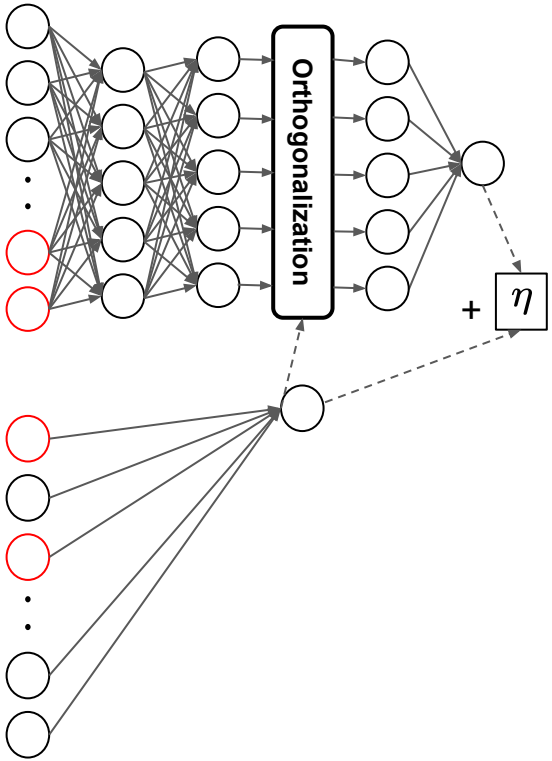
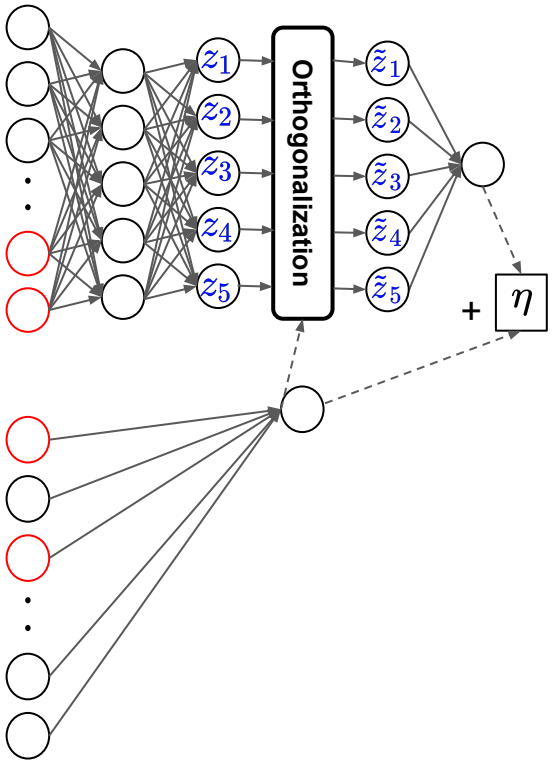


Rügamer et al., 2023,
The American Statistician

Non-Identifiability <-> Interpretability



[12] Rügamer et al., 2023,
The American Statistician

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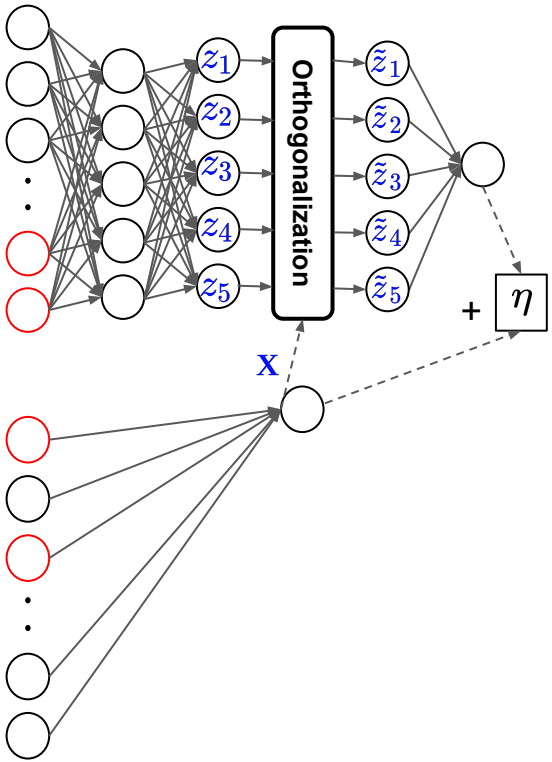

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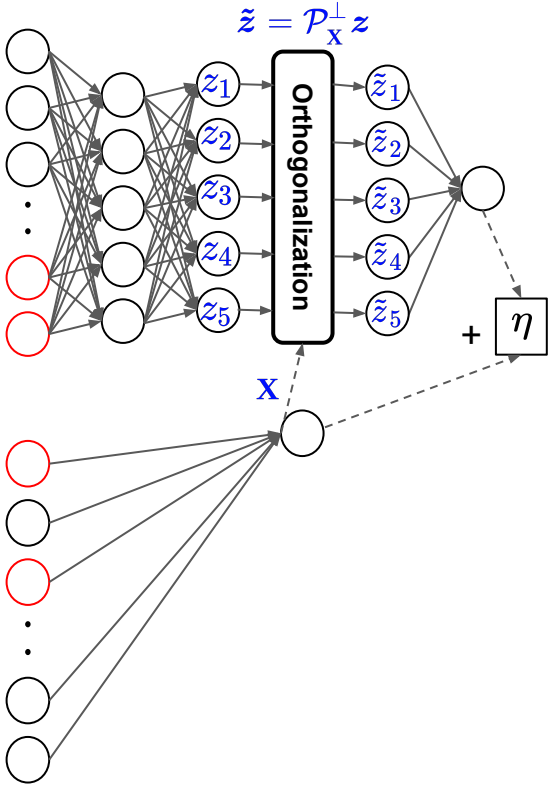

