Neural Networks

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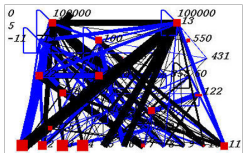
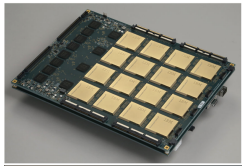
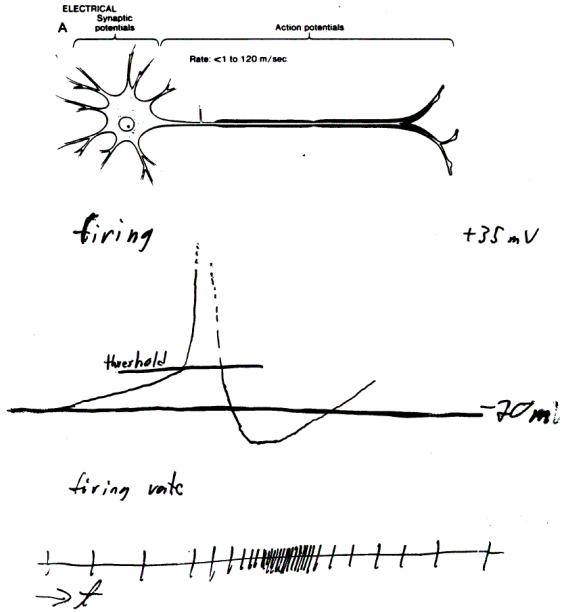
Motivation for Neural Networks



- Statistical machines with real-world applications
  - Pattern recognition, control, behavior
  - Biological and cognitive modeling
  - Usually simulated, but also hardware
- Motivation from biological neural networks
  - Abstracted into computational structures
  - Massively parallel, simple operations
  - Performance from scale



The Biological Neuron



Artificial Neuron

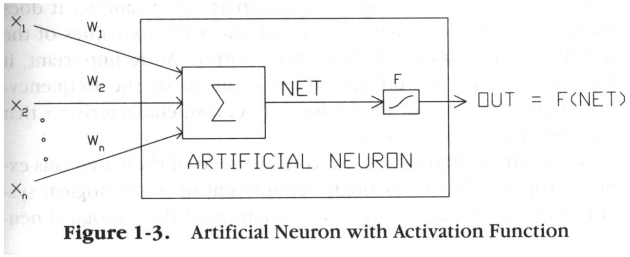
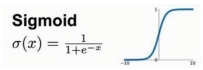


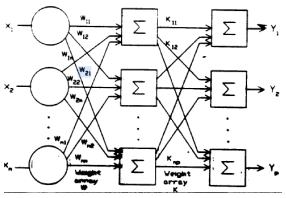
Figure 1-3. Artificial Neuron with Activation Function

- OUT = F(XW) = F($\sum w_i x_i$)
- Activity = Firing rate
- Nonlinear activation functions, e.g.:



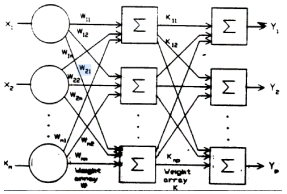
Feedforward Neural Networks (FNNs)

- Feedforward Neural Networks are the simplest type of artificial neural network.
- Consist of:
  - Input layer
  - One or more hidden layers
  - Output layer
- Information flows in one direction, from input to output, without loops or cycles.



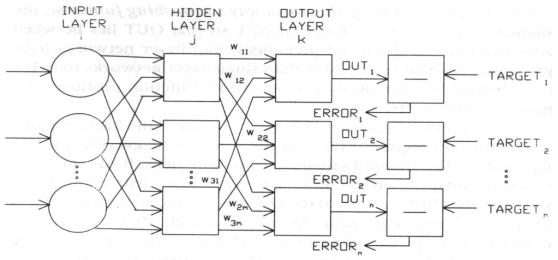
Details of Feedforward Neural Networks (FNNs)

- Input layer:
  - Receives raw data.
  - Each node corresponds to a feature or variable.
  - Passes input values to the next layer.
- Hidden layers:
  - Perform computations.
  - Each neuron calculates a weighted sum of inputs, passes through an activation function (e.g., ReLU, Sigmoid, Tanh).
- Output layer:
  - Produces the network's prediction.
  - Number of neurons matches the number of possible outputs.



