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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We have the Bias-Variance

Our Final Equation

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It represents the measure of the error between our machine $g(\boldsymbol{x}|\mathcal{D})$ and the expected output of the machine under $\boldsymbol{x}_i \sim p(\boldsymbol{x}|\Theta)$.

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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

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

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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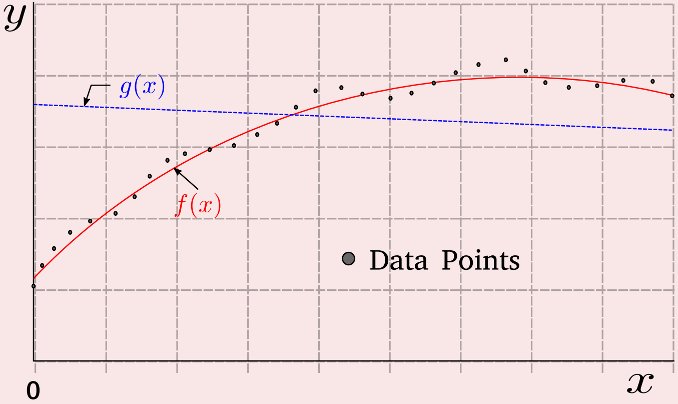

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Since $g(x)$ is fixed

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

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.

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

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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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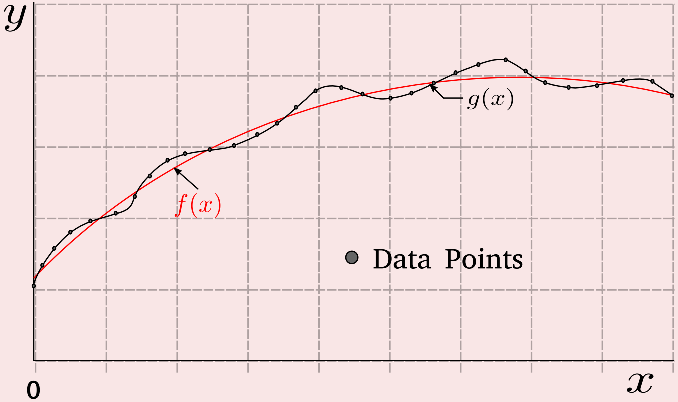

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Due to the zero mean of the noise source

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

Remark: At the training points the bias is zero.

However, the variance increases

$$\begin{aligned} E_D\left[\left(g_1\left(\boldsymbol{x}|\mathcal{D}\right) - E_D\left[g_1\left(\boldsymbol{x}|\mathcal{D}\right)\right]\right)^2\right] &= E_D\left[\left(f\left(x\right) + \epsilon - f\left(x\right)\right)^2\right] \\ &= \sigma_\epsilon^2, \text{ for } x = x_i, i = 1, 2, \dots, N \end{aligned}$$

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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 $h_{w}\left(x\right)$?

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 $h_{\boldsymbol{w}}\left(x\right)$?

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

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Regularization intuition is as follow

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

It implies

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

However handling such many parameters can be so difficult

Combinatorial problem in reality!!!

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Better, we can

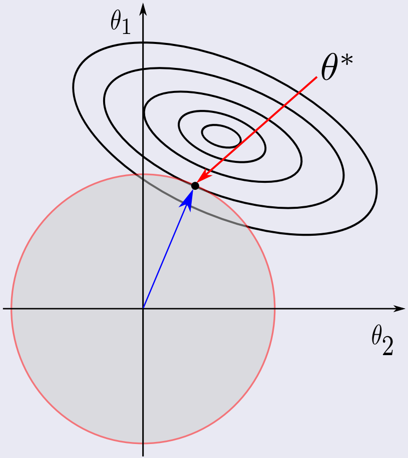
We better use the following

$$\min_{\boldsymbol{\theta}} \frac{1}{2} \sum_{i=1}^{N} \left(h_{\boldsymbol{\theta}}\left(x_i\right) - y_i\right)^2 + \lambda \sum_{i=1}^{d} \theta_i^2 \tag{9}$$

