# CS7015 (Deep Learning) : Lecture 8

## Regularization: Bias Variance Tradeoff, l2 regularization, Early stopping, Dataset augmentation, Parameter sharing and tying, Injecting noise at input, Ensemble methods, Dropout

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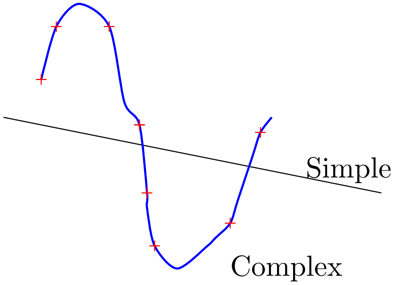
## Acknowledgements

- Chapter 7, Deep Learning book
- Ali Ghodsi's Video Lectures on Regularization[a]
- Dropout: A Simple Way to Prevent Neural Networks from Overfitting[b]

[a] Lecture 2.1 and Lecture 2.2
[b] Dropout

# Module 8.1 : Bias and Variance

We will begin with a quick overview of bias, variance and the trade-off between them.



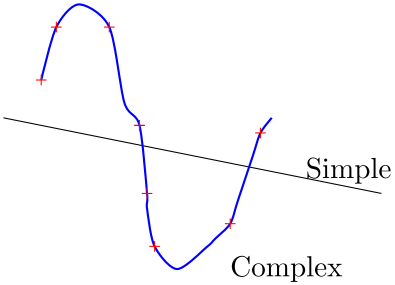

The points were drawn from a sinusoidal function (the true $f(x)$)

- Let us consider the problem of fitting a curve through a given set of points
- We consider two models :

$$\underset{(degree:1)}{Simple} \quad y = \hat{f}(x) = w_1 x + w_0$$

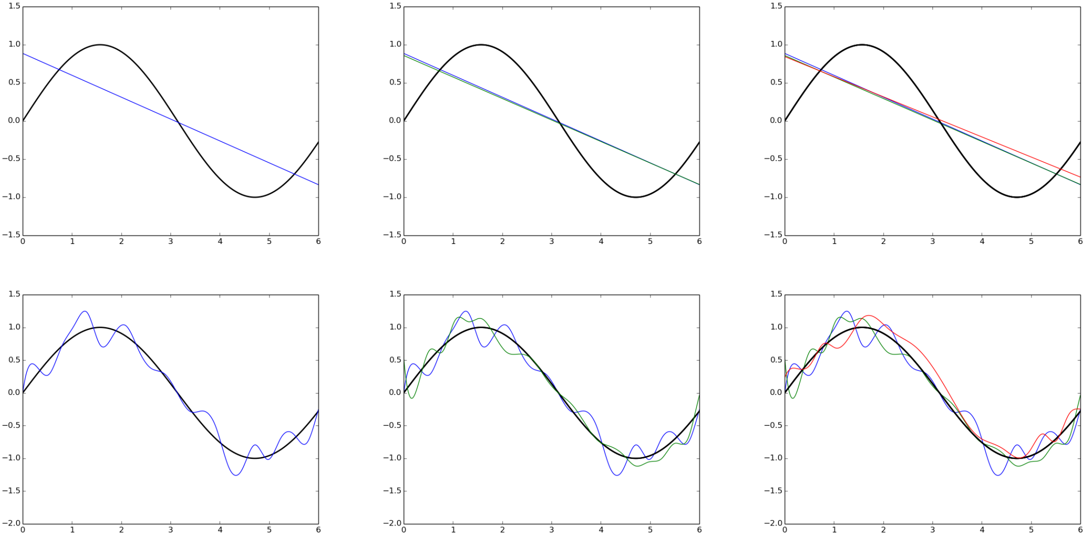
$$\underset{(degree:25)}{Complex} \quad y = \hat{f}(x) = \sum_{i=1}^{25} w_i x^i + w_0$$

- Note that in both cases we are making an assumption about how $y$ is related to $x$. We have no idea about the true relation $f(x)$
- The training data consists of 100 points




The points were drawn from a sinusoidal function (the true $f(x)$)

- We sample 25 points from the training data and train a simple and a complex model
- We repeat the process '$k$' times to train multiple models (each model sees a different sample of the training data)
- We make a few observations from these plots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2
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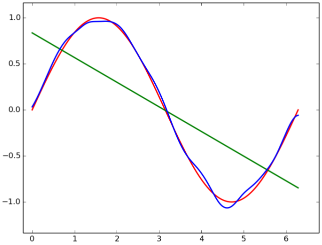
6

- Simple models trained on different samples of the data do not differ much from each other
- However they are very far from the true sinusoidal curve (under fitting)
- On the other hand, complex models trained on different samples of the data are very different from each other (high variance)

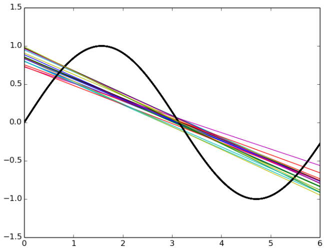


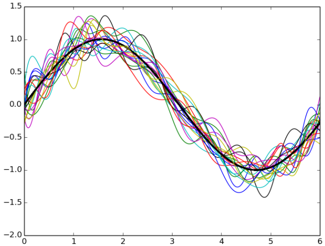

Green Line: Average value of $\hat{f}(x)$ for the simple model
Blue Curve: Average value of $\hat{f}(x)$ for the complex model
Red Curve: True model ($f$(x))

- Let $f(x)$ be the true model (sinusoidal in this case) and $\hat{f}(x)$ be our estimate of the model (simple or complex, in this case) then,

$$\text{Bias } (\hat{f}(x)) = E[\hat{f}(x)] - f(x)$$

- $E[\hat{f}(x)]$ is the average (or expected) value of the model
- We can see that for the simple model the average value (green line) is very far from the true value $f(x)$ (sinusoidal function)
- Mathematically, this means that the simple model has a high bias
- On the other hand, the complex model has a low bias



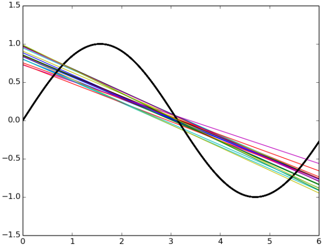

- We now define,

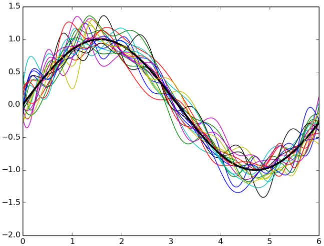
$$\text{Variance } (\hat{f}(x)) = E[(\hat{f}(x) - E[\hat{f}(x)])^2]$$

(Standard definition from statistics)

- Roughly speaking it tells us how much the different $\hat{f}(x)$'s (trained on different samples of the data) differ from each other

- It is clear that the simple model has a low variance whereas the complex model has a high variance




- In summary (informally)
- Simple model: high bias, low variance
- Complex model: low bias, high variance
- There is always a trade-off between the bias and variance
- Both bias and variance contribute to the mean square error. Let us see how

