Introduction to Neural Networks and Deep Learning

Deep Forward Neural Networks

Andres Mendez-Vazquez

June 17, 2025

Outline

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For this initial analysis

We will look at the paper by Bengio

- "Learning deep architectures for AI", Foundations and trends in Machine Learning 2, 1 (2009), pp. 1--127.

And for this, we will look at Boolean functions

- After Shanon pointed out the fact they are useful to represent complex problems [1].

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Example, Architecture

A two-layer circuit of logic gates can represent any boolean function [2]

- Any boolean function can be written as a sum of products, disjunctive normal form:
  - AND gates on the first layer with optional negation of inputs,
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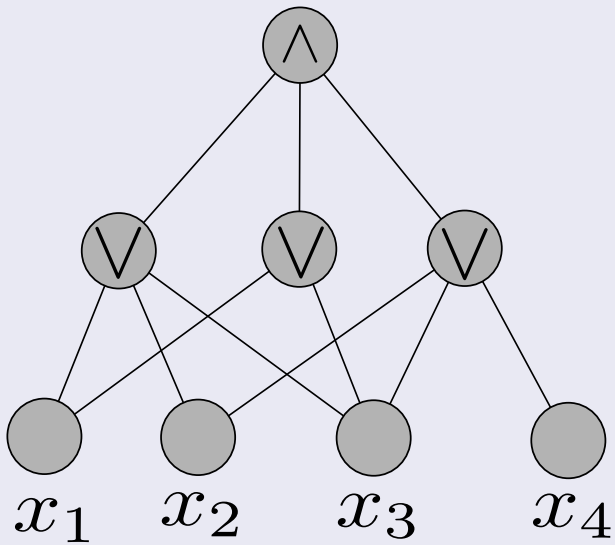

The Exponential Width

Here, we have a small problem

- There are functions computable with a polynomial-size logic gates circuit of depth k that require **exponential size** when restricted to depth $k-1$[3]
  - For Example

$$parity : (b_1, ..., b_d) \in \{0,1\}^d \mapsto \begin{cases} 1 & \text{if } \sum_{i=1}^{d} b_i \text{ is even} \\ -1 & \text{otherwise} \end{cases}$$

How this impact Deep Learning?

- Many of the results for boolean circuits can be generalized to architectures whose computational elements are linear threshold units

$$f(x) = 1_{wx+b>0}$$

  - The fan-in of a circuit is the maximum number of inputs of a particular element.

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How this impact shallow learning in Deep Learning?

- First, we define the concept of f_k function

Definition

- The function f_k is a function of N^{2k-2} variables. It is defined by a depth k circuit that is a tree. At the leaves of the tree there are unnegated variable, The i^{th} level from the bottom consists of $\wedge$-gates if i is even and otherwise it consists of $\vee$-gates.

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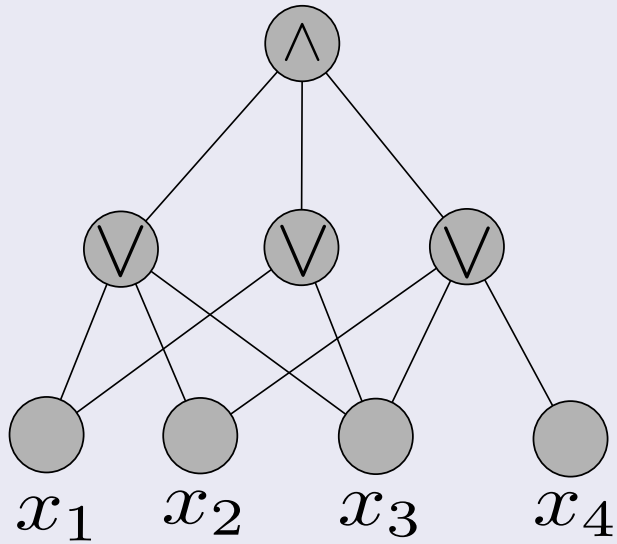

An Important Theorem

Of particular interest is the following theorem

- Monotone weighted threshold circuits (i.e. multi-layer neural networks with linear threshold units and positive weights)

Theorem [4]

- A monotone weighted threshold circuit of depth $k-1$ computing a function f_k has size at least 2^{cN} for some constant $c > 0$ and $N > N_0$.

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Meaning

This theorem does not fail any type of architecture

- But the question arises, Are the depth 1, 2 and 3 architectures (many Machine Learning algorithms) too shallow to represent efficiently more complicated functions?

What happens in Deep Architectures

- Bengio et al. argues that they can represent highly-varying functions [5]

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Highly-varying functions

Meaning

- We say that a function is highly-varying when a piecewise approximation of that function would require a large number of pieces.

Clearly

- Deeper Architectures can handle such functions in a easier way than shallow ones.

For Example

- The polynomial $\prod_{i=1}^{n} \sum_{j=1}^{m} a_{ij} x_j$ can be represented as a product of sums with only $O(nm)$ elements

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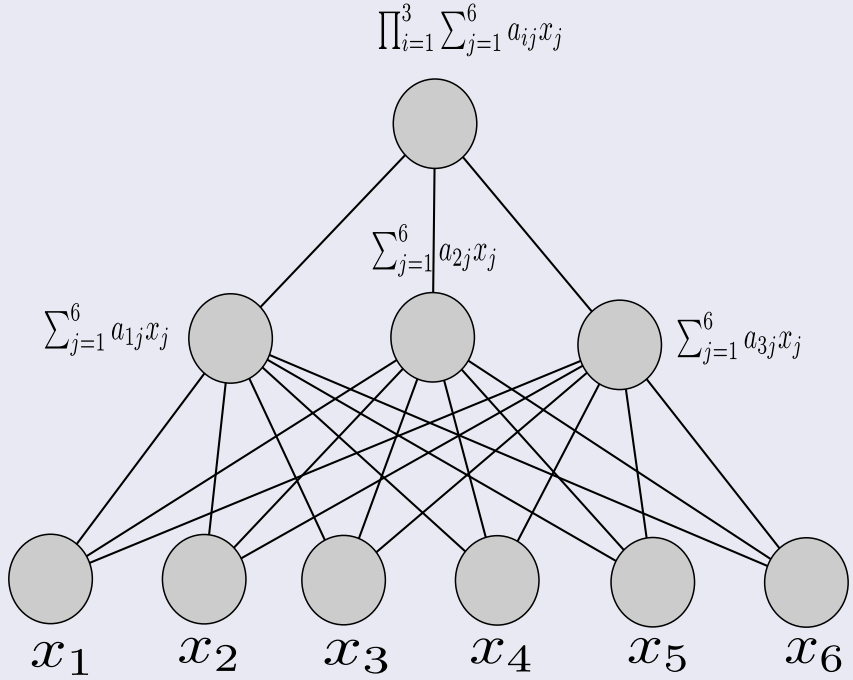
Basically

We have a Perceptron Layer and a Product Second Layer



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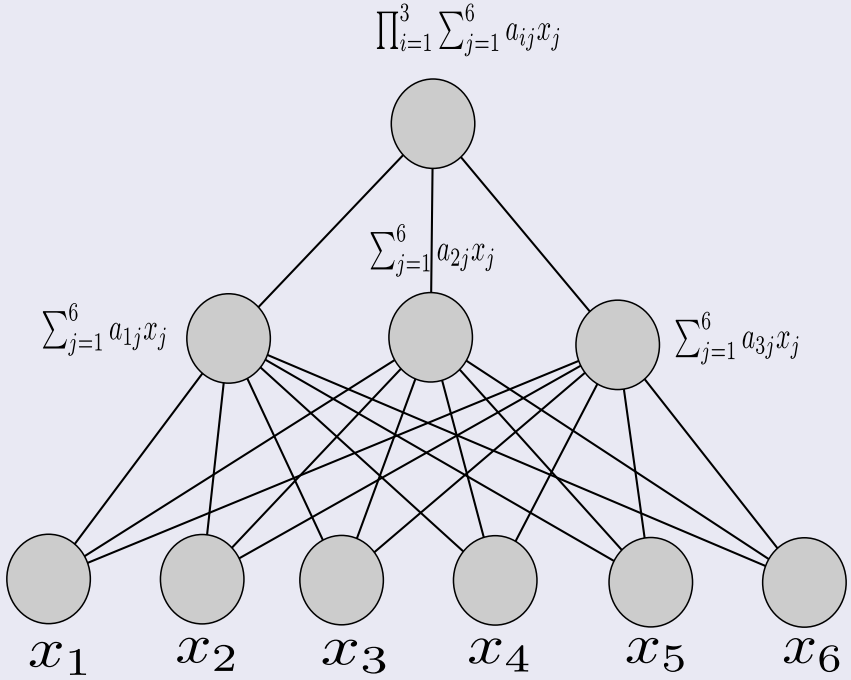

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Because for our case

$$\prod_{i=1}^{3}\sum_{j=1}^{6} a_{ij}x_j = \sum_{j=1}^{6}\prod_{i=1}^{3} a_{ij}x_j$$

We have the following problem $O(n^m)$

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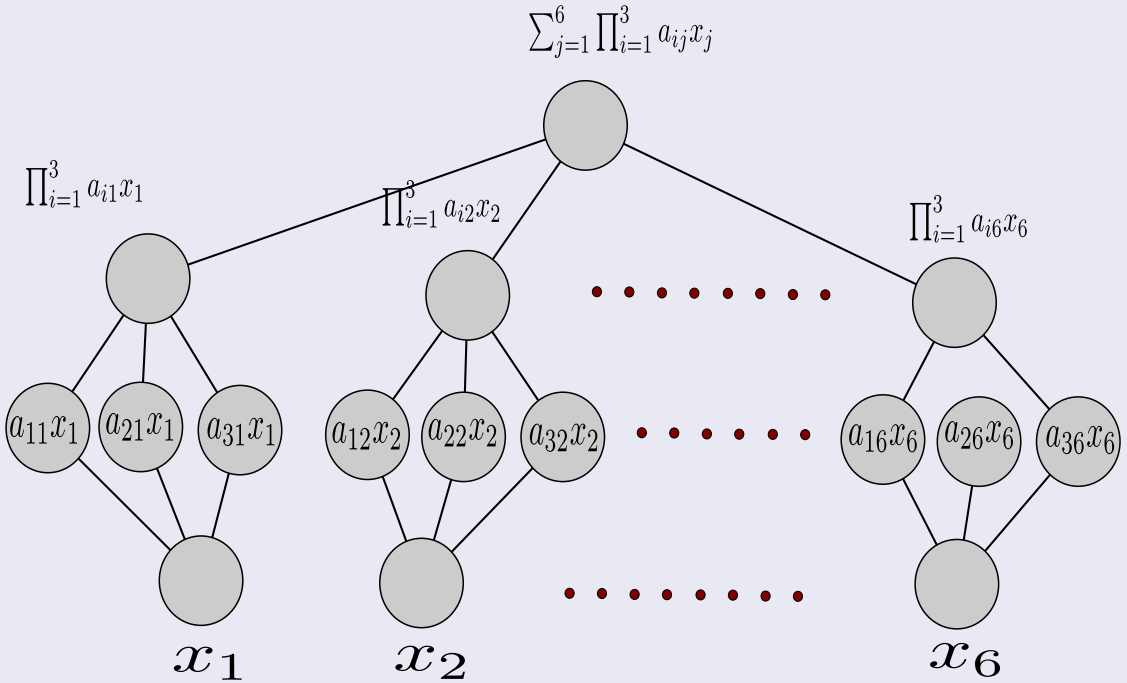

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You could claim

- Machine Learning shallow learning depends on complex computational units to handle complex functions

Deep Learning

- Proposes simpler units but deeper structures to handle complex functions

What about both ideas together

- Complex adaptive units
- Deeper architectures to helps such units
  - It seems to be the case of the human brain...!!!

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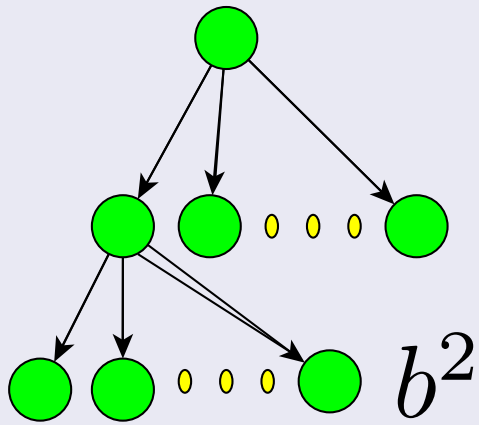
Actually making some numbers

If we allow Fan Out problem

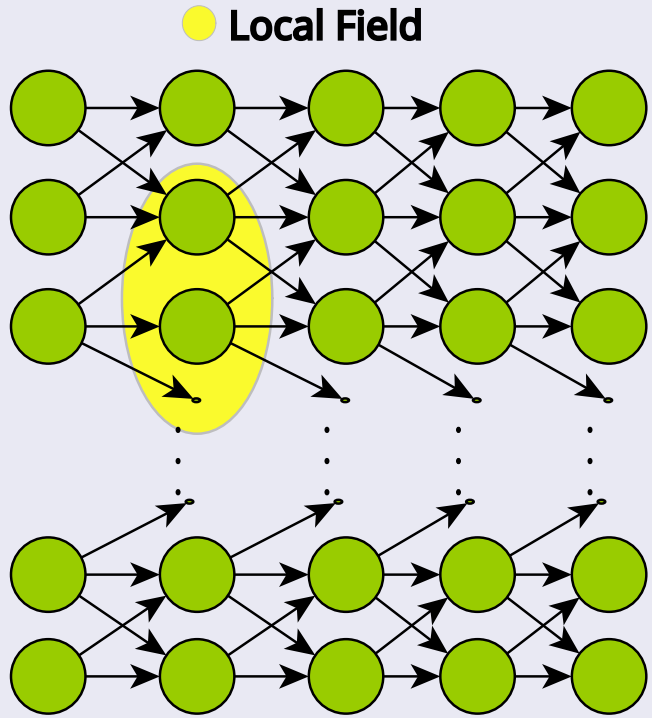
- Using a fully connected network with that allows a fanning out as



Yes, it allow more variability

This is what you try to do in shallow learning

- But other option avoid total fanout by using locality



Local vs Non-Local Generalization

We have smaller areas of information

- But we can go deeper

Avoid the Fan Out and Use Locality

- A local estimator partitions the input space in regions

Thus, local estimators are based on matching local templates

- It can be thought of as having two levels...

The first level

- It is made of a set of templates which can be matched to the input.

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A template unit will output a value that indicates the degree of matching

$$K(x|\Theta)$$

The second level combines these values

- Typically a simple linear combination or product combination

$$L(x) = \sum_{i=1}^{k} K(x|\Theta_i)$$

Classic Example, the kernel machine

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As you can see

The Kernel has a local influence based on the support vectors

- For example the Gaussian Kernel

$$K(x, x_i) = \exp\left\{-\frac{\|x - x_i\|^2}{\sigma^2}\right\}$$

The Problem of Kernel

- The assumption that the target function is smooth or can be well approximated with a smooth function.

