Introduction to Neural Networks and Deep Learning

Regularization

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Outline

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Introduction

What did we see until now?

The design of learning machines from two main points:

- Statistical Point of View
- Linear Algebra and Optimization Point of View

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- Something as curve fitting...

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Remark: Where the $\boldsymbol{x}_i \sim p(\boldsymbol{x}|\Theta)$!!!

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Outline

We have the Bias-Variance

Our Final Equation

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1. Increasing the bias decreases the variance and vice versa.
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If N grows we can have a more complex model to be fitted which reduces bias and ensures low variance.

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You always need to compromise

However, you always have some a priori knowledge about the data

Allowing you to impose restrictions

Lowering the bias and the variance

Nevertheless

We have the following example to grasp better the bothersome **bias–variance dilemma**.

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Assume

The data is generated by the following function

$$y = f(x) + \epsilon,$$
$$\epsilon \sim \mathcal{N}\left(0, \sigma_\epsilon^2\right)$$

We know that

The optimum regressor is $E[y|x] = f(x)$

Furthermore

Assume that the randomness in the different training sets, $\mathcal{D}$, is due to the y_i's (Affected by noise), while the respective points, x_i, are fixed.

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Sampling the Space [2]

Imagine that $\mathcal{D} \subset [x_1, x_2]$ in which x lies

For example, you can choose $x_i = x_1 + \frac{x_2 - x_1}{N-1}(i-1)$ with $i = 1, 2, ..., N$

Case 1

Choose the estimate of $f(x)$, $g(x|\mathcal{D})$, to be independent of $\mathcal{D}$

For example, $g(x) = w_1 x + w_0$

For example, the points are spread around $(x, f(x))$

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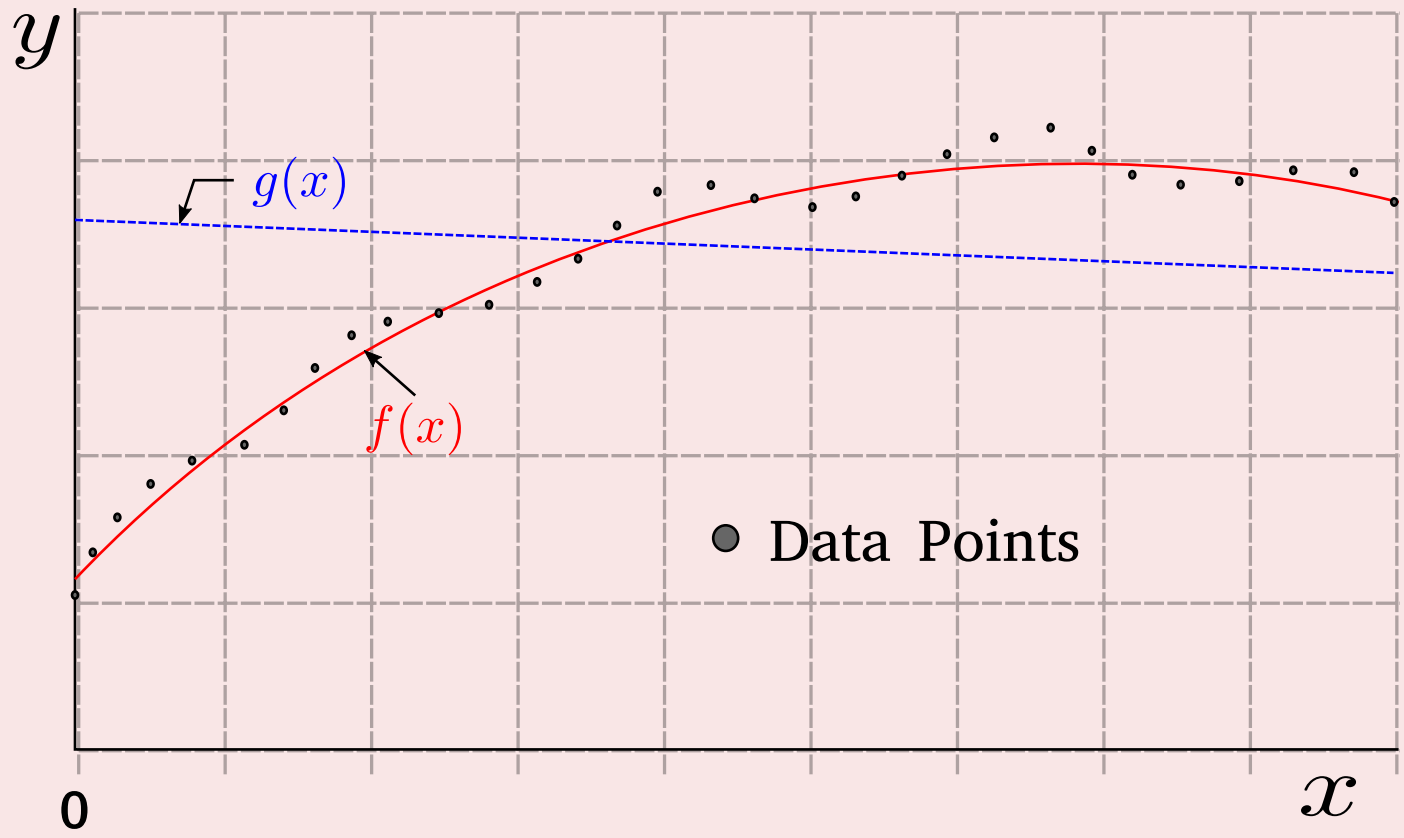

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$$E_{\mathcal{D}}\left[g\left(x|\mathcal{D}\right)\right] = g\left(x|\mathcal{D}\right) \equiv g\left(x\right) \tag{4}$$

With

$$Var_{\mathcal{D}}\left[g\left(x|\mathcal{D}\right)\right] = 0 \tag{5}$$

On the other hand

Because $g(x)$ was chosen arbitrarily the expected bias must be large.

$$\underbrace{\left(E_{\mathcal{D}}\left[g\left(\boldsymbol{x}|\mathcal{D}\right)\right] - E\left[y|\boldsymbol{x}\right]\right)^2}_{BIAS} \tag{6}$$

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Now, $g_1(x)$ corresponds to a polynomial of high degree so it can pass through each training point in $\mathcal{D}$.

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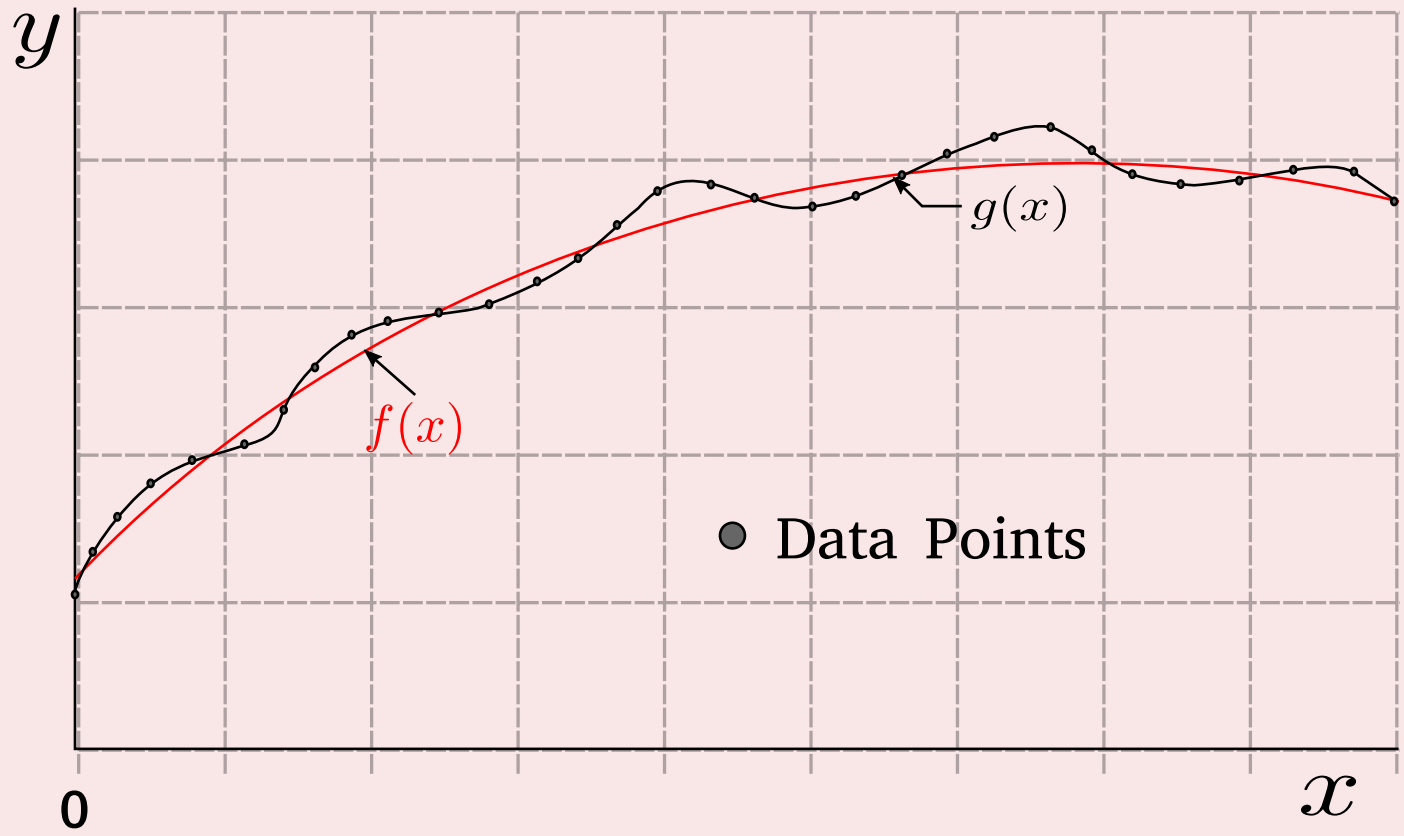

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Due to the zero mean of the noise source

$$E_D\left[g_1\left(\boldsymbol{x}|\mathcal{D}\right)\right] = f\left(x\right) = E\left[y|x\right] \text{ for any } x = x_i \tag{7}$$

Remark: At the training points the bias is zero.

However the variance increases

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The bias becomes zero (or approximately zero) but the variance is now equal to the variance of the noise source.

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Observations

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Everything that has been said so far applies to both the regression and the classification tasks.

However

Mean squared error is not the best way to measure the power of a classifier.

Think about

A classifier that sends everything far away of the hyperplane!!! Away from the values $+ -$ 1!!!

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Outline

The house example (From Andrew Ng Course)

Imagine the following data set

Now assume that we use a regressor

For the fitting

$$\frac{1}{2}\sum_{i=1}^{N}\left(h_{\boldsymbol{\theta}}\left(x_i\right)-y_i\right)^2$$

We can then run one of our machine to see what minimize better the previous equation

Question: Did you notice that I did not impose any structure to $h_w(x)$?

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For the fitting

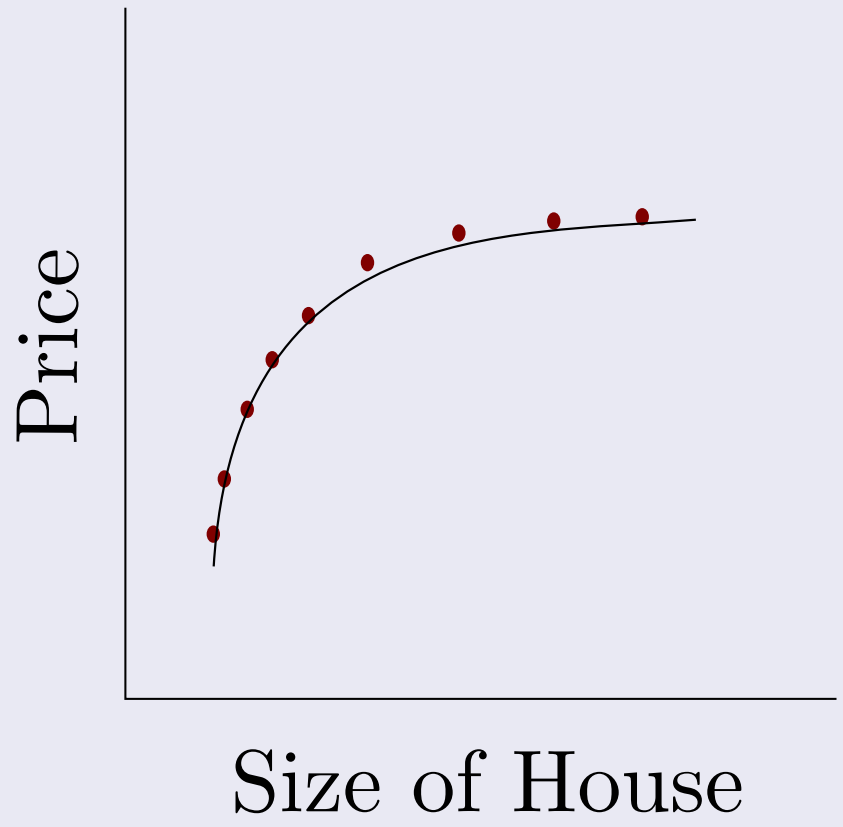
$$\frac{1}{2}\sum_{i=1}^{N}\left(h_{\boldsymbol{\theta}}\left(x_i\right)-y_i\right)^2$$

We can then run one of our machine to see what minimize better the previous equation

Question: Did you notice that I did not impose any structure to $h_{\boldsymbol{w}}\left(x\right)$?

Then, First fitting

What about using $h_1(x) = \theta_0 + \theta_1 x + \theta_2 x^2$?



Second fitting

What about using $h_2(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4 + \theta_5 x^5$?

Therefore, we have a problem

We get weird over fitting effects!!!

What do we do? What about minimizing the influence of $\theta_3, \theta_4, \theta_5$?

