

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

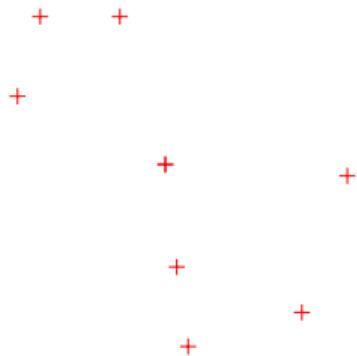
^a[Lecture 2.1](#) and [Lecture 2.2](#)

^b[Dropout](#)

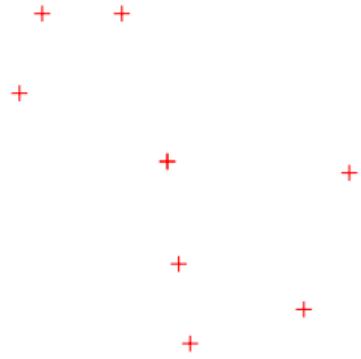
Module 8.1 : Bias and Variance

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

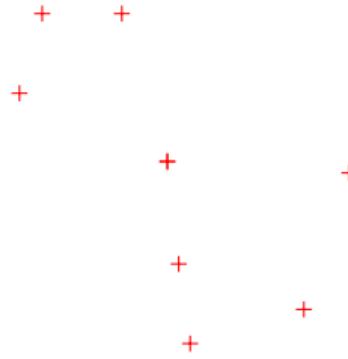


The points were drawn from a sinusoidal function (the true $f(x)$)



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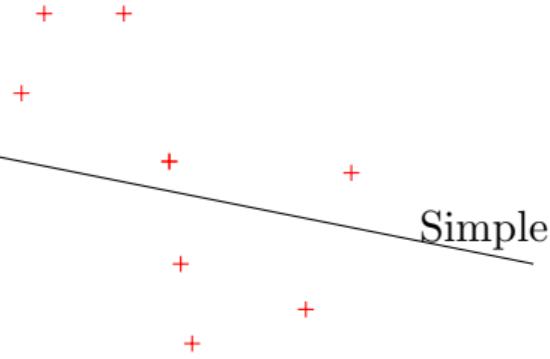
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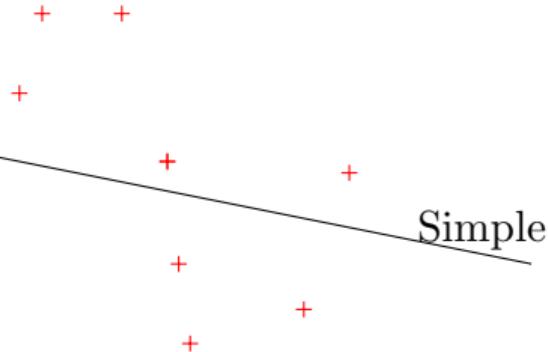
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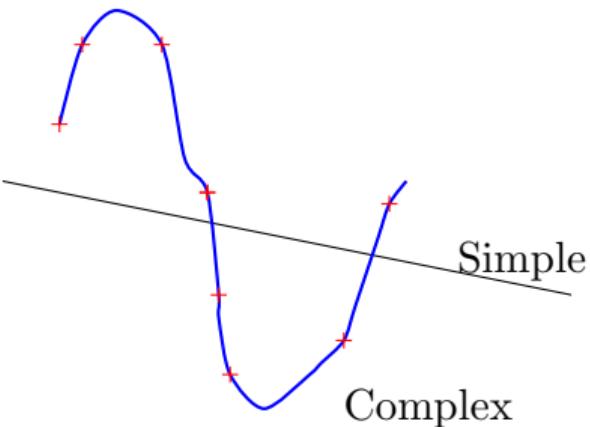
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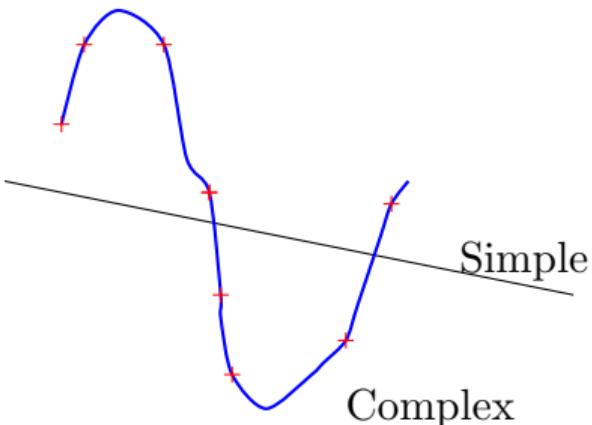
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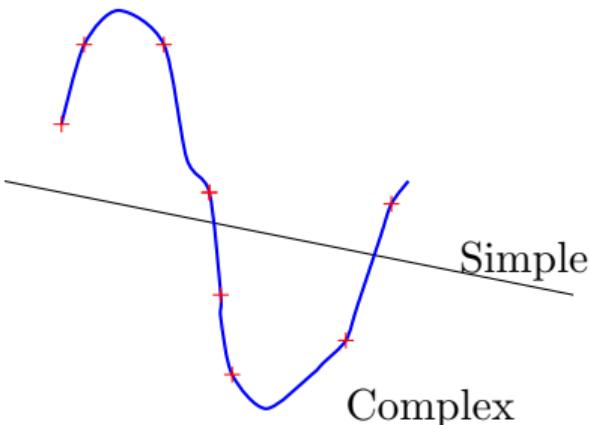
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- Note that in both cases we are making an assumption about how y is related to x . We have no idea about the true relation $f(x)$



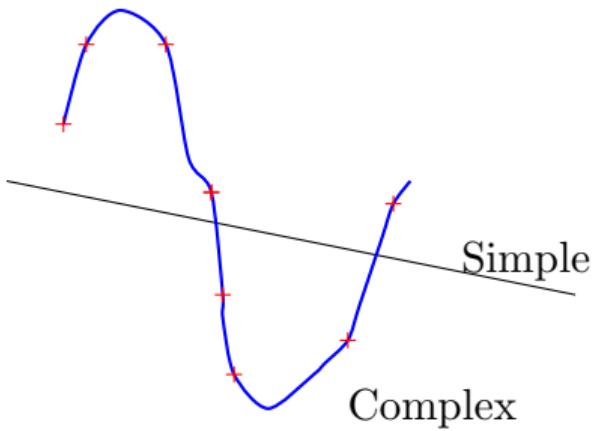
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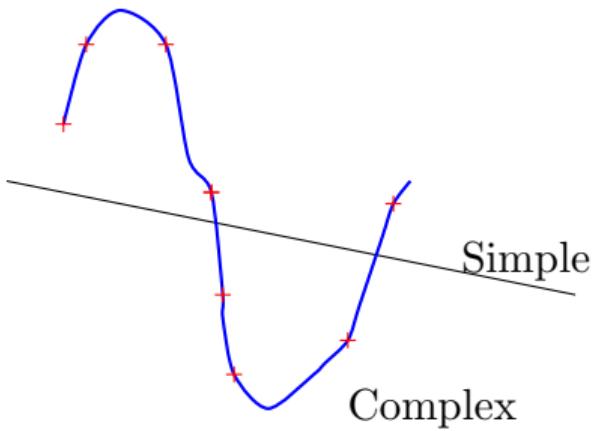
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- The training data consists of 100 points



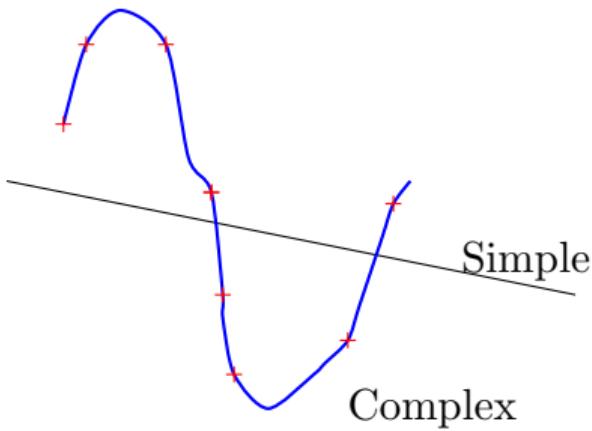
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- We sample 25 points from the training data and train a simple and a complex model



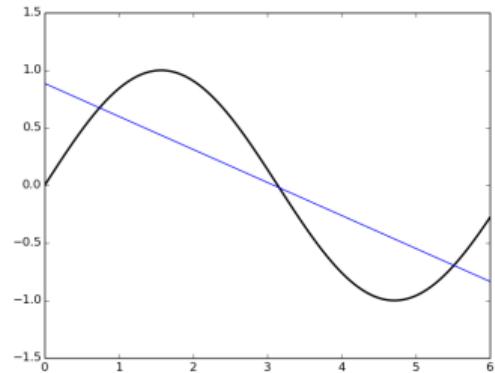
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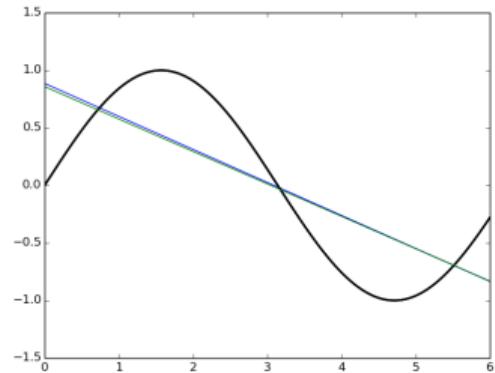
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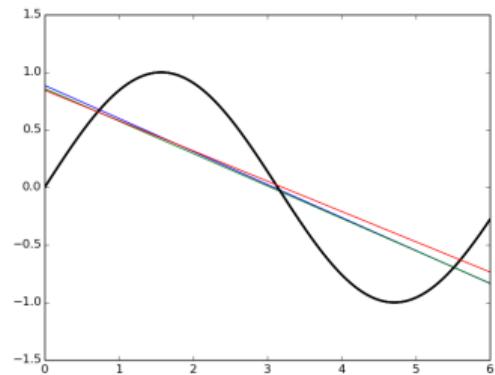


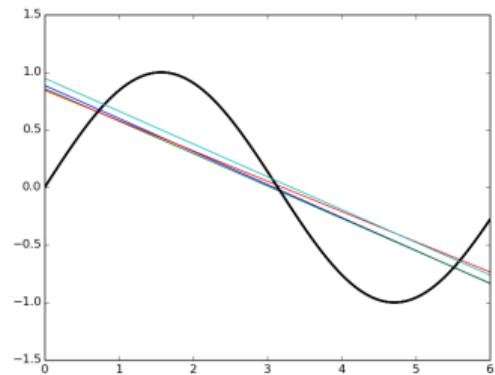
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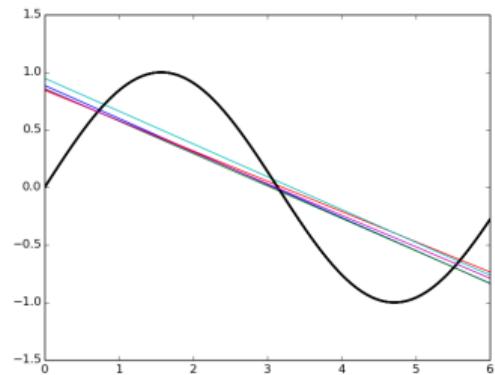
- We sample 25 points from the training data and train a simple and a complex model
- We repeat the process ' k ' times to train multiple models (each model sees a different sample of the training data)
- We make a few observations from these plots