# Module 8.2 : Train error vs Test error

- Consider a new point $(x, y)$ which was not seen during training
- If we use the model $\hat{f}(x)$ to predict the value of $y$ then the mean square error is given by

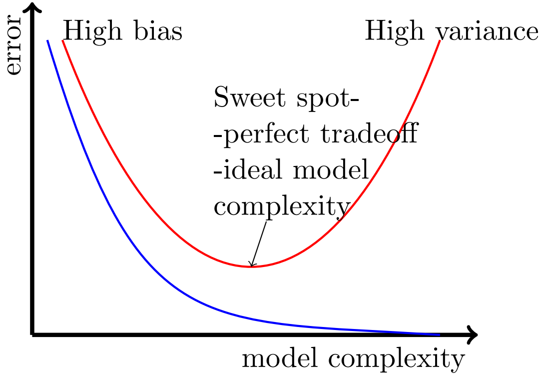
$$E[(y - \hat{f}(x))^2]$$

(average square error in predicting $y$ for many such unseen points)

- We can show that

$$\begin{aligned} E[(y - \hat{f}(x))^2] &= Bias^2 \\ &+ Variance \\ &+ \sigma^2 \text{ (irreducible error)} \end{aligned}$$

- See proof here




$$E[(y - \hat{f}(x))^2] = Bias^2 + Variance + \sigma^2 \text{ (irreducible error)}$$

- The parameters of $\hat{f}(x)$ (all $w_i$'s) are trained using a training set $\{(x_i, y_i)\}_{i=1}^n$
- However, at test time we are interested in evaluating the model on a validation (unseen) set which was not used for training
- This gives rise to the following two entities of interest:
  $train_{err}$ (say, mean square error)
  $test_{err}$ (say, mean square error)
- Typically these errors exhibit the trend shown in the adjacent figure

## Intuitions developed so far

- Let there be $n$ training points and $m$ test (validation) points

$$train_{err} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}(x_i))^2$$

$$test_{err} = \frac{1}{m}\sum_{i=n+1}^{n+m}(y_i - \hat{f}(x_i))^2$$

- As the model complexity increases $train_{err}$ becomes overly optimistic and gives us a wrong picture of how close $\hat{f}$ is to $f$
- The validation error gives the real picture of how close $\hat{f}$ is to $f$
- We will concretize this intuition mathematically now and eventually show how to account for the optimism in the training error

- Let D=$\{x_i, y_i\}_{i=1}^{m+n}$, then for any point $(x, y)$ we have,

$$y_i = f(x_i) + \varepsilon_i$$

- which means that $y_i$ is related to $x_i$ by some true function $f$ but there is also some noise $\varepsilon$ in the relation
- For simplicity, we assume

$$\varepsilon \sim \mathcal{N}(0, \sigma^2)$$

and of course we do not know $f$

- Further we use $\hat{f}$ to approximate $f$ and estimate the parameters using T $\subset$ D such that

$$y_i = \hat{f}(x_i)$$

- We are interested in knowing

$$E[(\hat{f}(x_i) - f(x_i))^2]$$

but we cannot estimate this directly because we do not know $f$

- We will see how to estimate this empirically using the observation $y_i$ & prediction $\hat{y}_i$

$$
\begin{aligned}
E[(\hat{y}_i - y_i)^2] &= E[(\hat{f}(x_i) - f(x_i) - \varepsilon_i)^2] \quad (y_i = f(x_i) + \varepsilon_i) \\
&= E[(\hat{f}(x_i) - f(x_i))^2 - 2\varepsilon_i(\hat{f}(x_i) - f(x_i)) + \varepsilon_i^2] \\
&= E[(\hat{f}(x_i) - f(x_i))^2] - 2E[\varepsilon_i(\hat{f}(x_i) - f(x_i))] + E[\varepsilon_i^2]
\end{aligned}
$$

$$
\therefore E[(\hat{f}(x_i) - f(x_i))^2] = E[(\hat{y}_i - y_i)^2] - E[\varepsilon_i^2] + 2E[\, \varepsilon_i(\hat{f}(x_i) - f(x_i)) \,]
$$

We will take a small detour to understand how to empirically estimate an Expectation and then return to our derivation

- Suppose we have observed the goals scored($z$) in $k$ matches as $z_1 = 2,\ z_2 = 1,\ z_3 = 0,\ \ldots\ z_k = 2$

- Now we can empirically estimate $E[z]$ i.e. the expected number of goals scored as

$$E[z] = \frac{1}{k}\sum_{i=1}^{k} z_i$$

- Analogy with our derivation: We have a certain number of observations $y_i$ & predictions $\hat{y}_i$ using which we can estimate

$$E[(\hat{y}_i - y_i)^2] = \frac{1}{m}\sum_{i=1}^{m} (\hat{y}_i - y_i)^2$$

... returning back to our derivation

$$E[(\hat{f}(x_i) - f(x_i))^2] = E[(\hat{y}_i - y_i)^2] - E[\varepsilon_i^2] + 2E[\ \varepsilon_i(\hat{f}(x_i) - f(x_i))\ ]$$

- We can empirically evaluate R.H.S using training observations or test observations

**Case 1**: Using test observations

$$\underbrace{E[(\hat{f}(x_i) - f(x_i))^2]}_{true\, error} = \underbrace{\frac{1}{m}\sum_{i=n+1}^{n+m}(\hat{y}_i - y_i)^2}_{empirical\, estimation\, of\, error} - \underbrace{\frac{1}{m}\sum_{i=n+1}^{n+m}\varepsilon_i^2}_{small\, constant} + 2\ \underbrace{E[\ \varepsilon_i(\hat{f}(x_i) - f(x_i))\ ]}_{=\, covariance\, (\varepsilon_i, \hat{f}(x_i) - f(x_i))}$$

$$\begin{aligned} \because \text{covariance}(X, Y) &= E[(X - \mu_X)(Y - \mu_Y)] \\ &= E[(X)(Y - \mu_Y)] (\text{if } \mu_X = E[X] = 0) \\ &= E[XY] - E[X\mu_Y] = E[XY] - \mu_Y E[X] = E[XY] \end{aligned}$$

$$\underbrace{E[(\hat{f}(x_i) - f(x_i))^2]}_{true\ error}$$

$$= \underbrace{\frac{1}{m}\sum_{i=n+1}^{n+m}(\hat{y}_i - y_i)^2}_{empirical\ estimation\ of\ error} - \underbrace{\frac{1}{m}\sum_{i=n+1}^{n+m}\varepsilon_i^2}_{small\ constant} + 2\ \underbrace{E[\ \varepsilon_i(\hat{f}(x_i) - f(x_i))\ ]}_{=covariance\,(\varepsilon_i,\hat{f}(x_i)-f(x_i))}$$