How do we do that?

$$\min_{\theta} \frac{1}{2} \sum_{i=1}^{N} \left(h_\theta \left(x_i \right) - y_i \right)^2$$

What about integrating those values to the cost function? Ideas

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Outline

We have

Regularization intuition is as follow

Small values for parameters $\theta_0, \theta_1, \theta_2, ..., \theta_n$

It implies

1. "Simpler" function
2. Less prone to overfitting

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We can do the previous idea for the other parameters

We can do the same for the other parameters

$$\min_{\boldsymbol{\theta}} \frac{1}{2} \sum_{i=1}^{N} \left(h_{\boldsymbol{\theta}} \left(x_i \right) - y_i \right)^2 + \sum_{i=1}^{d} \lambda_i \theta_i^2 \tag{8}$$

However handling such many parameters can be so difficult

Combinatorial problem in reality!!!

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Better, we can

We better use the following

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Graphically

Geometrically Equivalent to send our function to something quadratic

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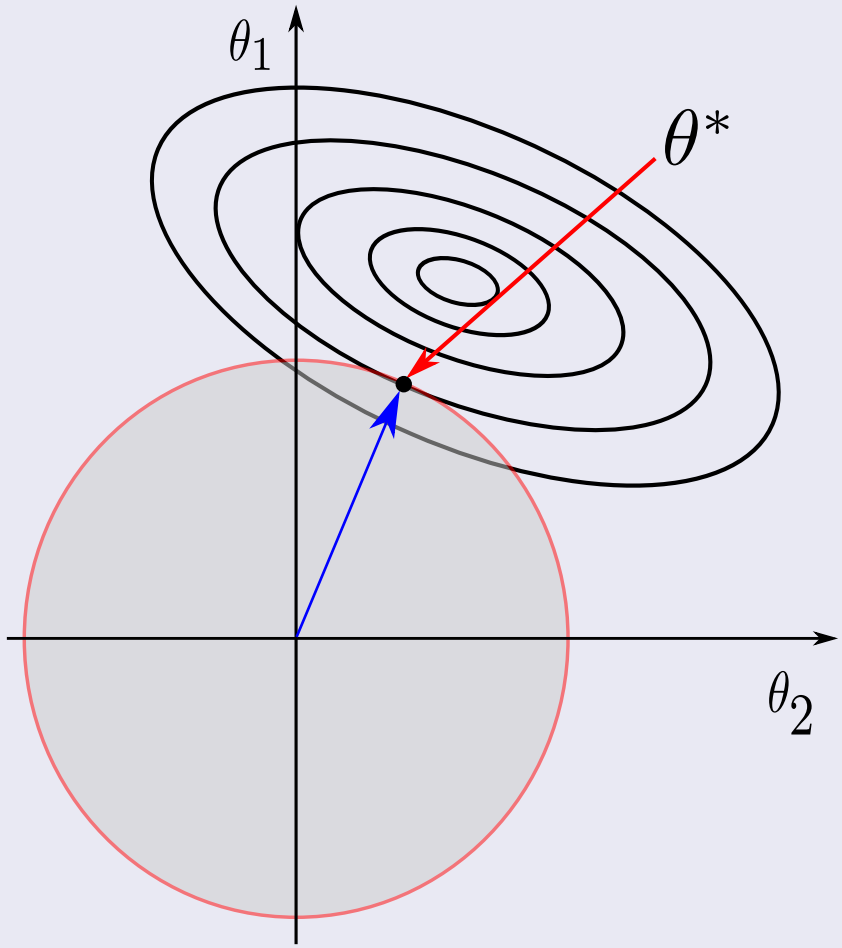

An interesting Observation, when using linear estimators

The function $\sum_{i=1}^{N}\left(\theta^T \boldsymbol{x}_i - y_i\right)^2$

- It is a convex function...

And also $\sum_{j=1}^{p}\theta_j$

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Therefore the final Lagrangian is a Convex function

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The game changes a lot

- When the estimator is a complex non-convex function

In our case

- Deep Learners

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Outline

Ridge Regression

Equation

$$\widehat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{w}} \left\{ \sum_{i=1}^{N} \left(y_i - \theta_0 - \sum_{j-1}^{d} x_{ij}\theta_j \right)^2 + \lambda \sum_{j=1}^{d} \theta_j^2 \right\}$$

Here

- $\lambda \geq 0$ is a complexity parameter that controls the amount of shrinkage

The Larger $\lambda \geq 0$

- The coefficients are shrunk toward zero (and each other).

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This is also can be written

Optimization Solution

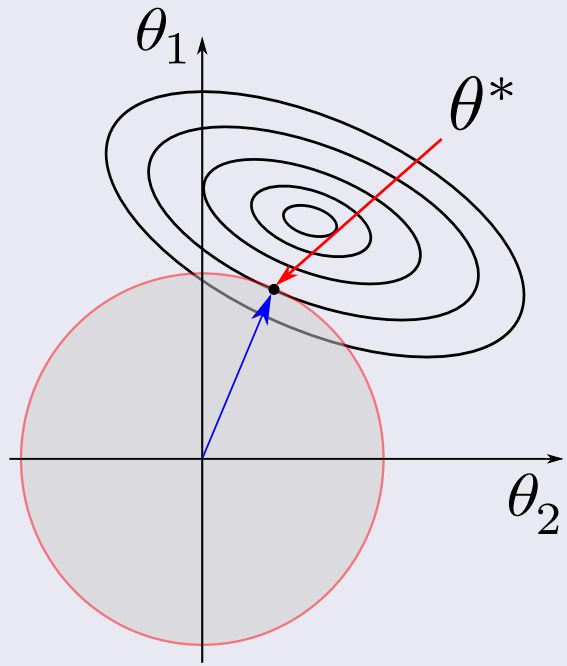
$$\arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{N} \left(y_i - \theta_0 - \sum_{j-1}^{d} x_{ij}\theta_j \right)^2$$

$$\text{subject to } \sum_{j=1}^{d} \theta_j^2 < t$$

Graphically

Geometrically Equivalent to

$$\arg\min \sum_{i=1}^{N} \left(y_i - \boldsymbol{x}_i^T \boldsymbol{\theta}\right)^2$$
$$\text{subject to } \sum_{i=1}^{d+1} \theta_i^2 < t$$



Outline

Least Absolute Shrinkage and Selection Operator (LASSO)

It was introduced by Robert Tibshirani in 1996 based on Leo Breiman's nonnegative garrote

$$\widehat{\boldsymbol{\theta}}^{garrote} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{N} \left(y_i - \theta_0 - \sum_{j=1}^{d} x_{ij}\theta_j \right)^2 + N\lambda \sum_{j=1}^{d} \theta_j$$

$$\text{s.t. } \theta_j > 0 \ \forall j$$

This is quite derivable

However, Tibshirani realized that you could get a more flexible model by using the absolute value at the constraint!!!

Robert Tibshirani proposed the use of the L_1 norm

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The Lagrangian

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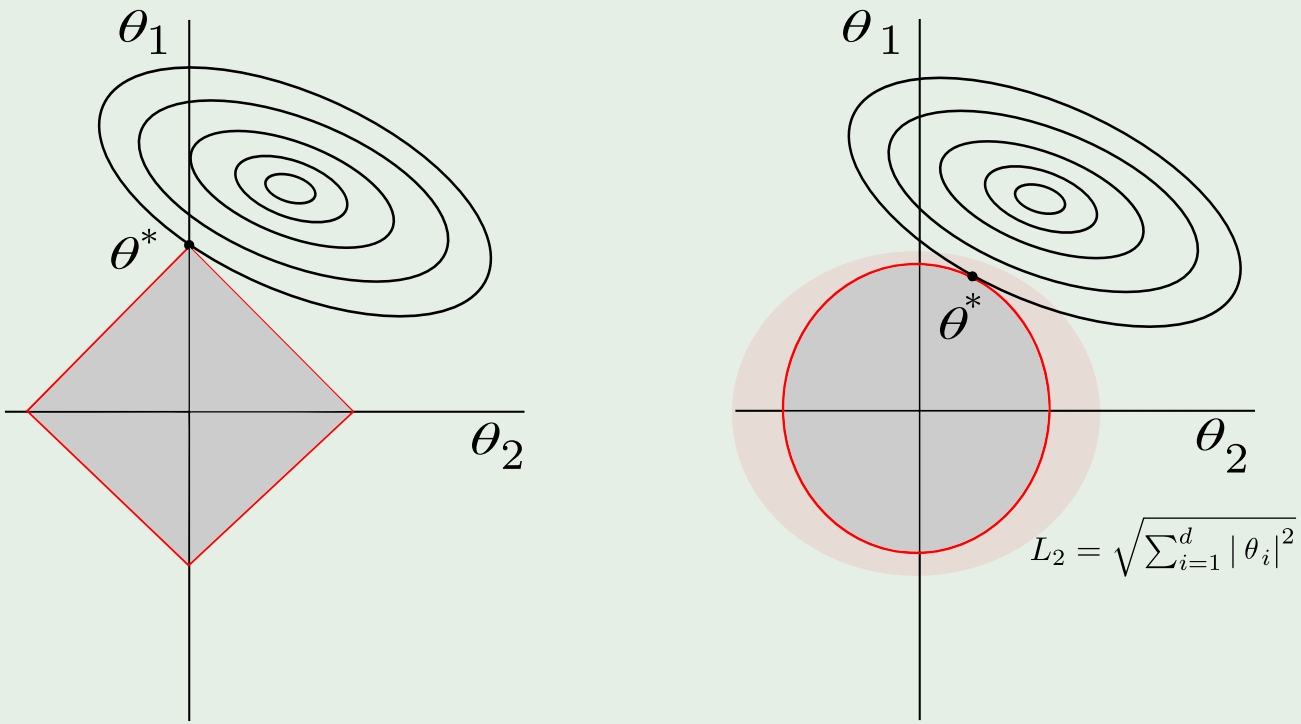
Graphically

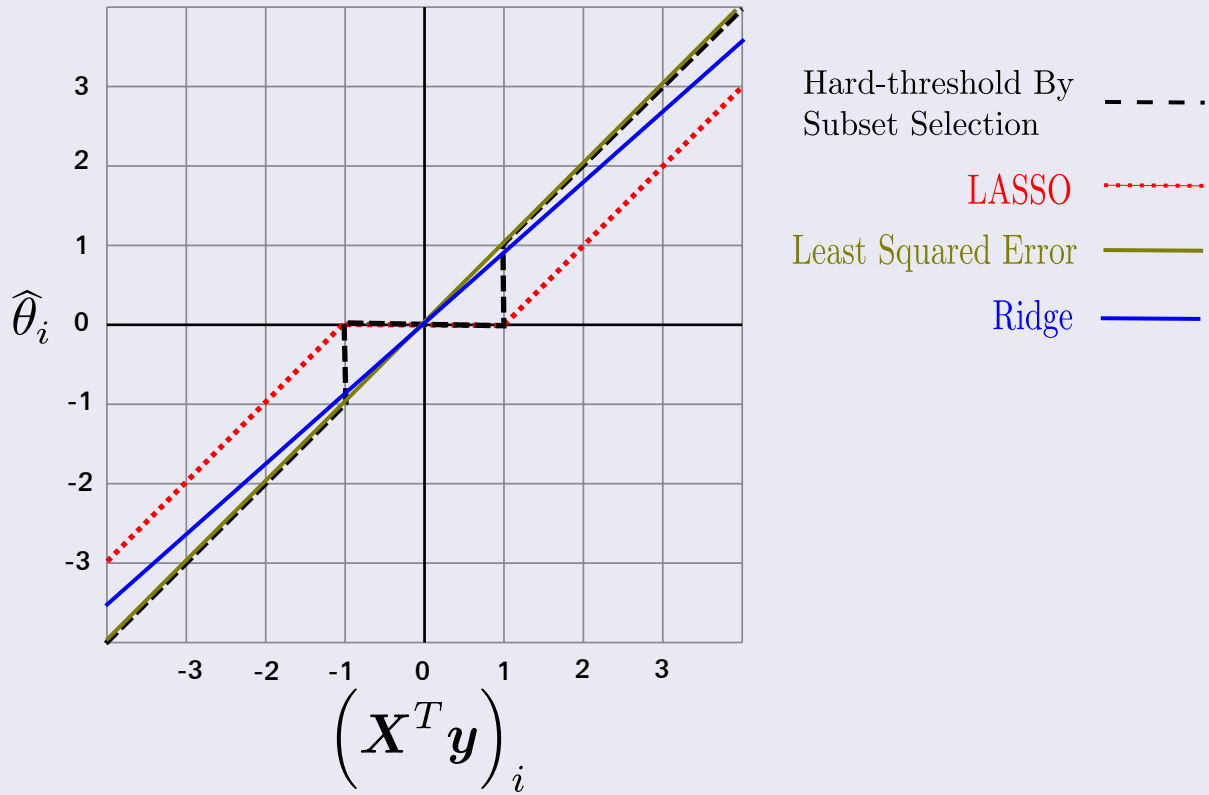
Yes the circle defined as $\|\boldsymbol{\theta}\|_2 = \sqrt{\sum_{i=1}^{d} |\theta_i|^2}$



For Example

In the Case of $\boldsymbol{X}$ is a Orthogonal Matrix, we have

$$\widehat{\theta}_i = sgn\left(X^T y\right)_i \left(\left(X^T y\right)_i - \sigma^2\alpha\right)_+$$