Graphically

Geometrically Equivalent to send our function to something quadratic

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



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

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The Larger $\lambda \geq 0$

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This is also can be written

Optimization Solution

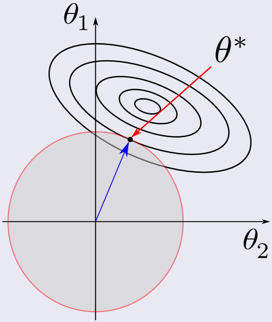
$$\arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{N} \left(y_i - \theta_0 - \sum_{j-1}^{d} x_{ij}\theta_j \right)^2$$

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

Graphically

Geometrically Equivalent to

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



Outline

Least Absolute Shrinkage and Selection Operator (LASSO)

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

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

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

$$\|\boldsymbol{\theta}\|_1 = \sum_{i=1}^{d} |\theta_i|$$

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The Final Optimization Problem

LASSO

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The Lagrangian Version

The Lagrangian

$$\widehat{\boldsymbol{\theta}}^{LASSO} = \arg\min_{\boldsymbol{\theta}} \left\{ \sum_{i=1}^{N} \left(y_i - \boldsymbol{x}^T \boldsymbol{\theta} \right)^2 + \lambda \sum_{i=1}^{d} |\theta_i| \right\}$$

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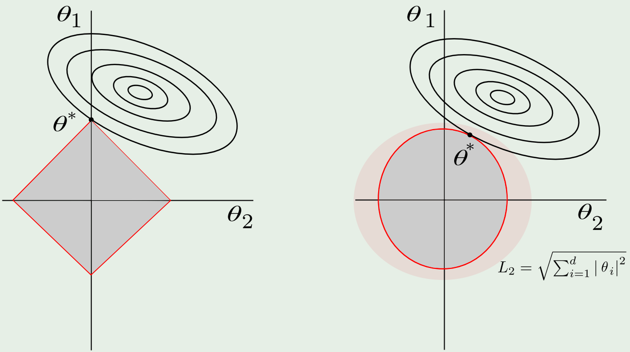
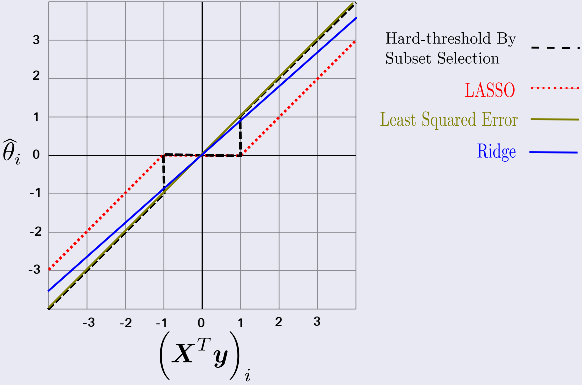
Graphically

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



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

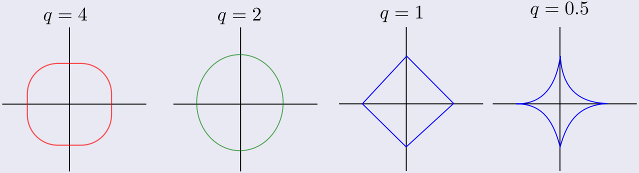
Furthermore

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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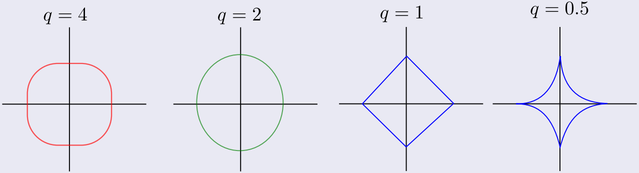

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Therefore

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

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

This is Basically

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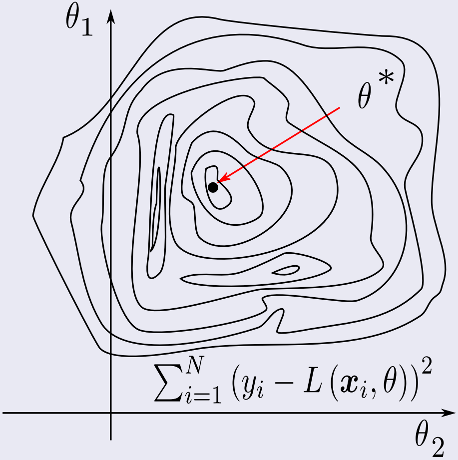
What can be done?