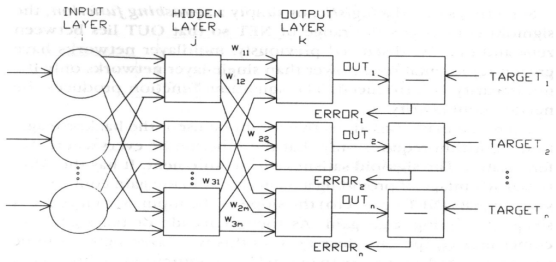
Learning Through Gradient Descent

- Weights typically trained with gradient descent (a.k.a. backpropagation)
  - Form a training corpus of input-target pairs
  - Initialize the weights to be small and random
  - Then train until convergence or out of time
  - Evaluate on a test corpus of unseen data



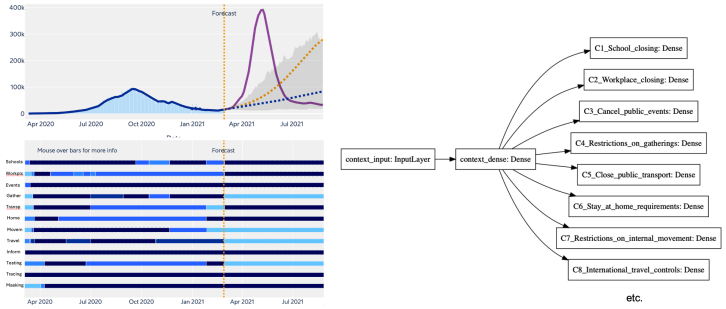
Learning Through Gradient Descent

- Gradient descent (online, i.e. stochastic version):
  - Select a training pair and present to the network
  - Compute output: $OUT = F(F(XU)W)$
  - Calculate error (i.e. loss): $\delta_k = F^{'}(NET_k) * (T_k - OUT_k)$
  - Backpropagate error through the network: $\delta_j = F^{'}(NET_j)\Sigma_k \delta_k W_{jk}$
  - Compute weight changes (i.e. the gradient): $\Delta W_{jk} = \eta \delta_k OUT_j; \quad \Delta U_{ij} = \eta \delta_j OUT_i$
- Demo: `https://playground.tensorflow.org`
- Alternatively, the weights can be discovered through evolution
  - Structure can be discovered through evolution as well



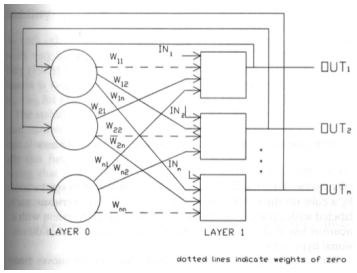
Example Evolved FFN: Pandemic Interventions

- The prescriptor receives an input vector of 21 days of past cases and NPIs
- It outputs stringency in 12 possible interventions
- Optimal strategy is not known; cannot use backprop
- Evolved with predictor as the fitness evaluator



Recurrent Neural Networks (RNNs)

- Recurrent Neural Networks (RNNs) are designed to recognize patterns in sequences of data.
- RNNs have connections that loop back, allowing information to persist.
- Well-suited for tasks where context and order matter, such as time series, text, or audio.

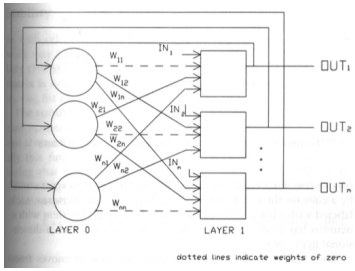


Details of Recurrent Neural Networks (RNNs)

- Neurons receive input from the previous layer and their previous states, allowing for memory.
- Process sequences one element at a time, maintaining a hidden state OUT_t that captures sequence information:

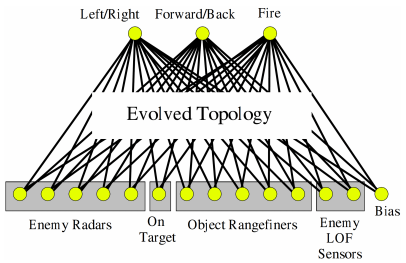
$$OUT_t = F(U \cdot IN_t + W \cdot OUT_{t-1})$$

