Machine learning in the string landscape

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CERN String Theory Seminar
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Based on [1706.07024]

UNIVERSITY OF OXFORD

Data sets in String Theory

- String theorists have produced large sets of data / samples of the string landscape over the years
  - Calabi-Yau manifolds
    - CICYs in 3D and 4D [Candelas,Dale,Lutken,Schimmrigk'88; Gray,Haupt,Lukas'13]
    - Kreuzer-Skarke database [Kreuzer,Skarke'00]
    - Toric bases for F-Theory [Morrison,Taylor'12]
  - String models
    - Type IIA/IIB models [Gmeiner,Blumenhagen,Honecker,Lust,Weigand'06; Davey,Hanany,Pasukonis'09; Franco,Lee,Seong,Vafa'16; …]
    - Heterotic on CY/Orbifolds/Free fermionic [Anderson,Constantin,Gray,Lukas,Palti'13; Nilles,Vaudrevange'14; Abel,Rizos'14; Blaszczyk,Groot Nibbelink,Loukas,FR'15; …]
    - F-Theory [Taylor,Wang'15; Halverson,Tian'16; Halverson,Long,Sung'17; …]

Study String Vacua

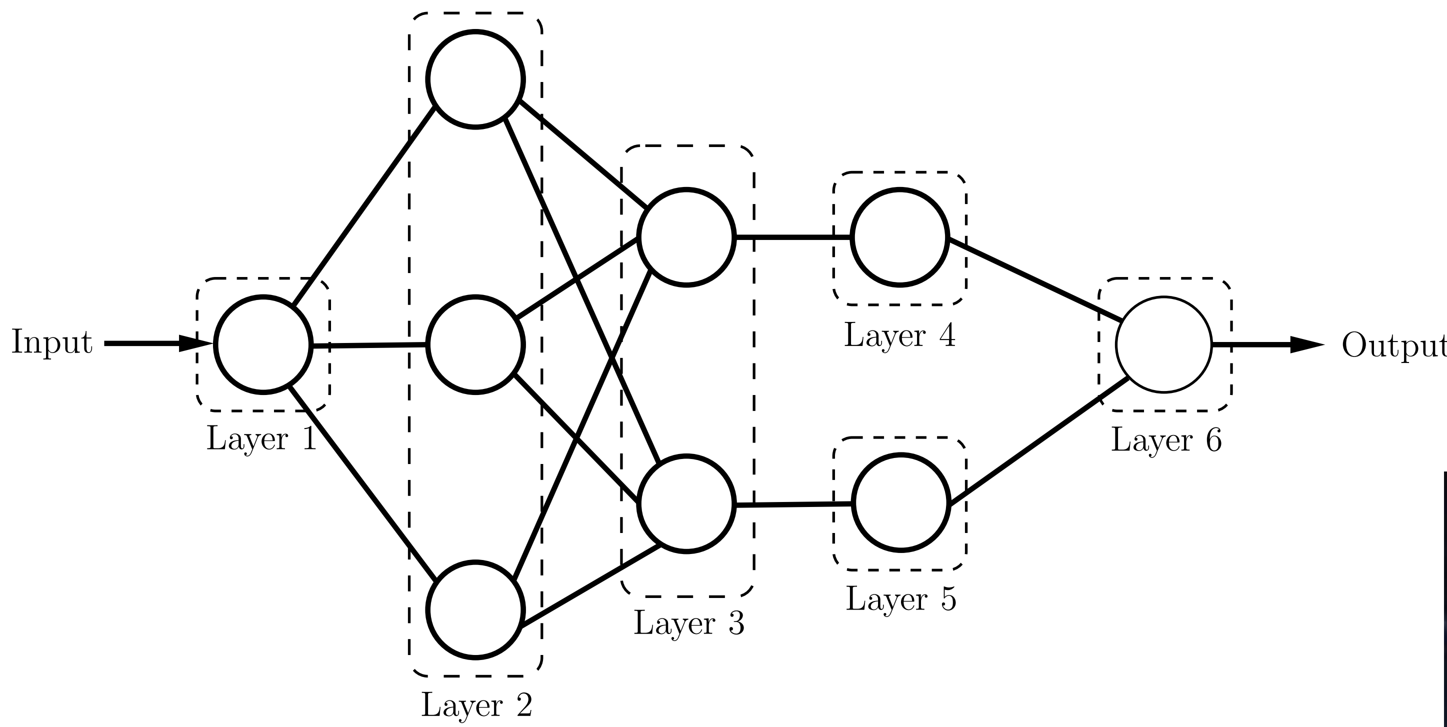
- Currently no selection mechanism for string vacua $\Rightarrow$ vast string landscape
- Long term goal for: Map out the landscape
  - Find string models in the landscape
  - Find generic / common features of string-derived model
  - Extract string theory predictions from the landscape
  - Are low energy manifestations of string vacua linked?
  - Find new relations/mathematical theorems from string theory
- Can we use neural networks (NNs) to answer or study such questions? [He'17; Krefl,Seong'17; FR'17; Carifio,Halverson,Krioukov,Nelson'17]

Study String Vacua

- Starting point: 12D/11D/10D F/M/I-IIA-IIB-HE-HS $\Rightarrow$ (rather) unique
- Phenomenology of the model encoded in discrete (background) choices / data (compactification space, fluxes, …)
- Given this data, can one decide whether a model has
  - SM gauge group
  - three generations with one pair of vector-like Higgs
  - correct Yukawa textures
  - 60 e-folds of slow-roll inflation
  - a Minkowski/de-Sitter vacuum solution
  - …
- In principle possible (computable for a given choice), but I cannot see it directly from the input data $\Rightarrow$ can a NN decide / compute (some of) these?
- If so, how can we find most efficient NNs for the job? $\Rightarrow$ Genetic algorithms

Outline

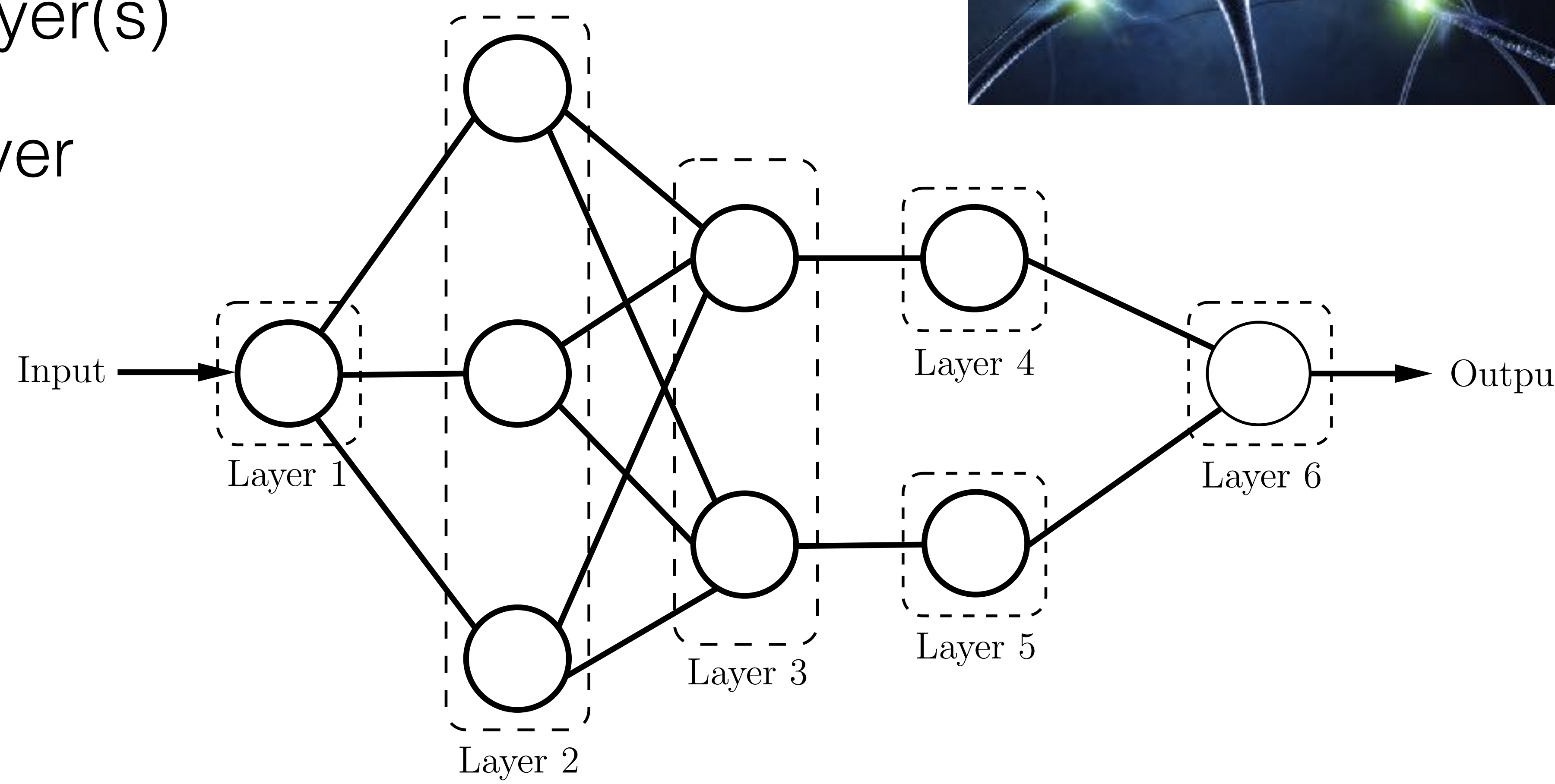
- Introduction to Neural Networks
  - Neural Networks 101 - How/why do they work
  - Where can we apply neural networks
- Genetic Algorithms 101
- Combining both approaches
  - Example: Classifying stable line bundles
  - Example: Computing line bundle cohomology
- Conclusions



Introduction to Neural Networks

Neural Networks 101

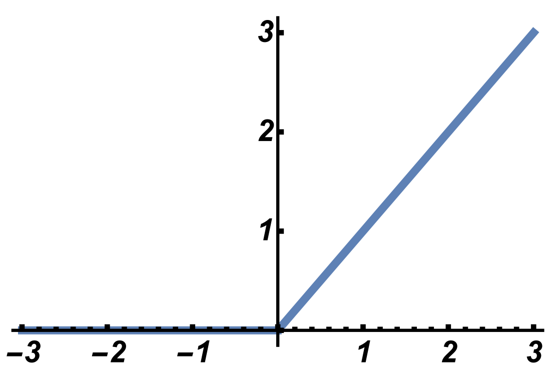
- Copy nature ⇒ modelled after human brain
- Building blocks
  - Input layer
  - Hidden layer(s)
  - Output layer



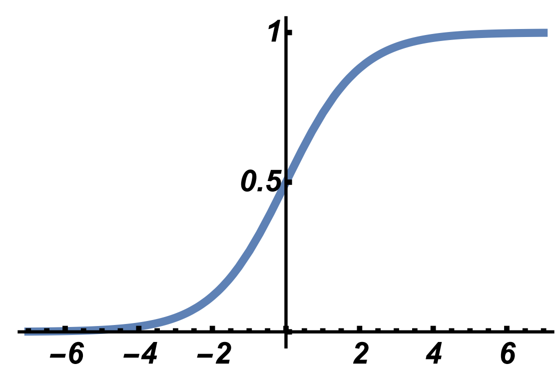
Neural Networks 101

- Connection between layers : Linear transformations L_i:
  Matrix multiplication $v^i_{\text{out}} = A^i v^i_{\text{in}} + b^i$
- Each layer applies a function (activation function) to its input to compute its output. Common choices are

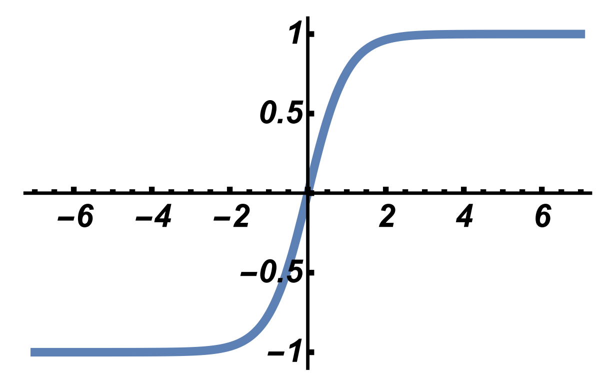
Ramp



Logistic Sigmoid



Tanh

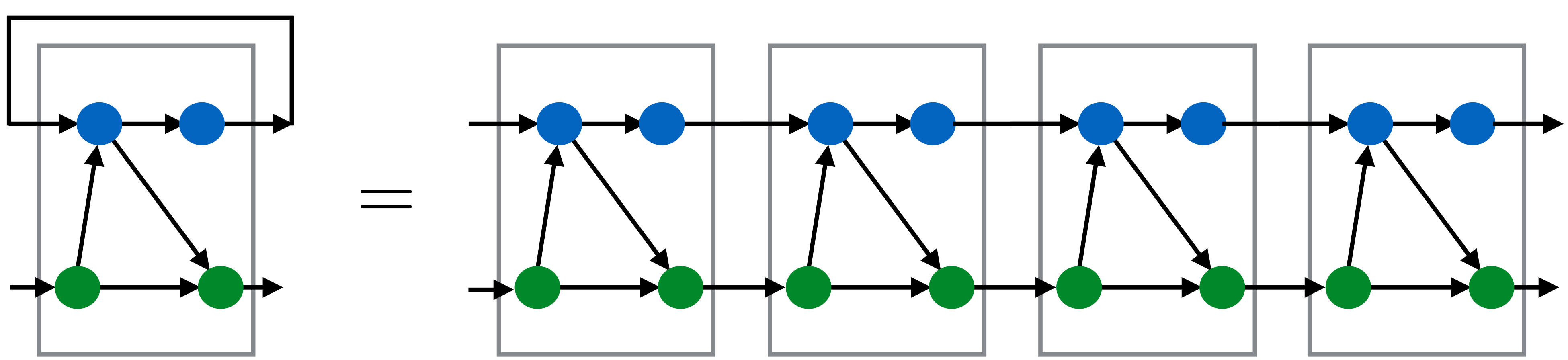


- Typical NN: $\mathbb{R}^M \rightarrow \mathbb{R}^N$

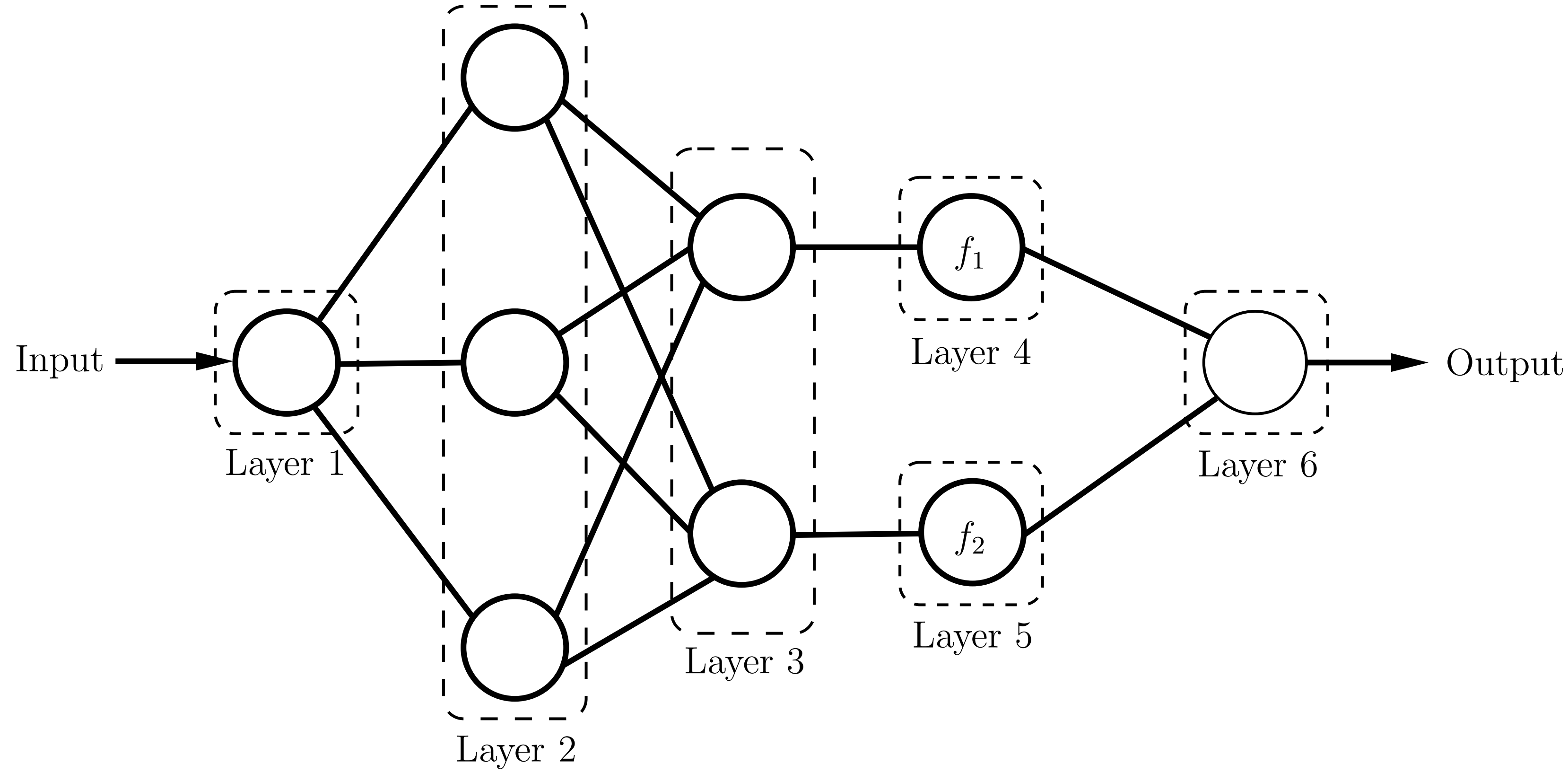
$$v \mapsto f_n \circ L_n \circ \ldots \circ f_0 \circ L_0$$