The seminal paper by Robert Tibshirani

An initial study of this regularization can be seen in

"Regression Shrinkage and Selection via the LASSO" by Robert Tibshirani - 1996

Outline

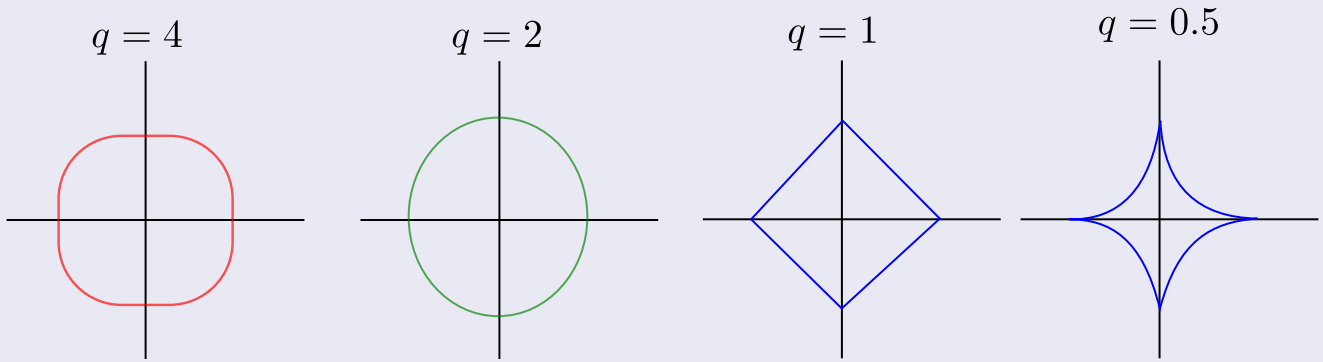
Furthermore

We can generalize ridge regression and the lasso, and view them as Bayes estimates

$$\widehat{\boldsymbol{\theta}}^{LASSO} = \arg\min_{\boldsymbol{w}} \left\{ \sum_{i=1}^{N} \left(y_i - L\left(\boldsymbol{x}_i, \boldsymbol{\theta} \right) \right)^2 + \lambda \sum_{i=1}^{d} |\theta_i|^q \right\} \text{ with } q \geq 0$$

For Example

We have when $d = 2$



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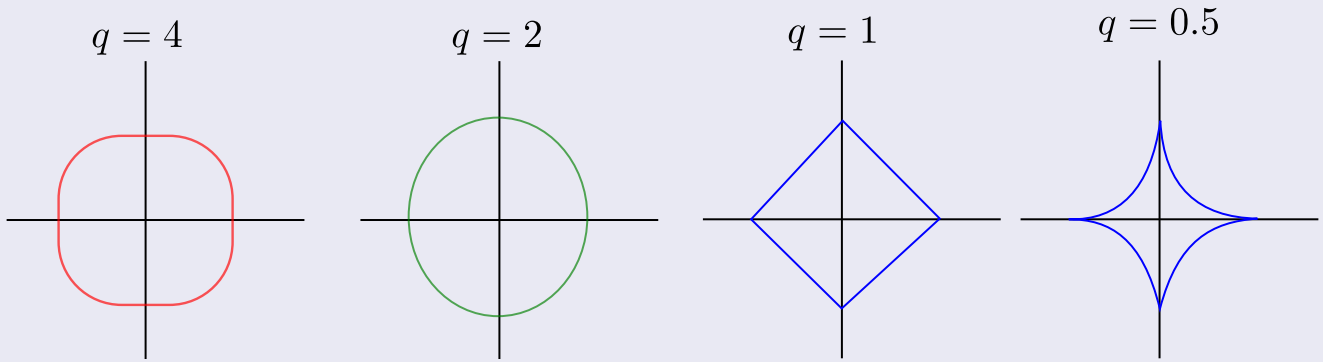

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Therefore

Zou and Hastie (2005) introduced the elastic-net penalty [3]

$$\lambda \sum_{i=1}^{d} \left\{ \alpha \theta_i^2 + (1-\alpha) |\theta_i| \right\}$$

This is Basically

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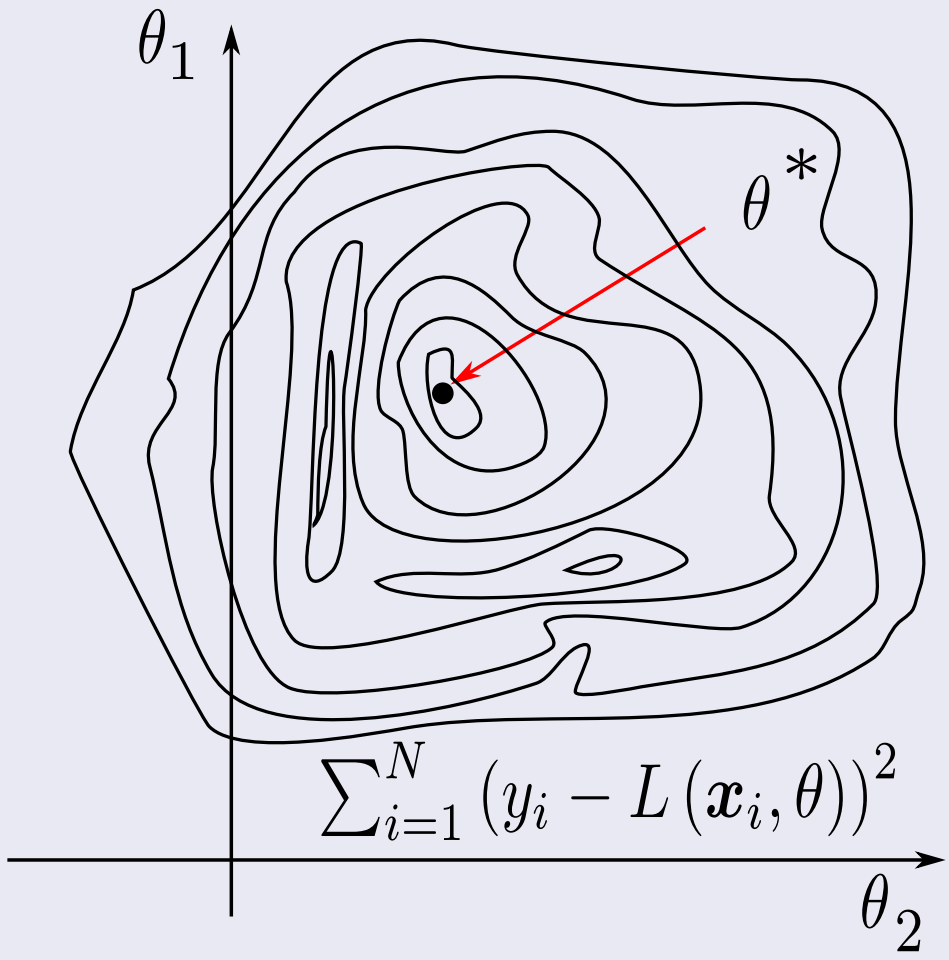
Outline

What can be done?

Remember that our optimization Landscape is highly variable



Over-fitting?

Basically (Intuition)

$$(y_i - L(\boldsymbol{x}_i, \theta))^2 = 0 \text{ for } i \in Training$$
$$(y_j - L(\boldsymbol{x}_i, \theta))^2 \gg 0 \text{ for } i \in Validation$$

At the other side, you have BIAS ←→ Simplification

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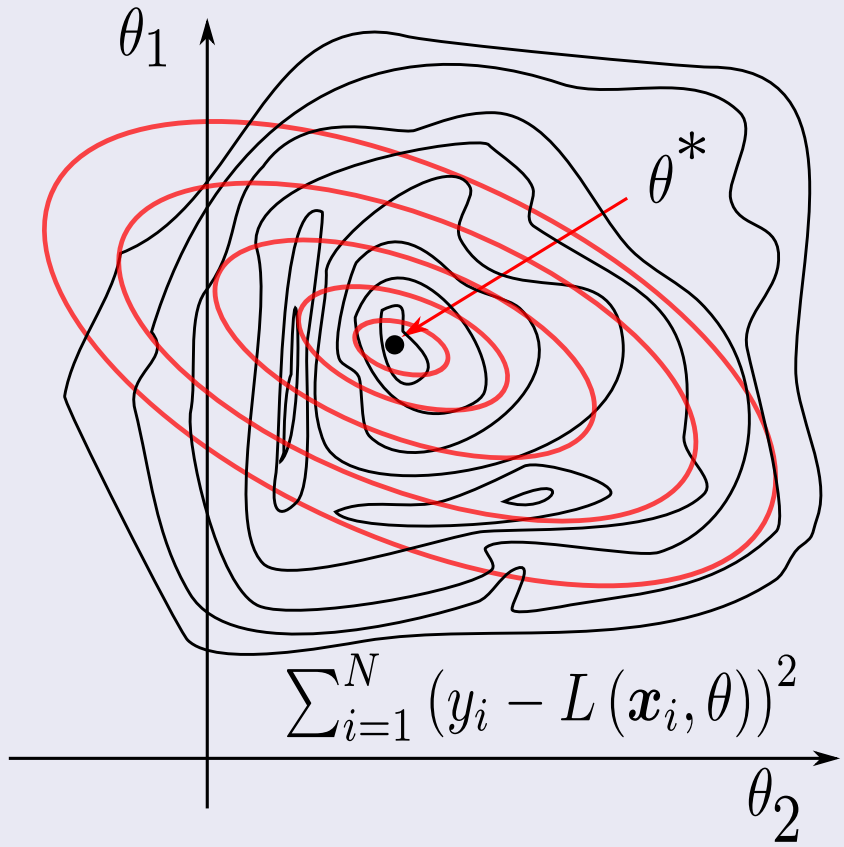
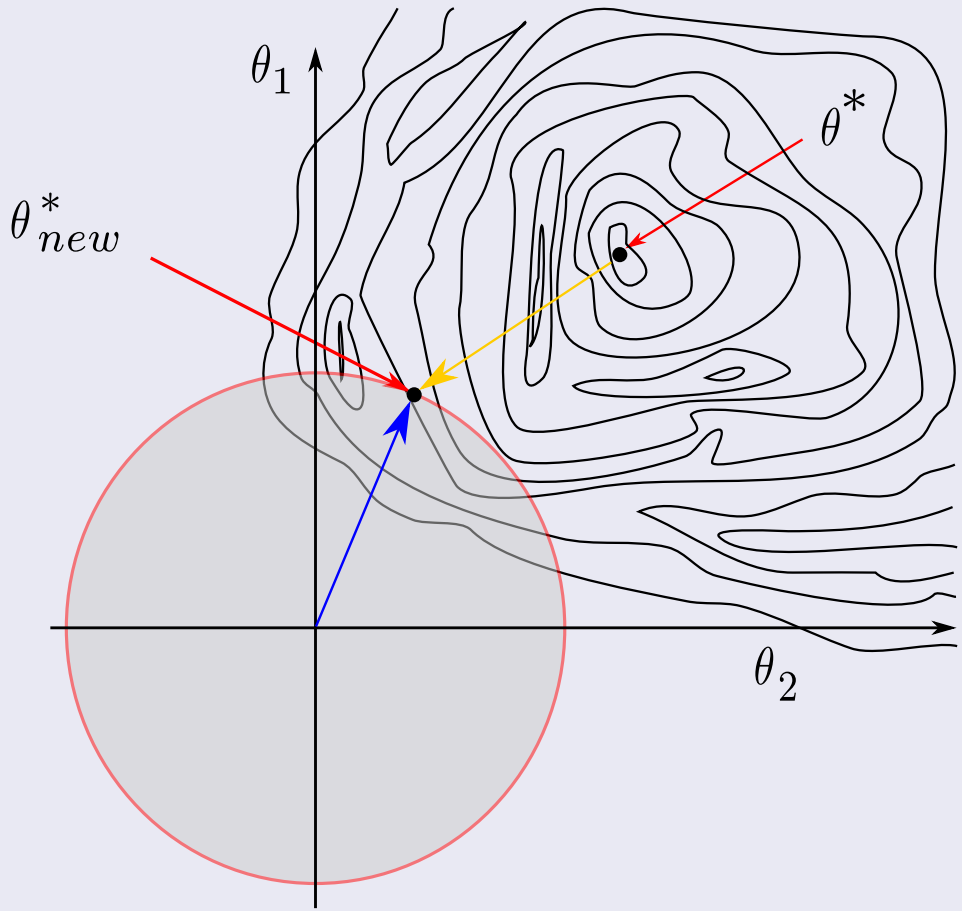
However, we do not want too much simplification

Look at this, the worst case Bias toward Red



Basically this simplification is due to the constrained optimization landscape

Basically our constraint is too Euclidean for Optimization Landscape



Well-Posed Problem

Definition by Hadamard (Circa 1902)

- Models of physical phenomenas should have the following properties
  1. A solution exists,
  2. The solution is unique,
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Any other problem that fails in any of this conditions

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The Deep Learners are highly ill-posed problems

- Ridge and LASSO have two possible effects

Too much simplification

- The Deep Learners losses power of representation.
  - Weights are eliminated

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DeVris and Taylor [5]

For many years

- Dataset augmentation has been a standard regularization technique used to reduce overfitting while training supervised learning models

For Example, LeCun et al. [4] when training the LeNet5

- They applied a series of transformations to the input images in order to improve the robustness of the model.

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In voice detection, adding

1. Gaussian noise to the input,
2. Shifting the pitch of the audio signal,
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They did something different

- First learning a data representation
- Then applying transformations to samples mapped to that representation.

They hypothesized

- Due to manifold unfolding in feature space, simple transformations applied to **encoded** rather than raw inputs
  - They will result in more plausible synthetic data.