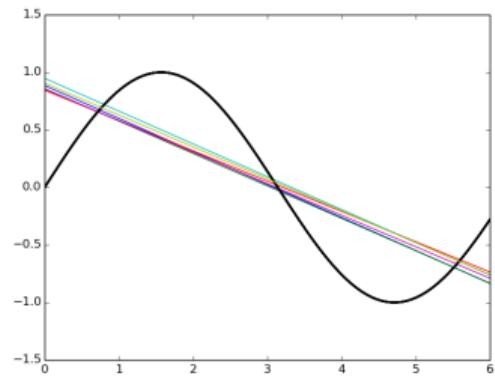


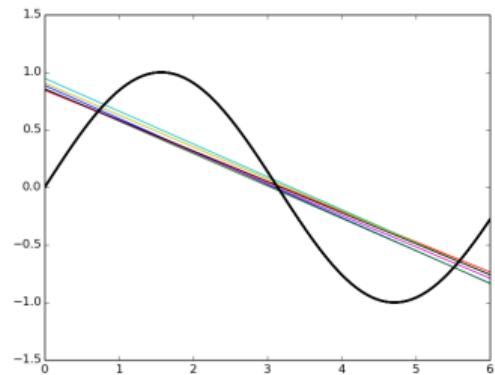


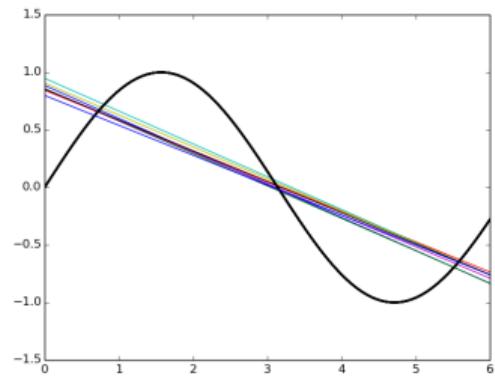


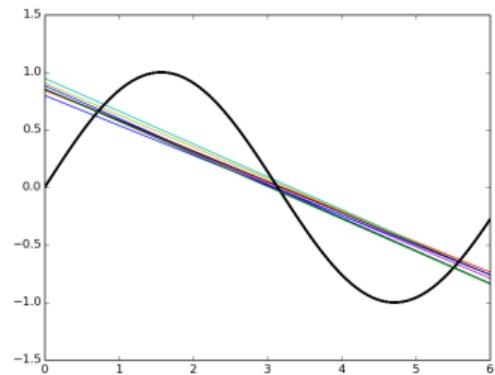


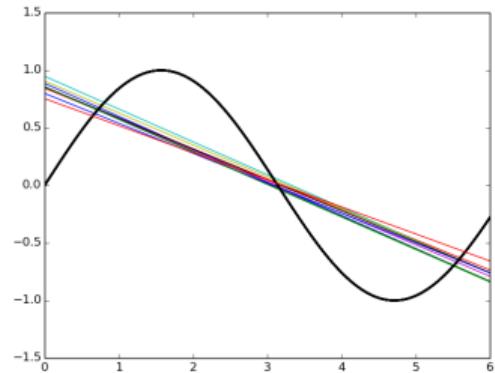


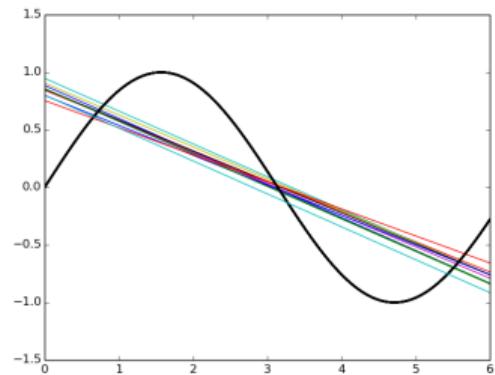


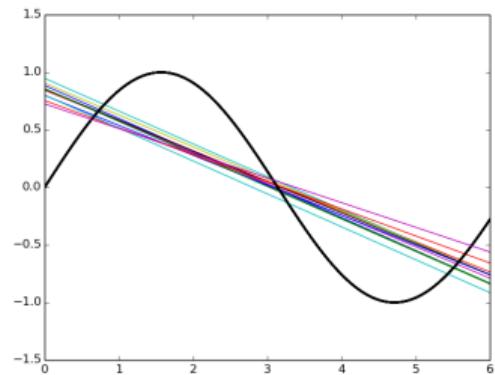


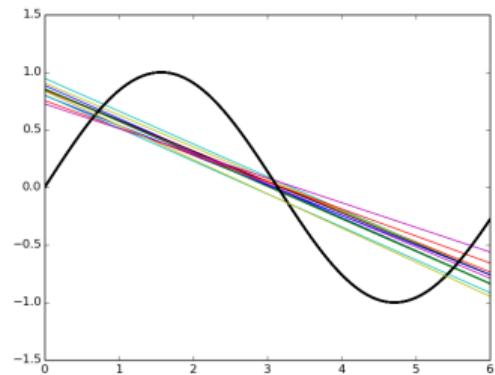


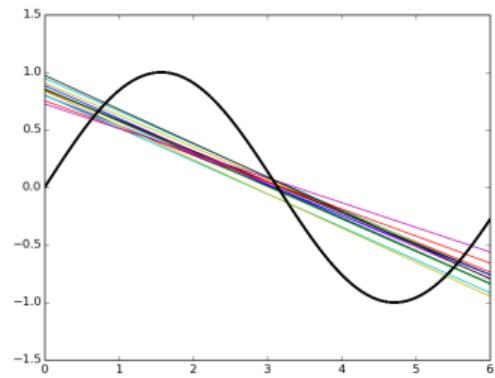


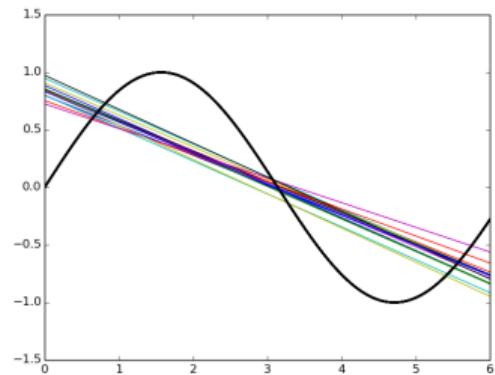


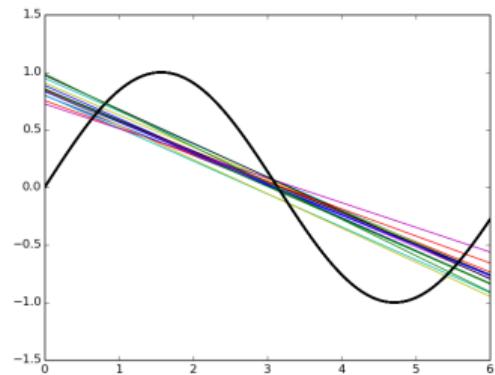


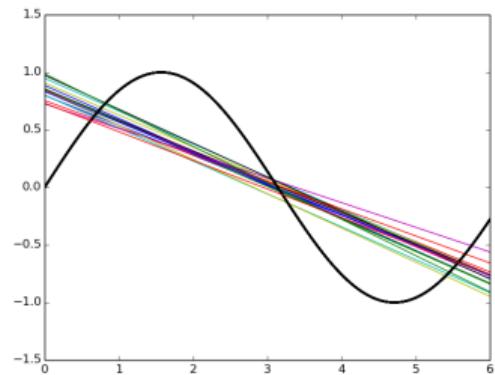


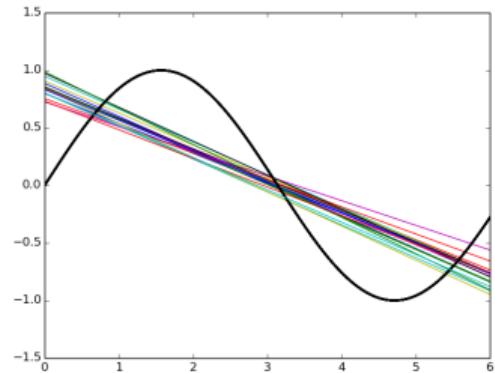


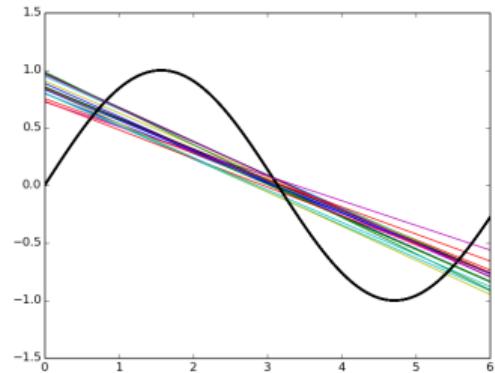


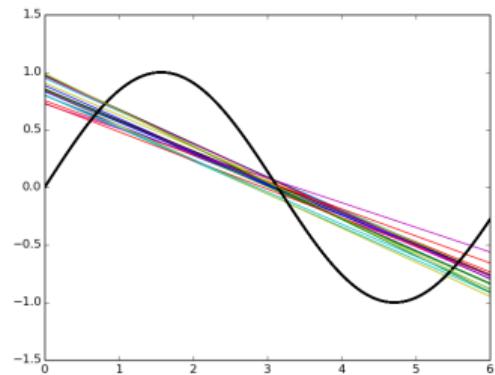


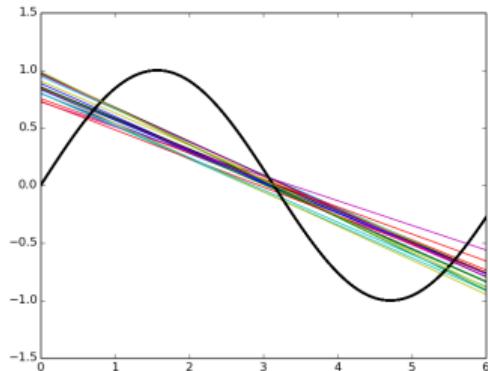




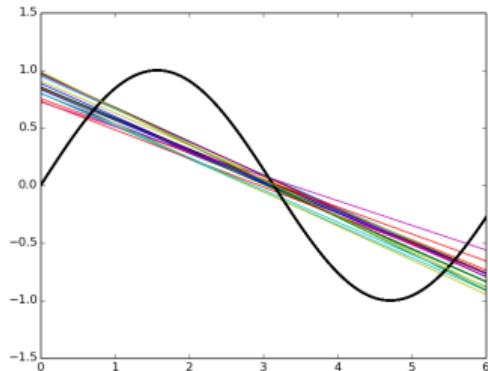




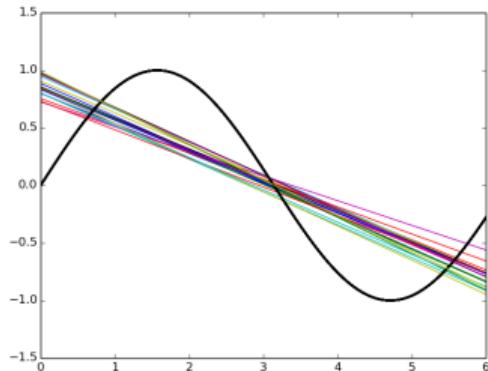




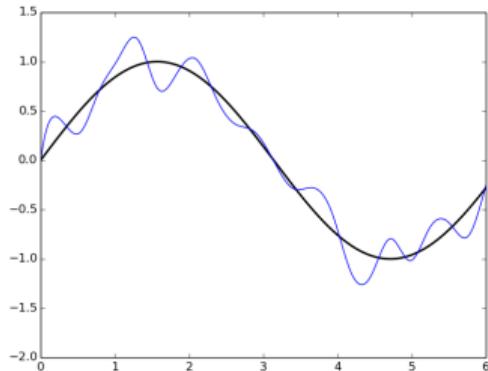
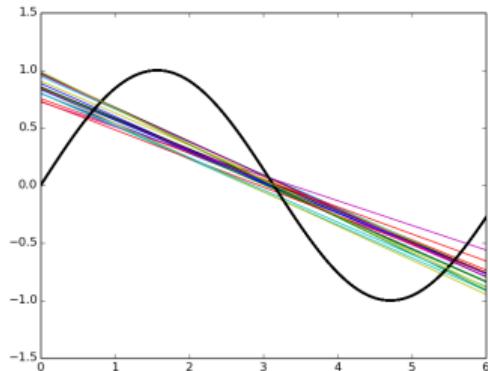
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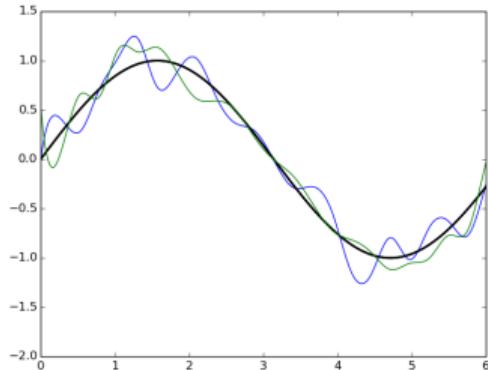
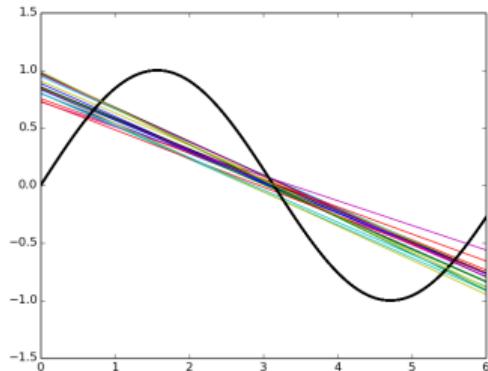
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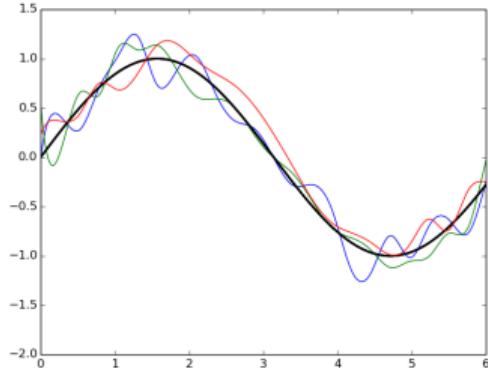
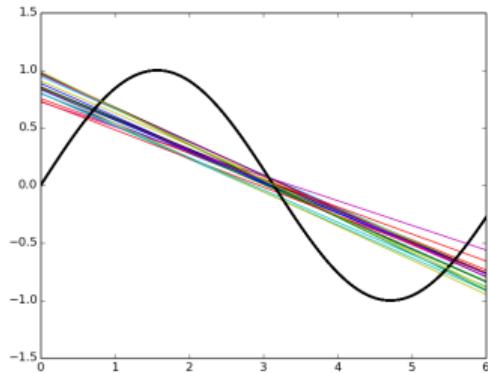
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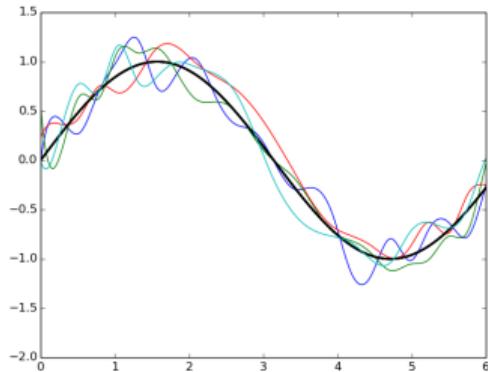
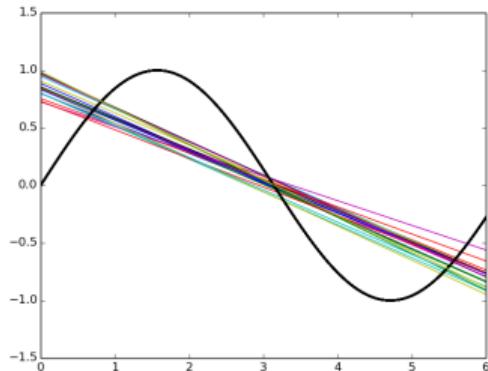
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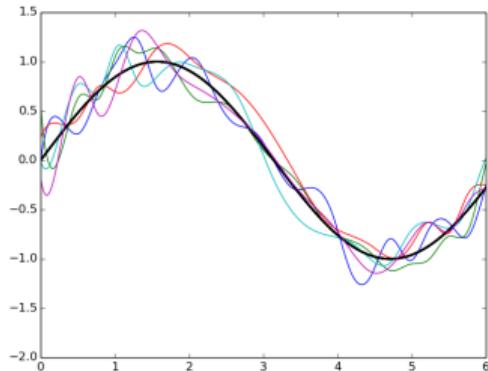
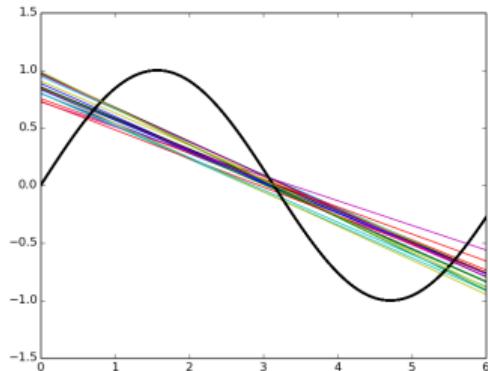
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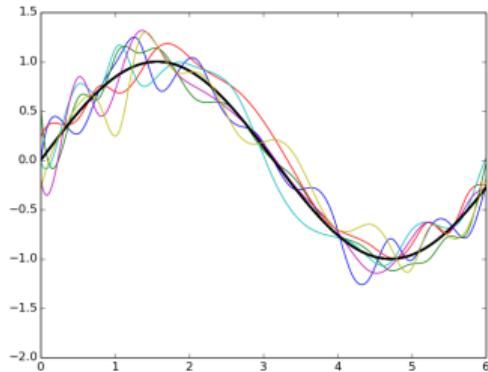
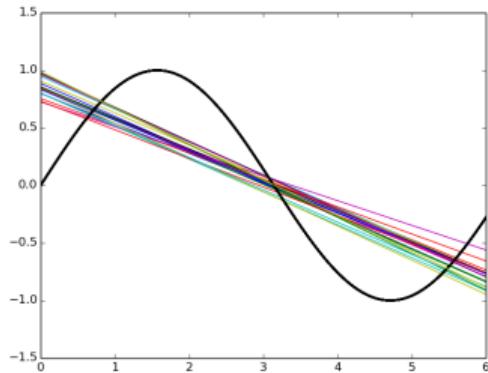
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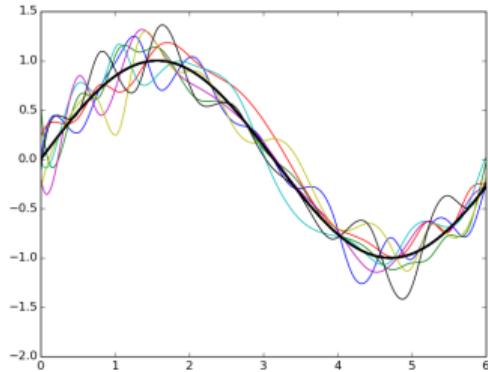
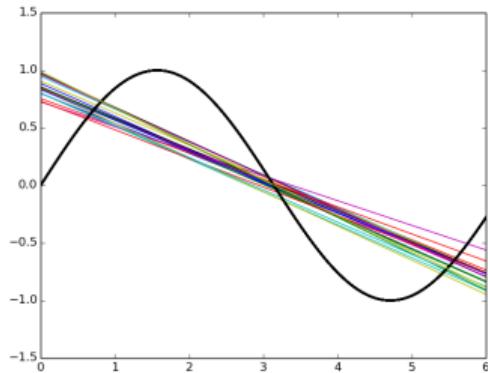
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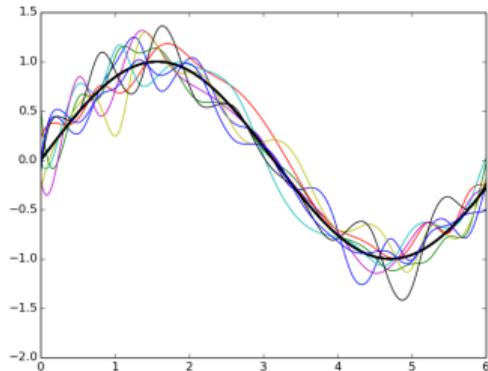
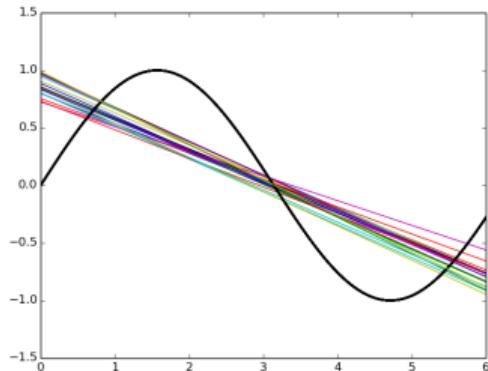
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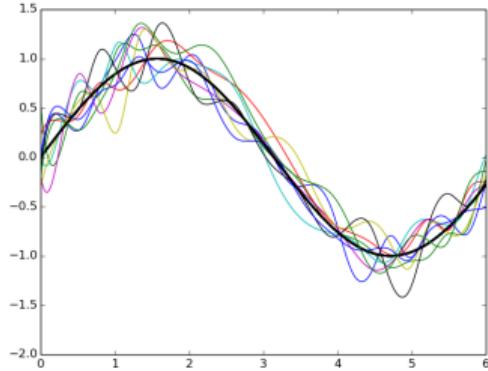
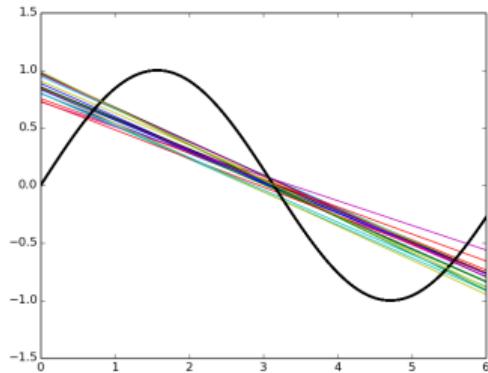
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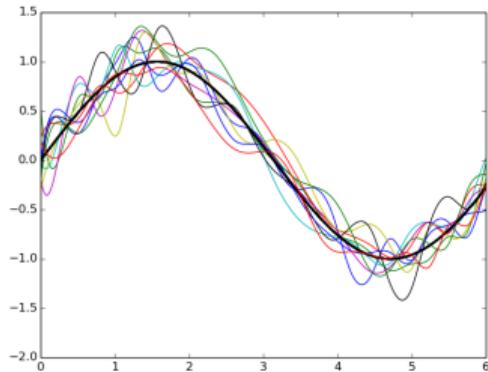