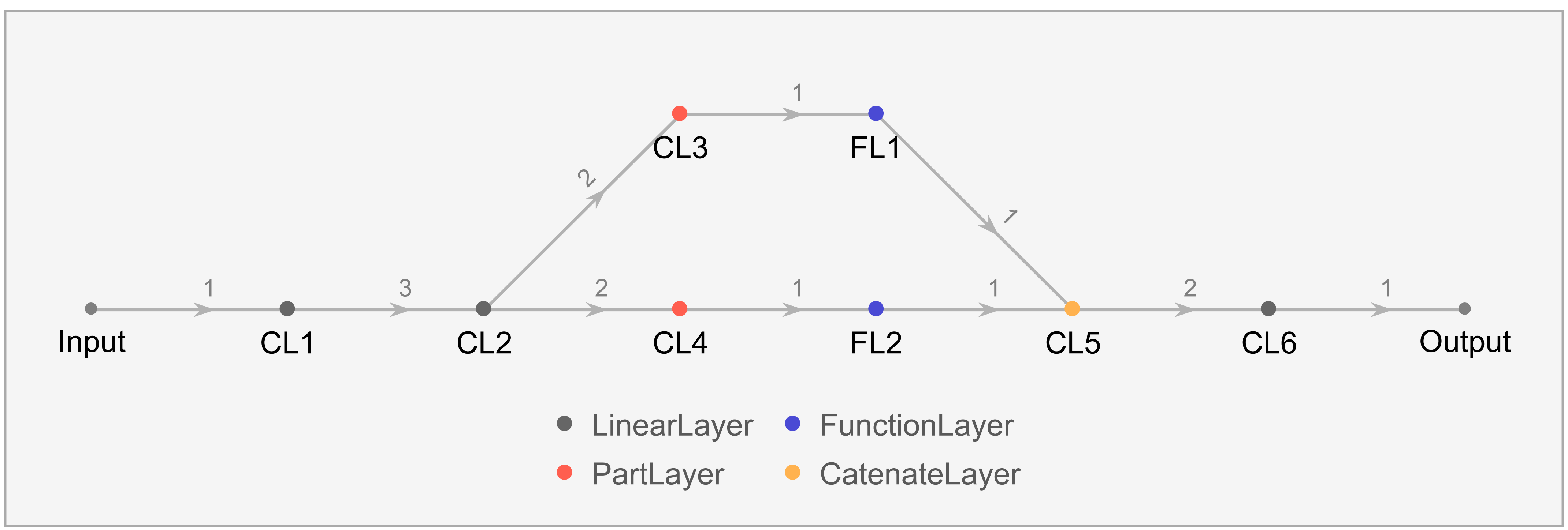
Modifications / Extensions

- Do not connect all outputs of layer i to all inputs of layer $i+1$
  - Add / multiply / concat results of parallel NN streams
- Create loops
  - Feed output of an NN layer back into its input
  - Recurrent NN $\Rightarrow$ Give the network a memory (LSTM layers)



Example NN


Input
Output
f_1
f_2
Layer 1
Layer 2
Layer 3
Layer 4
Layer 5
Layer 6


Input
CL1
CL2
CL3
CL4
FL1
FL2
CL5
CL6
Output
1
3
2
2
1
1
1
1
2
1
LinearLayer
FunctionLayer
PartLayer
CatenateLayer

Neural Networks - Training

- Precise way in which NN learn active field of research
- In *supervised* ML you show the network the correct results
- In *unsupervised* ML you let the network find common properties (clustering) and identify things that “don’t fit in” by itself
- In this talk: supervised ML:
    - Divide data set into a training set (30% of data) and validation set (70% of data)
    - Randomly initialize the trainable parameters of the NN (e.g. weights and biases of the connections)
    - Let the network look at the entire train set (inputs and outputs) and minimize the difference between its output and the output of the training set (w.r.t. some metric) “back-propagation”
    - Shuffle the training set and repeat until
        - Error is not significantly reduced anymore
        - Each training model has been used a set number of times
        - A certain amount of time has elapsed
    - Cross-check performance of trained NN against the validation set

Neural Networks - Applications

- Three ways of applying neural networks

  (A) To *find & bypass* implementations of algorithms (in combination with genetic algorithms)

  (B) To approximate functions (*predictor*)

  (C) To *classify* outcome of some complicated / unknown mathematical operation based on the structure of the input

- Once we have built a neural network to apply to (A) - (C) we need to train it

- Once trained NNs can perform very efficiently

  - They just apply simple functions to produce some output

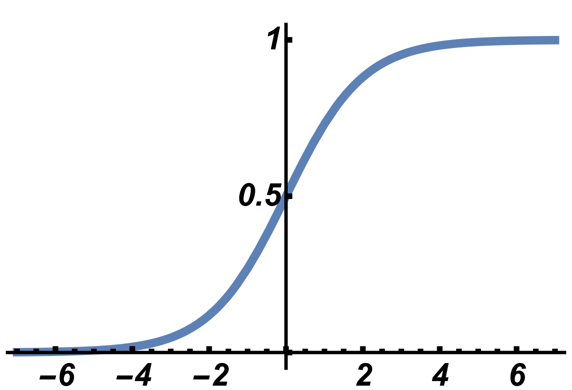
  - Computations are independent $\Rightarrow$ parallelizable

(A) Using NNs to implement algorithms

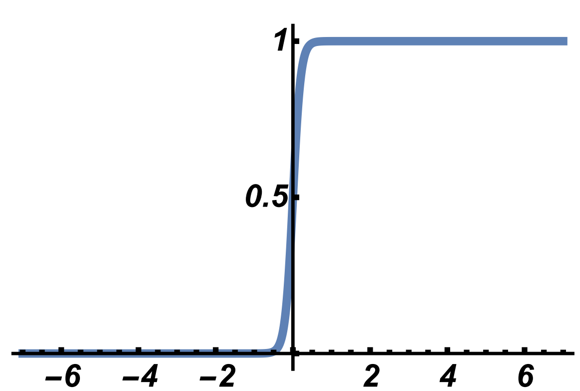
- This is more about abusing the modular nature of NN
- Each layer performs an action / applies a function
- Implement an arbitrary algorithm by
    - choosing the function appropriately
    - including a (possibly trained) NN that performs a specific algorithm (e.g. computes binomial coefficients)
    - emulating a computer using NNs (combine NN layers that perform bit-wise and/xor/not/… operations
- Like playing LEGO

(B) Using NN to approximate functions

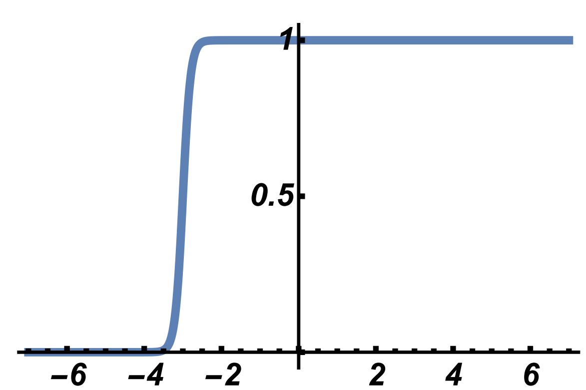
- Simple case: 1 layer, 1 node, logistic sigma function
    - Linear Layer: $x_{\text{int}} = a x_{\text{in}} + b$
    - Activation Function: $x_{\text{out}} = 1/(1 + \exp[x_{\text{int}}])$
      $= 1/(1 + \exp[a x_{\text{in}} + b])$
    - a : Steepness of step (step function for $a \to \infty$)
    - b : Position of step: (intersects y-axis at $y = 1/2$ for $b = 0$)



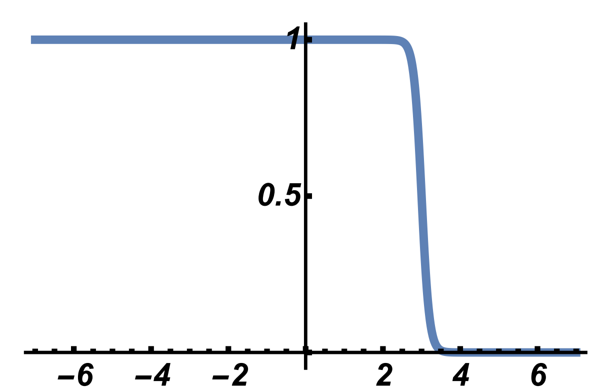
$a = 1, b = 0$



$a = 10, b = 0$

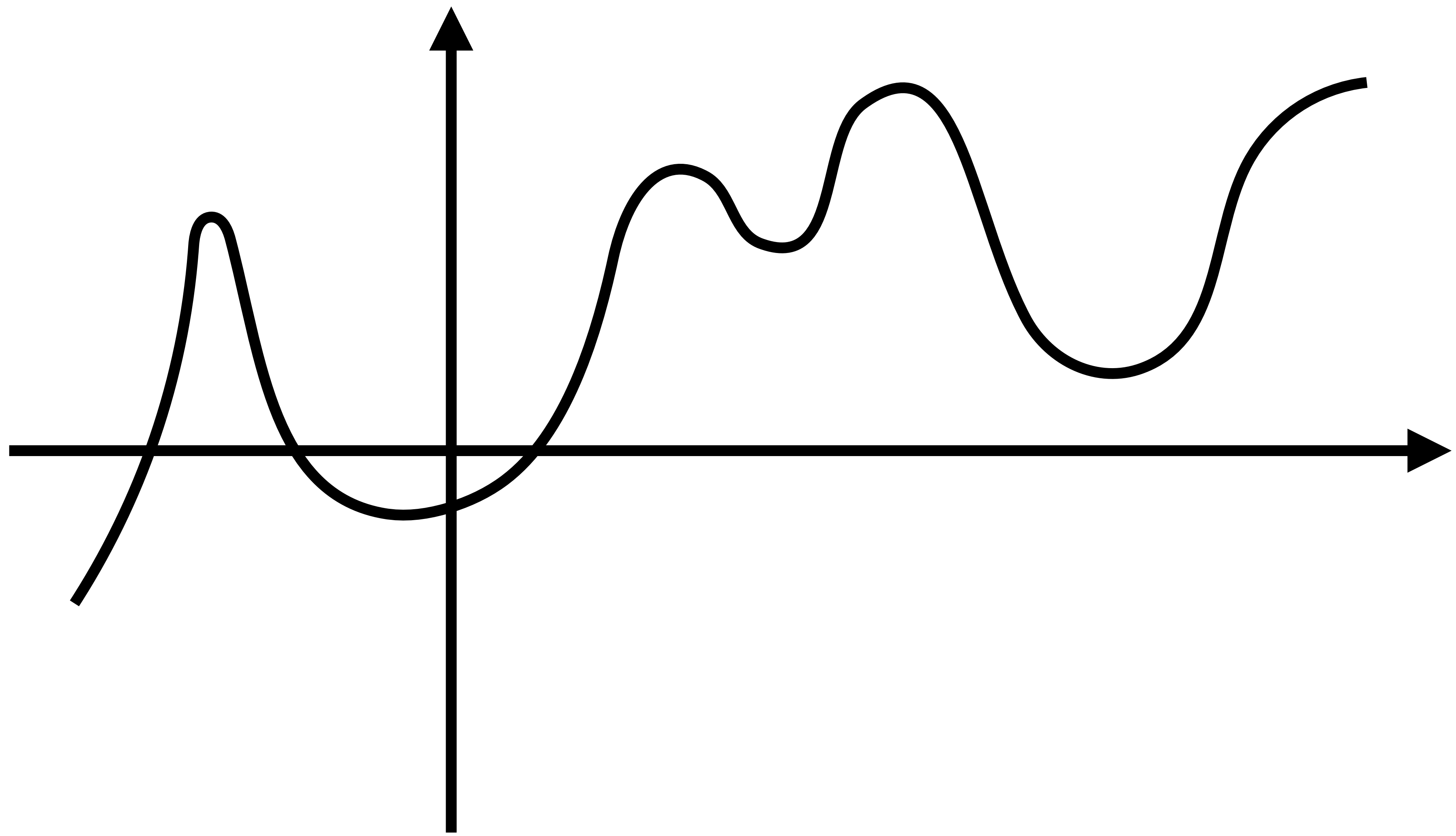


$a = 10, b = -30$

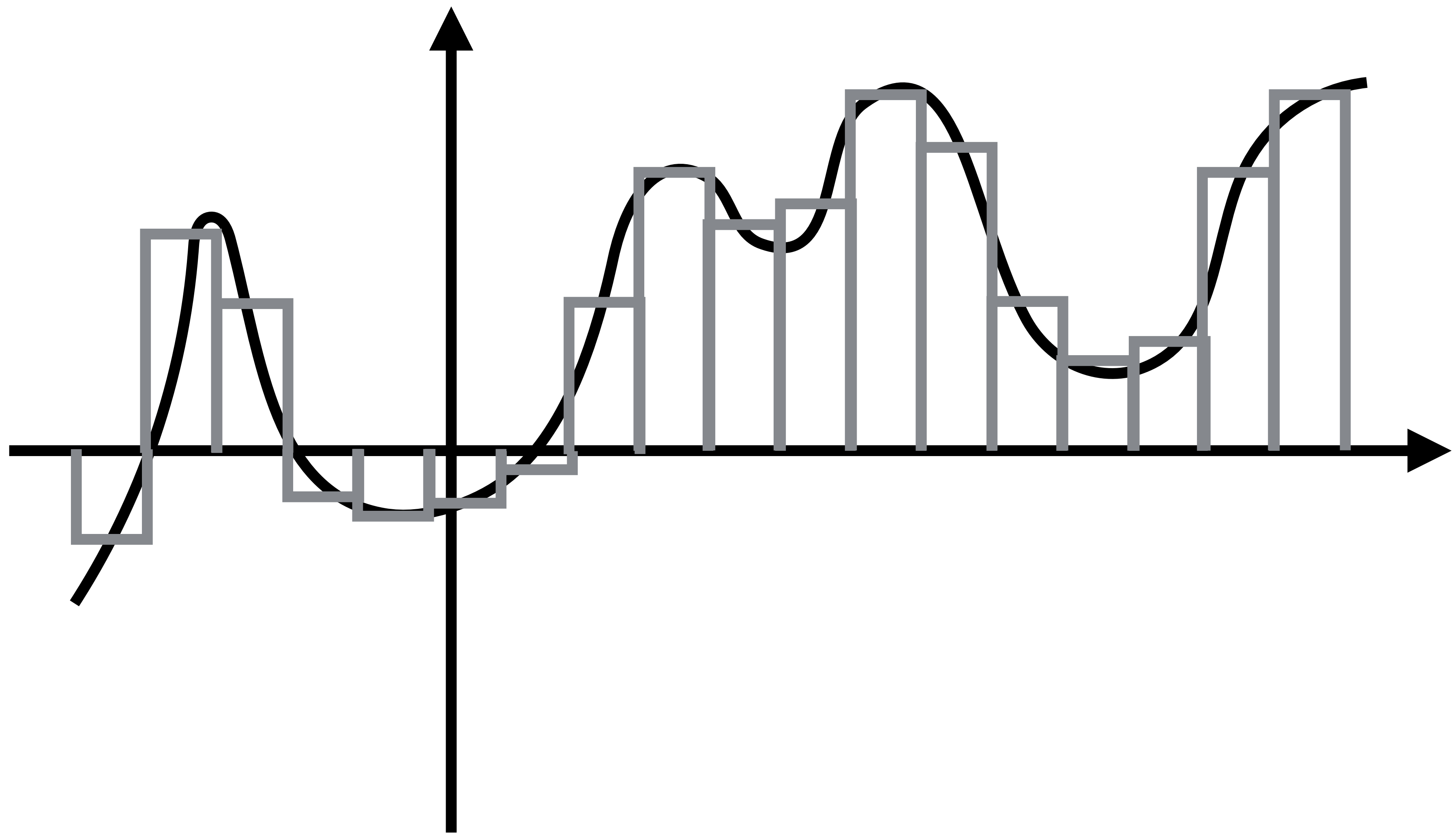


$a = -10, b = 30$

(B) Using NN to approximate functions



(B) Using NN to approximate functions

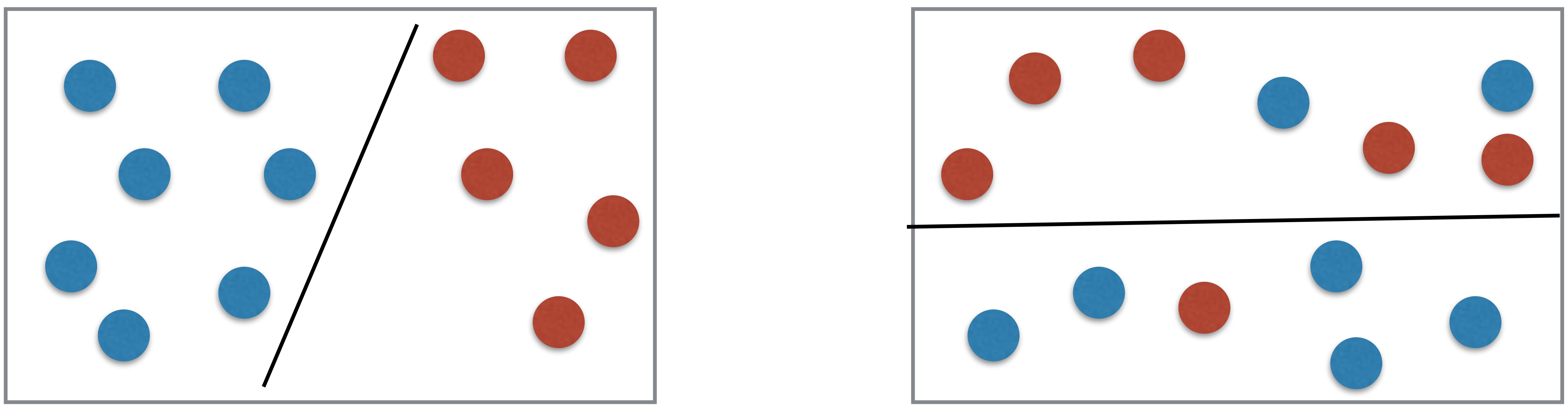


- More nodes $\Rightarrow$ more steps $\Rightarrow$ approximate any function (with one layer) “Universal Approximation Theorem”

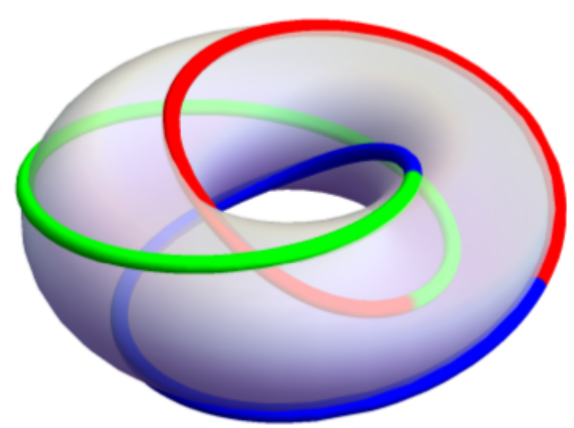
[Cybenko ’89; Hornik ’91; Nielsen‘15]

(C) Using NN to classify data

- Simple (feed-forward) NNs can classify data that is linearly separable, i.e. their convex hulls are disjoint



- When is data (linearly) separable? E.g. is the (3,2) torus knot linearly separable?