Remember that our optimization Landscape is highly variable



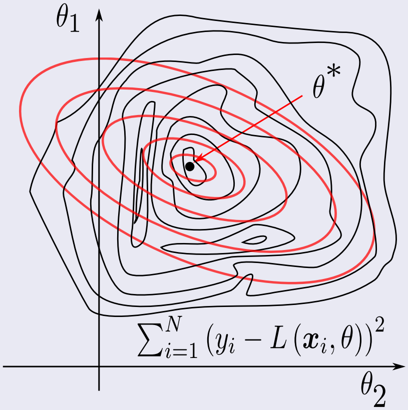
Overfitting?

Basically (Intuition)

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

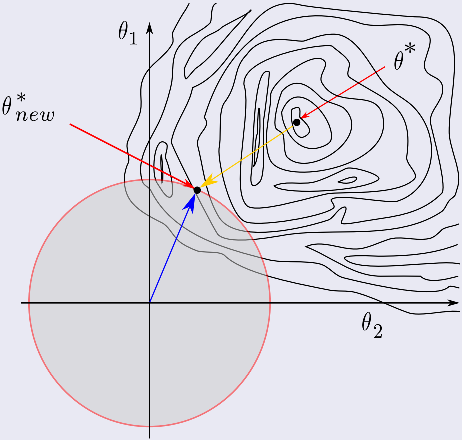
We do not want too much simplification

Look at this



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,
  3. The solution's behavior changes continuously with the initial conditions.

Any other problem that fails in any of this conditions

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It seems to be that

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

The constraints forces the $\theta's$

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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.

Unfortunately

- Dataset augmentation is not as straightforward to apply in all domains as it is for images.

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In voice detection, adding

1. Gaussian noise to the input,
2. Shifting the pitch of the audio signal,
3. Time stretching,
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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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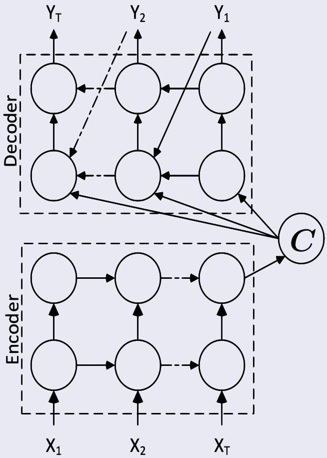
Outline

Decoder/Encoder Part

We have a Decoder and Encoder Architecture

$$\boldsymbol{C} = \text{Context Vector}$$



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

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

- σ a sigmoid function

The Update gate

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Where

The Activation Gate update

$$h_j^t = z_j h_j^{t-1} + (1 - z_j)\,\widetilde{h}_j^t$$

- Where $\widetilde{h}_j^t = \phi\left([\boldsymbol{W}\mathrm{x}]_j + [\boldsymbol{U}(\boldsymbol{r} \odot \boldsymbol{h}_{t-1})]_j\right)$

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

$$p\left(y_t | y_{t-1}, ..., y_1, \boldsymbol{c}\right) = \frac{\exp\left(W_o \boldsymbol{h}_t + U_o y_{t-1} + \boldsymbol{c}_{t-1}\right)}{\sum_{j=1}^{K} \exp\left(W_j \boldsymbol{h}_t + U_o y_{t-1} + \boldsymbol{c}_{t-1}\right)}$$

Then

- 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

$$\max_{\theta} \frac{1}{N} \sum_{n=1}^{N} p\left(y_n | x_n\right)$$

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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