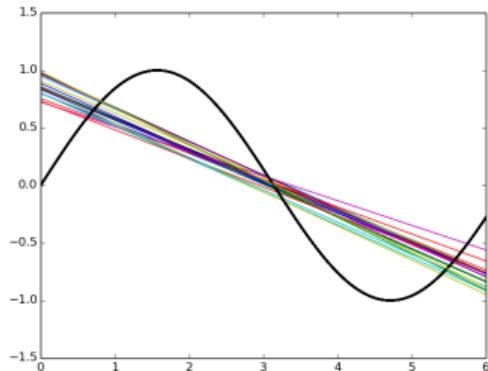
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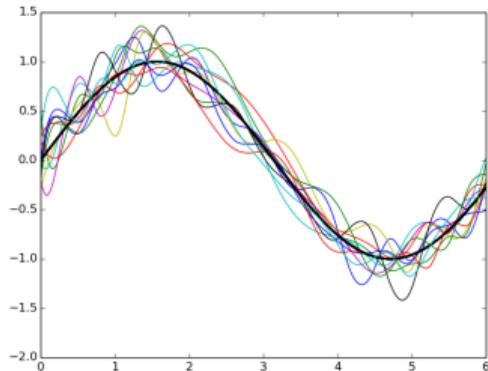
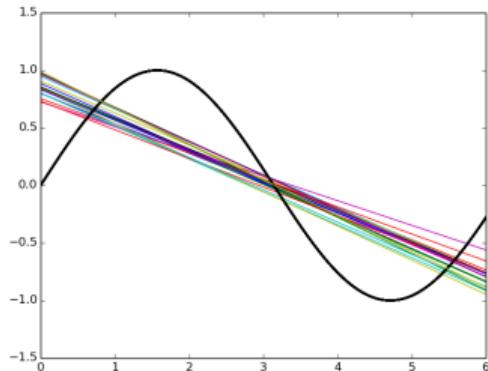
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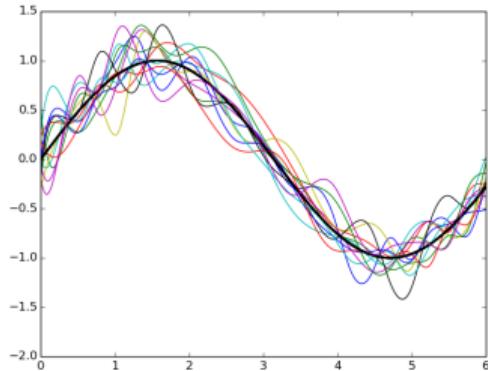
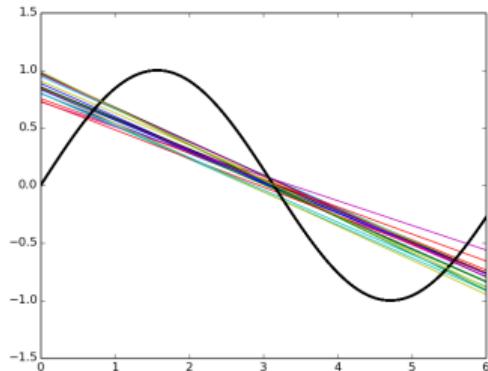
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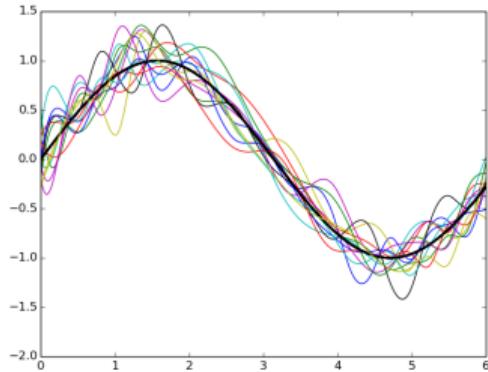
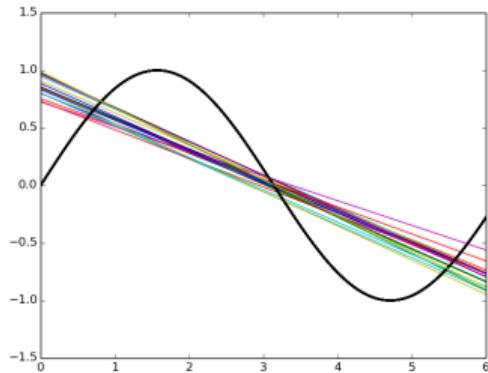
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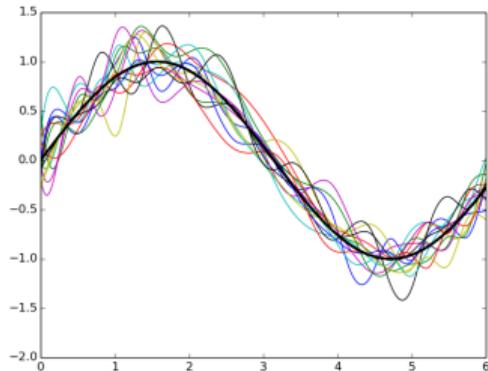
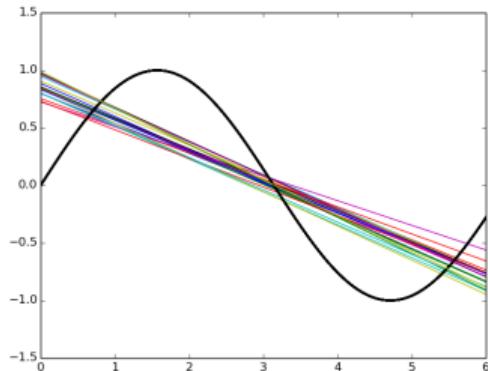
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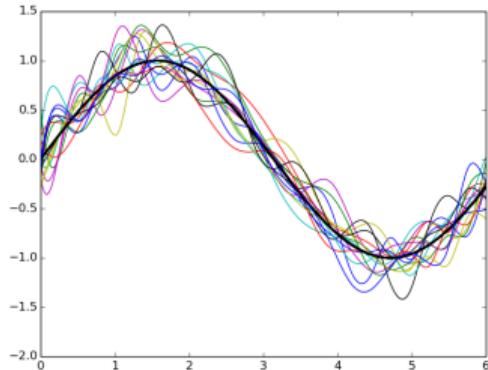
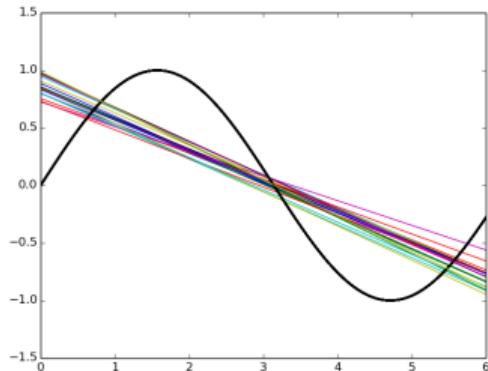
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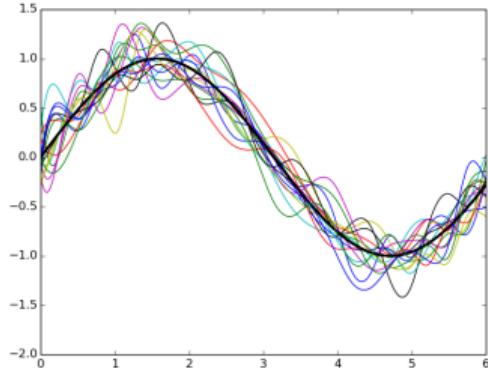
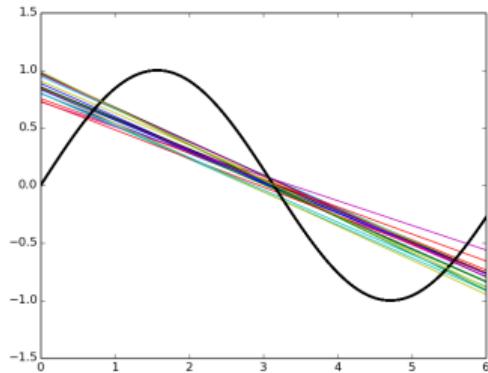
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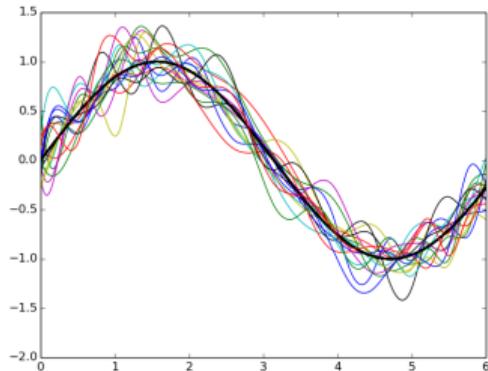
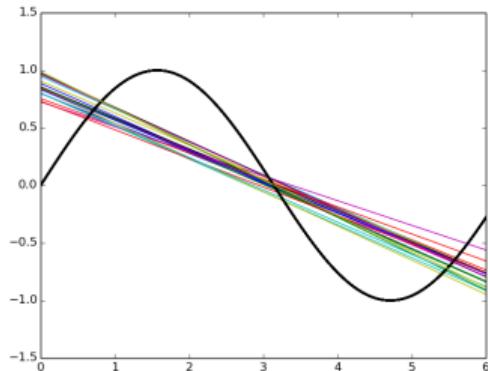
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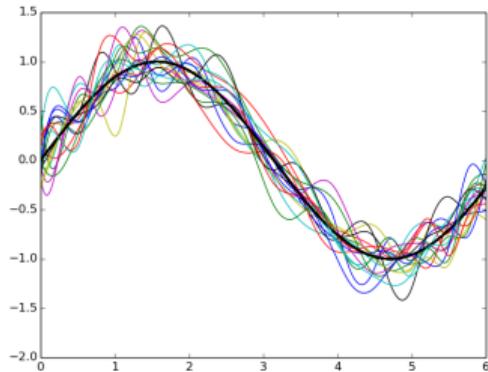
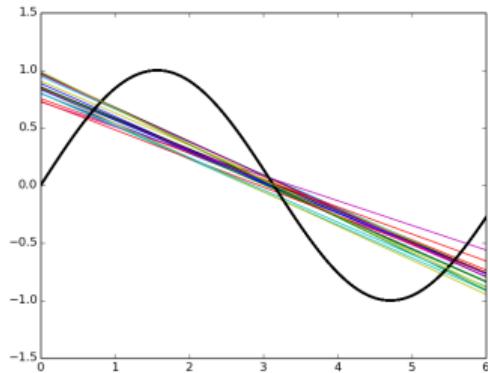
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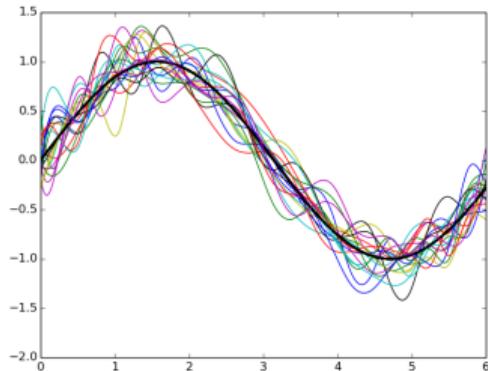
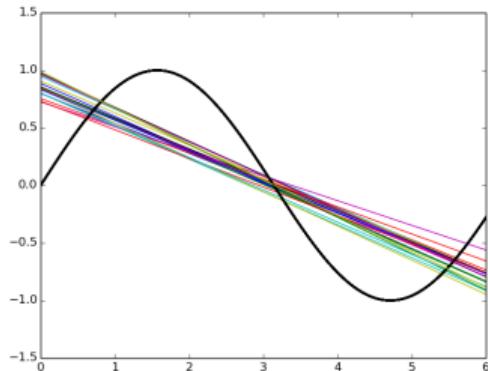
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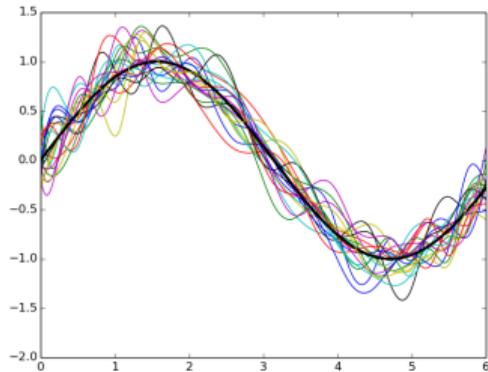
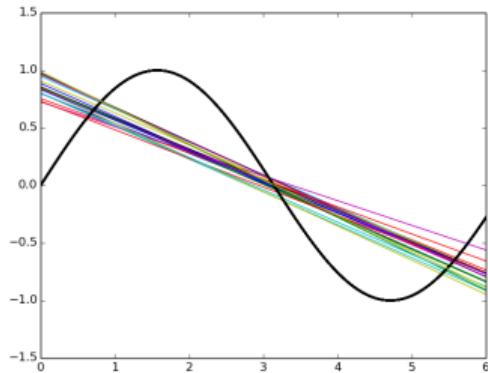
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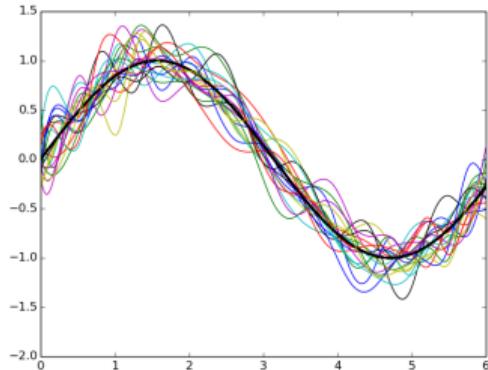
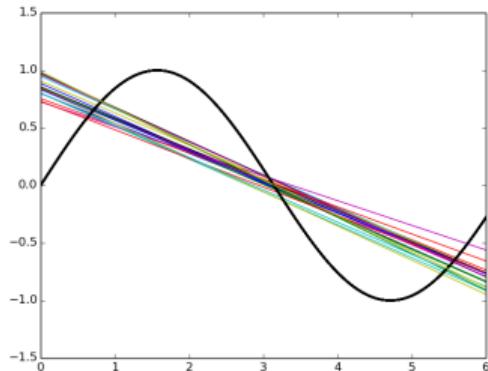
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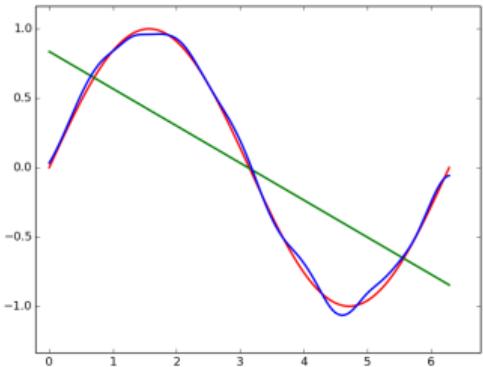
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- Simple models trained on different samples of the data do not differ much from each other
- However they are very far from the true sinusoidal curve (under fitting)
- On the other hand, complex models trained on different samples of the data are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



