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

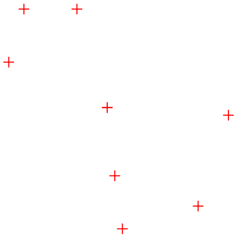
- Chapter 7, Deep Learning book
- Ali Ghodsi's Video Lectures on Regularization[a]
- Dropout: A Simple Way to Prevent Neural Networks from Overfitting[b]

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

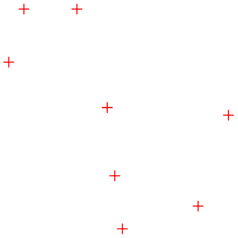
Module 8.1 : Bias and Variance

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

- Let us consider the problem of fitting a curve through a given set of points



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



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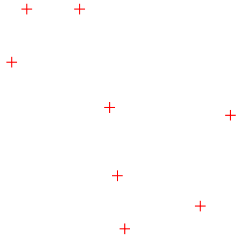
- Let us consider the problem of fitting a curve through a given set of points
- We consider two models :



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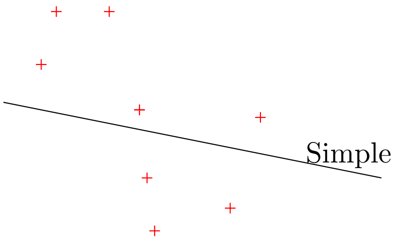
- Let us consider the problem of fitting a curve through a given set of points
- We consider two models :

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



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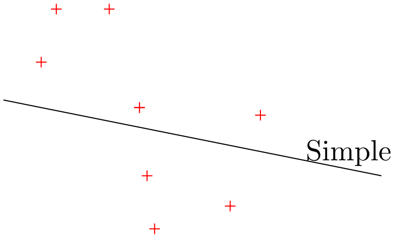

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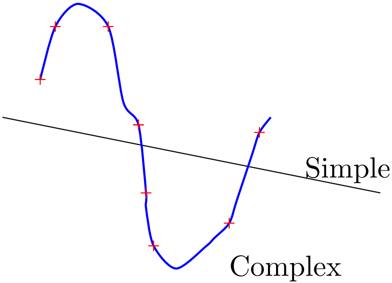
- Let us consider the problem of fitting a curve through a given set of points
- We consider two models :

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

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



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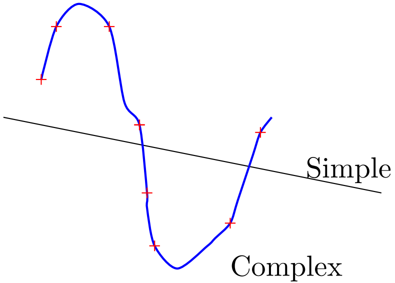

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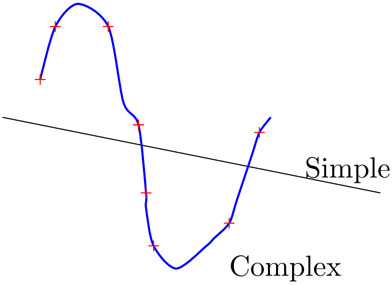
- Note that in both cases we are making an assumption about how y is related to x. We have no idea about the true relation $f(x)$



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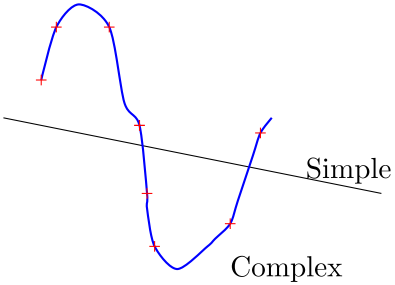
- Note that in both cases we are making an assumption about how y is related to x. We have no idea about the true relation $f(x)$
- The training data consists of 100 points



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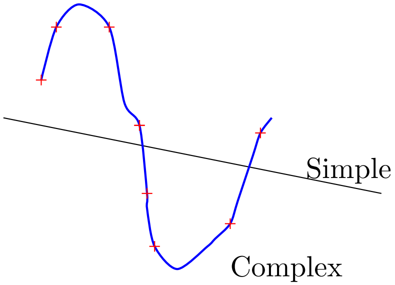
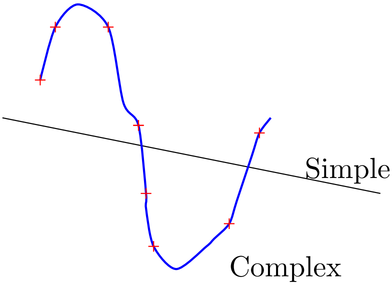
- We sample 25 points from the training data and train a simple and a complex model



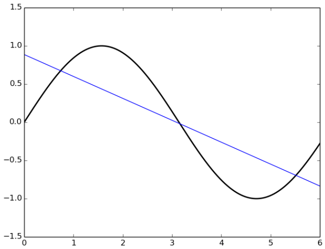
The points were drawn from a sinusoidal function (the true $f(x)$)

- 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)



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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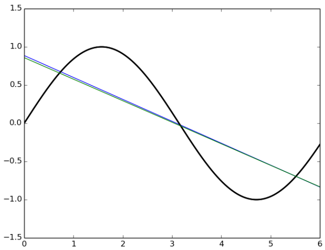

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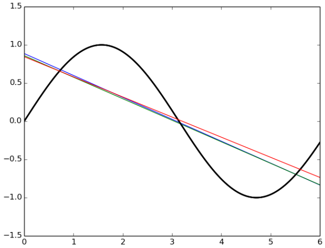
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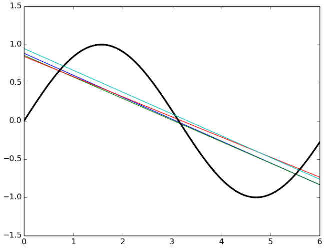
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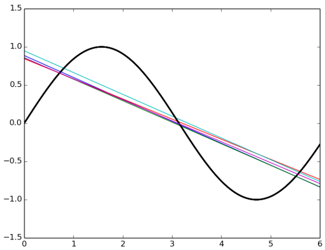
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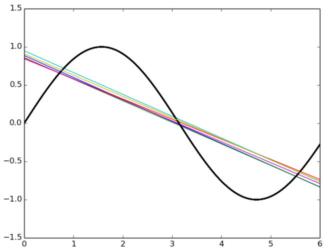
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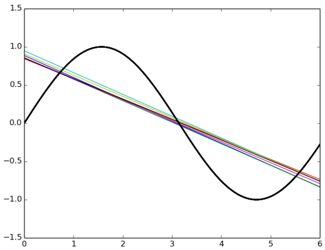
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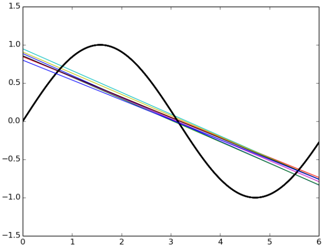
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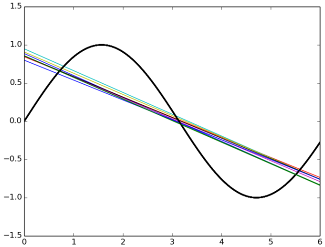
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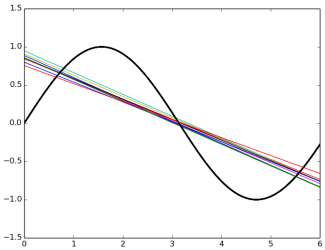
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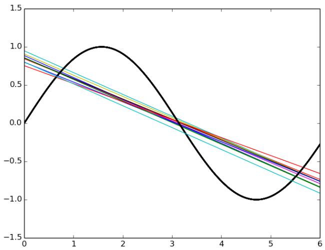
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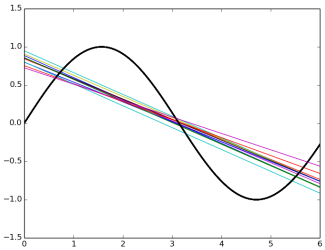
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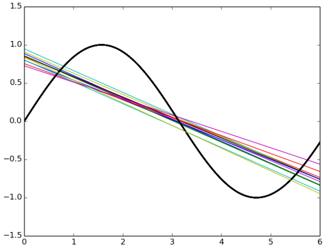
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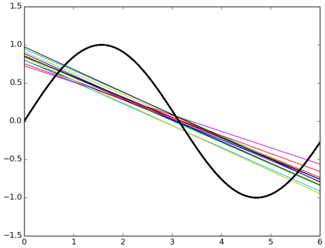
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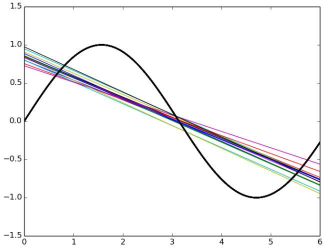
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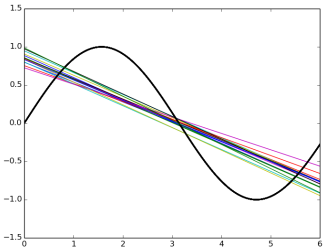
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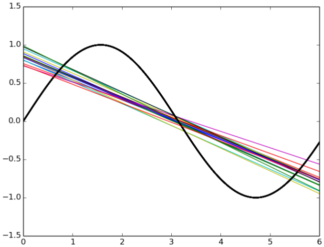
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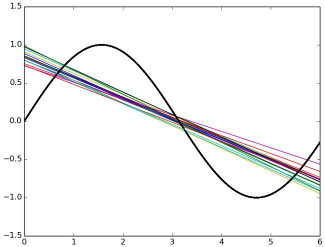
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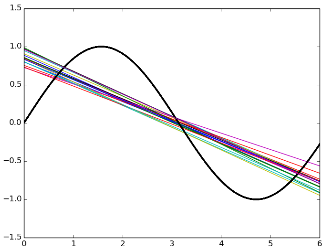
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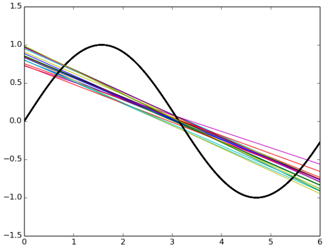
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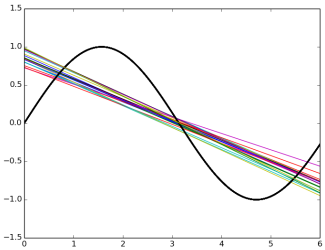

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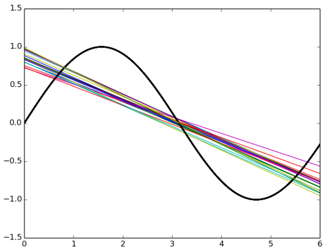

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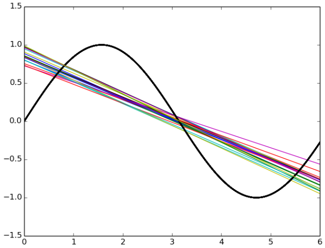
- However they are very far from the true sinusoidal curve (under fitting)



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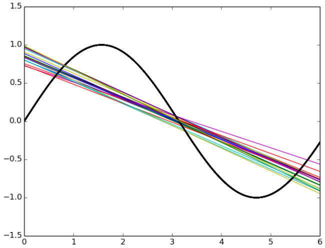

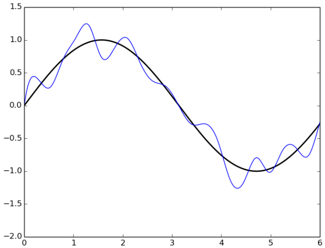

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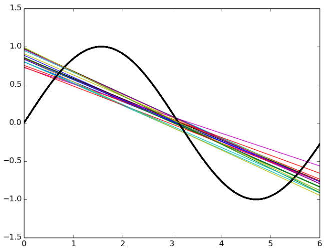

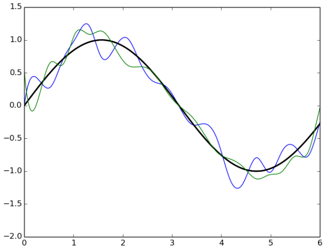

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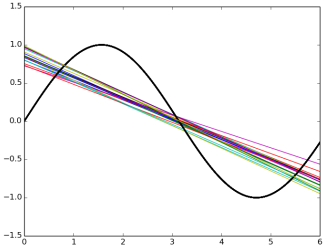

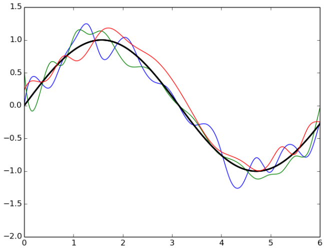

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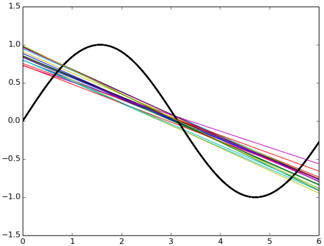