- None of the test observations participated in the estimation of $\hat{f}(x)$[the parameters of $\hat{f}$(x) were estimated only using training data]

$$\therefore \varepsilon \perp (\hat{f}(x_i) - f(x_i))$$

$$\therefore E[\varepsilon_i \cdot (\hat{f}(x_i) - f(x_i))] = E[\varepsilon_i] \cdot E[\hat{f}(x_i) - f(x_i))] = 0 \cdot E[\hat{f}(x_i) - f(x_i))] = 0$$

$$\therefore \text{true error} = \text{empirical test error} + \text{small constant}$$

- Hence, we should always use a validation set(independent of the training set) to estimate the error

**Case 2**: Using training observations

$$\underbrace{E[(\hat{f}(x_i) - f(x_i))^2]}_{true\ error}$$

$$= \underbrace{\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}_{empirical\ estimation\ of\ error} - \underbrace{\frac{1}{n}\sum_{i=1}^{n}\varepsilon_i^2}_{small\ constant} + 2\ \underbrace{E[\ \varepsilon_i(\hat{f}(x_i) - f(x_i))\ ]}_{=\ covariance\ (\varepsilon_i, \hat{f}(x_i) - f(x_i))}$$

Now, $\varepsilon \not\perp \hat{f}(\mathrm{x})$ because $\varepsilon$ was used for estimating the parameters of $\hat{f}(x)$

$$\therefore E[\varepsilon_i \cdot (\hat{f}(x_i) - f(x_i))] \neq E[\varepsilon_i] \cdot E[\hat{f}(x_i) - f(x_i))] \neq 0$$

Hence, the empirical train error is smaller than the true error and does not give a true picture of the error

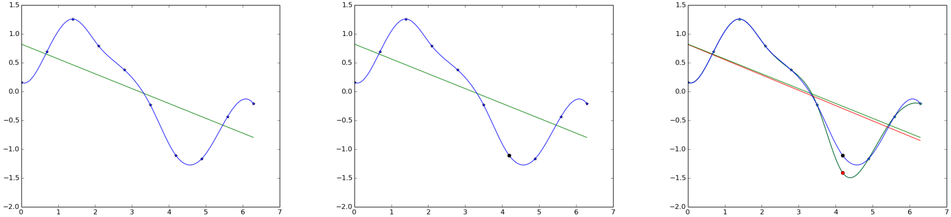
But how is this related to model complexity? Let us see

# Module 8.3 : True error and Model complexity

Using Stein's Lemma (and some trickery) we can show that

$$\frac{1}{n}\sum_{i=1}^{n}\varepsilon_i(\hat{f}(x_i) - f(x_i)) = \frac{\sigma^2}{n}\sum_{i=1}^{n}\frac{\partial \hat{f}(x_i)}{\partial y_i}$$

- When will $\frac{\partial \hat{f}(x_i)}{\partial y_i}$ be high? When a small change in the observation causes a large change in the estimation($\hat{f}$)
- Can you link this to model complexity?
- Yes, indeed a complex model will be more sensitive to changes in observations whereas a simple model will be less sensitive to changes in observations
- Hence, we can say that
  true error = empirical train error + small constant + $\Omega$(model complexity)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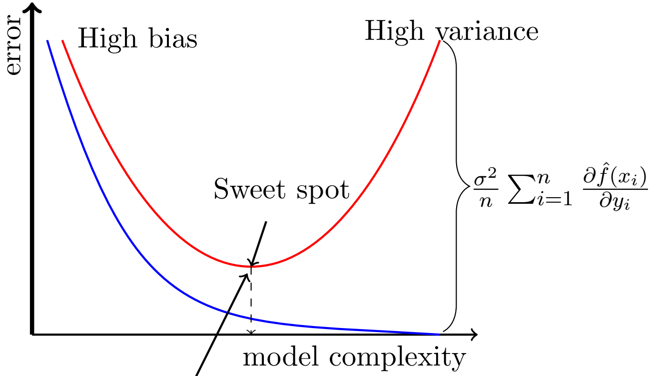
- Let us verify that indeed a complex model is more sensitive to minor changes in the data
- We have fitted a simple and complex model for some given data
- We now change one of these data points
- The simple model does not change much as compared to the complex model

- Hence while training, instead of minimizing the training error $\mathscr{L}_{train}(\theta)$ we should minimize

$$\min_{w.r.t\ \theta} \mathscr{L}_{train}(\theta) + \Omega(\theta) = \mathscr{L}(\theta)$$

- Where $\Omega(\theta)$ would be high for complex models and small for simple models
- $\Omega(\theta)$ acts as an approximate for $\frac{\sigma^2}{n} \sum_{i=1}^{n} \frac{\partial \hat{f}(x_i)}{\partial y_i}$
- This is the basis for all regularization methods
- We can show that $l_1$ regularization, $l_2$ regularization, early stopping and injecting noise in input are all instances of this form of regularization.




$\Omega(\theta)$ should ensure that model has reasonable complexity

- Why do we care about this bias variance tradeoff and model complexity?

- Deep Neural networks are highly complex models.
- Many parameters, many non-linearities.
- It is easy for them to overfit and drive training error to 0.
- Hence we need some form of regularization.

## Different forms of regularization

- $l_2$ regularization
- Dataset augmentation
- Parameter Sharing and tying
- Adding Noise to the inputs
- Adding Noise to the outputs
- Early stopping
- Ensemble methods
- Dropout

# Module 8.4 : $l_2$ regularization

## Different forms of regularization

- $l_2$ regularization
- Dataset augmentation
- Parameter Sharing and tying
- Adding Noise to the inputs
- Adding Noise to the outputs
- Early stopping
- Ensemble methods
- Dropout

- For $l_2$ regularization we have,

$$\widetilde{\mathscr{L}}(w) = \mathscr{L}(w) + \frac{\alpha}{2}\|w\|^2$$

- For SGD (or its variants), we are interested in

$$\nabla\widetilde{\mathscr{L}}(w) = \nabla\mathscr{L}(w) + \alpha w$$

- Update rule:

$$w_{t+1} = w_t - \eta\nabla\mathscr{L}(w_t) - \eta\alpha w_t$$

- Requires a very small modification to the code
- Let us see the geometric interpretation of this

- Assume $w^*$ is the optimal solution for $\mathscr{L}(w)$ [not $\widetilde{\mathscr{L}}(w)$] i.e. the solution in the absence of regularization ($w^*$ optimal $\rightarrow \nabla \mathscr{L}(w^*) = 0$)
- Consider $u = w - w^*$. Using Taylor series approximation (upto $2^{nd}$ order)

$$
\begin{aligned}
\mathscr{L}(w^* + u) &= \mathscr{L}(w^*) + u^T \nabla \mathscr{L}(w^*) + \frac{1}{2} u^T H u \\
\mathscr{L}(w) &= \mathscr{L}(w^*) + (w - w^*)^T \nabla \mathscr{L}(w^*) + \frac{1}{2}(w - w^*)^T H (w - w^*) \\
&= \mathscr{L}(w^*) + \frac{1}{2}(w - w^*)^T H (w - w^*) \qquad (\because \nabla L(w^*) = 0\ ) \\
\nabla \mathscr{L}(w) &= \nabla \mathscr{L}(w^*) + H(w - w^*) \\
&= H(w - w^*)
\end{aligned}
$$

