The Evolution of Machine Learning

Classical AI to Reinforced Learning

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Can a Computer Think?

1. The human brain is a remarkable organ. It has enabled us understand science and advance mankind.
2. The idea of mimicking the human brain or even improving the human cognitive functions is an alluring one and is an objective of Artificial Intelligence research.
3. But we are not even close in-spite of a century of research. However, it continues to have a major hold on our imagination given the potential of the rewards.
4. *The question of whether a computer can think is no more interesting than the question of whether a submarine can swim" - Dijkstra*
5. It is more interesting to understand the evolution of Machine Learning - how did it start, where are we today and where do we go from here.

Symbols & Reasoning

1. About 50,000 years ago, palaeontologists believe that some of us (1,000?), were able to deal with symbols - a major step in evolution.
2. Noam Chomsky thinks we were then able to create a new concept from 2 existing ideas without limiting the existing concepts.
3. Around 350 BC, Aristotle devised syllogistic logic, the first formal deductive reasoning system to model the way humans reason.
4. 2,000 years later, Bertrand Russel & Alfred Whitehead published Principia Mathematica that laid down the foundations for a formal representation of Mathematics.
5. John McCarthy, who championed the cause of mathematical logic in AI, was Aristotle of his day.
6. In 1942, Alan Turing showed that any form of mathematical reasoning could be processed by a machine.
7. By 1967, Marvin Minsky declared that "within a generation, the problem of creating Artificial Intelligence would substantially be solved".

Heuristic Reasoning & Model Backed Systems

1. In 1961, Minsky published "Steps towards Artificial Intelligence" and talked about search, matching, probability, learning. In 1986, Minsky wrote "The Society of Mind" and talked about heuristic programming,
2. McCarthy wanted to use logic to the extreme, Newel wanted to build cognitive models of problem solving and Simon believed that when we see something that is complicated in behavior, it is a consequence of a complex environment rather than because of a complex thinker.
3. Terry Winograd built a model backed system for dialog understanding, Patrick Winston built another model backed system for learning and Gerald Sussman built a model backed system for understanding blocks. And Roger Schank believed that understanding stories is the key to modeling human intelligence.
4. David Marr treated vision as an information processing system. Marr's hypothesis comprised of a computational level - what does the system do algorithmically, how does it do and a physical level - what neural structures and neuronal activities implement the visual system.

Expert Systems

1. In the 1980s, the expert systems were of great interest and focused on knowledge and inference mechanisms. While these systems did a pretty good job in their domains, they were narrow in specialization and were difficult to scale.
2. The field of AI was defined as computers performing tasks that were specifically thought of as something only humans can do. However, once these systems worked, they were no longer considered to be AI! For example, today the best chess players are routinely defeated by computers but chess playing is no longer really considered as AI!
3. McCarthy referred to as the "AI effect". IBM's Watson is a program at a level such as that of a human expert but it is not certainly not the first one.
4. Fifty years ago Jim Slagle's symbolic integration program at MIT was a tremendous achievement.
5. Nevertheless, it is very hard to build a program that has "common sense" and not just narrow domains of knowledge.

Perceptrons

1. Rosenblatt is credited with the concept of Perceptrons, “a machine which senses, recognizes, remembers, and responds like the human mind” as early as in 1957
2. In a critical book written in 1969, Marvin Minsky and Seymour Papert showed that Rosenblatt’s original system was painfully limited, literally blind to some simple logical functions like XOR. In the book they said: "... our intuitive judgment that the extension (to multilayer systems) is sterile".
3. This intuition was incorrect and the field of “Neural Networks” pretty much disappeared!

Neural Network

1. Geoff Hinton built more complex networks of virtual neurons that allowed a new generation of networks to learn more complicated functions (like the exclusive-or that had bedeviled the original Perceptron).
2. Even the new models had serious problems though. They learned slowly and inefficiently and couldn't master even some of the basic things that children do. By the late 1990s, neural networks had again begun to fall out of favor.
3. In 2006, Hinton developed a new technique that he dubbed deep learning, which extends earlier important work by Yann LeCun.
4. Deep learning's important innovation is to have models learn categories incrementally, attempting to nail down lower-level categories (like letters) before attempting to acquire higher-level categories (like words).

Deep Neural Networks

1. Today, at the core is the debate between logic inspired and neural network inspired paradigms for cognition.
2. LeCun, Bengio and Hinton state that succinctly in a review paper in Nature, dated 28th May 2015
   ... *"The issue of representation lies at the heart of the debate between the logic-inspired and the neural-network-inspired paradigms for cognition. In the logic-inspired paradigm, an instance of a symbol is something for which the only property is that it is either identical or non-identical to other symbol instances. It has no internal structure that is relevant to its use; and to reason with symbols, they must be bound to the variables in judiciously chosen rules of inference. By contrast, neural networks just use big activity vectors, big weight matrices and scalar non-linearities to perform the type of fast 'intuitive' inference that underpins effortless commonsense reasoning"*
   ...

Deep Learning

1. Almost everything you hear about artificial intelligence today is thanks to deep learning.
2. This category of algorithms works by using statistics to find patterns in data, and it has proved immensely powerful in mimicking human skills such as our ability to see and hear.
3. To a very narrow extent, it can even emulate our ability to reason. These capabilities power Google's search, Facebook's news feed, and Netflix's recommendation engine.
4. But though deep learning has singlehandedly thrust AI into the public eye, it represents just a small blip in the history of humanity's quest to replicate our own intelligence. It's been at the forefront of that effort for less than 10 years. When you zoom out on the whole history of the field, it's easy to realize that it could soon be on its way out.

arXiv papers

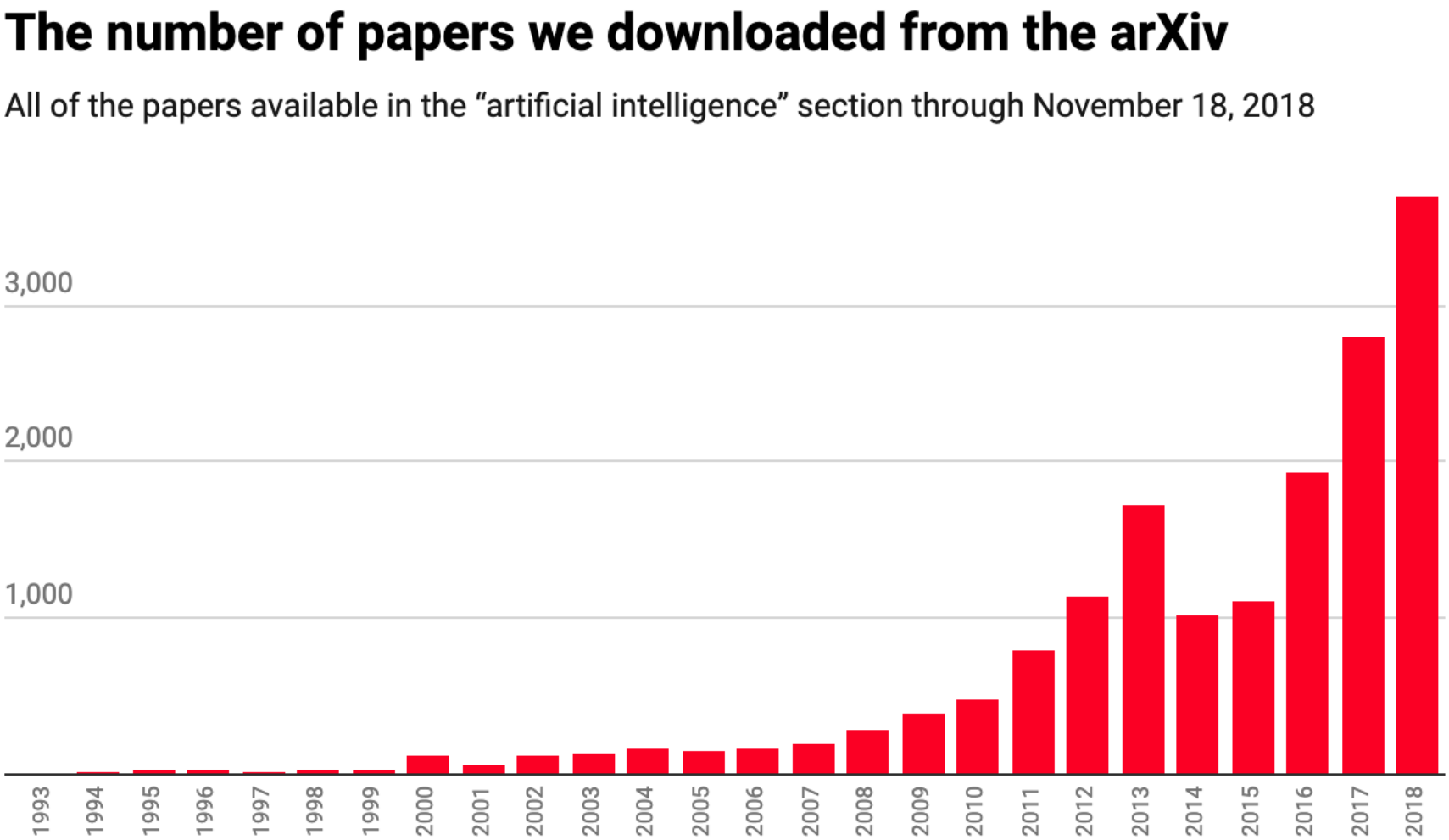


Figure: Number of papers - source Technology Review

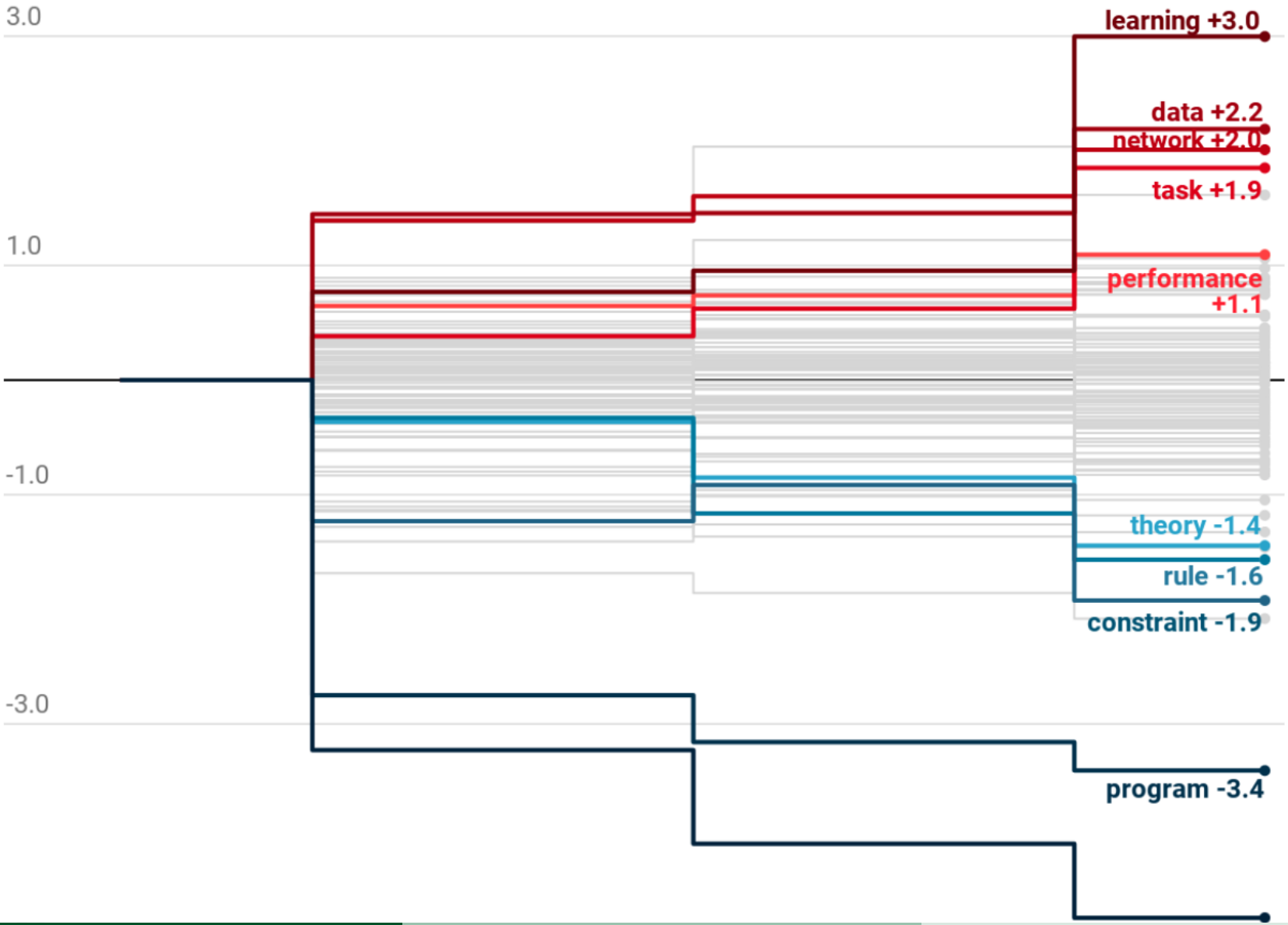
Trend

1. A shift toward machine learning during the late 1990s and early 2000s, a rise in the popularity of neural networks beginning in the early 2010s, and growth in reinforcement learning in the past few years.
2. arXiv's AI section goes back only to 1993, while the term "artificial intelligence" dates to the 1950s, so the database represents just the latest chapters of the field's history.
3. Second, the papers added to the database each year represent a fraction of the work being done in the field at that moment.
4. Nonetheless, the arXiv offers a great resource for gleaning some of the larger research trends and for seeing the push and pull of different ideas.

Paradigm Shift

1. The biggest shift we found was a transition away from knowledge-based systems by the early 2000s. These computer programs are based on the idea that you can use rules to encode all human knowledge. In their place, researchers turned to machine learning - the parent category of algorithms that includes deep learning.
2. Among the top 100 words mentioned, those related to knowledge-based systems - like “logic,” “constraint,” and “rule” - saw the greatest decline.
3. Those related to machine learning - like “data,” “network,” and “performance” - saw the highest growth.

Machine Learning eclipses Knowledge Based Reasoning



Machine Learning eclipses Knowledge Based Reasoning

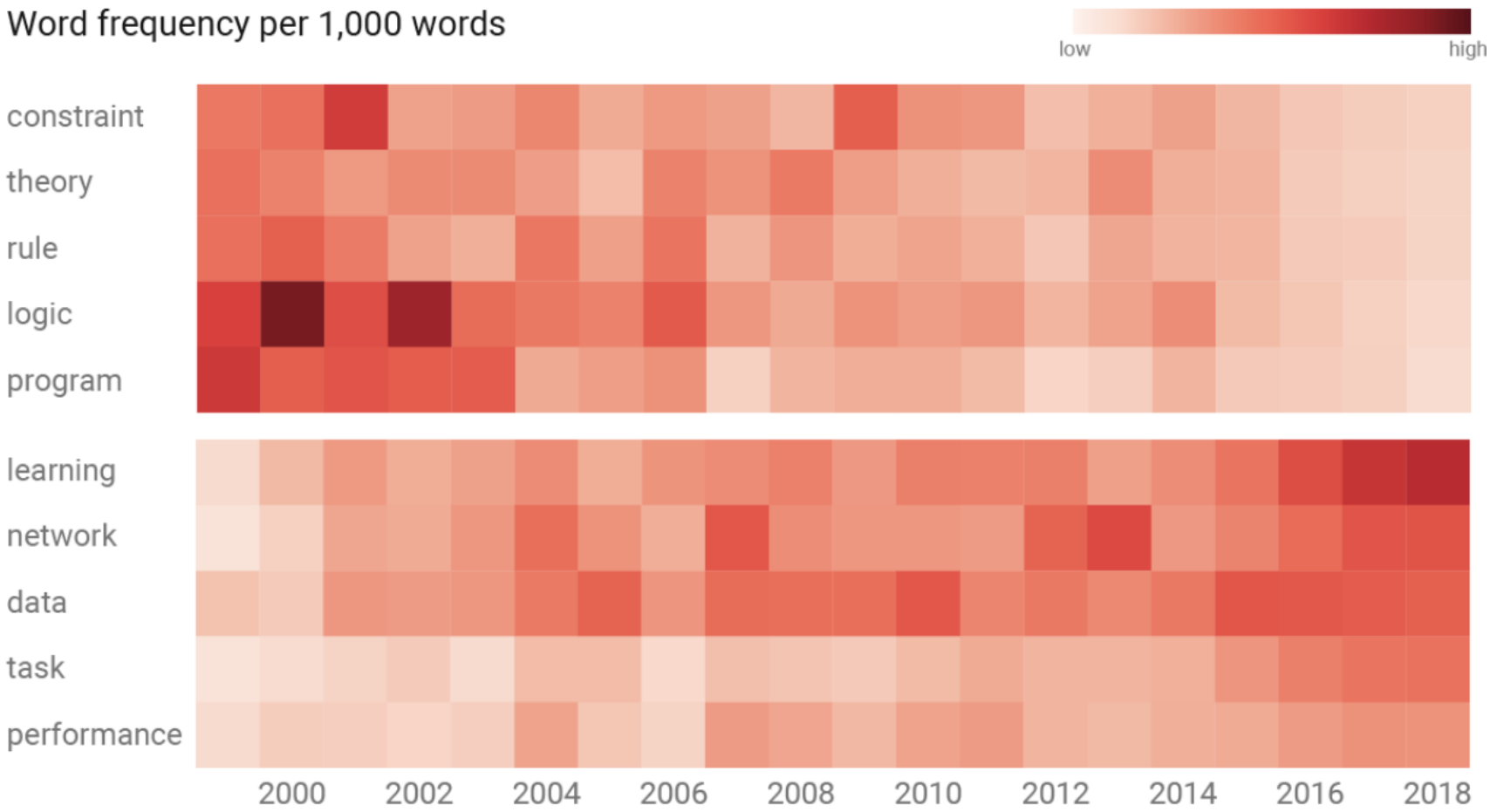


Figure: Word Frequency per 1,000 words - Source MIT Tech Review

The Reason for the Shift

1. In the '80s, knowledge-based systems amassed a popular following thanks to the excitement surrounding ambitious projects that were attempting to re-create common sense within machines.
2. But researchers hit a major problem: there were simply too many rules that needed to be encoded for a system to do anything useful.
3. Instead of requiring people to manually encode hundreds of thousands of rules, the ML approach programs machines to extract those rules automatically from piles of data. The field abandoned KB systems and turned to refining ML.
4. Under the new machine-learning paradigm, the shift to deep learning didn't happen immediately. Instead, as our analysis of key terms shows, researchers tested a variety of methods in addition to neural networks, the core machinery of deep learning.
5. Some of the other popular techniques included Bayesian networks, support vector machines, and evolutionary algorithms, all of which take different approaches to finding patterns in data.