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If we have the training example (x_i, y_i)

- We want to build predictor that output something near y_i when any other sample is near x_i

Basically the situation when regularizing

- Bengio and Le Cun claim this is not enough [8, 9]

Although, It is possible to argue

- That such highly varying space is due to a lack of the correct feature selection process.

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$$parity : (b_1, ..., b_d) \in \{0,1\}^d \mapsto \begin{cases} 1 & \text{if } \sum_{i=1}^{d} b_i \text{ is even} \\ -1 & \text{otherwise} \end{cases}$$

Theorem

- Let $f(x) = b + \sum_{i=1}^{2^d} \alpha_i K(x_i, x)$ be an affine combination of Gaussian with the same width σ centered on points $x_i \in \{-1,1\}^d$. If f solve the parity problem, then there are at least 2^{d-1} non-zero support vectors.

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Although, this function is not a representative

- The kind of functions we are more interested in AI.

It suggest that local based estimators

- They are not enough, but still not a conclusive result

After all

- More Memory could be added to those systems

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For example

Tensors have been used to add memory to SVM

$$\min_{\boldsymbol{U}_i^{(m)},\boldsymbol{K}^{(m)},\boldsymbol{\beta},b} \gamma \sum_{i=1}^{N} \left\| \mathcal{X}_i - \left[\!\left[\boldsymbol{K}^{(1)}\boldsymbol{U}_i^{(1)}, \cdots, \boldsymbol{K}^{(M)}\boldsymbol{U}_i^{(M)} \right]\!\right] \right\|_F^2 + \cdots$$

$$\lambda \boldsymbol{\beta}^T \widehat{\boldsymbol{K}} \boldsymbol{\beta} + \sum_{i=1}^{N} \left[1 - y_i \left(\widehat{\boldsymbol{k}}_i^T \boldsymbol{\beta} + b \right) \right]_+$$

- $\boldsymbol{K}^{(m)}$ are kernel matrices defined on each mode to capture the nonlinear part.
- $\boldsymbol{U}^{(m)} = \left[\boldsymbol{u}_1^{(m)}, \ldots, \boldsymbol{u}_R^{(m)} \right]$ are factor matrices of size $I_m \times R_m$

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A Problem

- You are limiting the Machine Learning operations to matrix additions and products and non-linear operations.
  - In a shallow way...

We need to add more complex functions

- After all deeper architectures construct complex functions layer by layer

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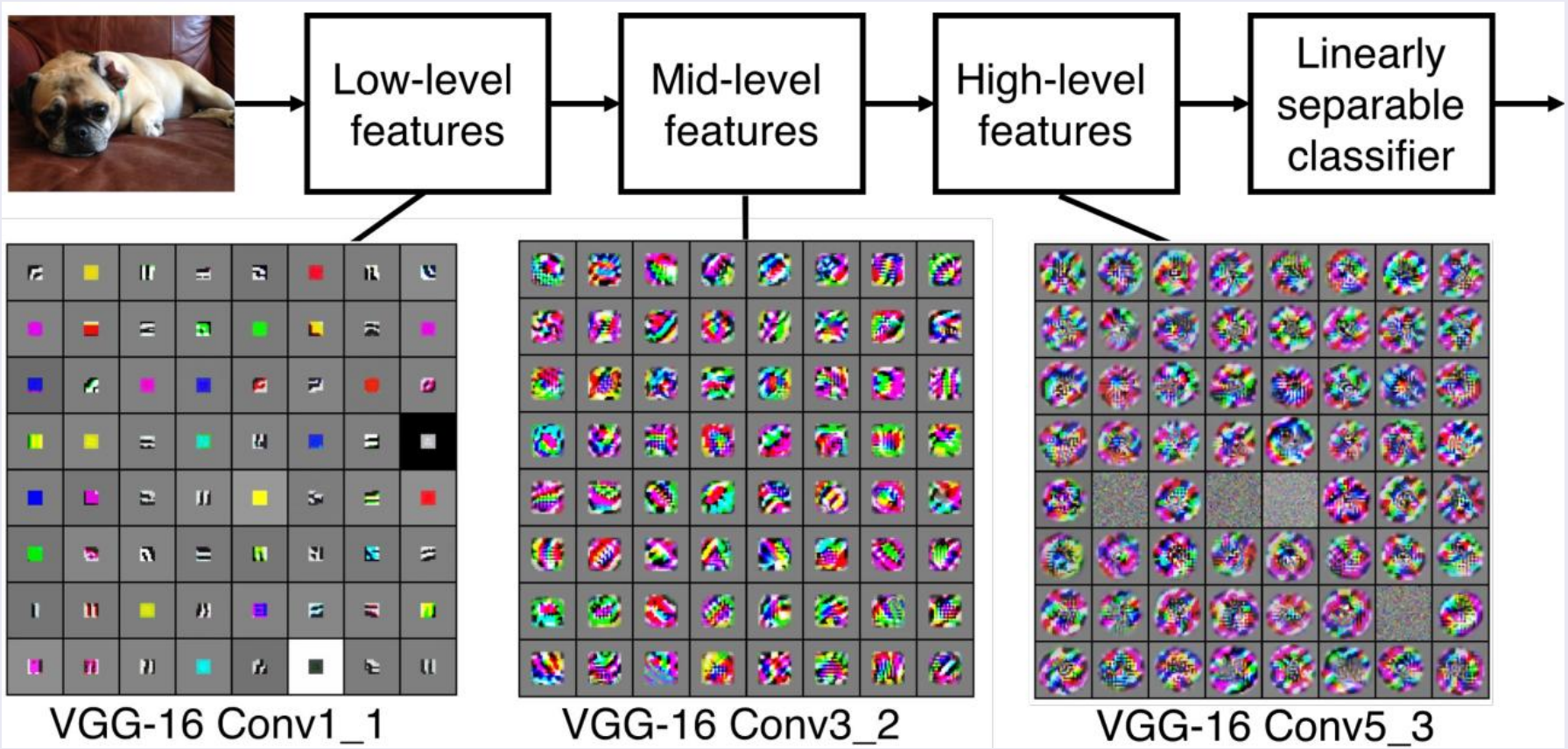
By Using Weights in Certain Deep Learners

The Application of each Layer increase the complexity of the features



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Some of the Models to be Reviewed

Convolutional Neural Networks

- The classic model that started the phenomena of Neural Networks.

Auto Encoder

- How to generate novel features by funneling.

Generative Models

- How to learn the underlaying models

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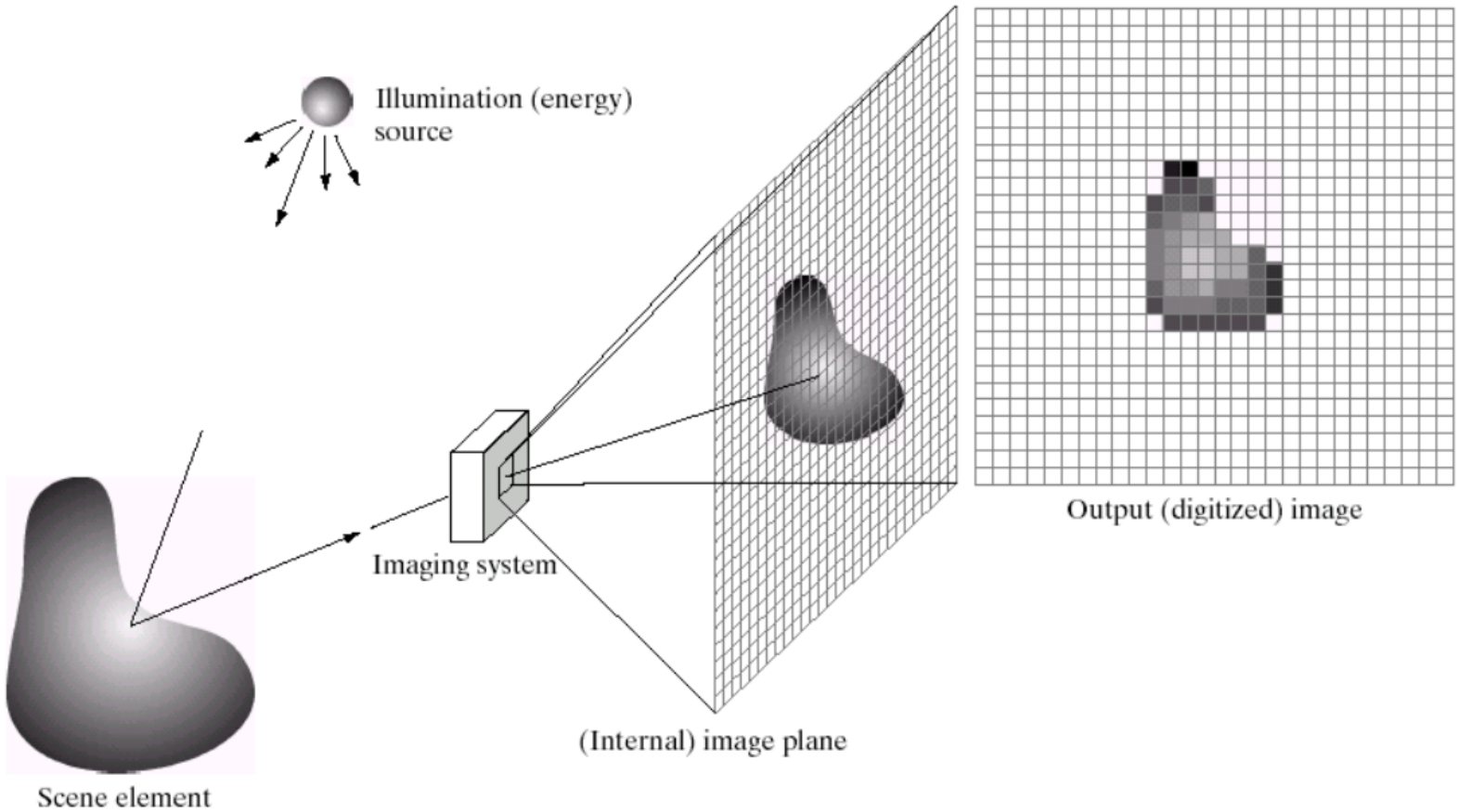
Digital Images as pixels in a digitized matrix



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Pixel values typically represent

- Gray levels, colours, heights, opacities etc

Something Notable

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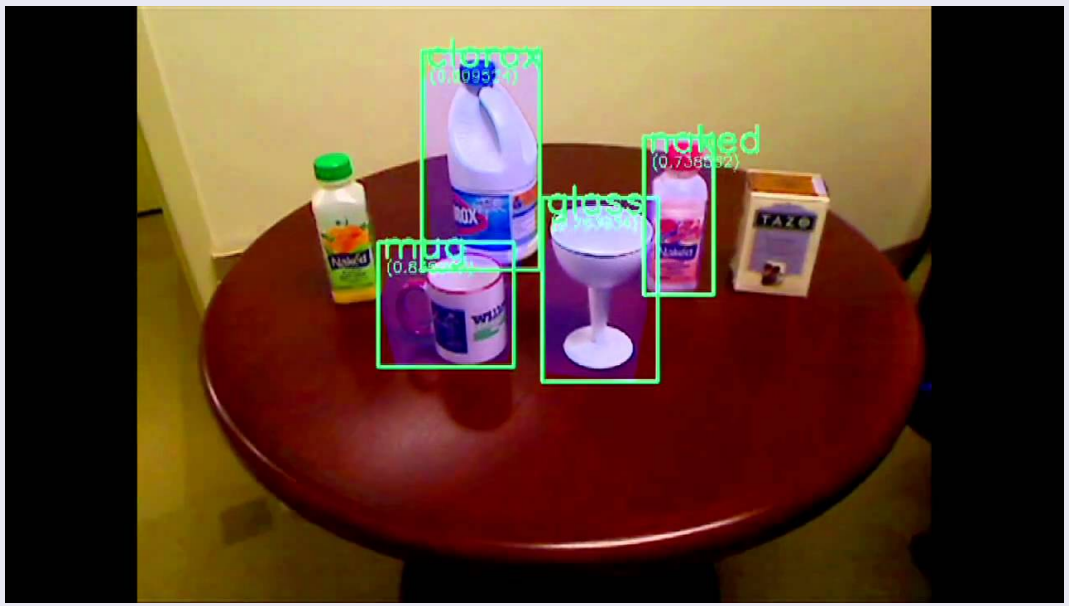

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Why not to use the data sets

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Work by Hubel and Wiesel in the 1950s and 1960s

- They showed that cat and monkey visual cortexes contain neurons that individually respond to small regions of the visual field.

After all more studies about the visual cortex happened

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Kunihiko Fukushima [10]

- Proposed a Hierarchical Network for image recognition with a convolution!!!

But it used a function φ

$$\varphi\left(\frac{1+\sum_{k_{l-1}=1}^{K_{l-1}}\sum_{v\in S_l}a_l\left(k_{l-1},v,k_l\right)u_{cl-1}\left(k_{l=1},n+v\right)}{1+\frac{2r_l}{1+r_l}b_l\left(k_l\right)v_{Cl-1}\left(n\right)}-1\right)$$

With a Relu function

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Weng et al. [11, 12]

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Basically they are deep learners based in convolutions or its variants

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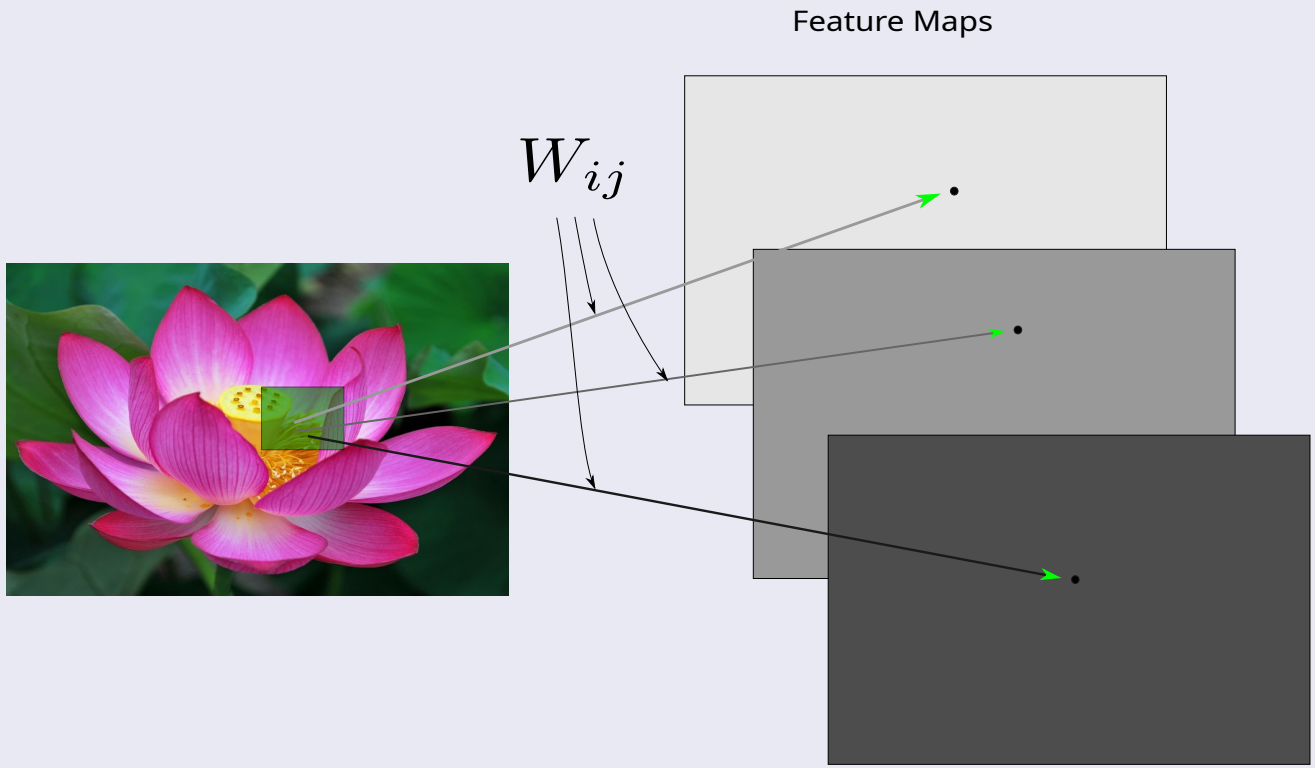

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Each Feature Map forms a 2D grid of features

That can be computed with a discrete convolution (*) of a kernel matrix k_{ij} which is the hidden weights matrix W_{ij} with rows and columns with its rows and columns flipped.