- Now,

$$
\begin{aligned}
\nabla \widetilde{\mathscr{L}}(w) &= \nabla \mathscr{L}(w) + \alpha w \\
&= H(w - w^*) + \alpha w
\end{aligned}
$$

- Let $\widetilde{w}$ be the optimal solution for $\widetilde{L}(w)$ [i.e regularized loss]

$$\because \nabla \widetilde{L}(\widetilde{w}) = 0$$

$$H(\widetilde{w} - w^*) + \alpha\widetilde{w} = 0$$
$$\therefore (H + \alpha\mathbb{I})\widetilde{w} = Hw^*$$
$$\therefore \widetilde{w} = (H + \alpha\mathbb{I})^{-1}Hw^*$$

- Notice that if $\alpha \to 0$ then $\widetilde{w} \to w^*$ [no regularization]
- But we are interested in the case when $\alpha \neq 0$
- Let us analyse the case when $\alpha \neq 0$

- If H is symmetric Positive Semi Definite

$$H = Q\Lambda Q^T \qquad [Q \text{ is orthogonal, } QQ^T = Q^TQ = \mathbb{I}]$$

$$\begin{aligned}
\widetilde{w} &= (H + \alpha\mathbb{I})^{-1}Hw^* \\
&= (Q\Lambda Q^T + \alpha\mathbb{I})^{-1}Q\Lambda Q^T w^* \\
&= (Q\Lambda Q^T + \alpha Q\mathbb{I}Q^T)^{-1}Q\Lambda Q^T w^* \\
&= [Q(\Lambda + \alpha\mathbb{I})Q^T]^{-1}Q\Lambda Q^T w^* \\
&= Q^{T^{-1}}(\Lambda + \alpha\mathbb{I})^{-1}Q^{-1}Q\Lambda Q^T w^* \\
&= Q(\Lambda + \alpha\mathbb{I})^{-1}\Lambda Q^T w^* \qquad (\because Q^{T^{-1}} = Q) \\
\widetilde{w} &= QDQ^T w^*
\end{aligned}$$

where $D = (\Lambda + \alpha\mathbb{I})^{-1}\Lambda$, is a diagonal matrix which we will see in more detail soon

$$\widetilde{w} = Q(\Lambda + \alpha\mathbb{I})^{-1}\Lambda Q^T w^*$$
$$= QDQ^T w^*$$

$$(\Lambda + \alpha\mathbb{I})^{-1} = \begin{bmatrix} \frac{1}{\lambda_1+\alpha} & & & \\ & \frac{1}{\lambda_2+\alpha} & & \\ & & \ddots & \\ & & & \frac{1}{\lambda_n+\alpha} \end{bmatrix}$$

$$D = (\Lambda + \alpha\mathbb{I})^{-1}\Lambda$$

$$(\Lambda + \alpha\mathbb{I})^{-1}\Lambda = \begin{bmatrix} \frac{\lambda_1}{\lambda_1+\alpha} & & & \\ & \frac{\lambda_2}{\lambda_2+\alpha} & & \\ & & \ddots & \\ & & & \frac{\lambda_n}{\lambda_n+\alpha} \end{bmatrix}$$

- So what is happening here?
- $w^*$ first gets rotated by $Q^T$ to give $Q^T w^*$
- However if $\alpha = 0$ then $Q$ rotates $Q^T w^*$ back to give $w^*$
- If $\alpha \neq 0$ then let us see what $D$ looks like
- So what is happening now?

$$\begin{aligned}\widetilde{w} &= Q(\Lambda + \alpha\mathbb{I})^{-1}\Lambda Q^T w^* \\ &= QDQ^T w^*\end{aligned}$$

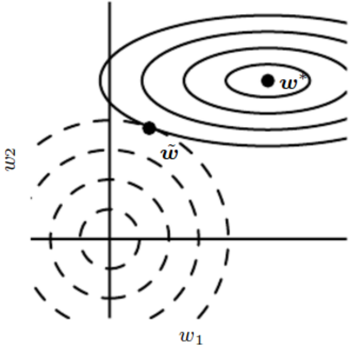
$$(\Lambda + \alpha\mathbb{I})^{-1} = \begin{bmatrix} \frac{1}{\lambda_1+\alpha} & & & \\ & \frac{1}{\lambda_2+\alpha} & & \\ & & \ddots & \\ & & & \frac{1}{\lambda_n+\alpha} \end{bmatrix}$$

$$D = (\Lambda + \alpha\mathbb{I})^{-1}\Lambda$$

$$(\Lambda + \alpha\mathbb{I})^{-1}\Lambda = \begin{bmatrix} \frac{\lambda_1}{\lambda_1+\alpha} & & & \\ & \frac{\lambda_2}{\lambda_2+\alpha} & & \\ & & \ddots & \\ & & & \frac{\lambda_n}{\lambda_n+\alpha} \end{bmatrix}$$

- Each element $i$ of $Q^T w^*$ gets scaled by $\frac{\lambda_i}{\lambda_i+\alpha}$ before it is rotated back by $Q$
- if $\lambda_i >> \alpha$ then $\frac{\lambda_i}{\lambda_i+\alpha} = 1$
- if $\lambda_i << \alpha$ then $\frac{\lambda_i}{\lambda_i+\alpha} = 0$
- Thus only significant directions (larger eigen values) will be retained.

$$\text{Effective parameters} = \sum_{i=1}^{n} \frac{\lambda_i}{\lambda_i + \alpha} < n$$

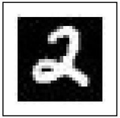



- The weight vector($w^*$) is getting rotated to ($\tilde{w}$)
- All of its elements are shrinking but some are shrinking more than the others
- This ensures that only important features are given high weights

# Module 8.5 : Dataset augmentation

## Different forms of regularization

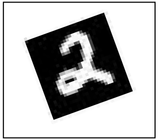
- $l_2$ regularization
- Dataset augmentation
- Parameter Sharing and tying
- Adding Noise to the inputs
- Adding Noise to the outputs
- Early stopping
- Ensemble methods
- Dropout



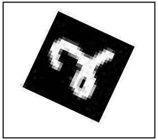
label = 2

[given training data]

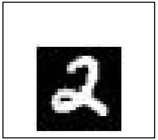
We exploit the fact that certain transformations to the image do not change the label of the image.