  - OUT_t: hidden state at time step t.
  - IN_t: input at time step t.
  - U, W: weight matrices.
  - F: activation function (e.g., *tanh*, *ReLU*).
- Weights learned through backprop (e.g. BP through time), or evolved
- The recurrent structure can be customized through evolution



Example Evolved RNN: Controlling a Game Agent

- Sensors convey information about the current state
- Recurrency provides information from the past
  - E.g. speed, an opponent disappearing behind a wall...
- Combined to make a decision, implemented by effectors
- Evolved with success in game play as a fitness



Long Short-Term Memory Networks (LSTMs)

- LSTMs are a special type of Recurrent Neural Network (RNN) designed to learn and retain long-term dependencies.
- Overcome the limitations of traditional RNNs, particularly in handling long sequences.
- Highly effective for tasks involving sequential data, such as language modeling, speech recognition, and time-series forecasting.

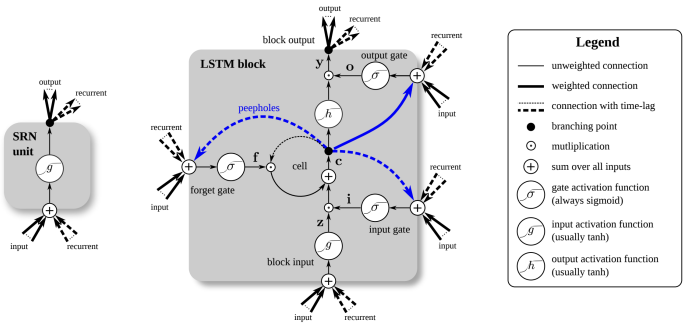
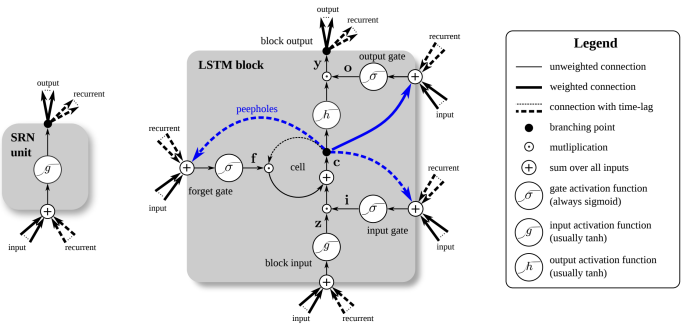


Figure: Left: Recurrent NN. Right: LSTM.

LSTM Cell Structure

- LSTM networks consist of LSTM cells, each with three main gates:
  - **Forget Gate:** Decides which parts of the cell's state to forget.
  - **Input Gate:** Determines which new information will be added to the cell state.
  - **Output Gate:** Controls the output based on the cell state.

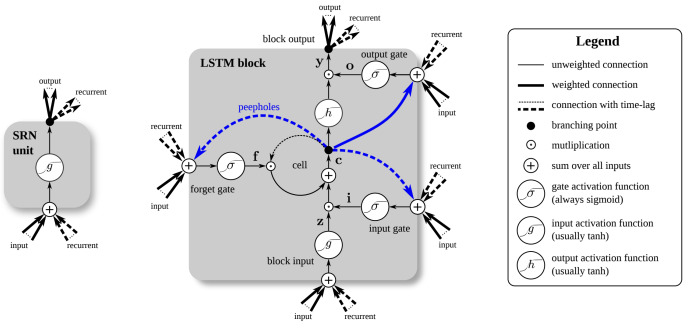


LSTM Gate Operations

- **Forget Gate:** $f_t = \sigma(W_f x_{f,t} + b_f)$
- **Input Gate:** $i_t = \sigma(W_i x_{i,t} + b_i)$

  $z_t = \tanh(W_z x_t + b_c)$
- **Cell State:** $c_t = f_t * c_{t-1} + i_t * z_t$
- **Output Gate:** $o_t = \sigma(W_o x_{o,t} + b_o)$

  $y_t = o_t * \tanh(c_t)$
- Weights can be learned through gradient descent, or evolved
- The internal structure can be optimized through evolution