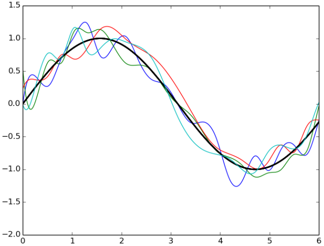

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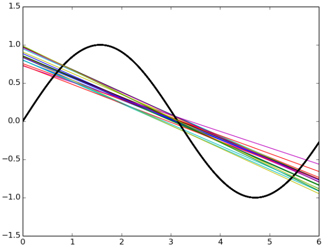

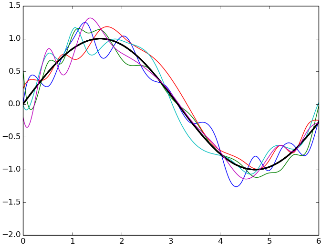

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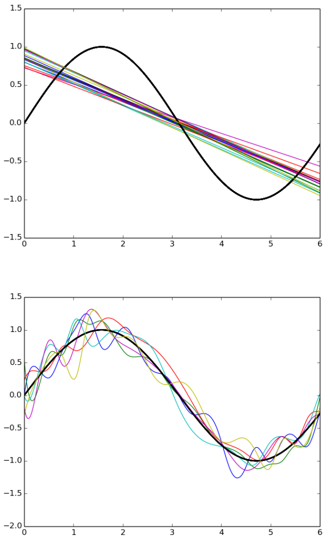

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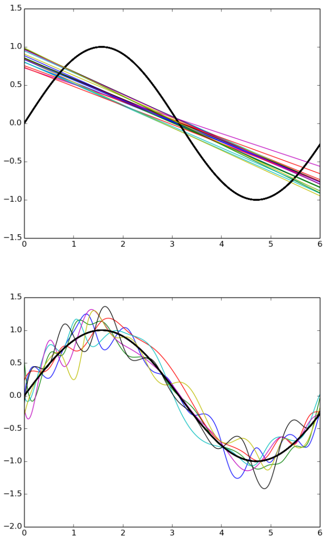

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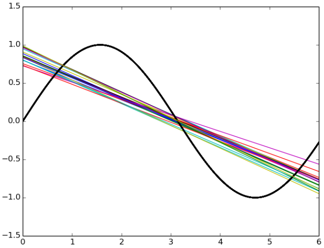

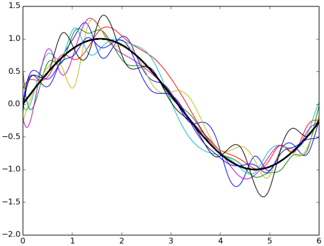

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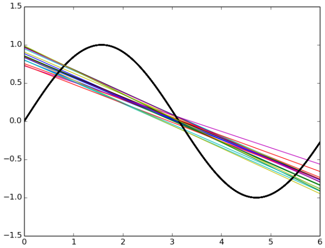

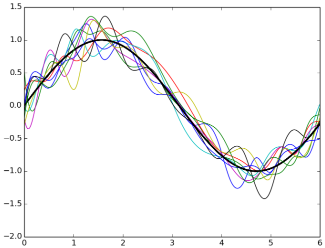

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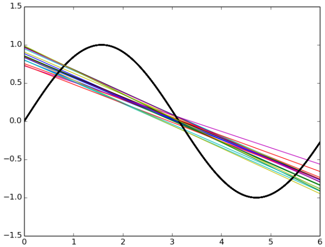

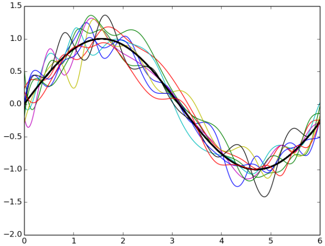

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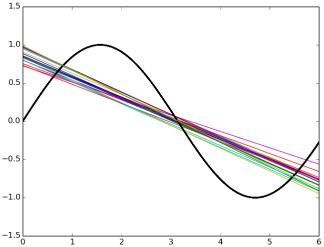

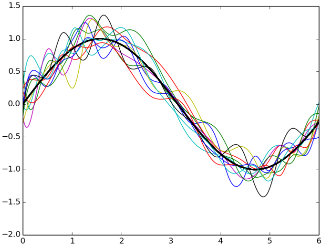

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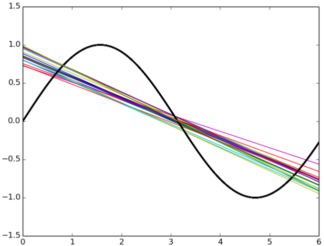

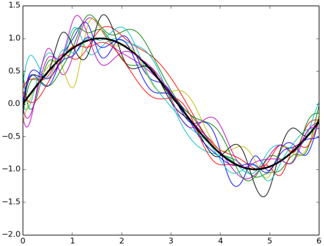

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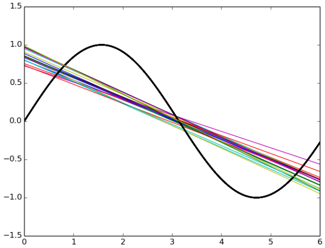

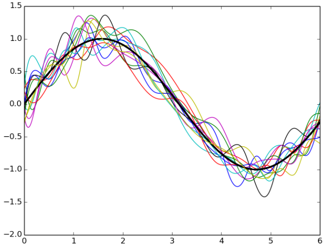

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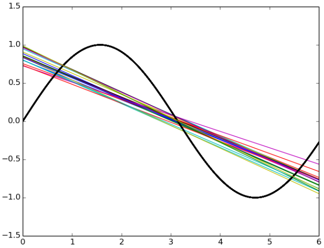

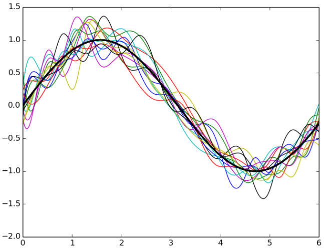

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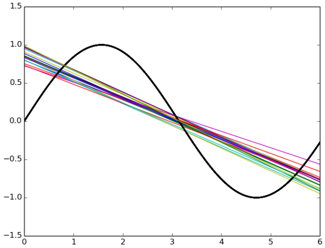

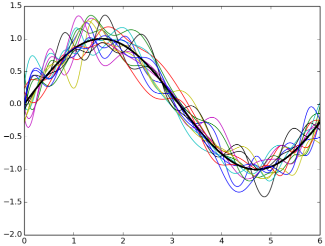

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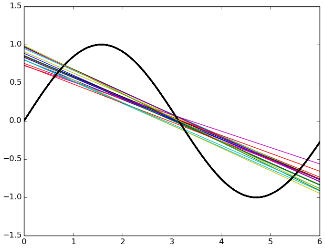

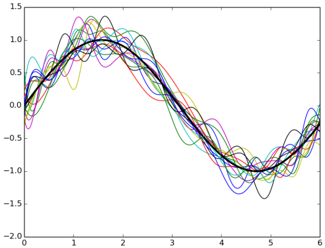

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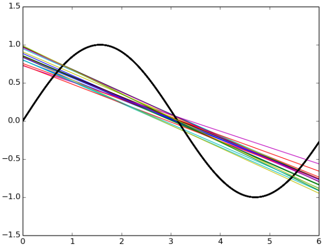

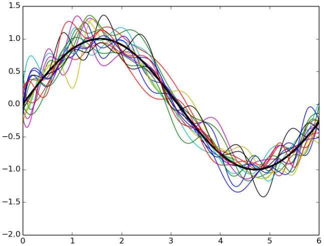

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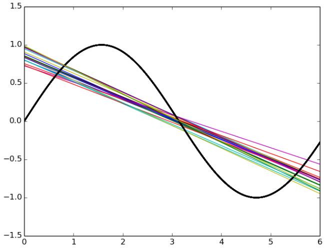

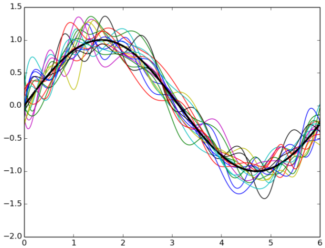

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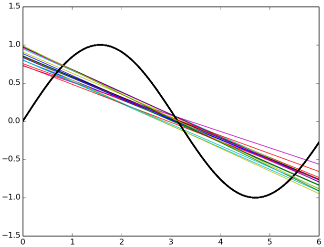

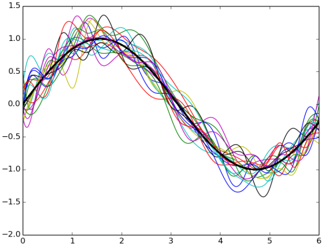

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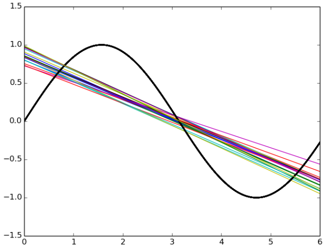

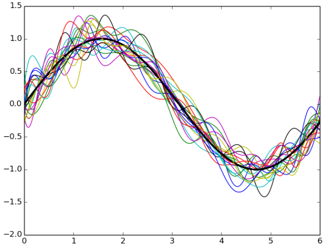

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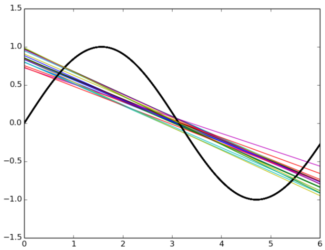
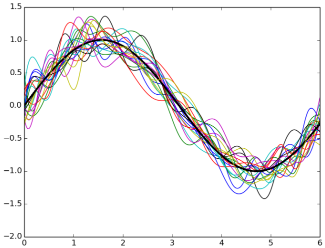
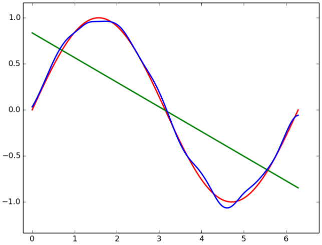




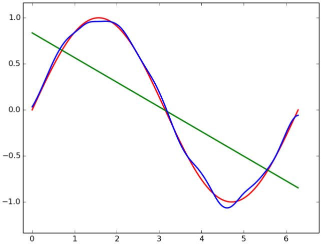
- Simple models trained on different samples of the data do not differ much from each other
- However they are very far from the true sinusoidal curve (under fitting)
- On the other hand, complex models trained on different samples of the data are very different from each other (high variance)



<u>Green Line</u>: Average value of $\hat{f}(x)$ for the simple model
<u>Blue Curve</u>: Average value of $\hat{f}(x)$ for the complex model
<u>Red Curve</u>: 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,

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



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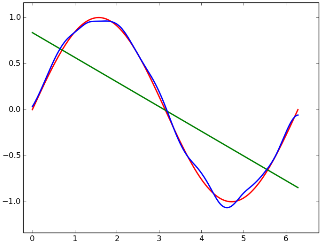

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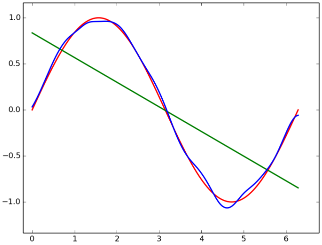

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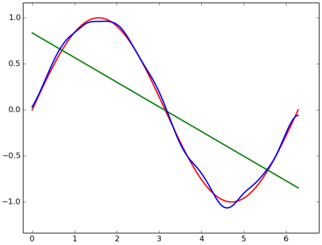
- Mathematically, this means that the simple model has a high bias



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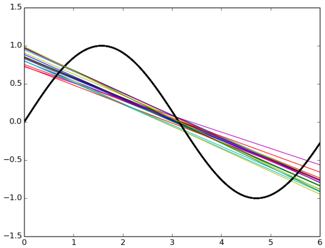
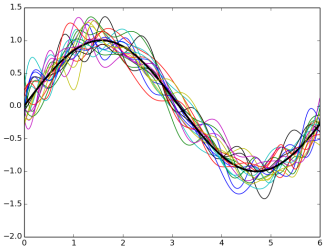
- On the other hand, the complex model has a low bias

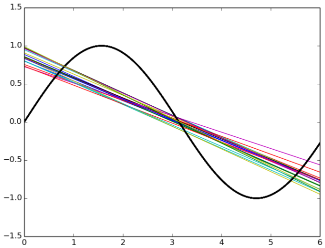


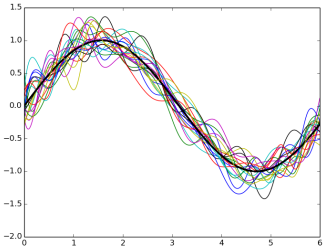


- We now define,

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

(Standard definition from statistics)





