

Course Materials for GEN-AI

Northeastern University

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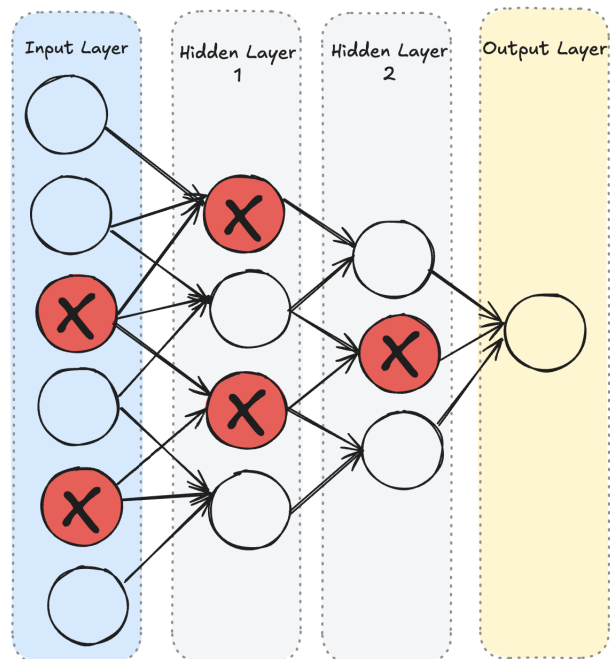
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Thank you for your understanding and collaboration.

Dropout

Introduction

Dropout is a regularization technique used in neural networks to prevent overfitting. It works by randomly "dropping out" (setting to zero) a subset of neurons during each forward pass of training. This forces the network to learn redundant data representations, improving its generalization performance.



Thinned network: A neural network consisting of all units that survived dropout.

A neural network with n units can create a collection of 2^n thinned networks. For each node, we have either drop or not(binary). For example, if you have 10 fingers, you can count from 0000000000 or 1111111111 or from 0 to $2^n - 1 = 1024$.

- **During training**, dropout samples from the number of thinned networks.
- **During testing**, we approximate the effect of averaging the predictions of all these thinned networks.

Consider a neural network with:

- L hidden layers,
- Z^i = input to layer i
- a^i = output to layer i
- w^i, b^i are weights and biases of layer i
- R_j^P = Bernouli value for node j in layer P

$$R_j^P \approx \text{Bernouli}(P)$$

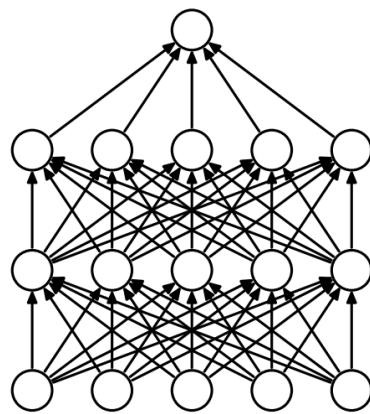
$$r^P = \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}_{S_P}$$

$$\tilde{a}^P = r^P \odot a^P$$

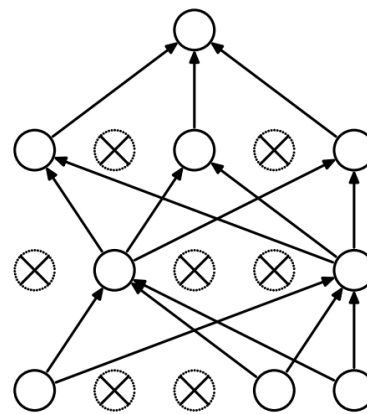
$$z_i^{P+1} = w_i^{P+1} \tilde{a}^P + b_i^{P+1}$$

$$\tilde{a}^{P+1} = f(z_i^{P+1})$$

We only back-propagate on each thinned network.



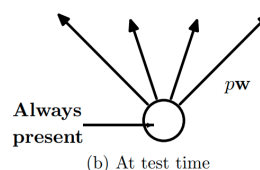
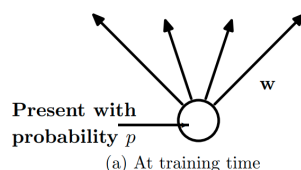
(a) Standard Neural Net



(b) After applying dropout.

Test Case

- use a single NN without dropout.
- Multiply all weights and biases by $P(\text{Bernoulli Parameter})$ because the weight/bias wasn't always available, so to ensure during the inference, that's also the case.
- every weight was used during the training with probability of $P(\text{Bernoulli})$ and was dropped with probability of $(1 - p)$.

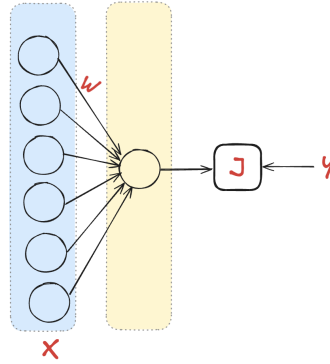


Left: A unit at training time that is present with probability p and is connected to units in the next layer

with weights w . Right: At test time, the unit is always present and the weights are multiplied by p . The output at test time is same as the expected output at training time.