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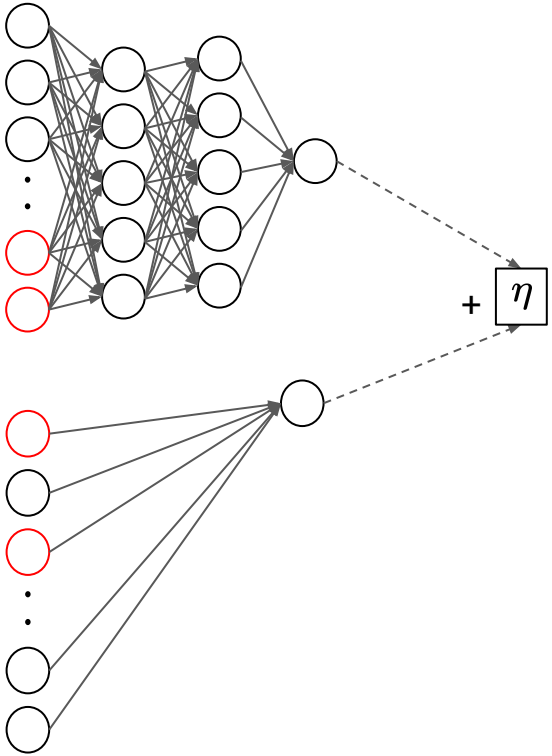
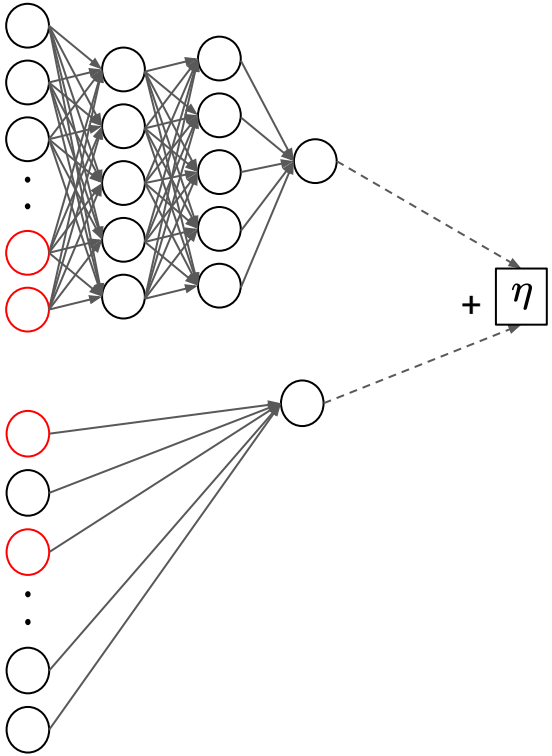


Post-hoc Orthogonalization
[13] Rügamer 2023, *ICML*

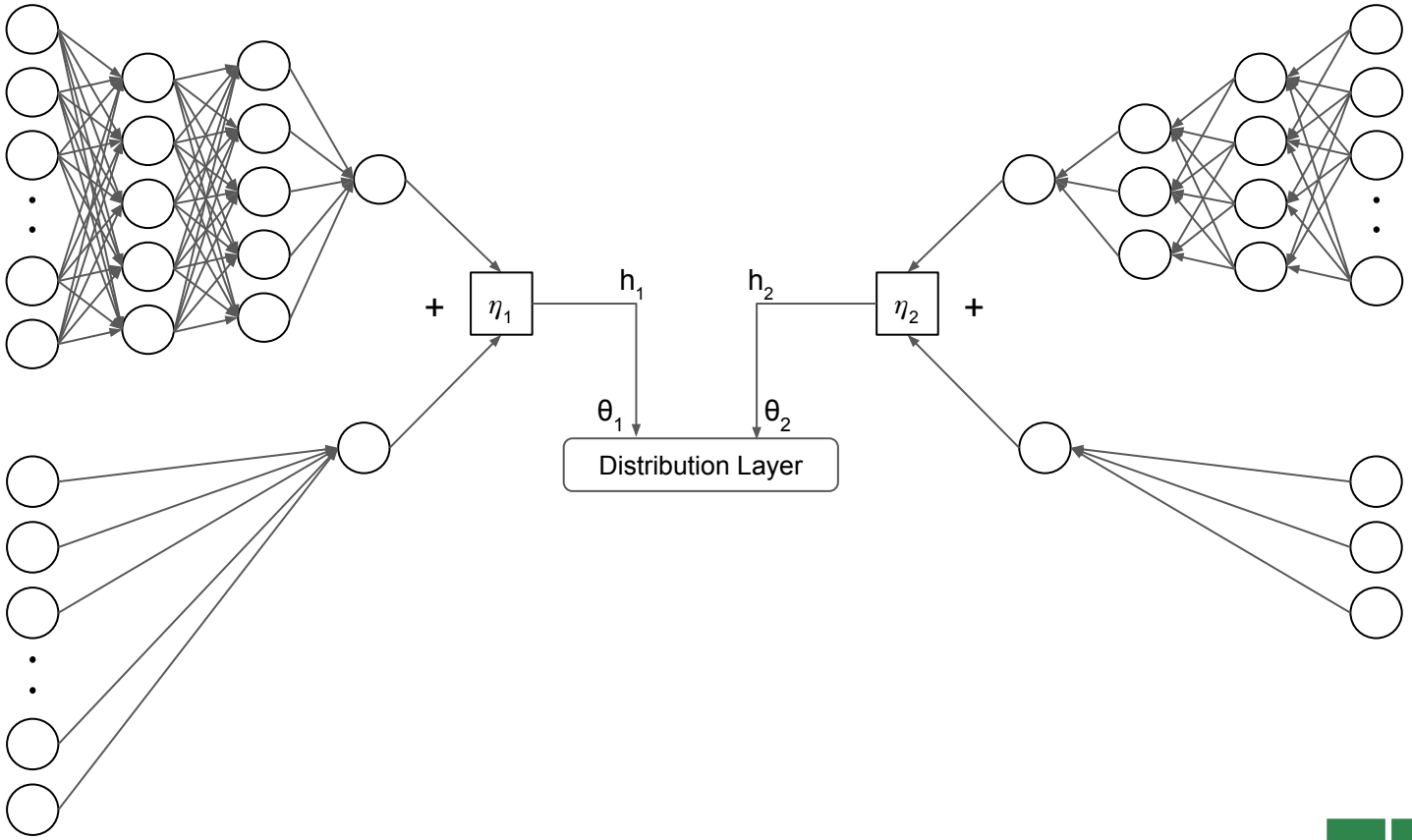
Non-Identifiability <-> Interpretability



Post-hoc Orthogonalization
[13] Rügamer 2023, *ICML*

- Fit network w/o constraints
- Orthogonalize after
- At costs of 1 forward pass
- More flexible
- Similar to functional ANOVA (Hooker)

Distributional Regression – Model the Variance



Expert Part:
Sparsity in Neural Networks

Expert Part: How can I obtain sparsity (in multimodal settings)?

Expert Part: How can I obtain sparsity (in multimodal settings)?

⇒ [11] **Sparse Modality Regression (Best Paper IWSM 2023)**

Why is sparse regularization not more common in DL?

- DL models are almost exclusively optimized "heuristically" using stoch. gradient descent (SGD) and variations (e.g., Adam)

Why is sparse regularization not more common in DL?