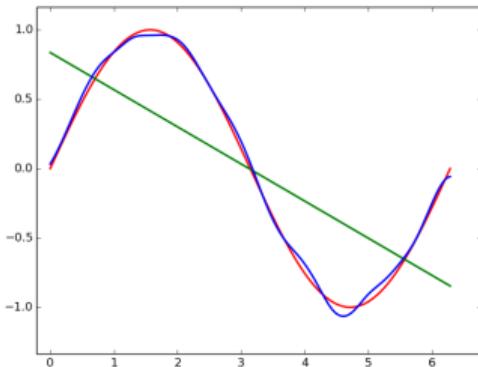
- Let $f(x)$ be the true model (sinusoidal in this case) and $\hat{f}(x)$ be our estimate of the model (simple or complex, in this case) then,

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

Green Line: Average value of $\hat{f}(x)$ for the simple model

Blue Curve: Average value of $\hat{f}(x)$ for the complex model

Red Curve: True model ($f(x)$)



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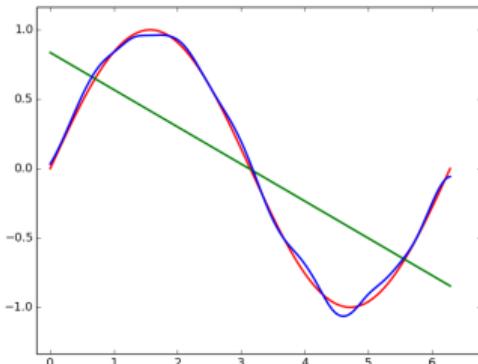
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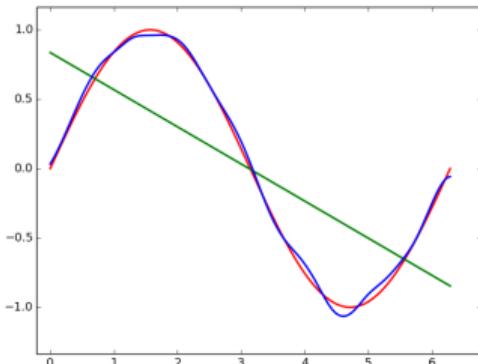
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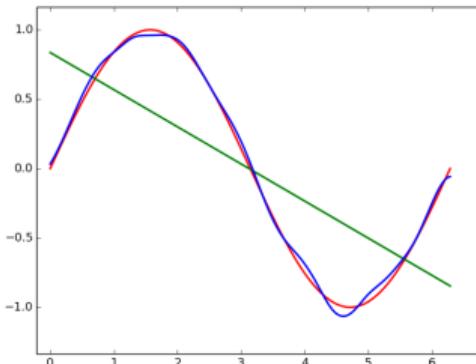
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- Mathematically, this means that the simple model has a high bias



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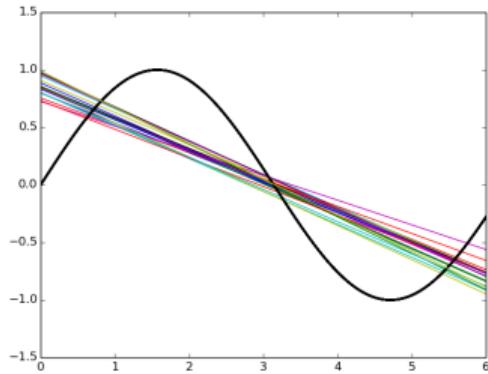
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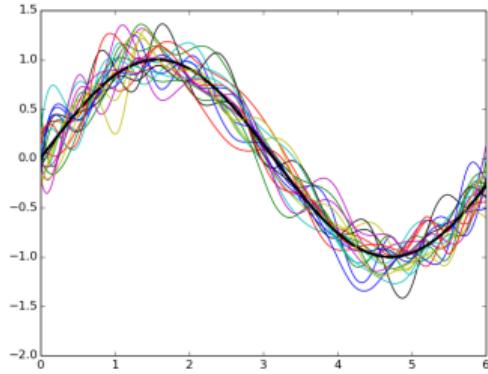
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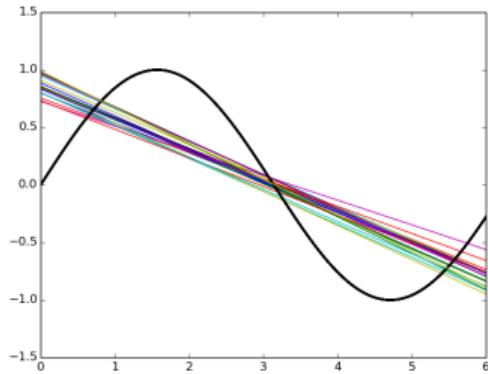
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- On the other hand, the complex model has a low bias