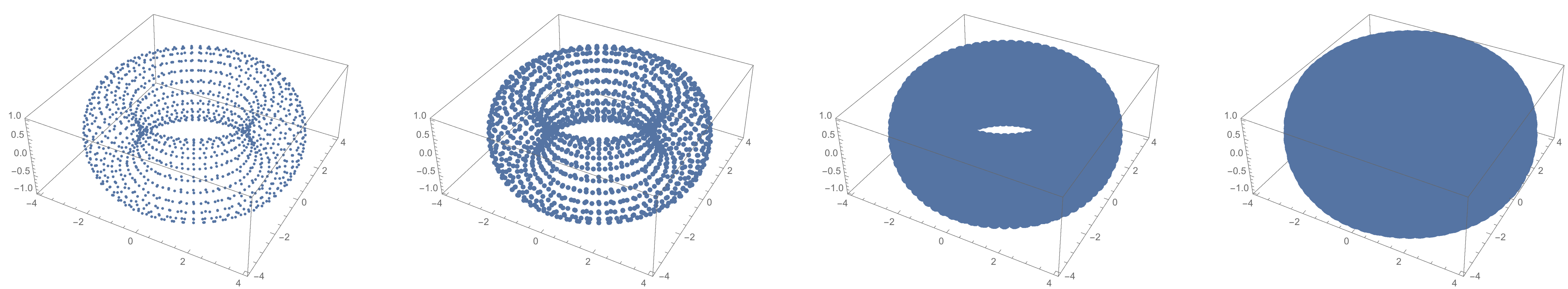


(C) Using NN to classify data

- Several ways to make data "linearly" separable
  - Go to higher dimensions (an n-dimensional knot can be disentangled in $2n+2$ dimensions)
  - Change / warp the geometry by applying non-linear functions (away from Euclidean, a "straight" line looks different)
  - Deform the data to make the error (i.e. the line that cuts through the entangled data) as small as possible

(C) Using NN to classify data

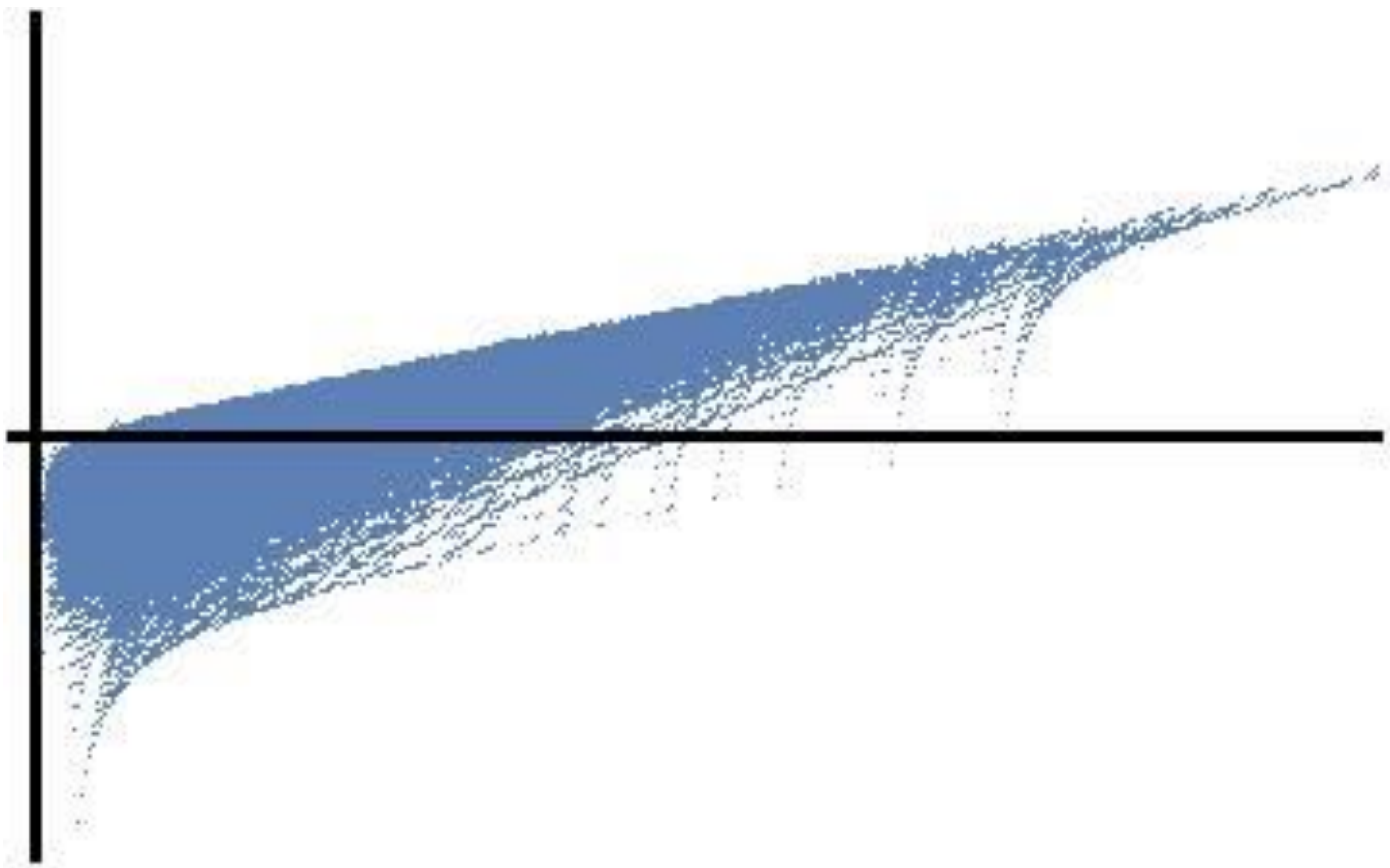
- Ways to identify "topology" of point set: Persistent homology
  - Has been applied to string vacua in [Cirafici '15]
  - Idea:
    - Replace data points by balls (several disconnected components)
    - As radius of points grow, components connect / form cycles / …
    - When radius grows further, cycles can disappear again



(C) Using NN to classify data

- For each k-cycle determine how long it exists as a function of the sphere radius $\Rightarrow$ barcode (Betti number vs radius)
- The longer a cycle exists the more likely it is to be a true feature
- In this talk we want to follow a different approach
  - The bar codes you obtain depend on the way you plot the data

(C) Using NN to classify data



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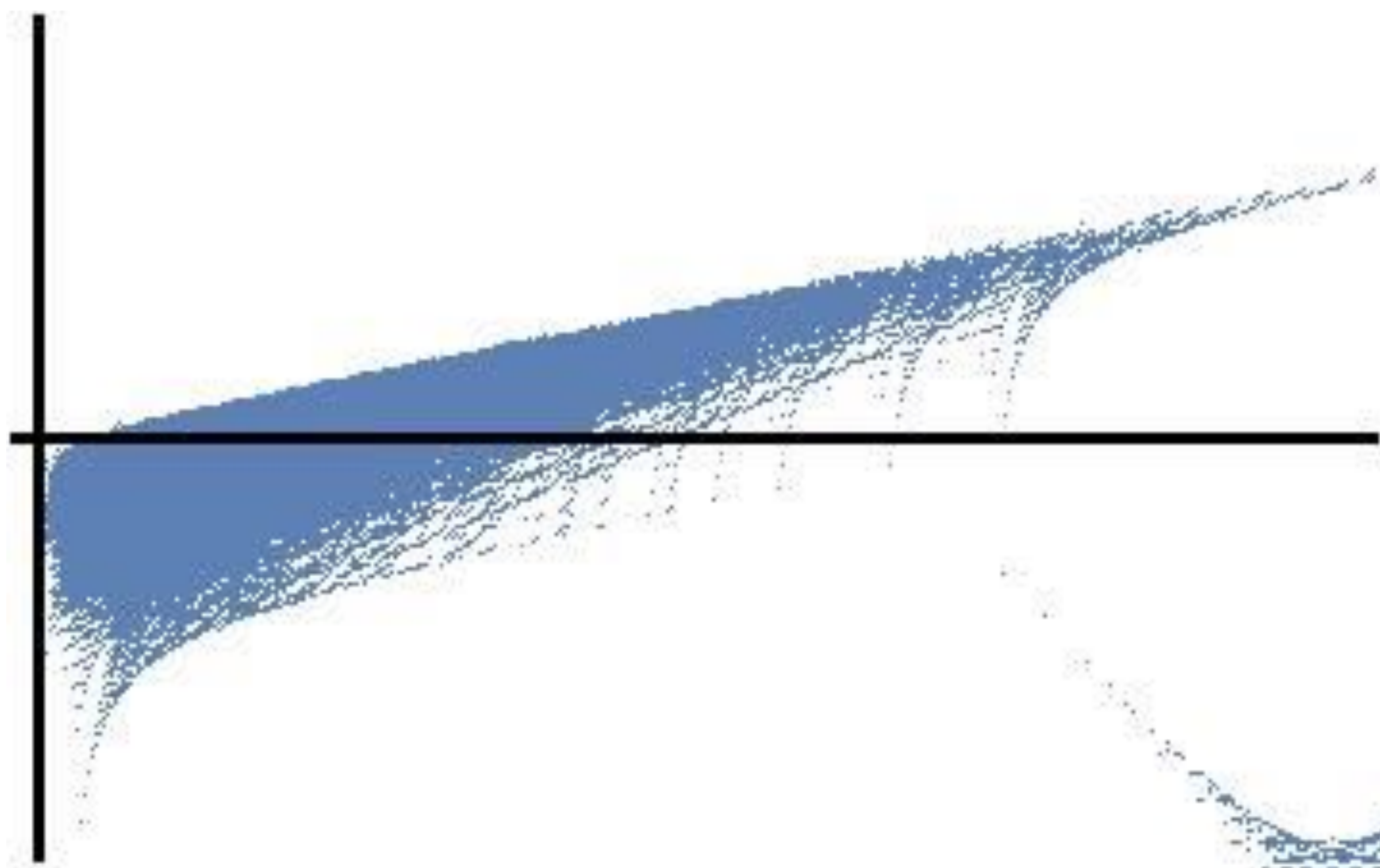

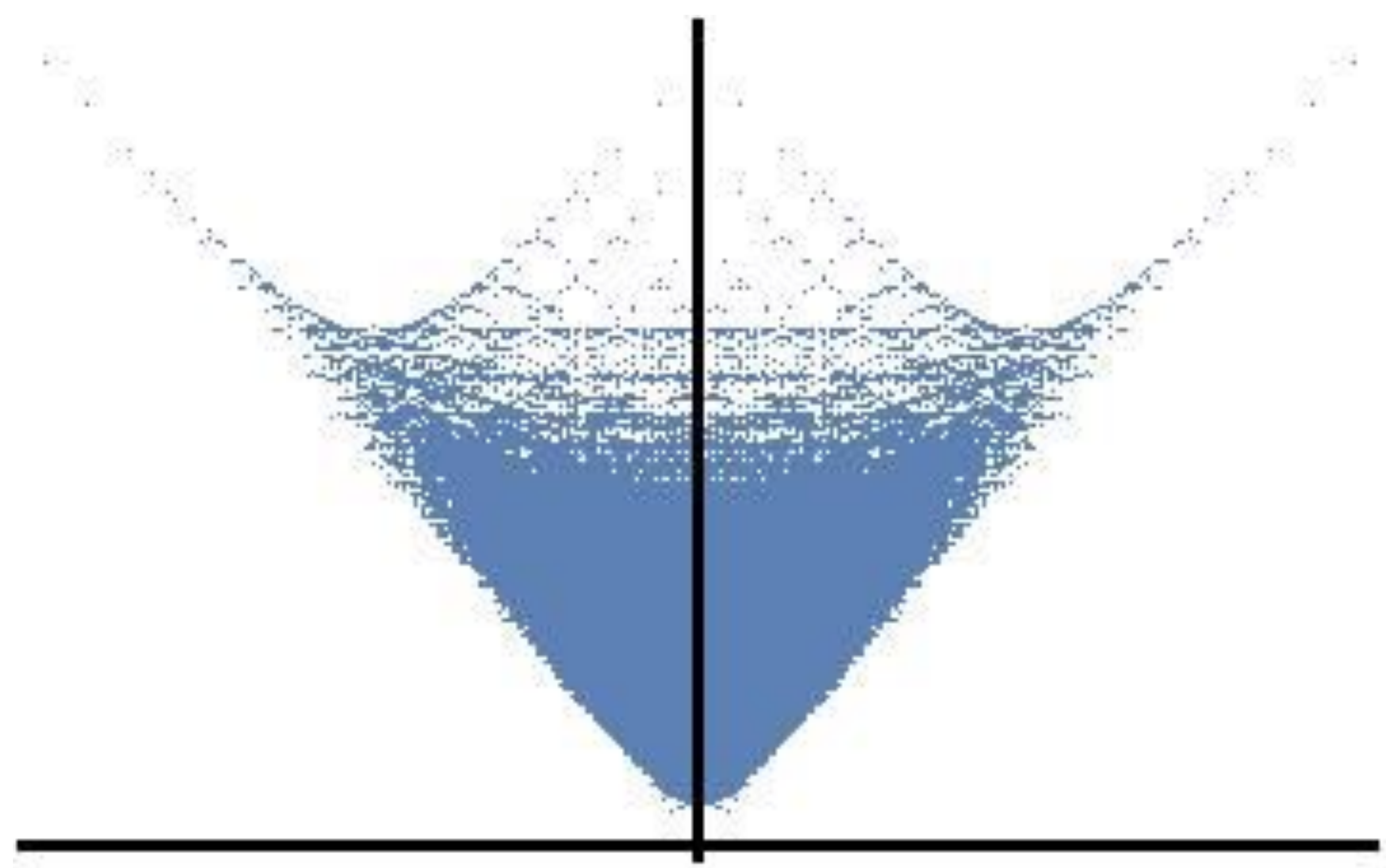

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    - For some applications we are only interested in a NN that works best

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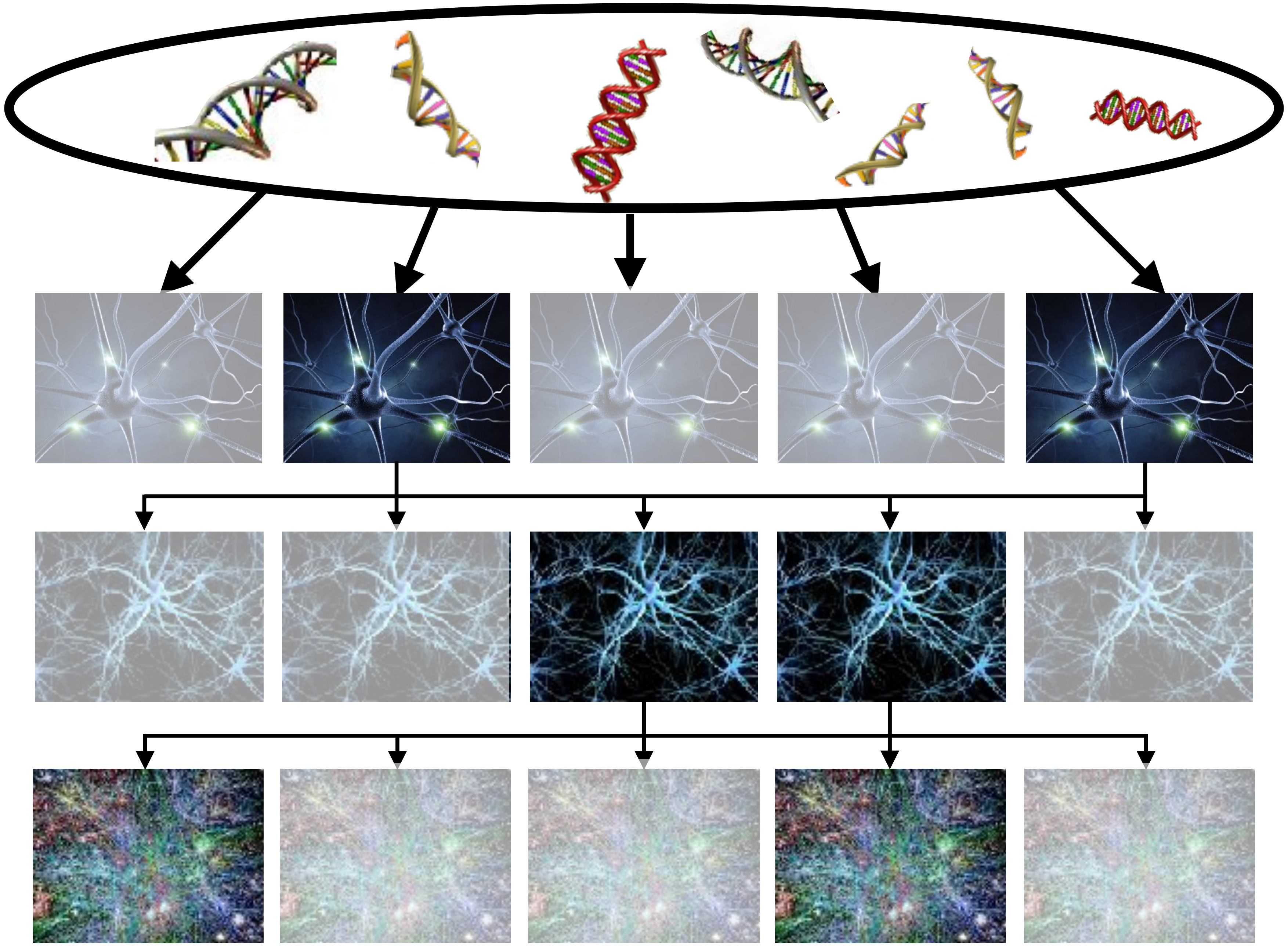
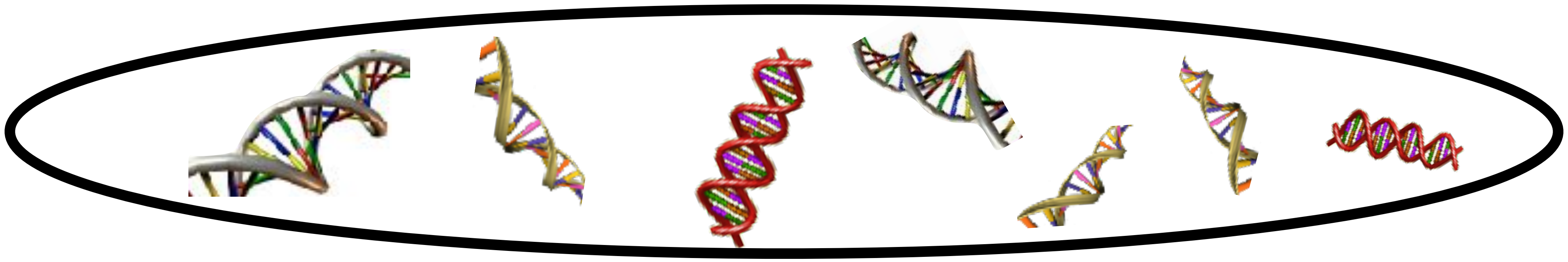
    - The bar codes you obtain depend on the way you plot the data
    - For some applications we are only interested in a NN that works best
- Instead of analyzing the data to decide the necessary complexity of the NN: Simply evolve a NN that works best