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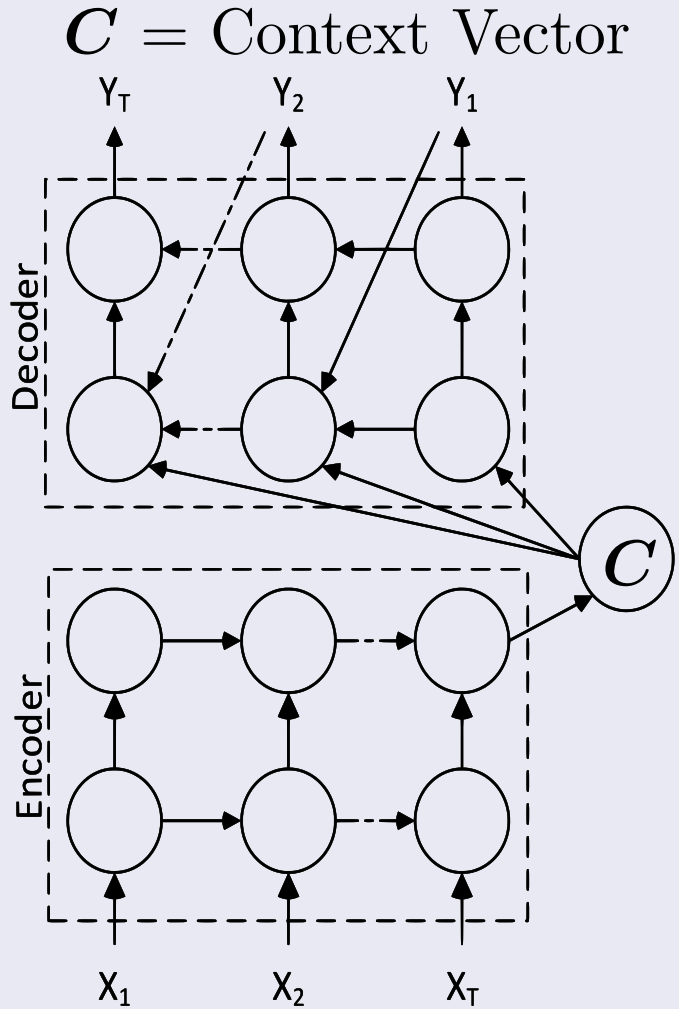
Outline

Decoder/Encoder Part

We have a Decoder and Encoder Architecture



Basically

They used a context C to pass information between the encoder and decoder

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Here

We have a K-coding symbol set

- The Encoder and Decoder are based in a novel hidden unit.

We have the following configuration per row element j

$$r_j = \sigma\left([\boldsymbol{W}_r \mathbf{x}]_j + [\boldsymbol{U}_r \mathbf{h}_{t-1}]_j\right) \leftarrow \text{Reset Gate}$$

- σ a sigmoid function

The Update gate

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In this formulation

- When the reset gate is close to 0, the hidden state is forced to ignore the previous hidden state!!!

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Finally, at output

We have a probability of producing a symbol of a set of at the Decoder

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Then, at the Encoder

- The encoder learns to predict the next symbol x_t based in the previous $x_{t-1},x_{t-2},...,x_1$ by using the maximization

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Here, the Noise

Generate noise by drawing from

- A Gaussian distribution with **zero mean** and **per-element standard deviation** calculated across all context vectors in the dataset

$$c_i' = c_i + \gamma X,\ X \sim N\left(0, \sigma_i^2\right)$$

We can generate this using a more direct approach

- For each sample in the dataset, we find its K nearest neighbors in feature space, then

$$c' = (c_k - c_j)\,\lambda + c_j$$

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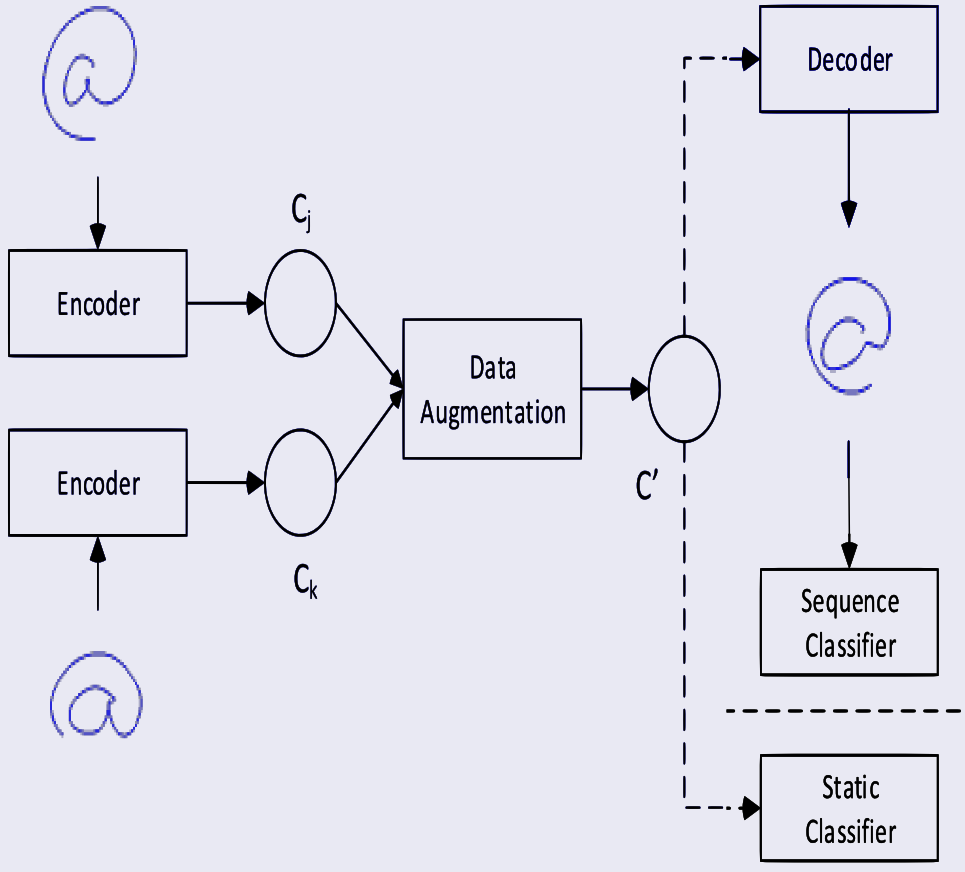
Then

Once this new augmented context vectors with noise are ready

- As input for a learning task,
- They can be decoded to generate new sequences

Finally, we have

The following architecture where two symbols are encoded



Results

Not so much improvement

Image Size	**Description**	**Test Error**	**Test Error** (Reconstructions of original data)
32×32	Original dataset	8.59 ± 0.24	-
24×24	Center crop	11.28 ± 0.25	18.54 ± 0.38
24×24	Center crop + extrapolation	13.90 ± 0.22	17.69 ± 0.39
24×24	Simple data augmentation	$\mathbf{7.33 \pm 0.17}$	13.60 ± 0.17
24×24	Simple data augmentation + extrapolation	8.80 ± 0.24	$\mathbf{12.00 \pm 0.23}$

Why is this happening?

It is the same problem at the exit point

- We are regularizing at the encoded input space... but the architecture is still there...

Therefore

- It is necessary to do something quite different...

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Regularization in Deep Forward

In Layers of a Deep Forward

- We want to find and estimation $\boldsymbol{x}_t^r$ to an input at $\boldsymbol{x}_0 \in \mathbb{R}^d$ in layer t satisfying

$$\sigma\left(A_t^I \boldsymbol{x}_t\right) = \boldsymbol{y}_{t+1}$$

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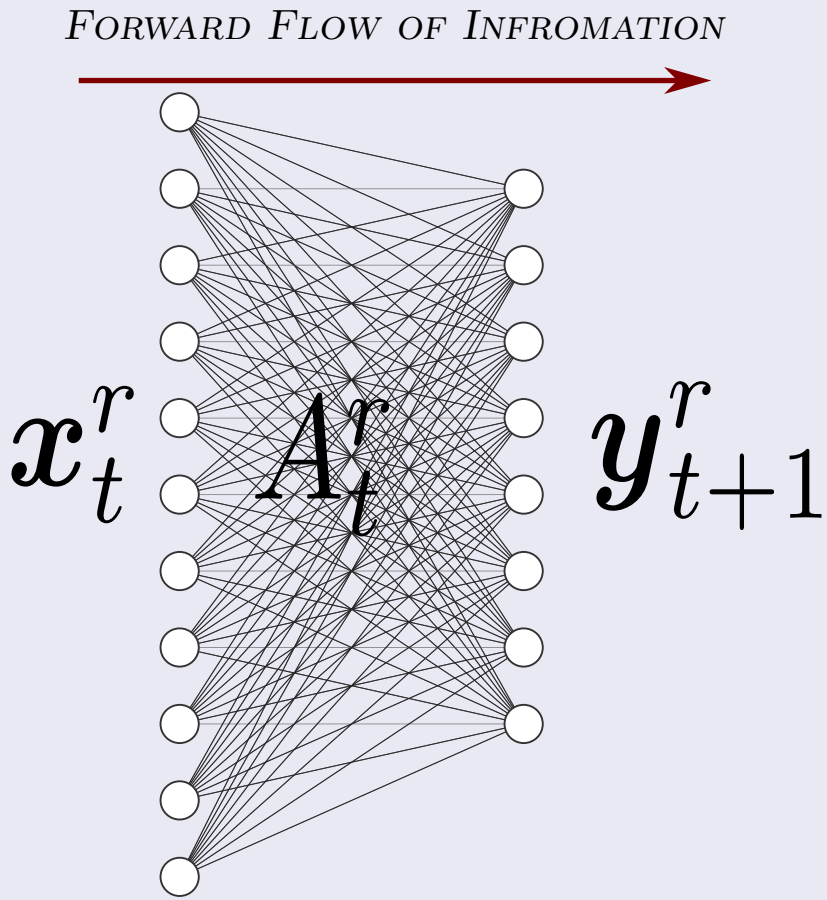
We can see this

A flow of information



In all such situations

The vector $\boldsymbol{x}_t$ is generated by $\boldsymbol{y}_{t+1}$ using back-propagation

$$A_t^r = A_t^{r-1} - \eta \frac{\partial L\left(A_T^{r-1}, ..., A_0^{r-1}, x_0\right)}{\partial A_t^{r-1}}$$

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- to x^* optimal at layer t for all possible inputs $x_0's$.

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We can see the Deep Forward Network as

$$y_T = \sigma\left(A_T\sigma\left(A_{T-1}\sigma\left(A_{T-2}\left(...\sigma\left(A_0x_0\right)\right)\right)\right)\right)$$

Here

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The Jacobian of the Gradient Descent

Here, we assume a Least Squared Error cost function

$$\frac{\partial L\left(A_T^{r-1},...,A_0^{r-1},x_0^i\right)}{\partial A_t^{r-1}} = -\left(z^i - y_T\right) \times \sigma'\left(A_{T-1}^r \boldsymbol{x}_{T-1}\right) \times \frac{\partial A_{T-1}^r \boldsymbol{x}_{T-1}}{\partial \boldsymbol{x}_{T-1}} \times ... \times \sigma'\left(A_t^r \boldsymbol{x}_t\right) \times \frac{\partial A_t^r \boldsymbol{x}_t}{\partial \boldsymbol{x}_t}$$

Where

$$\sigma'\left(A_k^r \boldsymbol{x}_k\right) = \begin{pmatrix} \sigma'\left(\boldsymbol{a}_{1k}^r \boldsymbol{x}_k\right) & 0 & \cdots & 0 \\ 0 & \sigma'\left(\boldsymbol{a}_{2k}^r \boldsymbol{x}_k\right) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma'\left(\boldsymbol{a}_{Mk}^r \boldsymbol{x}_k\right) \end{pmatrix}$$

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What will happen in the following situation?

Imagine that $A_k's$ are diagonal matrix

$$A_k^r = \begin{pmatrix} a_{1k} & 0 & \cdots & 0 \\ 0 & a_{2k} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{Mk} \end{pmatrix}$$

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Then, we have that

$$* = \begin{pmatrix} \prod_{k=T-1}^{t} \sigma'\left(a_{1k}^r x_{1k}\right) a_{1k} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \prod_{k=T-1}^{t} \sigma'\left(a_{Mk}^r x_{2k}\right) a_{2k} \end{pmatrix}$$

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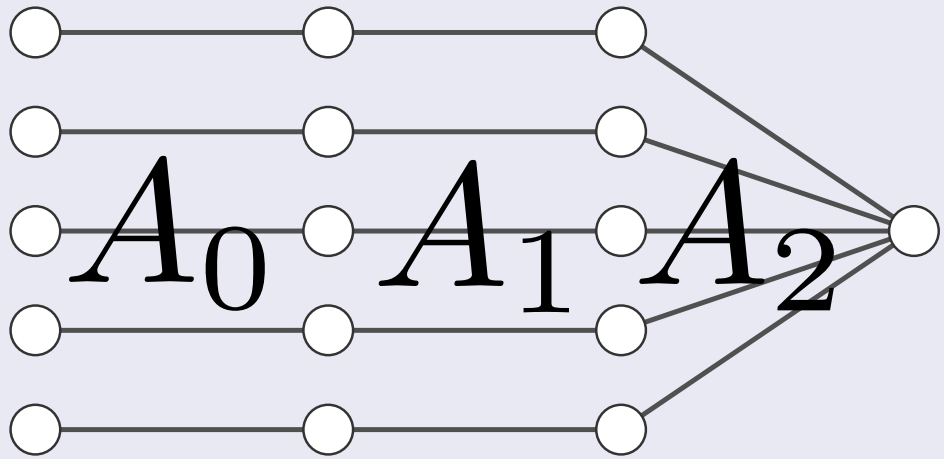
Actually

Choosing Matrices in such way

- It is like a heavy simplification of the Deep Forward Network



Something happens with the LASSO and Ridge

At the top of the Optimization Cost Function

- We do not know how such shallow regularization can affect the Neural Network

So heavy regularization

- It can not be a so good idea...

We need a new way of doing stuff

- For example, we could do the following...