- We now define,

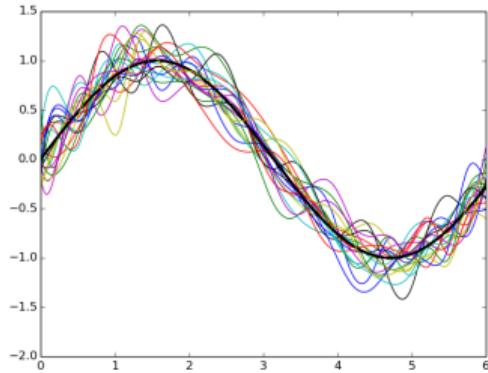
Variance ($\hat{f}(x)$) = $E[(\hat{f}(x) - E[\hat{f}(x)])^2]$
(Standard definition from statistics)



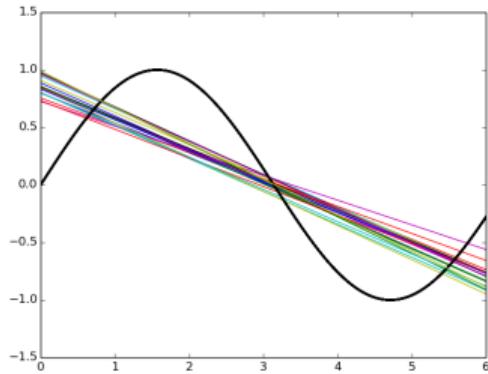


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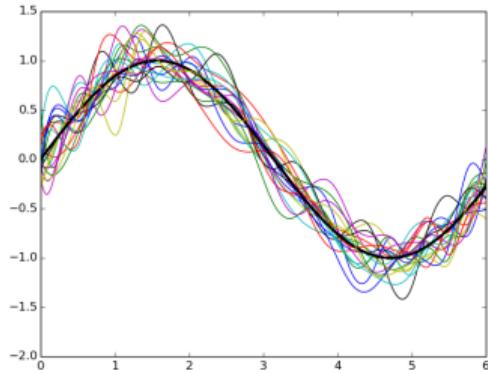


- Roughly speaking it tells us how much the different $\hat{f}(x)$'s (trained on different samples of the data) differ from each other

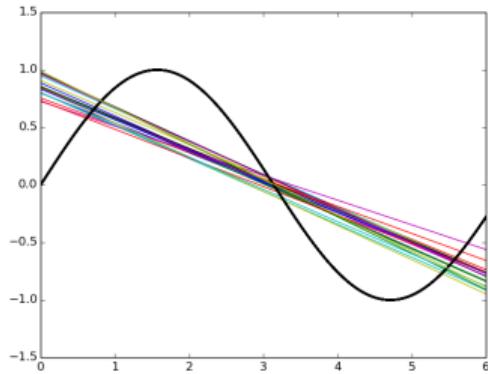


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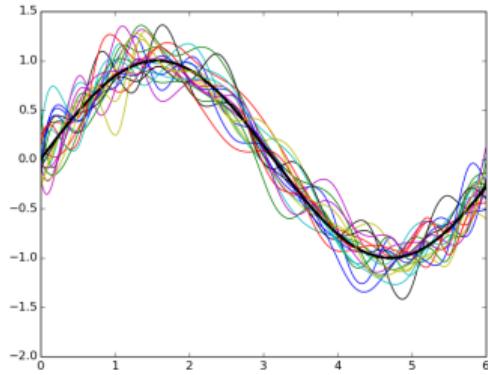
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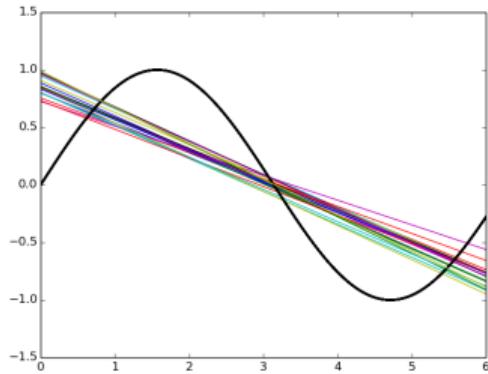


- Roughly speaking it tells us how much the different $\hat{f}(x)$'s (trained on different samples of the data) differ from each other
- It is clear that the simple model has a low variance whereas the complex model has a high variance

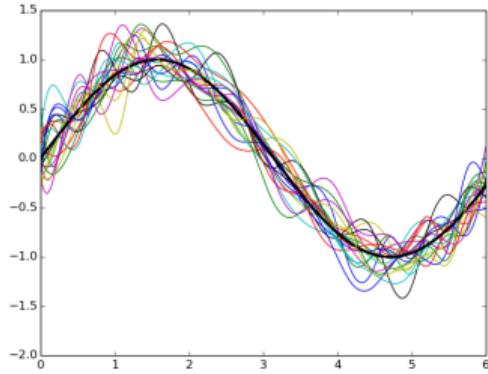


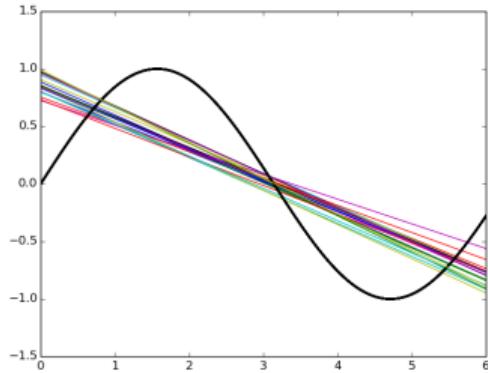
- In summary (informally)



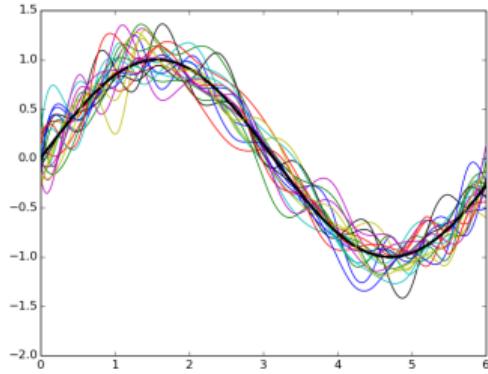


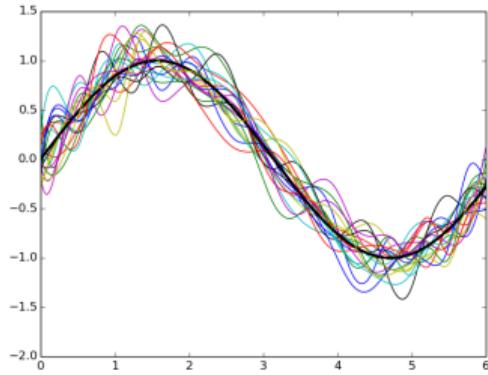
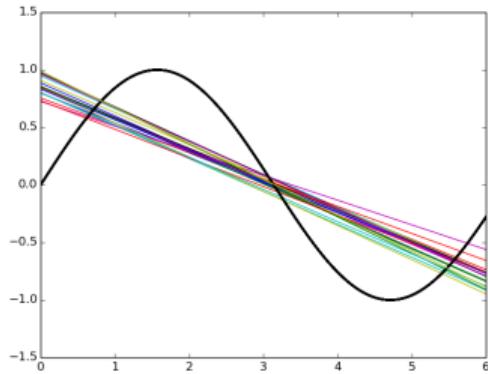
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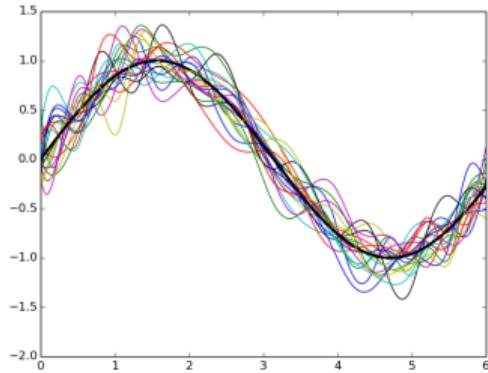
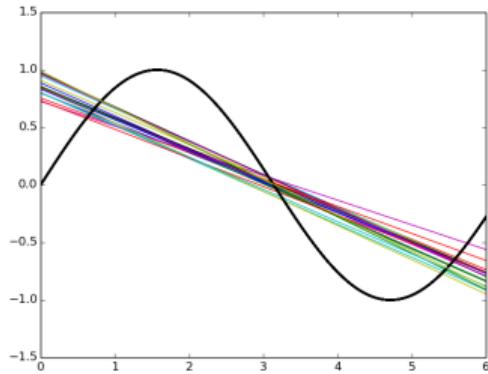


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- There is always a trade-off between the bias and variance
- Both bias and variance contribute to the mean square error. Let us see how

Module 8.2 : Train error vs Test error

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

- We can show that
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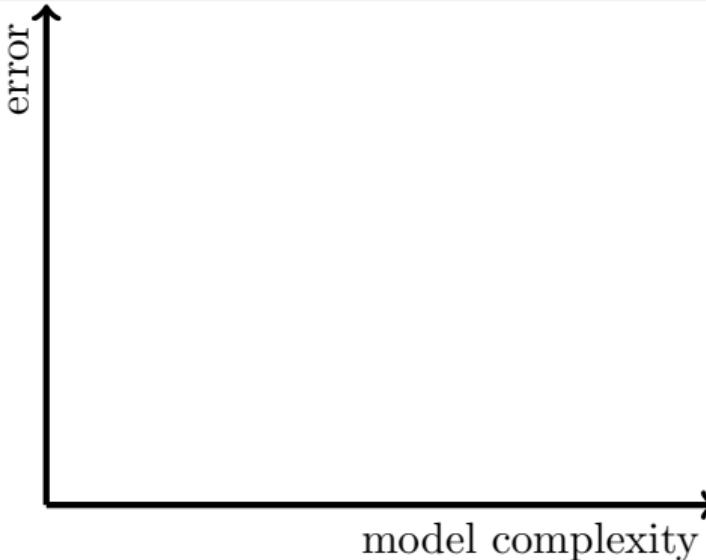
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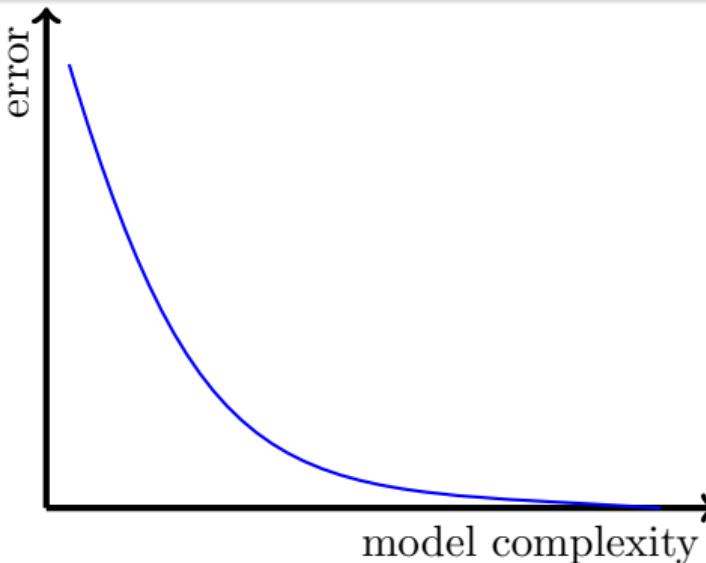
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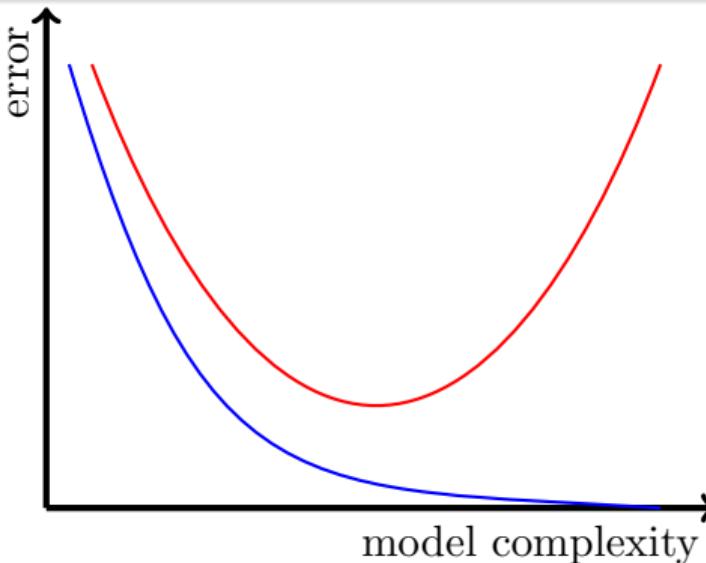
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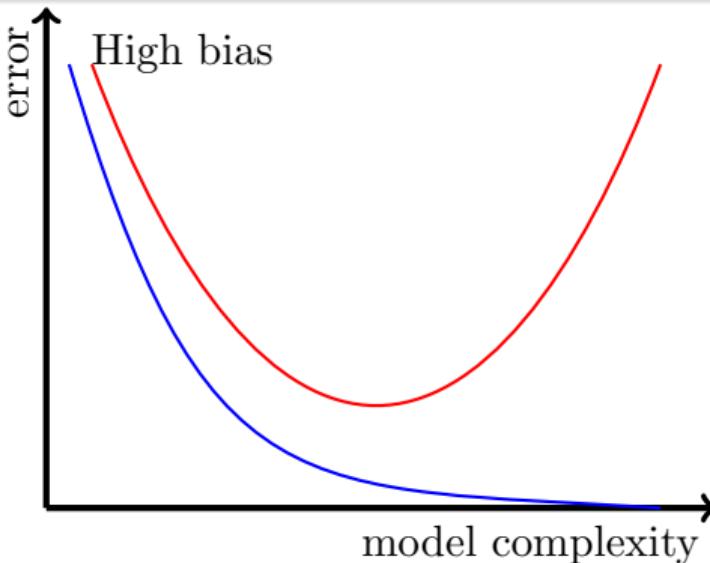
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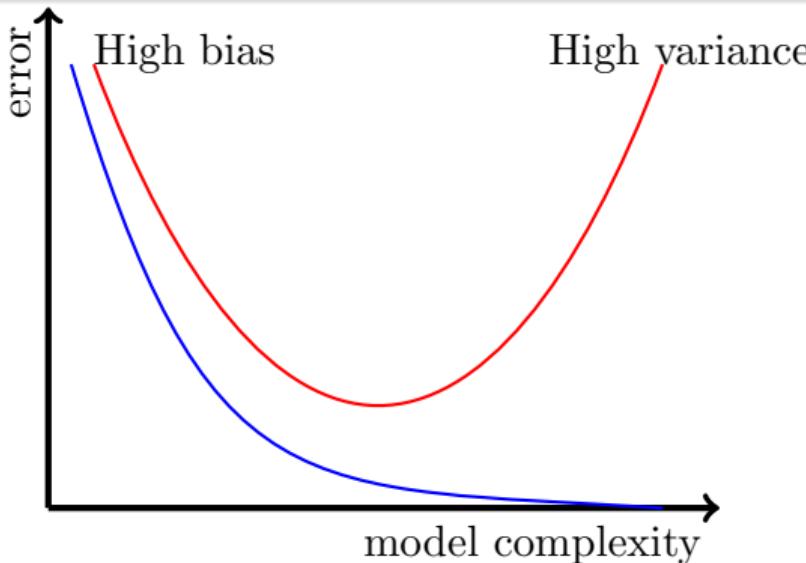
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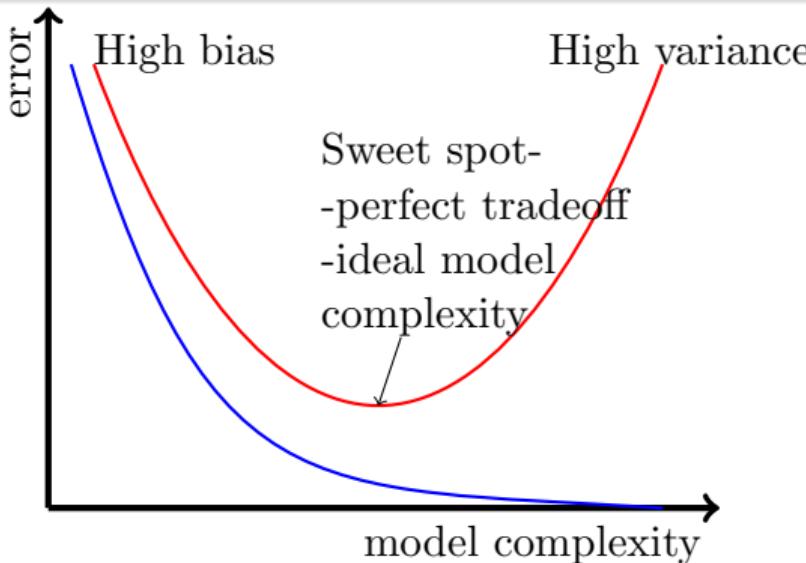
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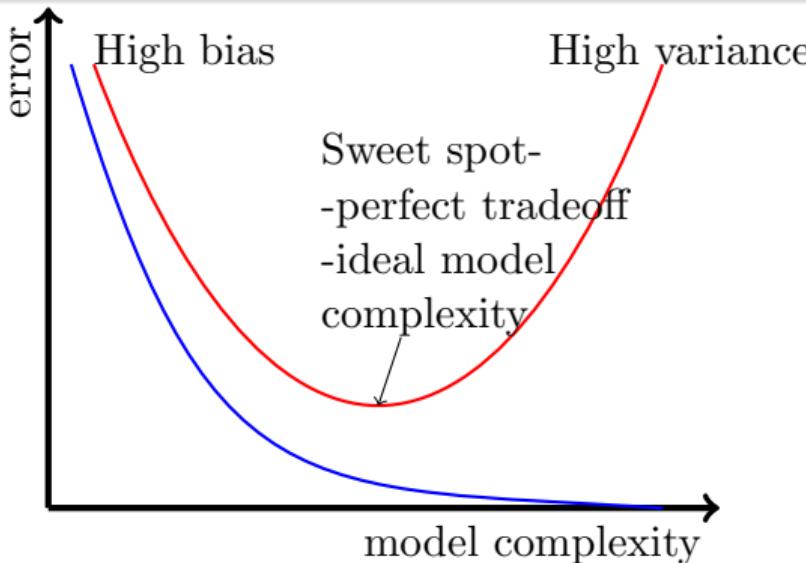
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Intuitions developed so far