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- Works well for non-convex objectives, but not for sparsity-inducing penalties

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problem for Deep Learning (DL)

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Our proposal: Hadamard product parameterization

- = Continuously differentiable surrogate penalty
- Smooth ⇒ off-the-shelf SGD

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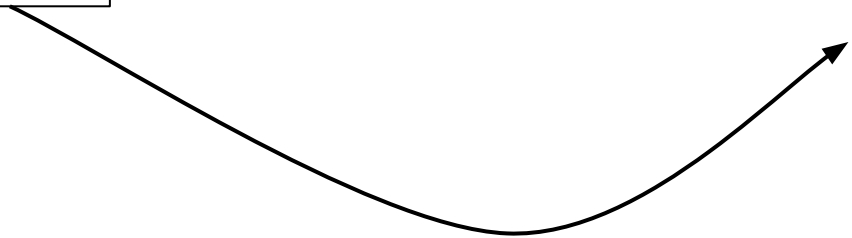

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⇒ Optimal solution is the same,
& introduces no additional local minima

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- “Truly” sparse solutions in neural networks using SGD
- Can be used for **anywhere** in the network
- Idea works for a large class of penalizations

$$\boldsymbol{\beta} \mapsto \sum_{j=1}^{L} \omega_j ||\boldsymbol{\beta}_j||_p^q \qquad 0 < q \leq p \leq 2,\ \omega_j > 0\ \forall\, j \in [L]$$

Empirical results: Linear model

$\beta = 0$

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L1 norm of coefficients β

Empirical results: Linear model

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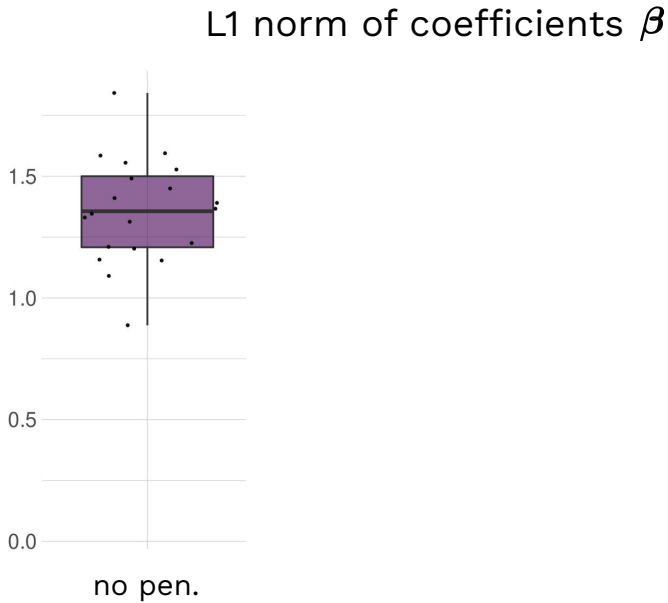

Empirical results: Linear model

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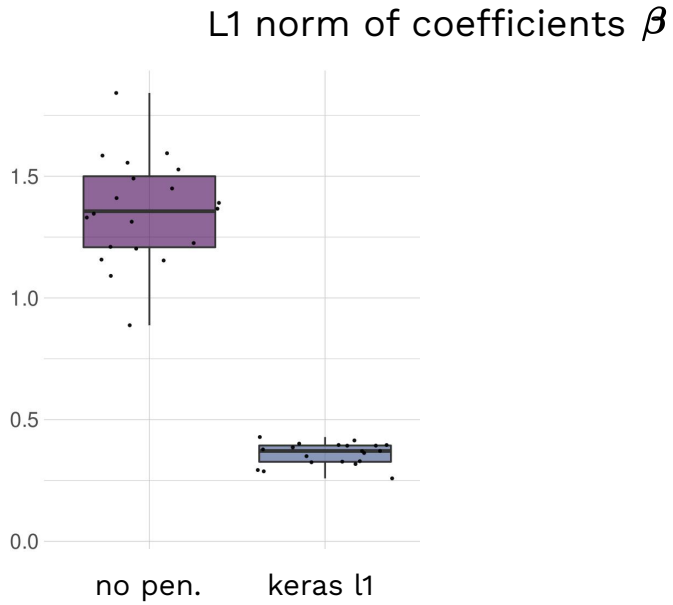

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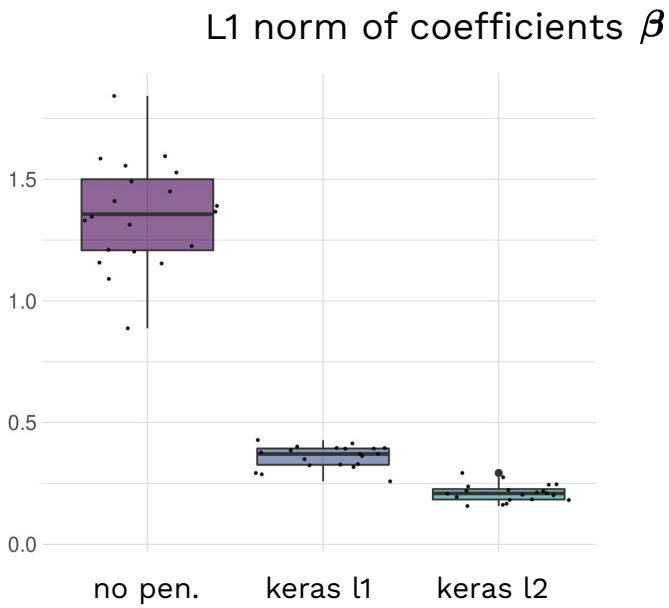

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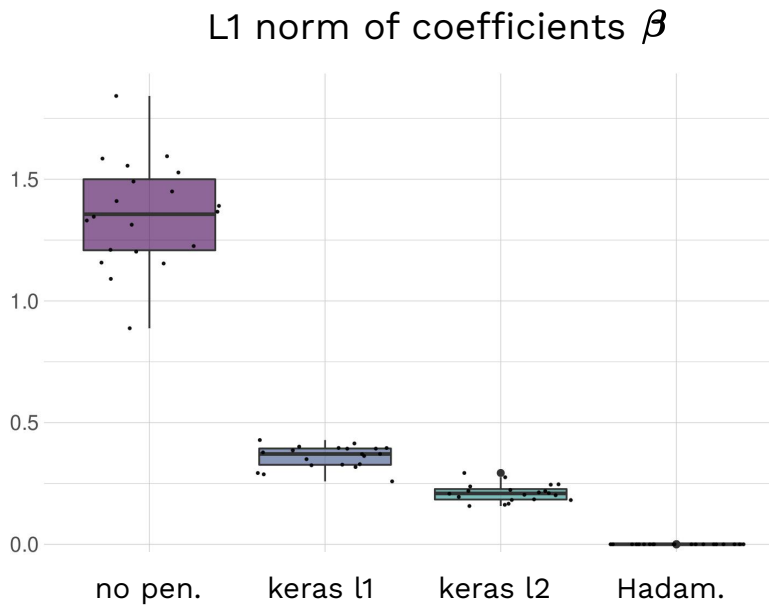