In addition

- x_i is the ith channel of input.
- k_{ij} is the convolution kernel.
- y_j is the hidden layer output.

Thus the total output

$$y_j = \sum_i k_{ij} * x_i \tag{2}$$

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That can be computed with a discrete convolution (*) of a kernel matrix k_{ij} which is the hidden weights matrix W_{ij} with rows and columns with its rows and columns flipped.

In addition

- x_i is the ith channel of input.
- k_{ij} is the convolution kernel.
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Thus the total output

$$y_j = \sum_i k_{ij} * x_i \tag{2}$$

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We have that

- A Convolutional Neural Network (CNN) directly accepts raw images as input.

Thus, their importance when training discrete filters

- Instead of assuming a certain comprehension of Computer Vision, one could think this is as a Silver Bullet.

However, you still

- You still need to be aware of :
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  - There initial works on how they work [14]

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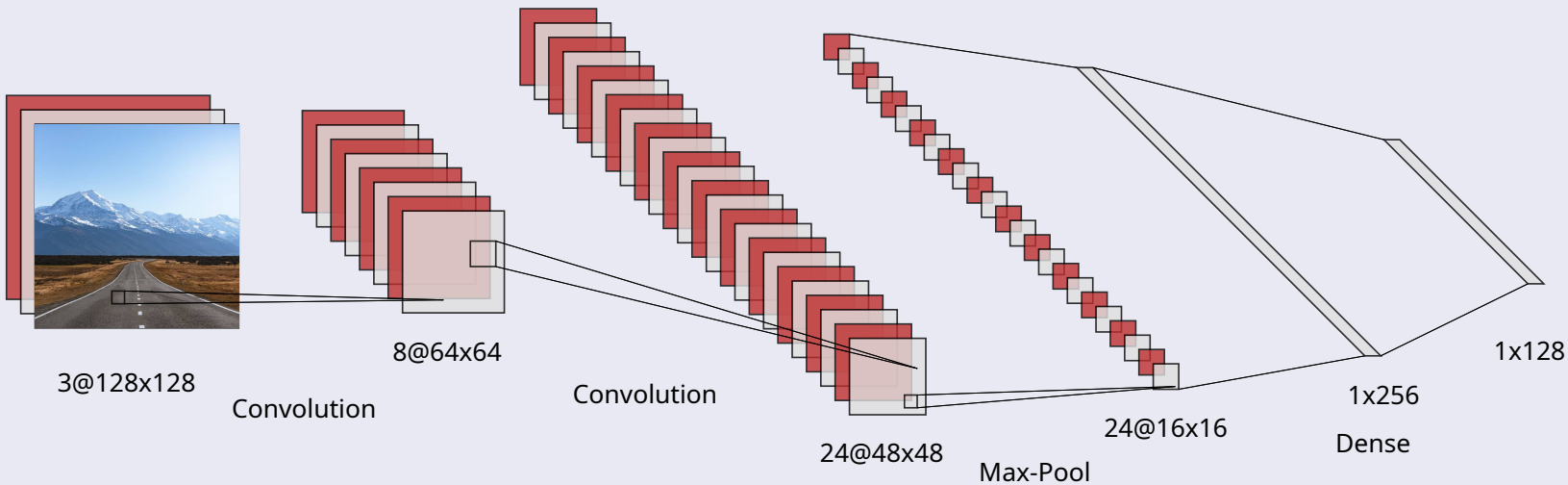
Example of CNN

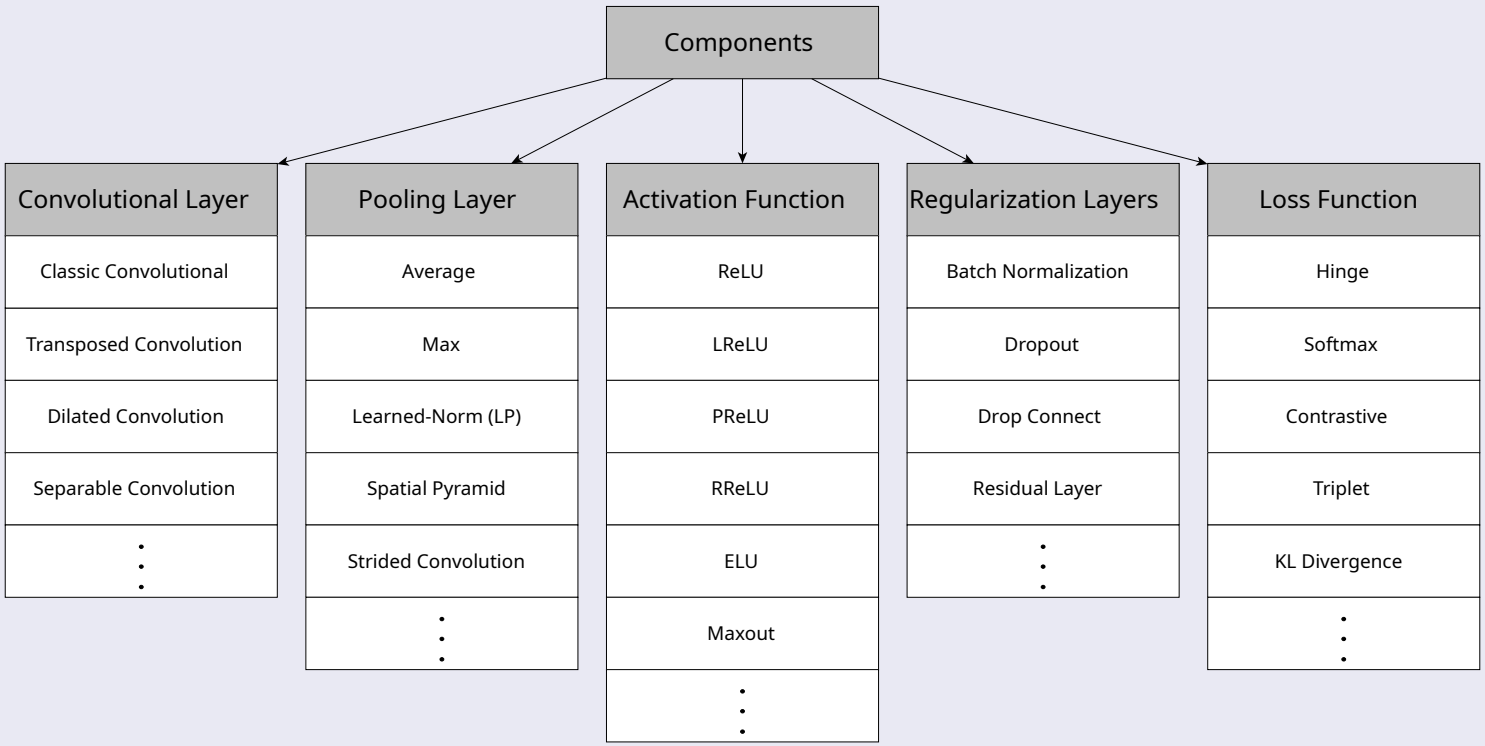
A Basic Convolutional Network



However

We will see that there are many possible architectures

- And different layers [15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25] :



Outline

We know that

Many of the existing machine learning algorithms

- They depend on the quality of the input characteristics to generate a good model.

Not only that

- The amount of these variables is also important, given that performance tends to decline as the input dimensionality increases.

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We have several techniques for that

Principal Component Analysis

$$L(\boldsymbol{u}_1) = \boldsymbol{u}_1^T S \boldsymbol{u}_1 + \lambda_1 \left(1 - \boldsymbol{u}_1^T \boldsymbol{u}_1\right)$$

Linear Locally Embeddings

$$\Phi(Y) = \sum_i \left| Y_i - \sum_j W_{ij} Y_j \right|^2$$

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- Uniform Manifold Approximation and Projection for Dimension Reduction [26]

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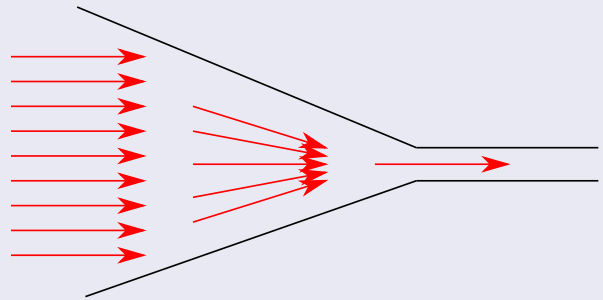
Therefore

We have the need to codify the original feature into better ones

- This can be done by a series of mappings that act as funnels, How?



Basically, we have a series of mappings

$$x \in \mathbb{R}^{n_1} \to f_1(x) \in \mathbb{R}^{n_2} \to f_2(x_1) \in \mathbb{R}^{n_3} \cdots \longrightarrow f_m(x_{m-1}) \in \mathbb{R}^{n_{m+1}}$$

Where

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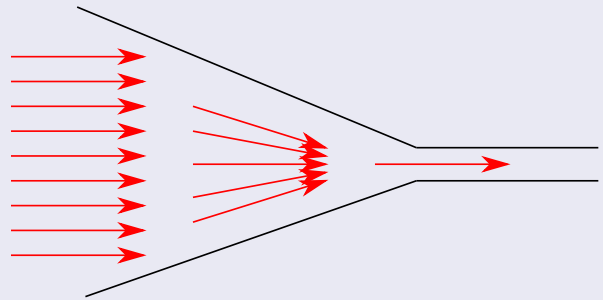

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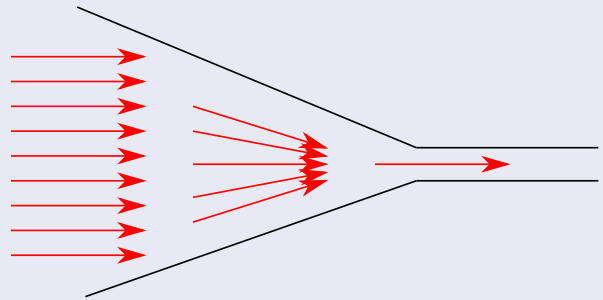

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Then, we can use linear mappings for this

With the following matrix functions

$$\sigma\left[f_{A_{i+1}}\left(x_i\right)\right] = \sigma\left(A_{i+1}x\right)$$

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- Therefore, we have the following architecture.

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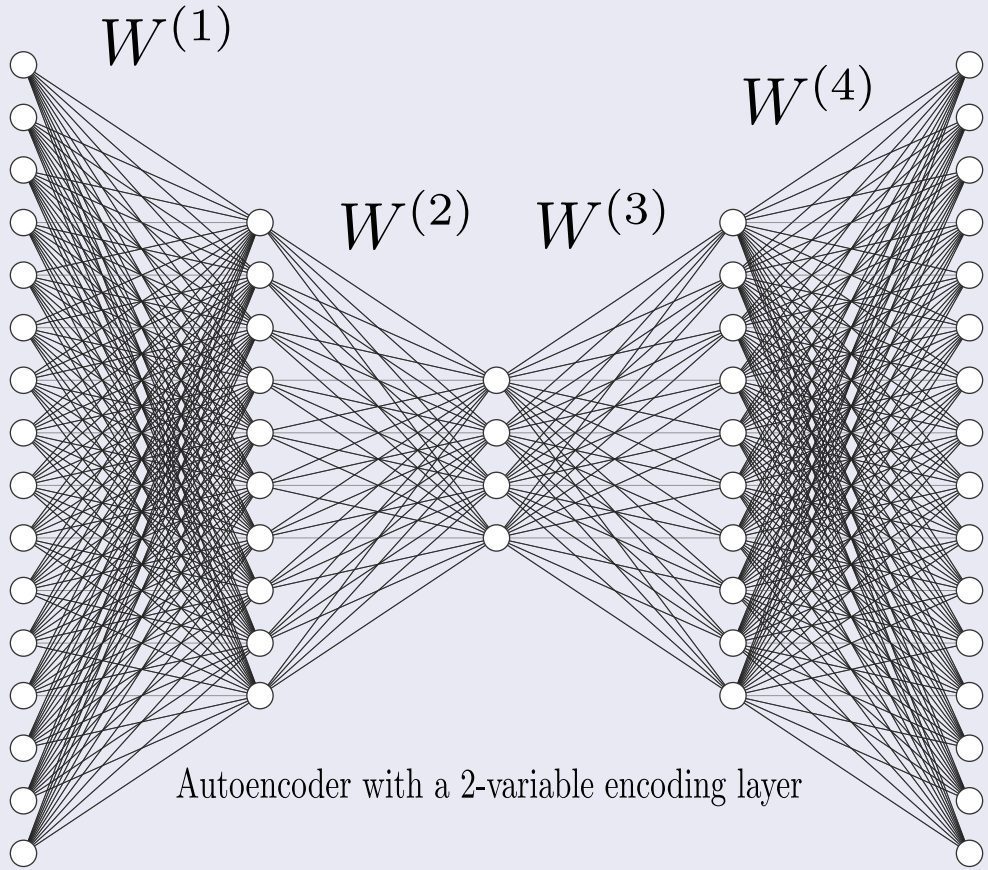
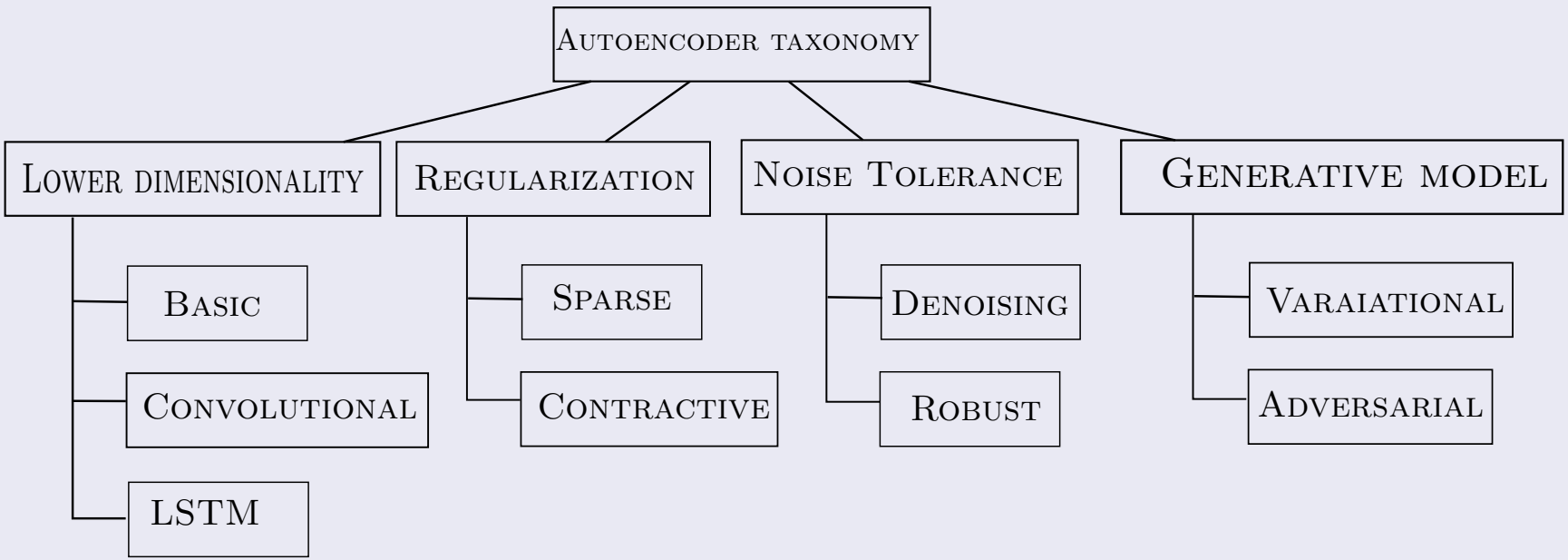
The Basic Auto Encoder Architecture