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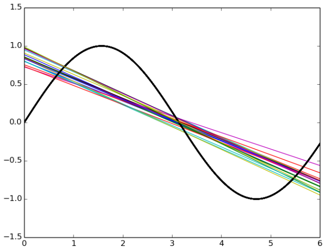

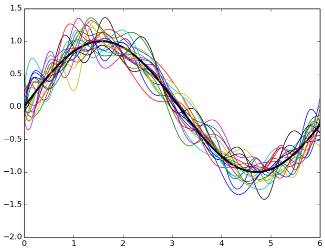

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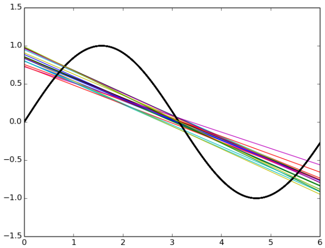
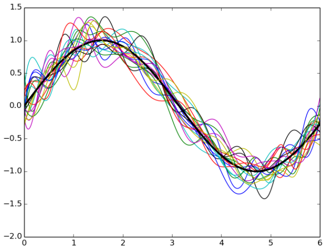
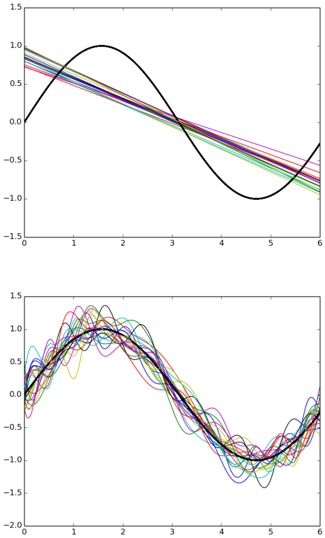
- It is clear that the simple model has a low variance whereas the complex model has a high variance

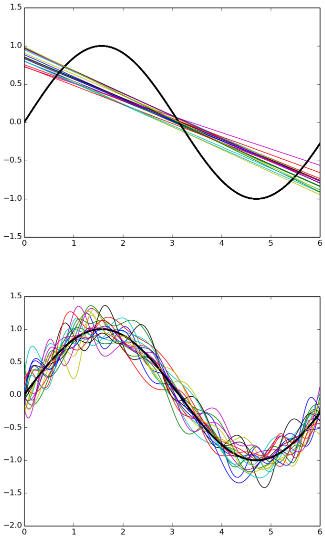




- In summary (informally)



- In summary (informally)
- Simple model: high bias, low variance



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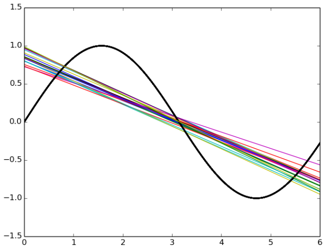

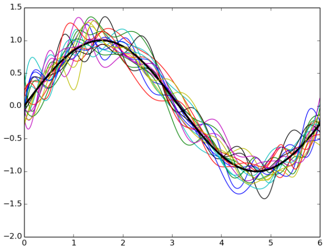

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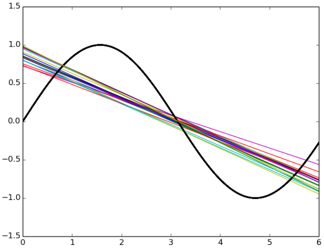
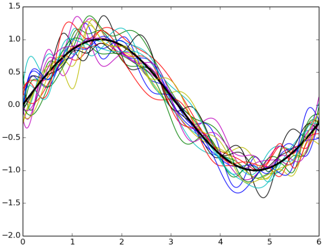
- There is always a trade-off between the bias and variance





- 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

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- See proof here

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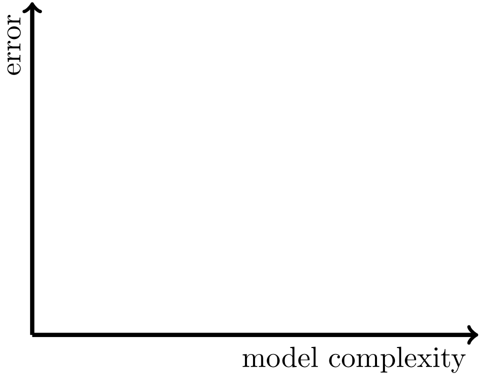

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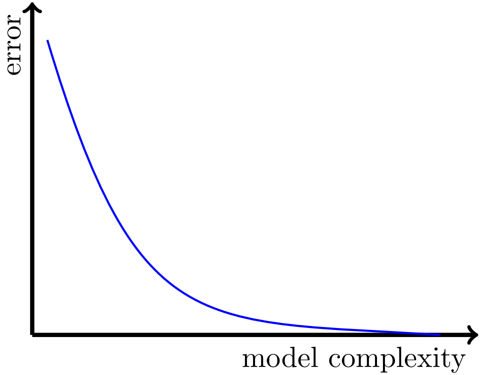

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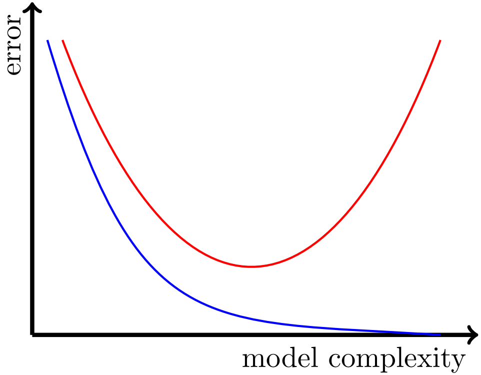

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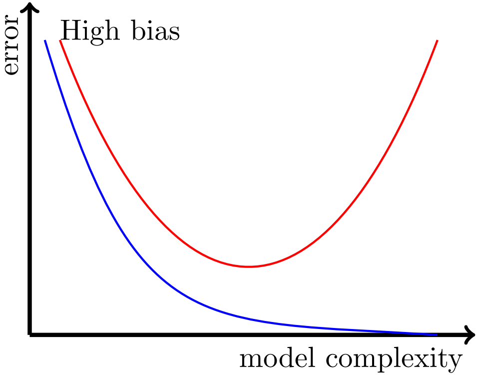

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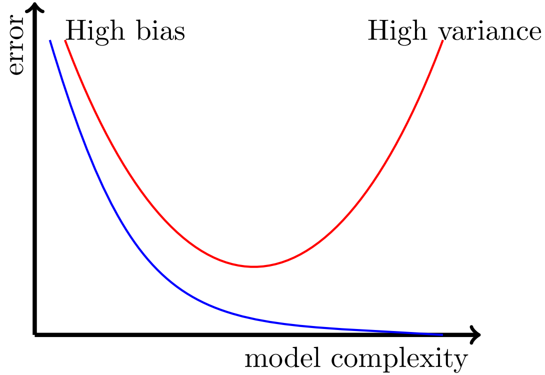

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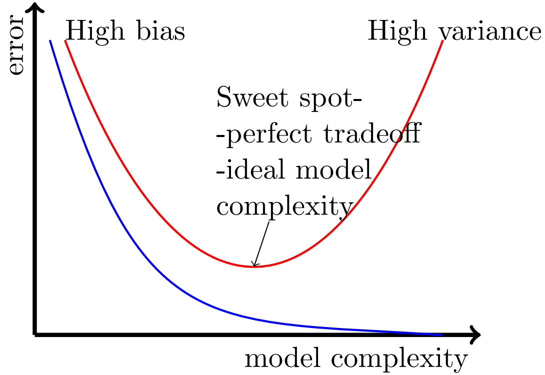

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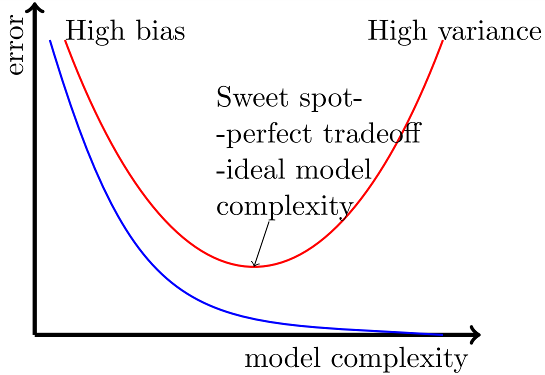

$$E[(y - \hat{f}(x))^2] = Bias^2 + Variance + \sigma^2 \text{ (irreducible error)}$$

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

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- We will concretize this intuition mathematically now and eventually show how to account for the optimism in the training error

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

$$E[(\hat{y}_i - y_i)^2]$$

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

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 $z_1 = 2,\ z_2 = 1,\ z_3 = 0,\ \ldots\ z_k = 2$

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... returning back to our derivation

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

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

Case 1: Using test observations

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$\because$ covariance(X, Y)

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- 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]

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

Case 2: Using training observations

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

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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

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

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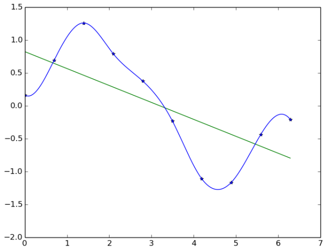
- Can you link this to model complexity?
- Yes, indeed a complex model will be more sensitive to changes in observations whereas a simple model will be less sensitive to changes in observations
- Hence, we can say that
  true error = empirical train error + small constant + Ω(model complexity)

- Let us verify that indeed a complex model is more sensitive to minor changes in the data



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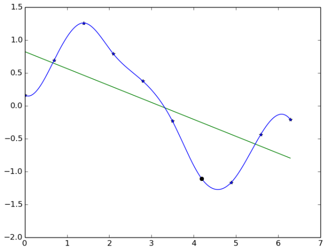

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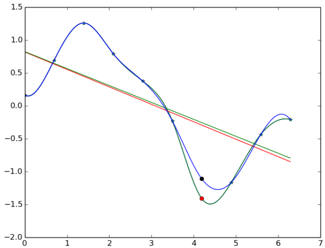

- Let us verify that indeed a complex model is more sensitive to minor changes in the data
- We have fitted a simple and complex model for some given data
- We now change one of these data points
- The simple model does not change much as compared to the complex model

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

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

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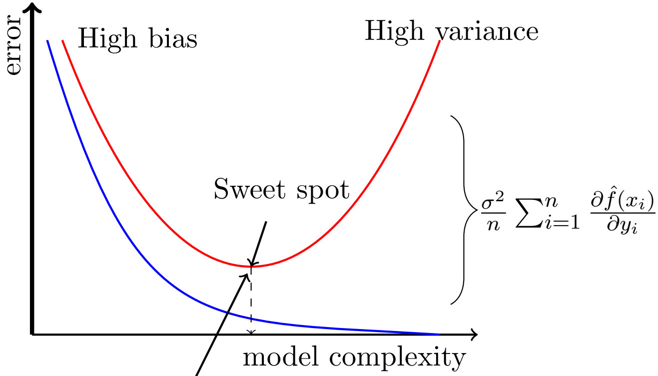
- This is the basis for all regularization methods
- We can show that L_1 regularization, L_2 regularization, early stopping and injecting noise in input are all instances of this form of regularization.



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

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- Hence we need some form of regularization.

Different forms of regularization

- L_2 regularization

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- Dataset augmentation

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- 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
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- Let us see the geometric interpretation of this

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- Let us analyse the case when $\alpha \neq 0$

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\end{aligned}$$

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

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

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

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

- So what is happening here?

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

- So what is happening here?
- w^* first gets rotated by Q^T to give $Q^T w^*$

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

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- w^* first gets rotated by Q^T to give $Q^T w^*$
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- 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

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

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\begin{aligned}
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&= Q D Q^T w^*
\end{aligned}
$$

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

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(\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}
$$

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

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- So what is happening now?