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

- $\lambda = 0.5$

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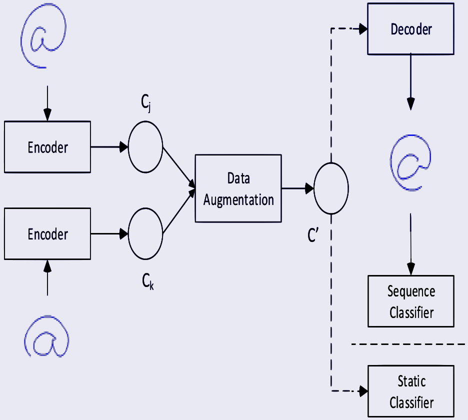
Then

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



Outline

Outline

Regularization in Deep Forward

In Layers of a Deep Forward

- We want to find and estimation x_t^r to an input at $x_0 \in \mathbb{R}^d$ in layer t satisfying

$$\sigma\left(A_t^T x_t\right) = y_{t+1}$$

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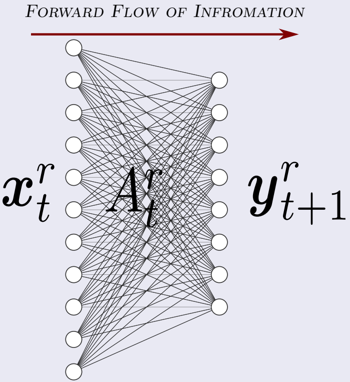
We can see this

A flow of information



In all such situations

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

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

It is usually a meaningless bad approximation

- 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

$$y_T = \sigma\left(A_T \sigma\left(A_{T-1} \sigma\left(A_{T-2}\left(\ldots \sigma\left(A_0 x_0\right)\right)\right)\right)\right)$$

Here

- The σ is applied to the generated vectors point wise...

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The Jacobian of the Gradient Descent

Here, we assume a Least Squared Error cost function

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

Where

$$\sigma'\left(A_k^r x_k\right) = \begin{pmatrix} \sigma'\left(a_{1k}^r x_k\right) & 0 & \cdots & 0 \\ 0 & \sigma'\left(a_{2k}^r x_k\right) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma'\left(a_{Mk}^r x_k\right) \end{pmatrix}$$

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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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First

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Then, we have that

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

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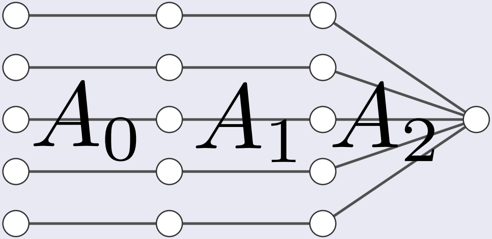
Actually

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

However, we could do the following at each layer

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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

- From [7] "Dropout training as adaptive regularization" by Wager et al.

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He comments that with unlimited computations

- "the best way to "regularize" a fixed-sized model is to average the predictions of all possible settings of the parameters"

Something like Boosting [1]

- By Using simpler and smaller models

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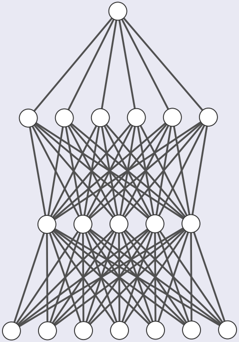

How it works?

You have forward layers

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\begin{aligned}
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)
\end{aligned}
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With dropout, the feed-forward operation becomes

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r_j^l &\sim Bernoulli\left(p\right) \\
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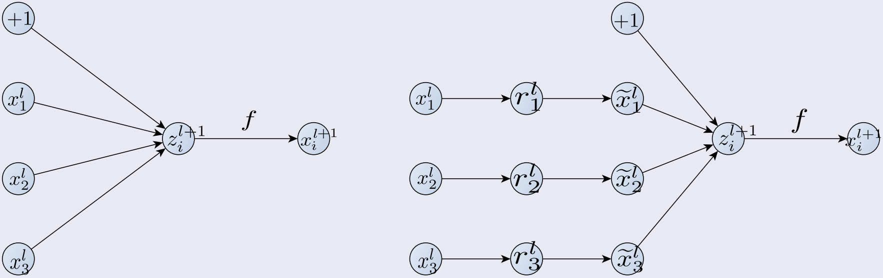
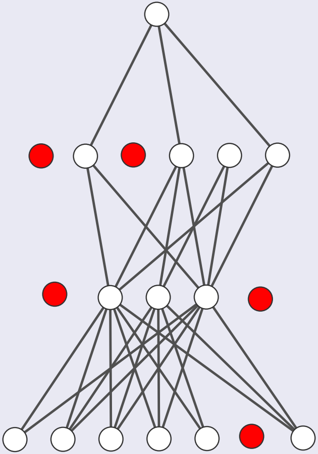
The Network