We have



Taxonomy

Most popular Auto Encoders



Outline

Generative Adversarial Networks

They can be seen as an Accept-Reject MCMC Model

- However, they do not require Markov Chains with the classic problem:
  - The independence between the samples to generate ergodic probabilities (The real one)

As in the Accept-Reject

- The **generator network** tries to produce realistic-looking samples
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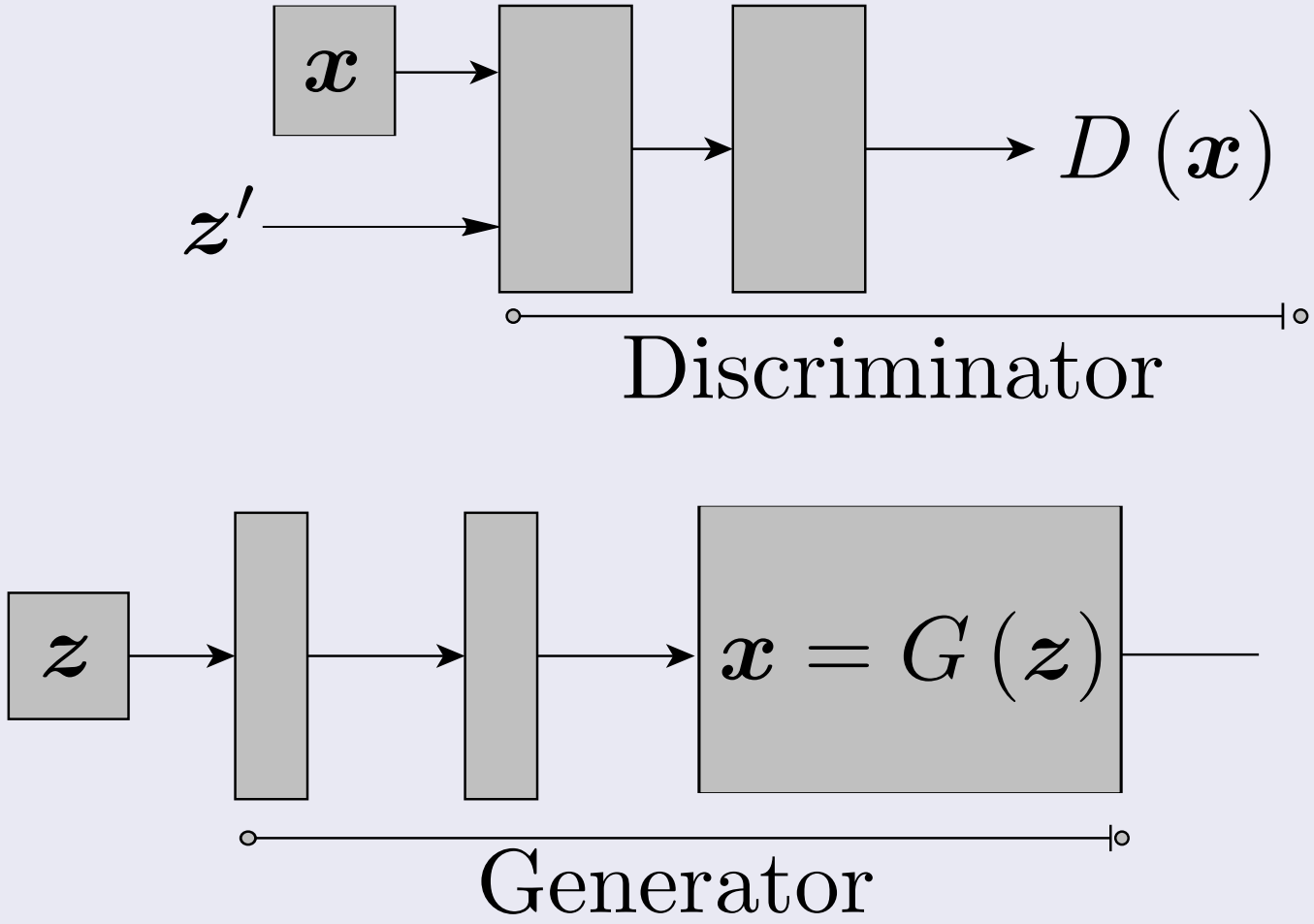
Graphically

We have the following Basic Model



Here

There is a need to join both functions

- So, we can use the idea of Backpropagation to obtain the desired minimization.

How can we do this?

- We can define a sensible learning criterion when the dataset is not linearly separable

For this, we can use the logistic cross-entropy loss (We will explain more about this later)

$$L_{LCE}(z,t) = L_{CE}(\sigma(z),t) = t\log(\sigma(z)) + (1-t)\log(1-\sigma(z))$$

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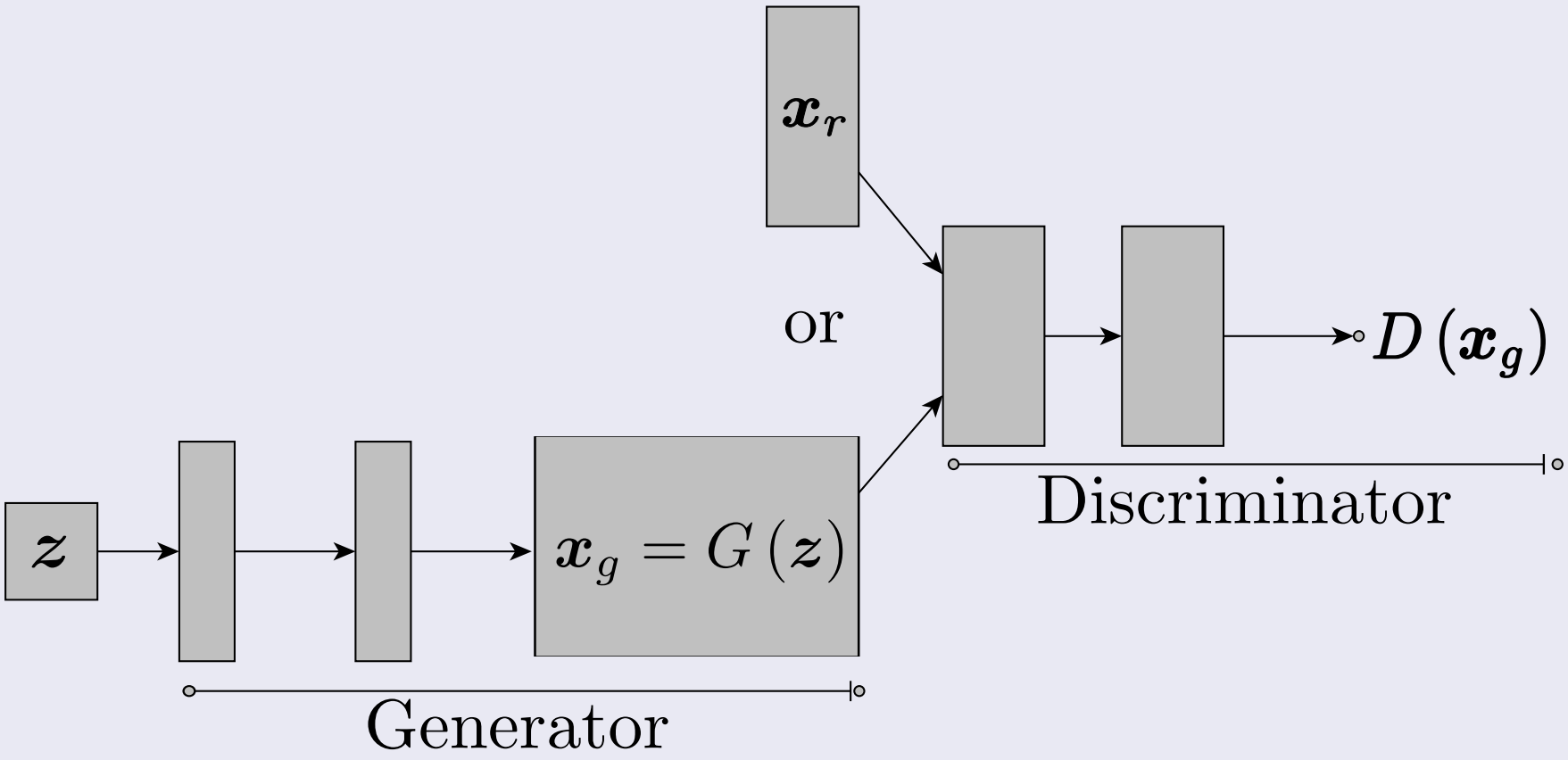
The following architecture use this idea



In this basic Generator

D denote the discriminator's predicted probability of being data

$$\mathcal{J}_D = E_{\boldsymbol{x}\sim\mathcal{D}}\left[-\log D\left(\boldsymbol{x}\right)\right] + E_{\boldsymbol{z}}\left[-\log\left(1 - D\left(G\left(\boldsymbol{z}\right)\right)\right)\right]$$

One possible cost function for the generator

$$\mathcal{J}_G = -\mathcal{J}_D = const + E_{\boldsymbol{z}}\left[\log\left(1 - D\left(G\left(\boldsymbol{z}\right)\right)\right)\right]$$

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The minimax formulation

- Since the generator and discriminator are playing a zero-sum game against each other.

Basically

$$\max_G \min_D \mathcal{J}_D$$

There are other examples using the LSE [27]

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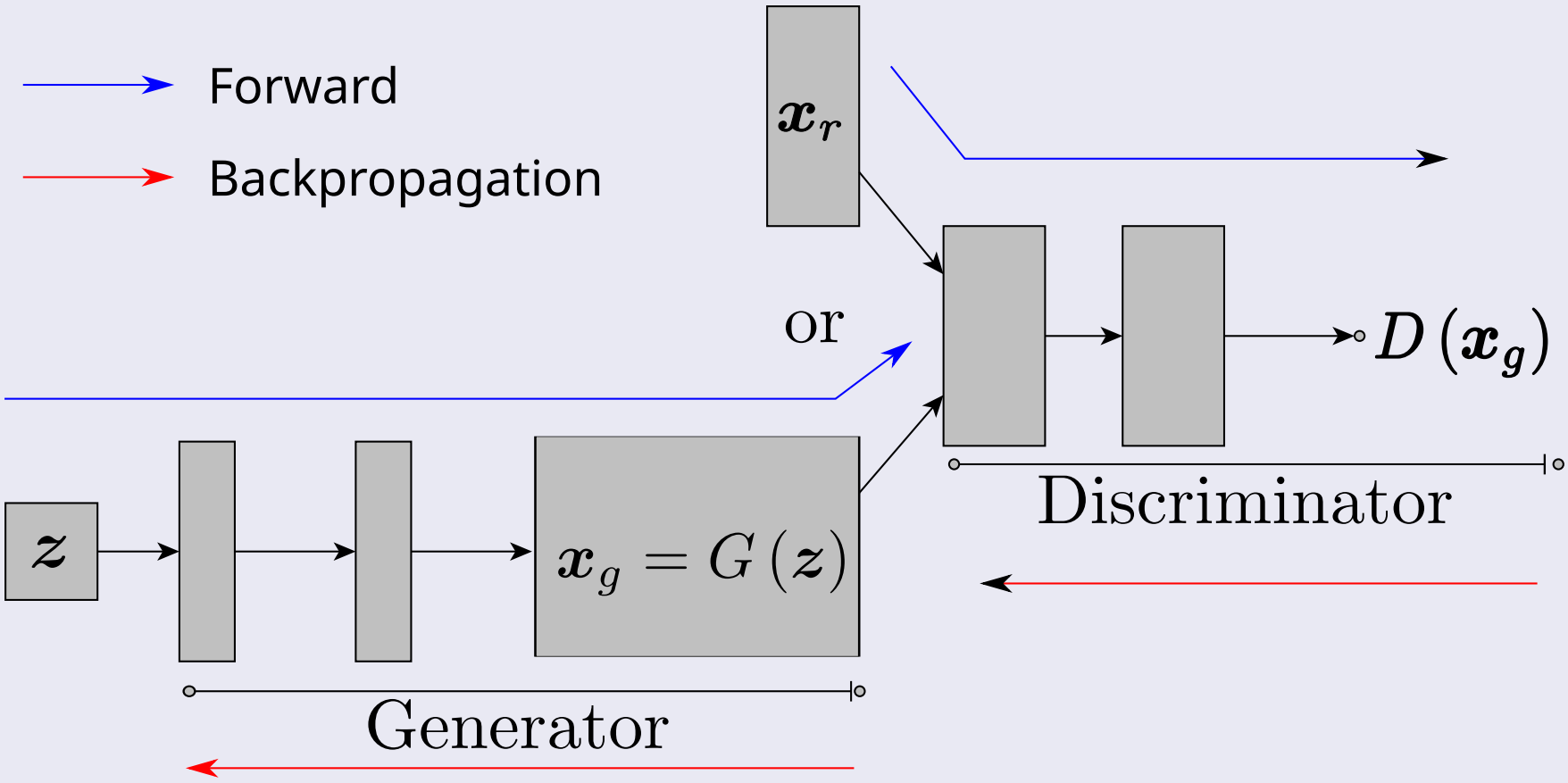
Therefore, we have two updates