Neural Nets take over ML methods

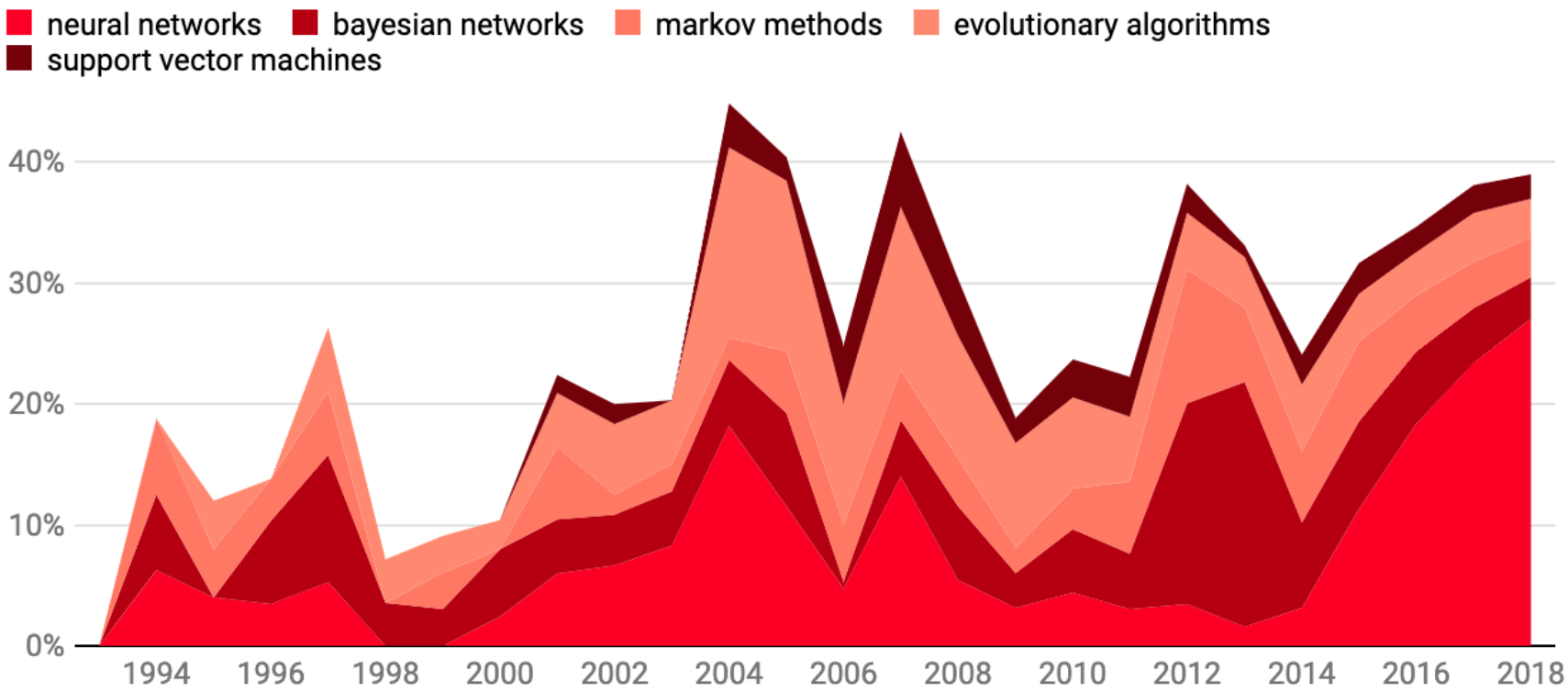


Figure: % of papers that mention each method - Source MIT Tech Review

The period 1990 - 2000

1. Through the 1990s and 2000s, there was steady competition between all of these methods.
2. Then, in 2012, a pivotal breakthrough led to another sea change. During the annual ImageNet competition, intended to spur progress in computer vision, a researcher named Geoffrey Hinton, along with his colleagues at the University of Toronto, achieved the best accuracy in image recognition by an astonishing margin of more than 10%.
3. The technique he used, deep learning, sparked a wave of new research - first within the vision community and then beyond.

The rise of Reinforcement Learning

1. In the few years since the rise of deep learning, a third and final shift has taken place in AI research.
2. In the last few years, however, reinforcement learning, which mimics the process of training animals through punishments and rewards, has seen a rapid uptick of mentions in paper abstracts.
3. The idea isn't new, but for many decades it didn't really work. But, just as with deep learning, one pivotal moment suddenly placed it on the map. That moment came in October 2015, when DeepMind's AlphaGo, trained with reinforcement learning, defeated the world champion in the ancient game of Go.
4. The effect on the research community was immediate!

Reinforcement Learning is gaining momentum

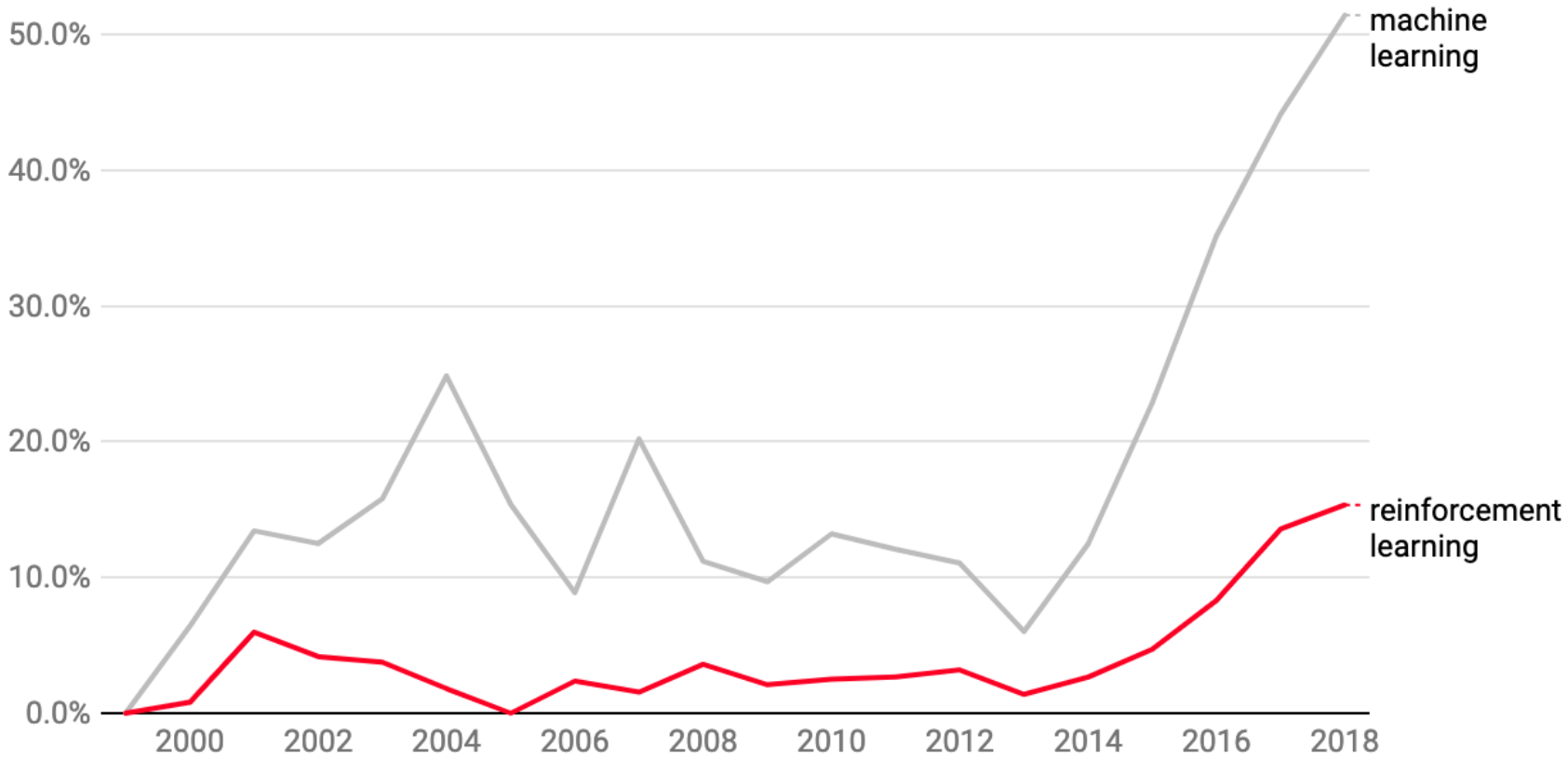


Figure: Share of papers that mention it compared to any type of machine learning - Source MIT Tech Review

The Next Decade

1. The analysis illustrates the fickleness of the quest to duplicate intelligence. "The key thing to realize is that nobody knows how to solve this problem".
2. Many of the techniques used in the last 25 years originated at around the same time, in the 1950s, and have fallen in and out of favor with the challenges and successes of each decade. Neural networks, for example, peaked in the '60s and briefly in the '80s but nearly died before regaining their current popularity through deep learning.
3. Every decade, in other words, has essentially seen the reign of a different technique: neural networks in the late '50s and '60s, various symbolic approaches in the '70s, knowledge-based systems in the '80s, Bayesian networks in the '90s, support vector machines in the '00s, and neural networks again in the '10s.
4. The 2020s should be no different, the era of deep learning may come to an end. The research community has competing ideas — an older technique may regain favor or an entirely new paradigm may emerge.

What is Machine Learning?

1. Machine Learning (ML) is a subset of Artificial Intelligence (AI).
2. In 1959, Arthur Samuel, one of the pioneers of machine learning, defined machine learning as a *"field of study that gives computers the ability to learn without being explicitly programmed".*
3. Machine Learning algorithms discover hidden patterns in data and make predictions about future data.
4. In mathematical terms, machine learning algorithms establishes a function, i.e., a relationship, between input X to output Y. In machine learning, a feature is an individual measurable attribute of a phenomenon that is being observed.
5. This means given training examples (X_i, Y_i) where X_i is the feature vector and Y_i the target variable, learn a function F to best fit the training data, i.e., $Y_i \approx F(X_i)$ for all i. For a new sample X with unknown Y, predict Y using $F(X)$.

The Model

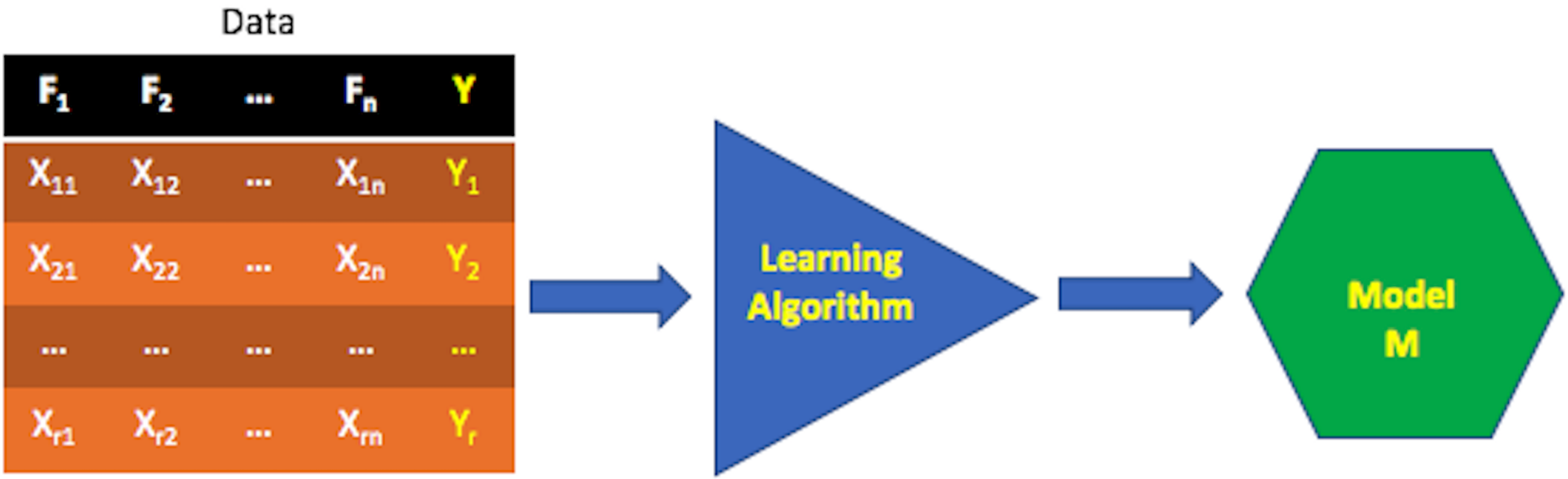


Figure: Model

Why Machine Learning?

1. For complex tasks where deterministic solution don't suffice, e.g., speech recognition, handwriting recognition, etc. Other examples include repetitive tasks needing human-like expertise such as recommendations, spam and fraud detection, personalization which cannot be solved manually in a large scale.

Types of Machine Learning

1. ML algorithms are classified as Supervised or Unsupervised depending on how it has been trained.
2. In supervised learning, the machine learns from data that has already been tagged with the correct answer by an expert. This data is typically termed as the training data or training set. Thereafter, when the machine is provided with a new set of data, it generates the answer based on its learning. The majority of practical machine learning uses supervised learning. An example of supervised learning is separating spam from legitimate email.
3. In unsupervised learning, the machine groups unsorted information according to similarities, patterns and differences without any prior training of data. The machine automatically figures out the patterns on its own. An example of unsupervised learning is playing the game of GO.

Definitions

Features are vectors and are represented as X. X_i represents the data corresponding to the ith data set and n is the number of features.

$$X_i = [x_{i1}\ x_{i2}\ x_{i3}\ \cdots\ x_{in}] \tag{1}$$

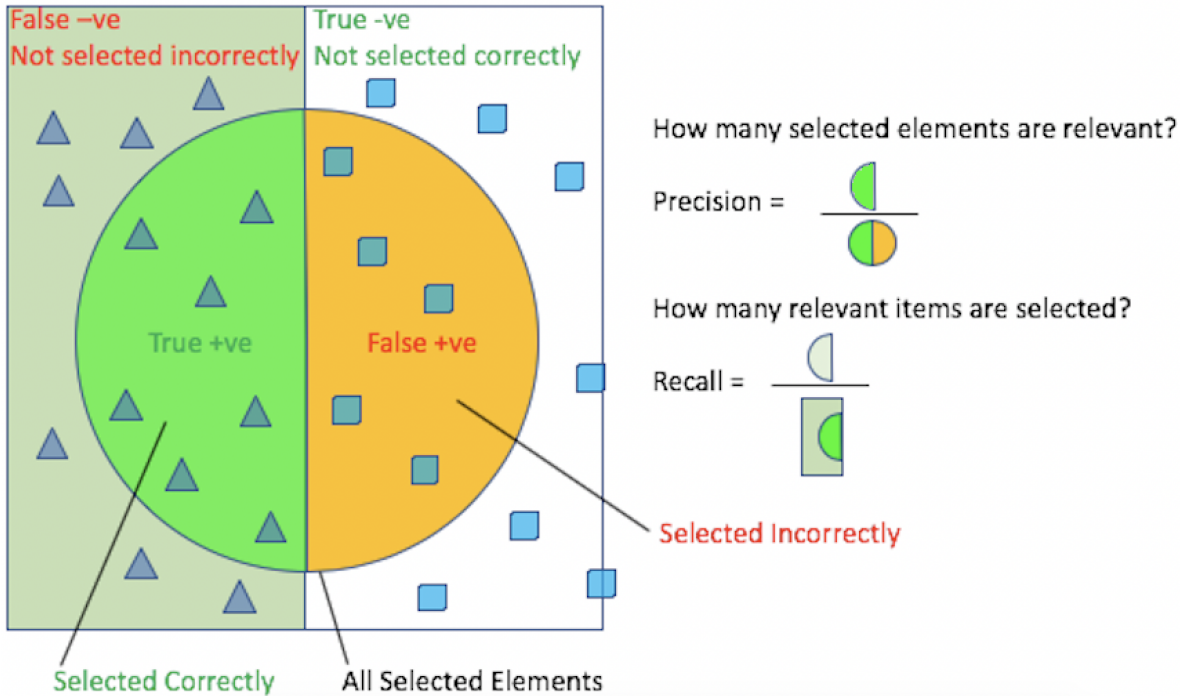


Figure: Precision & Recall

Definitions

$$Precision = \frac{t_p}{t_p + f_p} \tag{2}$$

$$Recall = \frac{t_p}{t_p + f_n} \tag{3}$$

$$Accuracy = \frac{t_p + t_n}{t_p + t_n + f_p + f_n} \tag{4}$$

F_1 is the harmonic mean of precision and recall and is given by:

$$F_1 = \frac{1}{2} \times \left(\frac{1}{Precision} + \frac{1}{Recall} \right) \tag{5}$$

Linear Regression

1. In machine learning, we often use Regression to establish a model. Regression is a measure of the relation between the mean value of one variable (e.g. output) and corresponding values of other variables. In machine learning, we use regression to determine the relation between X_i and Y_i.
2. A common function used to model training data is a linear regression model. The model is linear, i.e., the relationship does not involve any quadratic or other higher order terms. The model or the hypothesis is given by:

$$y_i = \theta_0 + \theta_1 x_{i1} + \theta_2 x_{i2} \cdots + \theta_n x_{in} \tag{6}$$

where x_{ij} is the observed value of the feature x_j, y_i is the predicted value of the outcome and θ_i are constants the values of which need to be determined. For now, we limit the the values of the features x_{ij} to numbers, positive or negative. Later on, we will study techniques on how to deal with the situation where the feature value is a string.