It looks like a series of gates



Then, we erase randomly connections through the network

We generate sparser version of the original one



Then assuming a Multilayer Perceptron

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

$$\min \frac{1}{N}\sum_{i=1}^{N}(z_i - t_i)^2$$

$$z_i = \sigma_1\left(W_{oh}\boldsymbol{y}_i\right)$$

$$\boldsymbol{y}_i = \sigma_2\left(W_{hi}\boldsymbol{x}_i\right)$$

Then, we get the following network after the sampling

$$L\left(W_{oh}, W_{hI}\right) = (t - z)^2$$

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Then, we have that

The Backpropagation at hidden weights

$$\frac{\partial L}{\partial W_{oh}} = -2\left(t - z\right) \times \frac{\partial \sigma_1'\left(net_{oh}\right)}{\partial net_{oh}} \times \left(\boldsymbol{r}^2 \odot \boldsymbol{y}\right)$$

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.

Something Notable

- These networks all share weights so that the total number of parameters is still $O(n^2)$, or less.

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.

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

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Mathematically

We have the following ideas

- Each node has associated matrices

$$W_{out} = \begin{pmatrix} w_1 & w_2 & \cdots & w_K \end{pmatrix}$$
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Then use the probability p

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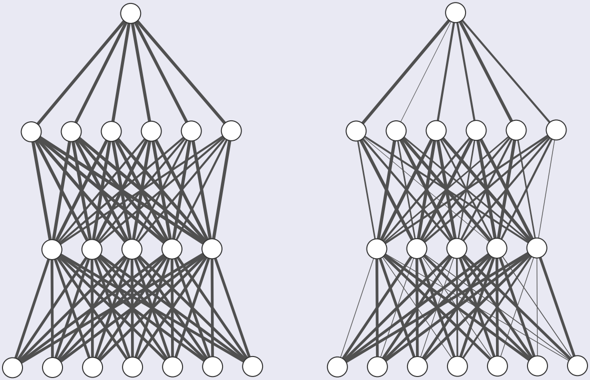
Then

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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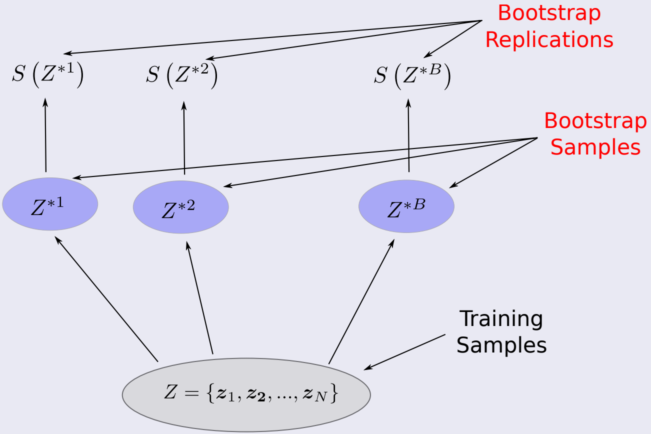
Bagging/Bootstrap Aggregation

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

Why not use for the Data for Sparsity?