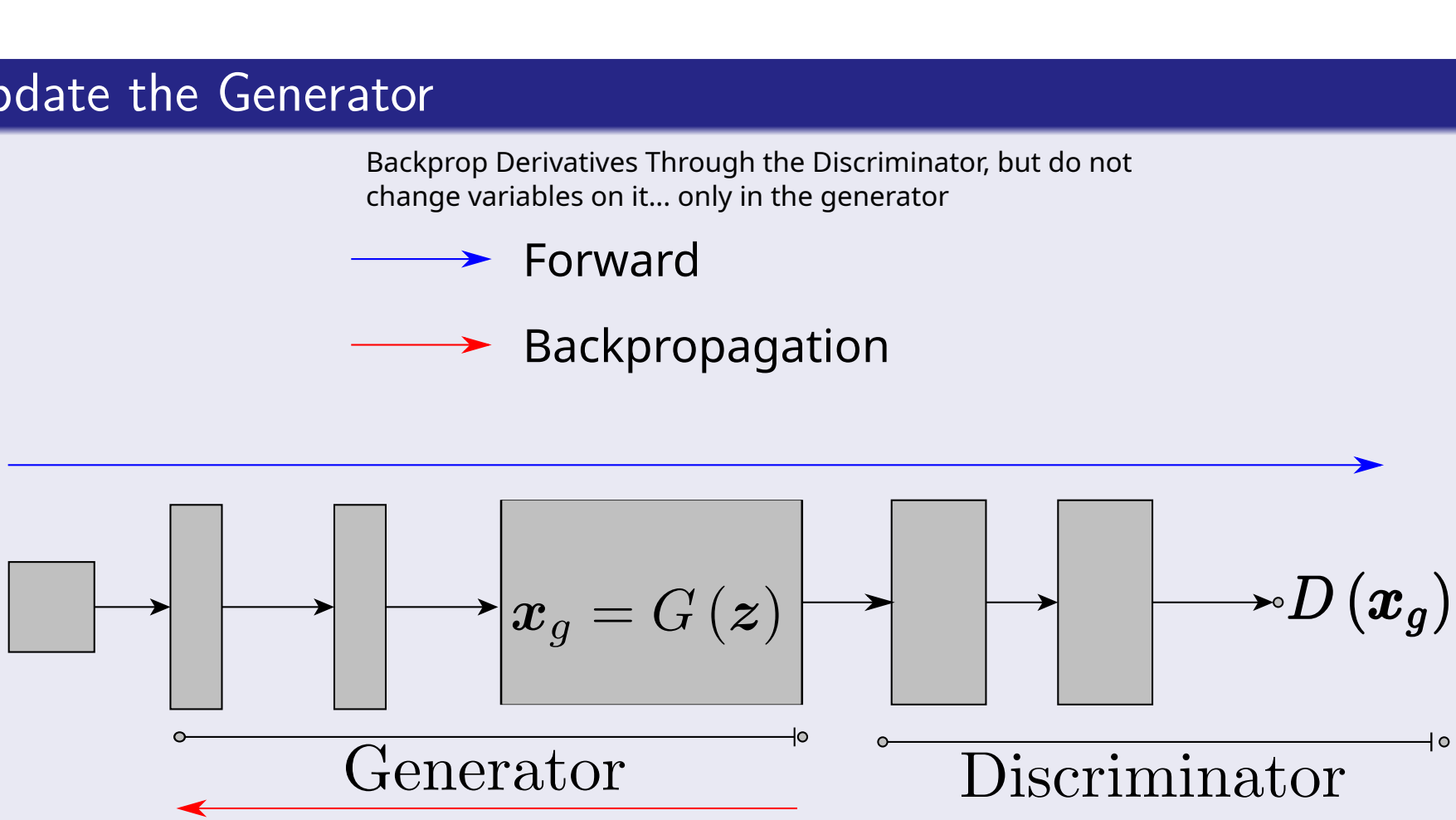
First update the Discriminator



Now

Update the Generator

Backprop Derivatives Through the Discriminator, but do not change variables on it... only in the generator



Outline

The Basic Energy Models

We have that the Boltzmann Machines

- A Boltzmann machine is a network of units that are connected to each other

Here, we have N be the number of units

- Each unit takes a binary value in $\{0, 1\}$
  - Represented by a random variable X_i, $i = 1, ..., N$.

Additionally, it has parameters

- Bias b_i
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The Energy Based Structure

The energy of the Boltzmann machine is defined by

$$E_{W,\boldsymbol{b}}[\boldsymbol{x}] = -\sum_{i=1}^{N} b_i x_i - \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} w_{ij} x_i x_j = -\boldsymbol{b}^T \boldsymbol{x} - \boldsymbol{x}^T W \boldsymbol{x}$$

This allows to define a probability distribution

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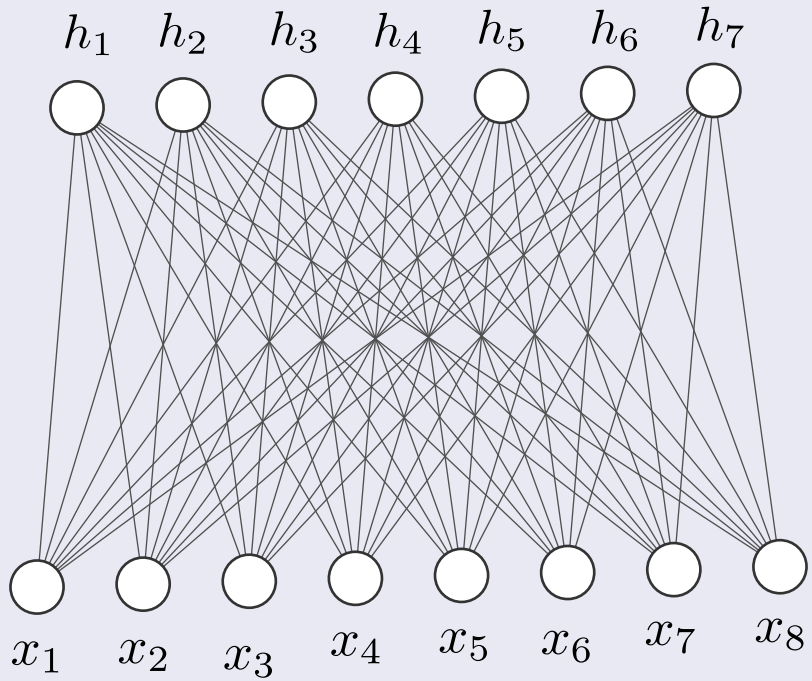
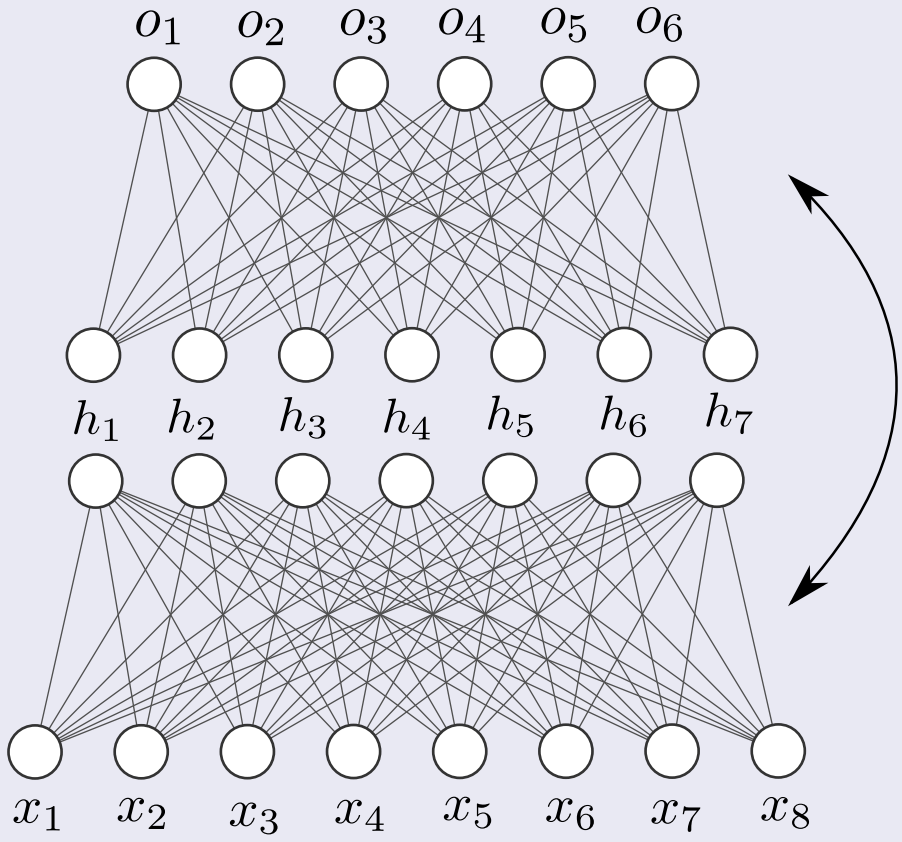
Example

Restricted Boltzmann Machines where the connectivity is layer by layer



Thus, using it as a basic model

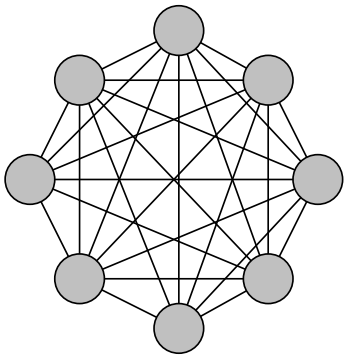
We can stack them into a multiple layer model



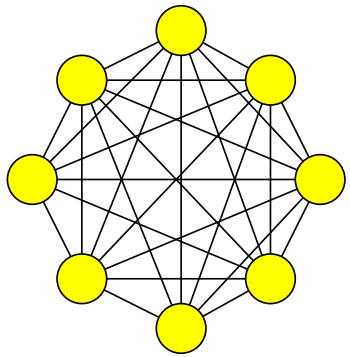
Outline

There Are Many More!!! Here a few more...

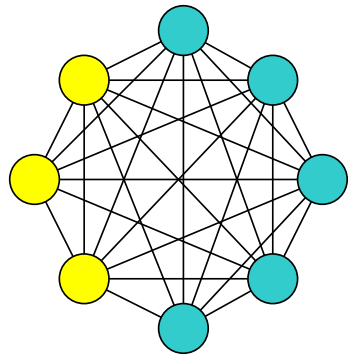
Markov Chain



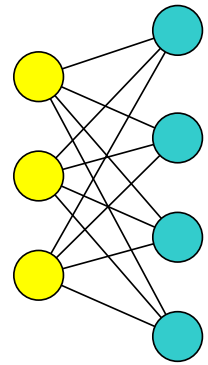
Hopfield Network



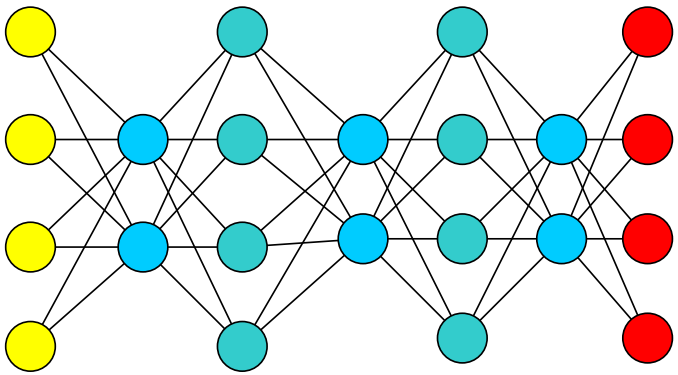
Boltzmann Machine



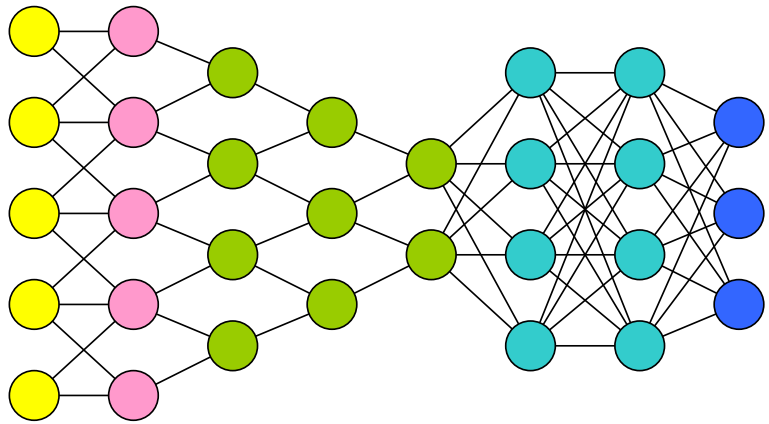
Restricted BM



Deep Belief Network

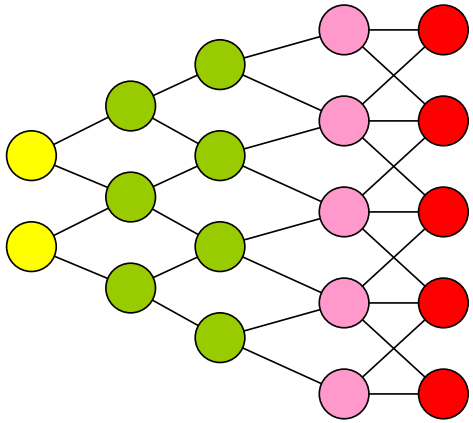


Convolutional Network

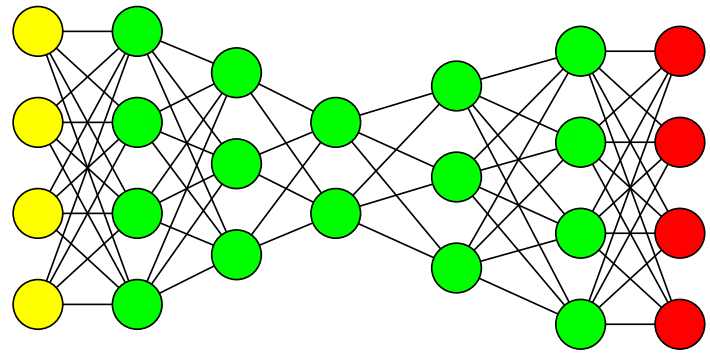


Furthermore

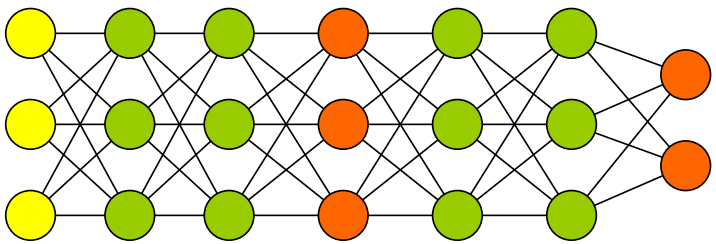
Deconvolutional Network



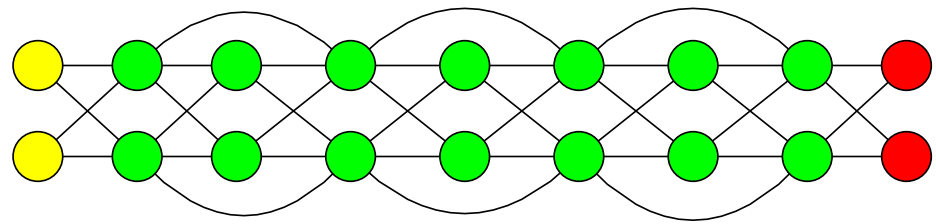
Autoencoder



Generative Adversarial Network



Deep Residual Network



Outline

Definition

Degradation Problem

- With the network depth increasing, accuracy gets saturated (which might be unsurprising) and then degrades rapidly.