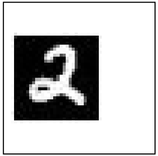
rotated by 20°



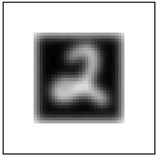
rotated by 65°



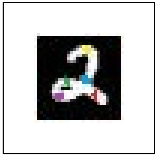
shifted vertically



shifted horizontally



blurred



changed some pixels

label = 2

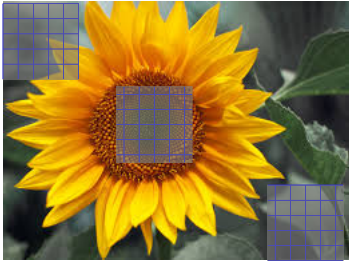
[augmented data = created using some knowledge of the task]

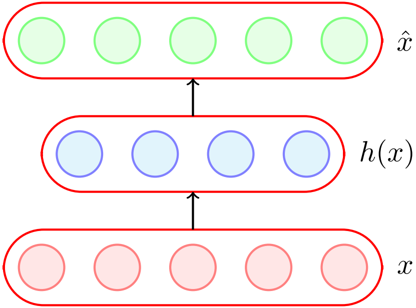
- Typically, More data = better learning
- Works well for image classification / object recognition tasks
- Also shown to work well for speech
- For some tasks it may not be clear how to generate such data

# Module 8.6 : Parameter Sharing and tying

## Other forms of regularization

- $l_2$ regularization
- Dataset augmentation
- Parameter Sharing and tying
- Adding Noise to the inputs
- Adding Noise to the outputs
- Early stopping
- Ensemble methods
- Dropout






## Parameter Sharing

- Used in CNNs
- Same filter applied at different positions of the image
- Or same weight matrix acts on different input neurons

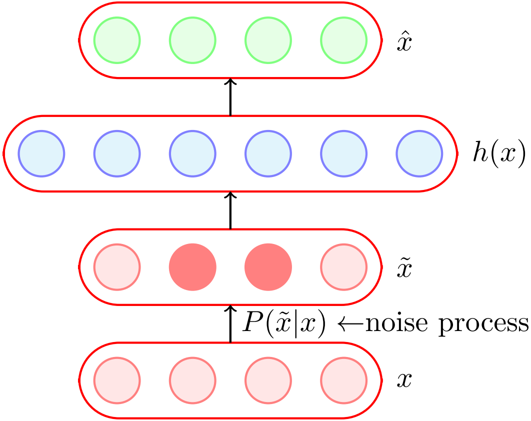
## Parameter Tying

- Typically used in autoencoders
- The encoder and decoder weights are tied.

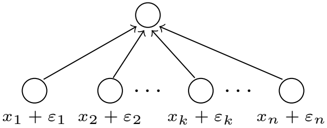
# Module 8.7 : Adding Noise to the inputs

## Other forms of regularization

- $l_2$ regularization
- Dataset augmentation
- Parameter Sharing and tying
- Adding Noise to the inputs
- Adding Noise to the outputs
- Early stopping
- Ensemble methods
- Dropout




- We saw this in Autoencoder
- We can show that for a simple input output neural network, adding Gaussian noise to the input is equivalent to weight decay ($L_2$ regularisation)
- Can be viewed as data augmentation




$$\varepsilon \sim \mathcal{N}(0, \sigma^2)$$

$$\widetilde{x}_i = x_i + \varepsilon_i$$

$$\widehat{y} = \sum_{i=1}^{n} w_i x_i$$

$$\widetilde{y} = \sum_{i=1}^{n} w_i \widetilde{x}_i$$

$$= \sum_{i=1}^{n} w_i x_i + \sum_{i=1}^{n} w_i \varepsilon_i$$

$$= \widehat{y} + \sum_{i=1}^{n} w_i \varepsilon_i$$

We are interested in $E[(\widetilde{y} - y)^2]$

$$E\left[(\widetilde{y} - y)^2\right] = E\left[\left(\widehat{y} + \sum_{i=1}^{n} w_i \varepsilon_i - y\right)^2\right]$$

$$= E\left[\left(\left(\widehat{y} - y\right) + \left(\sum_{i=1}^{n} w_i \varepsilon_i\right)\right)^2\right]$$

$$= E\left[(\widehat{y} - y)^2\right] + E\left[2(\widehat{y} - y)\sum_{i=1}^{n} w_i \varepsilon_i\right] + E\left[\left(\sum_{i=1}^{n} w_i \varepsilon_i\right)^2\right]$$

$$= E\left[(\widehat{y} - y)^2\right] + 0 + E\left[\sum_{i=1}^{n} w_i^2 \varepsilon_i^2\right]$$

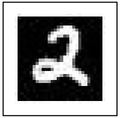
($\because$ $\varepsilon_i$ is independent of $\varepsilon_j$ and $\varepsilon_i$ is independent of ($\widehat{y}$-$y$) )

$$= (E\left[(\widehat{y} - y)^2\right] + \sigma^2 \sum_{i=1}^{n} w_i^2$$ (same as $L_2$ norm penalty)

# Module 8.8 : Adding Noise to the outputs

## Other forms of regularization

- $l_2$ regularization
- Dataset augmentation
- Parameter Sharing and tying
- Adding Noise to the inputs
- Adding Noise to the outputs
- Early stopping
- Ensemble methods
- Dropout



| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | Hard targets |

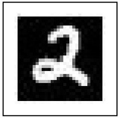
$$\text{minimize} : \sum_{i=0}^{9} p_i \log q_i$$

$$\text{true distribution} : p = \{0, 0, 1, 0, 0, 0, 0, 0, 0, 0\}$$

$$\text{estimated distribution} : q$$

**Intuition**

- Do not trust the true labels, they may be noisy
- Instead, use soft targets



| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $\frac{\varepsilon}{9}$ | $\frac{\varepsilon}{9}$ | $1-\varepsilon$ | $\frac{\varepsilon}{9}$ | $\frac{\varepsilon}{9}$ | $\frac{\varepsilon}{9}$ | $\frac{\varepsilon}{9}$ | $\frac{\varepsilon}{9}$ | $\frac{\varepsilon}{9}$ | $\frac{\varepsilon}{9}$ | Soft targets |

$$\varepsilon = \text{small positive constant}$$

$$\text{minimize} : \sum_{i=0}^{9} p_i \log q_i$$

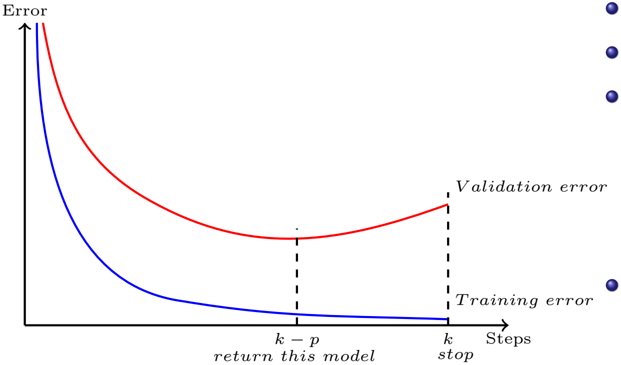
$$\text{true distribution + noise} : p = \left\{\frac{\varepsilon}{9}, \frac{\varepsilon}{9}, 1-\varepsilon, \frac{\varepsilon}{9}, \dots\right\}$$