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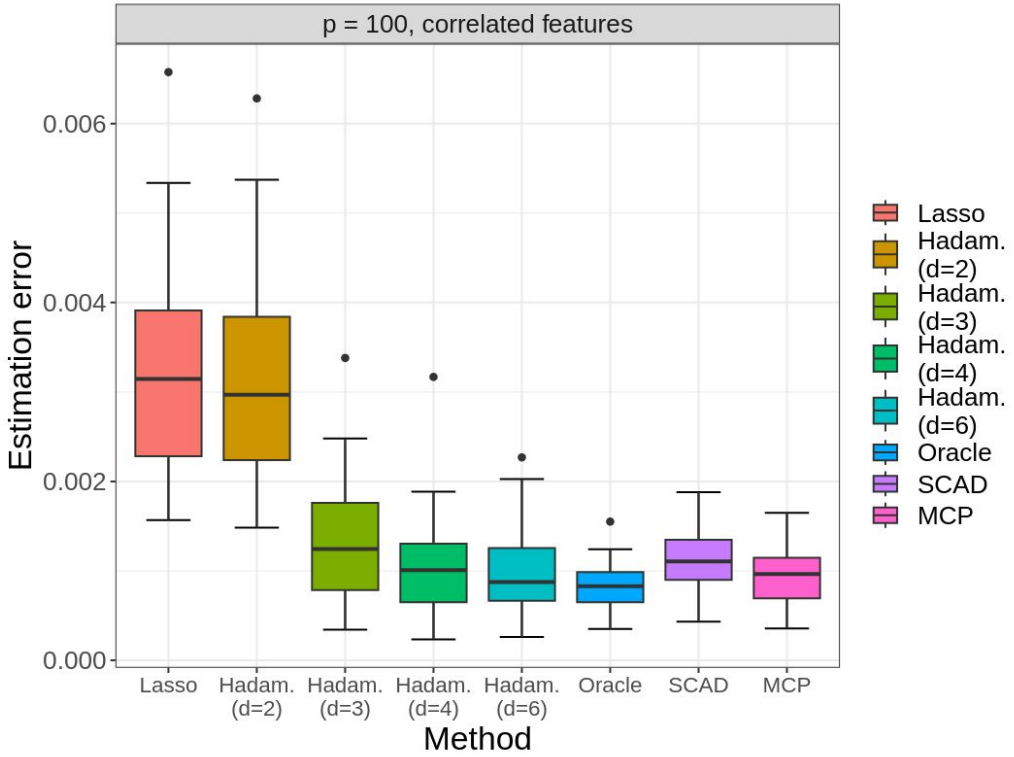

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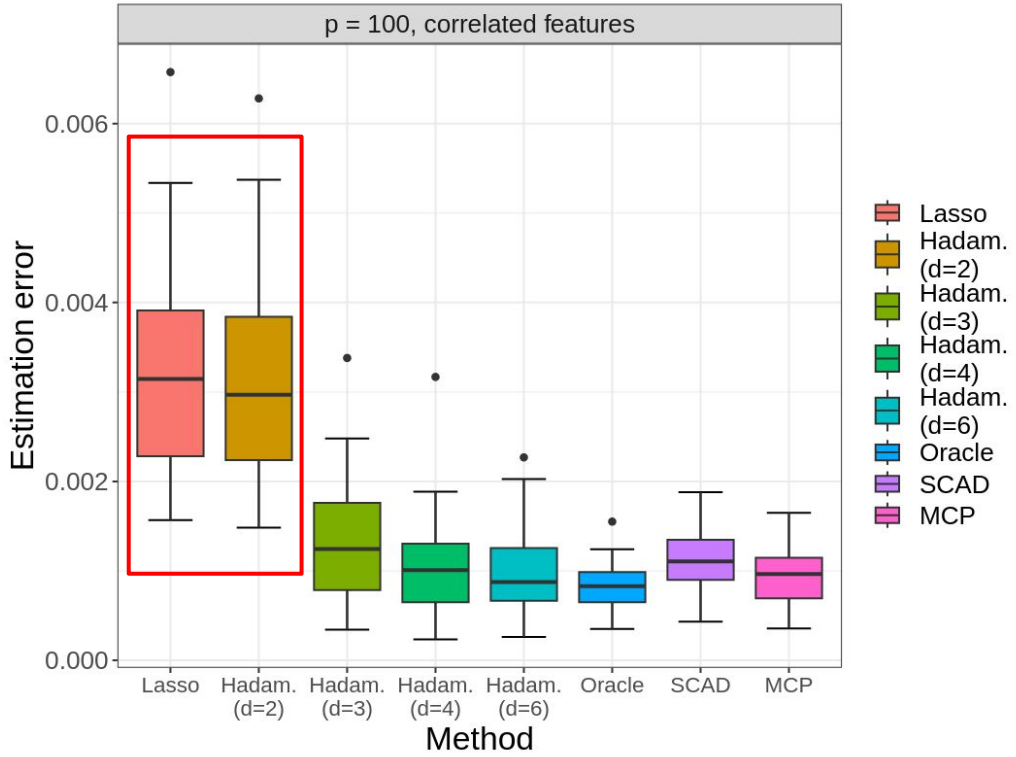

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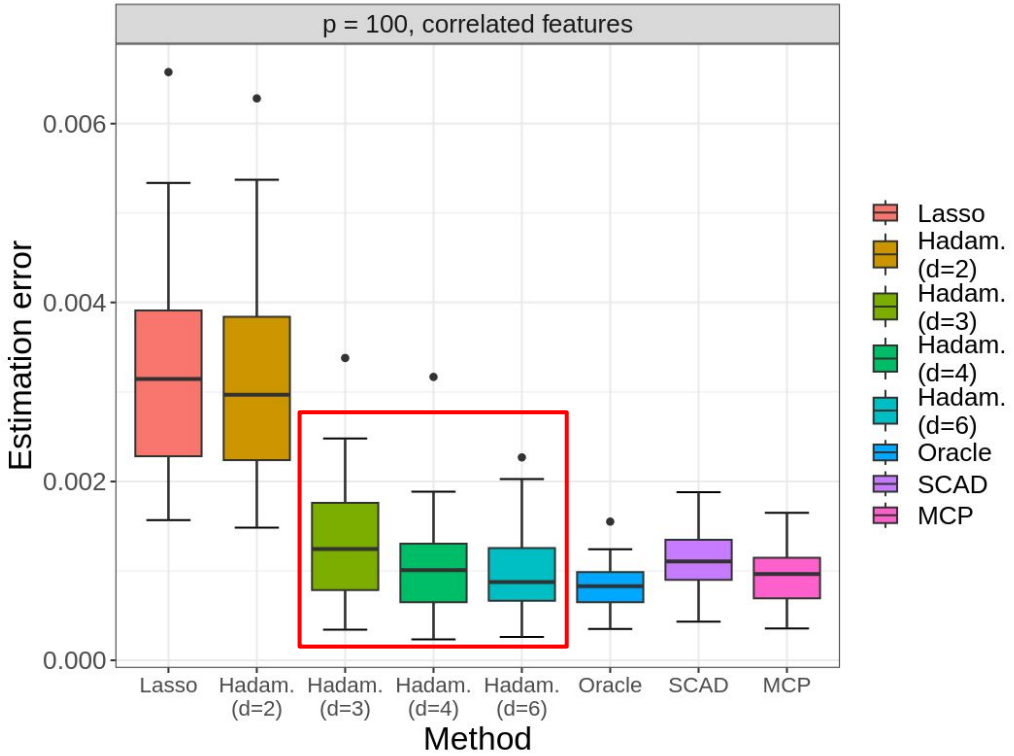
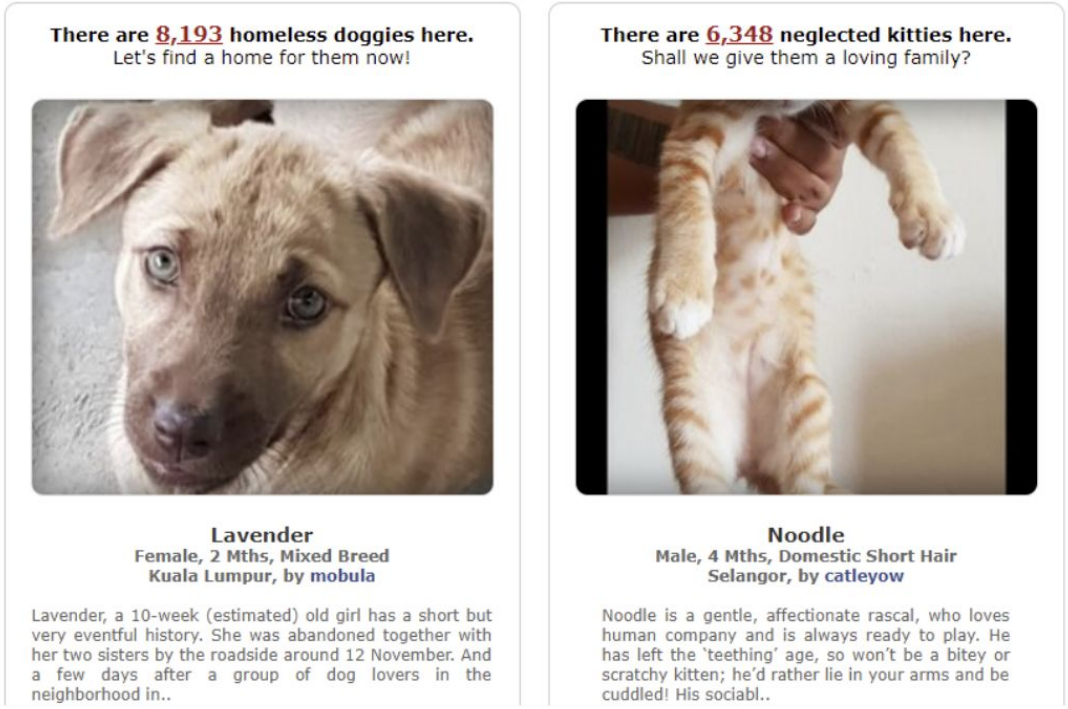