Examples of Evolved LSTM Designs

- Using the same components, but allowing more complexity
- More paths, nonlinearities, memory cells
- Still trained with gradient descent
- Improved 25-year old designs by 15% (in language modeling)

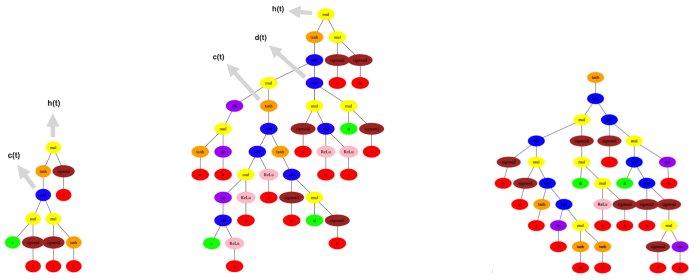
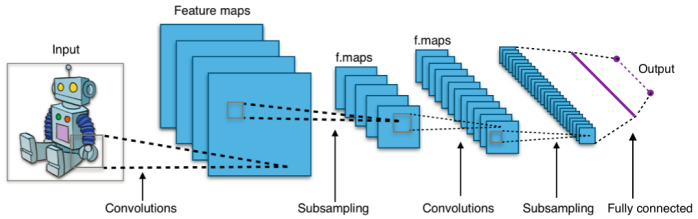


Figure: Original LSTM Language Music

Convolutional Neural Networks (CNNs)

- CNNs are deep learning models designed to process grid-like data structures, such as images.
- Effective for tasks involving spatial hierarchies, such as image recognition, object detection, and video analysis.
- Inspired by the visual cortex, where neurons respond to overlapping regions in the visual field.



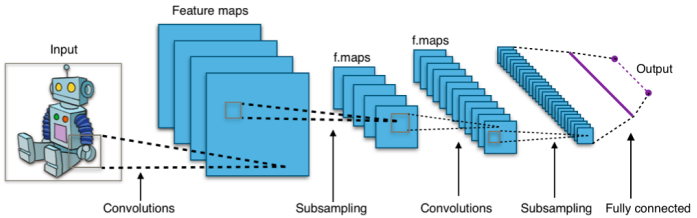
CNN Layers: Convolutional and Activation Layers

- **Convolutional Layer:**
  - Core component of a CNN.
  - Performs convolution operation using filters to extract spatial features.
  - With input I, kernel K, expressed as

$$(I * K)(x, y) = \sum_{i=1}^{m} \sum_{j=1}^{n} I(x + i, y + j) \cdot K(i, j)$$

- **Activation Function:**
  - Typically uses the Rectified Linear Unit (ReLU).
  - Introduces non-linearity:

$$f(x) = \max(0, x)$$



CNN Layers: Pooling and Fully Connected Layers

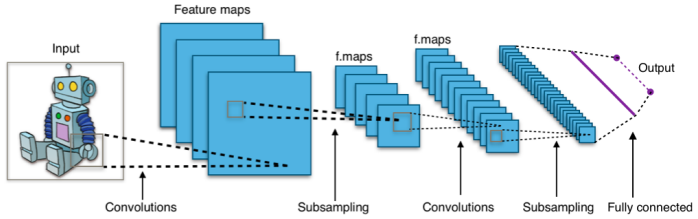
- **Pooling Layer:**
  - Reduces spatial dimensions of feature maps.
  - Commonly uses Max Pooling to retain prominent features:

$$P(x, y) = \max\{f(i, j) : i, j \in \text{window}(x, y)\}$$

- **Fully Connected Layer:**
  - High-level reasoning is performed.
  - Each neuron connects to every neuron in the previous layer.
  - Outputs class scores or other task-specific outputs:

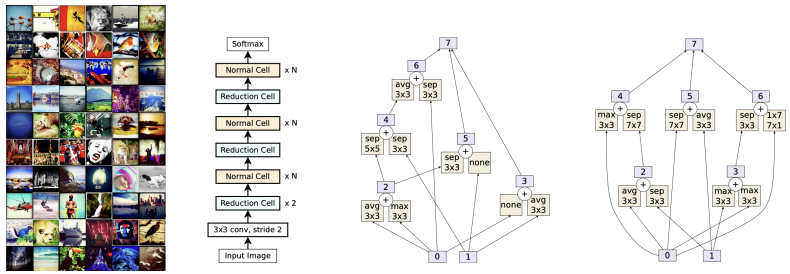
$$y = W \cdot x + b$$

- Weights learned through gradient descent (limited evolution)
- Structure can be optimized through evolution