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

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

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- 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 $\frac{\lambda_i}{\lambda_i+\alpha} = 1$

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

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

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

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

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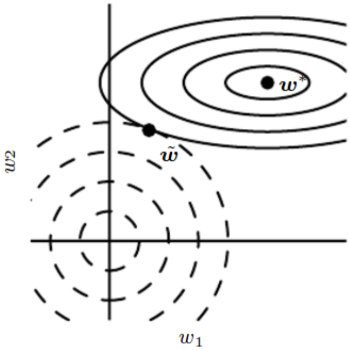
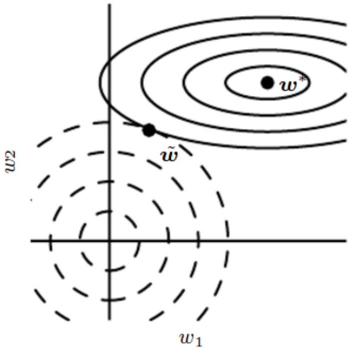
- Each element i of $Q^T w^*$ gets scaled by $\frac{\lambda_i}{\lambda_i+\alpha}$ before it is rotated back by Q
- if $\lambda_i >> \alpha$ then $\frac{\lambda_i}{\lambda_i+\alpha} = 1$
- if $\lambda_i << \alpha$ then $\frac{\lambda_i}{\lambda_i+\alpha} = 0$
- Thus only significant directions (larger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

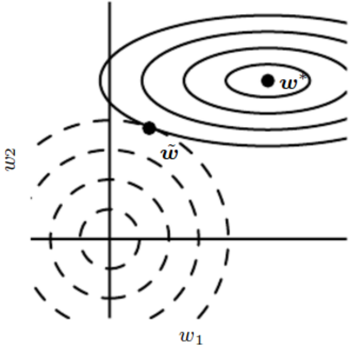
$$\text{Effective parameters} = \sum_{i=1}^{n} \frac{\lambda_i}{\lambda_i + \alpha} < n$$



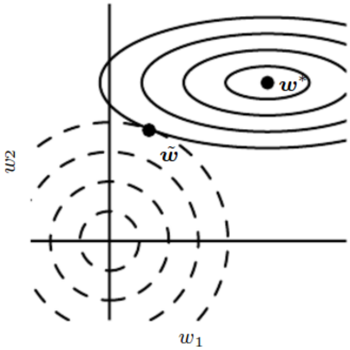
w^*
$\tilde{w}$
w_2
w_1



- The weight vector(w^*) is getting rotated to ($\tilde{w}$)



- The weight vector(w^*) is getting rotated to ($\tilde{w}$)
- All of its elements are shrinking but some are shrinking more than the others



- 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

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- L_2 regularization
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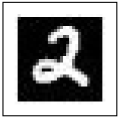

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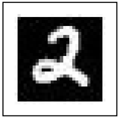

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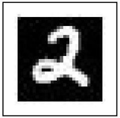
[given training data]



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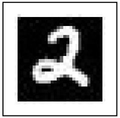
[given training data]



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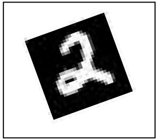
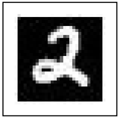
[given training data]



rotated by 20°



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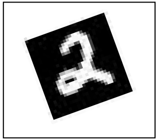
[given training data]



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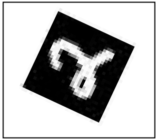
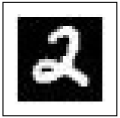
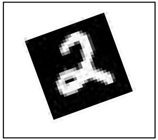


rotated by 65°

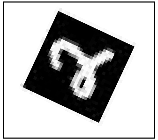


label = 2

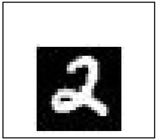
[given training data]



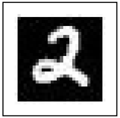
rotated by 20°



rotated by 65°



shifted vertically



label = 2

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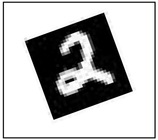

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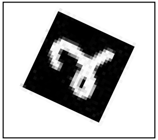

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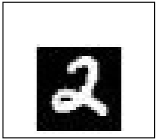
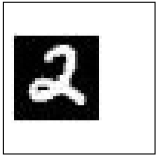
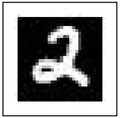


shifted vertically

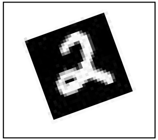


shifted horizontally

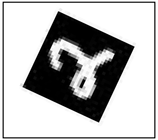


label = 2

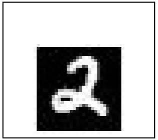
[given training data]



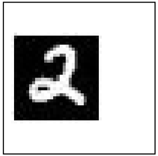
rotated by 20°



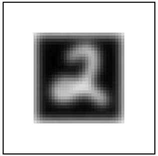
rotated by 65°



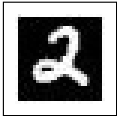
shifted vertically



shifted horizontally

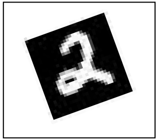


blurred

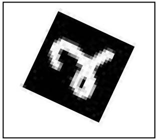


label = 2

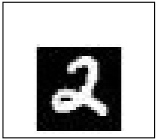
[given training data]



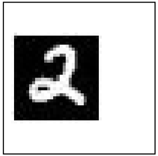
rotated by 20°



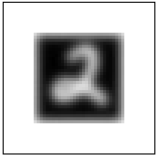
rotated by 65°



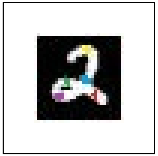
shifted vertically



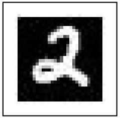
shifted horizontally



blurred

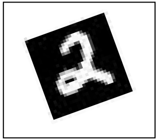


changed some pixels

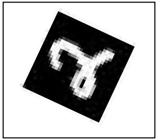


label = 2

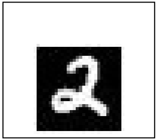
[given training data]



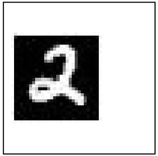
rotated by 20°



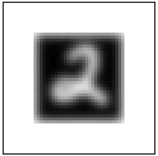
rotated by 65°



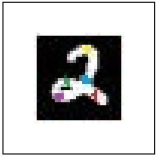
shifted vertically



shifted horizontally

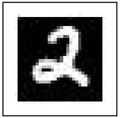


blurred



changed some pixels

label = 2



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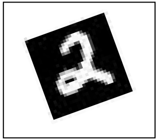
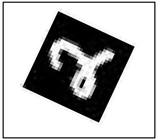
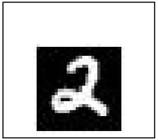
[given training data]



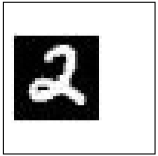
rotated by 20°



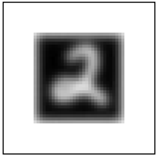
rotated by 65°



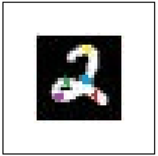
shifted vertically



shifted horizontally



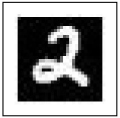
blurred



changed some pixels

label = 2

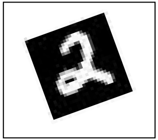
[augmented data = created using some knowledge of the task]



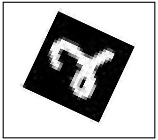
label $= 2$

[given training data]

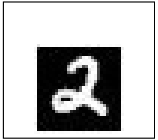
We exploit the fact that certain transformations to the image do not change the label of the image.



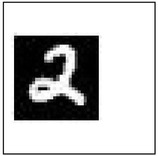
rotated by 20°



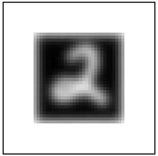
rotated by 65°



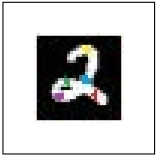
shifted vertically



shifted horizontally



blurred



changed some pixels

label $= 2$

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

- Typically, More data = better learning

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- Also shown to work well for speech

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- 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

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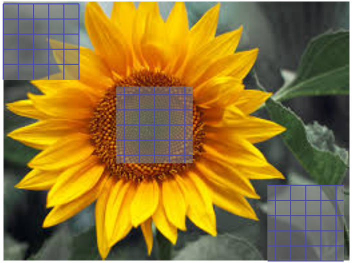
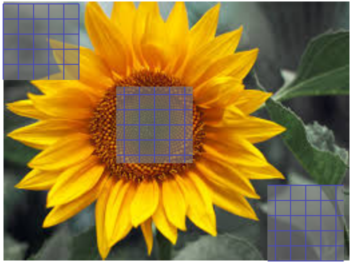
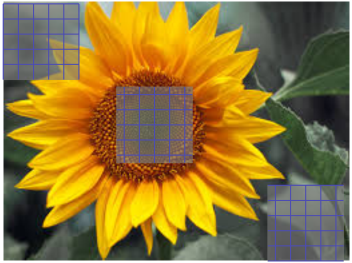


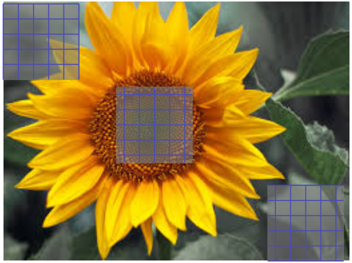


Parameter Sharing



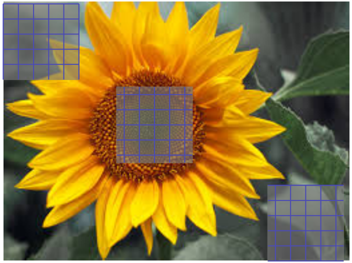
Parameter Sharing

- Used in CNNs



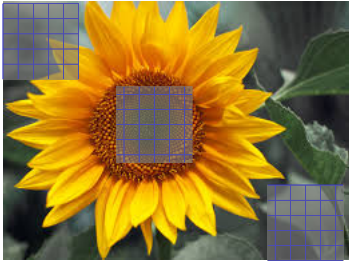
Parameter Sharing

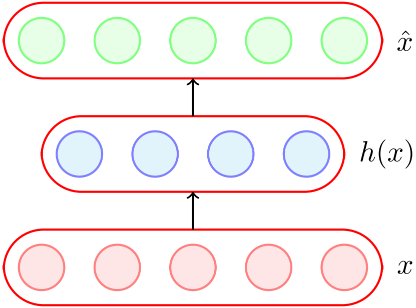
- Used in CNNs
- Same filter applied at different positions of the image



Parameter Sharing

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





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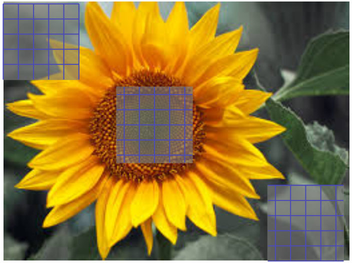

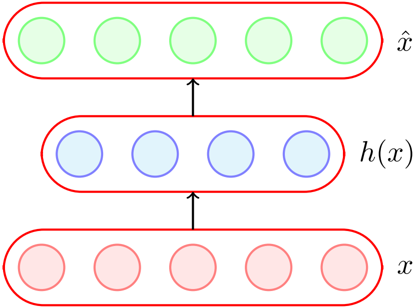

Parameter Sharing

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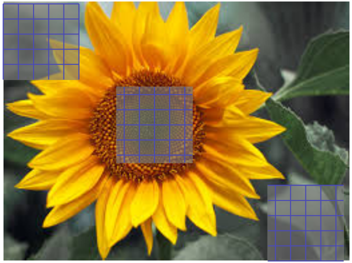
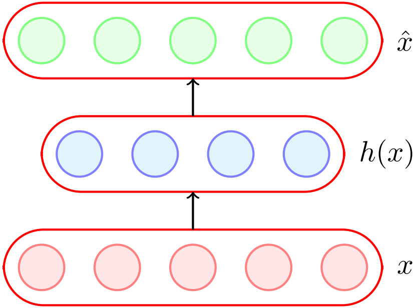
Parameter Tying