Something Notable

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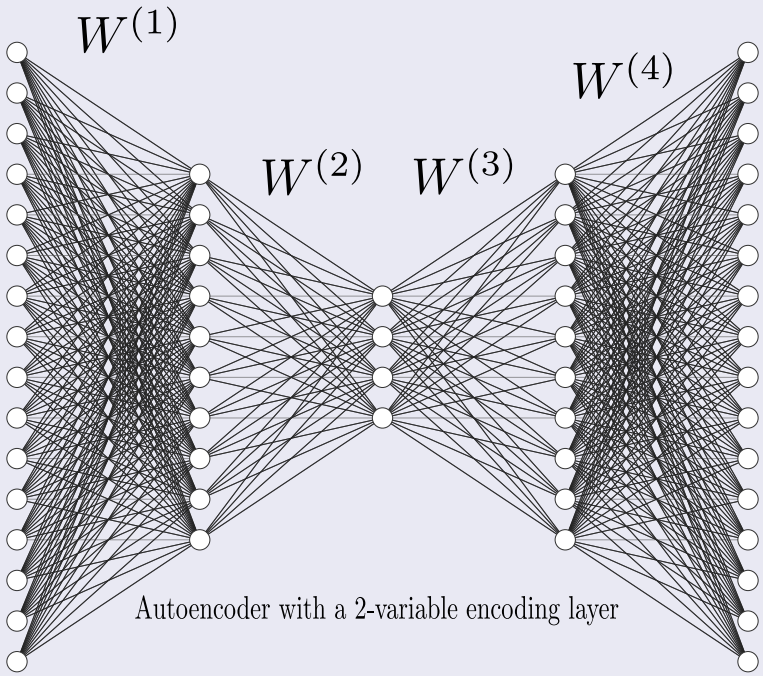
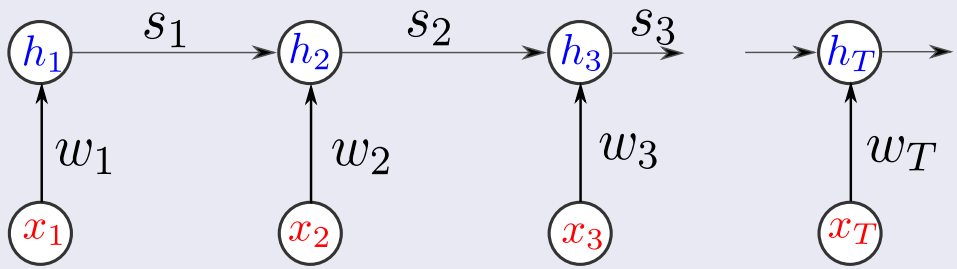


Consider a simple recurrent network

We have this simplified version using constants



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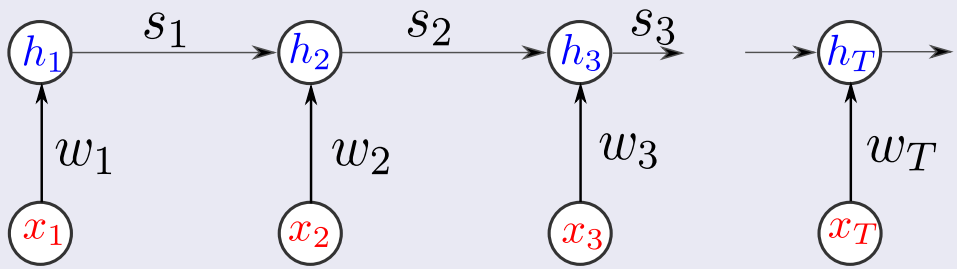

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Backpropagation Rules

Then, we get the following backpropagation rules

$$\frac{\partial h_t}{\partial w_i} = \frac{\partial h_t}{\partial h_{t-1}} \times \frac{\partial h_{t-1}}{\partial h_{t-2}} \times \ldots \times \frac{\partial h_i}{\partial w_i}$$

$$\frac{\partial h_t}{\partial s_i} = \frac{\partial h_t}{\partial h_{t-1}} \times \frac{\partial h_{t-1}}{\partial h_{t-2}} \times \ldots \times \frac{\partial h_{i+1}}{\partial s_i}$$

Then, we have

By Using Our simplifying assumption that

$$\frac{\partial h_t}{\partial h_{t-1}} = \frac{\partial \left(w_t x_t + s_{t-1} h_{t-1} \right)}{\partial h_{t-1}} = s_{t-1}$$

And for $\frac{\partial h_t}{\partial w_i}$

$$\frac{\partial h_i}{\partial w_i} = x_i$$

Finally, we have that

$$\frac{\partial h_t}{\partial w_i} = x_i \left[\prod_{k=t-1}^{i-1} s_k \right]$$

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It is clear that

Unless the s_k's are near to 1

- You have the vanishing gradient if $s_k \in [0, 1)$ for all k.
- You have the exploding gradient if $s_k \in (1, +\infty]$ for all k.

Even with activation functions

- These terms tend to appear in the Deep Learners when Backpropagation is done

In the case of Forward

- We have many activation function that squash the signal...

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Outline

Instead of doing this

Let us to do the following

$$f(x) = 3.5x(1-x)$$

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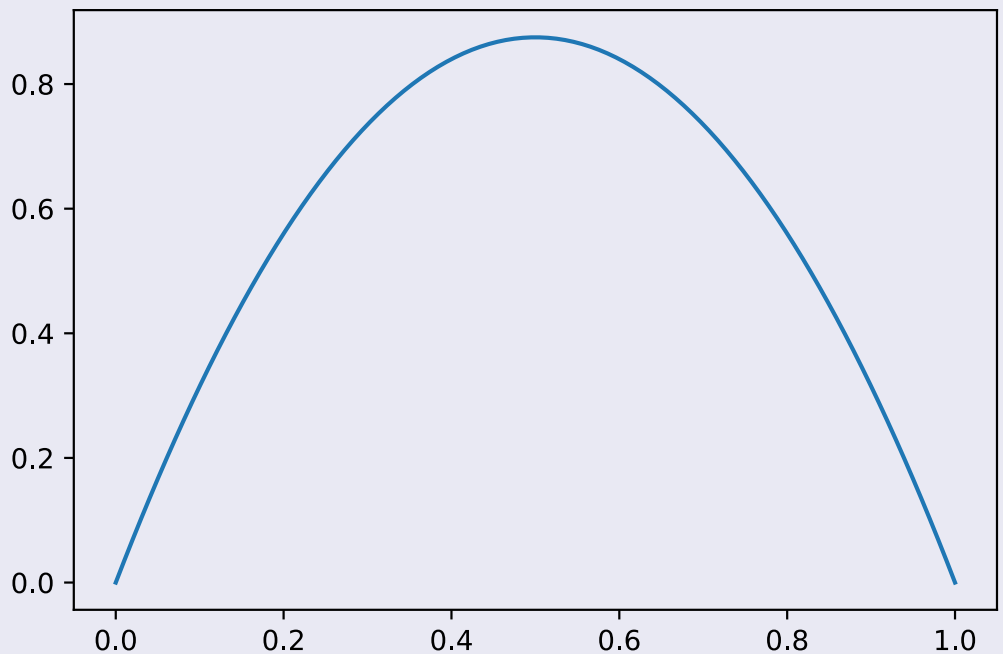
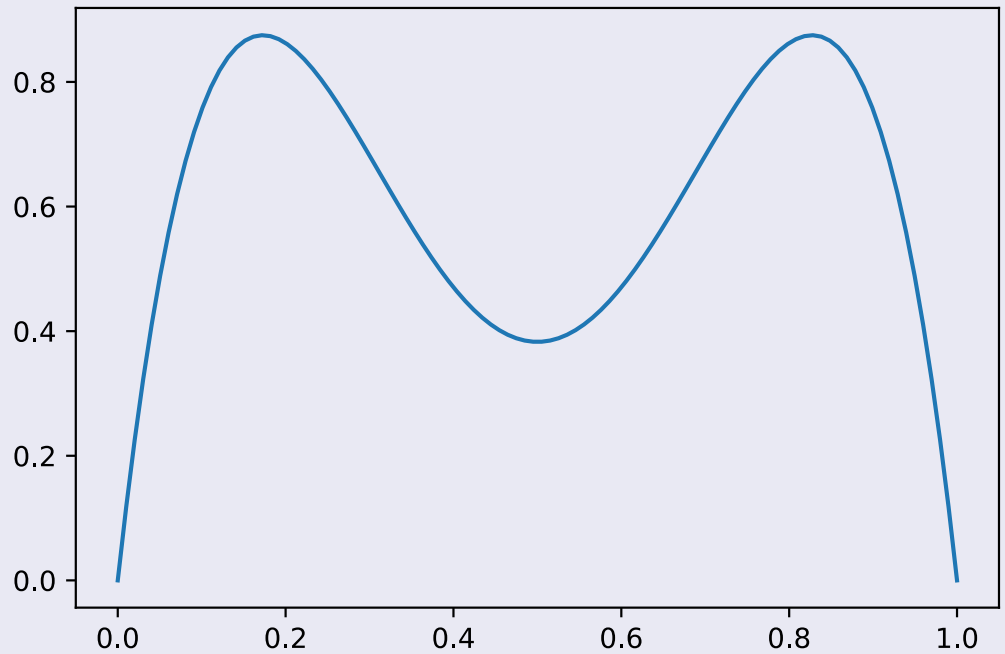