$$\boldsymbol{\beta} = \boldsymbol{u}_1 \odot \boldsymbol{u}_2 \odot \cdots \odot \boldsymbol{u}_d \longrightarrow \ell_{2/d}\text{-norm}$$

Empirical results: Sparse modality regression



Tabular + Image + Text Data

Source: Petfinder.my

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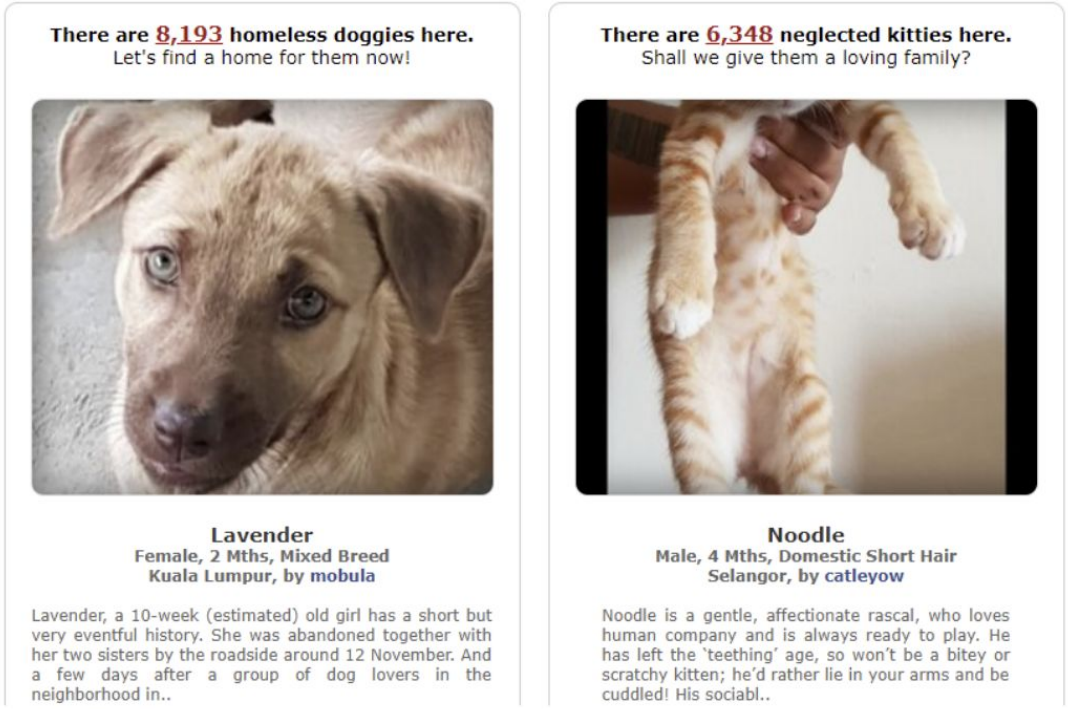
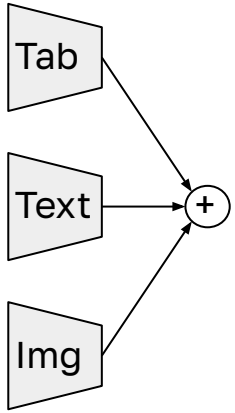