Linear Regression with Gradient Descent

In the previous chapter, we introduced linear regression and the squared error loss function.

$$y_i = \theta_0 + \theta_1 x_{i1} + \theta_2 x_{i2} \cdots + \theta_n x_{in} \tag{7}$$

$$\text{Squared Error Loss (L)} = \frac{1}{2} \times \sum_{i=1}^{r} (\hat{y}_i - y_i)^2 \tag{8}$$

Notice that the loss function is always positive, there is a minimum and is monotonically increasing from that minimum value in both positive and negative directions along the x-axis. Such a function is called a convex function.

Loss Function

Our objective is to find a good model that fits the training data. For that, we need to minimize some loss function over the training data D. Sometimes the word cost function is used in lieu of loss function. The total loss L corresponding to r set of data is given by:

$$L = Squared\ Error\ Loss = \frac{1}{2} \times \sum_{i=1}^{r} (\hat{y}_i - y_i)^2 \tag{9}$$

where $\hat{y}_i$ is the observed value of the ith outcome and n is the number of features. The factor $1/2$ is introduced to make subsequent computations simpler as will see in the next chapter. Note that the square of each error is considered so that positive and negative errors do not cancel out.

Gradient Descent

Mathematically, A convex function is a continuous function whose value at the midpoint of every interval in its domain does not exceed the arithmetic mean of its values at the ends of the interval.

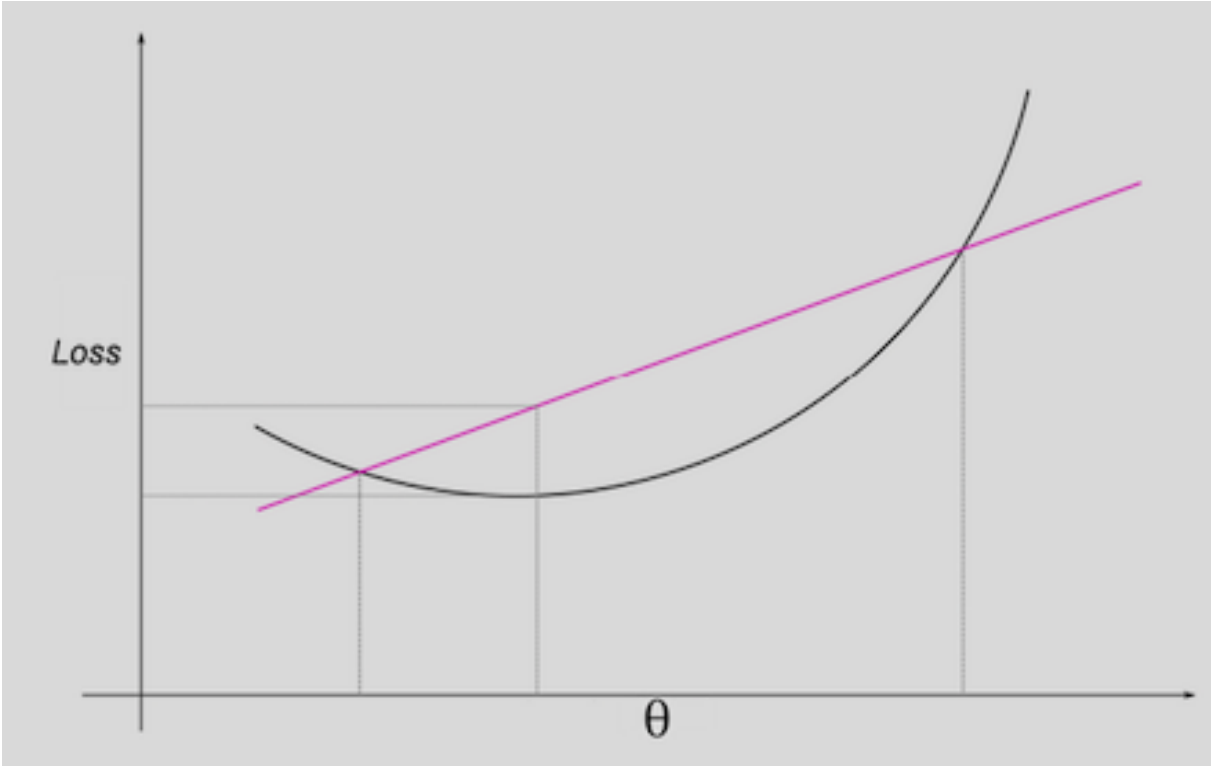


Figure: Convex Function

Gradient Descent

1. Such a loss function can be minimized by setting the partial derivative of the loss with respect to θ_j to zero. Using the chain rule in calculus, we have:

$$\frac{\partial L}{\partial \theta_0} = \sum_{i=1}^{r} (\hat{y}_i - y_i) = 0 \tag{10}$$

$$\frac{\partial L}{\partial \theta_j} = \sum_{i=1}^{r} (\hat{y}_i - y_i)\, x_{ij} = 0 \tag{11}$$

   Notice that the factor $1/2$ disappears. We will use these equations for determining θ_j.
2. We begin by randomly assigning values to θ_j. For a convex function it does not matter what the initial weights are as it will always converge to their correct values. Notice that in the above equations, $\hat{y}$ and x_{ij} are observed and y_i is computed. This means the slope of the loss function can be readily computed.

Gradient Descent

Now for a given θ_j, and keeping all other θ_i where $i \neq j$ constant, we change the value of θ_j slightly and compute a new value of θ_j

$$\triangle\theta_j = \alpha\theta_j$$
$$\theta_j^{'} = \theta_j + \triangle\theta_j$$

where α is small constant and is called the learning rate. Since the slope of $\frac{\partial L}{\partial \theta_j}$ is already calculated from the previous equations, we can compute the new value of the loss as follows:

$$L^{'} = L - \frac{\partial L}{\partial \theta_j}(\alpha\theta_j)$$

If $L^{'} < L$, we continue incrementing θ_j as long as the loss continues to decrease. When the direction changes and the loss increases, we have found the θ_j for which the loss is minimum. If $L^{'} > L$, we travel in the reverse direction and follow the same process. Like this, we compute the value of each and every θ_j.

Stochastic versus Batch Gradient Descent

1. The word stochastic means a system or a process that is linked with a random probability. In SGD, a single sample data is used to compute the θ_j. The sample is randomly shuffled and selected for performing the iteration.
2. In batch gradient descent, the the gradient is calculated from the whole training set and hence the word "batch". If we have a huge dataset with millions of data points, running the batch gradient descent can be quite costly since we need to reevaluate the whole training dataset each time we take one step towards the global minimum.

Stochastic versus Batch Gradient Descent

1. A compromise between computing the true gradient for the entire batch and the gradient at a single example is to compute the gradient for a mini batch at each step.
2. This can perform significantly better than stochastic gradient descent because the code can make use of vectorization libraries rather than computing each step separately.
3. It may also result in smoother convergence, as the gradient computed at each step uses more training examples. It is the algorithm of choice for neural networks with the batch sizes are usually between 50 and 256. Mini Batch Gradient Descent runs much faster than the Batch Gradient Descent.
4. In Batch Gradient Descent, the Batch Size refers to the total number of training examples present in a single batch and Epoch means that each sample in the training dataset has had an opportunity to update all the model parameters θ_j.

Momentum Method

Optimizing techniques such as the momentum method helps accelerate gradients vectors in the right directions for faster convergence. Instead of using only the gradient of the current step also accumulates the gradient of the past steps. Update terms:

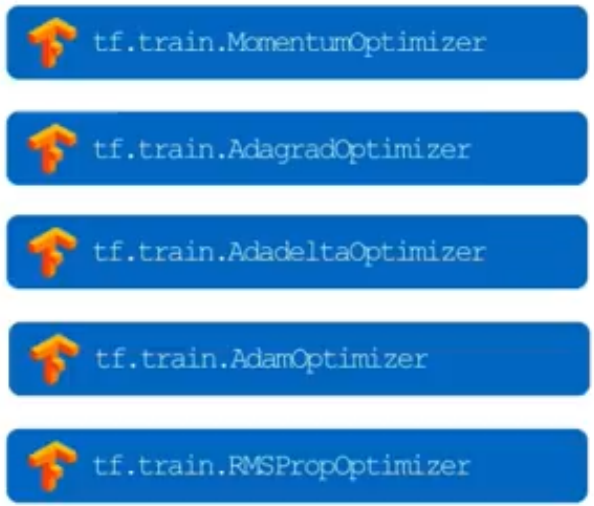
$$\begin{aligned} \text{update}_t &= \gamma \times \text{update}_{t-1} + \eta \nabla L \\ L_{t+1} &= L_t - \gamma \times \text{update}_t \end{aligned}$$

$$\begin{aligned} \text{update}_0 &= 0 \\ \text{update}_1 &= \gamma \times \text{update}_0 + \eta \nabla L_1 = \eta \nabla L_1 \\ \text{update}_2 &= \gamma \times \text{update}_1 + \eta \nabla L_2 = \gamma \eta \nabla L_1 + \eta \nabla L_2 \end{aligned}$$

where γ is slightly less than 1. This implies that we have the maximum faith in the latest gradient and an exponentially decaying faith in the previous gradients.

Adaptive Learning Rate Algorithms

- Momentum
- Adagrad
- Adadelta
- Adam
- RMSProp



Qian et al. "On the momentum term in gradient descent learning algorithms." 1999.

Duchi et al. "Adaptive Subgradient Methods for Online Learning and Stochastic Optimization." 2011.

Zeiler et al. "ADADELTA: An Adaptive Learning Rate Method." 2012.

Kingma et al. "Adam: A Method for Stochastic Optimization." 2014.

Figure: Common Learning Rate Algorithms

Logistic Regression

In many cases the value of y_i need to be bounded between 0 and 1. In such cases, we use the logistic regression model as given below:

$$y_i = \frac{1}{1 + e^{-z}} \tag{12}$$

where z is given by:

$$z_i = \theta_0 + \theta_1 x_1 + \theta_2 x_2 \cdots + \theta_n x_n \tag{13}$$

Equation 7 is known as sigmoid. Note that:

- for z is large +ve number, $\frac{1}{e^z} = 0$; $y_i = 1$
- for z $= 0$, $y_i = 0.5$
- for z is large -ve number, $y_i = 0$

Hence, the value of y_i is bounded between 0 and 1 for z between -∞ and ∞.

Sigmoid

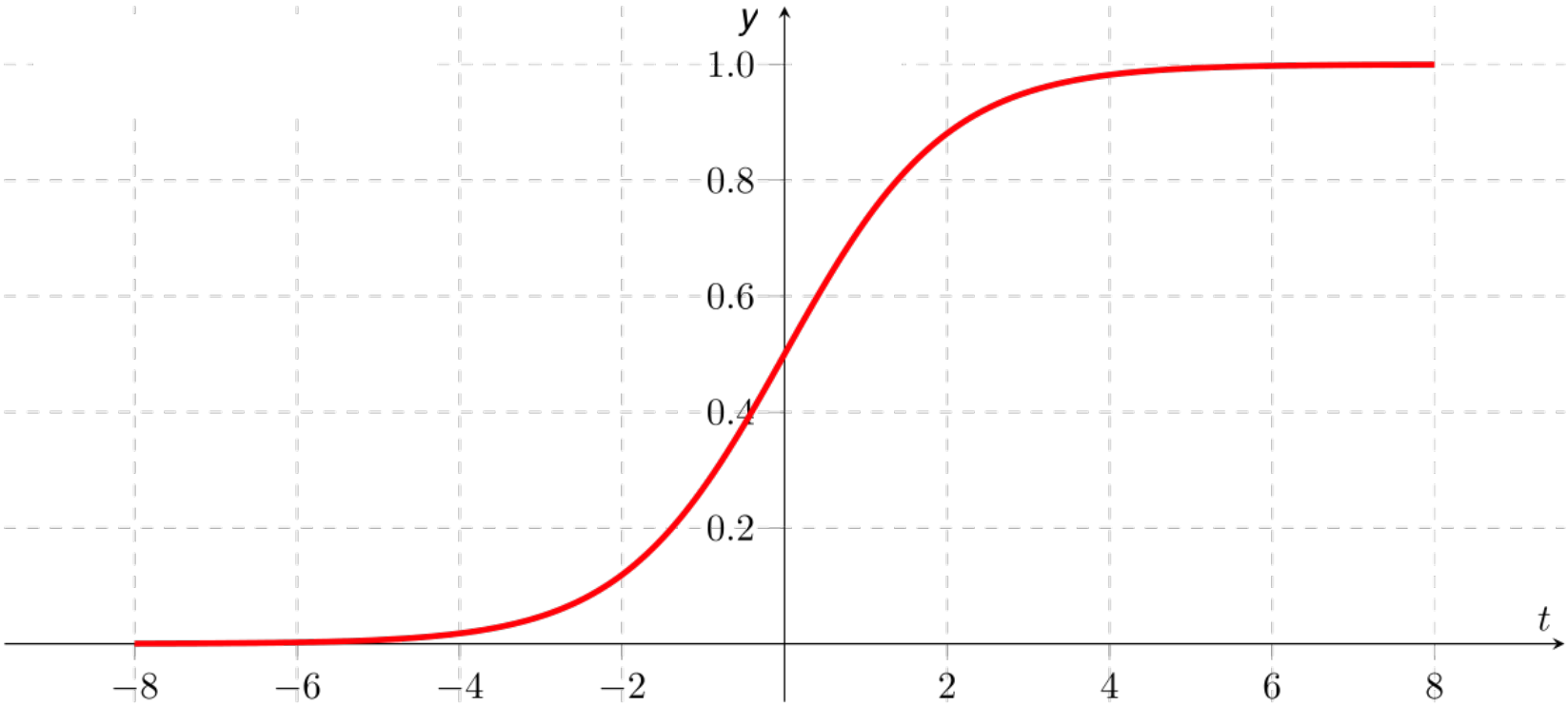


Figure: Sigmoid Curve

Logistic Regression

Logistic regression is modeled as follows:

$$P(y|x,\theta) = \begin{cases} h_\theta(x) & \text{if y} = 1 \\ (1 - h_\theta(x)) & \text{if y} = 0 \end{cases} \tag{14}$$

The above function can be written compactly as follows:

$$P(y|x,\theta) = (h_\theta(x))^y (1 - h_\theta(x))^{1-y} \tag{15}$$

Assuming that the r training examples were generated independently, we can then write down the likelihood L of the parameters as:

$$L(\theta) = p(\vec{y}|x,\theta) = \prod_{i=1}^{r} P(y^{(i)}|x^{(i)},\theta)$$

$$\boxed{L(\theta) = \prod_{i=1}^{r} (h_\theta(x^{(i)}))^{y^{(i)}} (1 - h_\theta(x^{(i)}))^{1-y^{(i)}}}$$

Log Likelihood

The log likelihood is given by:

$$l(\theta) = log\, L(\theta) = \prod_{i=1}^{r} y^{(i)} log(h(x^{(i)}) + (1 - y^{(i)}) log(1 - h(x^{(i)})) \quad (16)$$

Intuitively, we want to assign more punishment when the prediction is 1 while the actual is 0 and similarly when the prediction is 0 while the actual is 1. The loss function in logistic regression is doing exactly this and hence is called Logistic Loss.

The sigmoid function has an interesting property. It's derivative is given by:

$$g^{'}(x) = \frac{d}{dx}\left(\frac{1}{1+e^{-x}}\right) = \frac{e^{-x}}{(1+e^{-x})^2} = \frac{1}{1+e^{-x}} \times \left(1 - \frac{1}{1+e^{-x}}\right)$$
$$= \boxed{g(x)(1-g(x))} \quad (17)$$

Log Likelihood

Now, consider just one training example (x,y), and take derivatives to derive the stochastic gradient ascent rule:

$$\begin{aligned}\frac{\partial(l(\theta))}{\partial\theta_j} &= y\frac{1}{g(\theta^T x))} - (1-y)\frac{1}{1-g(\theta^T x)}\frac{\partial}{\partial\theta_j}g(\theta^T x) \\ &= y\frac{1}{g(\theta^T x))} - (1-y)\frac{1}{1-g(\theta^T x)}g(\theta^T x)(1-g(\theta^T x))x_j \\ &= y(1-g(\theta_T x) - (1-y)g(\theta^T x)x_j \\ &= y - h_\theta(x)x_j\end{aligned}$$

With the above equation, we are now in a position to compute the gradient and follow the same steps to determine θ_j corresponding to minimum loss as in the case of linear regression.