- 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

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

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

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

... returning back to our derivation

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

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

Case 1: Using test observations

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

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

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

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$\therefore \text{covariance}(X, Y)$

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

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$$\therefore \text{covariance}(X, Y) = E[(X - \mu_X)(Y - \mu_Y)]$$

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

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

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

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

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

Case 2: Using training observations

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

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

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

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

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

Case 2: Using training observations

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

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

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

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

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

Module 8.3 : True error and Model complexity

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

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

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- When will $\frac{\partial \hat{f}(x_i)}{\partial y_i}$ be high? When a small change in the observation causes a large change in the estimation(\hat{f})

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- When will $\frac{\partial \hat{f}(x_i)}{\partial y_i}$ be high? When a small change in the observation causes a large change in the estimation(\hat{f})
- Can you link this to model complexity?

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

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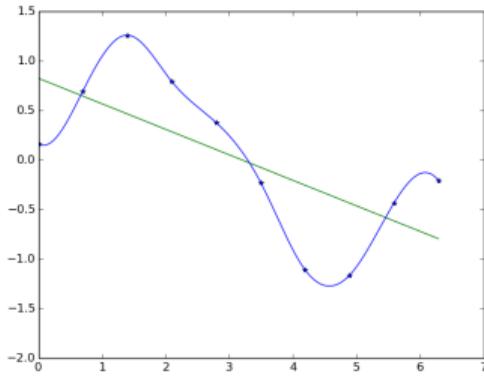
- When will $\frac{\partial \hat{f}(x_i)}{\partial y_i}$ be high? When a small change in the observation causes a large change in the estimation(\hat{f})
- Can you link this to model complexity?
- Yes, indeed a complex model will be more sensitive to changes in observations whereas a simple model will be less sensitive to changes in observations

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

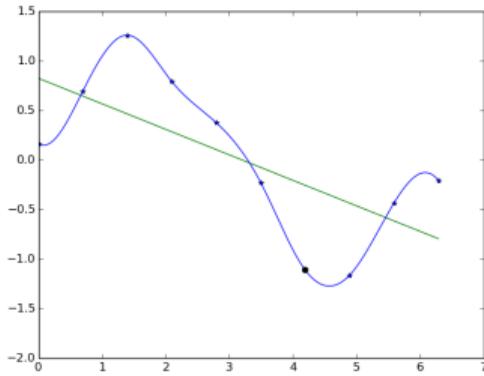
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- Can you link this to model complexity?
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- Hence, we can say that
true error = empirical train error + small constant + $\Omega(\text{model complexity})$

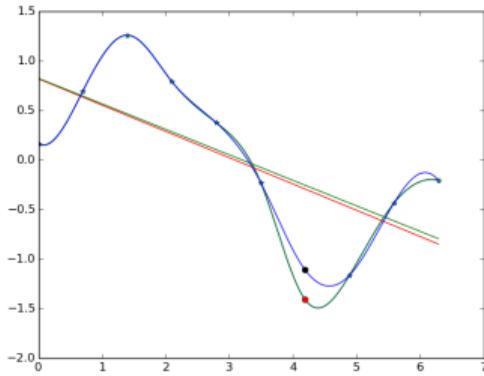
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- Let us verify that indeed a complex model is more sensitive to minor changes in the data
- We have fitted a simple and complex model for some given data
- We now change one of these data points
- The simple model does not change much as compared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

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

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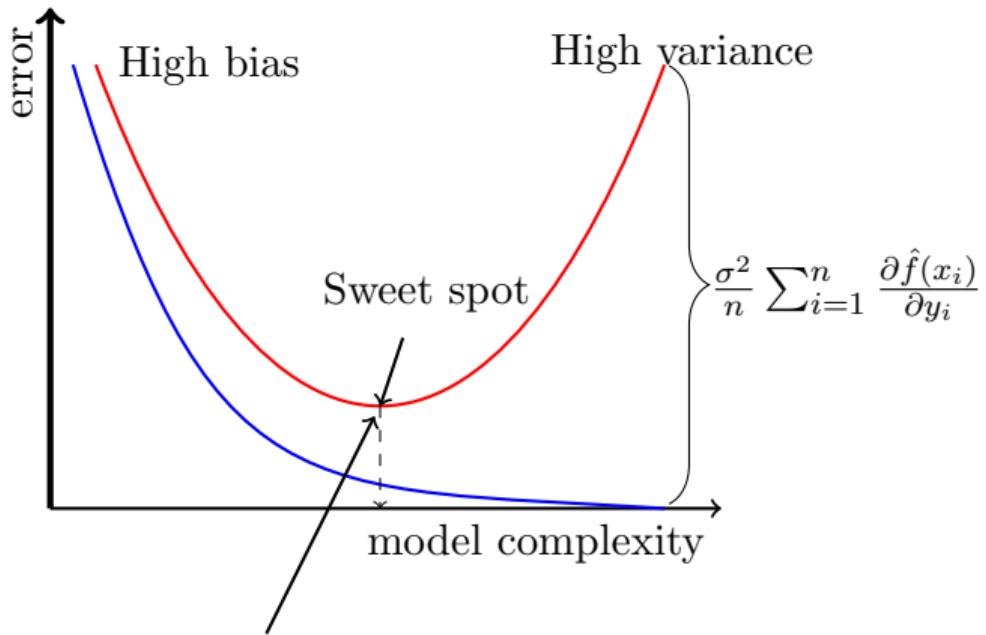
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- This is the basis for all regularization methods
- We can show that l_1 regularization, l_2 regularization, early stopping and injecting noise in input are all instances of this form of regularization.



$\Omega(\theta)$ should ensure
that model has rea-
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- Hence we need some form of regularization.

Different forms of regularization

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Module 8.4 : l_2 regularization

Different forms of regularization

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

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

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$$= QDQ^T w^*$$

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

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

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

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

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

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- So what is happening now?

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

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

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

$$= Q D Q^T w^*$$

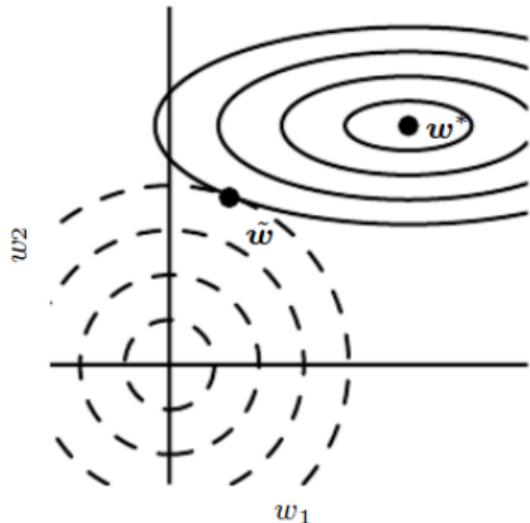
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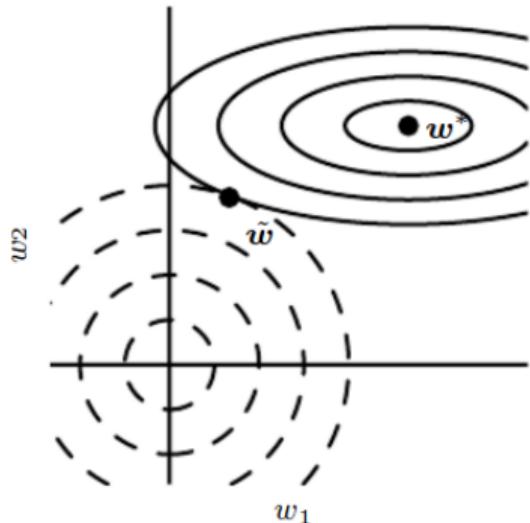
$$D = (\Lambda + \alpha \mathbb{I})^{-1} \Lambda$$

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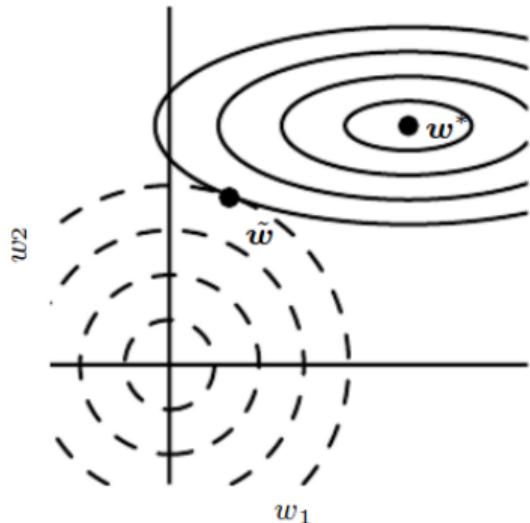
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- if $\lambda_i \gg \alpha$ then $\frac{\lambda_i}{\lambda_i + \alpha} = 1$
- if $\lambda_i \ll \alpha$ then $\frac{\lambda_i}{\lambda_i + \alpha} = 0$
- Thus only significant directions (larger eigen values) will be retained.