Example of an Evolved CNN Architecture

- $>$ 1M weights difficult to evolve directly
- But can evolve network structure and train it with gradient descent
  - Evolutionary Neural Architecture Search (NAS)!
- E.g. AmoebaNet: Given a search space of building blocks, evolve organization
- Scale up to more channels and widths
- State of the art in ImageNet in 2018



Transformer Networks

- Transformers are deep learning models that rely on self-attention mechanisms rather than traditional recurrent or convolutional layers.
- Highly effective for handling sequential data and long-range dependencies.
- Widely used in natural language processing (NLP) tasks such as machine translation, text generation, and summarization.

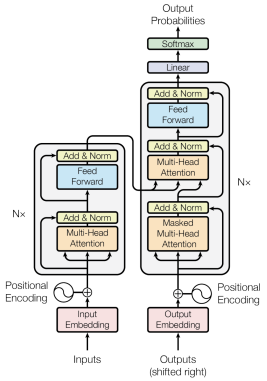
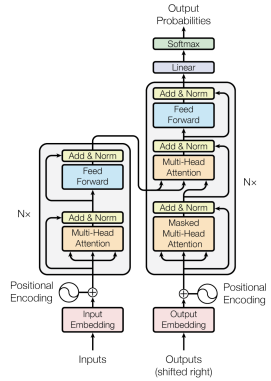
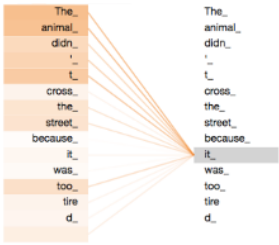


Figure: Transformer architecture: encoder (left) and decoder (right).

Transformer Architecture

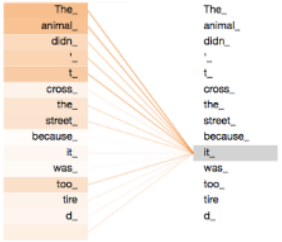
- Trained to predict the next token (e.g. word, symbol) by gradient descent
  - Initially designed to beat LSTMs on perplexity
- The core idea is transformations of token embeddings based on their relationships with other words
  - Many different relationships in parallel; Many stacked transformations
  - Transformations are learned and opaque
  - When scaled up, a powerful sequence processing architecture





Self-Attention Mechanism in Transformers

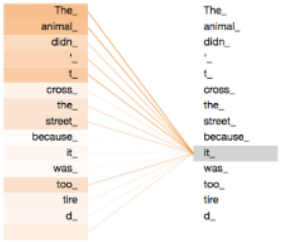
- **A single attention head:**
  - Computes a transformation of each token representation vector (i.e. embedding) based on its relation (i.e. attention) to other tokens.
  - Based on projecting embeddings in three ways:
    - Query $Q_i = X_i W_i^Q$ formed from current word embedding X_i
    - Keys $K_j = X_j W_j^K$ formed from nearby word embeddings X_j
    - Values $V_j = X_j W_j^V$ formed from nearby word embeddings X_j
  - Self-attention matches queries with keys and forms a representation by combining the values proportionally.
    - Could do it simply with embeddings themselves, but only once
    - Q, K V mappings make it possible in many different ways.
    - They are learned; the process becomes opaque.