Predictions

1. Our objective is to find a set of θ_j in 6 and 13 such that the loss is minimum. But before we do that, let us first understand the nature of potential errors.
2. Predictions from the model, i.e., the hypothesis will have differences or errors.The following diagram that depicts a correct fit.

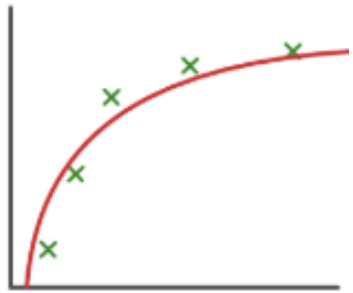


Figure: Correct Fit

Errors

1. Overfitting occurs when the model fits the training data well but does not generalize well to unseen data. In linear regression, overfitting will occur when an excessive number of features are used than required.

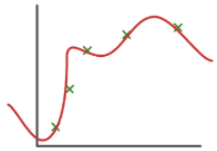


Figure: Overfit

2. Underfitting occurs when the model is simplistic and lacks expressive power to capture the entire phenomenon. The model fits the training data well but does not generalize well to unseen data. In linear regression, underfitting will occur when an insufficient number of features are used than required.

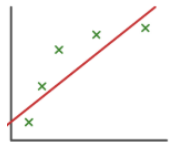


Figure: Underfit

Regularization

1. Regularization is a technique used to avoid problem of overfitting. It prevents overfitting in linear models by a penalty term that penalizes large weight values.
2. A regression model that uses L1 regularization (or L1 Norm) technique is called Lasso Regression and model that uses L2 regularization (or L2 Norm) is called Ridge Regression.
3. The key difference between these two is the penalty term.

Regularization - Lasso & Ridge

1. Lasso Regression (Least Absolute Shrinkage and Selection Operator) adds the absolute value of magnitude of coefficient as a penalty term to the loss function. Here the highlighted part represents L1 regularization element where λ is a constant.

$$L + \boxed{\lambda \sum_{j=1}^{n} |\theta_j|} \tag{18}$$

2. Ridge regression adds the squared magnitude of coefficient as a penalty term to the loss function. Here the highlighted part represents L2 regularization element.

$$L + \boxed{\lambda \sum_{j=1}^{n} \theta_j^2} \tag{19}$$

Regularization

1. Note that if λ is zero, the loss is the same as the squared error. The key difference between these techniques is that Lasso shrinks the less important feature's coefficient to zero thus removing some features altogether. Hence, this works well for feature selection where we have a large number of features.
2. Mathematically, L1 regularization produces sparse coefficients while L2 regularization produces non-sparse coefficients.
3. However, the L1-norm does not have an analytical solution, whereas the L2-norm does. This allows the L2-norm solutions to be computed efficiently.

Bias & Variance

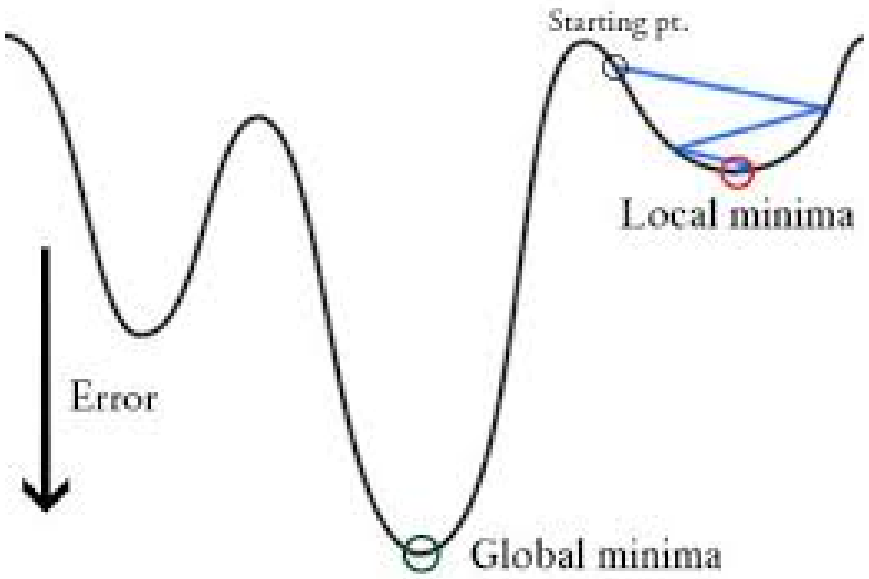
1. For a given model, bias is the difference between average model prediction and the true target value and variance is the variation in predictions across different training data samples.
2. Simple models with small number of features have high bias and low variance whereas complex models with large number of features have low bias and high variance.
3. We reduce bias by increasing model complexity, i.e., by adding more features and decreasing regularization.
4. We reduce variance by increasing training data and decreasing model complexity, i.e., by better feature selection and aggressive regularization.

Logistic Regression

In the previous chapter, we used a sigmoid function to model logistic regression as shown below:

$$h_\theta(x) = \frac{1}{1 + e^{-\theta^T X}} \tag{20}$$

For logistic regression, Least Squared Error will result in a *non-convex* graph with local minimums and hence is not feasible.



SoftMax

1. In the training data the values corresponding to the features x_j can have numerical values of different magnitudes. For example, one feature may have values ranging between $0 \ldots 10$, while another feature may have values ranging between $10,000 \cdots 100,000$. Some of these values can also be negative and the components will obviously not add up to 1.
2. The softmax function is a function that takes as input a vector of K real numbers, and normalizes it into a probability distribution consisting of K probabilities in the interval 0...1 with the components adding up to 1.

$$\sigma(z)_i = \frac{e_i^z}{\sum_{j=1}^{K} e^{z_j}} \tag{21}$$

The feature values are normalized with the softmax function prior to inputing in a regression model.

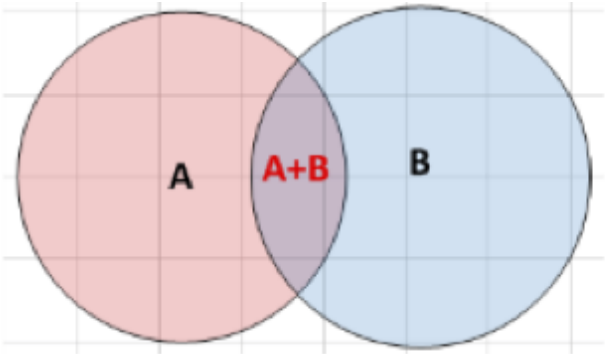
One Hot Encoding

1. In the linear regression and the logistic regression models that we studied so far can only deal with numerical data. It cannot handle features that have text as values. In one-hot encoding, the string encoded variable is replaced with new variables of boolean type. For example, a particular feature, say color, can have "red", "green" and "blue" as possible values. This feature color, will be replaced by 3 features, red, blue and green which hold the values 1 or 0. We can then encode color, in terms of red, blue and green as follows:

red	green	blue
1	0	0
0	1	0
0	0	1

Note that if the boolean value of the feature is 1, it must be 0 for all the other features

Conditional Probability



$$\mathbf{P(A|B)} = \frac{\boldsymbol{P}(\mathbf{A} \cap \boldsymbol{B})}{\boldsymbol{P}(\mathrm{B})}$$

Figure: Naive Bayes

$$P(A|B) \times P(B) = P(B|A) \times P(A)$$

$$\boxed{P(A|B) = P(B|A) \times \frac{P(A)}{P(B)}} \tag{22}$$

$$\boxed{P(B|A) = P(A|B) \times \frac{P(B)}{P(A)}}$$

Naive Bayes

Day	Outlook	Temperature	Humidity	Wind	Play Tennis
1	Sunny	Hot	High	Weak	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Weak	Yes
4	Rain	Mild	High	Weak	Yes
5	Rain	Cool	Normal	Weak	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Weak	No
9	Sunny	Cool	Normal	Weak	Yes
10	Rain	Mild	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Weak	Yes
14	Rain	Mild	High	Strong	No

Naive Bayes

$$
\begin{aligned}
P(Play = Yes) &= 9/14 \\
P(Play = No) &= 5/14 \\
P(Outlook = Sunny \mid Play = Yes) &= 2/9 \\
P(Temperature = Cool \mid Play = Yes) &= 3/9 \\
P(Humidity = High \mid Play = Yes) &= 3/9 \\
P(Wind = Strong \mid Play = Yes) &= 3/9
\end{aligned}
$$

$$
\begin{aligned}
P(Outlook = Sunny \mid Play = No) &= 3/5 \\
P(Temperature = Cool \mid Play = No) &= 1/5 \\
P(Humidity = High \mid Play = No) &= 4/5 \\
P(Wind = Strong \mid Play = No) &= 3/5
\end{aligned}
$$

Naive Bayes

Given, X = (Outlook=Sunny, Temperature=Cool, Humidity=High, Wind=Strong), do we play? Yes or No?

$$P(Yes \mid X) = P(Sunny \mid Yes) \times P(Cool \mid Yes) \times P(High \mid Yes) \times P(Strong \mid Yes) \times P(Play = Yes) = 0.0053$$

$$P(No \mid x) = P(Sunny \mid No) \times P(Cool \mid No) \times P(High \mid No) \times P(Strong \mid No) \times P(Play = No) = 0.0206$$

Since $P(Yes \mid X) < P(No \mid X)$, we label X to be No.

Latent Dirichlet Allocation (LDA)

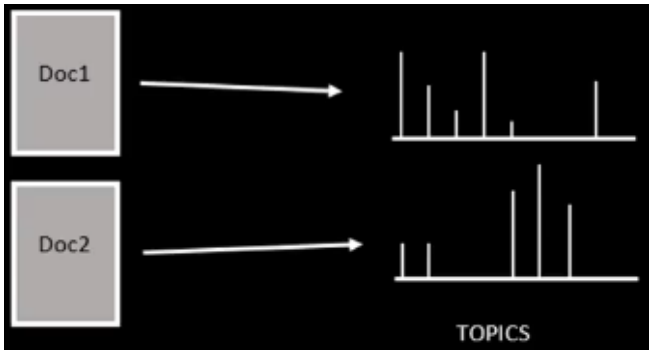


Figure: Topic Distribution

1. LDA is an unsupervised machine learning algorithm. LDA uses a generative process that treats a document as bag of words and learns the topics in the document.
2. The words are observable and the topics in the document are hidden and hence the term latent.
3. We are directly observing the words and not the topics, so the topics themselves are latent variables (along with the distributions themselves). Documents are probability distribution over latent topics and topics are probability distribution over words.

Latent Dirichlet Allocation (LDA)

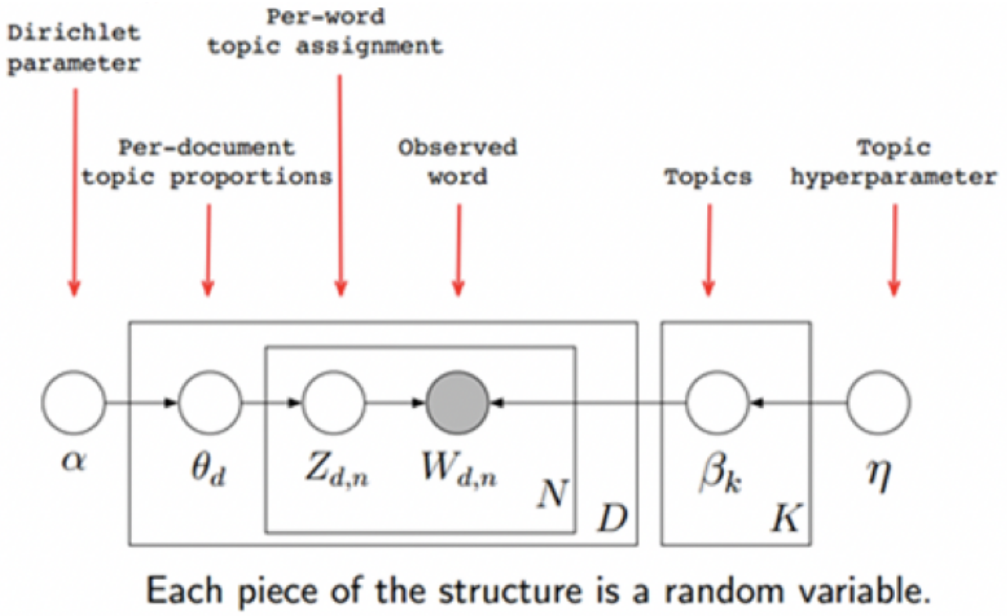


Figure: Plate Notation

The plate notation is a concise way of visually representing the dependencies among the model parameters. α is the parameter in the Dirichlet prior on the per document distribution. A high α implies that a document is likely to contain most of the topics. β is the parameter in the Dirichlet prior on the per topic word distribution. A high β implies that a topic is likely to contain most of the words.

LDA

1. w represents a word
2. W represents a document (a vector of words); $w = w_1, w_2, \cdots w_N$
3. α is the parameter of the Dirichlet distribution;

$$\alpha = (\alpha_1, \alpha_2, \cdots \alpha_n)$$

4. θ is per document topic proportions
5. Z is a vector of topics, where if the i th element of z is 1 then w draws from the i th topic D is the total set of documents
6. LDA assumes that new documents are generated by choosing a topic mixture for the document, (eg., 20% topic-1, 30%, topic-2 and 50% topic-3)) and generate words by first pick a topic based on the documnent's multinomial distribution and then pick a word based on the topics topic's multinomial distribution.

LDA Steps

1. The first step is to decide that there are k topics.
2. Next, from a given document, assign each word to of the k topics randomly.
3. Assume that all topic assignments except for the current word are correct. Calculate two ratios.
   - Proportion of words in the document d that are currently assigned to topic t.
   - Proportion of assignments to topic t over all documents that come from this word.
   - Assign the current word to the topic for which the probability p is maximum.

We continue repeating this process of re-assigning words until we reach a steady state. Mathematically, the LDA is expressed as follows:

$$\boxed{p(\theta, z|w, \alpha, \beta) \propto p(\theta, z, w|\alpha, \beta) = p(w|z, \beta)p(z|\theta)p(\theta|\alpha)} \quad (23)$$

Now, given a new document, how do we determine what topics does it consist of? We can score potential topics using the cross-entropy, i.e., KL

Information & Uncertainty

1. In Clause Shannon's information theory, one bit of information reduces the uncertainty by 2. Similarly, if 3 bits of information are sent, then the reduction in uncertainly by 2^3, i.e., 8. This is intuitive. With 3 bits, there could be 8 possible values and so if a particular set of bits are transmitted, 8 possibilities are eliminated with 1 certainty.
2. Information Content When the information is probabilistic, the self-information I_x, or Information Content of *measuring a random variable X as outcome x is defined as:*

$$I_x = log\left(\frac{1}{p(x)}\right) = -log(p(x)) \tag{24}$$

where $p(x)$ is probability mass function.
3. Shannon Entropy of the random variable X is defined as:

$$H(X) = \sum_x -p(x)log(p(x)) = E(I_x) \tag{25}$$

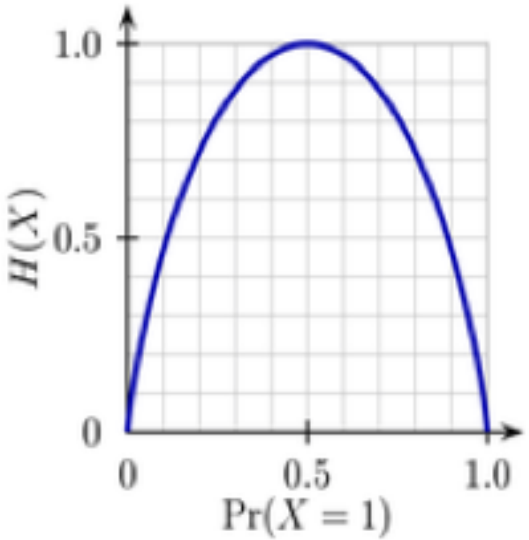
It is the *expected information content* of the measurement of X.

Example

1. Suppose S has 25 examples, 15 positive and 10 negatives [15+, 10-]. Then the entropy of S relative to this classification is computed as:

$$E(S) = -(15/25)log_2(15/25) - (10/25)log_2(10/25) = 0.67$$

In a 2 class system, The entropy is 0 if the outcome is *certain*. The entropy is maximum if we have no knowledge of the system, i.e., whemn any outcome is equally possible.



Cross Entropy - Kullback–Leibler (KL) divegence

1. Cross-Entropy is defined as:

$$H(p, q) = -\sum_i p(i) log_2 q(i) \tag{26}$$

where p is the true distribution and q is the predicted distribution. If the predictions are perfect, then the cross-entropy is same as the entropy. If the prediction differs, then there is a divergence which is known as *Kullback–Leibler (KL) divergence*. Hence,

$$Cross\ Entropy = Entropy + KL\ Divergence$$

or,

$$KL\ Divergence = H(p, q) - H(p)$$

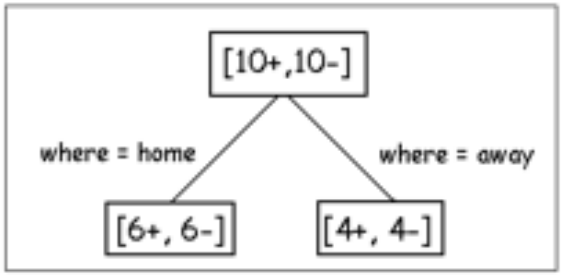
Hence, if the predicted distribution is closer to true distribution when KL divergence is low.