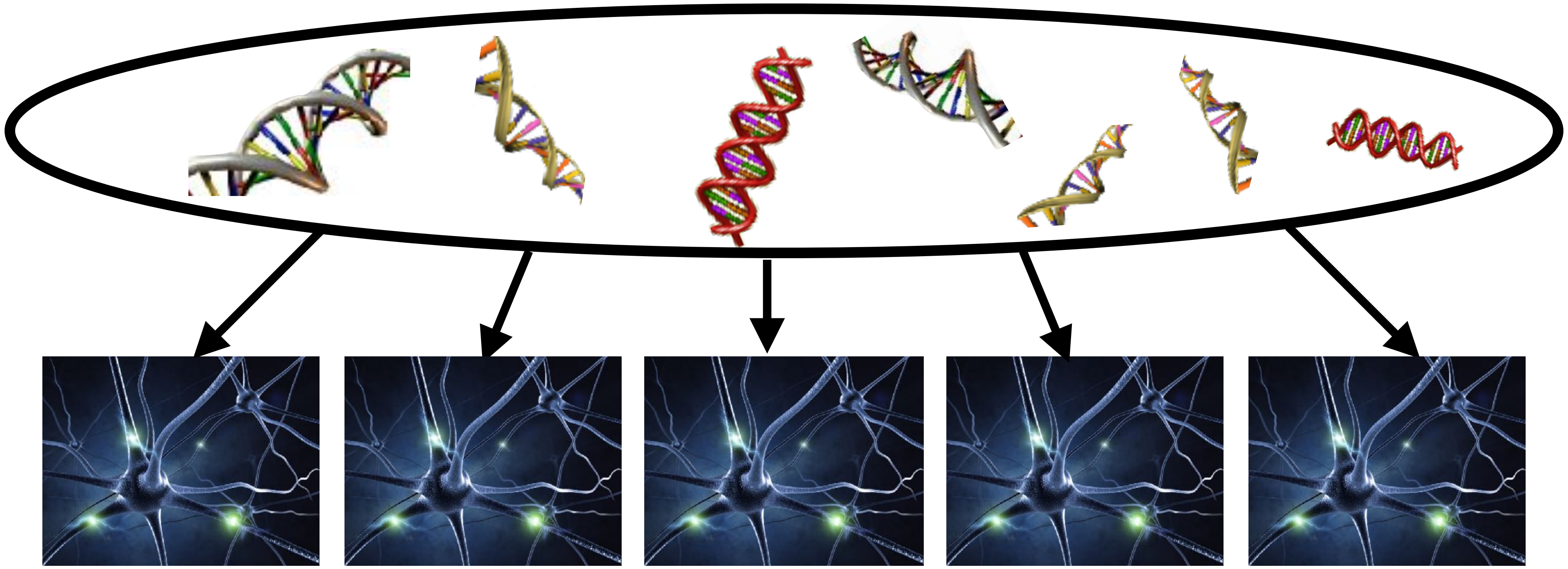


Introduction to Genetic Algorithms

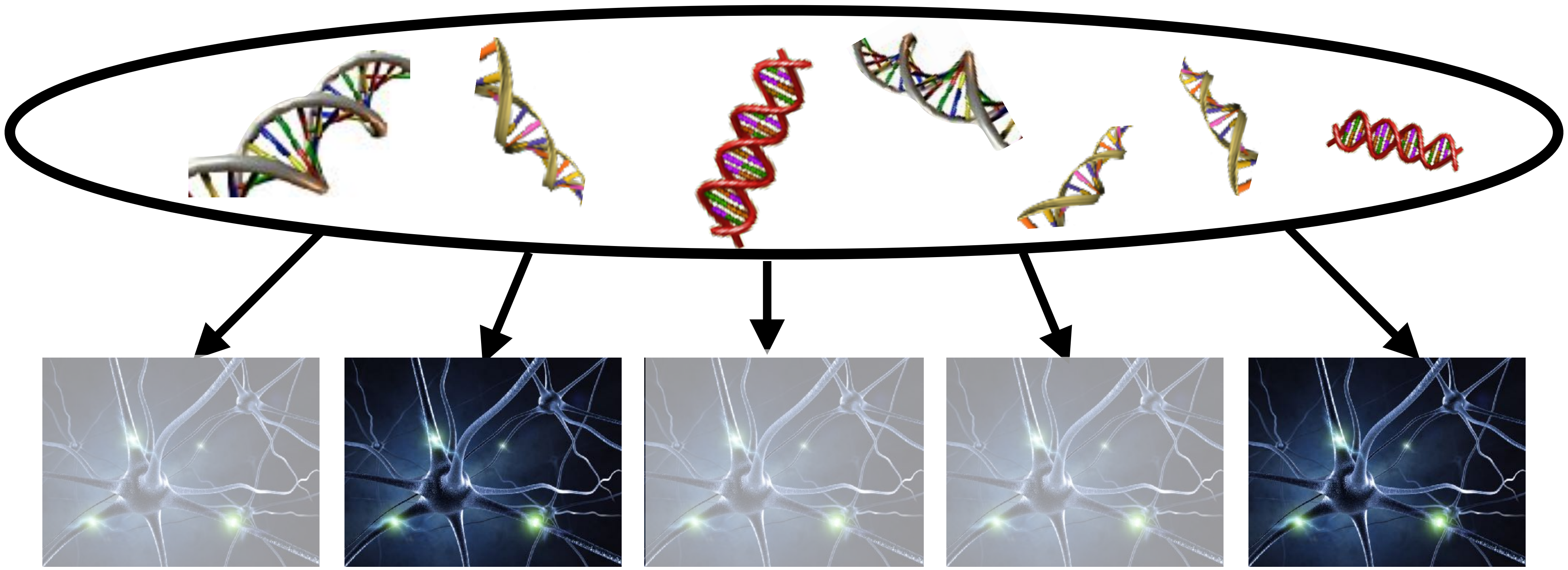
Genetic Algorithms 101



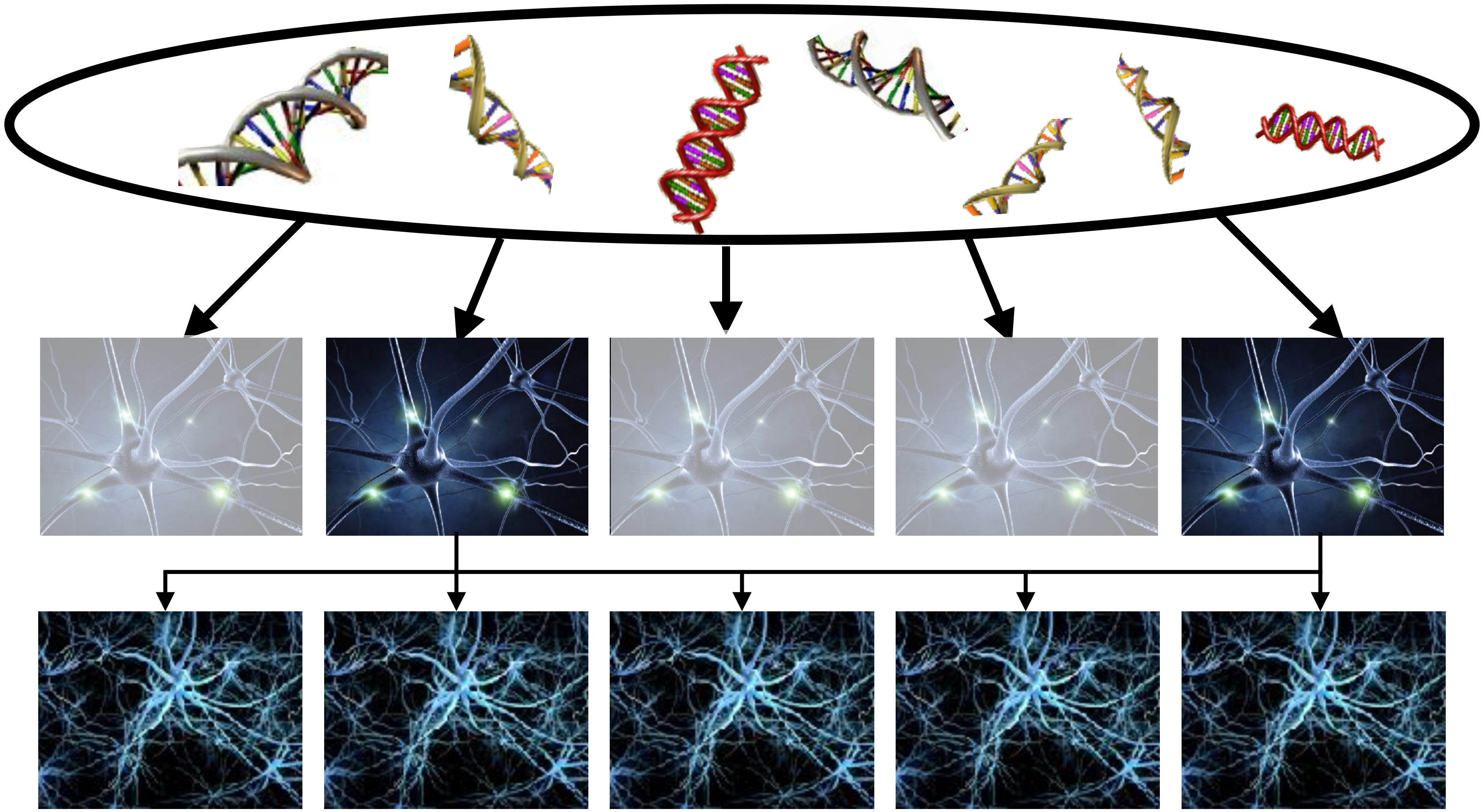
Genetic Algorithms 101



Genetic Algorithms 101



Genetic Algorithms 101



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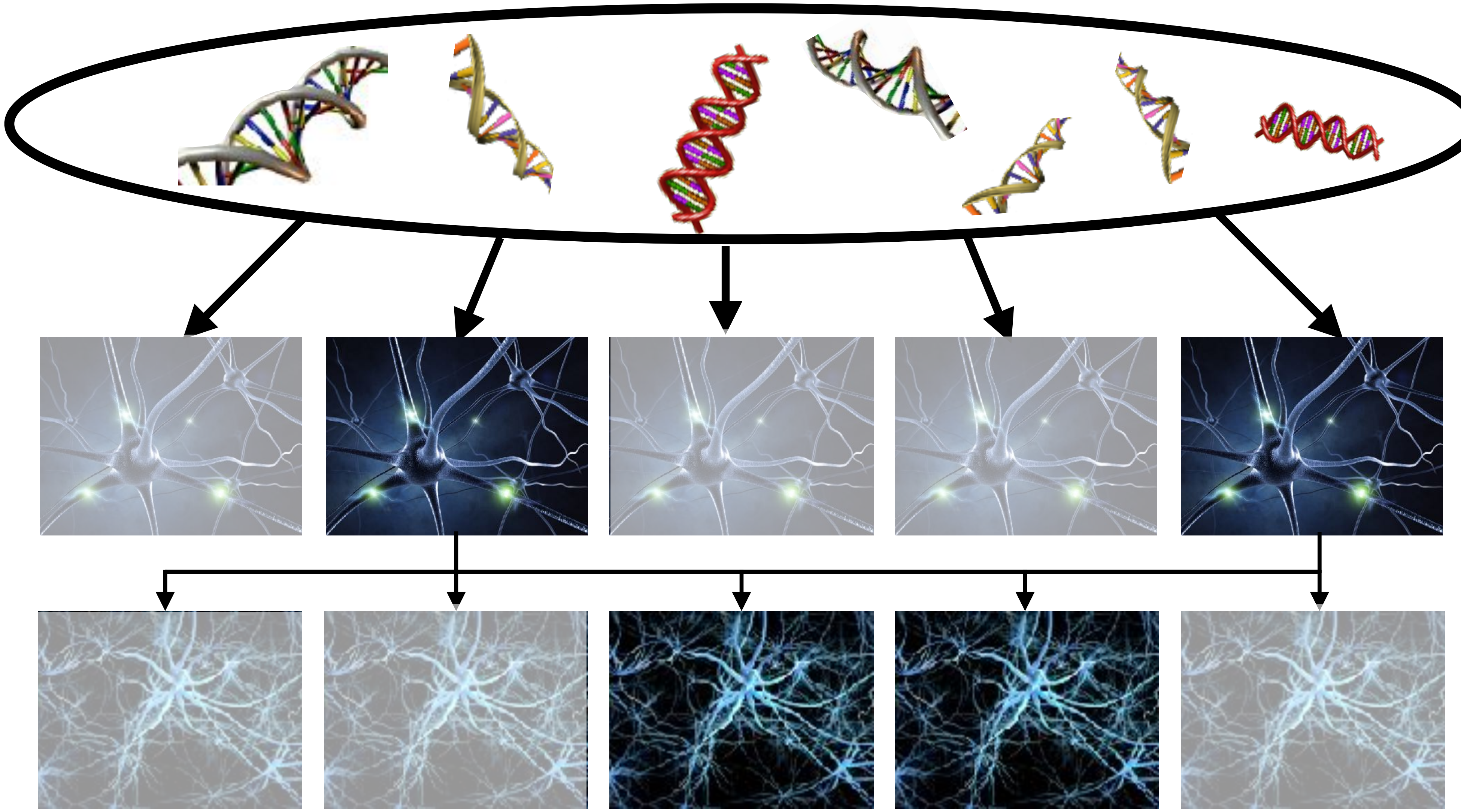

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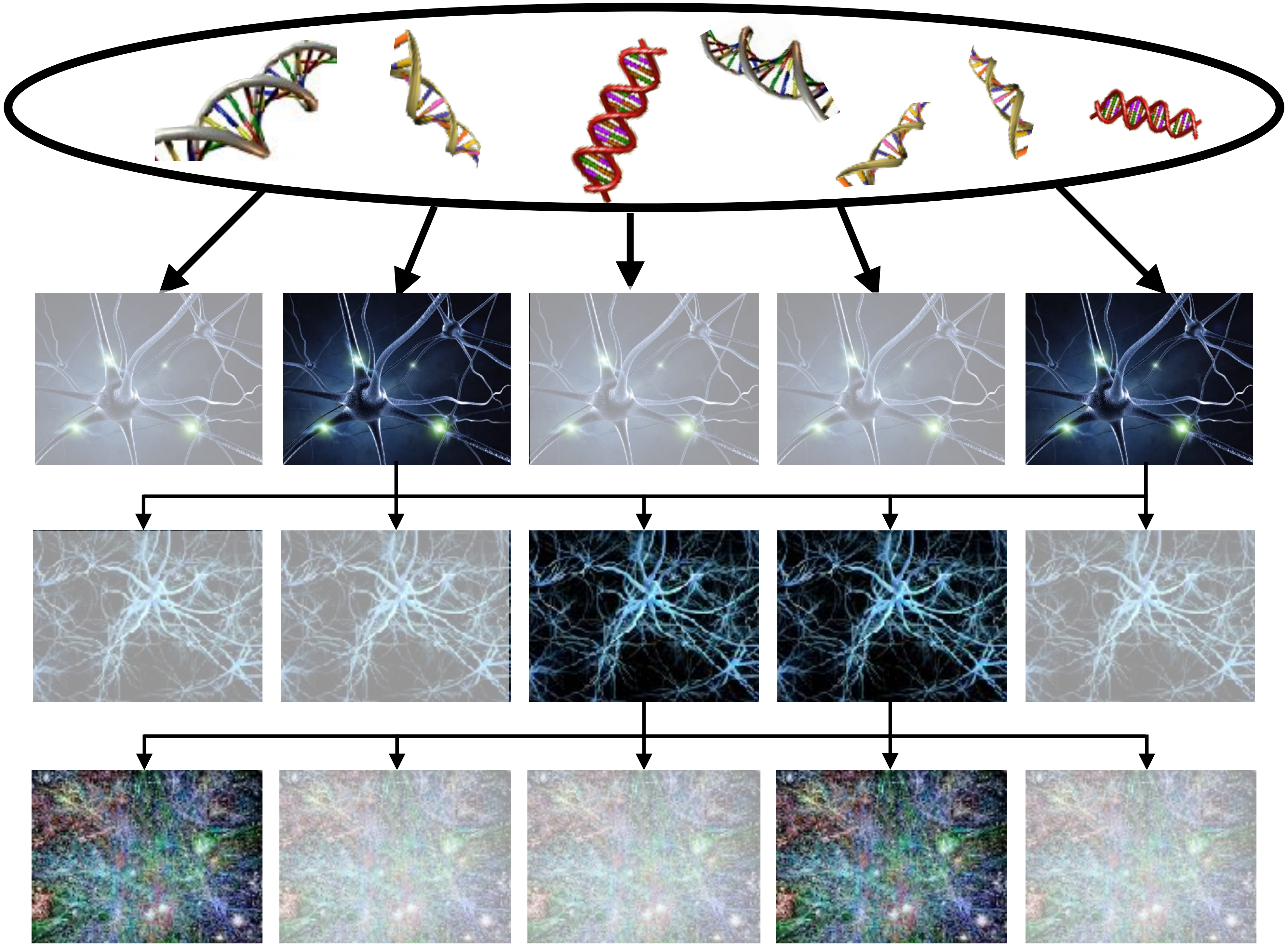
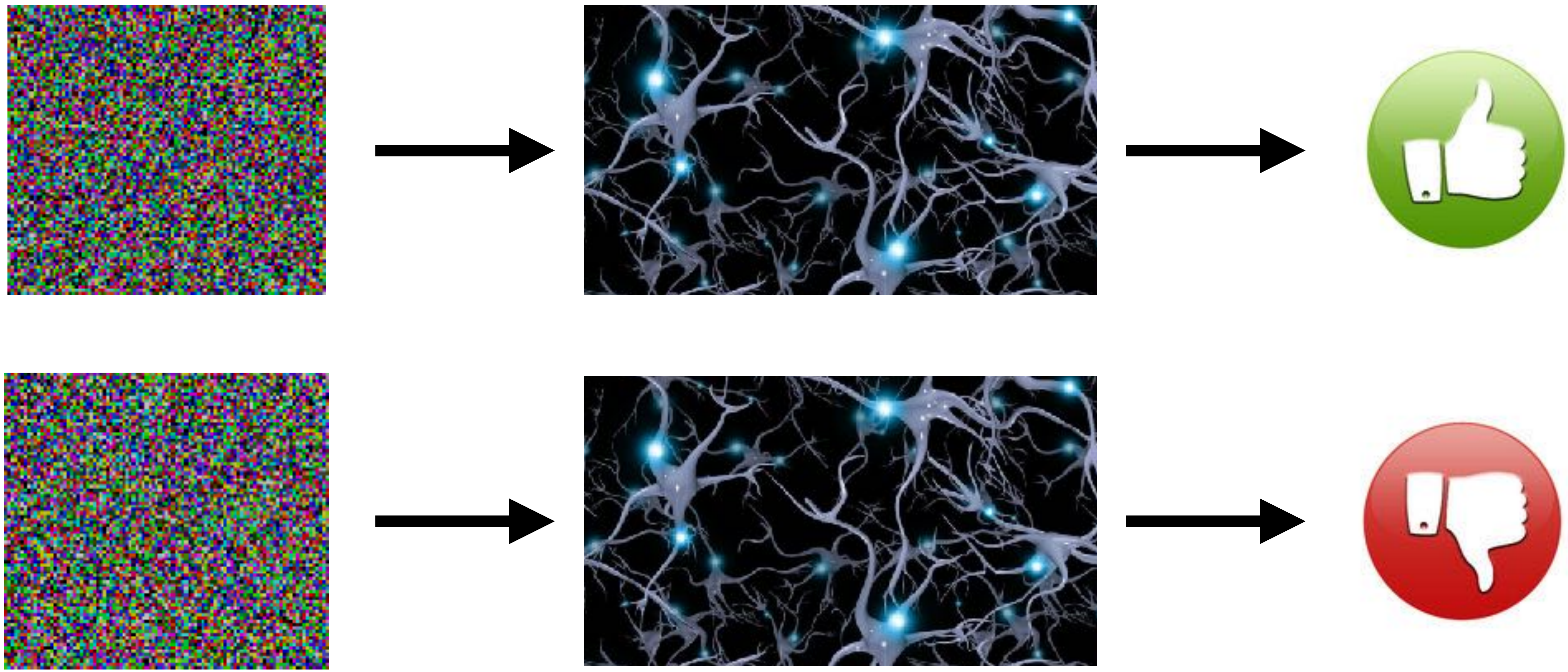


Genetic Algorithms 101

- Idea: Copy nature again $\Rightarrow$ dynamically evolve models [Darwin 1859]
- Applied in string theory to find models [Allanach,Grellscheid,Quevedo'04; Abel,Rizos'14]
- Pros:
  - Evolve / improve themselves 24/7 (automated trial & error)
  - Evolution/fitness evaluation parallelizable within a generation
- Possible applications:
  - Evolve connections rather than weighting them by training - similar to evolution of nerve connections between synapses in the human brain
  - Evolve training/validation set (important if the set cannot be easily randomized: the train set might accidentally have a feature which is picked up by the NN)
  - Evolve entire NNs (topology, activation function, no of layers, no of nodes per layer,…) - similar to evolving entire species in a computer