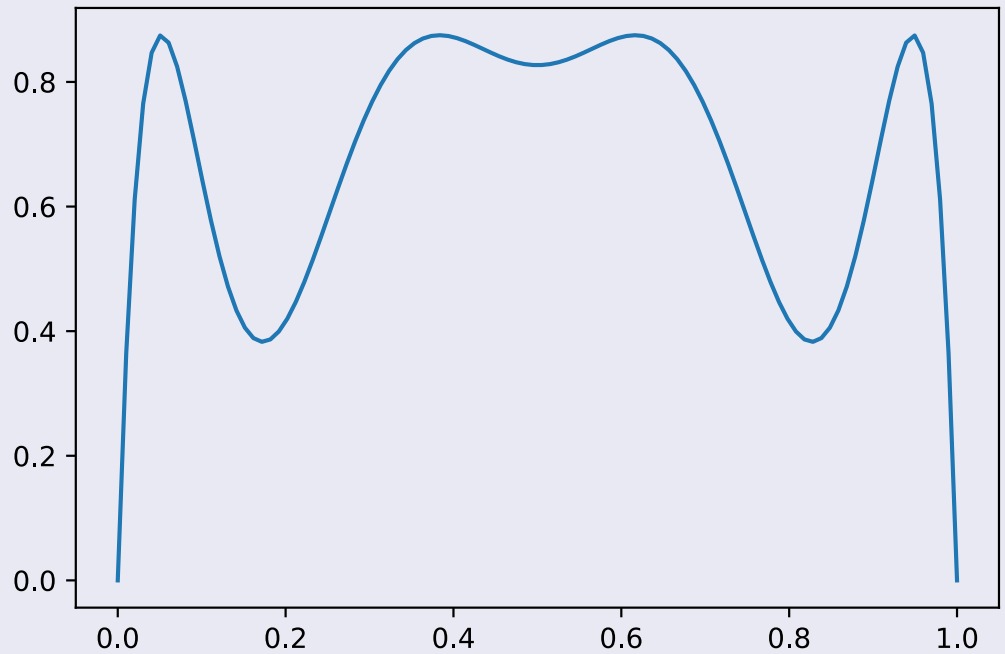
Now, as we compound the function

Second one, $y = f \circ f\,(x)$



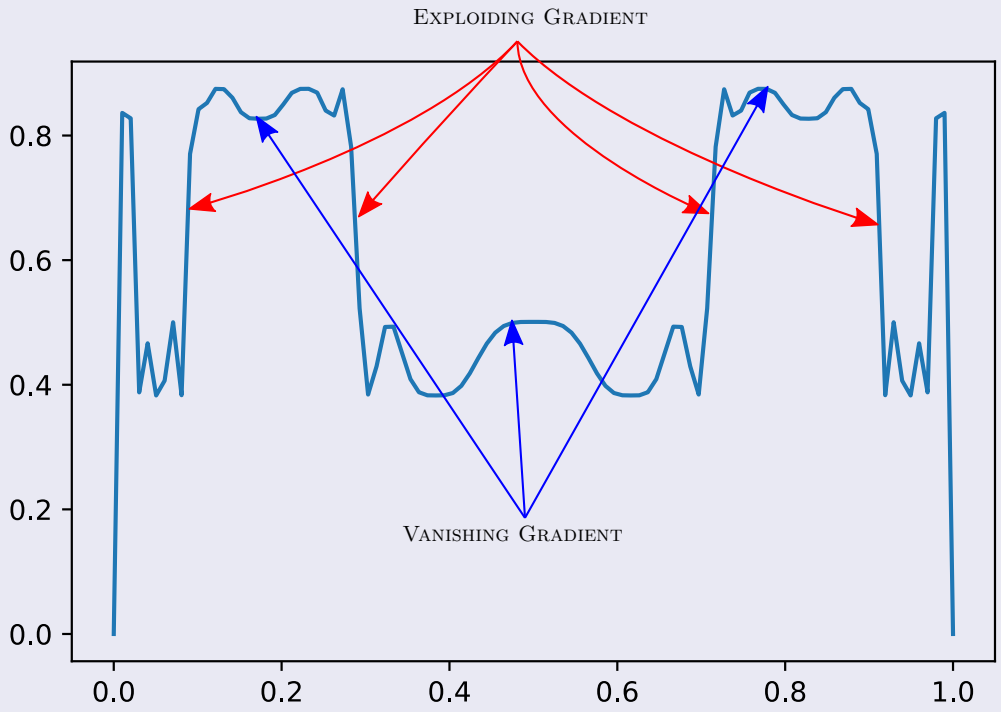
Now, as we increment iterations

Third one, $y = f \circ f \circ f\,(x)$



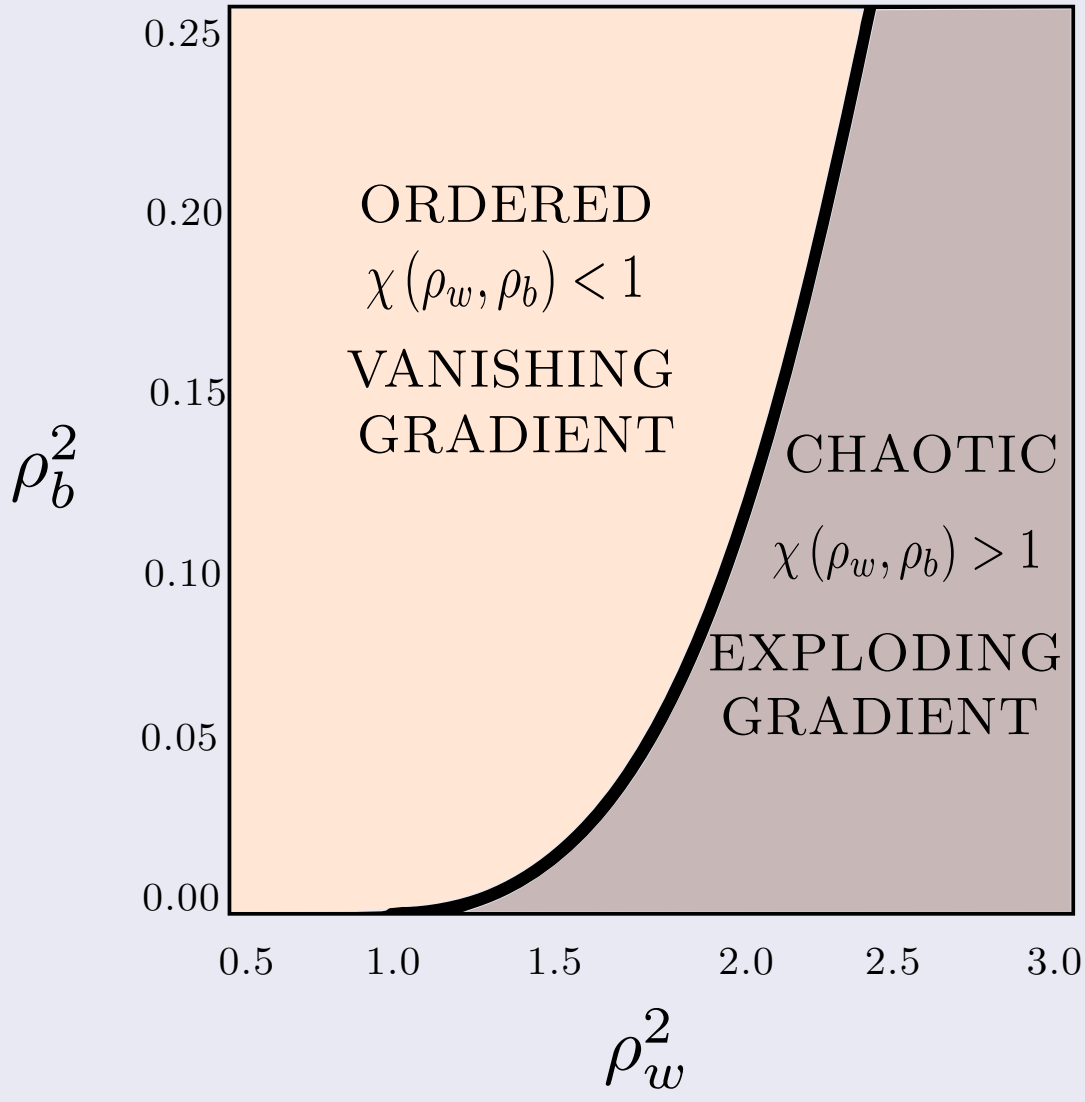
Finally

We see the increment in the gradient part negative or positive



Actually, we have

A Frontier defining the Vanishing and Exploding Gradient [28]



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Actually

Eventually, the iterates go to infinity or zero OR

- They wind up at a fixed point...

A Fixed Point?

$$x = f(x)$$

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Basically, Attractors and Repulsors

The fixed points can be thought

- Some fixed points repel the iterates; **these are called sources.**
- Other fixed points attract the iterates; **these are called sinks.**

Basically $f'(x) < 1$ are sinks and $f'(x) > 1$ are sources

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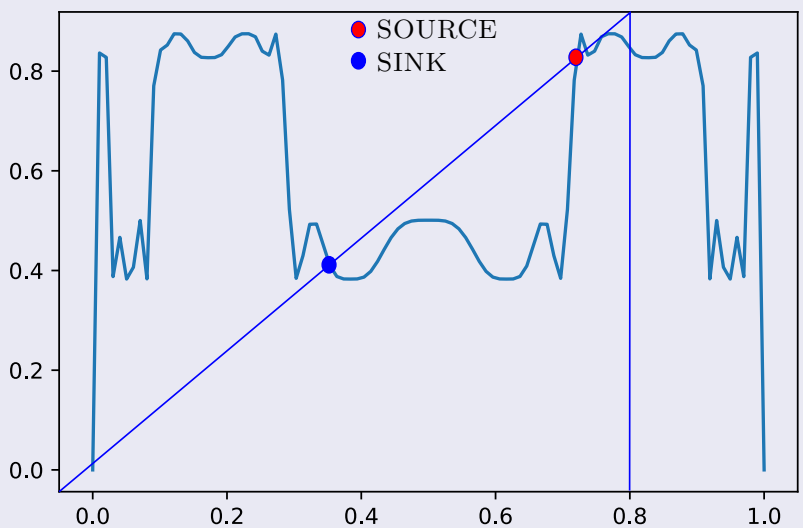
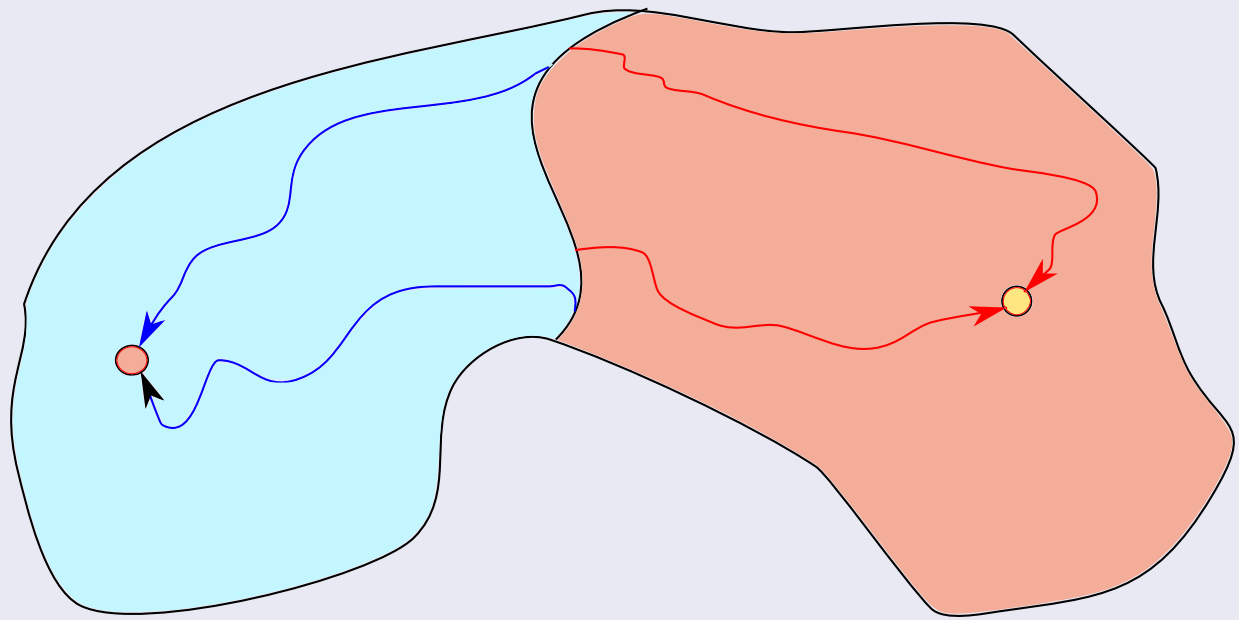


Areas of attraction

Basically, we have that there are areas the pull in the iterations of the function



These fixed points

In Deep Structures as RNN without sigmoid functions

$$\boldsymbol{h}_t = W_{sd}\boldsymbol{x}_t + U_{ss}\boldsymbol{h}_{t-1}$$
$$\boldsymbol{y}_t = V_{os}\boldsymbol{h}_t$$

We have that for a fixed point

$$\boldsymbol{x}_t = V_{os}\left[W_{sd}\boldsymbol{x}_t + U_{ss}\boldsymbol{h}_{t-1}\right]$$

Then, we have that

$$\boldsymbol{x}_t = V_{os}W_{sd}\boldsymbol{x}_t + V_{os}U_{ss}\boldsymbol{h}_{t-1} = I\boldsymbol{x}_t + 0$$

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Therefore

We have that

$$V_{os}W_{sd} \approx I \text{ and } \boldsymbol{h}_{t-1} \approx 0$$

They define an area

Where V_{os} and W_{sd}

- They are the inverse of each other

And the hidden state is almost zero

- Basically they fixed point converts a RNN without activation functions into a linear model

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Gradient Clipping

We prevent gradient from blowing up by rescaling to a certain value

$$\|\nabla_\theta L\| > \eta \Longrightarrow \nabla_\theta L = \frac{\eta \nabla_\theta L}{\|\nabla_\theta L\|}$$

We have a series of nice analysis at [29]

- "Analysis of Gradient Clipping and Adaptive Scaling with a Relaxed Smoothness Condition" by Zhang et al.

$$\min_{x \in \mathbb{R}^d} f(x)$$

In general this problem is intractable

- We look for locality i.e. we search fro a point x such that for a small ϵ,

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For this, we assume that

We have that the following conditions are true in the following neighborhood with initial point $\boldsymbol{x}_o$

$$S = \{\boldsymbol{x} | \exists \boldsymbol{y} \text{ such that } f(\boldsymbol{y}) \leq f(\boldsymbol{x}_o), \text{ and } \|\boldsymbol{x} - \boldsymbol{y}\| \leq 1\}$$

Assumption 1

- Function f is lower bounded by f^* i.e. $f^*(\boldsymbol{x}) \leq f(\boldsymbol{x})$ for all $\boldsymbol{x} \in S$

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In addition, they added the following assumption

New relaxed smoothness assumption

- Assumption 3 (L_0, L_1) −smoothness
  - f is (L_0, L_1) −smooth, if there exist positive constants L_0 and L_1 such that $\left\|\nabla^2 f(\boldsymbol{x})\right\| \leq L_0 + L_1 \|\nabla f(\boldsymbol{x})\|$.

Using the former two Assumptions

They proposed bounds of convergence for the clipped version of gradient descent

$$x_{k+1} = x_k - \eta \nabla f(x_k)$$

The Clipped Gradient Descent (CGD)

$$x_{k+1} = x_k - h_c \nabla f(x_k), \text{ where } h_c = \min\left\{\eta_c, \frac{\gamma \eta_c}{\|\nabla f(x)\|}\right\}$$

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Remark

Clipped GD and NGD are almost equivalent

- If we set $\gamma\eta_c = \eta_n$ and $\eta_c = \frac{\eta_n}{\beta}$ then

$$\frac{1}{2}h_c \leq h_n \leq 2h_c$$

A Natural Question

Definition

- The objective f is called L-smooth if $\|\nabla f(x) - \nabla f(y)\| \leq L \|x - y\|$ for all $x, y \in \mathbb{R}^d$

This is equivalent under a twice differentiable function f

$$\left\|\nabla^2 f(x)\right\| \leq L$$

Then, if you expand the function using the second order Taylor expansion

$$f(y) \approx f(x) + \nabla^T f(x)(y - x) + \frac{1}{2}(y - x)^T \nabla^2 f(x)(y - x)$$

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Then, it is possible to use the 3^{rd} Assumption

We have that

$$f(y) \leq f(x) + \nabla^T f(x)(y-x) + \frac{1}{2}L\|y-x\|^2$$

Then fixing all the other variables and assuming $y = x - h\nabla f(x)$

$$h^* = \arg\min_h \left[f(x) - h\|\nabla f(x)\|^2 + \frac{1}{2}Lh^2\|\nabla f(x)\|^2 \right] = \frac{1}{L}$$

Basically

- This choice of h leads to GD with a fixed step.

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- "Is clipped gradient descent optimized for a different smoothness condition?"

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Then, we have

$$L(x) = \frac{\|\nabla f(x)\| + \beta}{\eta}$$

Assumption 3 by using $\|\nabla^2 f(x)\| \leq L$

- (L_0, L_1)-smoothness. f is (L_0, L_1)-smooth, if there exist positive L_0 and L_1 such that $\|\nabla^2 f(x)\| \leq L_0 + L_1\|\nabla f(x)\|$
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The final Theorem

Theorem (CGD) [29]

- Assume that Assumptions 1, 2, and 3 hold in set S. With parameters

$$\eta_c = \frac{1}{10L_o} \text{ and } \gamma = \min\left\{\frac{1}{\eta_c}, \frac{1}{10L_o\eta_c}\right\},$$

  - Then Clipped GD terminates in

$$\frac{20L_0\left(f\left(x_0\right)-f^*\right)}{\epsilon^2} + \frac{20\max\left\{1, L_1^2\right\}\left(f\left(x_0\right)-f^*\right)}{L_0} \text{ iterations}$$

Remarks

The paper

- It points out to a high correlation between the Jacobian and the Hessian

There are more work to be done

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Another way to stabilize the network

Data Normalization

- Standardization is the most popular form of preprocessing
  - Normally mean subtraction and subsequent scaling by the standard deviation.

Mean subtraction

$$\mu = \frac{1}{N}\sum_{i=1}^{N} x_i \text{ then } x_i^c = x_i - \mu$$

Finally

- Standardization refers to altering the data dimensions such that they are of approximately the same scale.

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$$x_i^s = \frac{x_i - \mu}{\sigma}$$

However, there other tricks, Bengio et al [30]

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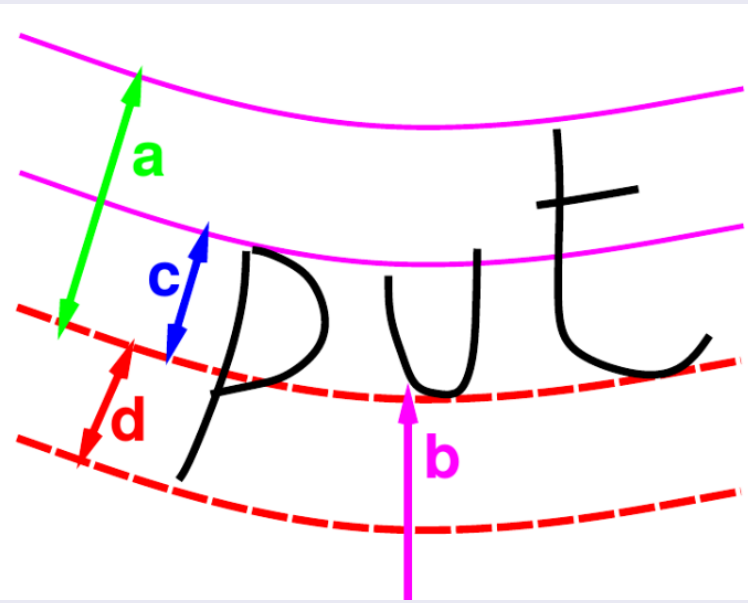

a - ascender curve height relative to baseline
b - baseline absolute vertical position
c - core line position
d - descenders curve position
κ - curvature
s - angle

Softmax Scaling

Thus

- All new features have zero mean and unit variance.