We have

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

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

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

$$p\left(\tau|\gamma\right)=\left(\frac{\gamma}{2}\right)^{d}\prod_{i=1}^{d}\exp\left\{-\frac{\gamma}{2}\tau_{i}\right\}$$

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How do we build such distribution

Given that each w_i has a zero-mean Gaussian prior

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

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Then, we have

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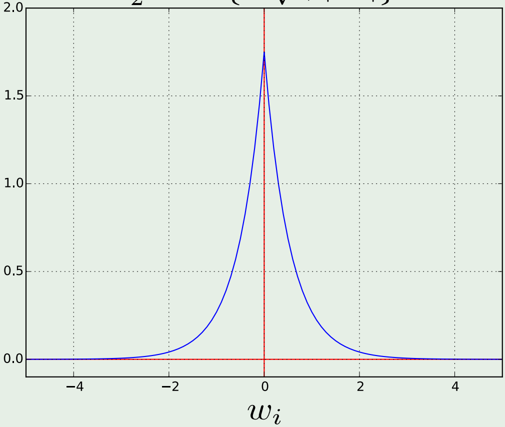
Example

The double exponential

$$\frac{\sqrt{\gamma}}{2}\exp\left\{-\sqrt{\gamma}\,|\,w_i|\right\}$$



Then using the Monte Carlo Method

We have

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

Then, we use the mini batch per epoch to decide if we drop a weight

- Basically, the previous

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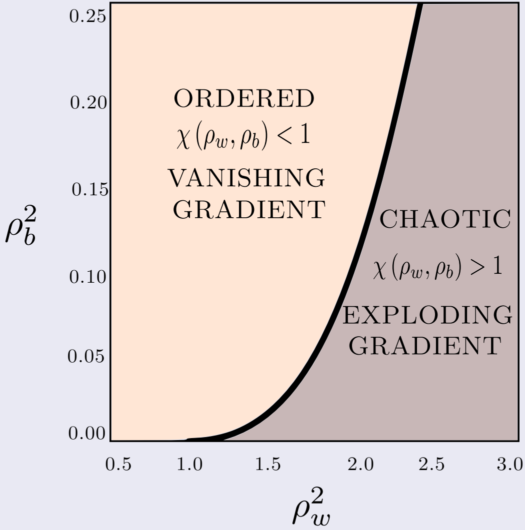
We are using the following idea

Basically, we are using the fact that



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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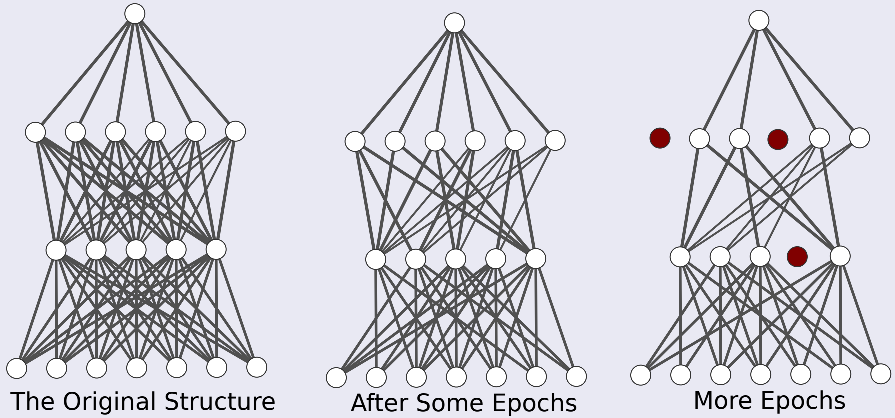
As the process progress

Once the weights fall below certain level we shutdown the weight



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]

Bouthillier et al.[8]

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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 $M \sim \mathcal{B}(p_h)$

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

- 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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Outline

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

- It is to augment the data using noise:
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Outline

Augmenting by Noise [8]

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

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

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

$$L\left(\boldsymbol{x}, \boldsymbol{x}^*\right) = \left[(f \circ h)(\boldsymbol{x}^*) - \left(\widetilde{f} \circ h\right)(\boldsymbol{x}^*)\right]^2$$