Genetic Algorithms - Modifications

- Adjust *fitness*
  - accuracy of prediction
  - computation time
- Change *reproduction*
  - cell division or cloning
  - *n* fittest get to reproduce via mating
  - all get to reproduce weighted by their fitness
  - mixture of cell division and mating depending on complexity of evolved species
- Change *mutation*
  - change rate
  - adjust complexity of genes that can mutate
  - change gene properties instead of exchanging entire genes
- Change *complexity* of genes in the *gene pool*
  - include higher level NNs
  - include trained NNs

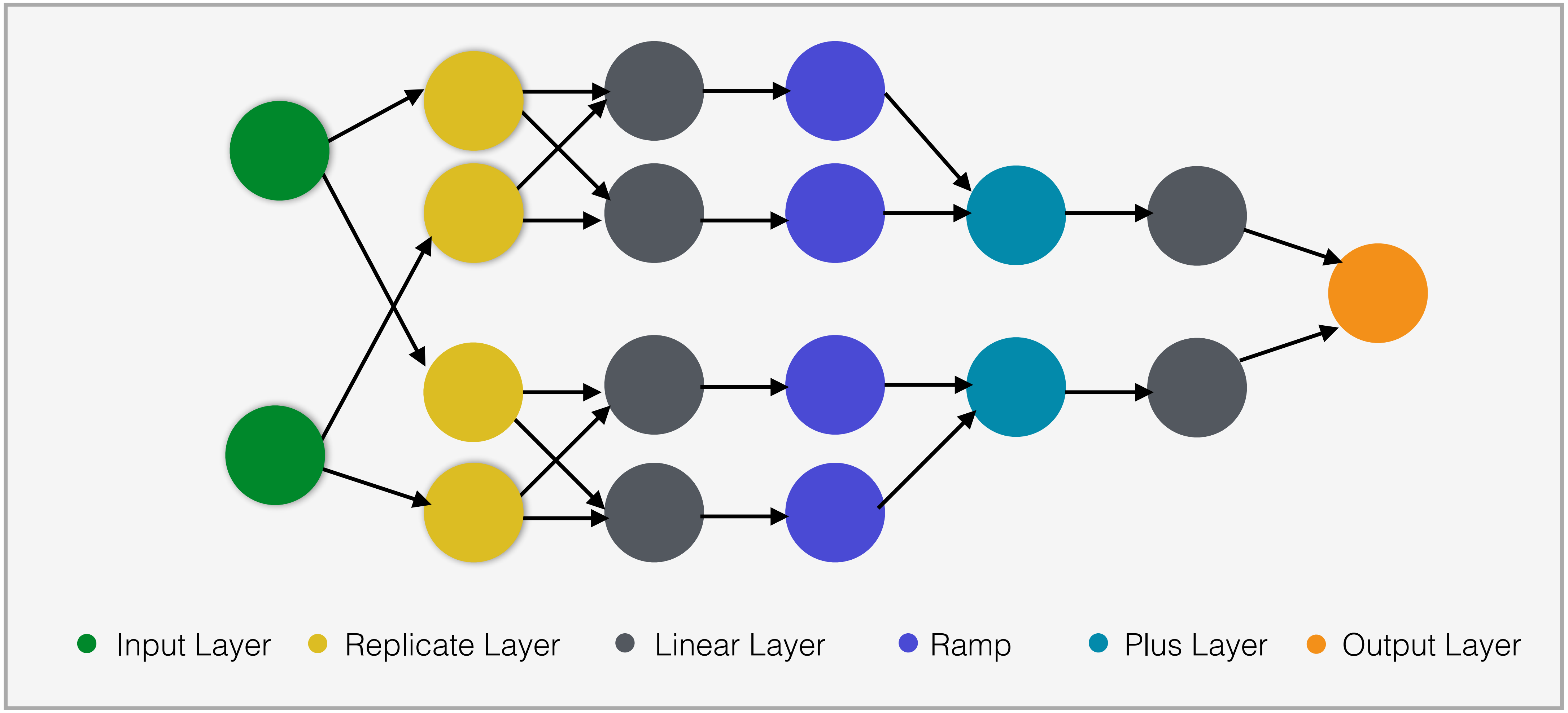


Combining both approaches

Example: Classify stable bundles

- Line bundle D-flat if $\int_X c_1(\mathcal{L}) \wedge J \wedge J = \kappa_{ijk} k^i t^j t^k = 0$
- Stability restricts Kahler cone to sub-region
- Still bounded by hyperplanes $\Rightarrow$ well-suited for NNs
- Simple example: CICY on $\mathbb{P}^2 \times \mathbb{P}^2$:
  - $h^{1,1} = 2$ (from the two $\mathbb{P}^2$ factors)
  - Kahler cone: $t^1, t^2 > 0$
  - Line bundle: $c_1(\mathcal{L}) = \mathcal{O}_X(k_1, k_2)$
  - Intersection numbers: $\kappa_{112} = \kappa_{122} = 3$, $\kappa_{111} = \kappa_{222} = 0$
  - Stable iff $k_1 > 0, k_2 < 0$ or $k_1 < 0, k_2 > 0$

Example: Classify stable bundles



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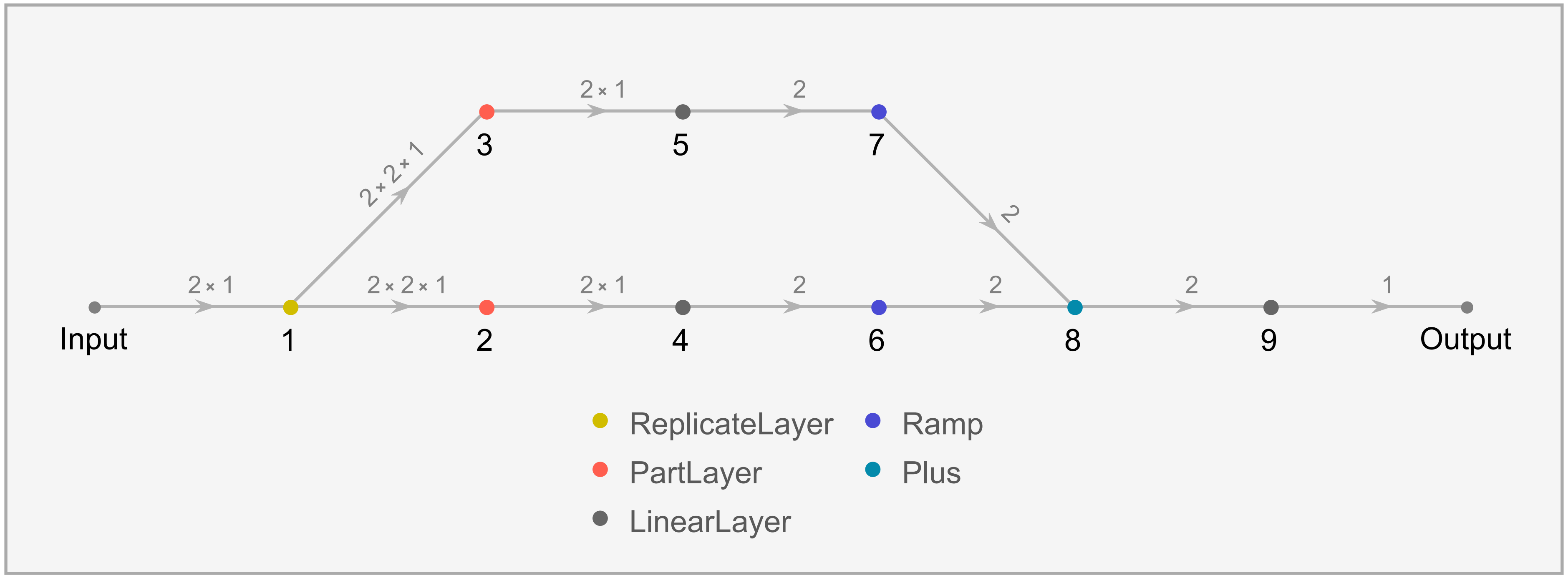

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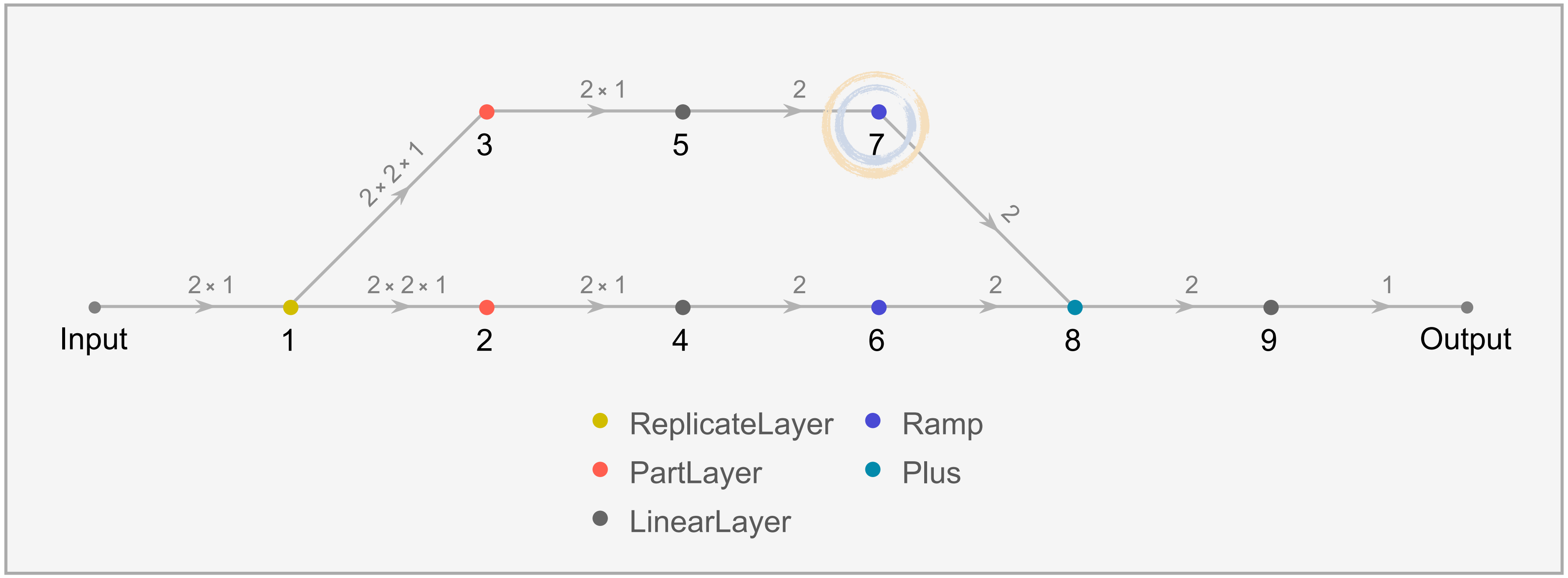

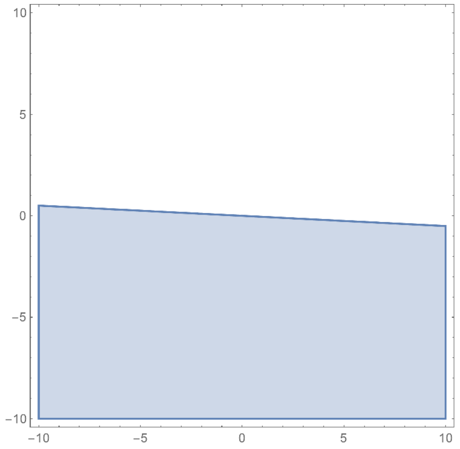

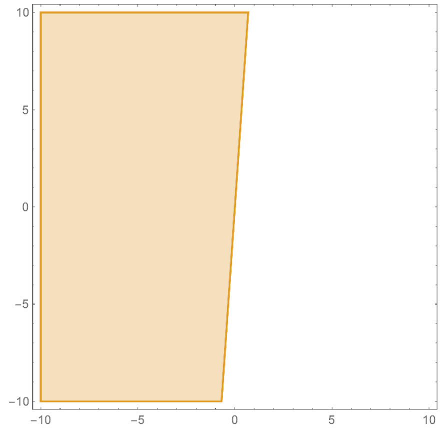

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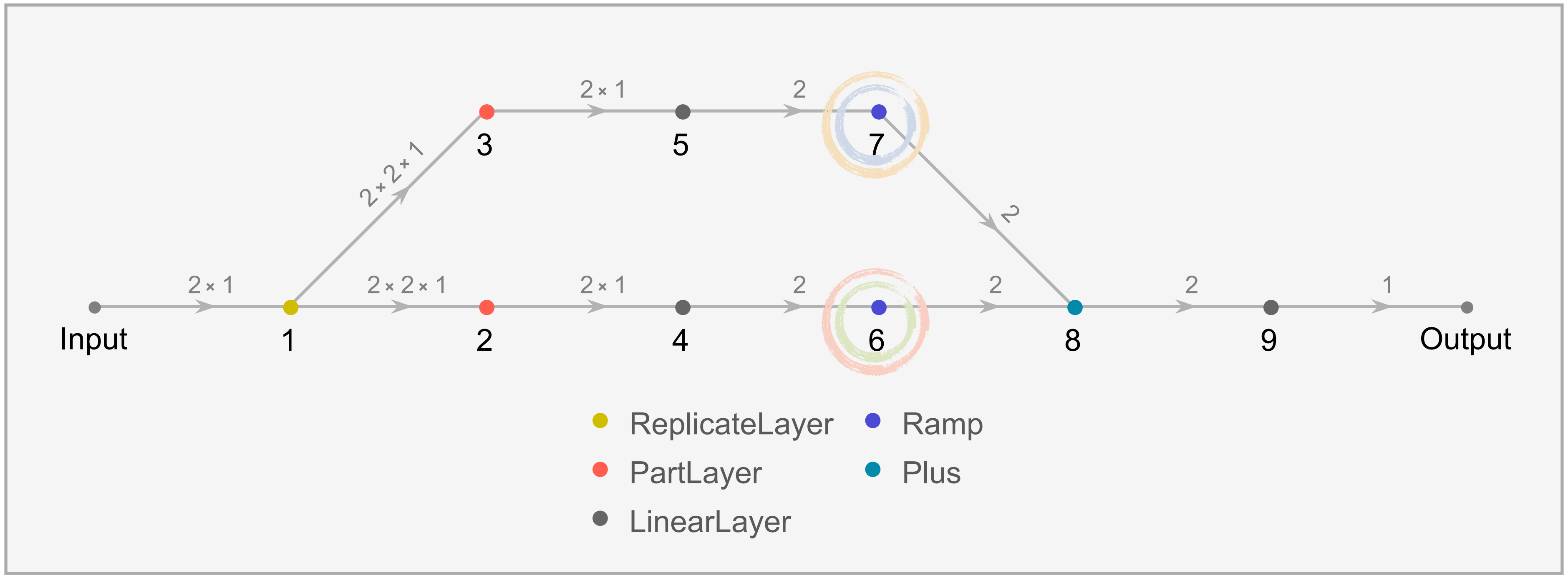

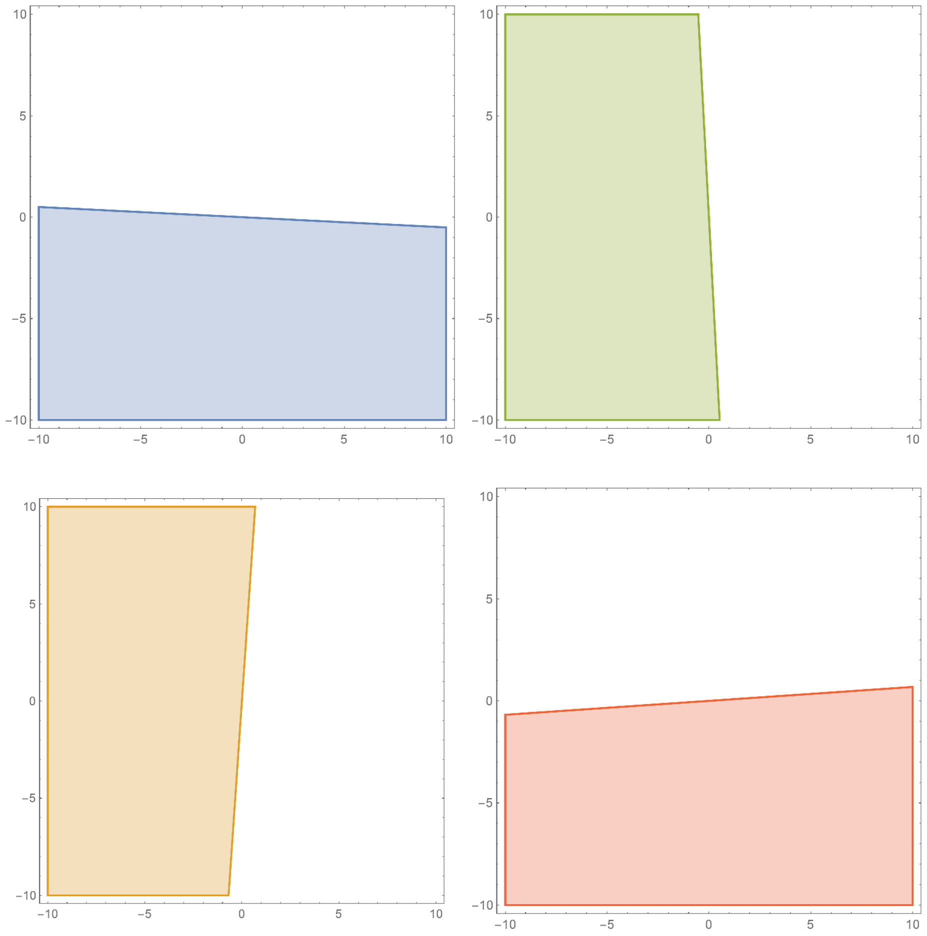

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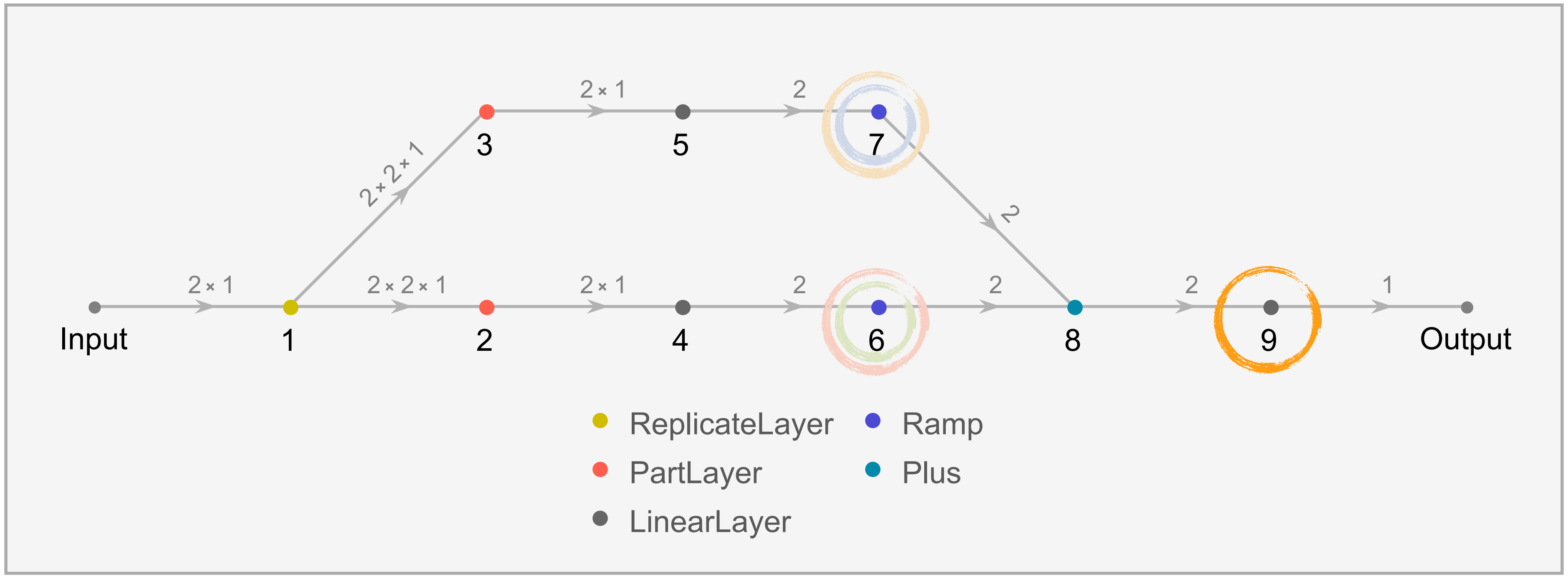