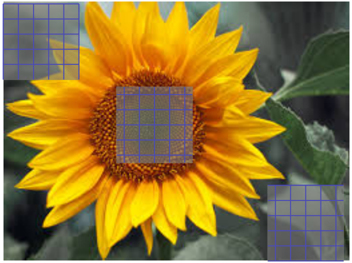


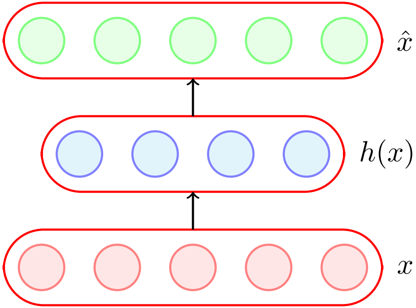
Parameter Sharing

- 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





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
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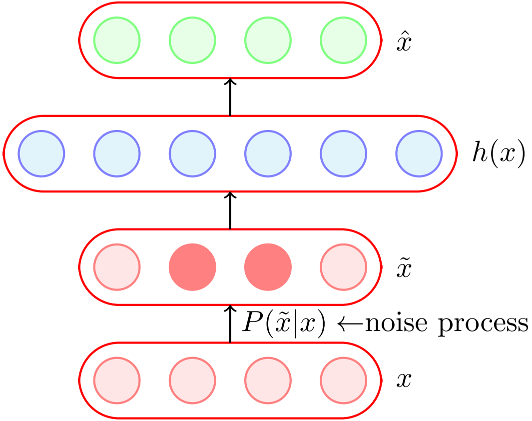
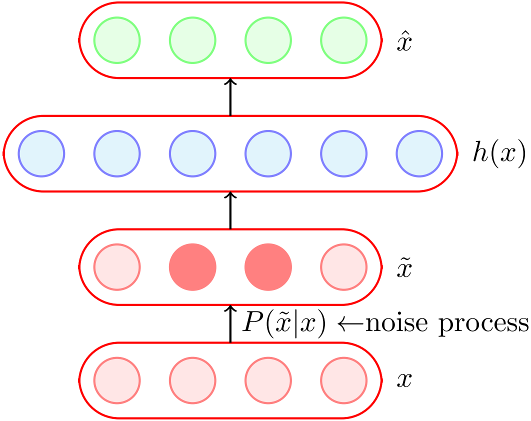
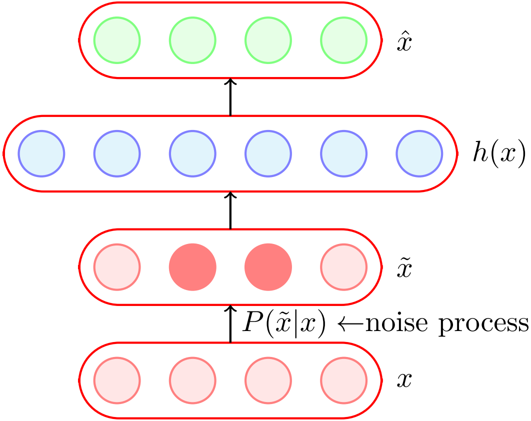
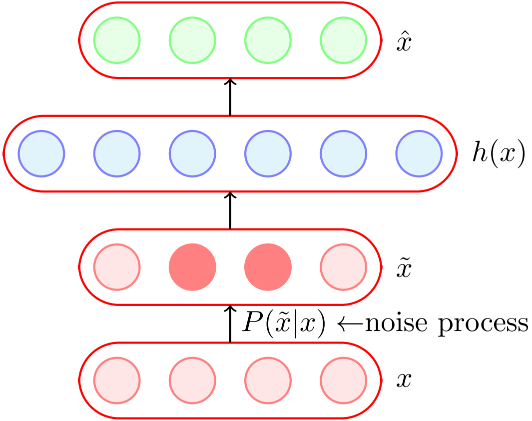

$\hat{x}$
$h(x)$
$\tilde{x}$
$P(\tilde{x}|x)$ ←noise process
x

- We saw this in Autoencoder

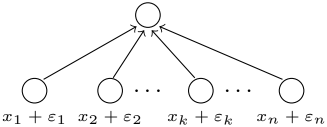




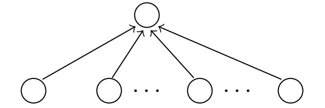
- We saw this in Autoencoder
- We can show that for a simple input output neural network, adding Gaussian noise to the input is equivalent to weight decay (L_2 regularisation)



- 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

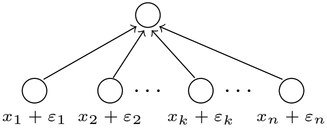


$$\varepsilon \sim \mathcal{N}(0, \sigma^2)$$



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

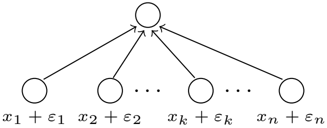
$$\widetilde{x}_i = x_i + \varepsilon_i$$



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

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

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



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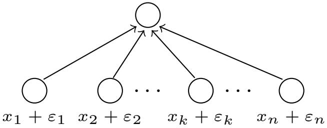
$$\widetilde{y} = \sum_{i=1}^{n} w_i \widetilde{x}_i$$



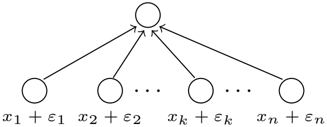
$$\varepsilon \sim \mathcal{N}(0, \sigma^2)$$

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

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

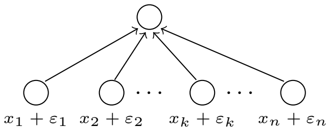
$$\widetilde{y} = \sum_{i=1}^{n} w_i \widetilde{x}_i$$

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



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

$$\begin{aligned}
\widetilde{x}_i &= x_i + \varepsilon_i \\
\widehat{y} &= \sum_{i=1}^{n} w_i x_i \\
\widetilde{y} &= \sum_{i=1}^{n} w_i \widetilde{x}_i \\
&= \sum_{i=1}^{n} w_i x_i + \sum_{i=1}^{n} w_i \varepsilon_i \\
&= \widehat{y} + \sum_{i=1}^{n} w_i \varepsilon_i
\end{aligned}$$



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

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

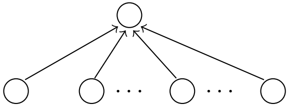
$$\widehat{y} = \sum_{i=1}^{n} w_i x_i$$

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

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

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

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



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

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

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

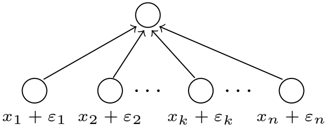
$$\widetilde{y} = \sum_{i=1}^{n} w_i \widetilde{x}_i$$

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

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

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

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



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

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

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

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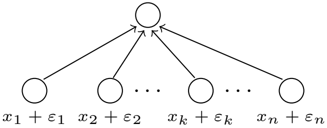
We are interested in $E[(\widetilde{y} - y)^2]$

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

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



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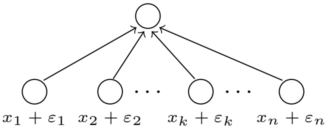

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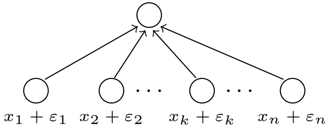
$$= E\left[(\widehat{y} - y)^2\right] + 0 + E\left[\sum_{i=1}^{n} w_i^2\varepsilon_i^2\right]$$

($\because$ ε_i is independent of ε_j and ε_i is independent of ($\widehat{y}$-y))



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

($\because$ ε_i is independent of ε_j and ε_i is independent of ($\widehat{y}$-y))

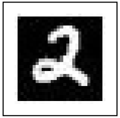
$$= (E\left[(\widehat{y} - y)^2\right] + \sigma^2 \sum_{i=1}^{n} w_i^2$$

(same as L_2 norm penalty)

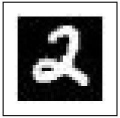
Module 8.8 : Adding Noise to the outputs

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

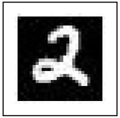


0	0	1	0	0	0	0	0	0	0	Hard targets



0	0	1	0	0	0	0	0	0	0	Hard targets

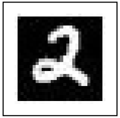
$$\text{minimize} : \sum_{i=0}^{9} p_i \log q_i$$



0	0	1	0	0	0	0	0	0	0	Hard targets

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

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



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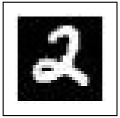
$$\text{estimated distribution} : q$$



0	0	1	0	0	0	0	0	0	0	Hard targets

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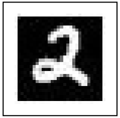
Intuition

- Do not trust the true labels, they may be noisy



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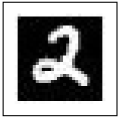
$$\text{true distribution} : p = \{0, 0, 1, 0, 0, 0, 0, 0, 0, 0\}$$

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

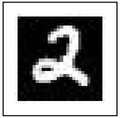
Intuition

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



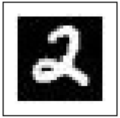
$\frac{\varepsilon}{9}$	$\frac{\varepsilon}{9}$	$1-\varepsilon$	$\frac{\varepsilon}{9}$	$\frac{\varepsilon}{9}$	$\frac{\varepsilon}{9}$	$\frac{\varepsilon}{9}$	$\frac{\varepsilon}{9}$	$\frac{\varepsilon}{9}$	$\frac{\varepsilon}{9}$

Soft targets



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

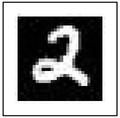
$\varepsilon =$ small positive constant



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

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

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

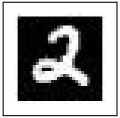


$\frac{\varepsilon}{9}$	$\frac{\varepsilon}{9}$	$1-\varepsilon$	$\frac{\varepsilon}{9}$	$\frac{\varepsilon}{9}$	$\frac{\varepsilon}{9}$	$\frac{\varepsilon}{9}$	$\frac{\varepsilon}{9}$	$\frac{\varepsilon}{9}$	$\frac{\varepsilon}{9}$	Soft targets

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

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

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



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

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

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

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

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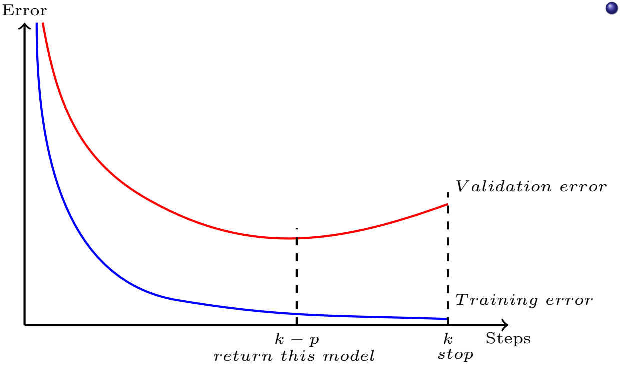
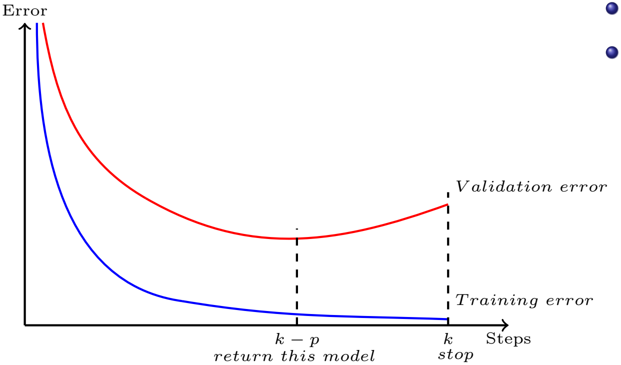
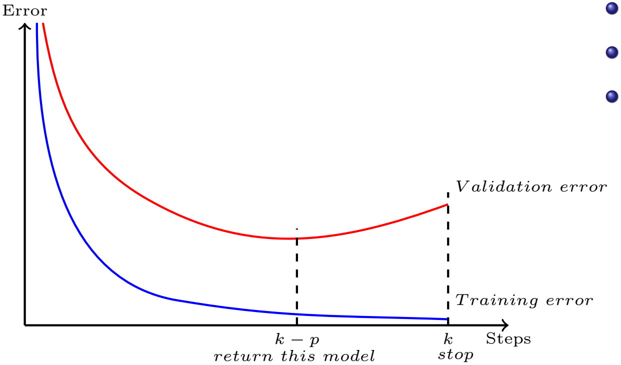


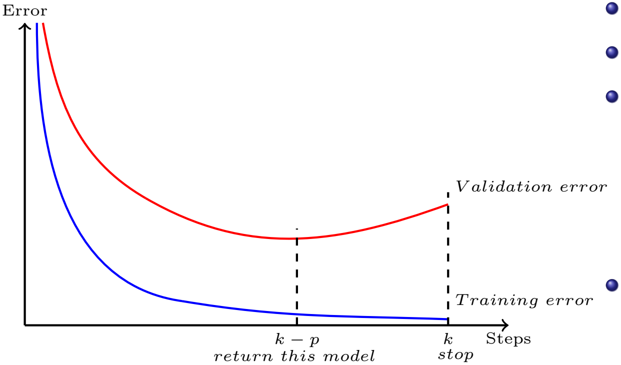
- Track the validation error



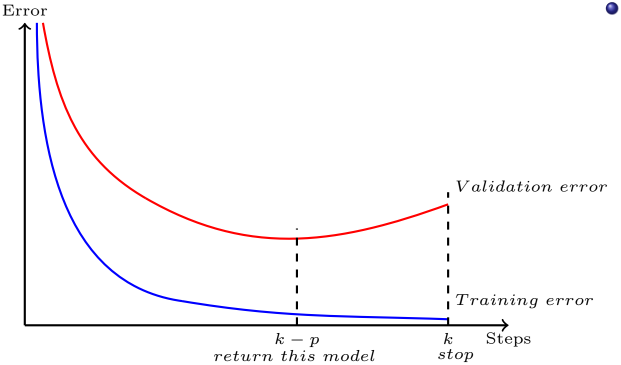
- Track the validation error
- Have a patience parameter p



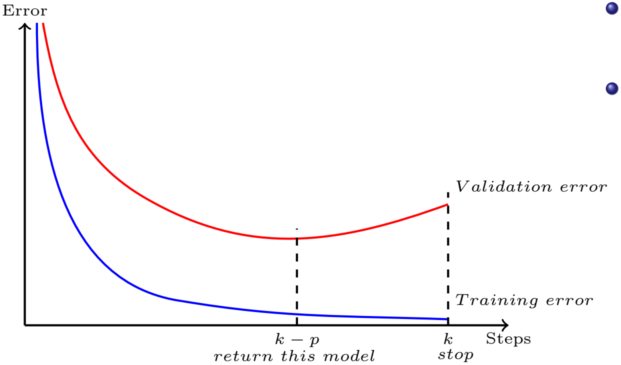
- Track the validation error
- Have a patience parameter p
- If you are at step k and there was no improvement in validation error in the previous p steps then stop training and return the model stored at step $k - p$