$$\text{estimated distribution} : q$$

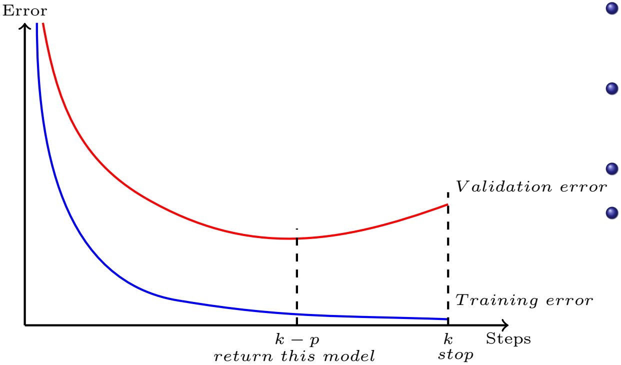
# Module 8.9 : Early stopping

## Other forms of regularization

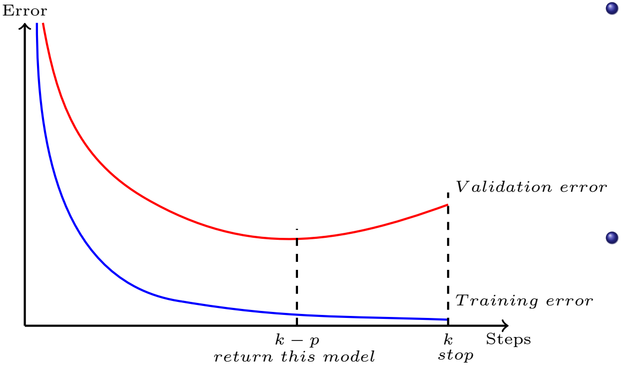
- $l_2$ regularization
- Dataset augmentation
- Parameter Sharing and tying
- Adding Noise to the inputs
- Adding Noise to the outputs
- Early stopping
- Ensemble methods
- Dropout




- Track the validation error
- Have a patience parameter $p$
- If you are at step $k$ and there was no improvement in validation error in the previous $p$ steps then stop training and return the model stored at step $k-p$
- Basically, stop the training early before it drives the training error to 0 and blows up the validation error




- Very effective and the mostly widely used form of regularization
- Can be used even with other regularizers (such as $l_2$)
- How does it act as a regularizer ?
- We will first see an intuitive explanation and then a mathematical analysis




- Recall that the update rule in SGD is

$$w_{t+1} = w_t - \eta \nabla w_t$$
$$= w_0 - \eta \sum_{i=1}^{t} \nabla w_i$$

- Let $\tau$ be the maximum value of $\nabla w_i$ then

$$|w_{t+1} - w_0| \leq \eta t |\tau|$$

- Thus, $t$ controls how far $w_t$ can go from the initial $w_0$
- In other words it controls the space of exploration

We will now see a mathematical analysis of this

- Recall that the Taylor series approximation for $\mathscr{L}(w)$ is

$$\mathscr{L}(w) = \mathscr{L}(w^*) + (w - w^*)^T \nabla \mathscr{L}(w^*) + \frac{1}{2}(w - w^*)^T H (w - w^*)$$

$$= \mathscr{L}(w^*) + \frac{1}{2}(w - w^*)^T H (w - w^*) \qquad [\ w^* \ \textit{is optimal so} \ \nabla \mathscr{L}(w^*) \ \textit{is} \ 0\ ]$$

$$\nabla(\mathscr{L}(w)) = H(w - w^*)$$

Now the SGD update rule is:

$$\begin{aligned} w_t &= w_{t-1} - \eta \nabla \mathscr{L}(w_{t-1}) \\ &= w_{t-1} - \eta H(w_{t-1} - w^*) \\ &= (I - \eta H) w_{t-1} + \eta H w^* \end{aligned}$$

$$w_t = (I - \eta H)w_{t-1} + \eta H w^*$$

- Using EVD of $H$ as $H = Q\Lambda Q^T$, we get:

$$w_t = (I - \eta Q\Lambda Q^T)w_{t-1} + \eta Q\Lambda Q^T w^*$$

- If we start with $w_0 = 0$ then we can show that (See Appendix)

$$w_t = Q[I - (I - \varepsilon\Lambda)^t]Q^T w^*$$

- Compare this with the expression we had for optimum $\tilde{W}$ with $L_2$ regularization

$$\tilde{w} = Q[I - (\Lambda + \alpha I)^{-1}\alpha]Q^T w^*$$

- We observe that $w_t = \tilde{w}$, if we choose $\varepsilon$,$t$ and $\alpha$ such that

$$(I - \varepsilon\Lambda)^t = (\Lambda + \alpha I)^{-1}\alpha$$

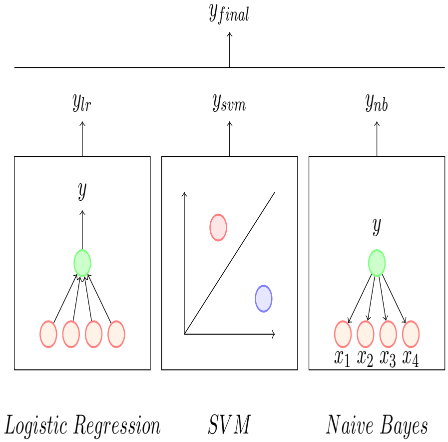
### Things to be remember

- Early stopping only allows $t$ updates to the parameters.
- If a parameter $w$ corresponds to a dimension which is important for the loss $\mathscr{L}(\theta)$ then $\frac{\partial \mathscr{L}(\theta)}{\partial w}$ will be large
- However if a parameter is not important ($\frac{\partial \mathscr{L}(\theta)}{\partial w}$ is small) then its updates will be small and the parameter will not be able to grow large in '$t'$ steps
- Early stopping will thus effectively shrink the parameters corresponding to less important directions (same as weight decay).

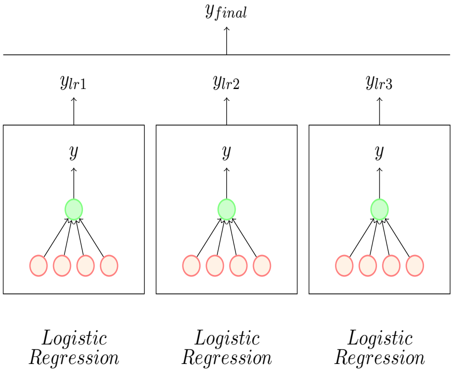
# Module 8.10 : Ensemble methods

## Other forms of regularization

- $l_2$ regularization
- Dataset augmentation
- Parameter Sharing and tying
- Adding Noise to the inputs
- Adding Noise to the outputs
- Early stopping
- Ensemble methods
- Dropout




- Combine the output of different models to reduce generalization error
- The models can correspond to different classifiers
- It could be different instances of the same classifier trained with:
  - different hyperparameters
  - different features
  - different samples of the training data




Each model trained with a different sample of the data (sampling with replacement)

- Bagging: form an ensemble using different instances of the same classifier
- From a given dataset, construct multiple training sets by sampling with replacement $(T_1, T_2, ..., T_k)$
- Train $i^{th}$ instance of the classifier using training set $T_i$