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Extending to n layers

For this, we define

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

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

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

$$L\left(\boldsymbol{x}, \boldsymbol{x}^{(1)^{*}}, \ldots, \boldsymbol{x}^{(n)^{*}}\right) = \sum_{i=1}^{n} \lambda_i \left[g^{(i)}\left(\boldsymbol{x}^{(i)^{*}}\right) - \widetilde{g}^{(i)}\left(\boldsymbol{x}\right)\right]^2$$

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However

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

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

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Finally

$$rect\left(h^{(i)}\left(g^{(i-1)}\left(\boldsymbol{x}^*\right)\right)\right) = M^{(i)} \odot rect\left(h^{(i)}\left(g^{(i-1)}\left(\boldsymbol{x}^*\right)\right)\right)$$

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Therefore

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.
  - $d_{(i)}$ is the number of of hidden units.
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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 x^* for each hidden layer

by providing multiple inputs

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

However

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

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Outline

Co-adaptation/Overfitting

Definition

- Co-adaptation is the accumulation of interacting genes in the gene pool of a population by selection.
  - Selection pressures on one of the genes will affect its interacting proteins, after which compensatory changes occur.

In Neural Networks

- In neural network, co-adaptation means that some neurons are highly dependent on others:
  - Getting into over-fitting!!!

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This is not trivial given that

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Therefore

We can then

- Modifying the probability distribution is the most straightforward way to improve the set of transformations.

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Define

$$M_{hij} \sim \mathcal{B}(\rho_h) \text{ (Bernoulli)}$$
$$\rho_h \sim U(0, p_h) \text{ (Uniform)}$$

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

Here, the authors use the same ρ for all the layers of the neurons, then

$$\widetilde{f}(h) = \frac{1}{1-\rho} M \odot rect(h)$$

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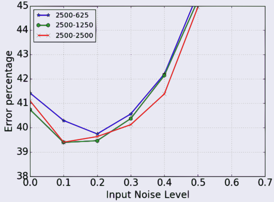
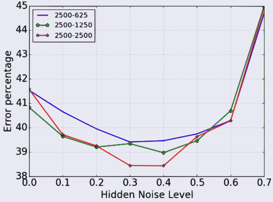
Results

Something Notable

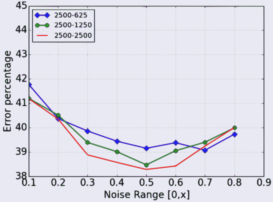
Using dropout with varying input noise and fixed hidden noise of 0.5.



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.

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

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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 $h_i^{l+1} = f\left(y_i^l + b_i^l\right)$

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We have that

- All the hidden units in a layer share the same normalization terms μ and σ
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Layer normalization does not impose any constraint

- On the size of a mini-batch and it can be used in the pure on-line regime with batch size 1.

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The Flow of Information through time

First, the new $\boldsymbol{h}^t$ with a gain vector $\boldsymbol{g}$

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

The Temporal Layer Mean Normalization

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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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In the other hand

Layer normalization

- It is not invariant to the individual scaling of the single weight vectors.

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

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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

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

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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

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

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

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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

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

Basically

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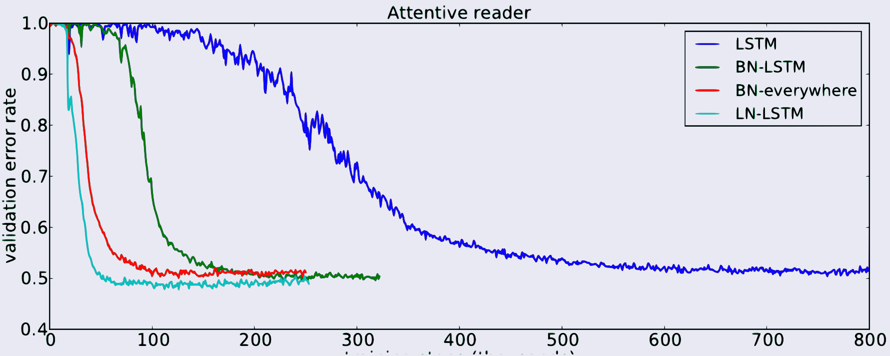
Results

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.

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