- w_i^L , out of 10 epochs maybe, x times was used in training, we multiply $\frac{x}{10} * w_i^L$, by doing so we are getting on average results from 10 NNs. Technically each iteration we had a new NN as they were different in nodes. (like bagging)

Applying dropout to linear regression



Given,

$$X \in \mathbb{R}^{m \times d}; w \in \mathbb{R}^{d \times I}; y \in \mathbb{R}^m$$

In Linear regression our goal is to minimize:

$$J = \|\mathbf{y} - X\mathbf{w}\|^2$$

$$R \in \mathbb{R}^{m \times d}, \quad R = \begin{bmatrix} R_{1,1} & R_{1,2} & \dots & R_{1,d} \\ R_{2,1} & R_{2,2} & \dots & R_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ R_{m,1} & R_{m,2} & \dots & R_{m,d} \end{bmatrix},$$

where each element $R_{i,j} \sim \text{Bernoulli}(p)$, i.e.,

$$R_{i,j} = \begin{cases} 1, & \text{with probability } p, \\ 0, & \text{with probability } 1 - p. \end{cases}$$

our objective function becomes:

$$\min_{\mathbf{w}} \mathbb{E}_{R \sim \text{Bernoulli}(p)} [\|\mathbf{y} - (R * X)\mathbf{w}\|^2]$$

$$|y - Xw|^2$$

⇒ we apply dropout using Bernoulli p

$$\Rightarrow |y - R \odot Xw|^2$$

applying Bernoulli to x, so some of the weights will drop

$$\Rightarrow |y - Mw|^2$$

the goal is to understand the expectation of $R \odot X$

In each iteration R changes (Bernoulli \approx p), so some w will drop.

We want to see what is the expected value of w_i^L if we drop/keep it randomly after n epochs.

$$= (y - Mw)^T (y - Mw) = y^T y - y^T m w - w^T m^T y + w^T m^T m w$$

$$= y^T y - 2w^T m^T y + w^T m^T m w$$

⇒ we want to find:

$$E[(y - Mw)^2] \text{ w.r.t. } R$$

$$\Rightarrow E[y^T y - 2w^T m^T y + w^T m^T m w]$$

$$= E[y^T y] - 2w^T (E[m])^T y + w^T E[m^T m] w$$

break down:

$$E[\mathbf{M}] = \begin{bmatrix} E[M_{11}] & E[M_{12}] & \cdots & E[M_{1d}] \\ E[M_{21}] & E[M_{22}] & \cdots & E[M_{2d}] \\ \vdots & \vdots & \ddots & \vdots \\ E[M_{m1}] & E[M_{m2}] & \cdots & E[M_{md}] \end{bmatrix} \Rightarrow E[M_{ij}] = p \cdot X_{ij}$$

$$\Rightarrow E[R \odot X] = E[M] = p \cdot X$$

$$\Rightarrow E[(M^T M)_{ij}] = \sum_k E(R_{ki} R_{kj}) X_{ki} X_{kj}$$

$$\text{where } E[R_{ki} R_{kj}] = \begin{cases} \text{if } i \neq j; p^2 \\ \text{if } i=j; p \end{cases}$$

Considering the above

$$\Rightarrow E[y^T y] - 2w^T (E[m])^T y + w^T E[m^T m] w = y^T y - 2p w^T X^T y + w^T E[m^T m] w$$

We could solve it by directly multiplying P by X,

$$|y - pXw|^2 = y^T y - 2p w^T X^T y + p^2 w^T X^T X w$$

So we can express:

$$[\|y - (R \odot X)w\|^2] = |y - pXw|^2 - p^2 w^T X^T X w + w^T E[m^T m] w$$

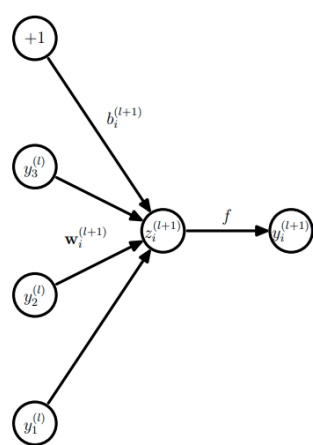
$$\Rightarrow |y - pXw|^2 + w^T [-p^2 X^T X + E[m^T m]] w$$

$$\text{considering that: } \begin{cases} \text{if } i \neq j; E[m^T m] = p^2 X^2 \\ \text{if } i=j; E[m^T m] = p \cdot \text{diagonal}(X^2) \end{cases}$$

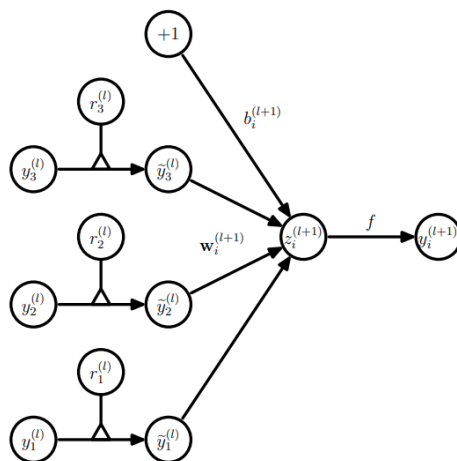
$$\Rightarrow |y - pXw|^2 + w^T [-p^2 X^T X + pX^2] w$$

$$\Rightarrow |y - pXw|^2 + w^T [p * (1 - p) \text{diagonal}(X^2)] w$$

In general applying the dropout to linear regression is similar to Ridge Regression.



(a) Standard network



(b) Dropout network