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Outline

Dropout

It was introduced by Hinton and Google [6]

- To avoid the problem of over-fitting

You can see it as a regularization

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He comments that with unlimited computations

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Something like Boosting [1]

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Problem

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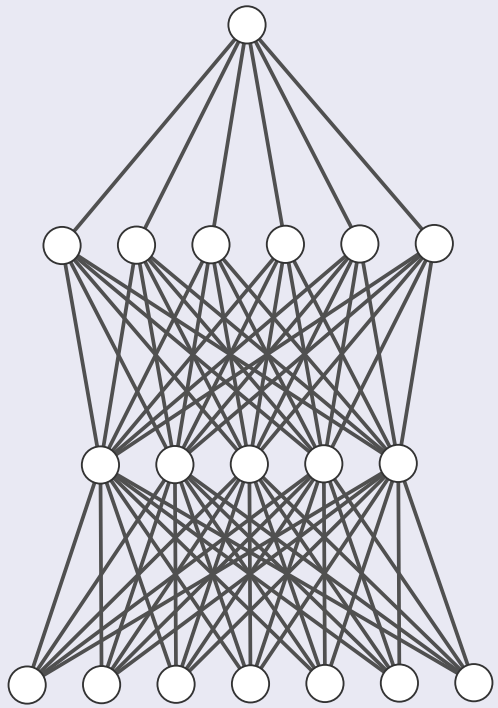

How it works?

You have forward layers

$$z_i^{l+1} = W_i^{l+1} \boldsymbol{x}^l + b_i^{l+1}$$
$$x_i^{l+1} = \sigma\left(z_i^{l+1}\right)$$

With dropout, the feed-forward operation becomes

$$r_j^l \sim Bernoulli\,(p)$$
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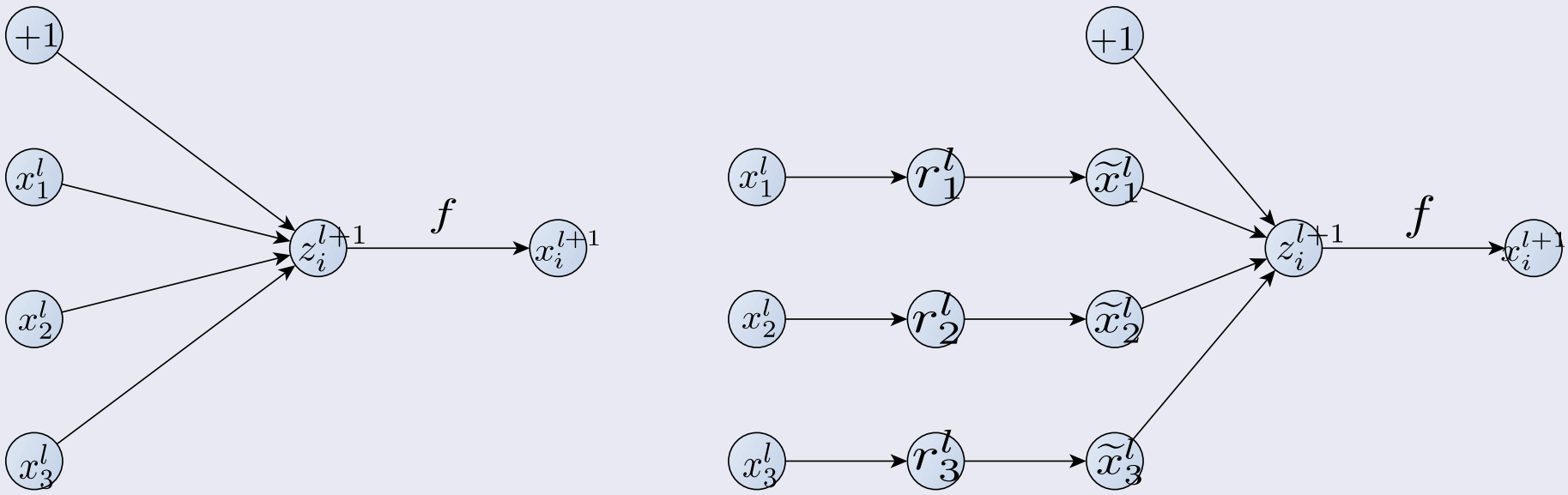
The Network

It looks like a series of gates



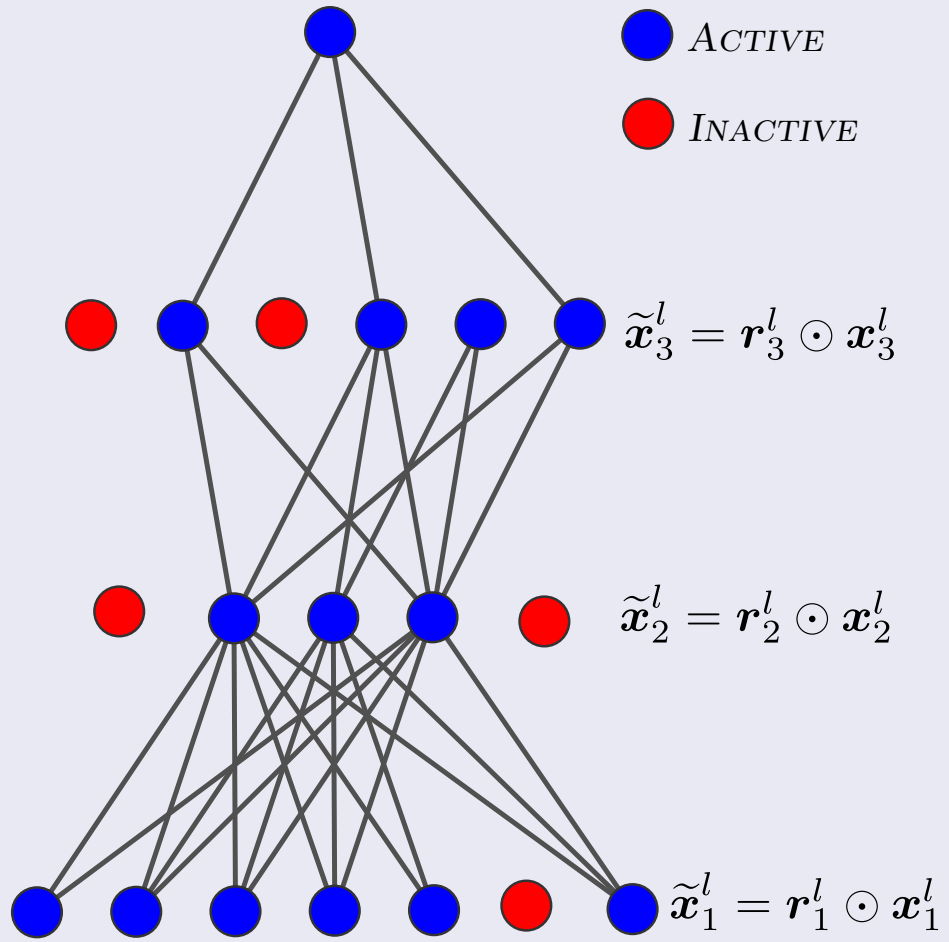
Therefore

We have that sampling is done in a Bernoulli to generate the $\boldsymbol{r}^l$, a vector of Bernoulli random variables

- Then, the layers are thinned by the wise multiplication with the nodes at each layer

Then, we erase randomly connections through the network

We generate sparser version with input layer such that $p^1_{1j} \rightarrow 1.0$



Then assuming a Multilayer Perceptron

We have the following Architecture without bias to simplify with a single output

$$\min \frac{1}{N} \sum_{i=1}^{N} (z_i - t_i)^2$$
$$z_i = \sigma_1 (W_{oh} \boldsymbol{y}_i)$$
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Then, we get the following network after the sampling

$$L(W_{oh}, W_{hI}) = (t - z)^2$$
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The Backpropagation at hidden weights

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Basically

$$\left(W_{oh}^{t+1}\right)_j = \begin{cases} \left(W_{oh}^{t}\right)_j + \eta 2\left(t-z\right) \times \frac{\partial \sigma_1'\left(net_{oh}\right)}{\partial net_{oh}} \left(\boldsymbol{y}\right)_j & \text{if } r_j = 1 \\ \left(W_{oh}^{t}\right)_j & \text{if } r_j = 0 \end{cases}$$

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However, At Testing

There are a exponential number of possible sparse networks

- A neural net with n units, can be seen as a collection of 2^n possible thinned neural networks.

Assuming

- These networks all share weights so that the total number of parameters is still $O(n^2)$ given that you this many connections

$$\frac{n\left(n-1\right)}{2}=O\left(n^2\right)$$

Problem, we cannot average such amount of sub-networks

- We average over the different passes to obtain a p for each node in the network
  - Meaning the probability of being active in the network.

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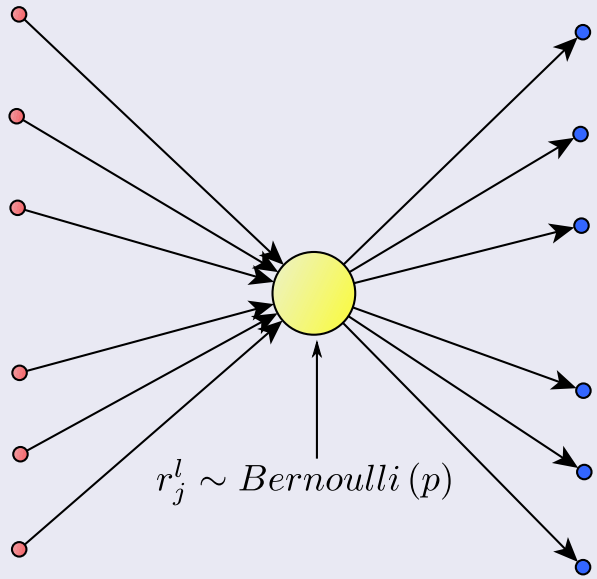
At Training



The mixture of the models

We know that

$$E\left(w_{ik}\right) = \sum_{m=1}^{M} w_{ik}^{m} p\left(w_{ik}^{m} | \text{BackProp}_{M}, \boldsymbol{X}\right)$$

Clearly, we need to get $p\left(w_{ik}^{m} | \text{BackProp}_{M}, \boldsymbol{X}\right)$

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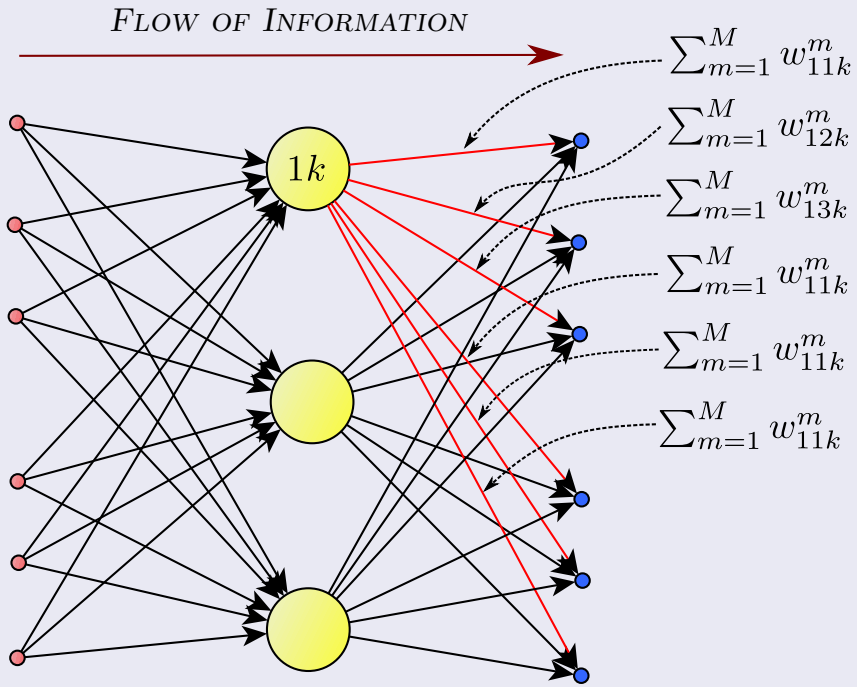
Therefore, Using the fact that Forward has a Flow of Information

Add flow of information between all the different generated trained networks



Mathematically

We have the following ideas

- Each node has associated matrices for exit weights

$$W_{out} = \begin{pmatrix} \sum_{i=1}^{m} w_{i1k}^{m} \\ \sum_{i=1}^{m} w_{i2k}^{m} \\ \vdots \\ \sum_{i=1}^{m} w_{iJk}^{m} \end{pmatrix}$$

Then use the probability p to get the new final weights

$$p_{ik} W_{out} = \begin{pmatrix} \sum_{i=1}^{m} w_{i1k}^{m} p_{ik} \\ \sum_{i=1}^{m} w_{i2k}^{m} p_{ik} \\ \vdots \\ \sum_{i=1}^{m} w_{iJk}^{m} p_{ik} \end{pmatrix}$$

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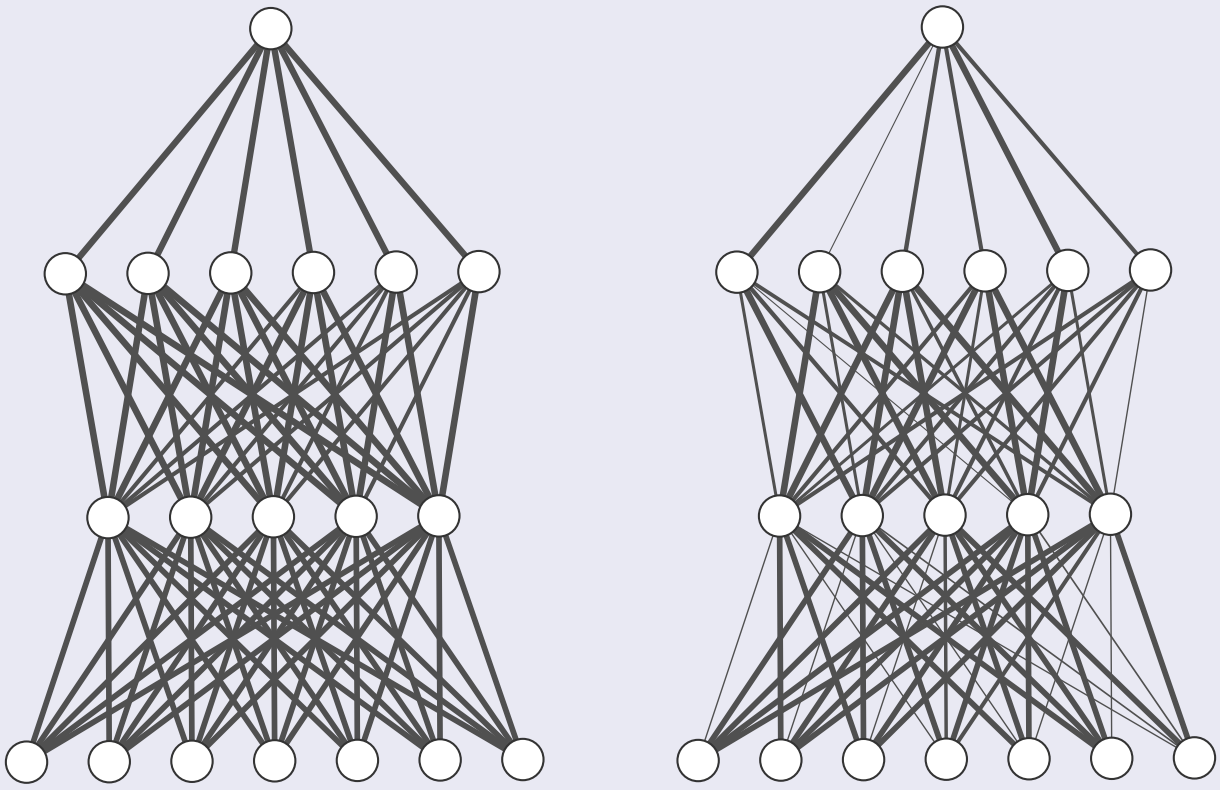
Then

We have the following structure where thiner lines represent smaller weights



The Original Structure

At Testing

Outline

Why dropout?