Decision Tree

1. Decision Tree is a supervised machine learning algorithm. In decision trees, the goal is to tidy the data. You try to separate your data and group the samples together in the classes they belong to. You know their label since you construct the trees from the training set. You maximize the purity of the groups as much as possible each time you create a new node of the tree (meaning you cut your set in two). Of course, at the end of the tree, you want to have a clear answer.
2. At each step, each branching, you want to decrease the entropy, so this quantity is computed before the cut and after the cut. If it decreases, the split is validated and we can proceed to the next step, otherwise, we must try to split with another feature or stop this branch.
3. Before and after the decision, the sets are different and have different sizes. Still, entropy can be compared between these sets, using a weighted sum.

Example

Consider the following table for win/loss of soccer games at home and away.



The entropy is:

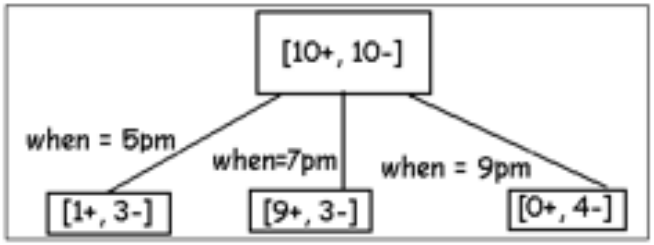
$$H\left(\frac{6}{12},\frac{6}{12}\right) = -\frac{6}{12}log_2\left(\frac{6}{12}\right) - \frac{6}{12}log_2\left(\frac{6}{12}\right) = 0.69$$

$$H\left(\frac{4}{8},\frac{4}{8}\right) = -\frac{4}{8}log_2\left(\frac{4}{8}\right) - \frac{4}{8}log_2\left(\frac{4}{8}\right) = 0.69$$

$$H = -\frac{12}{20} \times H\left(\frac{6}{12},\frac{6}{12}\right) - \frac{8}{20}H\left(\frac{4}{8},\frac{4}{8}\right) = 0.69$$

Example

Partitioning by when, we have:



$$H(5pm) = H\left(\frac{1}{4}, \frac{3}{4}\right) = -\frac{1}{4}log_2\left(\frac{1}{4}\right) - \frac{3}{4}log_2\left(\frac{3}{4}\right) = 0.56$$

$$H(7pm) = H\left(\frac{9}{12}, \frac{3}{12}\right) = -\frac{9}{12}log_2\left(\frac{9}{12}\right) - \frac{3}{12}log_2\left(\frac{3}{12}\right) = 0.56$$

$$H(9pm) = H\left(\frac{0}{4}, \frac{4}{4}\right) = -\frac{0}{4}log_2\left(\frac{0}{4}\right) - \frac{4}{4}log_2\left(\frac{4}{4}\right) = 0.00$$

Entropy after partition is:

$$H = -\frac{4}{20}H\left(\frac{1}{4}, \frac{3}{4}\right) - \frac{12}{20}H\left(\frac{12}{20}, \frac{3}{4}\right) - \frac{4}{20}H\left(\frac{4}{20}, \frac{3}{4}\right) = 0.45$$

Hence, the Information gain is 0.69 - 0.45 = 0.24.

Decision Trees

1. We can apply the same approach for other columns to find the most dominant factor on decision. This way we construct the decision tree that has the least entropy.
2. Decision trees can generate understandable rules and classify without much computation. It can handle both continuous and categorical variables. Also, it provides a clear indication of which fields are most important for prediction or classification.
3. However, it is not suitable for prediction of continuous attributes. It performs poorly with many class and small data. It is computationally expensive to train.

Random Forest

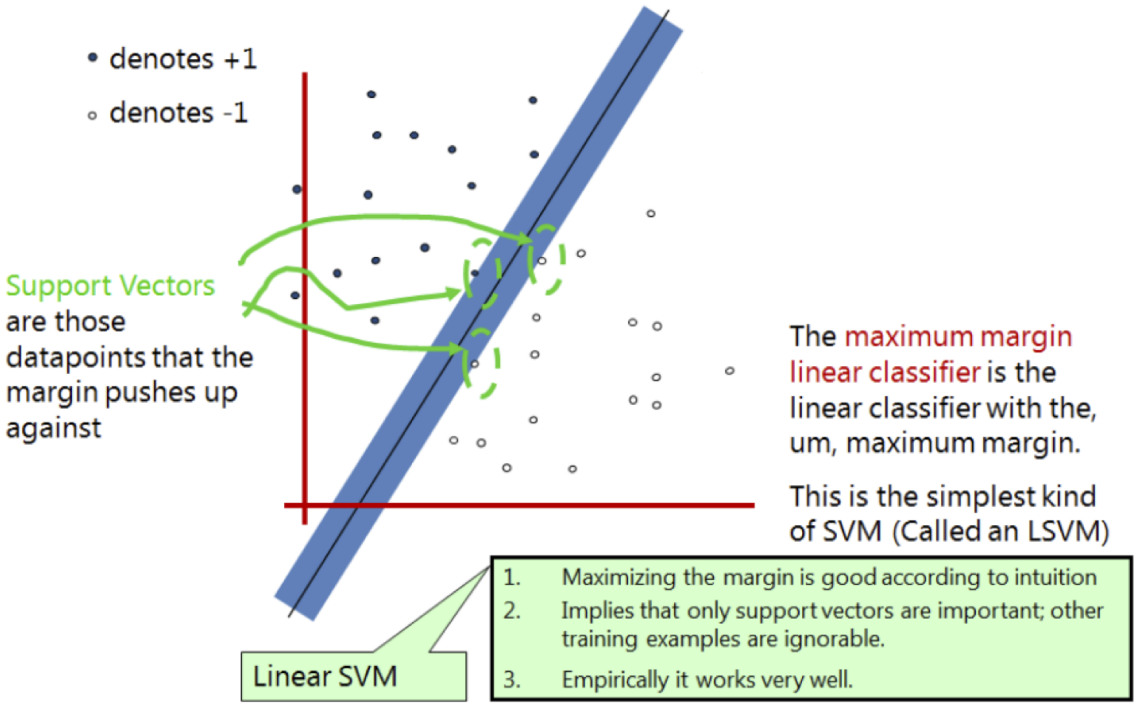
1. Random forest builds multiple decision trees and merges them together to get a more accurate and stable prediction. The fundamental idea behind a random forest is to combine many decision trees into a single model. Individually, predictions made by decision trees (or humans) may not be accurate, but combined together, the predictions will be closer to the mark on average.
2. Why the name 'random forest?' Well, much as people might rely on different sources to make a prediction, each decision tree in the forest considers a random subset of features when forming questions and only has access to a random set of the training data points.
3. This increases diversity in the forest leading to more robust overall predictions and the name 'random forest.' When it comes time to make a prediction, the random forest takes an average of all the individual decision tree estimates. (This is the case for a regression task, such as our problem where we are predicting a continuous value of temperature.

Clustering

1. Create the first K initial clusters from the dataset by choosing K rows of data randomly from the dataset.
2. Each record is assigned to the nearest cluster (the cluster which it is most similar to) using a measure of distance or similarity.
3. Re-calculate the arithmetic mean for each cluster.
4. Repeat step 2.
5. Stop when arithmetic mean for the clusters stabilize.

Support Vector Machines (SVM)

1. SVM is a supervised machine learning algorithm. SVM performs classification tasks by constructing hyperplanes in a multidimensional space that separates cases of different class labels.
2. SVM supports both regression and classification tasks and can handle multiple continuous and categorical variables.



SVM

Figure: Plane

Figure: Normal to the Plane

SVM

1. The equation of a plane is given by:

$$w^T x + b = 0 \tag{27}$$

For two points x' and x'' on the plane, we have:

$$w^T x^{'} + b = 0$$
$$w^T x^{''} + b = 0$$
$$w^T (x^{'} - x^{''}) = 0$$

The normal distance d of a point x_n from x is given by:

$$d = ||\hat{w}(x_n - x)|| = \frac{1}{||w||}(w^T x_n + b - w^T x - b) = \frac{2}{||w||} \tag{28}$$

SVM

Our goal is to maximize the distance which is the same as minimizing $\frac{1}{2}w^T w$ subject to the condition:

$$wx_i + b \geq 1 \text{ for } y_i = +1 \tag{29}$$

$$wx_i + b \leq 1 \text{ for } y_i = -1 \tag{30}$$

i.e., for all i:

$$y_i(wx_i + b) \geq 1 \tag{31}$$

We will now use the Lagrange formulation to minimize:

$$\mathcal{L}(w, b, \alpha) = \frac{1}{2}w^T w - \sum^{N} \alpha_n(y_n(w^T x_n + b) - 1) \tag{32}$$

with respect to w and b and maximize with respect to each $\alpha_n > 0$

SVM

$$\nabla \mathcal{L} = w - \sum_{n=1}^{N} \alpha_n y_n x_n = 0 \tag{33}$$

$$\frac{\partial \mathcal{L}}{\partial b} = - \sum_{n=1}^{N} \alpha_n y_n = 0 \tag{34}$$

$$w = \sum_{n=1}^{N} \alpha_n y_n x_n \tag{35}$$

$$\sum_{n=1}^{N} \alpha_n y_n = 0 \tag{36}$$

$$\boxed{\mathcal{L}(\alpha) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} - \sum_{n=1}^{N} \sum_{m=1}^{N} y_n y_m \alpha_n \alpha_m x_n^T x_m} \tag{37}$$

maximize above eqn w.r.t α subject to $\alpha_x > 0$ *for* $n = 1, 2, \cdots N$.

SVM

$$\max_{\alpha} \sum_{n=1}^{N} \alpha_n - \frac{1}{2} - \sum_{n=1}^{N}\sum_{m=1}^{N} y_n y_m \alpha_n \alpha_m x_n^T x_m \quad (38)$$

$$\min_{\alpha} \frac{1}{2} \sum_{n=1}^{N}\sum_{m=1}^{N} y_n y_m \alpha_n \alpha_m x_n^T x_m - \sum_{n=1}^{N} \alpha_n \quad (39)$$

$$\min_{\alpha} \frac{1}{2}\alpha^T] \begin{vmatrix} y_1 y_1 x_1^T x_1 & y_1 y_2 x_1^T x_2 & \cdots & y_1 y_N x_1^T x_N \\ y_2 y_1 x_2^T x_1 & y_2 y_2 x_2^T x_2 & \cdots & y_2 y_N x_2^T x_N \\ \cdots & \cdots & \cdots & \cdots \\ y_N y_1 x_N^T x_1 & y_N y_2 x_N^T x_2 & \cdots & y_N y_N x_N^T x_N \end{vmatrix} \alpha + (-1^T)\alpha \quad (40)$$

subject to $y^T \alpha = 0; 0 < \alpha \leq \infty$.

$$\min_{\alpha} \boxed{\frac{1}{2}\alpha^T Q \alpha - 1^T \alpha} \quad (41)$$

SVM

subject to Karush Kuhn Tucker (KKT) condition: $y^T \alpha = 0; \alpha \geq 0$. We then compute w:

$$\boxed{w = \sum_{n=1}^{N} \alpha_n y_n x_n} \tag{42}$$

and solve for b:

$$\boxed{y_n(wx_n + b) = 1} \tag{43}$$

Non Linearity

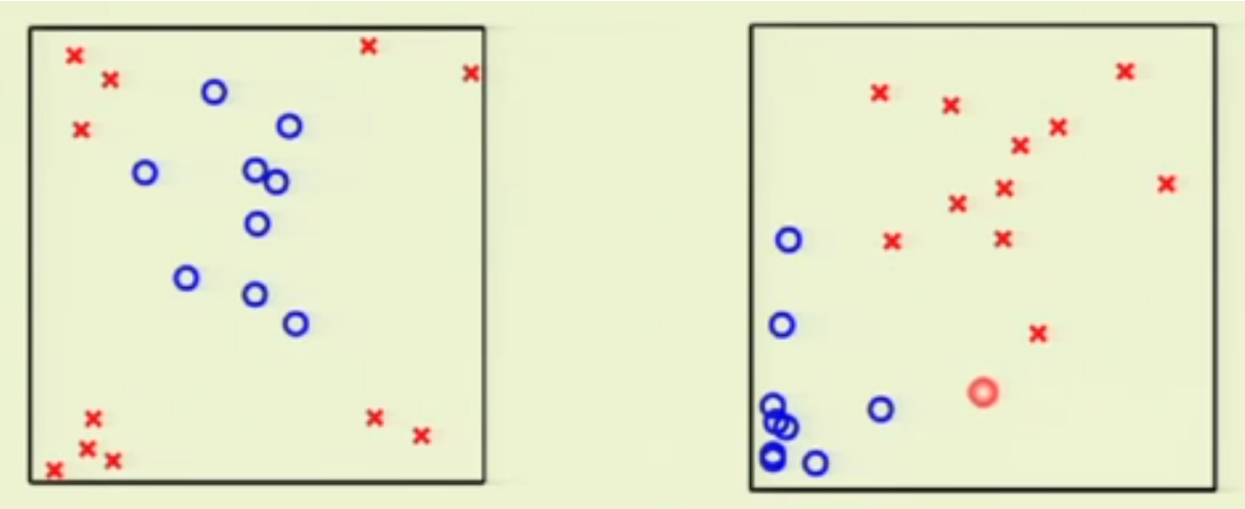


Figure: Transform to linear space

For non-linear systems, we transform to z space:

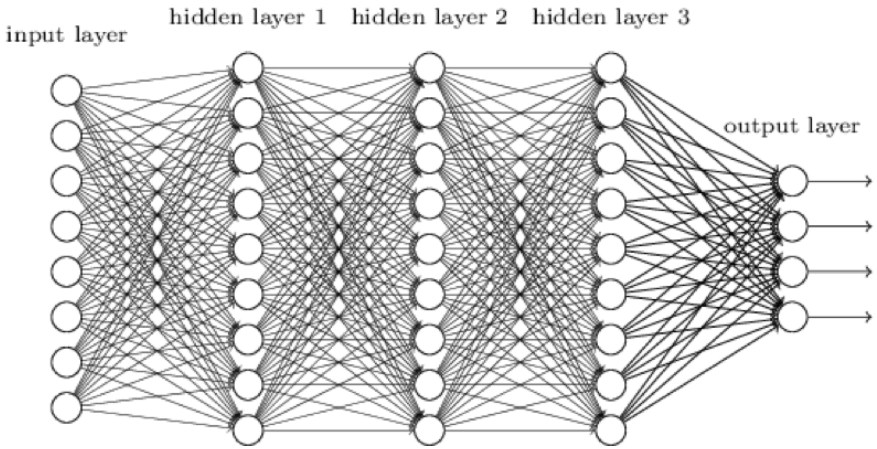
$$\mathcal{L}(\alpha) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} - \sum_{n=1}^{N} \sum_{m=1}^{N} y_n y_m \alpha_n \alpha_m z_n^T z_m \tag{44}$$

and we will have support vectors in the transformed space.

Deep Neural Net

1. Deep Learning Success - Image Recognition, Speech Comprehension, Chatbot
2. DNNs are suitable where the raw underlying features are not individually interpretable. This success is attributed to their ability to learn hierarchical representations, unlike traditional methods that rely upon hand-engineered features.
3. DNNs are greedily built by stacking restricted Boltzmann machines, and Convolutional Neural Networks, which exploit the local dependency of visual information, and have demonstrated record-setting results on many important applications.
4. Neural networks are powerful learning models that achieve state-of-the-art results in a wide range of supervised and unsupervised machine learning tasks for classification & regression.
5. Simple linear models tend to under-fit, and often under utilize computing resources with 8-GPU Hydra.