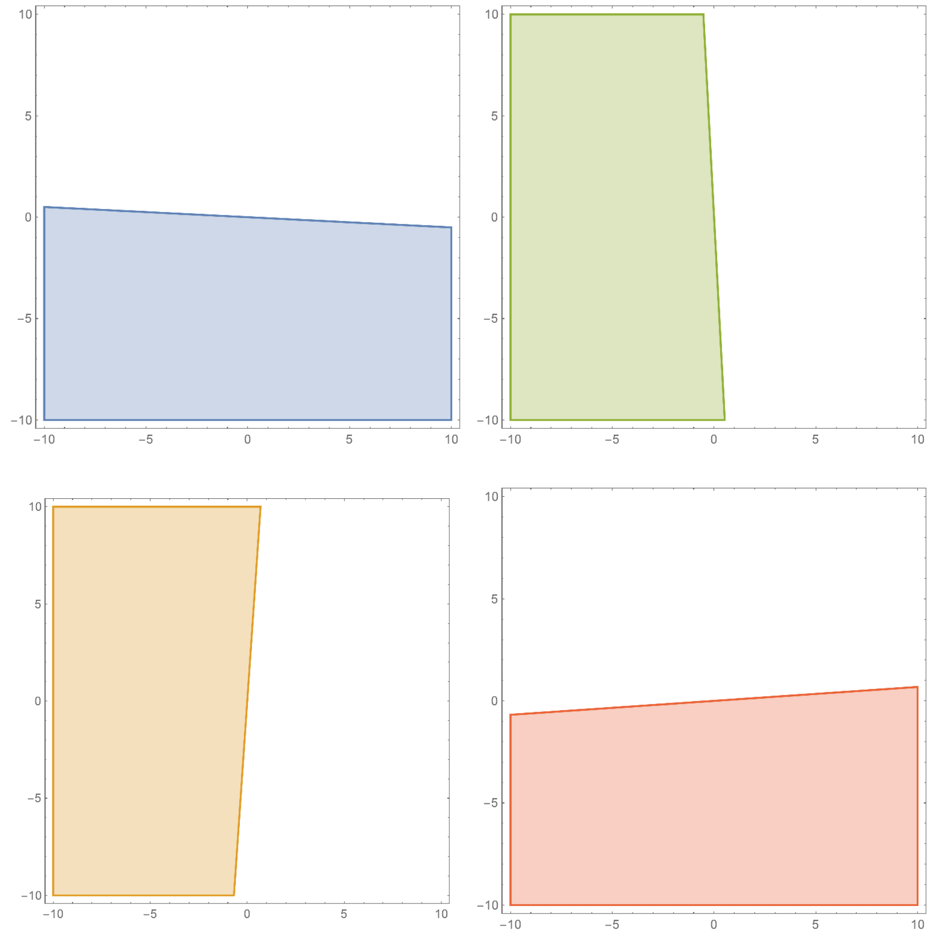

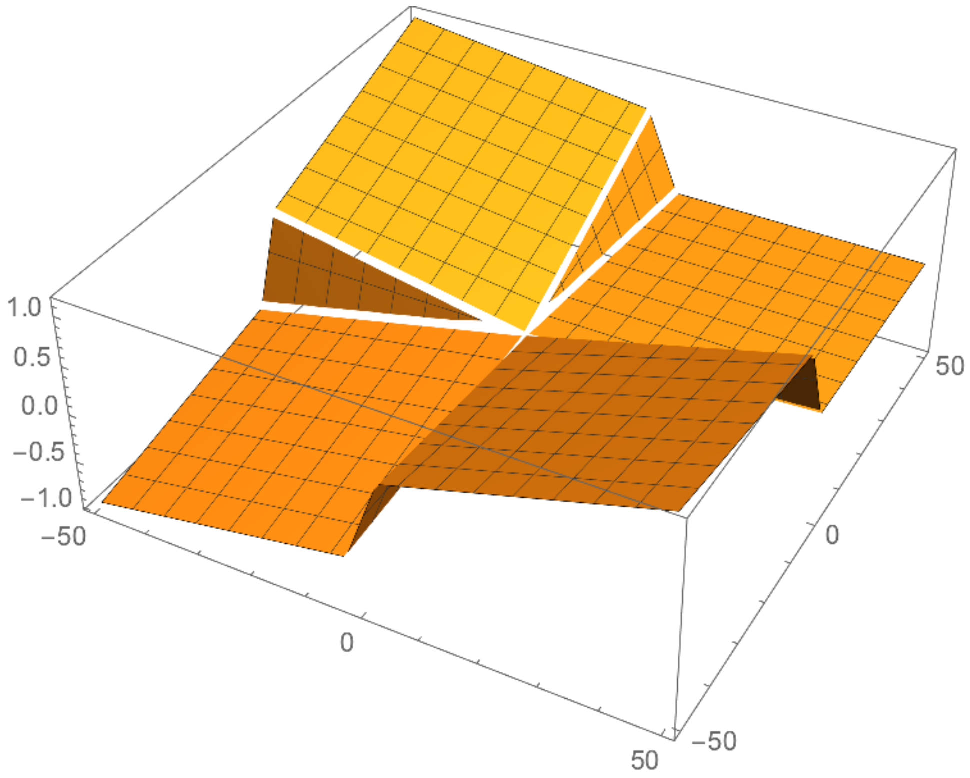

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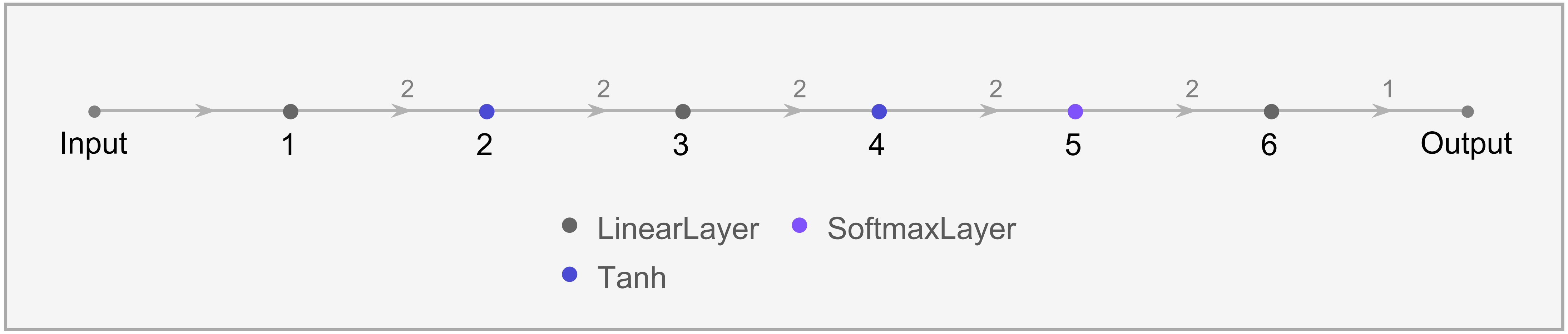

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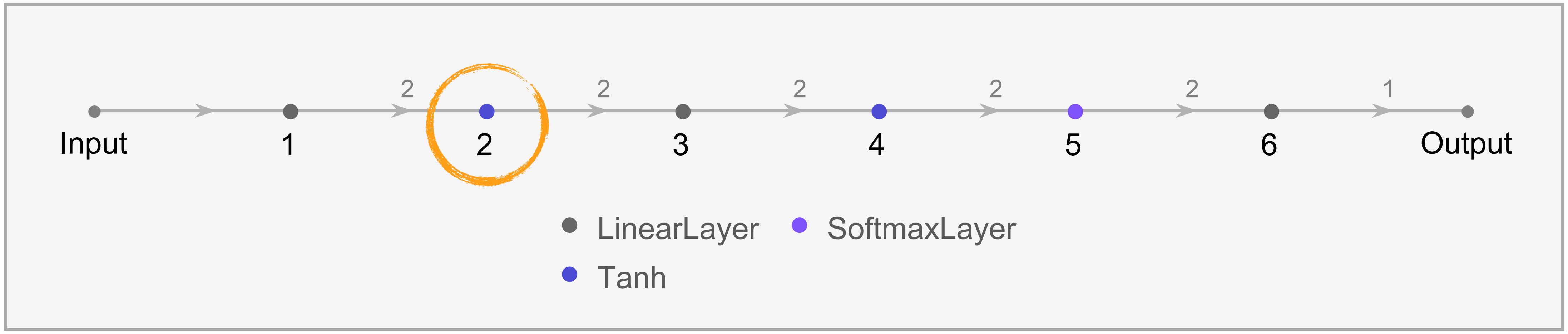

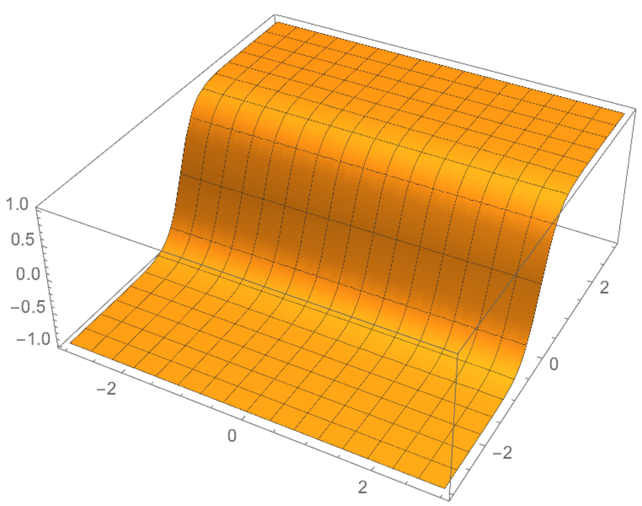

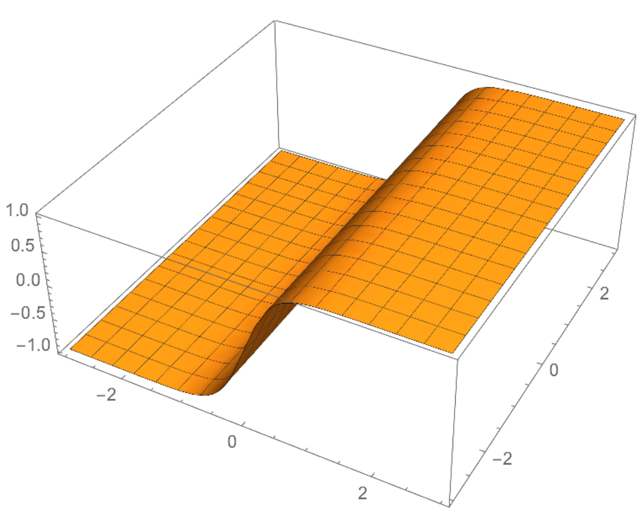

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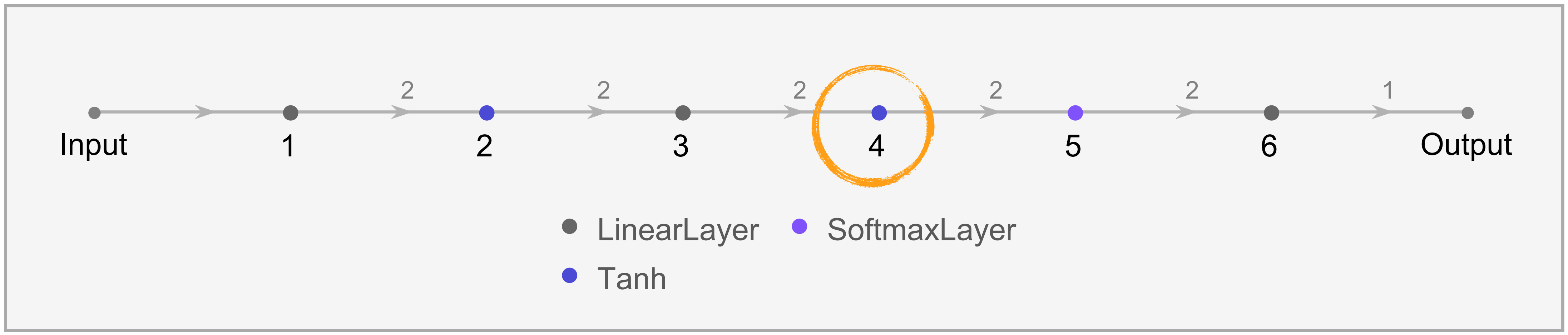