Semi-structured Neural Network



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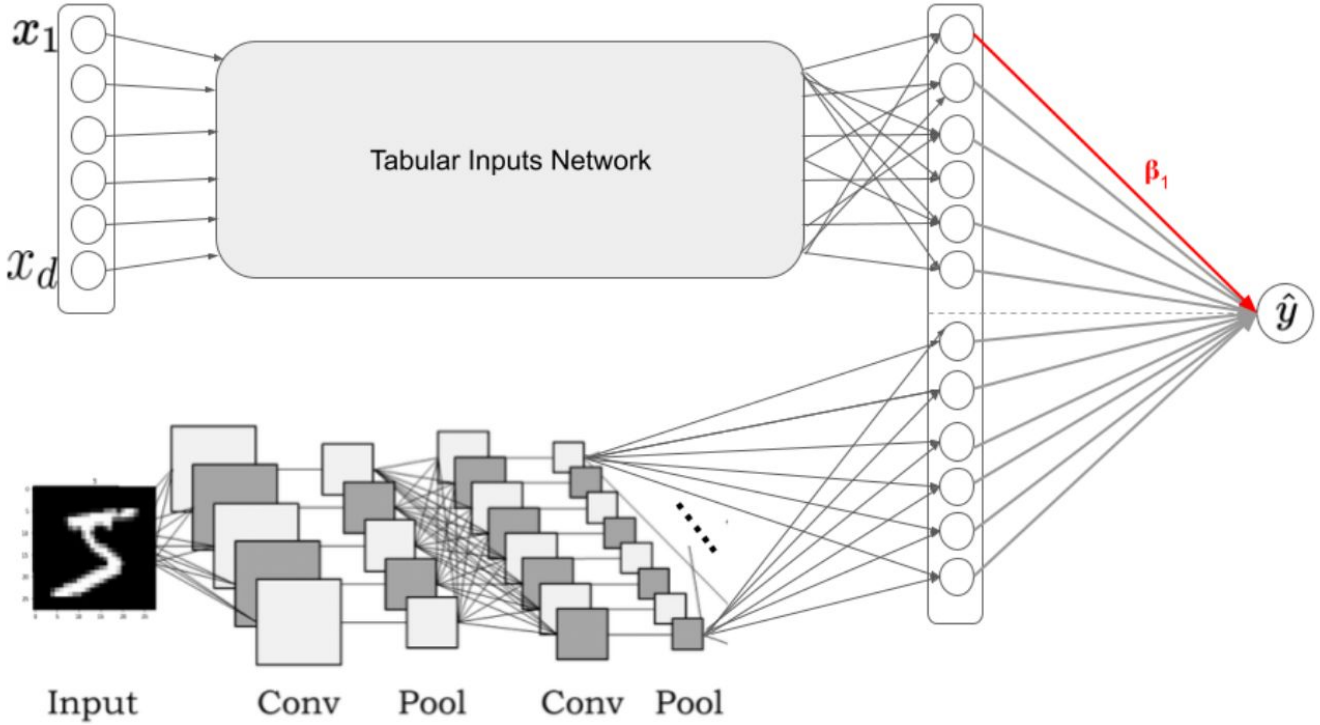

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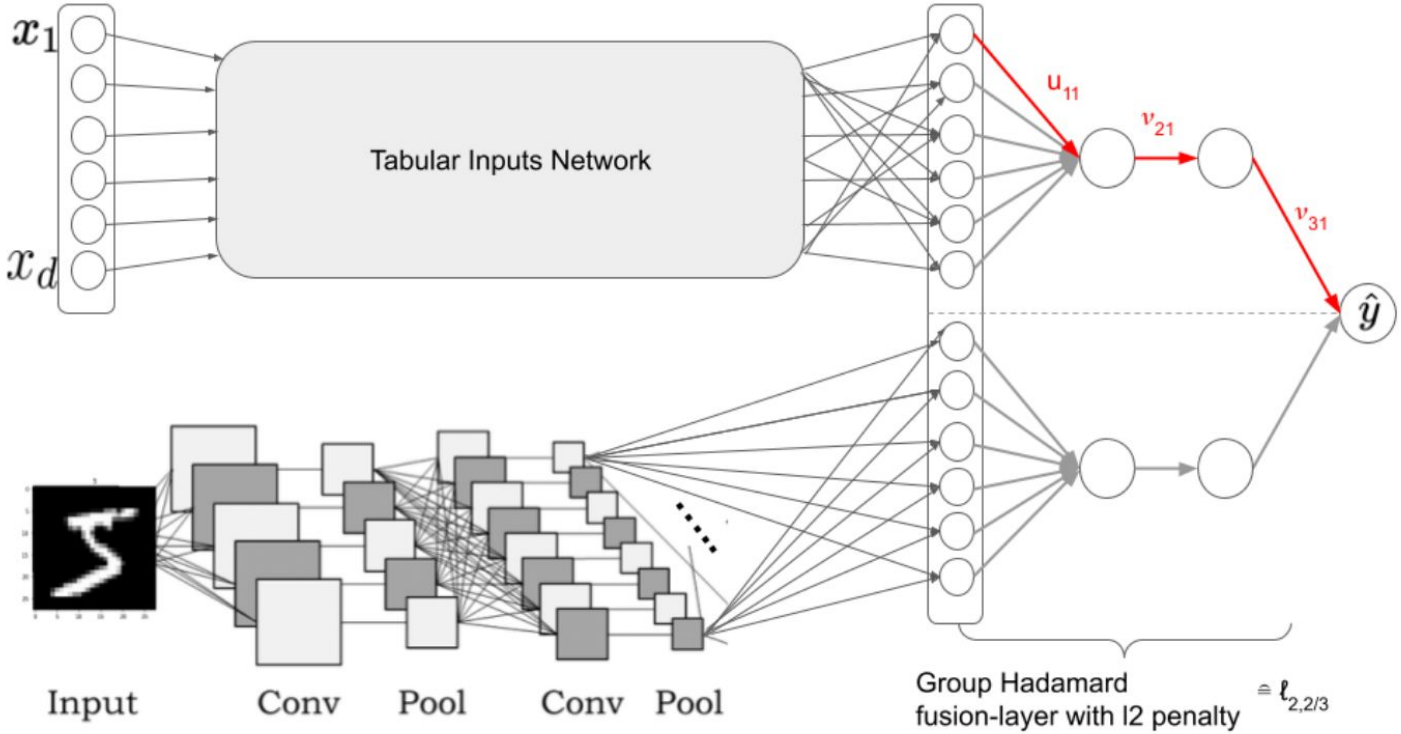

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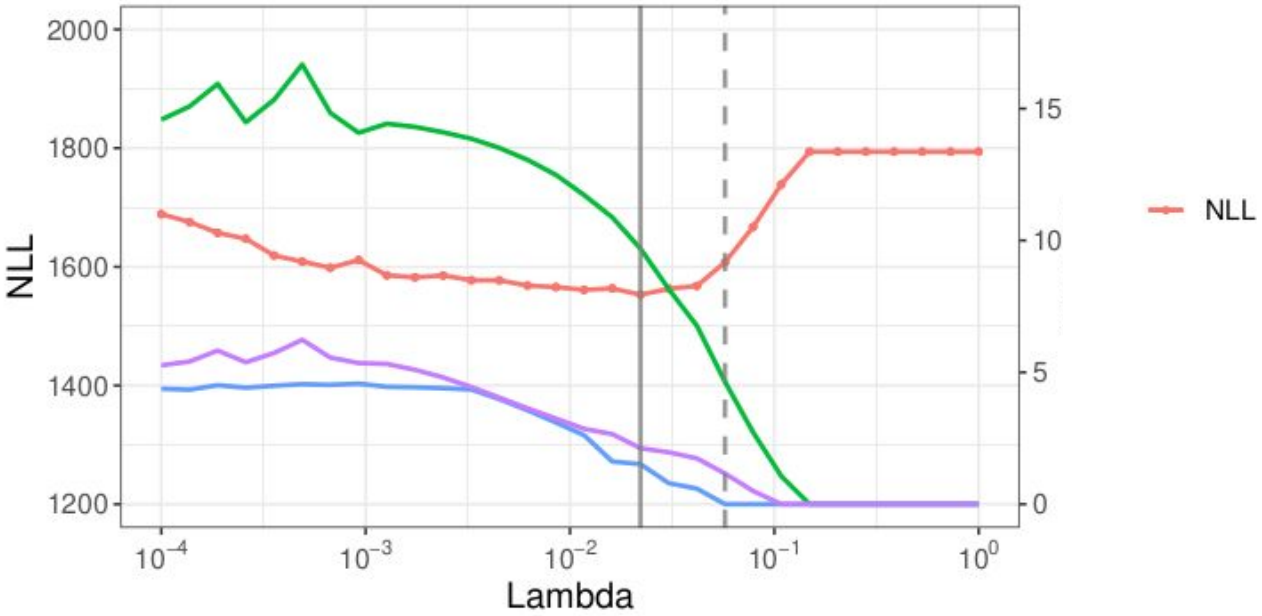