Deep Neural Net



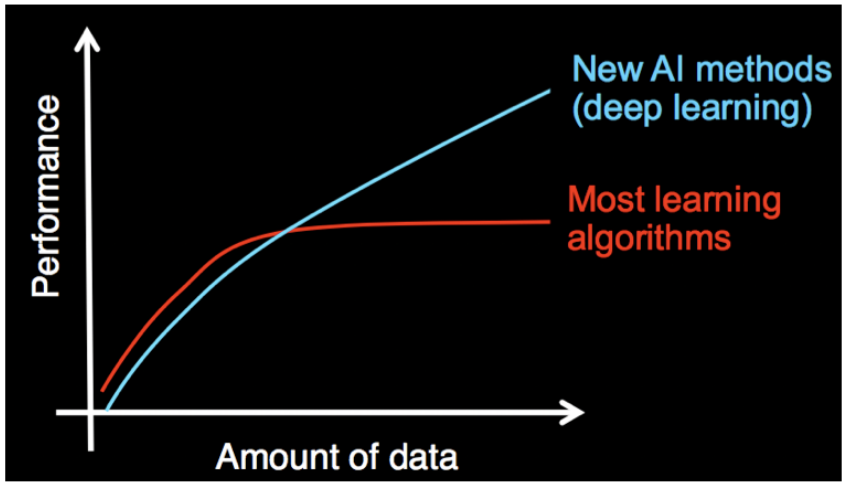
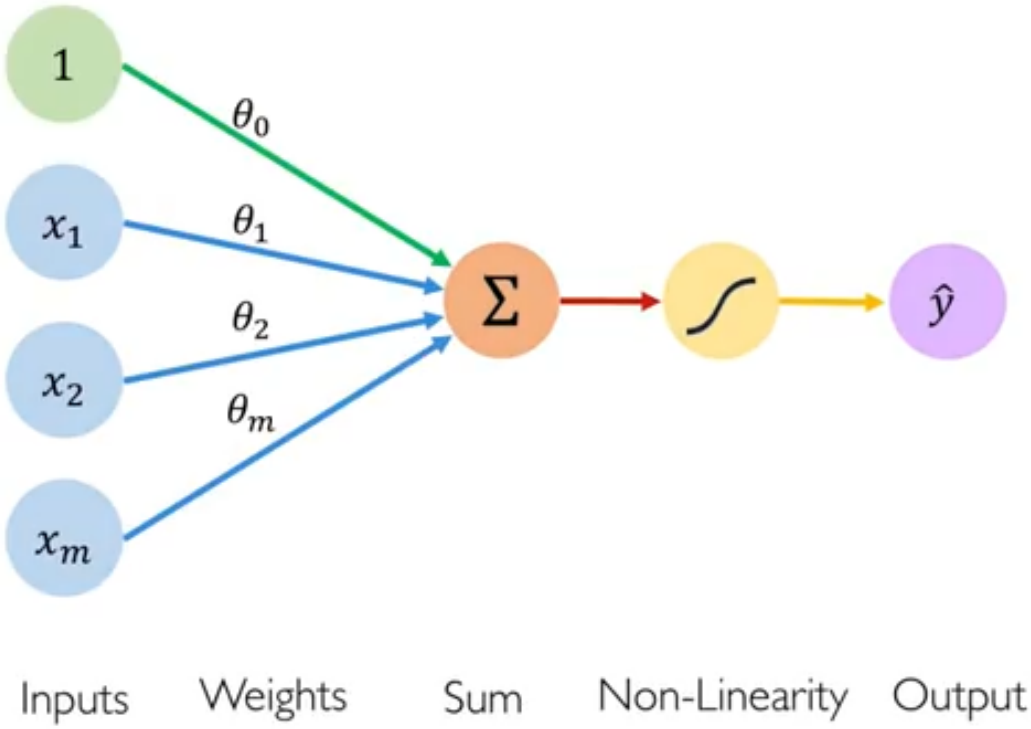


Figure: Deep Learning

Deep Neural Net



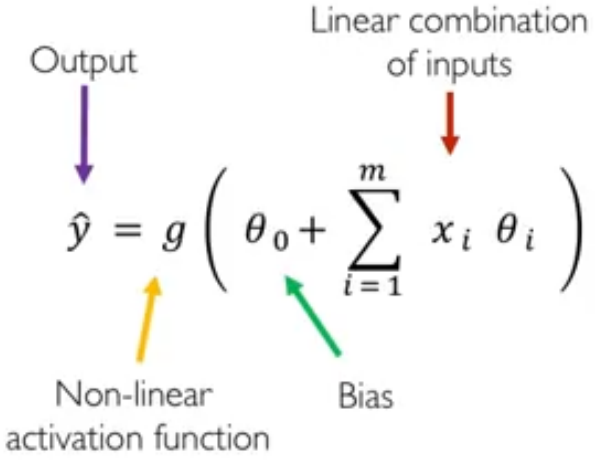
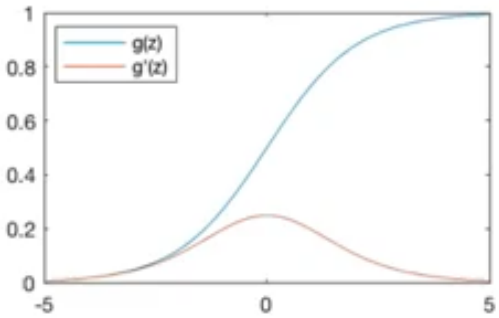


Figure: Forward Propagation

Source: MIT 6.S191 (2018) - Introduction to Deep Learning

Deep Neural Net

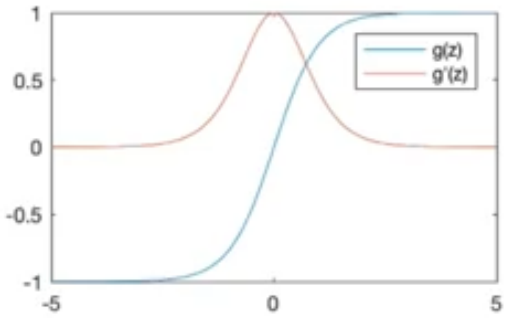
Sigmoid Function



$$g(z) = \frac{1}{1 + e^{-z}}$$

$$g'(z) = g(z)(1 - g(z))$$

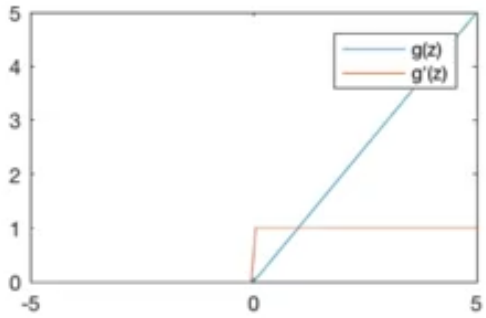
Hyperbolic Tangent



$$g(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$

$$g'(z) = 1 - g(z)^2$$

Rectified Linear Unit (ReLU)



$$g(z) = \max(0, z)$$

$$g'(z) = \begin{cases} 1, & z > 0 \\ 0, & \text{otherwise} \end{cases}$$

Figure: Activation Functions

Back Propagation

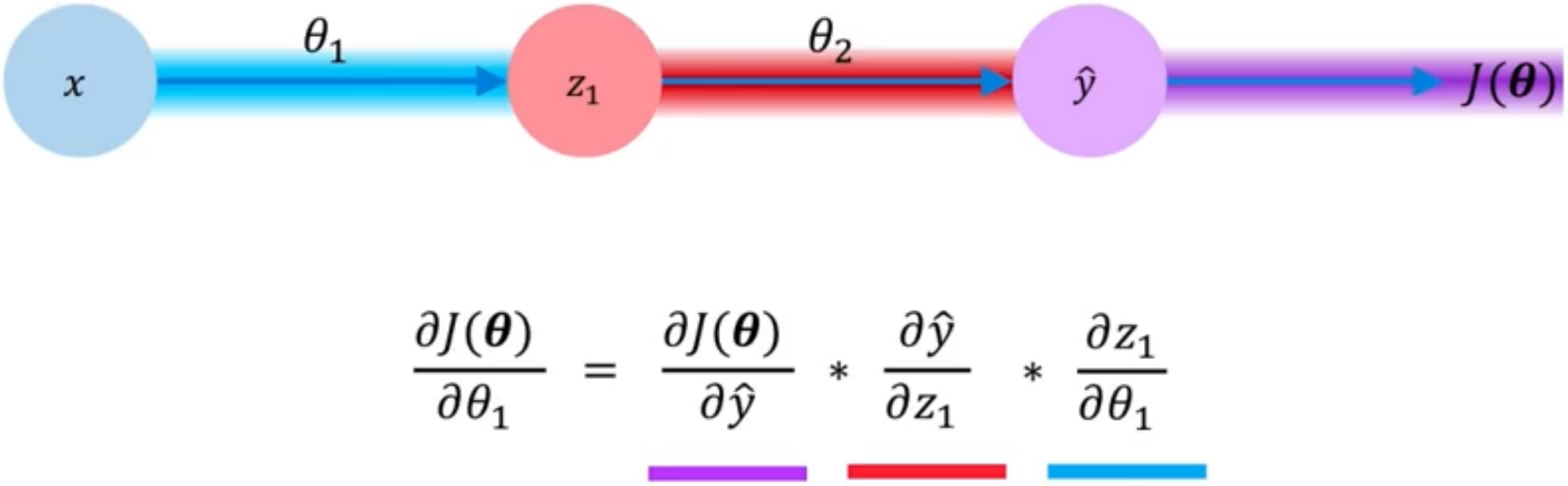


Figure: Loss Minimization

Repeat this for every weight in the network using gradients from later layers.

Loss Surface

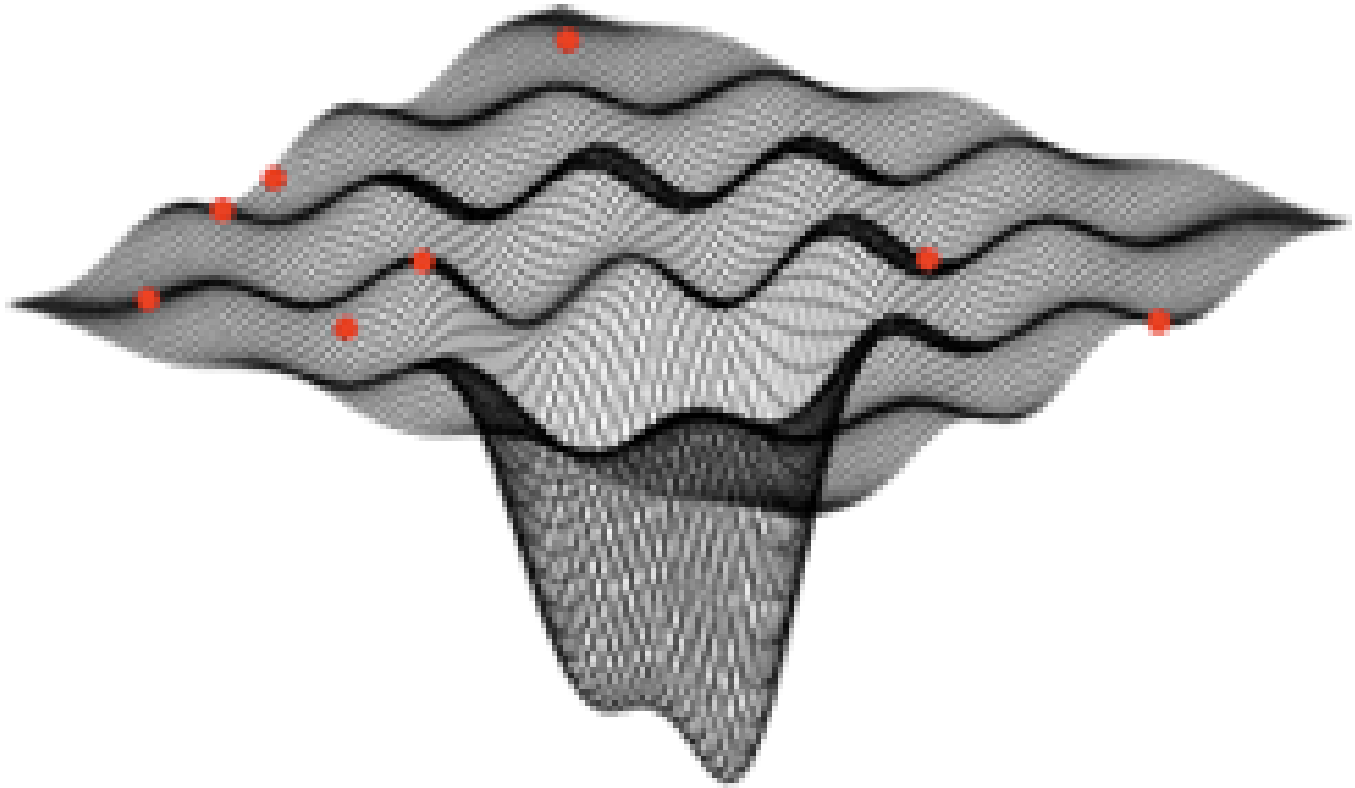


Figure: Global versus Local Minima

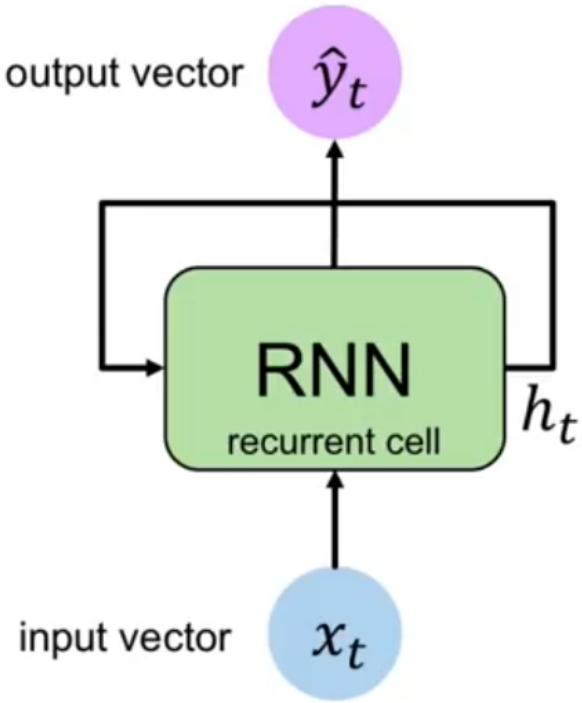
Recurrent Neural Network (RNN)

1. Dialogue systems, self-driving cars, robotic surgery, speech, etc. among others require an explicit model of sequentiality or time – a combination of classifiers or regressors cannot provide these functionalities.
2. SVM, logistic regression, feedforward networks have proved very useful without explicitly modeling time. But the assumption of independence precludes modeling long range dependencies.
3. Frames from video, snippets of audio, and words pulled from sentences – the independence assumption fails.
4. RNNs are connectionist models with the ability to selectively pass information across sequence steps while processing sequential data one element at a time. They can model input and/or output consisting of sequences of elements that are not independent.

Sequence Modeling Criteria)

1. Handle variable length sequences.
2. Track long term dependencies.
3. Maintain information about order.
4. Share parameters across the sequence.

RNN



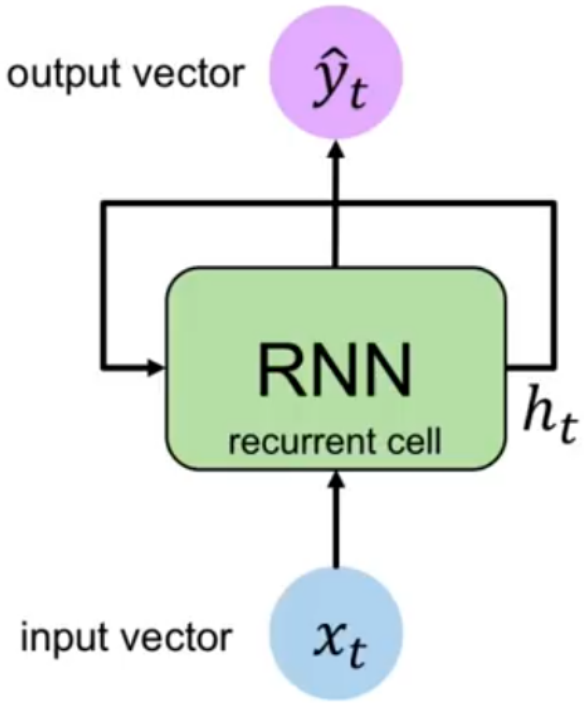
Apply a **recurrence relation** at every time step to process a sequence:

$$\underbrace{h_t}_{\text{cell state}} = \underbrace{f_W}_{\substack{\text{function} \\ \text{parameterized} \\ \text{by W}}} (\underbrace{h_{t-1}}_{\text{old state}}, x_t)$$