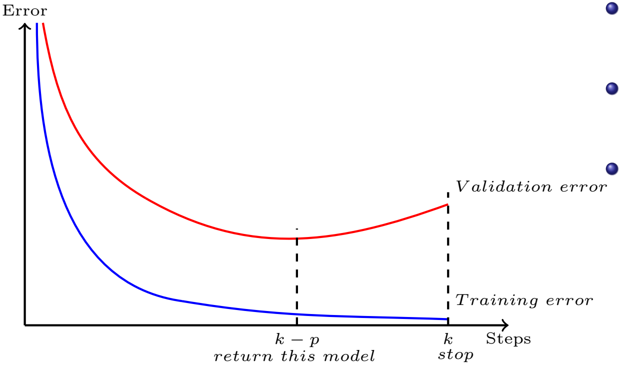
- Track the validation error
- Have a patience parameter p
- If you are at step k and there was no improvement in validation error in the previous p steps then stop training and return the model stored at step $k-p$
- Basically, stop the training early before it drives the training error to 0 and blows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



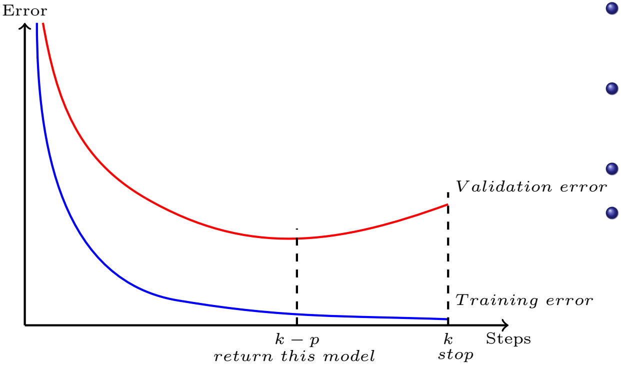
- Very effective and the mostly widely used form of regularization



- Very effective and the mostly widely used form of regularization
- Can be used even with other regularizers (such as L_2)



- 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 ?



- Very effective and the mostly widely used form of regularization
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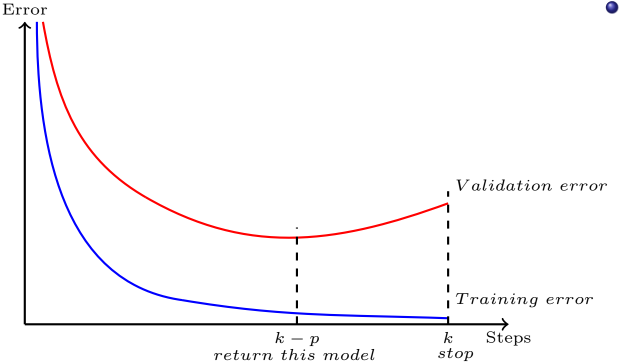
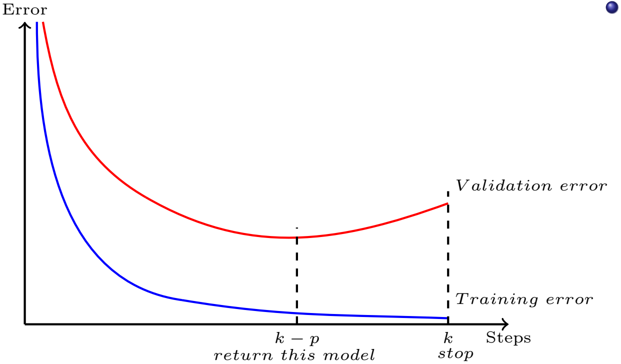
- How does it act as a regularizer ?
- We will first see an intuitive explanation and then a mathematical analysis



- Recall that the update rule in SGD is :-



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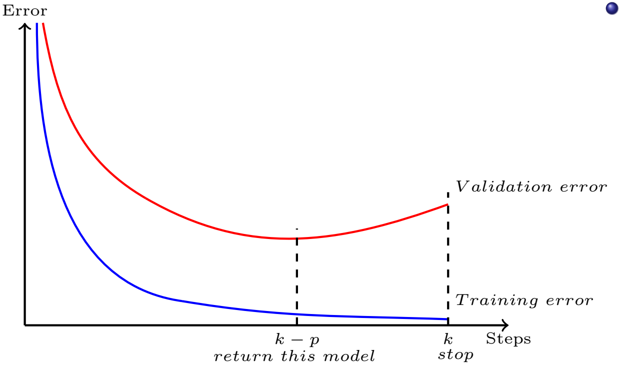
$$\omega_{t+1} = \omega_t + \eta \nabla \omega_t$$



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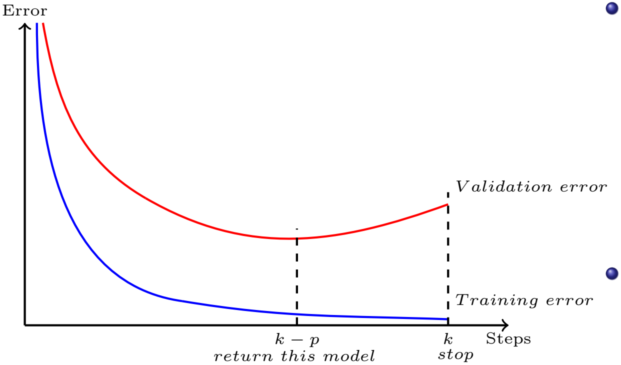

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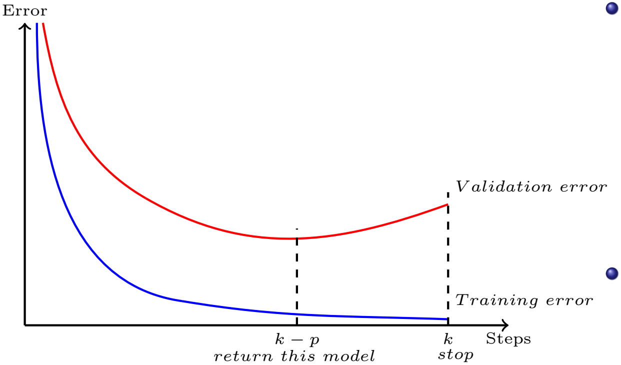
- Let τ be the maximum value of $\nabla \omega_i$ then



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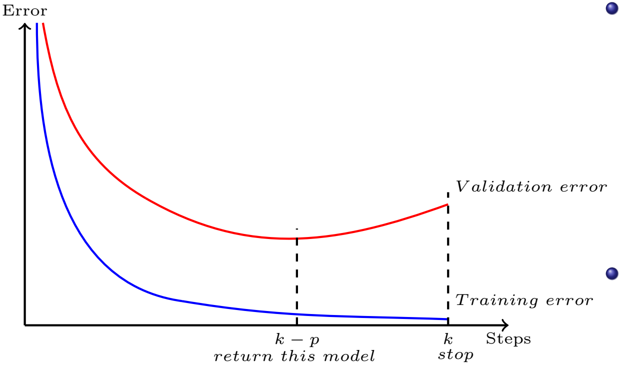
- Let τ be the maximum value of $\nabla \omega_i$ then

$$\omega_{t+1} \leq \omega_0 + \eta t \tau$$



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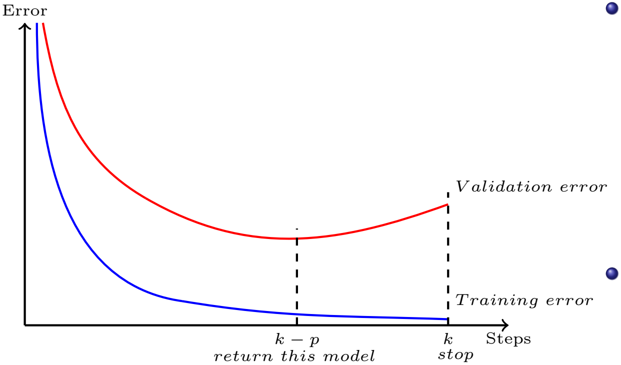
- Thus, t controls how far ω_t can go from the initial ω_0



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- Thus, t controls how far ω_t can go from the initial ω_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 $J(\omega)$ is

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$$J(\omega) = J(\omega^*) + (\omega - \omega^*)^T \nabla J(\omega^*) + \frac{1}{2}(\omega - \omega^*)^T H(\omega - \omega^*)$$

- Recall that the Taylor series approximation for $J(\omega)$ is

$$
\begin{aligned}
J(\omega) &= J(\omega^*) + (\omega - \omega^*)^T \nabla J(\omega^*) + \frac{1}{2}(\omega - \omega^*)^T H (\omega - \omega^*) \\
&= J(\omega^*) + \frac{1}{2}(\omega - \omega^*)^T H (\omega - \omega^*) \qquad [\ \omega^* \ \textit{is optimal so}\ \nabla J(\omega^*)\ \textit{is}\ 0\ ]
\end{aligned}
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\nabla(J(\omega)) &= H(\omega - \omega^*)
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$$\nabla(J(\omega)) = H(\omega - \omega^*)$$

Now the SGD update rule is:

$$\omega_t = \omega_{t-1} + \eta \nabla J(\omega_{t-1})$$

- Recall that the Taylor series approximation for $J(\omega)$ is

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\begin{aligned}
J(\omega) &= J(\omega^*) + (\omega - \omega^*)^T \nabla J(\omega^*) + \frac{1}{2}(\omega - \omega^*)^T H(\omega - \omega^*) \\
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$$
\begin{aligned}
\omega_t &= \omega_{t-1} + \eta \nabla J(\omega_{t-1}) \\
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\end{aligned}
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\begin{aligned}
J(\omega) &= J(\omega^*) + (\omega - \omega^*)^T \nabla J(\omega^*) + \frac{1}{2}(\omega - \omega^*)^T H(\omega - \omega^*) \\
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\omega_t &= \omega_{t-1} + \eta \nabla J(\omega_{t-1}) \\
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&= (I + \eta H)\omega_{t-1} - \eta H \omega^*
\end{aligned}
$$

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- Let us see the derivation

- To prove: The below two equations are equivalent

$$\omega_t = (I + \eta Q\Lambda Q^T)\omega_{t-1} - \eta Q\Lambda Q^T \omega^*$$
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- Proof by induction:
- Base case: $t = 1$ and ω_0=0:
- ω_1 according to the first equation:

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- ω_1 according to the second equation:

$$\begin{aligned}\omega_1 &= Q(I - (I - \eta\Lambda)^1)Q^T w^* \\ &= \eta Q \Lambda Q^T w^*\end{aligned}$$

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

$$\begin{aligned}\therefore \omega_t &= (I + \eta Q\Lambda Q^T)\omega_{t-1} - \eta Q\Lambda Q^T\omega^* \\ &= Q[I - (I - \varepsilon\Lambda)^t]Q^T\omega^*\end{aligned}$$

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$$\begin{aligned} \omega_{t+1} &= (I - \eta Q \Lambda Q^T)\omega_t + \eta Q \Lambda Q^T \omega^* \\ &\quad (\text{using } \omega_t = Q[I - (I - \varepsilon\Lambda)^t]Q^T \omega^*) \\ &= \color{red}{(I - \eta Q \Lambda Q^T)}Q(I - (I - \eta\Lambda)^t)Q^T \omega^* + \eta Q \Lambda Q^T \omega^* \\ &\quad (\text{Opening this bracket}) \end{aligned}$$

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$$= (I - \eta Q\Lambda Q^T)Q(I - (I - \eta\Lambda)^t)Q^T\omega^* + \eta Q\Lambda Q^T\omega^*$$
$$(\text{Opening this bracket})$$
$$= {\color{red}I}Q(I - (I - \eta\Lambda)^t)Q^T\omega^* - {\color{red}\eta Q\Lambda Q^T}Q(I - (I - \eta\Lambda)^t)Q^T\omega^* + \eta Q\Lambda Q^T\omega^*$$

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$$\omega_{t+1} = (I - \eta Q\Lambda Q^T)\omega_t + \eta Q\Lambda Q^T\omega^*$$

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

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

(Opening this bracket)

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

- Continuing

$$\omega_{t+1} = Q(I-(I-\eta\Lambda)^t)Q^T\omega^* - \eta Q\Lambda Q^T Q(I-(I-\eta\Lambda)^t)Q^T\omega^* + \eta Q\Lambda Q^T\omega^*$$

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\omega_{t+1} &= Q(I-(I-\eta\Lambda)^t)Q^T\omega^* - \eta Q\Lambda Q^T Q(I-(I-\eta\Lambda)^t)Q^T\omega^* + \eta Q\Lambda Q^T\omega^* \\
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\end{aligned}$$

- Continuing

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\end{aligned}$$

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- Continuing

$$
\begin{aligned}
\omega_{t+1} &= Q(I-(I-\eta\Lambda)^t)Q^T\omega^* - \eta Q\Lambda Q^T Q(I-(I-\eta\Lambda)^t)Q^T\omega^* + \eta Q\Lambda Q^T\omega^* \\
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&= Q(I-(I-\eta\Lambda)^{t+1})Q^T\omega^*
\end{aligned}
$$

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\begin{aligned}
\omega_{t+1} &= Q(I-(I-\eta\Lambda)^t)Q^T\omega^* - \eta Q\Lambda Q^T Q(I-(I-\eta\Lambda)^t)Q^T\omega^* + \eta Q\Lambda Q^T\omega^* \\
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\end{aligned}
$$

Hence, proved!