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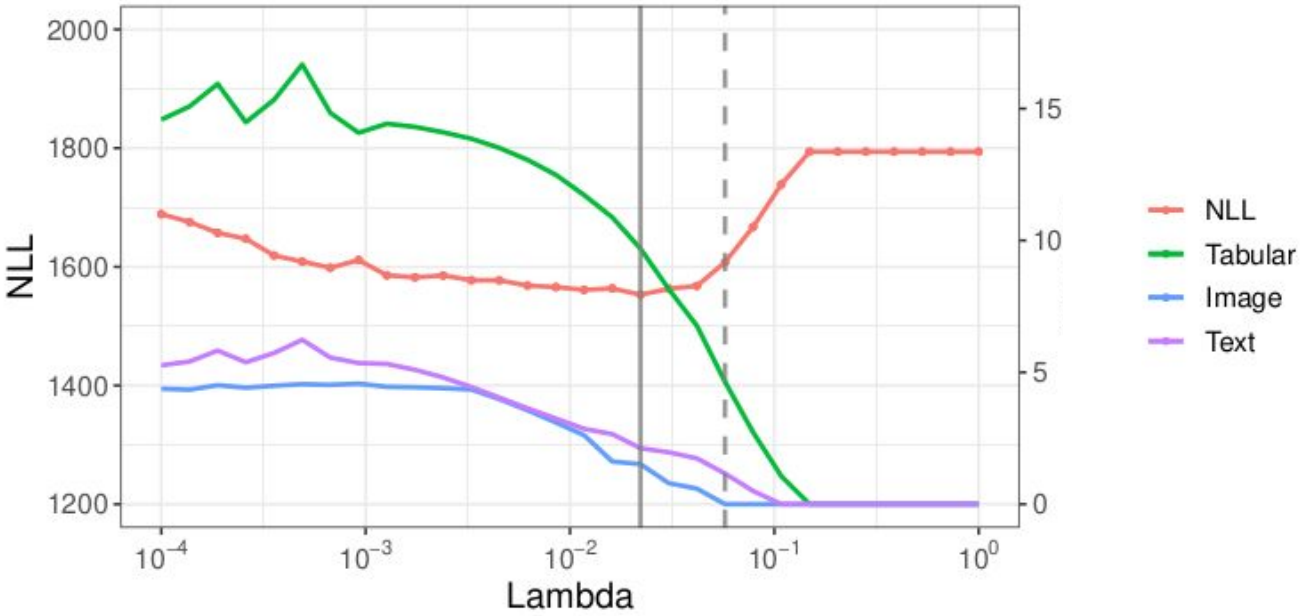

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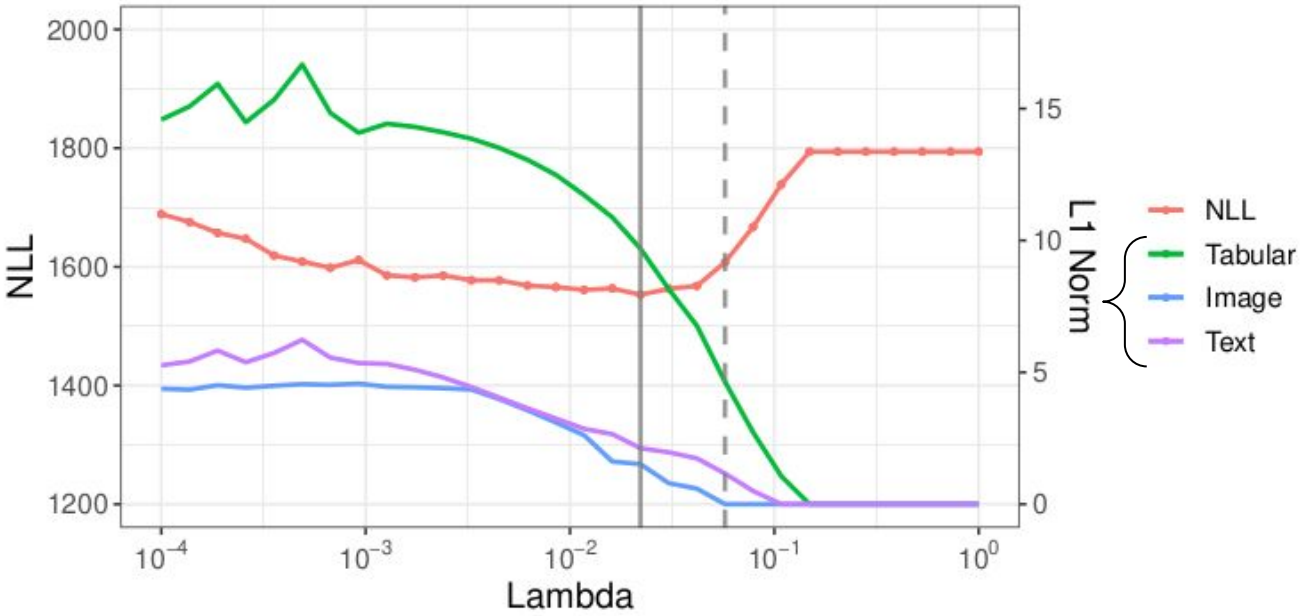