- The error made by the average prediction of all the models is $\frac{1}{k}\sum_i \varepsilon_i$
- The expected squared error is :

$$
\begin{aligned}
mse =& E[(\frac{1}{k}\sum_i \varepsilon_i)^2] \\
=& \frac{1}{k^2}E[\sum_i \sum_{i=j} \varepsilon_i \varepsilon_j + \sum_i \sum_{i\neq j} \varepsilon_i \varepsilon_j] \\
=& \frac{1}{k^2}E[\sum_i \varepsilon_i^2 + \sum_i \sum_{i\neq j} \varepsilon_i \varepsilon_j] \\
=& \frac{1}{k^2}(\sum_i E[\varepsilon_i^2] + \sum_i \sum_{i\neq j} E[\varepsilon_i \varepsilon_j]) \\
=& \frac{1}{k^2}(kV + k(k-1)C) \\
=& \frac{1}{k}V + \frac{k-1}{k}C
\end{aligned}
$$

- When would bagging work?
- Consider a set of $k$ LR models
- Suppose that each model makes an error $\varepsilon_i$ on a test example
- Let $\varepsilon_i$ be drawn from a zero mean multivariate normal distribution
- $Variance = E[\varepsilon_i^2] = V$
- $Covariance = E[\varepsilon_i \varepsilon_j] = C$

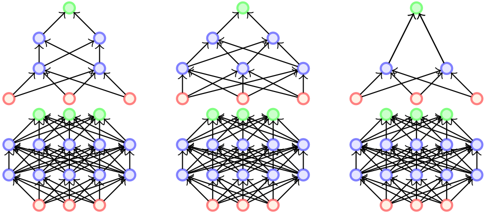
$$mse = \frac{1}{k}V + \frac{k-1}{k}C$$

- When would bagging work ?
- If the errors of the model are perfectly correlated then $V = C$ and $mse = V$ [bagging does not help: the mse of the ensemble is as bad as the individual models]
- If the errors of the model are independent or uncorrelated then $C = 0$ and the mse of the ensemble reduces to $\frac{1}{k}V$
- On average, the ensemble will perform at least as well as its individual members

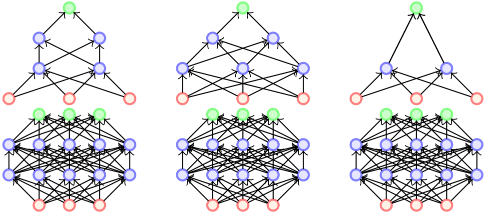
# Module 8.11 : Dropout

## Other forms of regularization

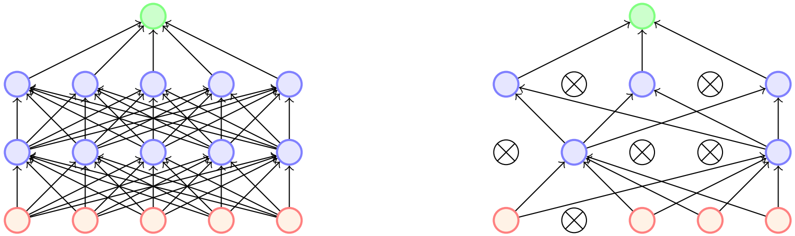
- $l_2$ regularization
- Dataset augmentation
- Parameter Sharing and tying
- Adding Noise to the inputs
- Adding Noise to the outputs
- Early stopping
- Ensemble methods
- Dropout



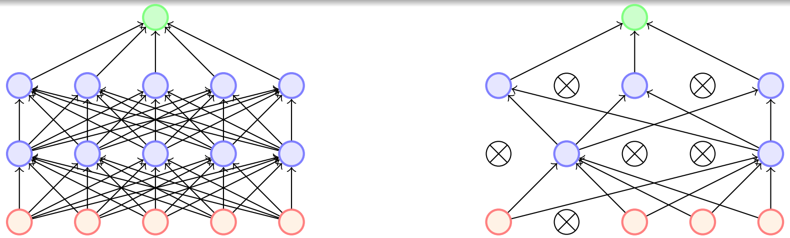
- Typically model averaging(bagging ensemble) always helps
- Training several large neural networks for making an ensemble is prohibitively expensive
- Option 1: Train several neural networks having different architectures(obviously expensive)
- Option 2: Train multiple instances of the same network using different training samples (again expensive)
- Even if we manage to train with option 1 or option 2, combining several models at test time is infeasible in real time applications



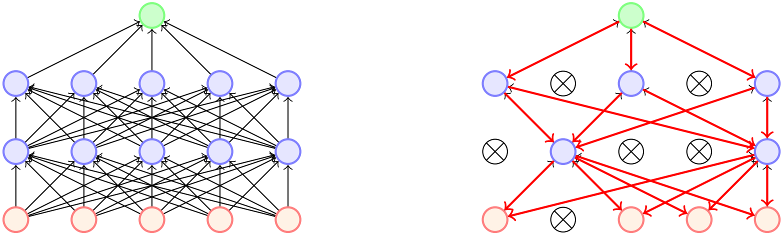
- Dropout is a technique which addresses both these issues.
- Effectively it allows training several neural networks without any significant computational overhead.
- Also gives an efficient approximate way of combining exponentially many different neural networks.



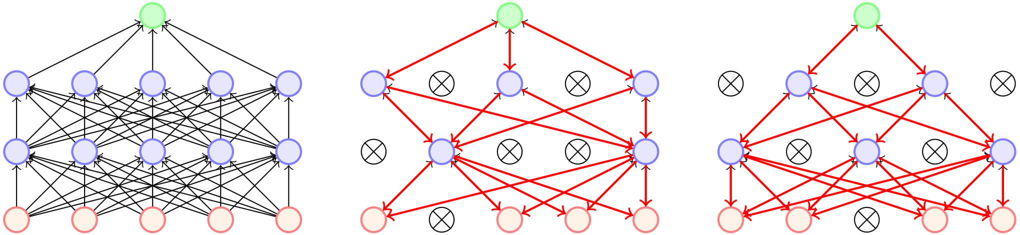
- Dropout refers to dropping out units
- Temporarily remove a node and all its incoming/outgoing connections resulting in a thinned network
- Each node is retained with a fixed probability (typically $p = 0.5$) for hidden nodes and $p = 0.8$ for visible nodes



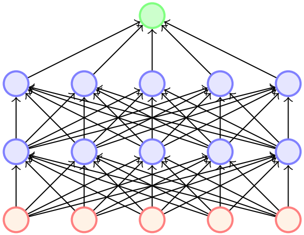
- Suppose a neural network has $n$ nodes
- Using the dropout idea, each node can be retained or dropped
- For example, in the above case we drop 5 nodes to get a thinned network
- Given a total of $n$ nodes, what are the total number of thinned networks that can be formed? $2^n$
- Of course, this is prohibitively large and we cannot possibly train so many networks
- **Trick:** (1) Share the weights across all the networks
  (2) Sample a different network for each training instance
- Let us see how?