Srivastava et al. [6]

- A motivation for dropout comes from the theory of evolution!!!
  - Yes a original network and after a mutated one!!!

The most accepted interpretation of dropout

- It is implicitly bagging at test time a large number of neural networks which share parameters.

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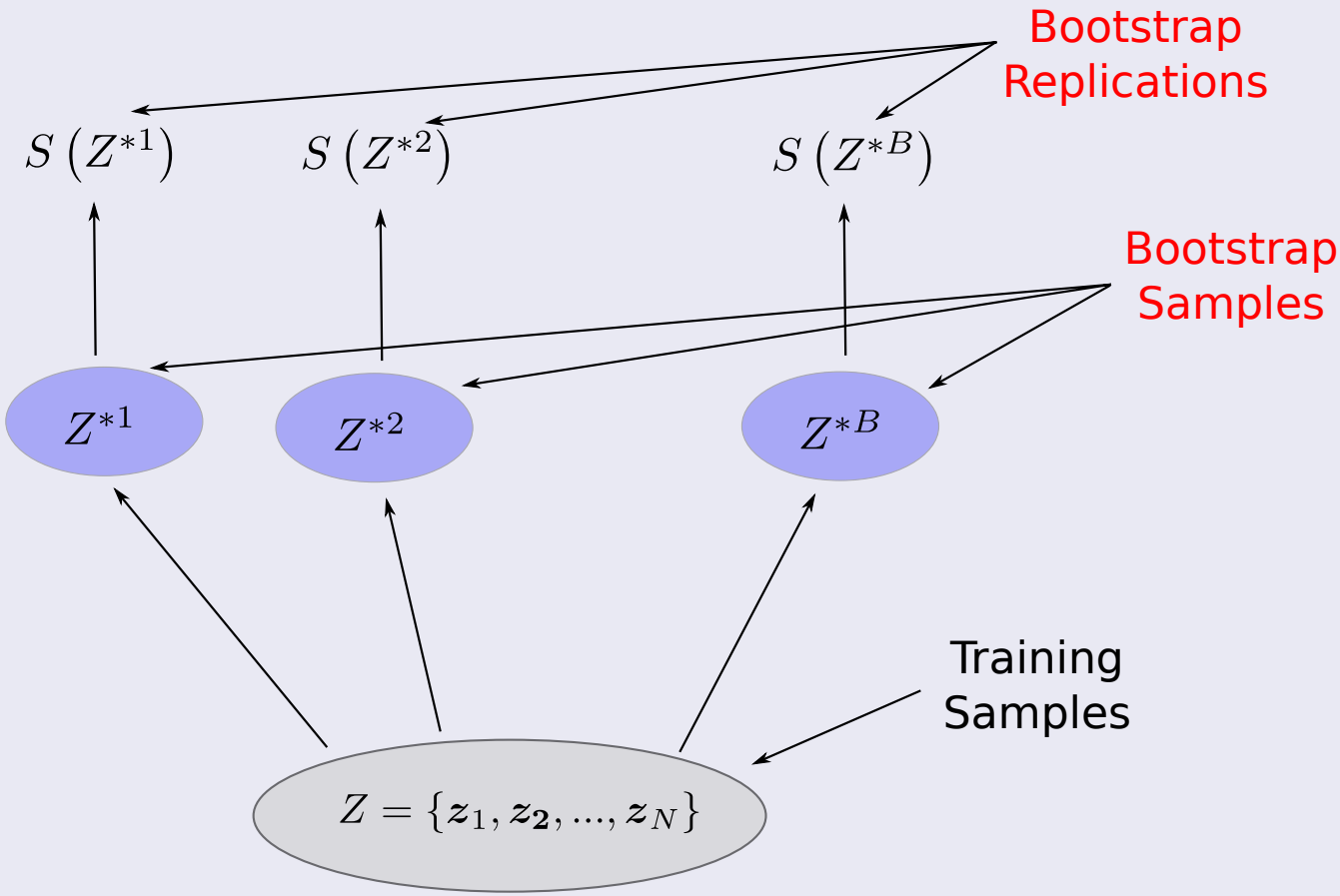
Bagging/Bootstrap Aggregation

Schematic of the Bootstrap Aggregation process [1]



Thus

Use each of them to train a copy $y_b(\boldsymbol{x})$ of a predictive regression model to predict a single continuous variable

$$y_{com}(\boldsymbol{x}) = \frac{1}{B}\sum_{b=1}^{B} y_b(\boldsymbol{x})$$

Results

We have that

Method	CIFAR-10 Error	CIFAR-100 Error
CNN+max pooling (hand tuned)	15.60%	43.48%
CNN+stochastic pooling (Zeiler and Fergus, 2013)	15.13%	42.51%
CNN+max pooling (Snoek et al., 2012)	14.98%	-
CNN+max pooling + dropout fully connected layers	14.32%	41.26%
CNN+max pooling + dropout in all layers	12.61%	37.20%
CNN+maxout (Goodfellow et al., 2013)	11.68%	38.57%

Outline

Given the previous ideas

Why not to use the Data Flow for Sparsity?

- Basically, we can assume that a pattern exist in the data you are looking at
  - The shifts on the weights are not so great...

$p_{\forall k}$ is to broad because it does not represents the real $p\left(w_{ijk}^{M} | \text{BackProp}_{M}, \mathbf{X}\right)$

- Actually, you should use the min-batch values, x_t and y_{t+1}, to generate the real distribution

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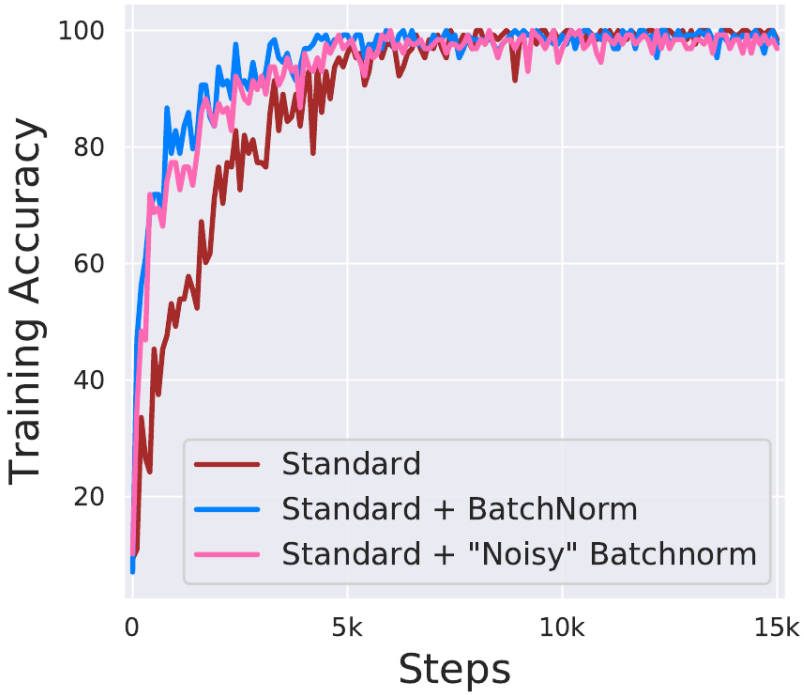
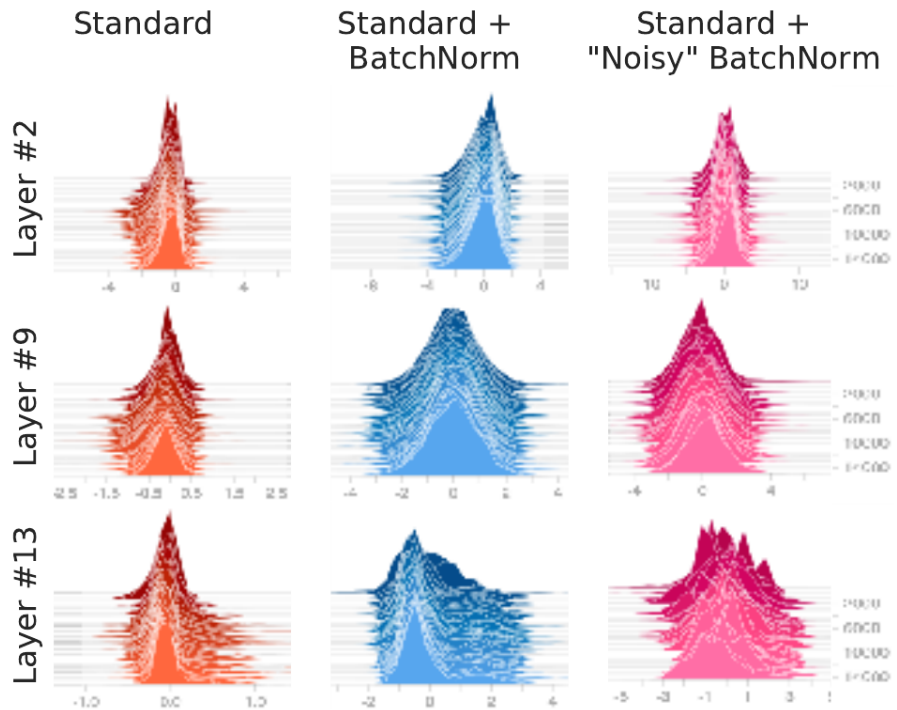
Based in the paper

"How does batch normalization help optimization?", in Advances in Neural Information Processing Systems (2018), pp. 2483--2493.





Then, we can use a Gaussian Distribution to model this

Actually, the paper is telling us that, given the noise that is injected at each time step t

$$\mu^t \sim U\left(-n_\mu, n_\mu\right)$$
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Why not use for the Data for enforcing Sparsity?

We have

$$p\left(\boldsymbol{y}^{l+1}|\boldsymbol{x}^{l},W\right)=\mathcal{N}\left(\sigma\left(W\boldsymbol{x}^{l}\right),\sigma^{2}I\right)$$

$$p\left(\sigma^{2}\right)\propto "constant"$$

$$p\left(W^{l}|\tau\right)=\prod_{i=1}^{d}\mathcal{N}\left(w_{j}^{l}|0,\tau_{j}^{l}\right)=\mathcal{N}\left(W^{l}|0,\left(\Upsilon\left(\tau\right)\right)^{-1}\right)$$

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How do we build such distribution

Given that each w_i has a zero-mean Gaussian prior

$$p(w_i|\tau_i) = \mathcal{N}(w_i|0, \tau_i) \tag{10}$$

Where τ_i has the following exponential hyper-prior

$$p(\tau_i|\gamma) = \frac{\gamma}{2} \exp\left\{-\frac{\gamma}{2}\tau_i\right\} \text{ for } \tau_i \geq 0 \tag{11}$$

Then, we have

$$w_i \sim p(w_i|\gamma) = \int_0^\infty p(w_i|\tau_i)\, p(\tau_i|\gamma)\, d\tau_i = \frac{\sqrt{\gamma}}{2} \exp\left\{-\sqrt{\gamma}\,|w_i|\right\} \tag{12}$$