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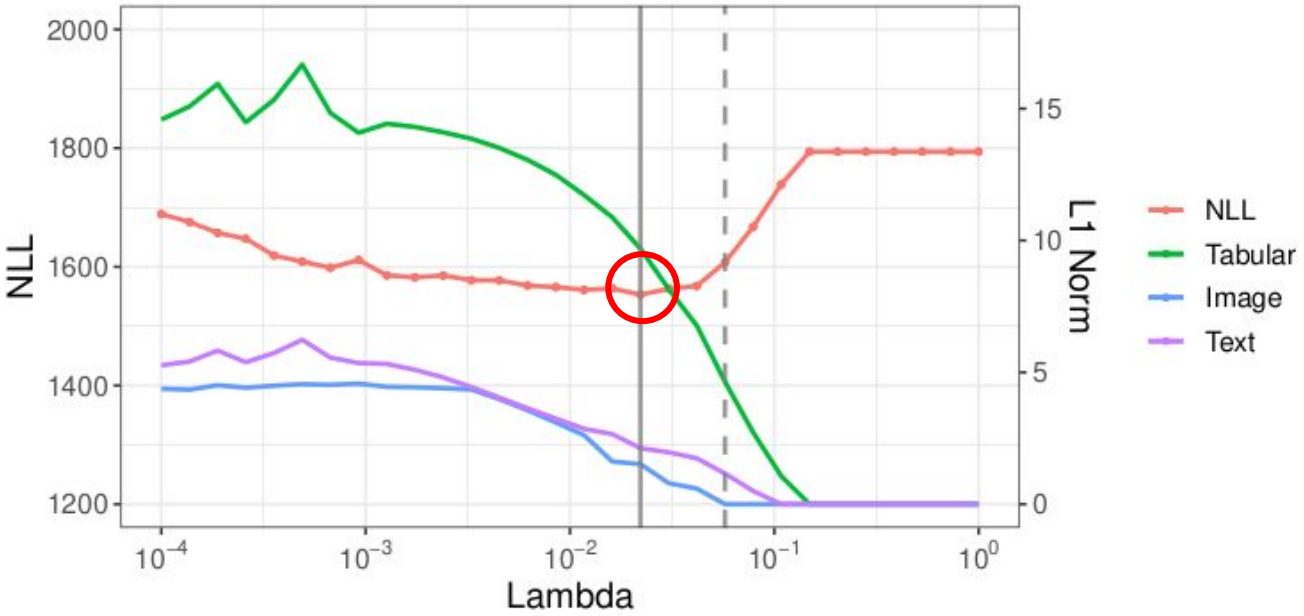

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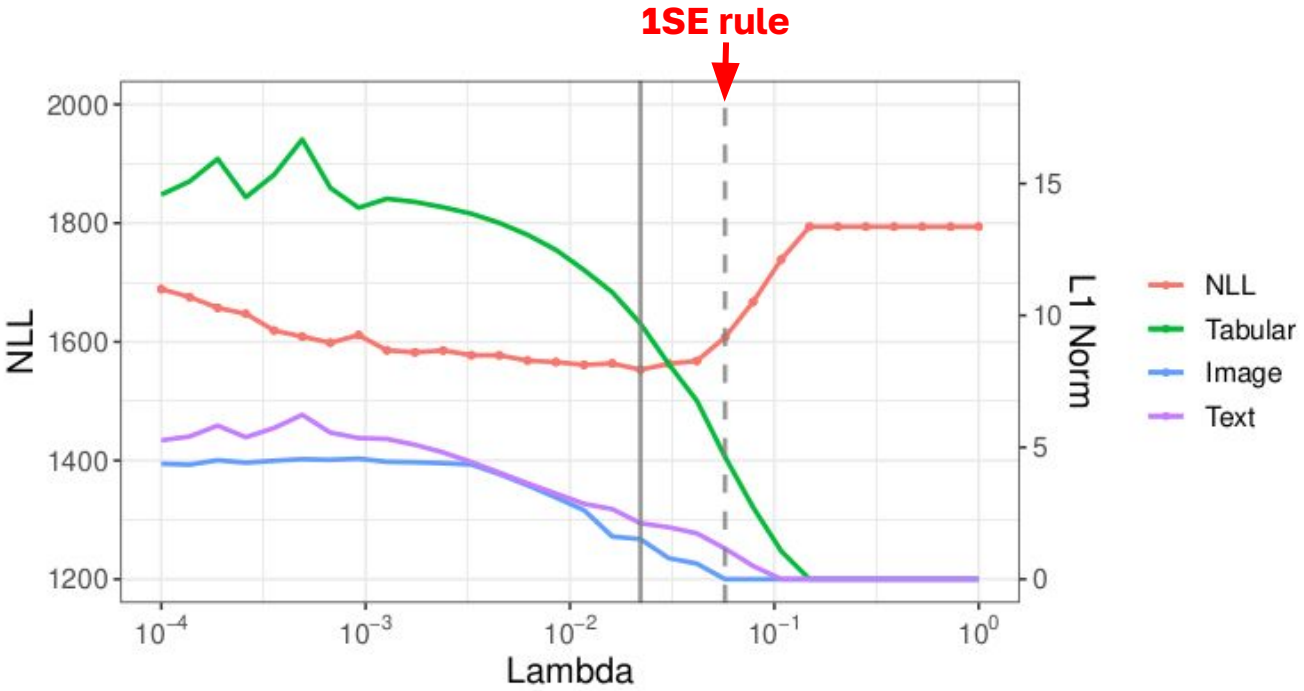

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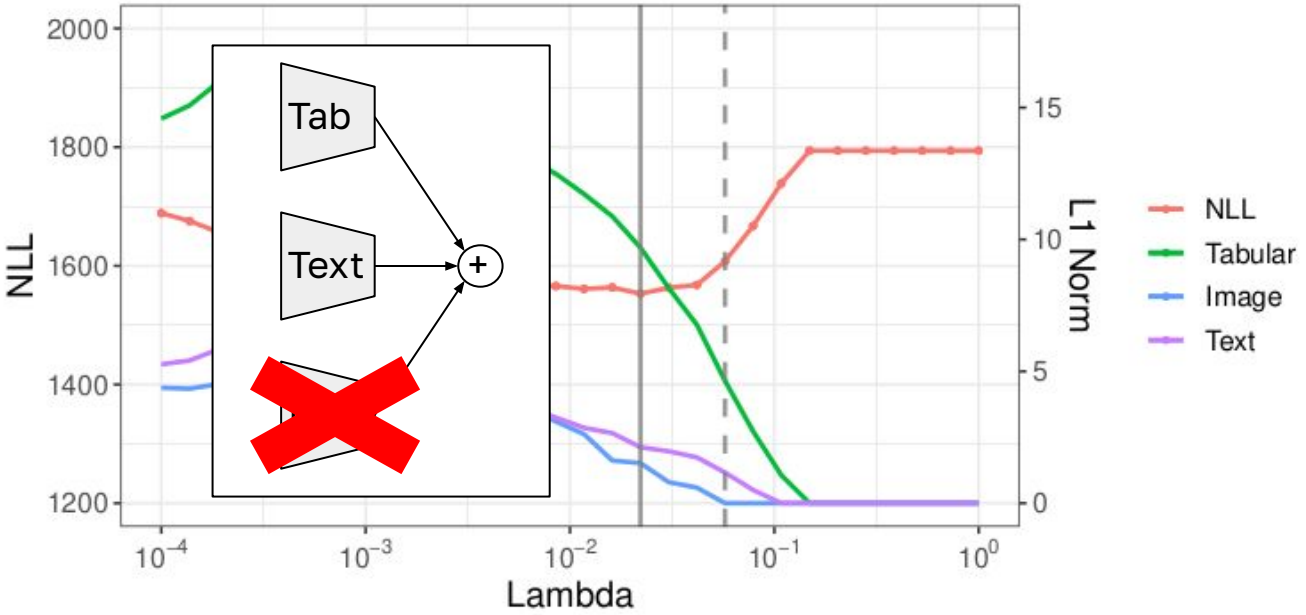

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