Self-Attention Mechanism in Transformers

- **Calculating attention scores:**
  - Take the dot product of Q and K, measuring relevance of each nearby word to the current word.
  - Scale by the square root of the dimensionality of K.
  - Take a softmax to scale between 0..1.
  - Interpret the result as weights determining how much each token j influences the transformed representation for token i

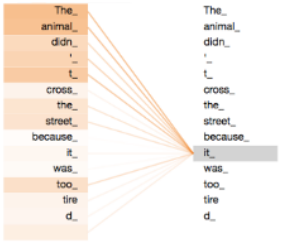
$$\text{AttentionScore}(Q, K) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)$$



Self-Attention Mechanism in Transformers

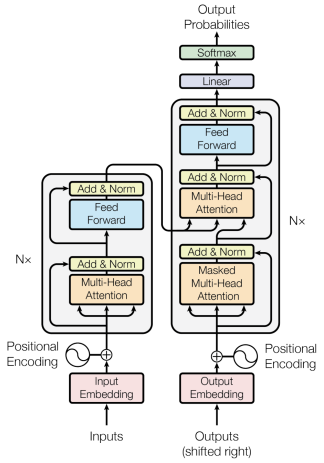
- **Calculating the transformation:**
  - Form an AttentionScore-weighted sum of value vectors V_j.
  - The result is an attention-based representation for token i.
  - The collection of these representations for all tokens j is the output of the attention head.
  - It is a transformation of the token embeddings based on their relationships with other tokens, i.e. attention.

$$\text{AttentionRepresentation}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$



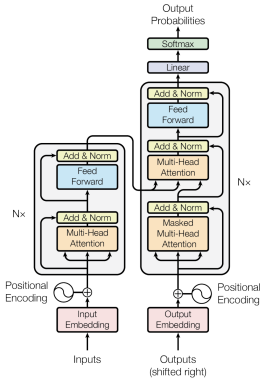
Self-Attention Mechanism in Transformers

- **Multihead attention:**
  - Multiple attention heads calculate different transformations in parallel, attending to different aspects (e.g. verb/subject, semantics, style, etc.)
  - Their outputs are combined in a feed-forward layer.
  - The output is passed on as input to the next layer
  - Many such transformations are stacked, forming more complex representations.



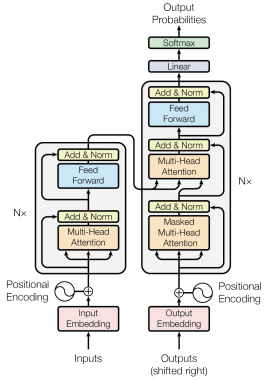
Transformer Encoder-Decoder Structure

- **Encoder-Decoder Structure:**
  - The encoder processes the input sequence into an internal representation.
  - The decoder generates an output sequence, based on input so far and the encoder's representation.
  - Depending on the task, only the encoder, only the decoder, or both may be needed.



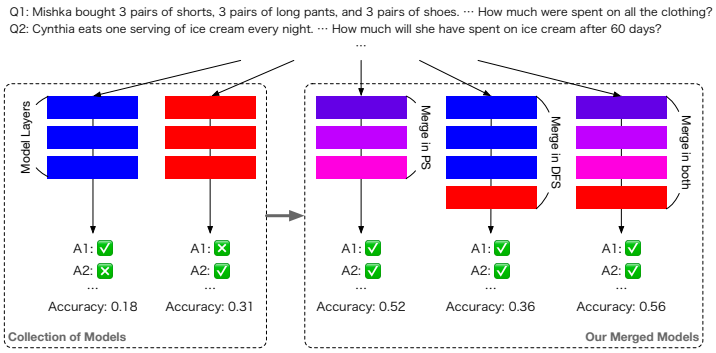
Making it Work

- **Positional Encoding**
  - Sequential structure is encoded into initial embeddings.
- **Gradient descent:**
  - Matrices W^Q, W^K, W^V, feedforward parameters.
  - The resulting representations are opaque and hard to understand.
- **Layer Normalization and Residual Connections:**
  - Layer normalization stabilizes and speeds up training.
  - Residual connections help prevent the vanishing gradient problem.



Example of an Evolved LLM Model Merging

- LLMs are large trainsformer models trained with language
- With 70B weights, difficult to train or evolve
- But can evolve an optimal way of combining existing models
  - Recombine layers, or recombine weights
- E.g. a model fine-tuned for Japanese and another for math
- The merged model can do both



Conclusion

- Neural networks include several designs in size and complexity
- They make many difficult applications possible
- The common training method of gradient descent only works in known domains
  - Where the optimal outputs are known
- Neuroevolution allows training neural networks with only fitness information
- Can also be combined with gradient descent to find optimal designs
- Makes impactful applications possible that otherwise would not be.