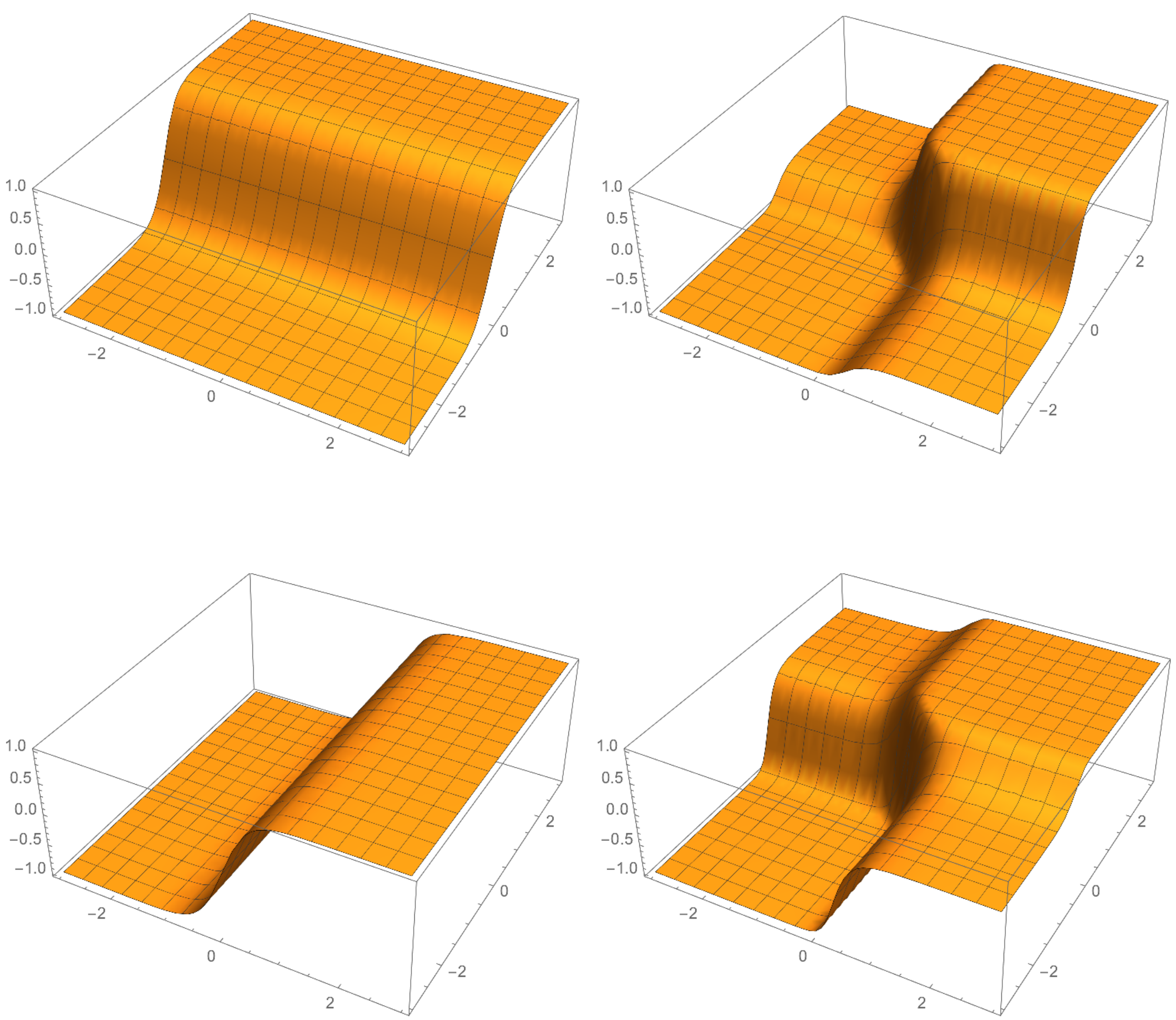

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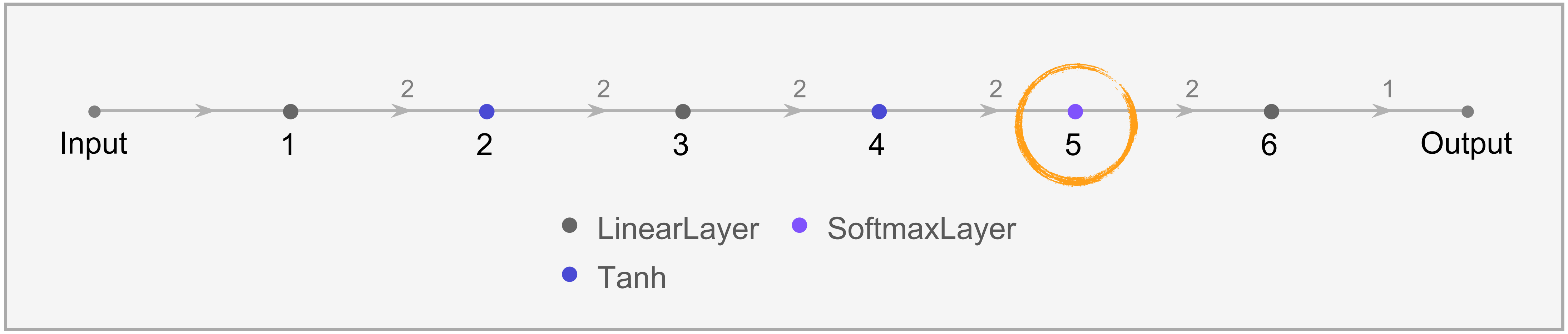
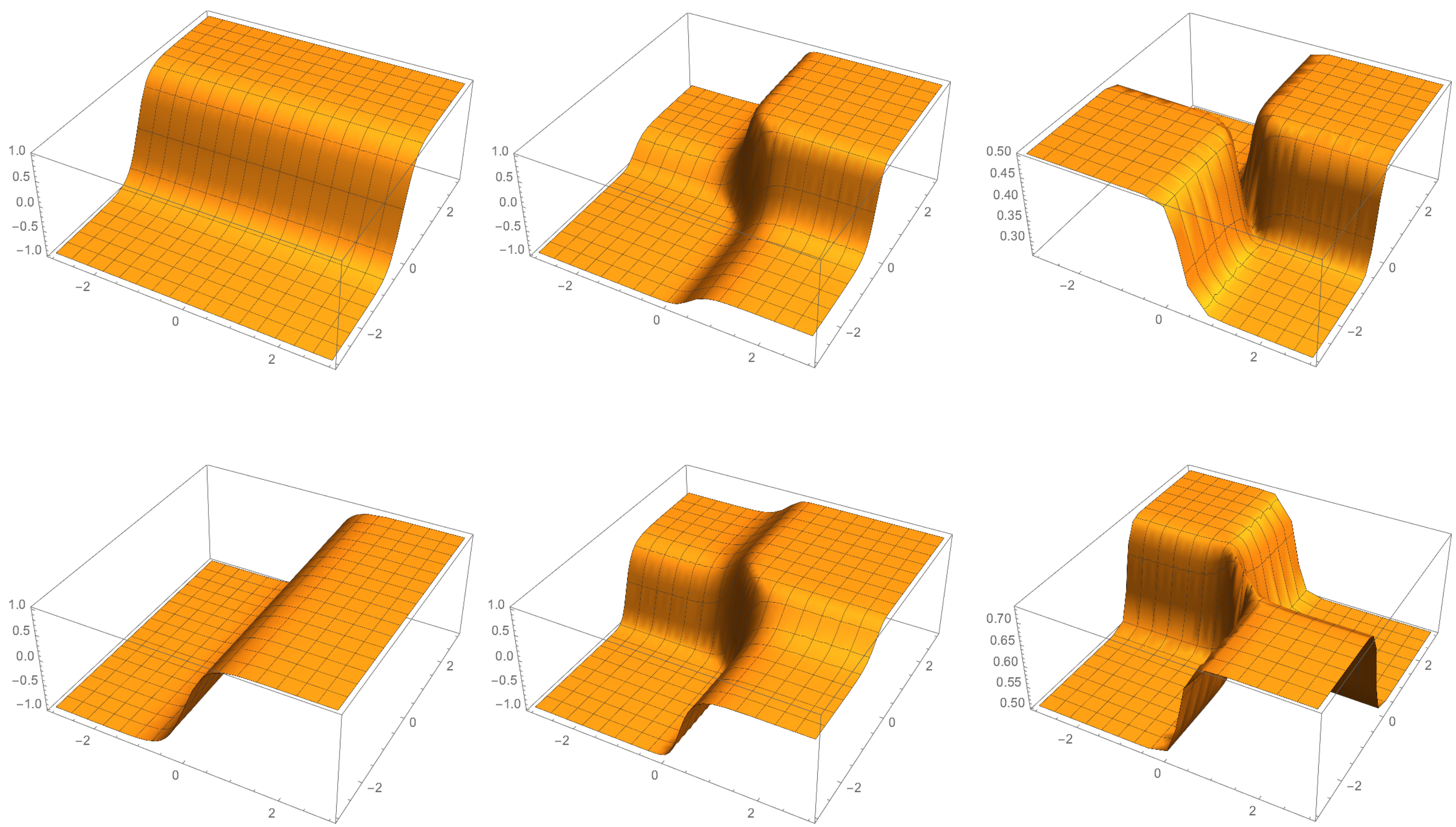
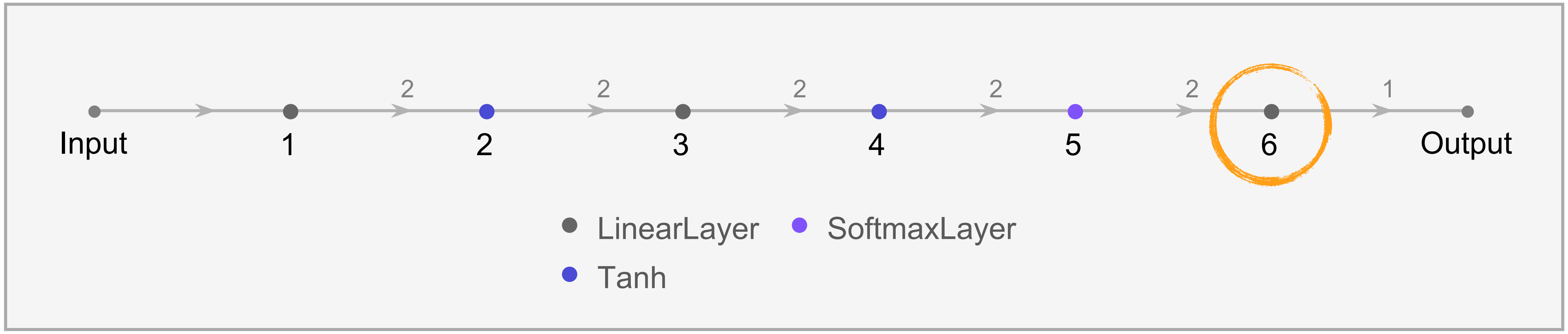
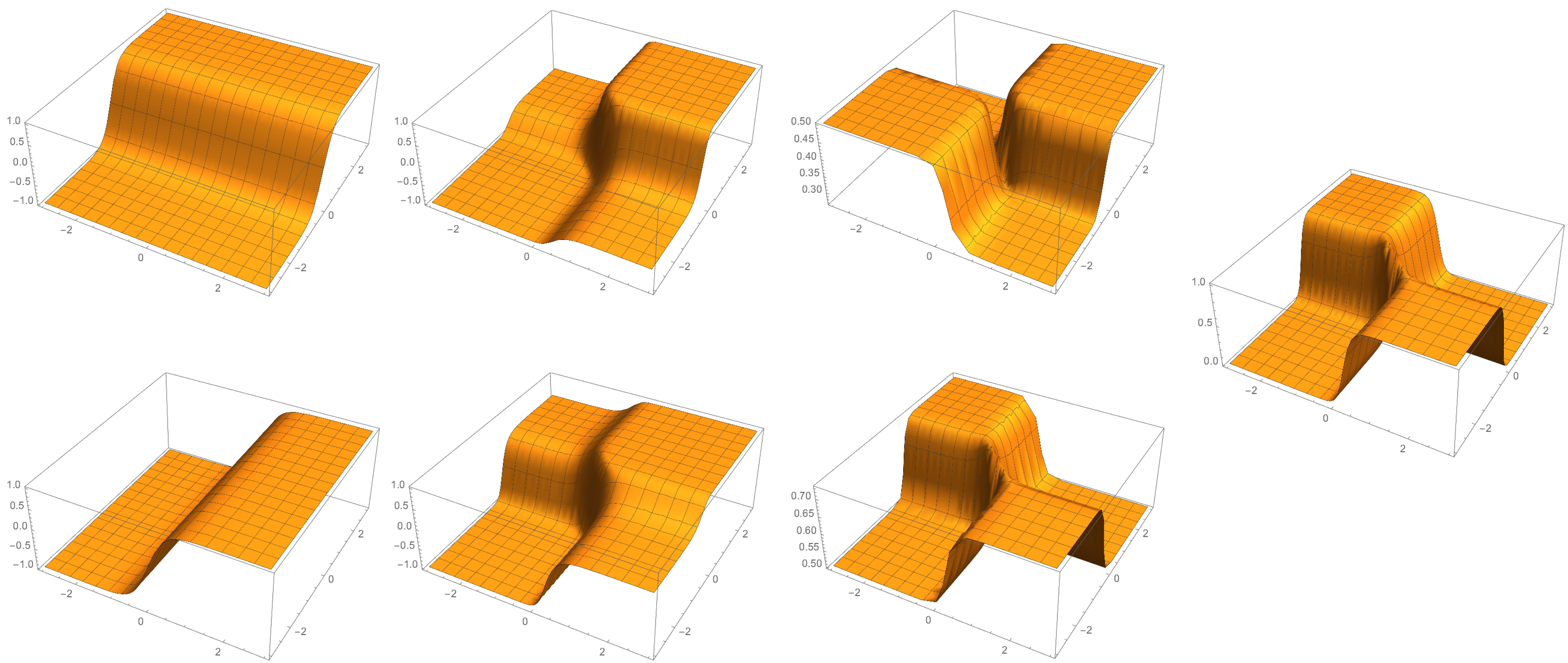