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

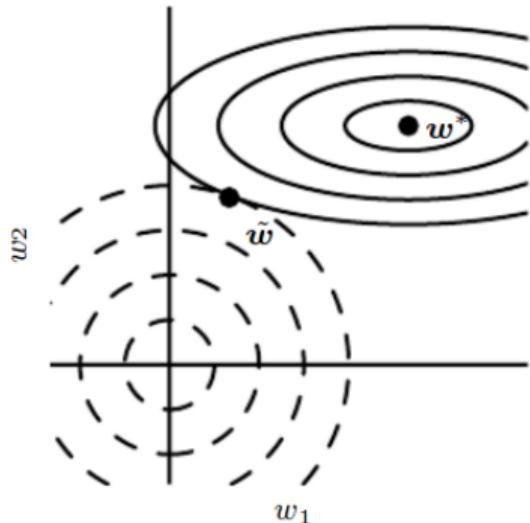




- The weight vector(w^*) is getting rotated to (\tilde{w})



- 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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label = 2



label = 2

[given training data]



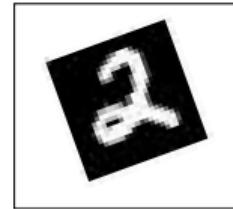
label = 2

[given training data]



label = 2

[given training data]

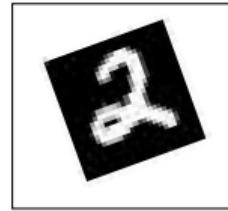


rotated by 20°

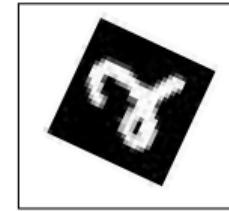


label = 2

[given training data]



rotated by 20°

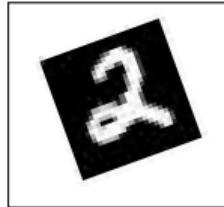


rotated by 65°

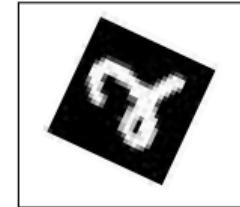


label = 2

[given training data]



rotated by 20°



rotated by 65°



shifted vertically

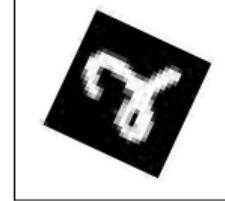


label = 2

[given training data]



rotated by 20°



rotated by 65°



shifted vertically



shifted horizontally

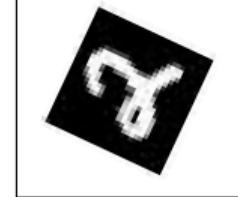


label = 2

[given training data]



rotated by 20°



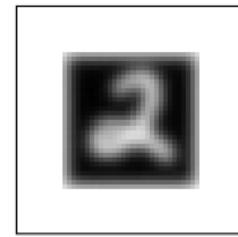
rotated by 65°



shifted vertically



shifted horizontally



blurred

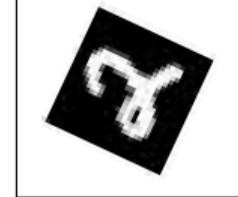


label = 2

[given training data]



rotated by 20°



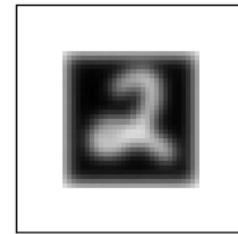
rotated by 65°



shifted vertically



shifted horizontally



blurred



changed some pixels

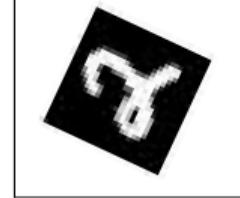


label = 2

[given training data]



rotated by 20°



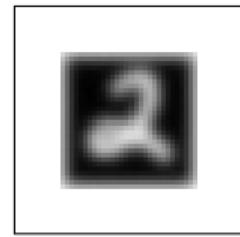
rotated by 65°



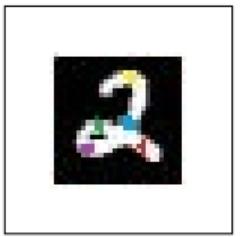
shifted vertically



shifted horizontally



blurred



changed some pixels

label = 2

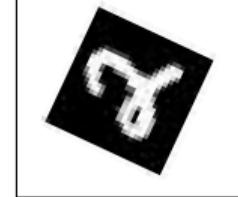


label = 2

[given training data]



rotated by 20°



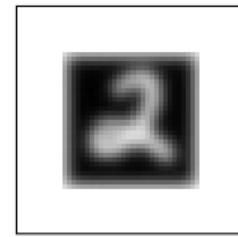
rotated by 65°



shifted vertically



shifted horizontally



blurred



changed some pixels

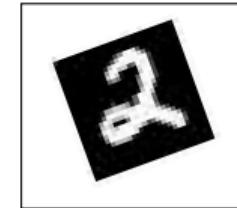
label = 2

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

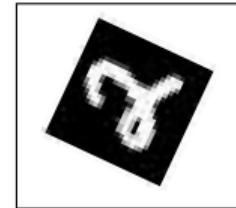


label = 2

[given training data]
We exploit the fact that certain transformations to the image do not change the label of the image.



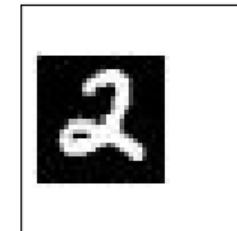
rotated by 20°



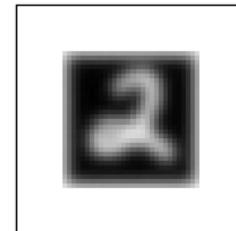
rotated by 65°



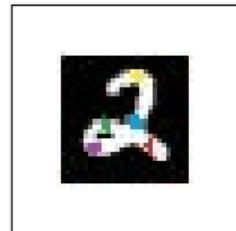
shifted vertically



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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 - Works well for image classification / object recognition tasks

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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

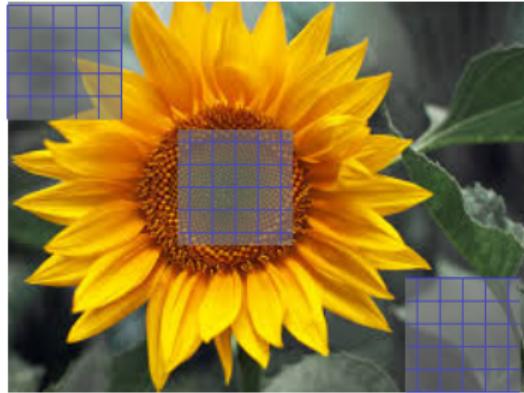
Module 8.6 : Parameter Sharing and tying

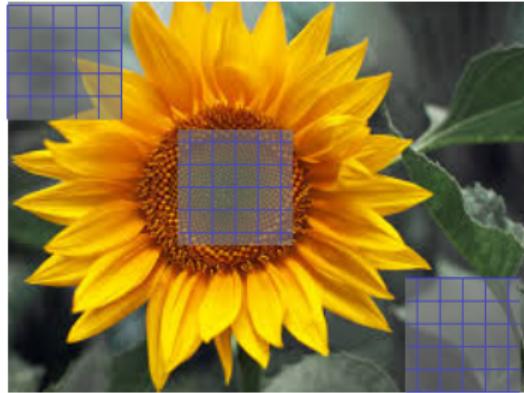
Other forms of regularization

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

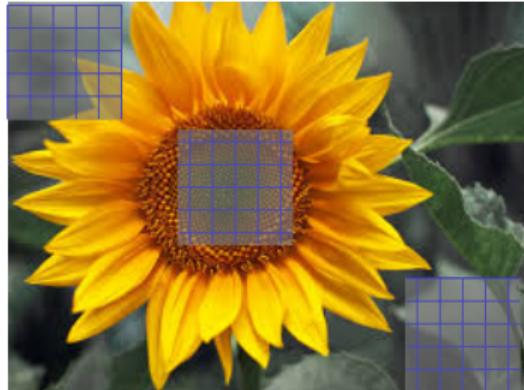
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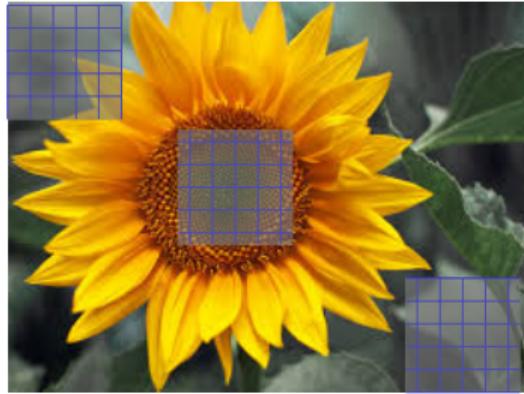


Parameter Sharing



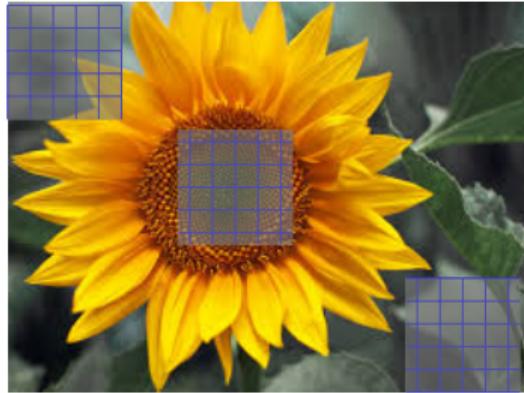
Parameter Sharing

- Used in CNNs



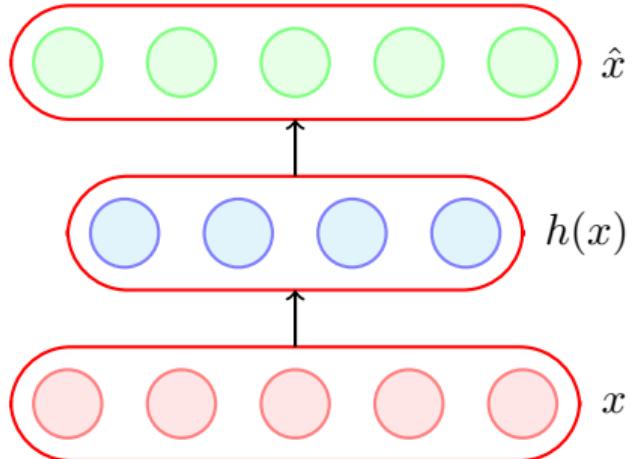
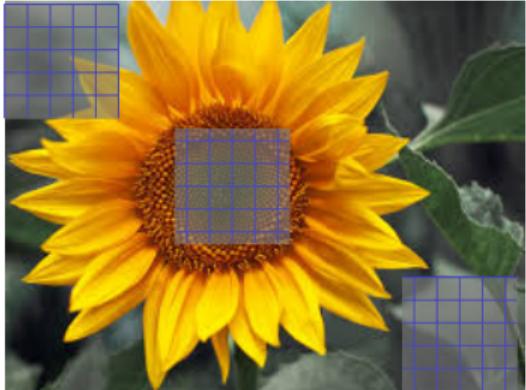
Parameter Sharing

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



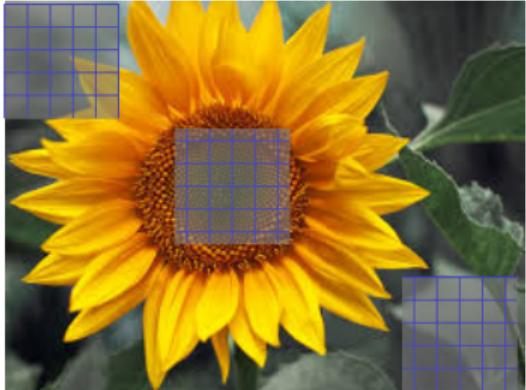
Parameter Sharing

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



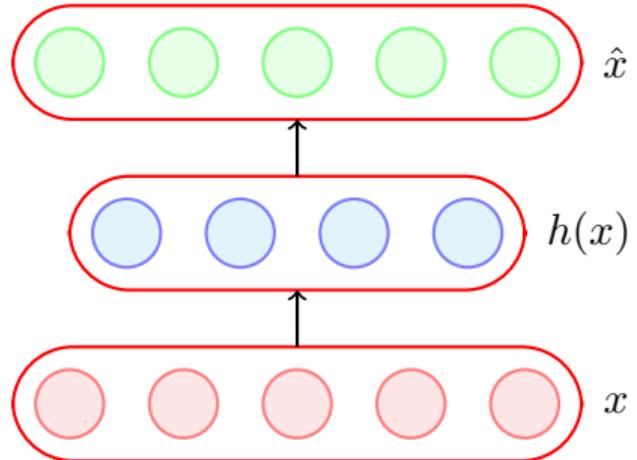
Parameter Sharing

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

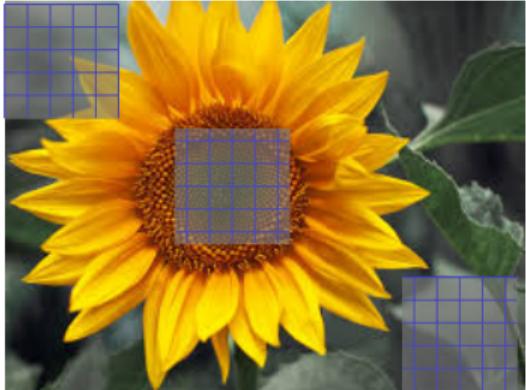


Parameter Sharing

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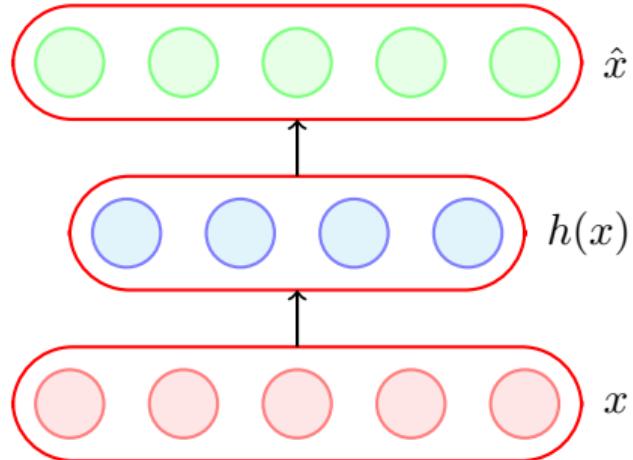