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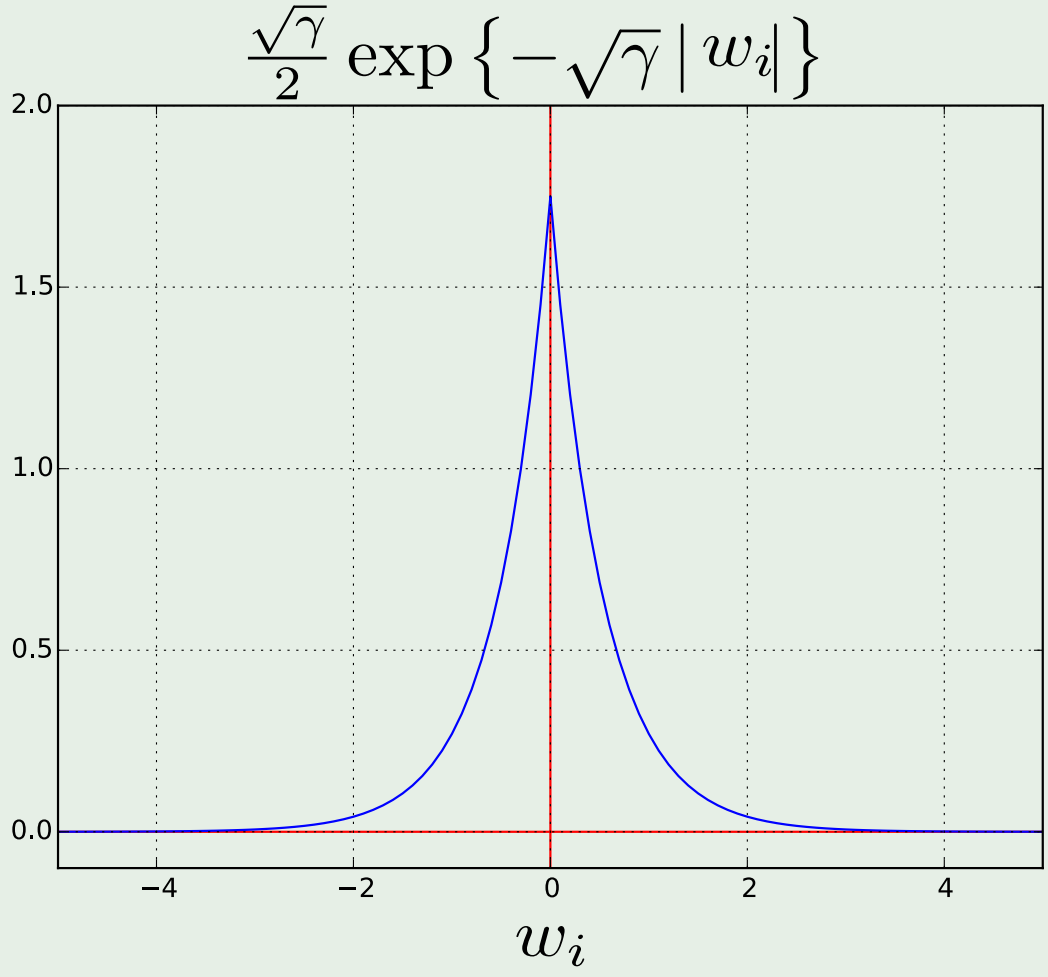
Example

The double exponential



Then using the Monte Carlo Method

We have

$$E\left[W^t|f\left(W_b^{tl}\boldsymbol{x}_b\right),\sigma^2 I\right]=\frac{p\left(\sigma^2\right)}{B}\sum_{b=1}^{B}\mathcal{N}\left(f\left(W_b^{tl}\boldsymbol{x}_b\right),\sigma^2 I\right)p\left(W_b^{tl}|\tau_i\right)p\left(\tau_i|\gamma\right)$$

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We are using the following idea

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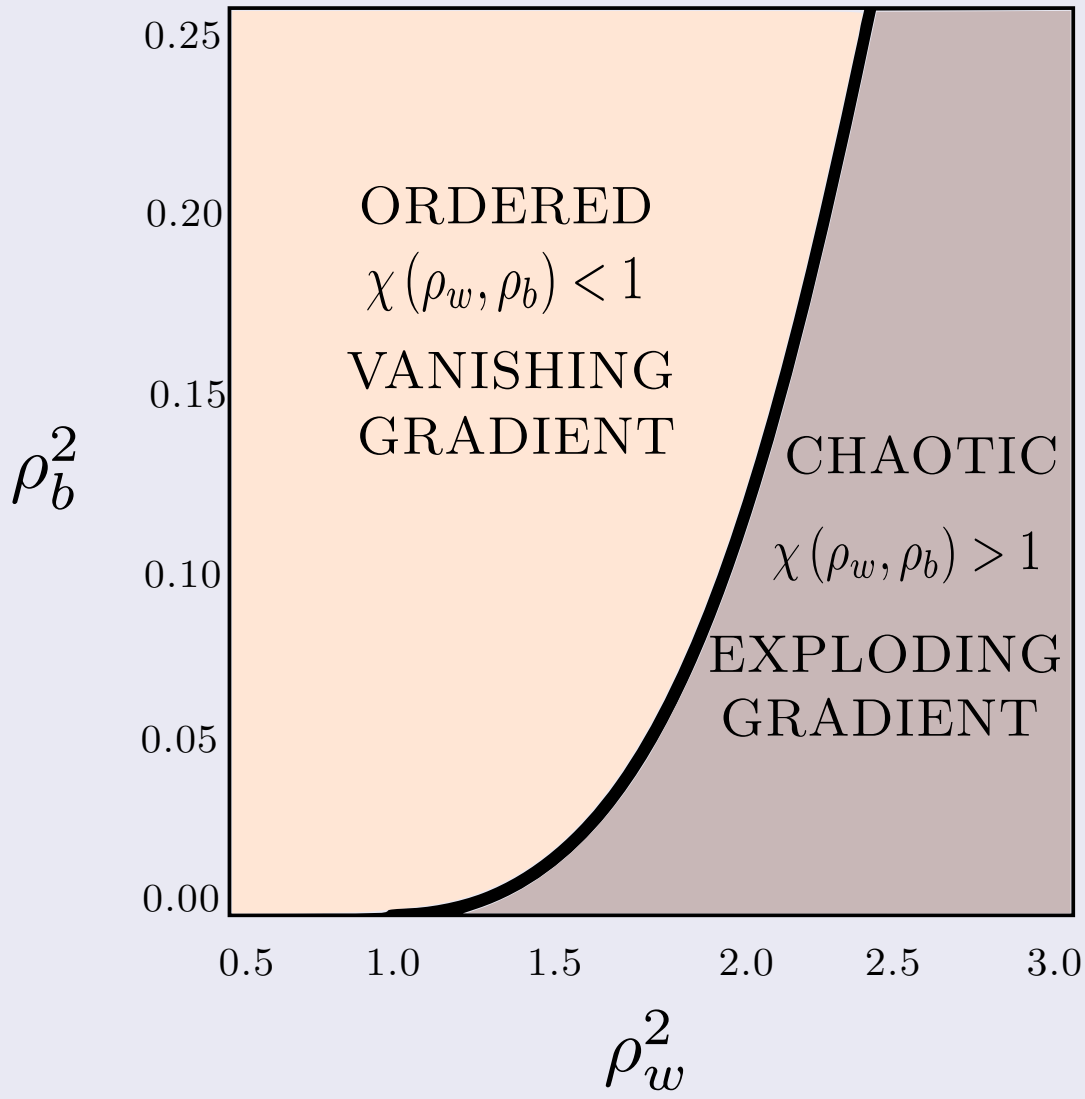

Thus, we have that

The layer output can be bounded by

$$\mathcal{N}\left(f\left(W_b^{tl}\boldsymbol{x}_b\right), \sigma^2 I\right)$$

The other part of the equation is the sparsity part

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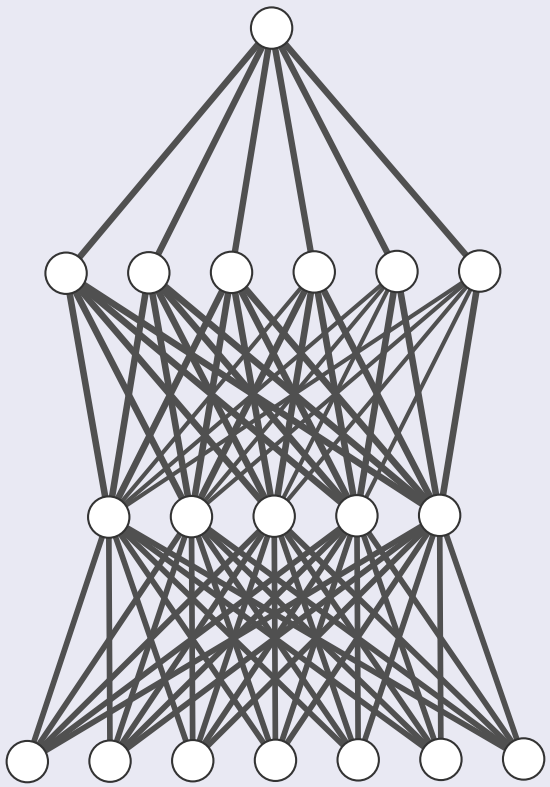
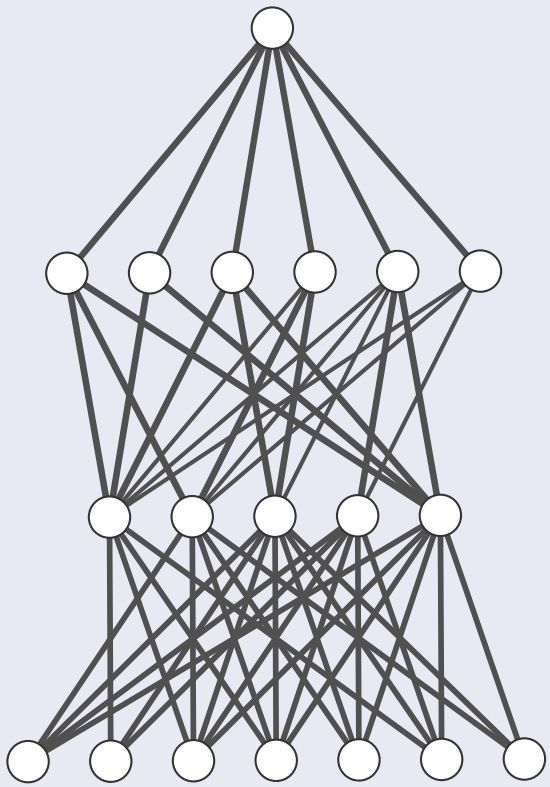
As the process progress

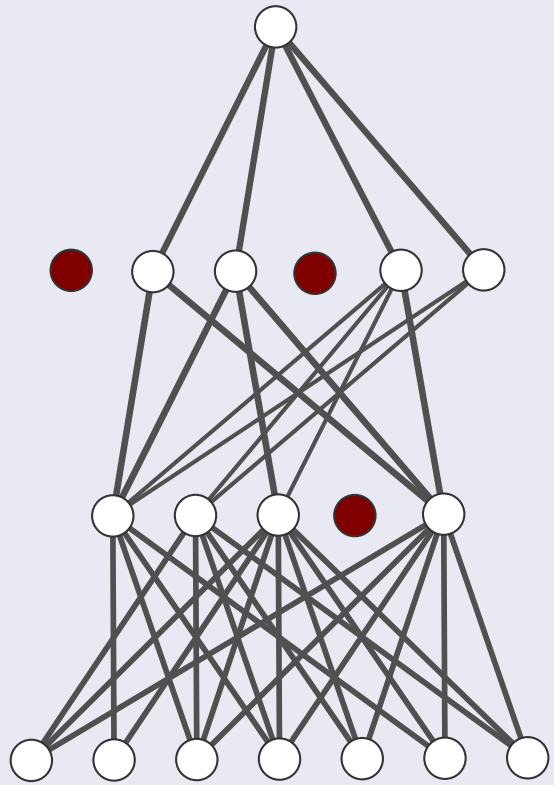
Once the weights fall below certain level we shutdown the weight



The Original Structure



After Some Epochs



More Epochs

Outline

Bouthillier et al.[8]

The main goal when using dropout

- It is to regularize the neural network we are training

Those random modifications of the network's stucture

- They are believed to avoid co-adaptation of neurons by making it impossible for two subsequent neurons to rely solely on each other [6]

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Therefore

We have a function that projects from a dimensional space to another

$$h(\boldsymbol{x}) = W\boldsymbol{x} + \boldsymbol{b}$$

Then, given the noisy version of an activation function where $M \sim \mathcal{B}(p_h)$

$$\tilde{f}(h) = M \odot rect(h) \text{ (Training)}$$

- Where $f(h) = rect(h)$ (Testing)

Actually Srivastava et al. [6]

- He mentions to use

$$p_{ijk} = \frac{\#\text{of subnets wehre node } ijk \text{ was active}}{\#\text{Of total subnets}}$$

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Data Augmentation

In many previous works [5, 4]

- It has been shown that augmenting data by using domain specific transformations helps in learning better models

Therefore, the main idea

- It is to map input data to output labels

One way to learn such a mapping function

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We assume that for a given $\widetilde{f}(h)$, there is an optimal $\boldsymbol{x}^*$

$$(f \circ h)(\boldsymbol{x}^*) = rect(h(\boldsymbol{x}^*)) :\approx M \odot rect(h) = \left(\widetilde{f} \circ h\right)(\boldsymbol{x}^*)$$

This $\boldsymbol{x}^*$ can be found by minimizing by stochastic gradient descent

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Extending to n layers

For this, we define

$$\widetilde{g}^{(i)}(\boldsymbol{x}) = \left[\widetilde{f}^{(i)} \circ h^{(i)} \circ \cdots \circ \widetilde{f}^{(1)} \circ h^{(1)}\right](\boldsymbol{x})$$

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Then, it is possible to compute the back propagation projection corresponding to all hidden layer activations at once

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Small Problem

- It is possible to show by contradiction that one is unlikely to find a single $\boldsymbol{x}^* = \boldsymbol{x}^{(1)^*} = \cdots = \boldsymbol{x}^{(n)^*}$
  - Such that you can significantly reduce L

Proof of the unlikeness of $\boldsymbol{x}^* = \boldsymbol{x}^{(1)^*} = \cdots = \boldsymbol{x}^{(n)^*}$

By the associative property of function composition

$$g^{(i)}\left(\boldsymbol{x}^*\right) = \left(f^{(i)} \circ h^{(i)}\right)\left(g^{(i-1)}\left(\boldsymbol{x}^*\right)\right)$$

Suppose there exist $\boldsymbol{x}^* = \boldsymbol{x}^{(1)^*} = \cdots = \boldsymbol{x}^{(n)^*}$ an such that

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This is only true if $M^{(i)} = 1$

- When $rect_j \left(h^{(i)} \left(g^{(i-1)} \left(\boldsymbol{x}^* \right) \right) \right) > 0$

This only happens with a probability $p_{(i)}^{d_{(i)} s_{(i)}}$

- Where:
  - $p_{(i)}$ is the Bernoulli success probability.
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Which is quite low!!!