Figure: Same function and set of parameters are used in every step

Source - MIT 6.S191- Recurrent Neural Networks

RNN



Output Vector

$$\hat{y}_t = \boldsymbol{W_{hy}} h_t$$

Update Hidden State

$$h_t = \tanh(\boldsymbol{W_{hh}} h_{t-1} + \boldsymbol{W_{xh}} x_t)$$

Input Vector

Figure: State Update and Output

RNN

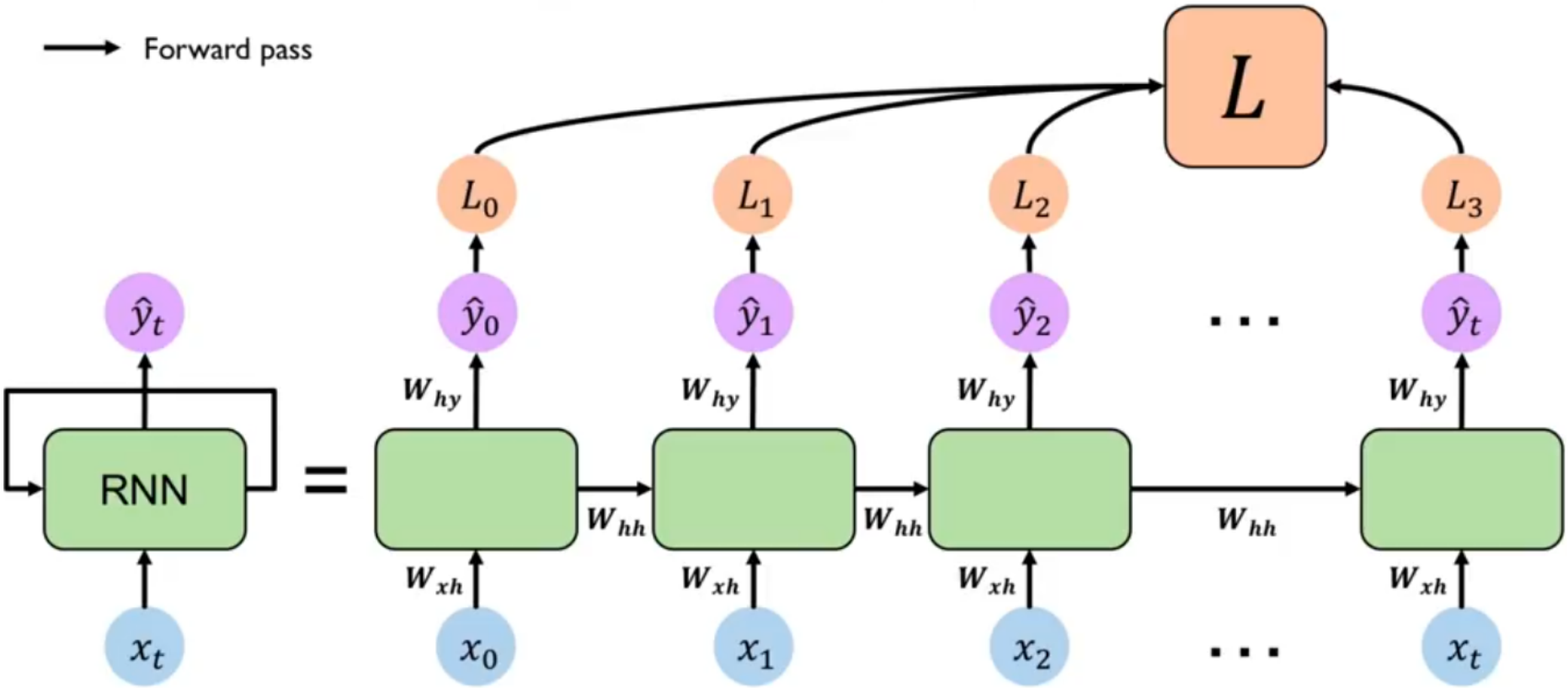


Figure: Computational Graph

RNN

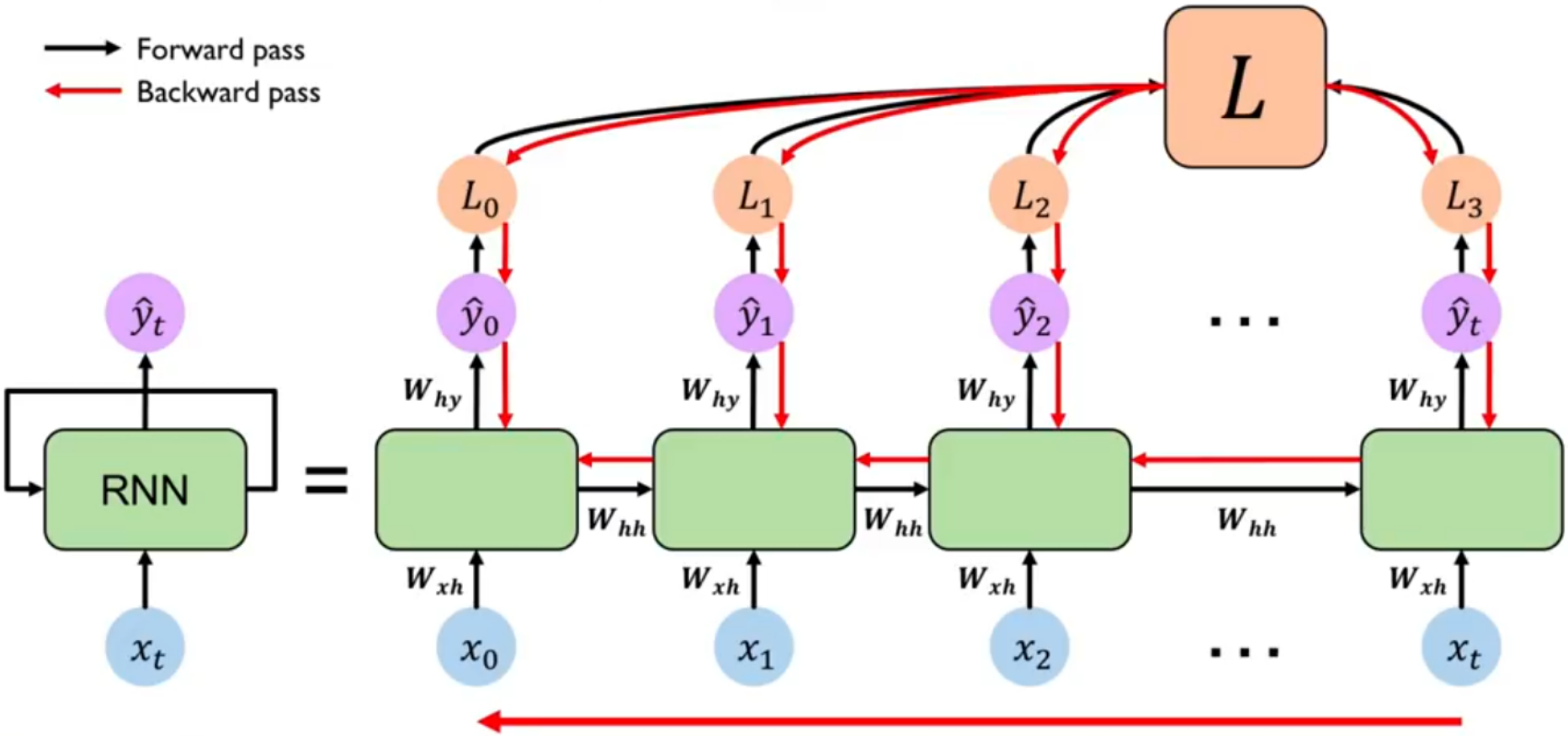


Figure: Backpropagation over time

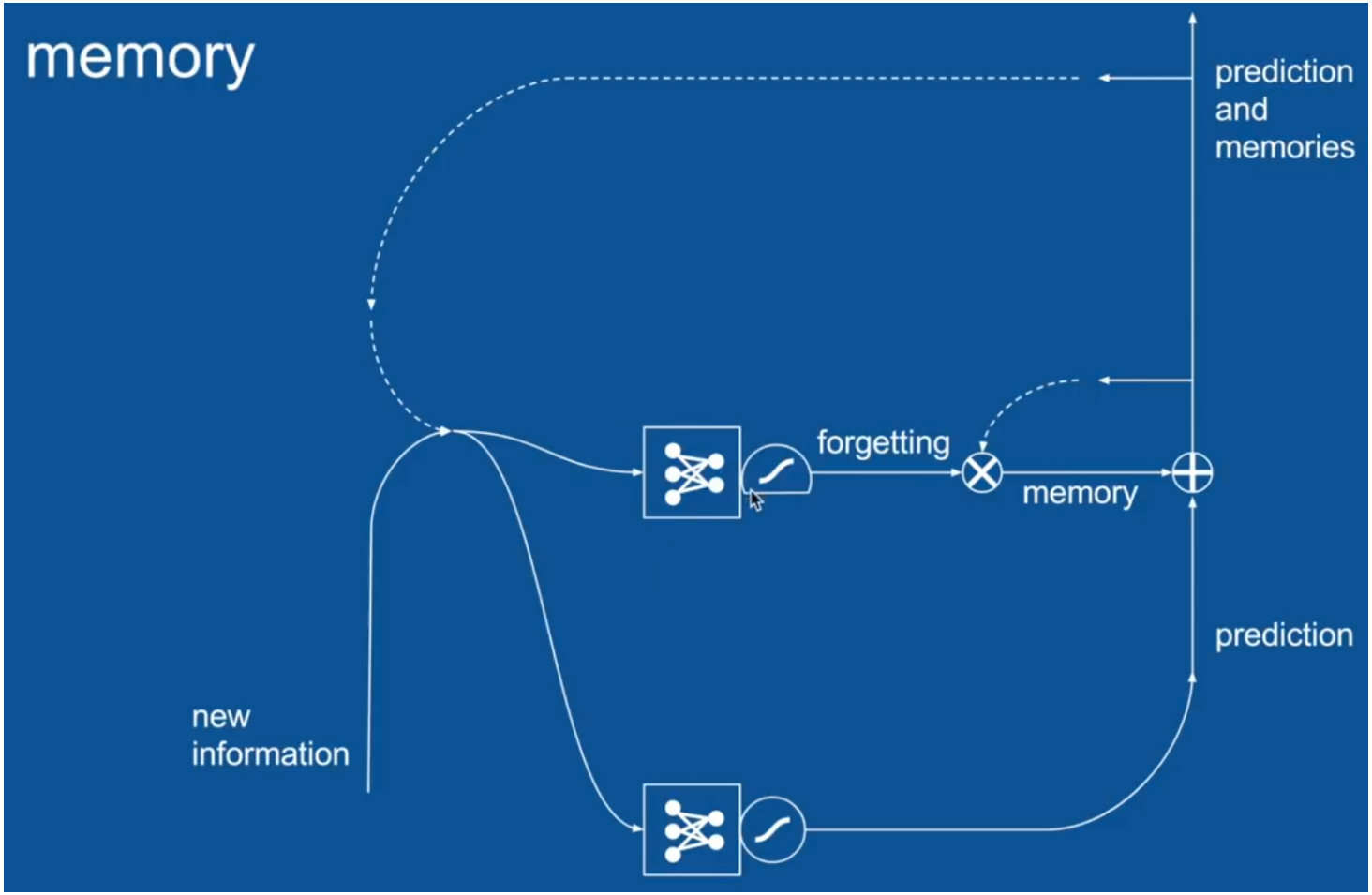
Vanishing / Exploding Gradients

1. Learning with recurrent networks is challenging due to the difficulty of learning long-range dependencies, [Bengio et al. 1994], [Hochreiter et al, 2001].
2. Problems of vanishing and exploding gradients occur when backpropagating errors across many time steps.
3. Which of the two phenomena occurs depends on whether the weight of the recurrent edge $|wjj| > 1$ or $|wjj| < 1$ and on the activation function in the hidden node. For a sigmoid activation function, the vanishing gradient problem is more pressing, but with a rectified linear unit $max(0, x)$, it is easier to imagine the exploding gradient.

Long Short Term Memory (LSTM) - Hochreiter & Schmidhuber

1. Maintain a separate cell state
2. Use gates
    1. Forget
    2. Selectively update
    3. Ouput
3. Backpropagation does not require matrix multiplication

LSTM



Source: Recurrent Neural Networks (RNN) and Long Short-Term Memory (LSTM) - Brandon Rohrer