- Coming back...

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

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

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

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

- We observe that $\omega_t = \tilde{\omega}$, if we choose ε,t and α such that

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

Things to be remember

- Early stopping only allows t updates to the parameters.

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- However if a parameter is not important ($\frac{\partial \mathscr{L}(\theta)}{\partial \omega}$ 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

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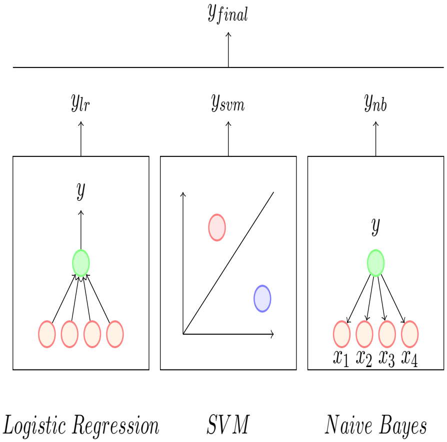
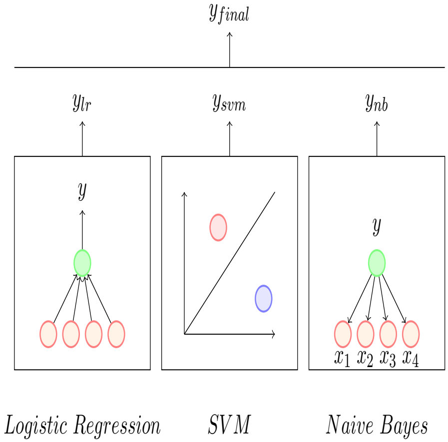
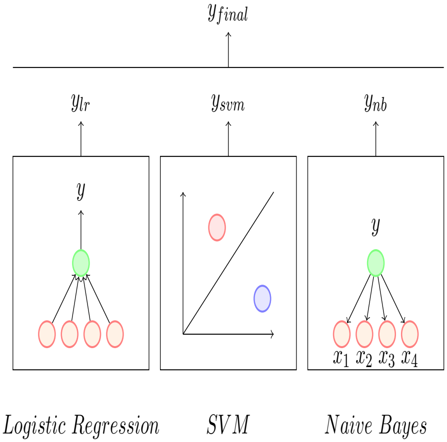


- Combine the output of different models to reduce generalization error



- Combine the output of different models to reduce generalization error
- The models can correspond to different classifiers



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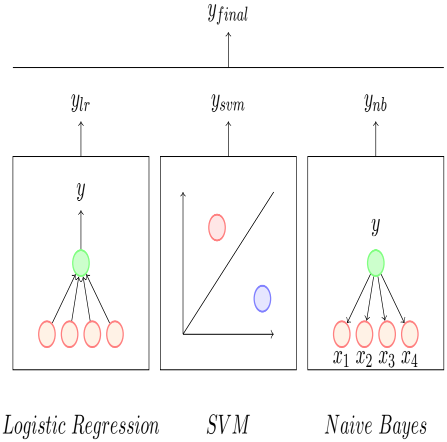

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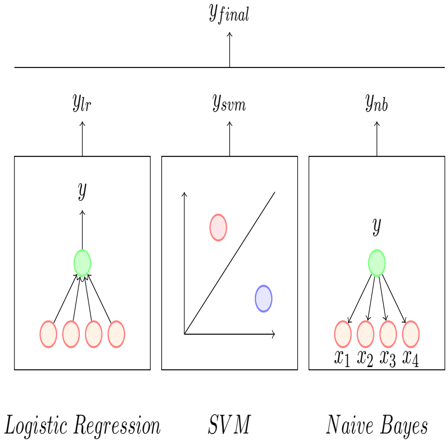

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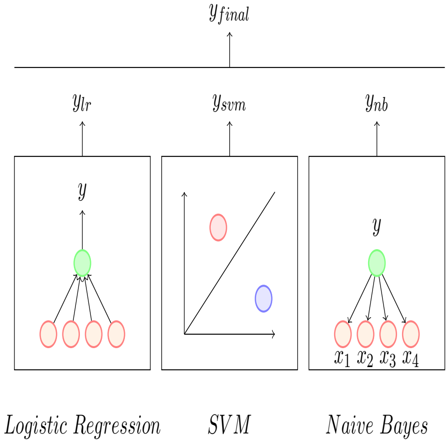

- Combine the output of different models to reduce generalization error
- The models can correspond to different classifiers
- It could be different instances of the same classifier trained with:
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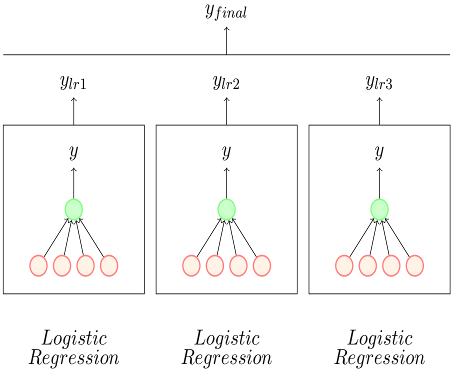
  - different features
  - different samples of the training data


y_{final}
y_{lr1}
y_{lr2}
y_{lr3}
y
y
y
Logistic Regression
Logistic Regression
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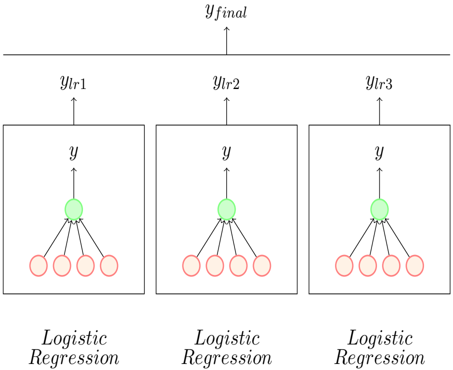

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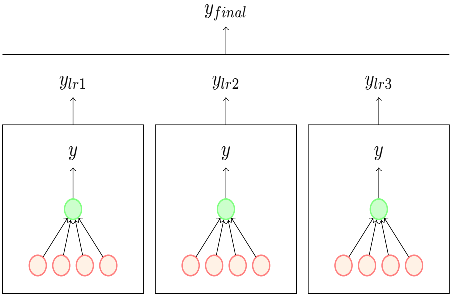
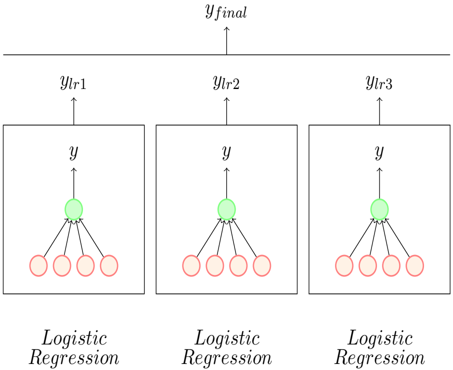


Logistic Regression *Logistic Regression* *Logistic Regression*

- Bagging: form an ensemble using different instances of the same classifier



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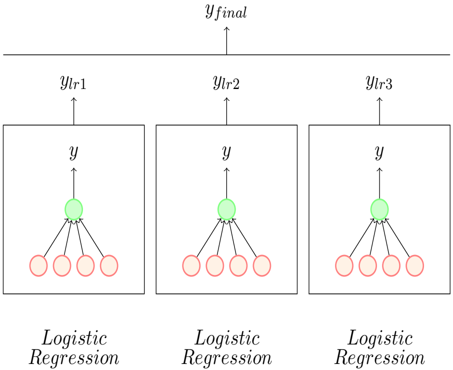
- From a given dataset, construct multiple training sets by sampling with replacement $(T_1, T_2, ..., T_k)$



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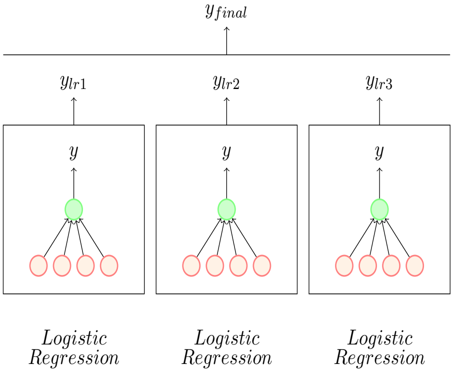

Each model trained with a different sample of the data (sampling with replacement)

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$$mse = E[(\frac{1}{k}\sum_i \varepsilon_i)^2]$$
$$= \frac{1}{k^2}E[\sum_i \sum_{i=j} \varepsilon_i \varepsilon_j + \sum_i \sum_{i \neq j} \varepsilon_i \varepsilon_j]$$
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- When would bagging work?
- Consider a set of k LR models
- Suppose that each model makes an error ε_i on a test example
- Let ε_i be drawn from a zero mean multivariate normal distribution
- $Variance = E[\varepsilon_i^2] = V$
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- 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

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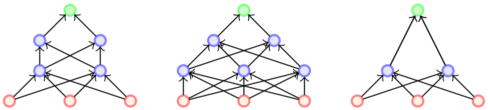

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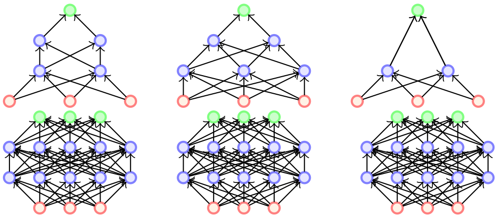

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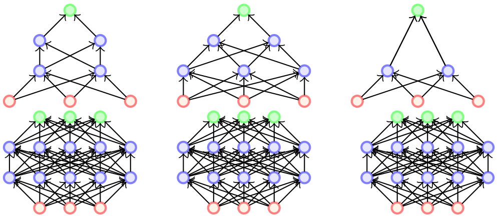

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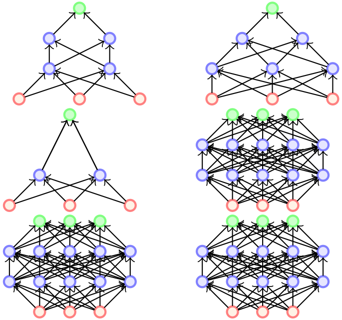
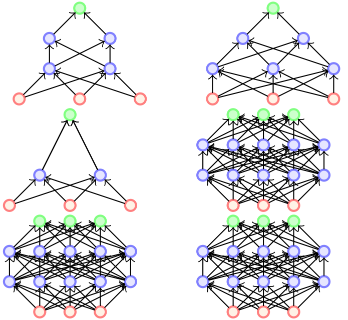
- Training several large neural networks for making an ensemble is prohibitively expensive
- Option 1: Train several neural networks having different architectures(obviously expensive)
- Option 2: Train multiple instances of the same network using different training samples (again expensive)
- Even if 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.



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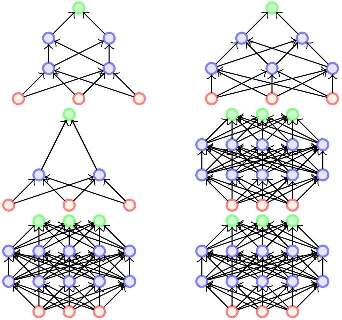
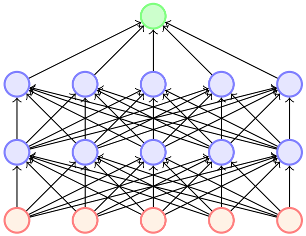
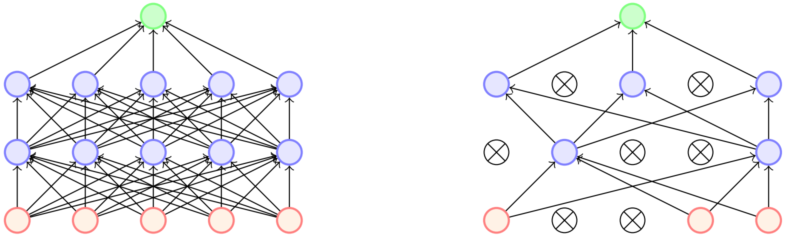
- Effectively it allows training several neural networks without any significant computational overhead.