This probability is very low for standard hyper-parameters values

- With $p_{(i)} = 0.5$, $d_{(i)} = 1000$ and $s_{(i)} = 0.15$

$$p_{(i)}^{d_{(i)}s_{(i)}} = 10^{-47}$$

However

Fortunately

- It is easy to find a different $\boldsymbol{x}^*$ for each hidden layer

by providing multiple inputs

$$\left(\boldsymbol{x}, \boldsymbol{x}^{(1)^*}, \boldsymbol{x}^{(2)^*}, \ldots, \boldsymbol{x}^{(n)^*}\right)$$

However

- This raises the question whether we can train the network deterministically on the $\boldsymbol{x}^{(i)^*}$ instead of using dropout

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Co-adaptation/Overfitting

Definition

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  - Selection pressures on one of the genes will affect its interacting proteins, after which compensatory changes occur.

In Neural Networks

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- where h defines the layer, i the sample, and j the layer's neuron.

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Results

Something Notable

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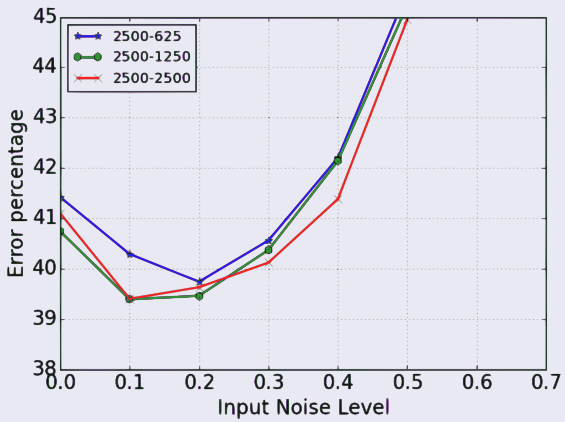
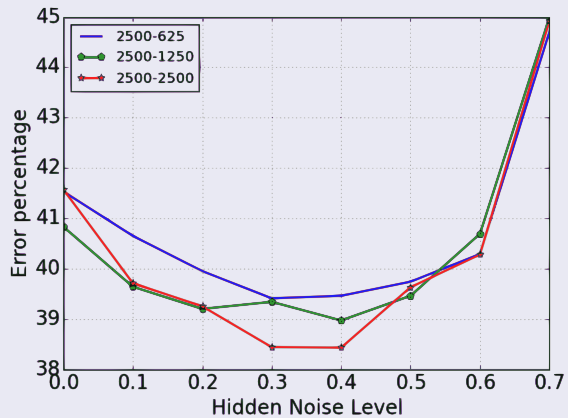
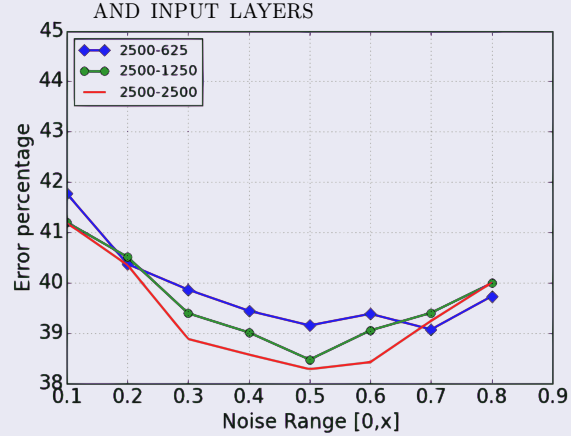


Using dropout with varying input noise and fixed hidden noise of 0.2.



Using Random-dropout with varying noise range [0, x] used at hidden and input layers



Outline

Here, the people at Google [9] 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

- Internal Covariate Shift as the change in the distribution of network activations due to the change in network parameters during training.

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Transformation

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. $\mu_{\mathcal{B}} = \frac{1}{m}\sum_{i=1}^{m} x_i$
2. $\sigma_{\mathcal{B}}^2 = \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2$
3. $\widehat{x} = \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}}$
4. $y_i = \gamma^{(k)}\widehat{x}_i + \beta = BN_{\gamma,\beta}(x_i)$

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Remember

Using Min-Batch inputs, we have

$$\mu_{\mathcal{B}} = \frac{1}{m}\sum_{i=1}^{m} \boldsymbol{x}_i$$

And Variance

$$\sigma_{\mathcal{B}}^2 = \frac{1}{m}\sum_{i=1}^{m} \left(\boldsymbol{x}_i - \mu_{\mathcal{B}}\right)^2$$

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$$\sigma^2_{\mathcal{B}} = \frac{1}{m}\sum_{i=1}^{m} (\boldsymbol{x}_i - \mu_{\mathcal{B}})^2$$

Therefore, Ba et al. [10]

We get the mean over the output of the layer l with H number of hidden units

$$\mu^l = \frac{1}{H}\sum_{i=1}^{H} y_i^l$$

- Basically, do the forward process then add over the output $y_i^l = w_i^{lT} h^l$ where $h_i^{l+1} = f\left(y_i^l + b_i^l\right)$

Then the standard deviation layer l

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We have that

- All the hidden units in a layer share the same normalization terms μ and σ
  - but different training cases have different normalization terms.

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The Flow of Information through time

First, the new h^t with a gain vector g

$$\boldsymbol{h}^t = f\left[\frac{\boldsymbol{g}}{\sigma^t} \odot \left(\boldsymbol{y}^t - \mu^t\right) + b\right]$$

The Temporal Layer Mean Normalization

$$\mu^t = \frac{1}{H}\sum_{i=1}^{H} y_i^t$$

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Outline

Weight re-scaling and re-centering

Observe that under batch normalization and weight normalization

- Any re-scaling to the incoming weights w_i of a single neuron has no effect on the normalized summed inputs to a neuron.

Meaning

- If the weight vector is scaled by δ_i the two scalars μ and σ will also be scaled by δ

Properties

- The batch and weight normalization are invariant to the re-scaling of the weights.

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- Layer normalization is invariant to scaling of the entire weight matrix.
- Also it is invariant to a shift to all of the incoming weights in the weight matrix.

How?

Imagine the following

- Let there be two sets of model parameters θ, θ' with weigh matrices

$$W' = \delta W + 1\gamma^T$$

We have

Given that $y_i^l = w_i^{lT} \boldsymbol{x}^l$

$$y_i^{'l} = \left(\delta W + 1\gamma^T\right)_i \boldsymbol{x}^l$$

Then, we have

$$\mu^{'l} = \frac{\delta}{H}\sum_{i=1}^{H} W_i \boldsymbol{x}^l + \frac{1}{H}\sum_{i=1}^{H}\left(1\gamma^T\right)_i \boldsymbol{x}^l = \delta\mu + \left(1\gamma^T\right)_i \boldsymbol{x}^l$$

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Now

Standard Deviation

$$\sigma' = \sqrt{\frac{1}{H}\sum_{i=1}^{H}\left(y_i'^{l} - \mu'\right)^2} = \delta\sqrt{\frac{1}{H}\sum_{i=1}^{H}\left(y_i^{l} - \mu\right)^2}$$

Finally, Under Layer Normalization, we have the same output

$$\begin{aligned} h' &= f\left[\frac{g}{\sigma'}\left(W'x - \mu'\right) + b\right] \\ &= f\left[\frac{g}{\sigma'}\left(\left[\delta W + 1\gamma^T\right]x - \mu'\right) + b\right] \\ &= f\left[\frac{g}{\sigma}\left(Wx - \mu\right) + b\right] = h \end{aligned}$$

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=& f\left[\frac{\boldsymbol{g}}{\sigma}\left(W\boldsymbol{x} - \mu\right) + \boldsymbol{b}\right] = \boldsymbol{h}
\end{aligned}$$

Remarks

Something Notable

- if normalization is only applied to the input before the weights, the model will not be invariant to re-scaling and re-centering of the weights.

Data re-scaling and re-centering

We can show

- All the normalization methods are invariant to re-scaling the dataset

Layer normalization is invariant to re-scaling of individual training cases

$$h_i' = f\left[\frac{g_i}{\sigma'}\left(w_i^T \boldsymbol{x}' - \mu'\right) + b_i\right] = f\left[\frac{g_i}{\delta\sigma}\left(\delta w_i^T \boldsymbol{x} - \delta\mu\right) + b_i\right] = h_i$$

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Additionally

Layer Normalization has a relation with the Fisher Information Matrix

$$F(\theta) = E_{\boldsymbol{x}\sim P(\boldsymbol{x}),y\sim P(y|\boldsymbol{x})}\left[\frac{\partial \log P(y|\boldsymbol{x})}{\partial \theta}\left(\frac{\partial \log P(y|\boldsymbol{x})}{\partial \theta}\right)^T\right]$$

Basically, we can write the generalized linear model as

$$\log P(y|\boldsymbol{x}, w, b) = \frac{(a+b)\,y - \eta(a+b)}{\Phi} + c(y, \Phi)$$

$$E[y|\boldsymbol{x}] = f(a+b) = f\left(w^T\boldsymbol{x} + b\right)$$

$$Var[y|\boldsymbol{x}] = \Phi f'(a+b)$$

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The curvature of a Riemannian manifold

It is entirely captured by its Riemannian metric

$$ds^2 \approx \frac{1}{2}\delta^T F(\theta)\,\delta$$

- where, δ is a small change to the parameters.

Then, under Layer Normalization, we have

$$F(\theta) = \frac{1}{\Phi^2} E_{x\sim P(x)} \begin{bmatrix} Cov(y_1, y_2|x)\frac{(a_1-\mu)^2}{\sigma^2} & \cdots & Cov(y_1, y_H|x)\frac{(a_1-\mu)(a_H-\mu)}{\sigma^2} \\ \vdots & \ddots & \vdots \\ Cov(y_H, y_1|x)\frac{(a_1-\mu)(a_H-\mu)}{\sigma^2} & \cdots & Cov(y_H, y_H|x)\frac{(a_H-\mu)^2}{\sigma^2} \end{bmatrix}$$

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Where

We have that $a_i = w_i^T \boldsymbol{x}$

- We project the gradient updates to the gain parameter δ_{gi} of the i^{th} neuron to its weight vector as

$$\frac{\delta_{gi}\delta_{gj}}{2\Phi^2} E_{x\sim P(\boldsymbol{x})}\left[Cov\left(y_i, y_j|\boldsymbol{x}\right)\frac{\left(a_1-\mu\right)\left(a_H-\mu\right)}{\sigma^2}\right]$$

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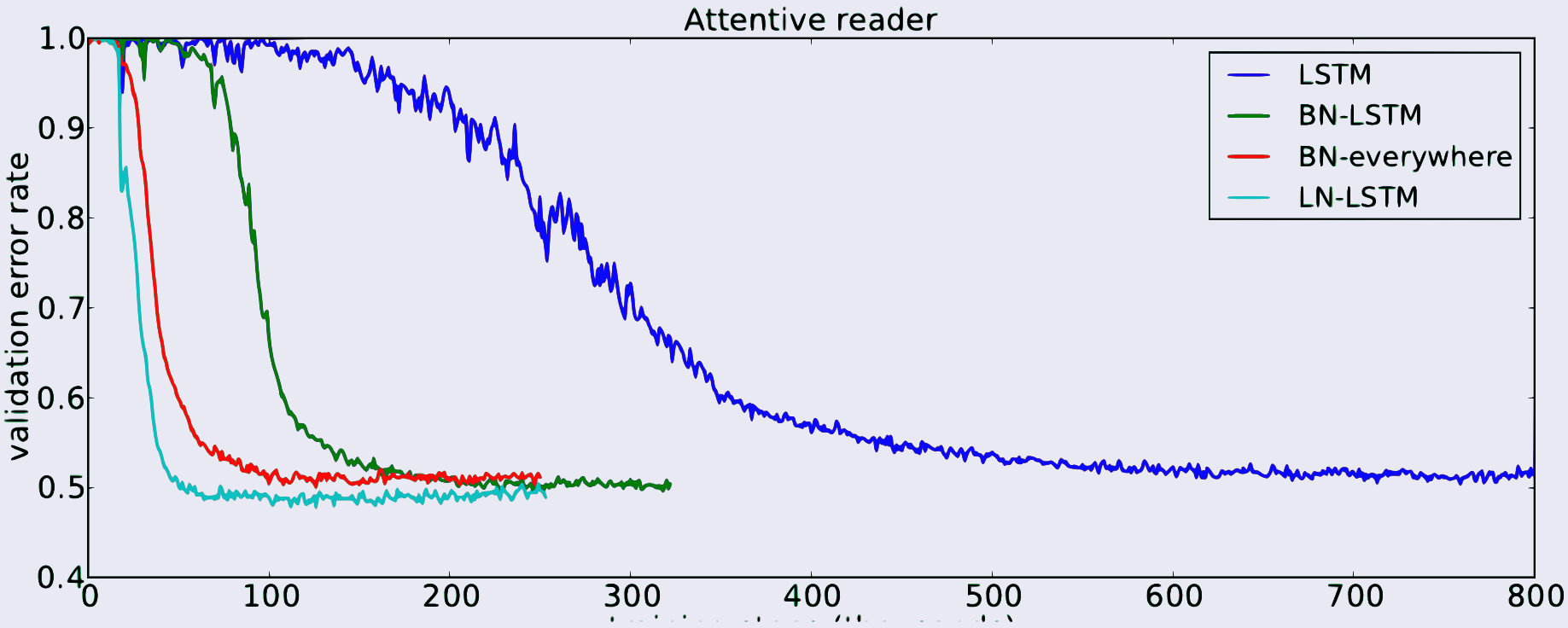
Results

In a LSTM



Outline

We have the following paper

Please Take a Look

- Kukačka, J., Golkov, V., & Cremers, D. (2017). Regularization for deep learning: A taxonomy. arXiv preprint arXiv:1710.10686.

Conclusions

There is still a lot to understand on the Deep Learning Architectures

- The Last 10 years have shown us a lot on the need of regularization...

Therefore

- When connecting with the paper
  - "How Does Batch Normalization Help Optimization?" by Santurkar, Tsipras, Ilyas and Madry

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