LSTM

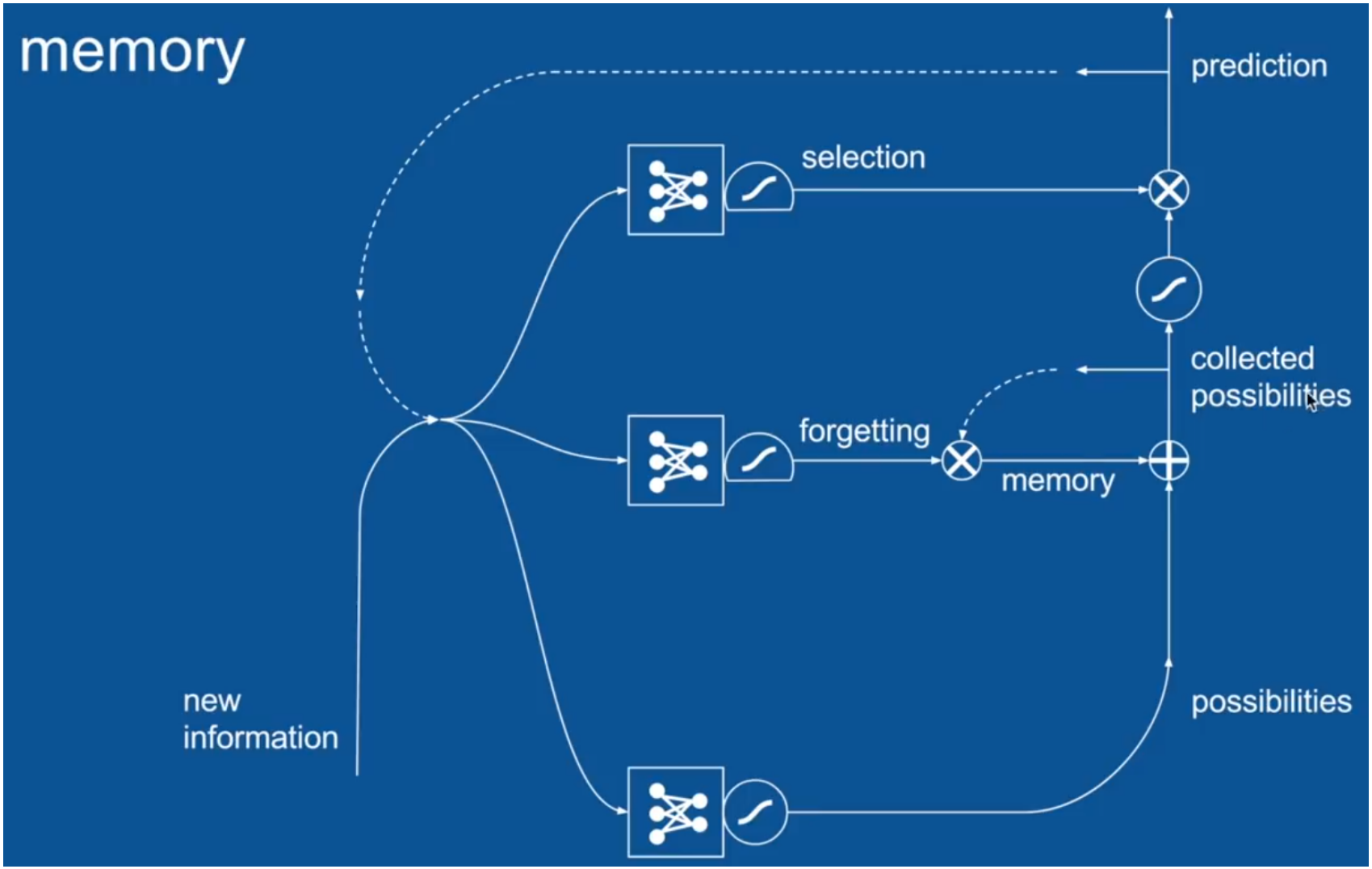


Figure: Memory & Selection

Long Short Term Memory

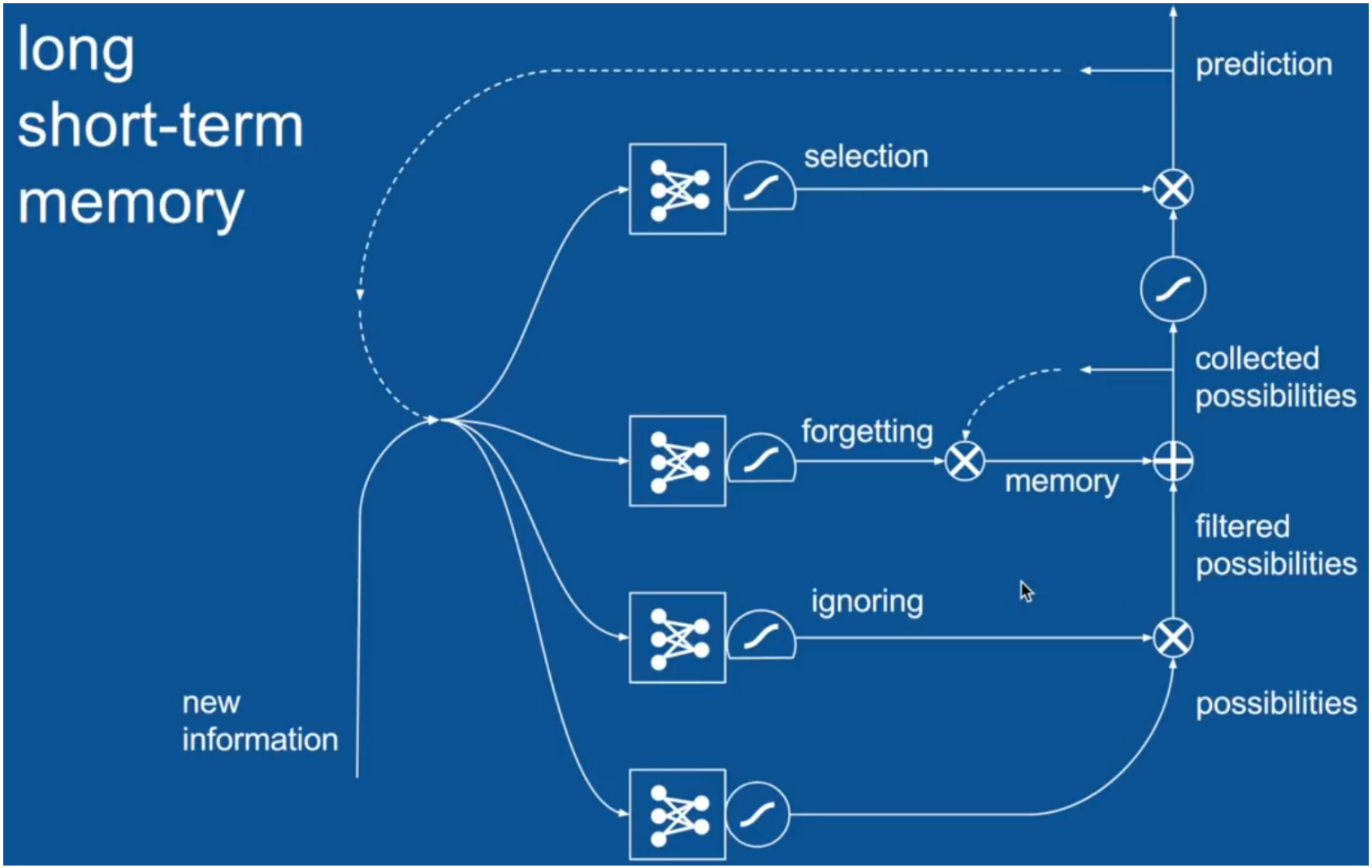


Figure: Memory, Selection & Ignoring

Long Short Term Memory

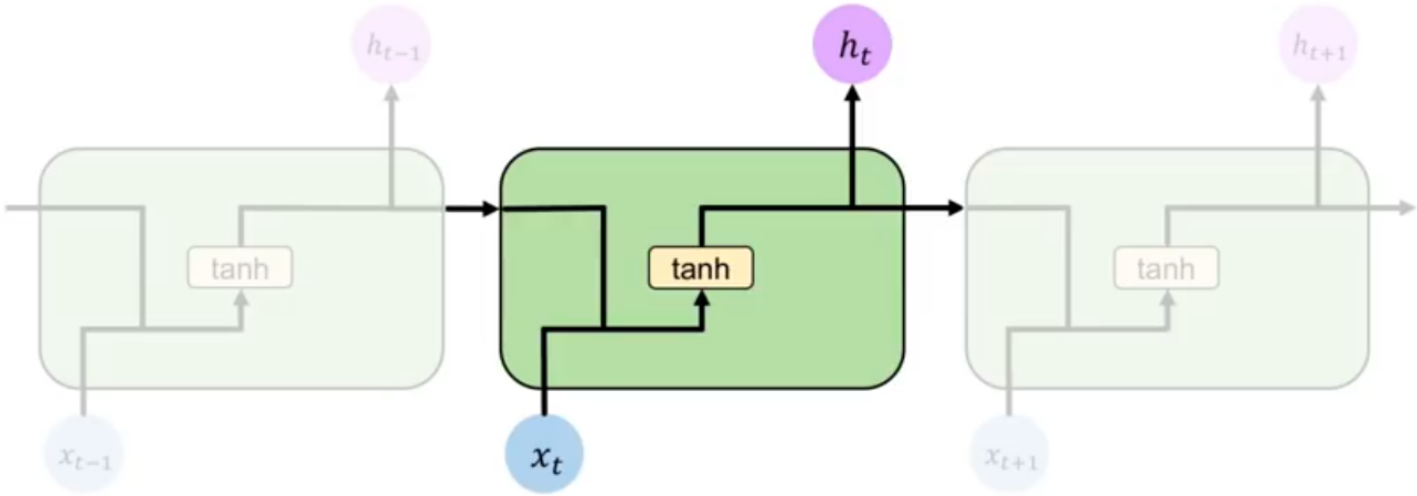
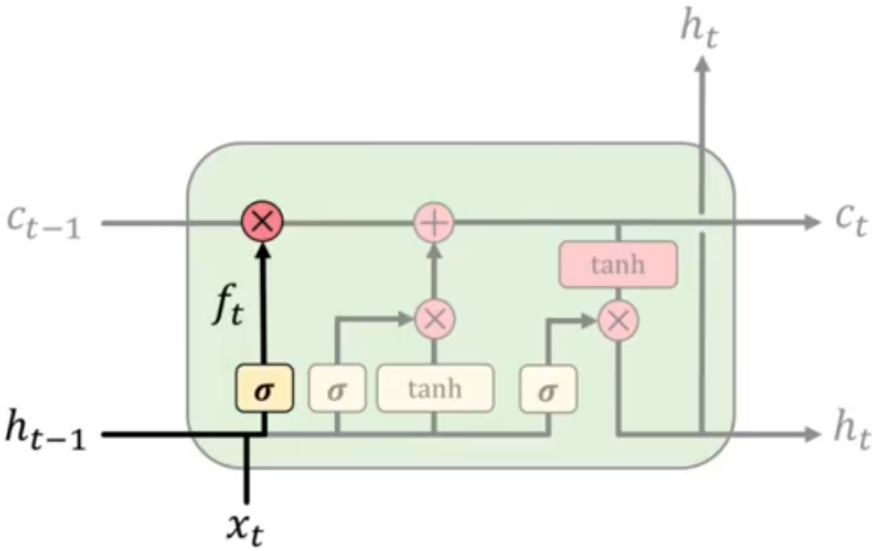


Figure: A Standard RNN

Source - MIT 6.S191- Recurrent Neural Networks

Long Short Term Memory

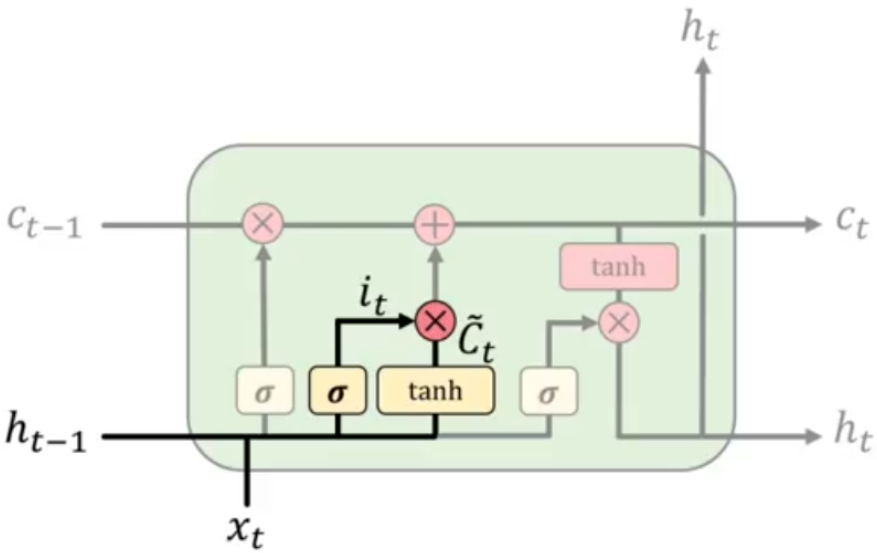


$$f_t = (\boldsymbol{W_f} \cdot \sigma\,[\,h_{t-1}, x_t\,] + b_f)$$

- Use previous cell output and input
- Sigmoid: value 0 and 1 – "completely forget" vs. "completely keep"

Figure: Forget

Long Short Term Memory



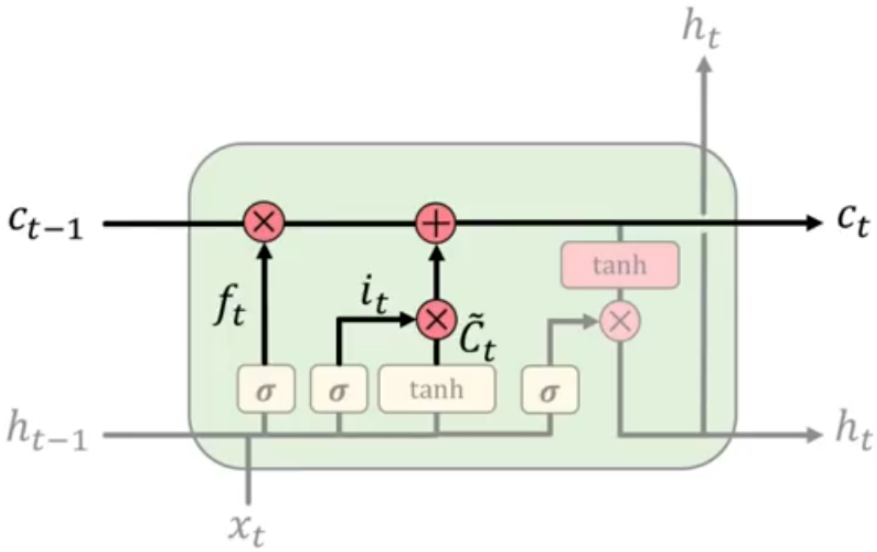
$$i_t = \sigma(\boldsymbol{W_i}[\, h_{t-1}, x_t \,] + b_i)$$

$$\tilde{C}_t = \tanh(\boldsymbol{W_C}[\, h_{t-1}, x_t \,] + b_C)$$

- Sigmoid layer: decide what values to update
- Tanh layer: generate new vector of "candidate values" that could be added to the state

Figure: New vector of candidate values

Long Short Term Memory

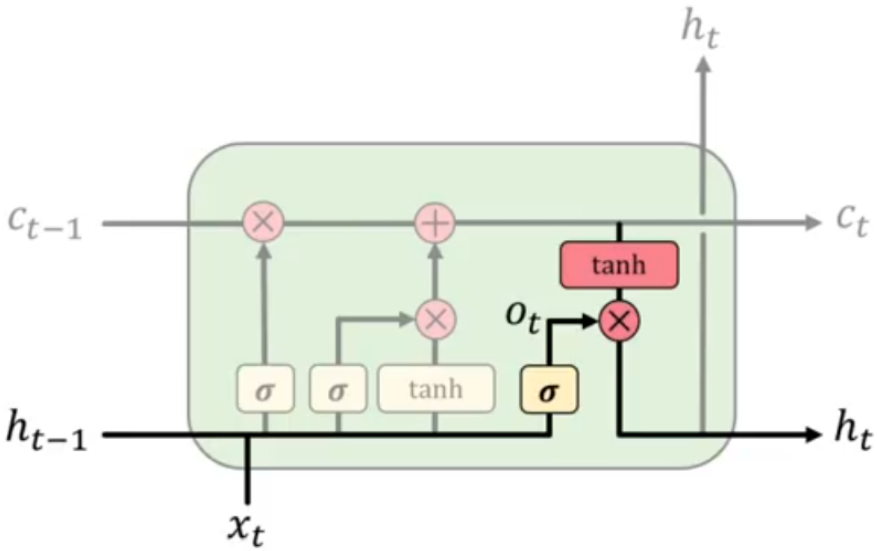


$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

- Apply forget operation to previous internal cell state: $f_t * C_{t-1}$
- Add new candidate values, scaled by how much we decided to update: $i_t * \tilde{C}_t$

Figure: Decide what parts of state to output

Long Short Term Memory



$$o_t = \sigma(\boldsymbol{W_o}[\, h_{t-1}, x_t \,] + b_o)$$

$$h_t = o_t * \tanh(C_t)$$

- Sigmoid layer: decide what parts of state to output
- Tanh layer: squash values between -1 and 1
- $o_t * \tanh(C_t)$: output filtered version of cell state

Figure: Output filtered version of cell state

Long Short Term Memory

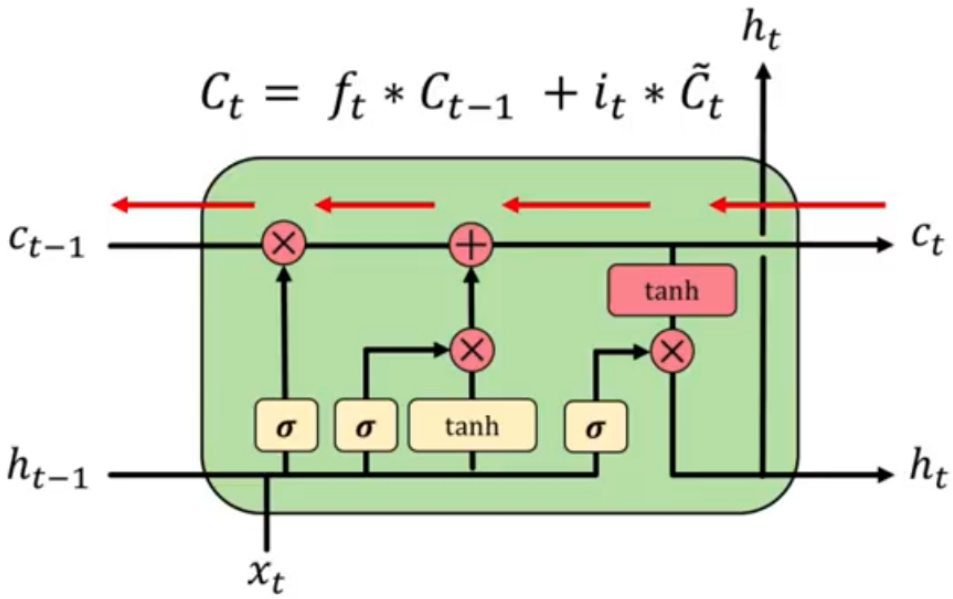


Figure: LSTM Gradient Flow

Long Short Term Memory

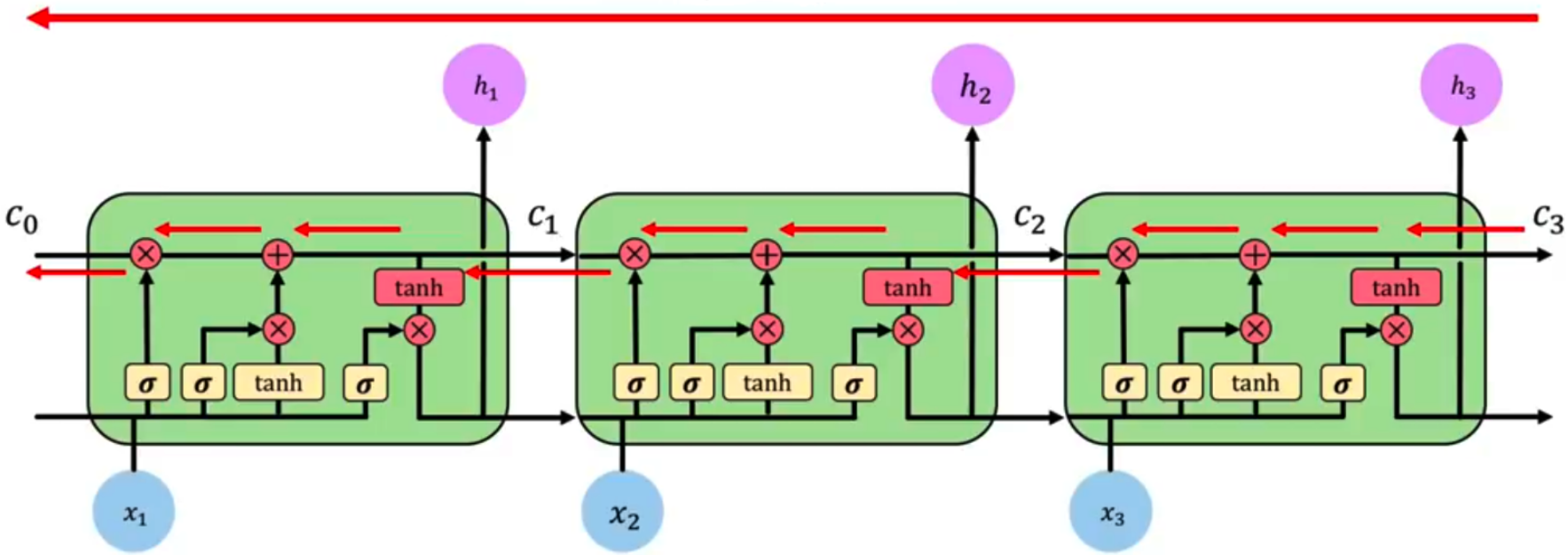


Figure: Uninterrupted Gradient Flow

Reinforcement Learning

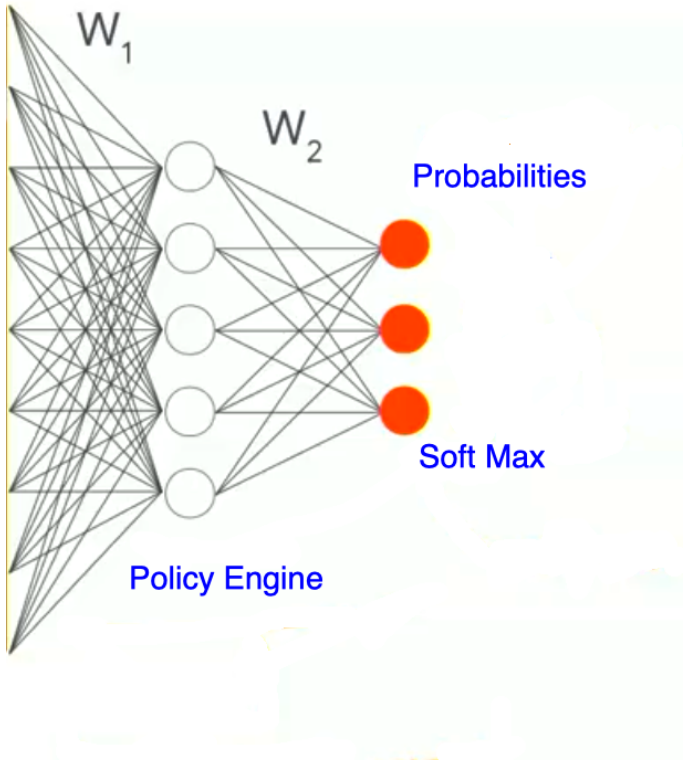


Figure: Reinforcement Learning

$$Cross\ Entropy\ Loss = -(\hat{P}_1 log P_1 + \hat{P}_2 log P_2 \cdots \hat{P}_n log P_n) \quad (45)$$

Reinforcement Learning

1. $\hat{P}$ is sampled.
2. P_i is predicted and is a function of the weights and is differentiable with respect to the weights.
3. Cross Entropy Loss has to be minimized, this will lead to determining the weights.
4. Policy Gradients
   1. Discounted Rewards for the i^{th} move. R_i reduces geometrically over previous steps.
   $$loss_i = -R_i log(P_i^{chosen}) \tag{46}$$
   2. Normalized Rewards across a batch of moves
   $$R_i = \frac{R_i - \bar{R}}{stdev(R)} \tag{47}$$