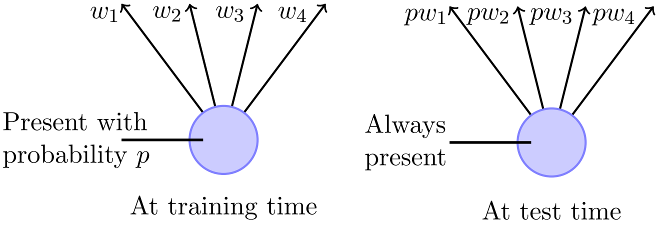


- We initialize all the parameters (weights) of the network and start training
- For the first training instance (or mini-batch), we apply dropout resulting in the thinned network
- We compute the loss and backpropagate
- Which parameters will we update? Only those which are active

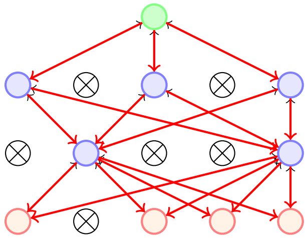


- For the second training instance (or mini-batch), we again apply dropout resulting in a different thinned network
- We again compute the loss and backpropagate to the active weights
- If the weight was active for both the training instances then it would have received two updates by now
- If the weight was active for only one of the training instances then it would have received only one updates by now
- Each thinned network gets trained rarely (or even never) but the parameter sharing ensures that no model has untrained or poorly trained parameters

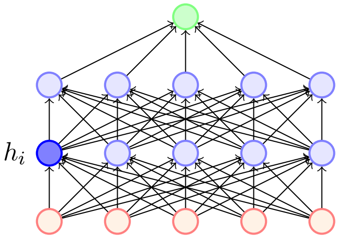





- What happens at test time?
- Impossible to aggregate the outputs of $2^n$ thinned networks
- Instead we use the full Neural Network and scale the output of each node by the fraction of times it was on during training



- Dropout essentially applies a masking noise to the hidden units
- Prevents hidden units from co-adapting
- Essentially a hidden unit cannot rely too much on other units as they may get dropped out any time
- Each hidden unit has to learn to be more robust to these random dropouts




- Here is an example of how dropout helps in ensuring redundancy and robustness
- Suppose $h_i$ learns to detect a face by firing on detecting a nose
- Dropping $h_i$ then corresponds to erasing the information that a nose exists
- The model should then learn another $h_i$ which redundantly encodes the presence of a nose
- Or the model should learn to detect the face using other features

## Recap

- $l_2$ regularization
- Dataset augmentation
- Parameter Sharing and tying
- Adding Noise to the inputs
- Adding Noise to the outputs
- Early stopping
- Ensemble methods
- Dropout

# Appendix

- To prove: The below two equations are equivalent

$$w_t = (I - \eta Q\Lambda Q^T)w_{t-1} + \eta Q\Lambda Q^T w^*$$
$$w_t = Q[I - (I - \varepsilon\Lambda)^t]Q^T w^*$$

- Proof by induction:
- Base case: $t = 1$ and $w_0$=0:
- $w_1$ according to the first equation:

$$\begin{aligned} w_1 &= (I - \eta Q\Lambda Q^T)w_0 + \eta Q\Lambda Q^T w^* \\ &= \eta Q\Lambda Q^T w^* \end{aligned}$$

- $w_1$ according to the second equation:

$$\begin{aligned} w_1 &= Q(I - (I - \eta\Lambda)^1)Q^T w^* \\ &= \eta Q\Lambda Q^T w^* \end{aligned}$$

- Induction step: Let the two equations be equivalent for $t^{th}$ step

$$\therefore w_t = (I - \eta Q \Lambda Q^T) w_{t-1} + \eta Q \Lambda Q^T w^*$$
$$= Q[I - (I - \varepsilon \Lambda)^t] Q^T w^*$$

- Proof that this will hold for $(t+1)^{th}$ step

$$w_{t+1} = (I - \eta Q \Lambda Q^T) w_t + \eta Q \Lambda Q^T w^*$$

(using $w_t = Q[I - (I - \varepsilon \Lambda)^t] Q^T w^*$)

(using $w_t = Q[I - (I - \varepsilon \Lambda)^t] Q^T w^*$)

$$= (I - \eta Q \Lambda Q^T) Q(I - (I - \eta \Lambda)^t) Q^T w^* + \eta Q \Lambda Q^T w^*$$

$$= (I - \eta Q \Lambda Q^T) Q(I - (I - \eta \Lambda)^t) Q^T w^* + \eta Q \Lambda Q^T w^*$$

$$= (I - \eta Q \Lambda Q^T) Q(I - (I - \eta \Lambda)^t) Q^T w^* + \eta Q \Lambda Q^T w^*$$

(Opening this bracket)

$$= IQ(I - (I - \eta \Lambda)^t) Q^T w^* - \eta Q \Lambda Q^T Q(I - (I - \eta \Lambda)^t) Q^T w^* + \eta Q \Lambda Q^T w^*$$

- Continuing

$$
\begin{aligned}
w_{t+1} &= Q(I-(I-\eta\Lambda)^t)Q^Tw^* - \eta Q\Lambda Q^TQ(I-(I-\eta\Lambda)^t)Q^Tw^* + \eta Q\Lambda Q^Tw^* \\
&= Q(I-(I-\eta\Lambda)^t)Q^Tw^* - \eta Q\Lambda(I-(I-\eta\Lambda)^t)Q^Tw^* + \eta Q\Lambda Q^Tw^* (\because Q^TQ = I \\
&= Q(I-(I-\eta\Lambda)^t)Q^Tw^* - \eta Q\Lambda(I-(I-\eta\Lambda)^t)Q^Tw^* + \eta Q\Lambda Q^Tw^* \\
&= Q\big[(I-(I-\eta\Lambda)^t) - \eta\Lambda(I-(I-\eta\Lambda)^t) + \eta\Lambda\big]Q^Tw^* \\
&= Q(I-(I-\eta\Lambda)^t)Q^Tw^* - \eta Q\Lambda(I-(I-\eta\Lambda)^t)Q^Tw^* + \eta Q\Lambda Q^Tw^* \\
&= Q\big[(I-(I-\eta\Lambda)^t) - \eta\Lambda(I-(I-\eta\Lambda)^t) + \eta\Lambda\big]Q^Tw^* \\
&= Q\big[(I-(I-\eta\Lambda)^t) - \eta\Lambda(I-(I-\eta\Lambda)^t) + \eta\Lambda\big]Q^Tw^* \\
&= Q\big[I-(I-\eta\Lambda)^t + \eta\Lambda(I-\eta\Lambda)^t\big]Q^Tw^* \\
&= Q\big[I-(I-\eta\Lambda)^t + \eta\Lambda(I-\eta\Lambda)^t\big]Q^Tw^* \\
&= Q\big[I-(I-\eta\Lambda)^t + \eta\Lambda(I-\eta\Lambda)^t\big]Q^Tw^* \\
&= Q\big[I-(I-\eta\Lambda)^t(I-\eta\Lambda)\big]Q^Tw^* \\
&= Q\big[I-(I-\eta\Lambda)^t(I-\eta\Lambda)\big]Q^Tw^*
\end{aligned}
$$