Further

- Other linear techniques limit the feature values in the range of $[0, 1]$ or $[-1, 1]$ by proper scaling.

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Softmax Scaling

Thus

- All new features have zero mean and unit variance.

Further

- Other linear techniques limit the feature values in the range of $[0, 1]$ or $[-1, 1]$ by proper scaling.

However

- We can nonlinear mapping. For example the softmax scaling.

Steps of Softmax Scaling

Softmax Scaling

- It consists of two steps

First one

$$y_{ik} = \frac{x_{ik} - \overline{x}_k}{\sigma} \tag{3}$$

Second one

$$\hat{x}_{ik} = \frac{1}{1 + \exp\{-y_{ik}\}} \tag{4}$$

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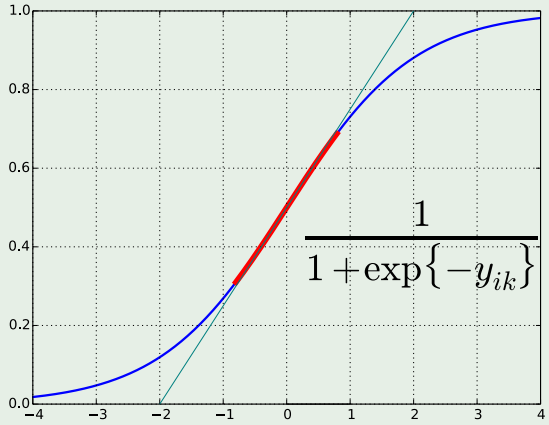
Explanation

Notice the red area is almost flat!!!



Thus, we have that

- The red region represents values of y inside of the region defined by the mean and variance (small values of y).
- Then, if we have those values x behaves as a linear function.

And values too away from the mean

- They are squashed by the exponential part of the function.

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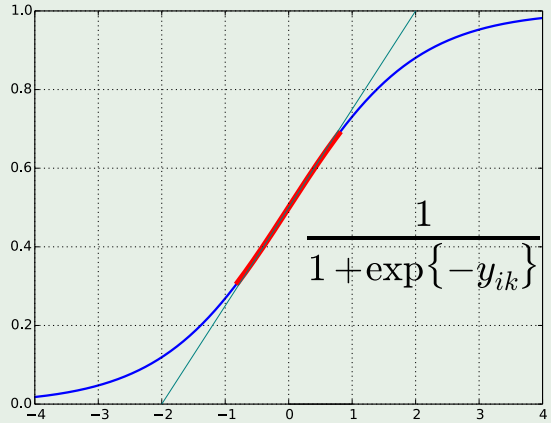

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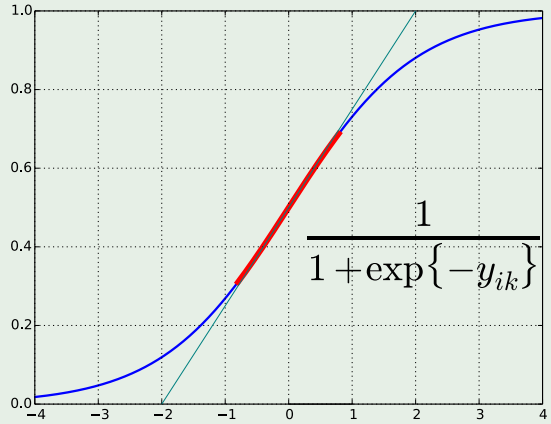

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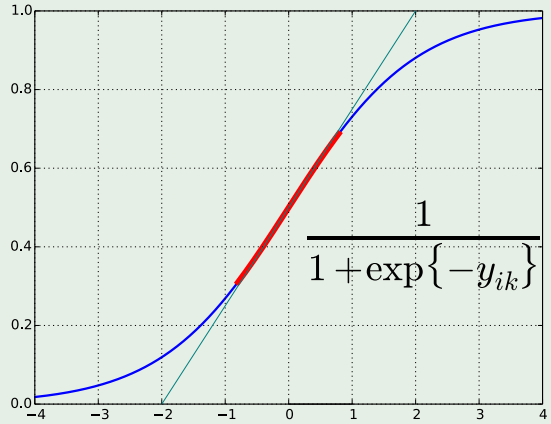

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Outline

Here, the people at Google [22] around 2015

They commented in the "Internal Covariate Shift Phenomena"

- Due to the change in the distribution of each layer's input

They claim

- The min-batch forces to have those changes which impact on the learning capabilities of the network.

In Neural Networks, they define this

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They gave the following reasons

Consider a layer with the input u that adds the learned bias b

- Then, it normalizes the result by subtracting the mean of the activation over the training data:

$$\widehat{\boldsymbol{x}} = \boldsymbol{x} - E\left[\boldsymbol{x}\right]$$

  - $\mathcal{X} = \{\boldsymbol{x}, ..., \boldsymbol{x}_N\}$ the data samples and $E\left[\boldsymbol{x}\right] = \frac{1}{N}\sum_{i=1}^{N} \boldsymbol{x}_i$

Now, if the gradient ignores the dependence of $E\left[\boldsymbol{x}\right]$ on b

- Then $b = b + \Delta b$ where $\Delta b \propto -\frac{\partial l}{\partial \widehat{x}}$

Finally

$$u + (b + \Delta b) - E[u + (b + \Delta b)] = u + b - E[u + b]$$

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Normalization via Mini-Batch Statistic

It is possible to describe the normalization as a transformation layer

$$\widehat{\boldsymbol{x}} = Norm\left(\boldsymbol{x}, \mathcal{X}\right)$$

- Which depends on all the training samples $\mathcal{X}$ which also depends on the layer parameters

For back-propagation, we will need to generate the following terms

$$\frac{\partial Norm\left(\boldsymbol{x}, \mathcal{X}\right)}{\partial \boldsymbol{x}} \text{ and } \frac{\partial Norm\left(\boldsymbol{x}, \mathcal{X}\right)}{\partial \mathcal{X}}$$

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Normalization via Mini-Batch Statistic

Problem!!!

- whitening the layer inputs is expensive, as it requires computing the covariance matrix

$$Cov\left[\boldsymbol{x}\right] = E_{\boldsymbol{x}\in\mathcal{X}}\left[\boldsymbol{x}\boldsymbol{x}^T\right] \text{ and } E\left[\boldsymbol{x}\right]E\left[\boldsymbol{x}\right]^T$$

  - To produce the whitened activations

Therefore

A Better Options, we can normalize each dimension

$$\widehat{\boldsymbol{x}}^{(k)} = \frac{\boldsymbol{x}^{(k)} - \mu}{\sigma}$$

- with $\mu = E\left[\boldsymbol{x}^{(k)}\right]$ and $\sigma^2 = Var\left[\boldsymbol{x}^{(k)}\right]$

This allows to speed up convergence

- Simply normalizing each input of a layer may change what the layer can represent.

So, we need to insert a transformation in the network

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The Linear transformation

$$\boldsymbol{y}^{(k)} = \gamma^{(k)}\widehat{\boldsymbol{x}}^{(k)} + \beta^{(k)}$$

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Batch Normalizing Transform

Input: Values of $\boldsymbol{x}$ over a mini-batch: $\mathcal{B} = \{\boldsymbol{x}_{1\ldots m}\}$, Parameters to be learned: γ, β

Output: $\{y_i = BN_{\gamma,\beta}(\boldsymbol{x}_i)\}$

1. $\mu_{\mathcal{B}} = \frac{1}{m}\sum_{i=1}^{m} \boldsymbol{x}_i$
2. $\sigma_{\mathcal{B}}^2 = \frac{1}{m}\sum_{i=1}^{m} (\boldsymbol{x}_i - \mu)^2$
3. $\widehat{x} = \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}}$
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Backpropagation

We have the following equations by using the loss function l

1. $\frac{\partial l}{\partial \widehat{\boldsymbol{x}}_i} = \frac{\partial l}{\partial \boldsymbol{y}_i} \times \gamma$
2. $\frac{\partial l}{\partial \sigma_{\mathcal{B}}^2} = \sum_{i=1}^{m} \frac{\partial l}{\partial \widehat{x}_i} \times (x_i - \mu_{\mathcal{B}}) \times \left(-\frac{1}{2}\right) \times (\sigma_{\mathcal{B}}^2 + \epsilon)^{-\frac{3}{2}}$
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Training Batch Normalization Networks

Input: Network N with trainable parameters Θ; subset of activations $\left\{x^{(k)}\right\}_{k=1}^{K}$

Output: Batch-normalized network for inference N_{BN}^{inf}

1. $N_{BN}^{tr} = N$ // Training BN network
2. for $k = 1 \ldots K$ do
3. Add transformation $y^{(k)} = BN_{\gamma^{(k)},\beta^{(k)}}\left(x^{(k)}\right)$ to N_{BN}^{tr}
4. Modify each layer in N_{BN}^{tr} with input $x^{(k)}$ to take $y^{(k)}$ instead
5. Train N_{BN}^{tr} to optimize the parameters $\Theta \cup \left\{\gamma^{(k)}, \beta^{(k)}\right\}_{k=1}^{K}$
6. $N_{BN}^{inf} = N_{BN}^{tr}$ // Inference BN network with frozen parameters
7. for $k = 1 \ldots K$ do
8. Process multiple training mini-batches $\mathcal{B}$, each of size m, and average over them
9. $E[x] = E_{\mathcal{B}}[\mu_{\mathcal{B}}]$ and $Var[x] = \frac{m}{m-1} E_{\mathcal{B}}\left[\sigma_{\mathcal{B}}^2\right]$
10. In N_{BN}^{inf}, replace the transform $y = BN_{\gamma,\beta}(x)$ with
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- They found thats is not the covariance shift the one affected by it!!!

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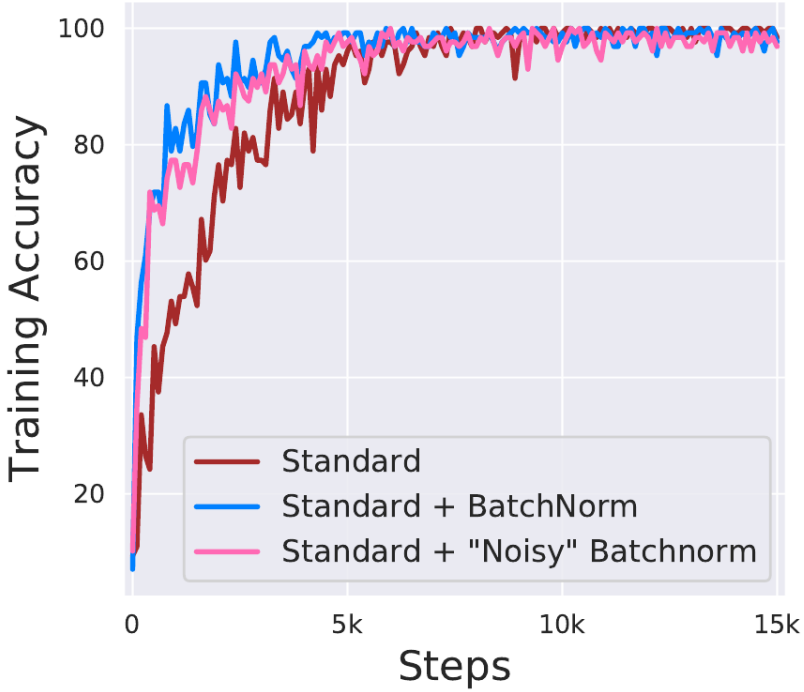
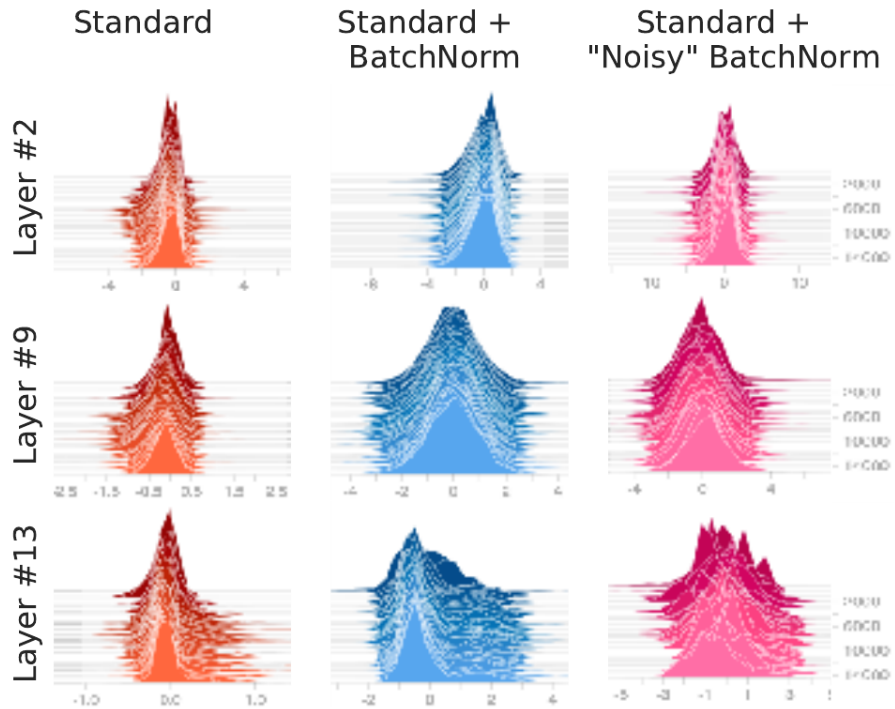
The following facts





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It does not do anything to the Internal Covariate Shift

- Actually smooth the optimization manifold
  - It is not the only way to achieve it!!!

They suggest that

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To the analysis of gradient clipping!!!

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Theorem (The effect of BatchNorm on the Lipschitzness of the loss)

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$$\left\|\nabla_{y_j}\widehat{\mathcal{L}}\right\|^2 \leq \frac{\gamma^2}{\sigma_j^2}\left[\left\|\nabla_{y_j}\mathcal{L}\right\|^2 - \frac{1}{m}\left\langle \mathbf{1}, \nabla_{y_j}\mathcal{L}\right\rangle^2 - \frac{1}{\sqrt{m}}\left\langle \nabla_{y_j}\mathcal{L}, \widehat{\boldsymbol{y}}_j\right\rangle^2\right]$$

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Outline

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- Although a simple idea

They represent a rich field of study

- Basically... From Lower Complexity Features toward more complex more informative!!!

In conclusion

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