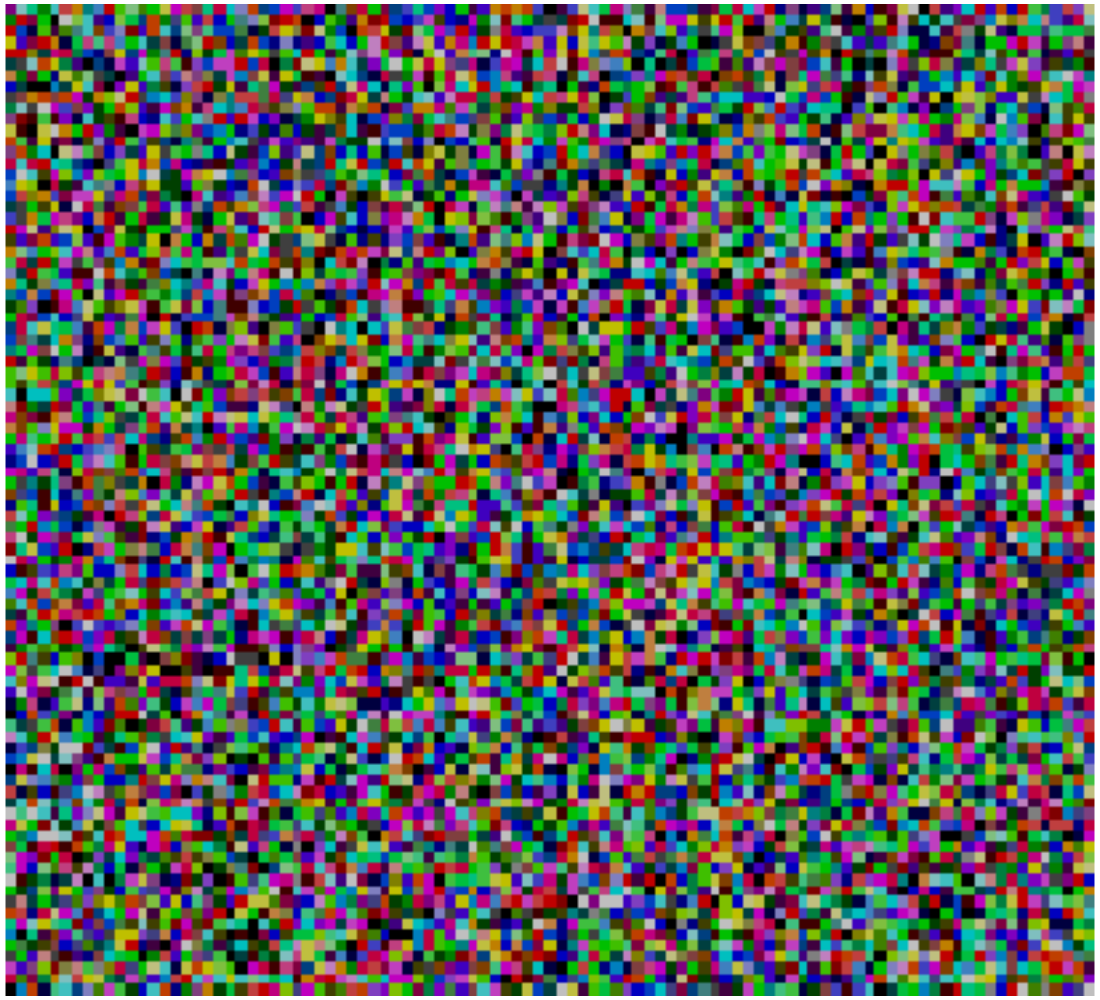


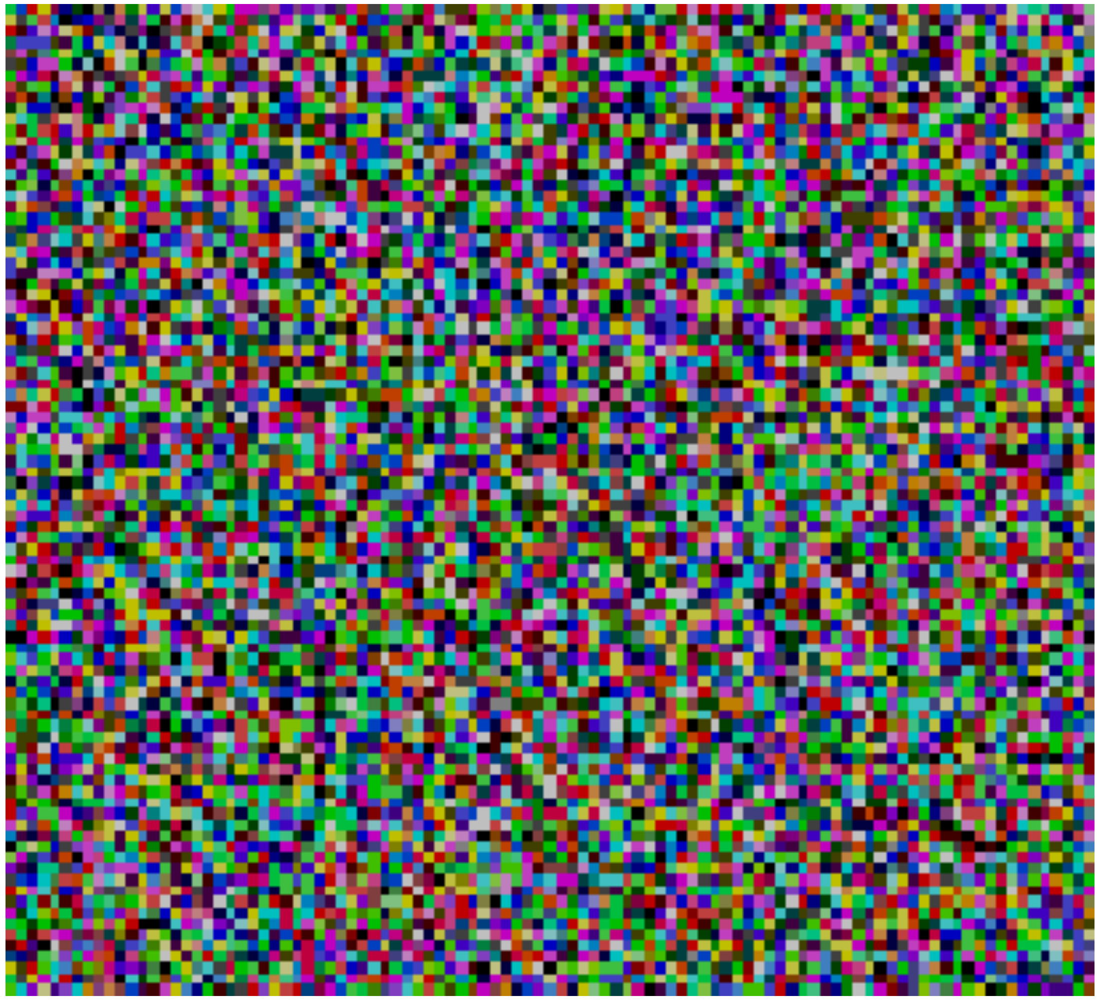
Example: Classify stable bundles



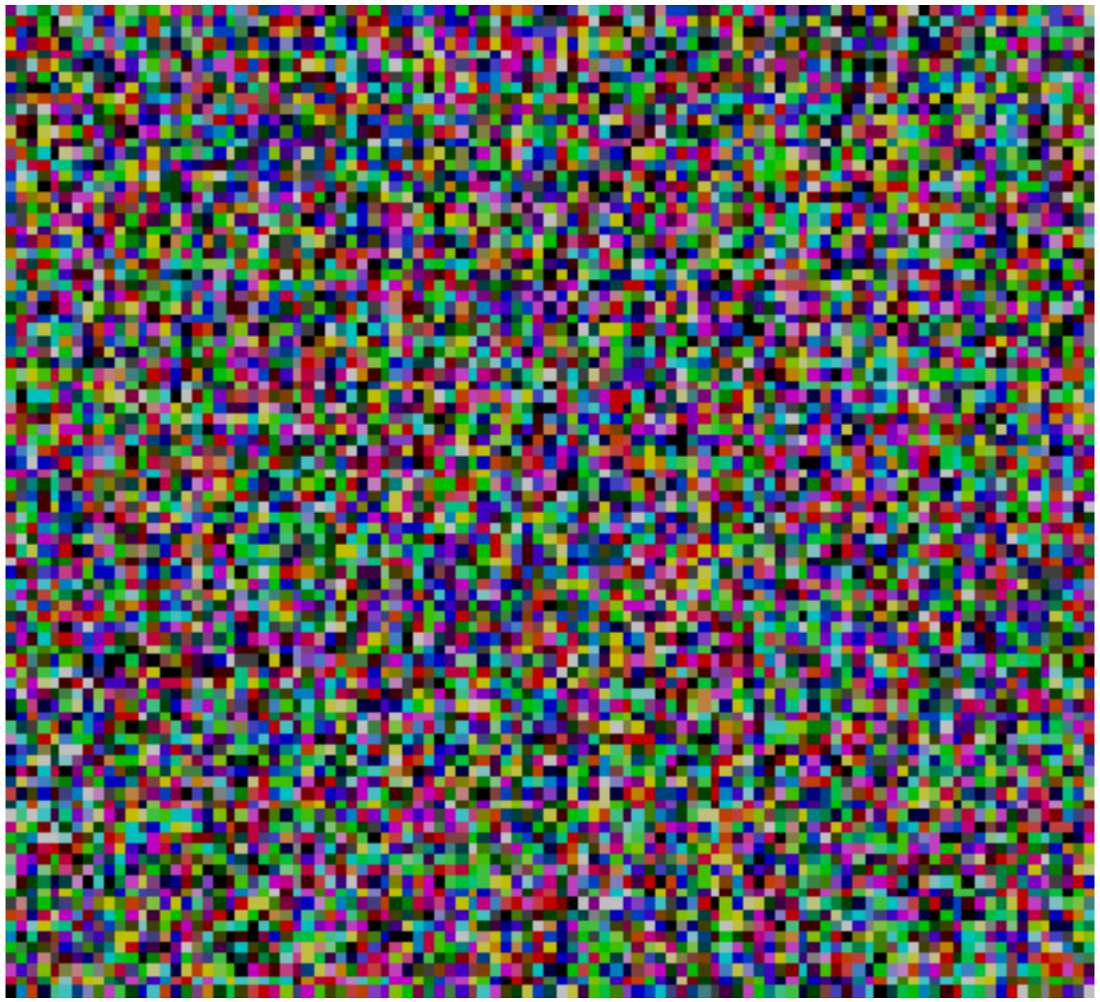


Example: Classify stable bundles

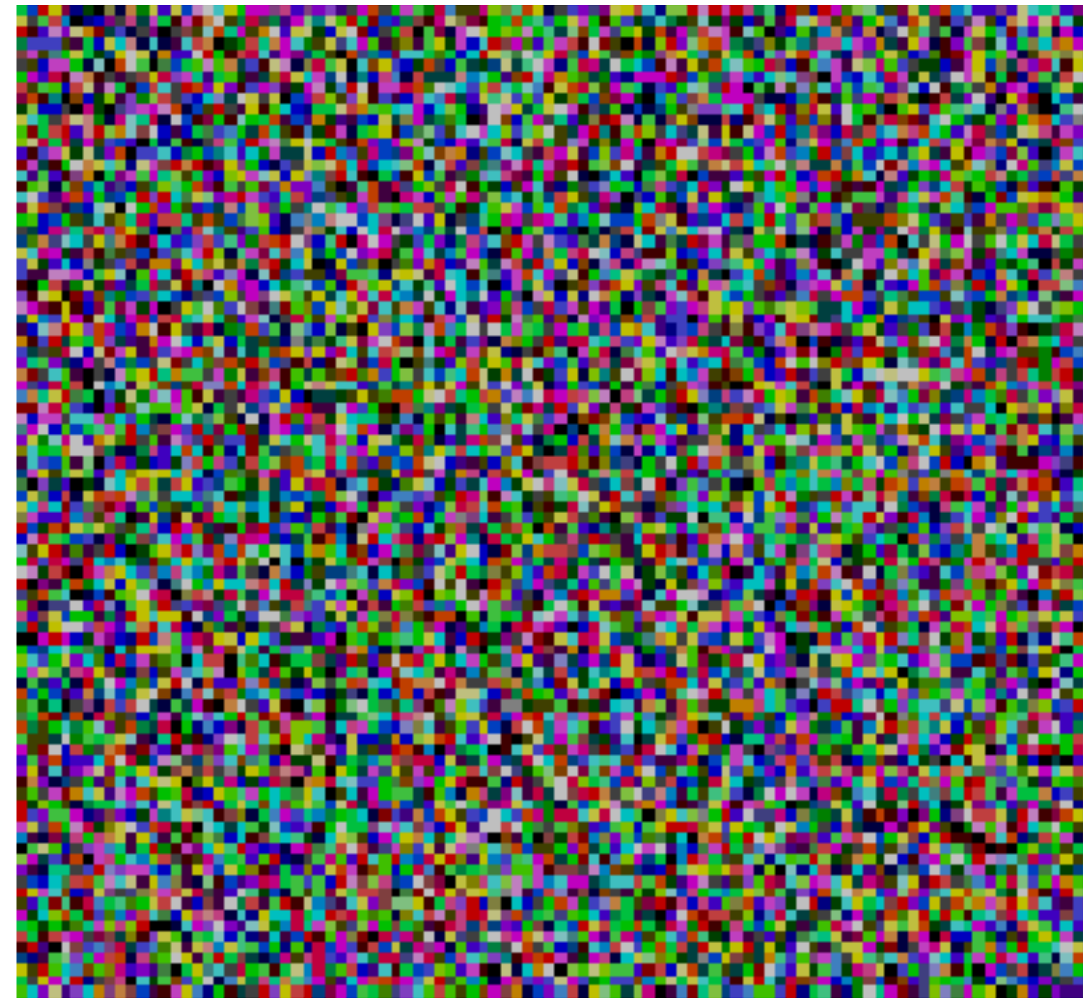




Example: Classify stable bundles



stable



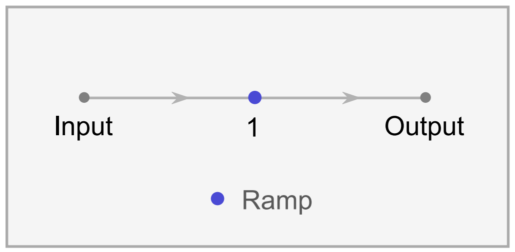
unstable

Example: Compute bundle cohomology

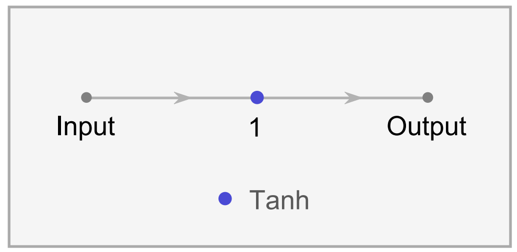
- Species computing $h^1(\mathcal{L})$ for Complete Intersection Calabi-Yau (codim 3) on $\mathbb{P}^1 \times \mathbb{P}^1 \times \mathbb{P}^1 \times \mathbb{P}^3$
- 10 Generations
- Fittest 2 survive
- Reproduction via cell division
- Mutation rate 10%
- During mutation, insert/replace genes at any position ("gene splicing")
- Training time 45 seconds on 3000 bundles
- Fitness evaluated on another 7000 bundles

Example: Compute bundle cohomology

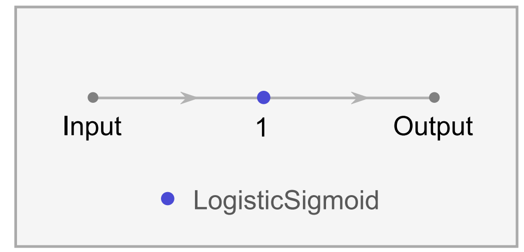
Available gene pool



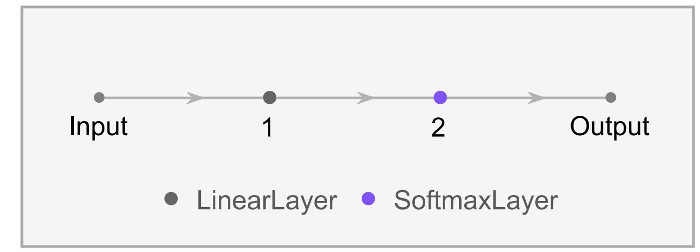
Ramp Layer



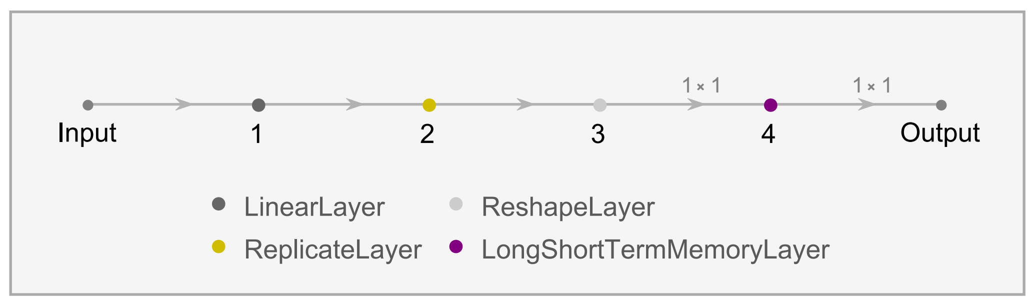
Tanh Layer



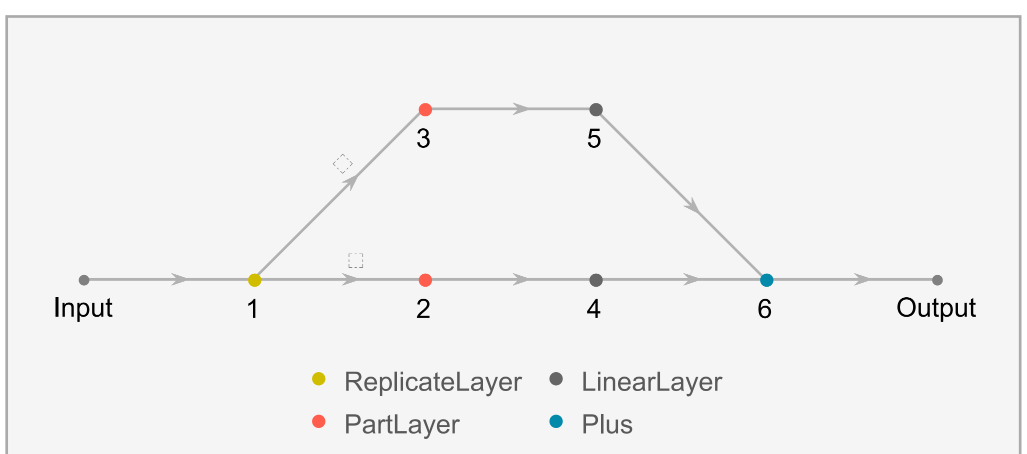
Logistic Sigmoid Layer



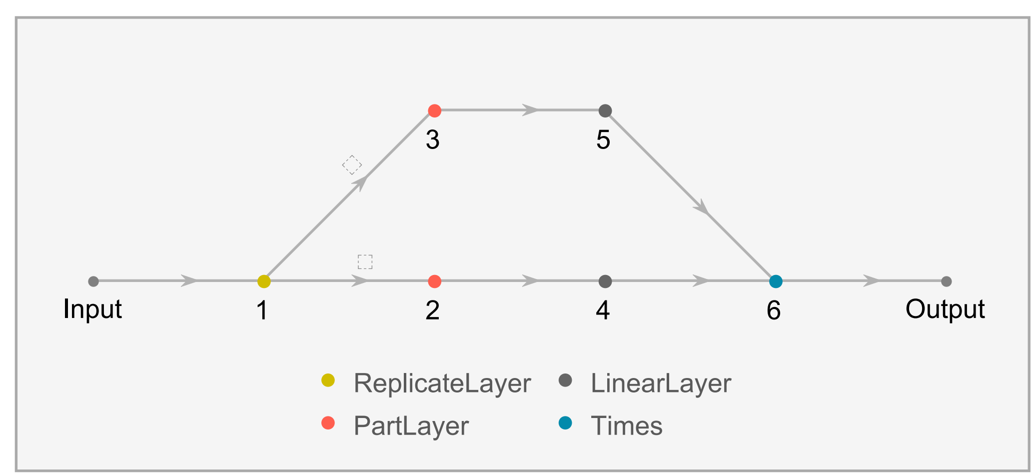
Softmax Layer



LSTM Layer

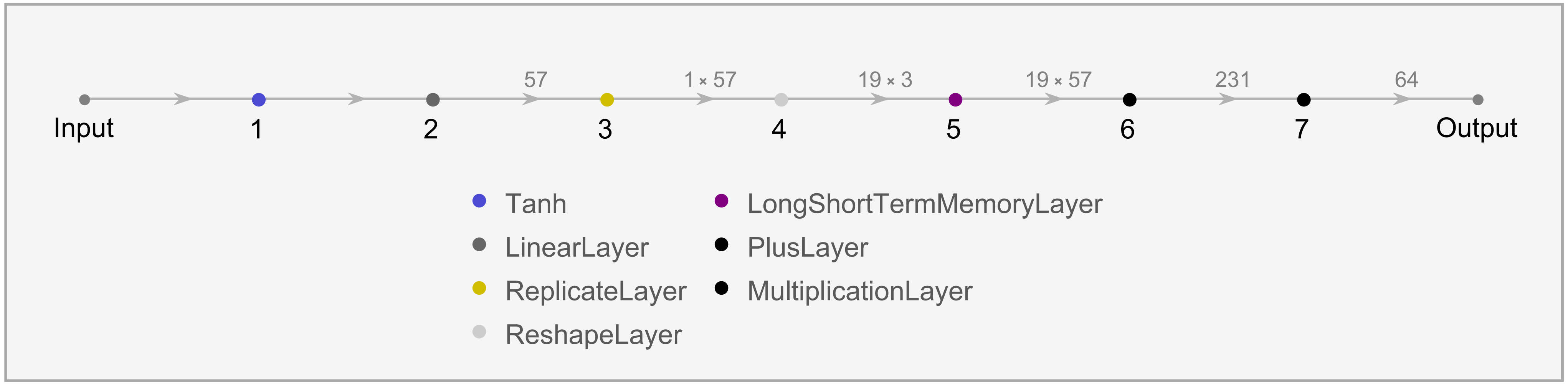


Addition Layer

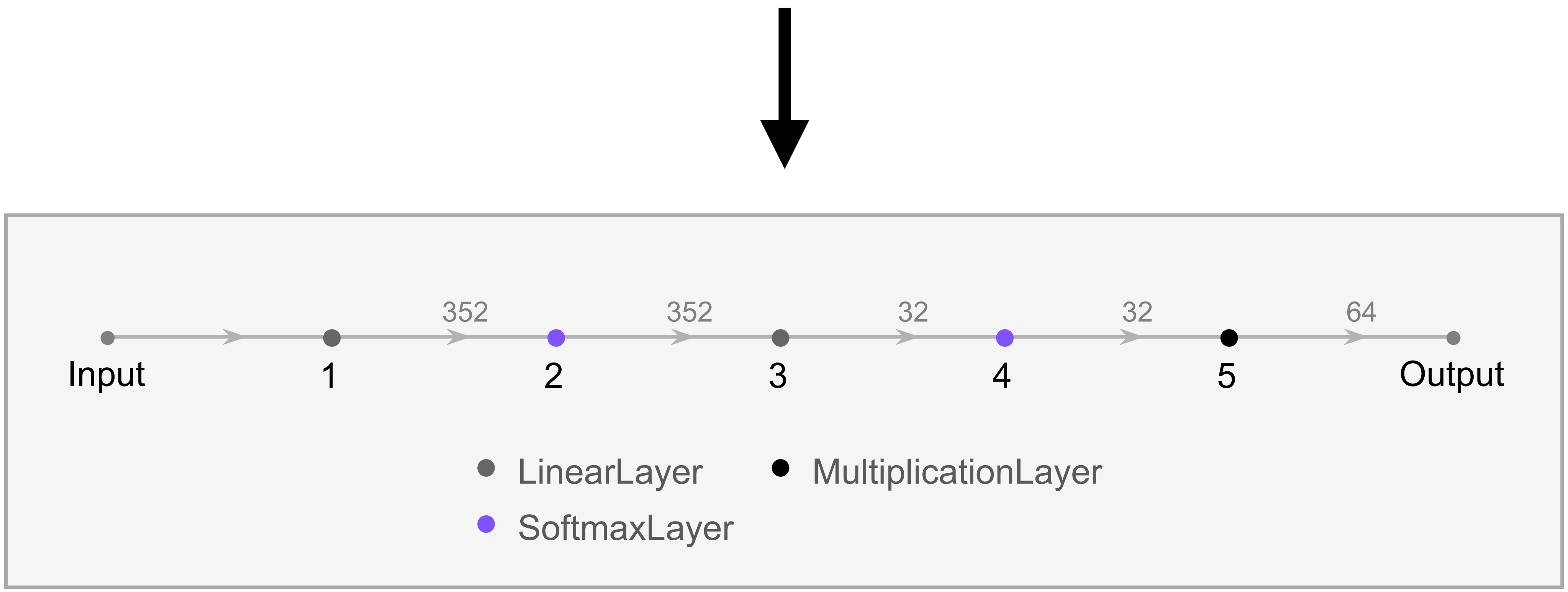


Multiplication Layer

Example: Compute bundle cohomology

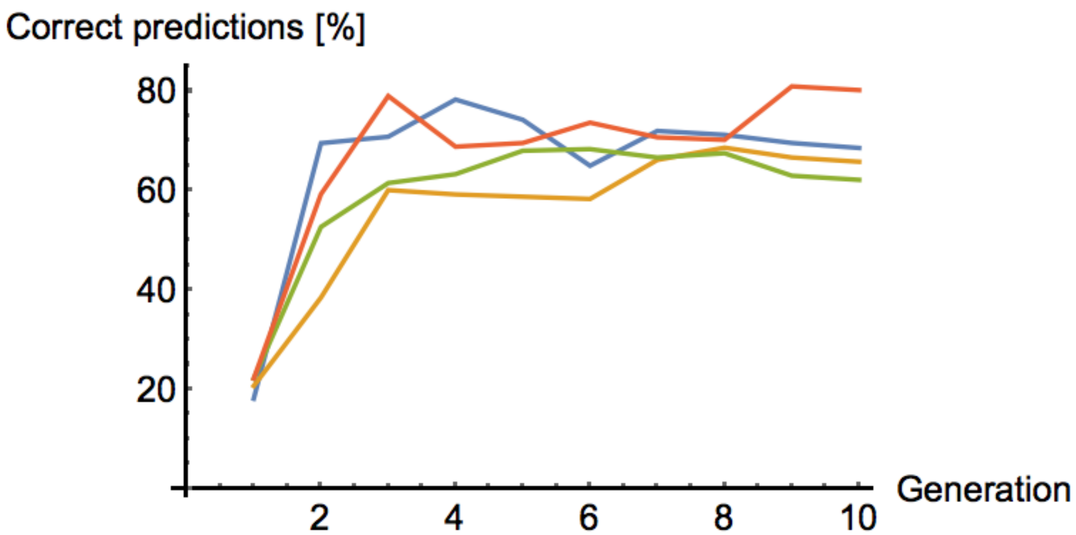


Species: $h^1(\mathcal{L})$, Generation: 1, Fitness 0.59

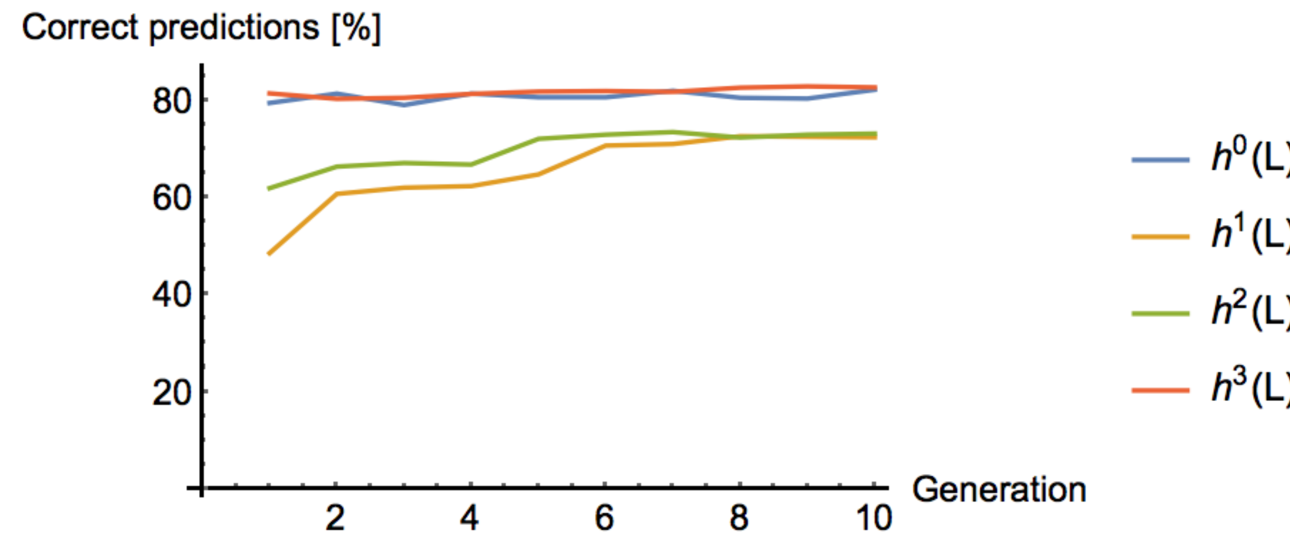


Species: $h^1(\mathcal{L})$, Generation: 10, Fitness 0.71

Example: Compute bundle cohomology



Average Fitness



Maximal Fitness

- $h^0(\mathcal{L})$ and $h^3(\mathcal{L})$ max out at 83%, $h^1(\mathcal{L})$ and $h^2(\mathcal{L})$ max out at 72%
- $h^1(\mathcal{L})$ and $h^2(\mathcal{L})$ more complex, evolve LSTM Layer
- Longer training of winner does not improve results
- Computation of 10 000 cohomologies takes
    - 5 hours using Koszul / Leray spectral sequences
    - 30 seconds with trained network
- Same network works on other CICYs (with same ambient space dimension) if trained with their data

Conclusion

- We have large sets of data in string theory with (potentially) interesting structure
  - Geometry (Calabi-Yaus)
  - String models
- Machine learning / NN can be applied to

  (A) Find & bypass implementations of algorithms

  (B) Approximate functions (predictor)

  (C) Classify data
- Tasks are versatile $\Longrightarrow$ dynamically evolve NN that is best equipped to handle individual situations
  - Feasible to evolve NN to compute bundle cohomologies
  - These NNs can be applied to different manifolds (if trained on them)

Thank you for your attention!