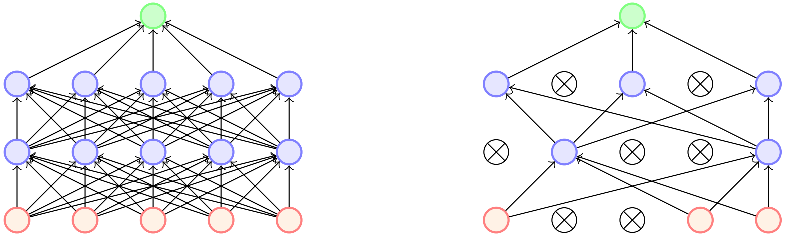
- Dropout is a technique which addresses both these issues.
- Effectively it allows training several neural networks without any significant computational overhead.
- Also gives an efficient approximate way of combining exponentially many different neural networks.



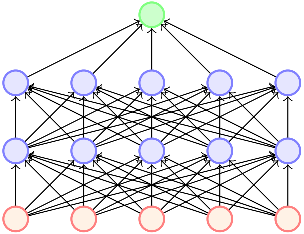
- Dropout refers to dropping out units

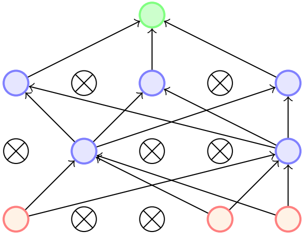


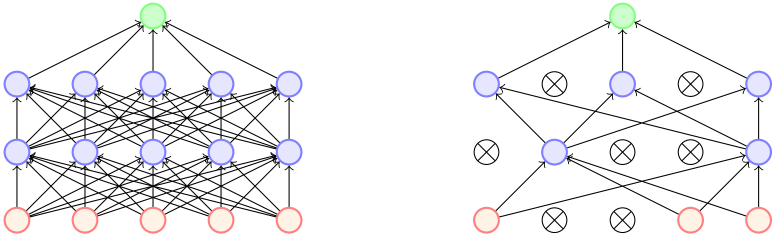
- Dropout refers to dropping out units
- Temporarily remove a node and all its incoming/outgoing connections resulting in a thinned network



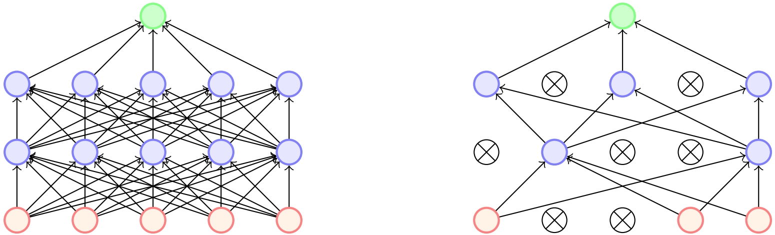
- Dropout refers to dropping out units
- Temporarily remove a node and all its incoming/outgoing connections resulting in a thinned network
- Each node is retained with a fixed probability (typically $p = 0.5$) for hidden nodes and $p = 0.8$ for visible nodes



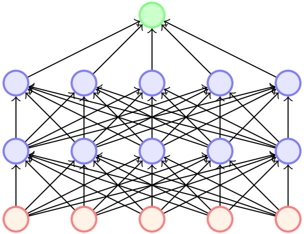
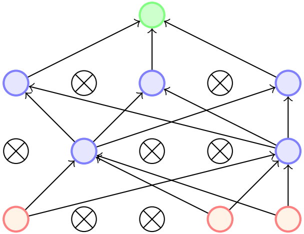




- A neural network with n nodes can be seen as a collection of 2^n possible thinned networks



- A neural network with n nodes can be seen as a collection of 2^n possible thinned networks
- The weights in these networks are shared

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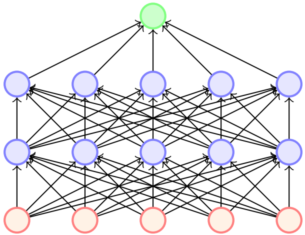
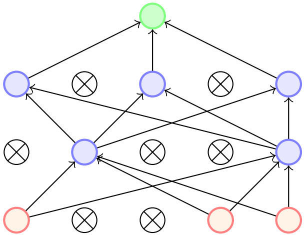
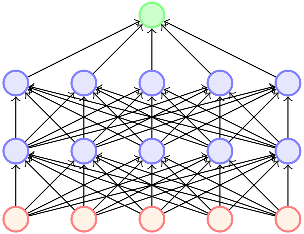
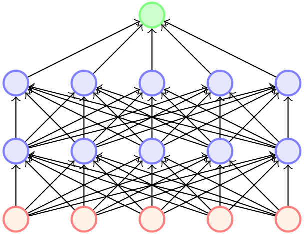
- For each training instance, a different thinned network is sampled and trained

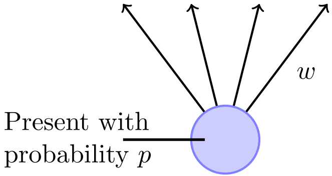




- A neural network with n nodes can be seen as a collection of 2^n possible thinned networks
- The weights in these networks are shared
- For each training instance, a different thinned network is sampled and trained
- Each thinned network gets trained rarely (or even never) but the parameter sharing ensures that no model has untrained or poorly trained parameters

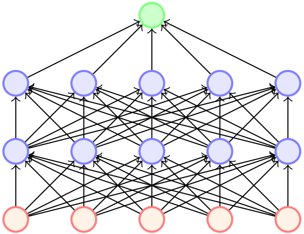




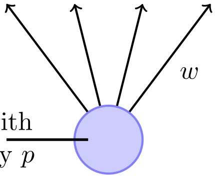


At training time

- What happens at test time?

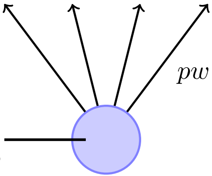


Present with probability p



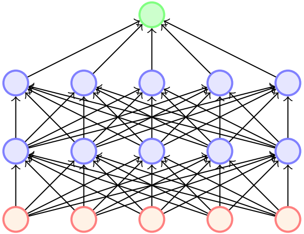
At training time

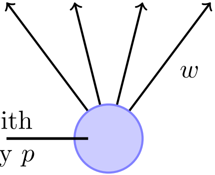
Always present

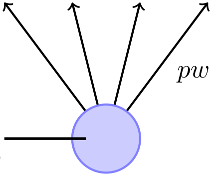


At test time

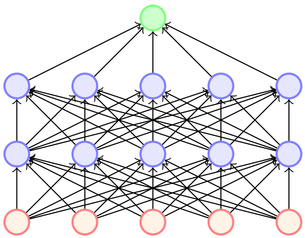
- What happens at test time?
- Impossible to aggregate the outputs of 2^n thinned networks.

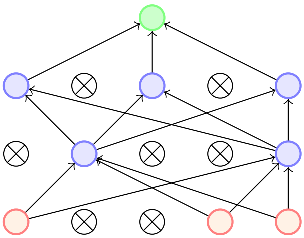


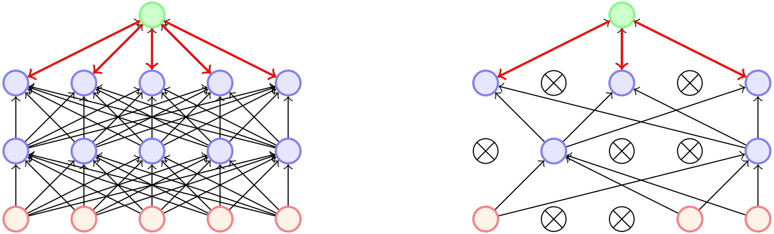




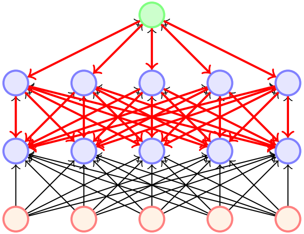
- What happens at test time?
- Impossible to aggregate the outputs of 2^n thinned networks.
- Instead we use the full Neural Network and scale the output of each node by the fraction of times it was on during training.

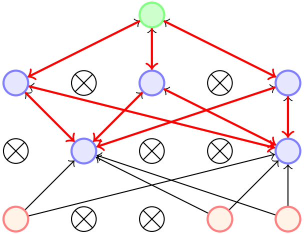






- How do you do backpropagation in such a noisy network which changes for each training instance (or batch)





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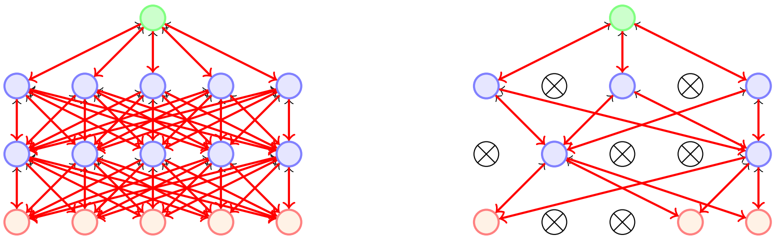
- Simple: we only backpropagate over the paths which are active and only update those weights which are active in the current thinned network



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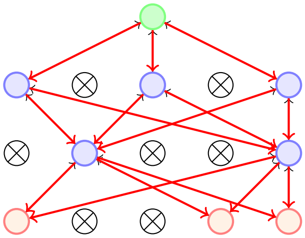
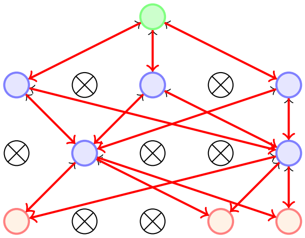


- Dropout essentially applies a masking noise to the hidden units



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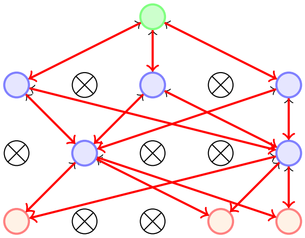
- Prevents hidden units from co-adapting



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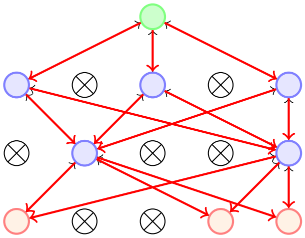
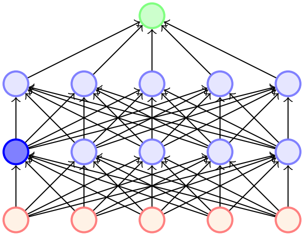
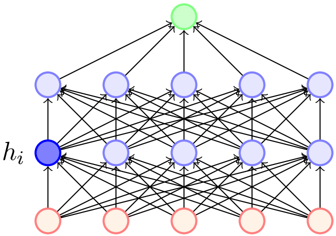
- Essentially a hidden unit cannot rely too much on other units as they may get dropped out any time



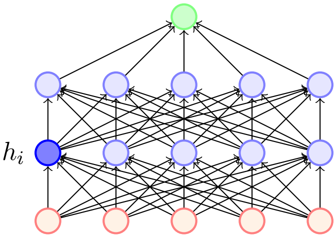
- Dropout essentially applies a masking noise to the hidden units
- Prevents hidden units from co-adapting
- Essentially a hidden unit cannot rely too much on other units as they may get dropped out any time
- Each hidden unit has to learn to be more robust to these random dropouts

h_i





- Here is an example of how dropout helps in ensuring redundancy and robustness



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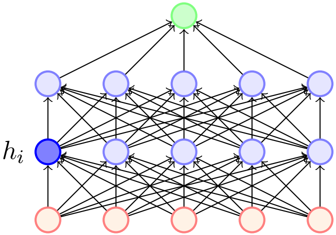
- Suppose h_i learns to detect a face by firing on detecting a nose



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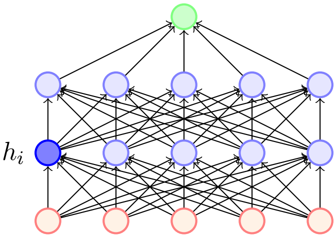
- Suppose h_i learns to detect a face by firing on detecting a nose
- Dropping h_i then corresponds to erasing the information that a nose exists



- 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
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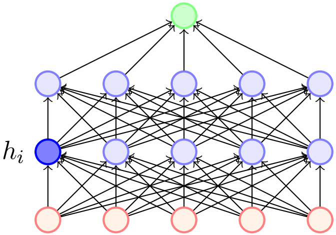
- The model should then learn another h_i which redundantly encodes the presence of a nose



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- 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