Parameter Tying



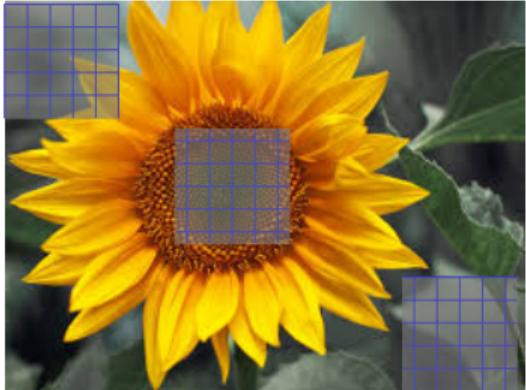
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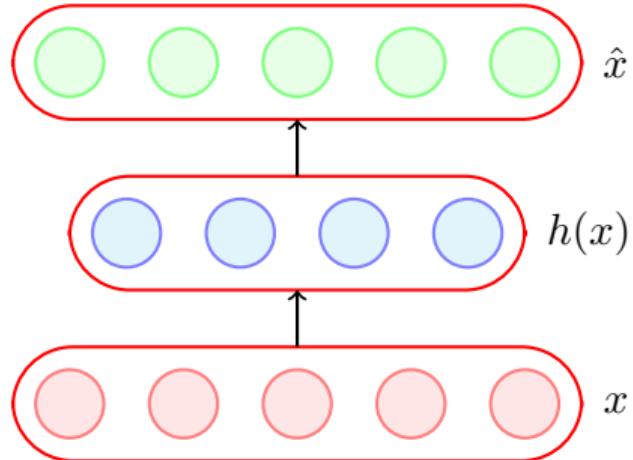
Parameter Tying

- 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.

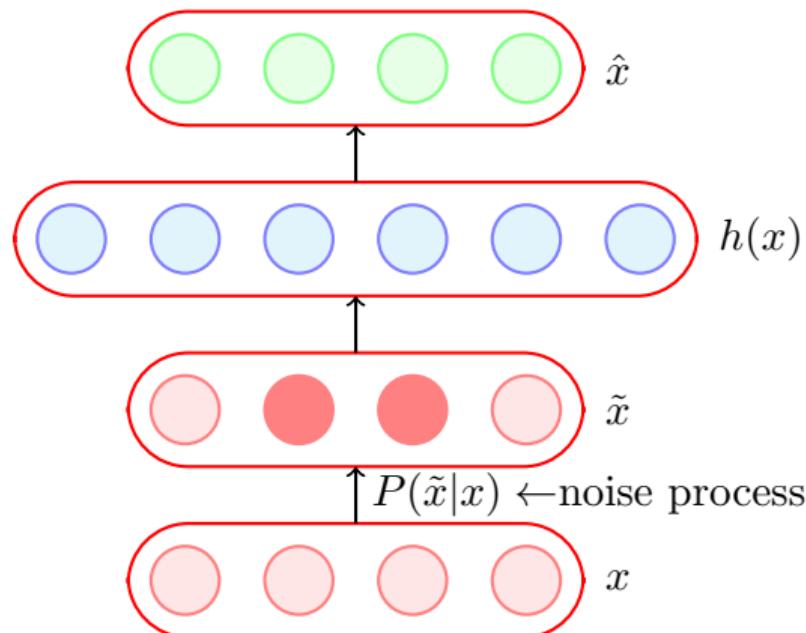
Module 8.7 : Adding Noise to the inputs

Other forms of regularization

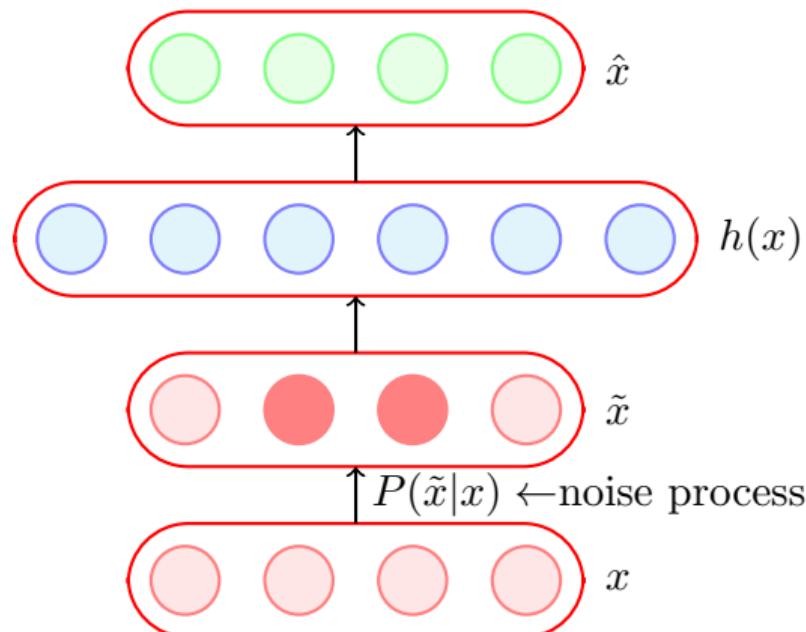
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Other forms of regularization

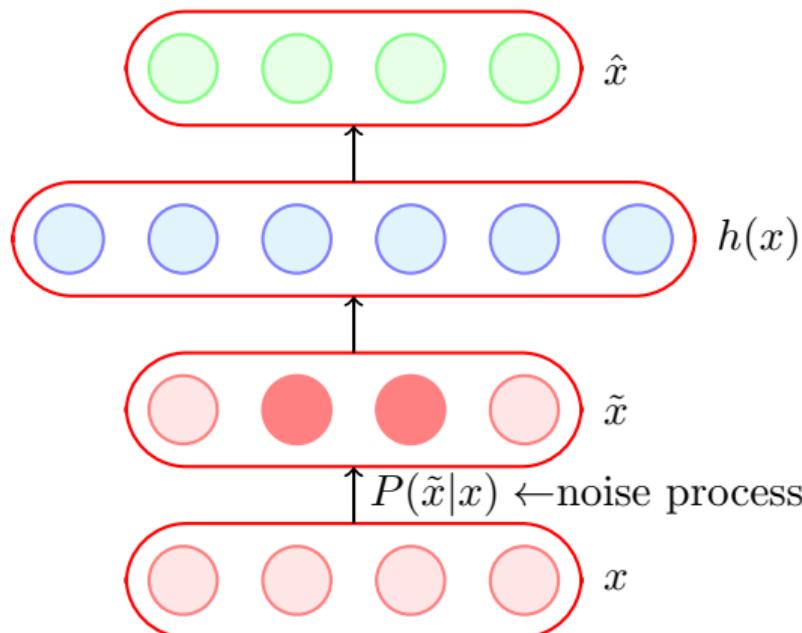
- l_2 regularization
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- Dropout



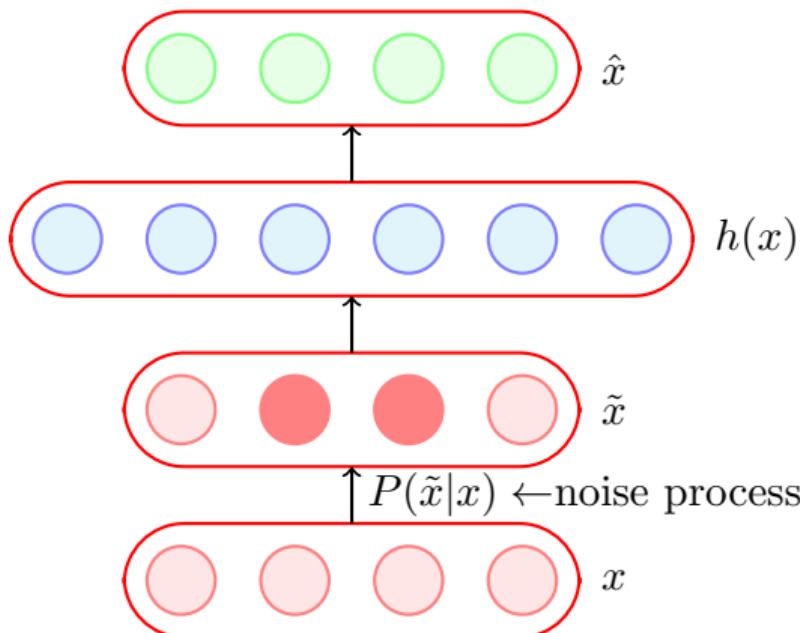
- We saw this in Autoencoder

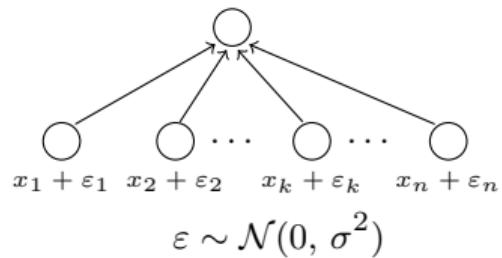


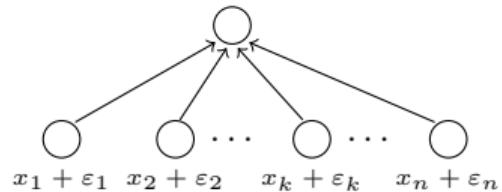
- We saw this in Autoencoder
- We can show that for a simple input output neural network, adding Gaussian noise to the input is equivalent to weight decay (L_2 regularisation)



- 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

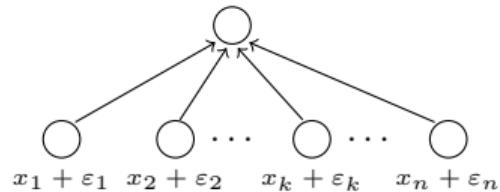






$$\varepsilon \sim \mathcal{N}(0, \sigma^2)$$

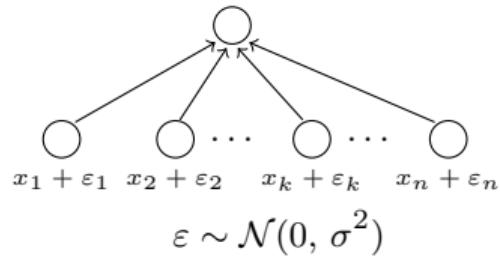
$$\tilde{x}_i = x_i + \varepsilon_i$$



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

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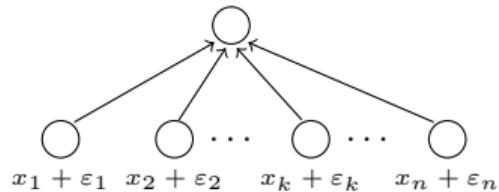
$$\hat{y} = \sum_{i=1}^n w_i x_i$$



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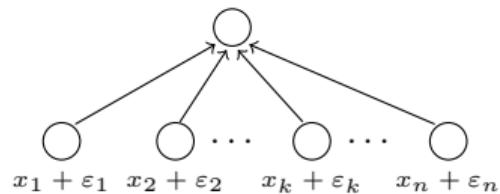
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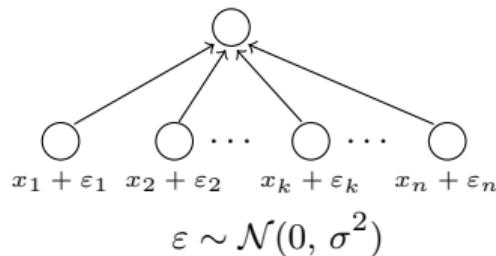
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We are interested in $E[(\tilde{y} - y)^2]$



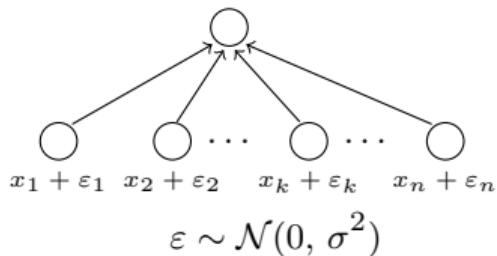
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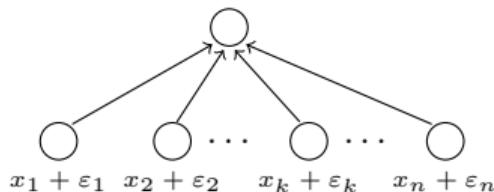
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$$E[(\tilde{y} - y)^2] = E \left[\left(\hat{y} + \sum_{i=1}^n w_i \varepsilon_i - y \right)^2 \right]$$



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

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

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

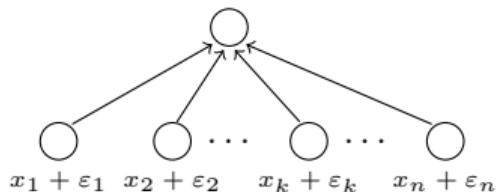
$$\tilde{y} = \sum_{i=1}^n w_i \tilde{x}_i$$

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

$$\begin{aligned} E[(\tilde{y} - y)^2] &= E \left[\left(\hat{y} + \sum_{i=1}^n w_i \varepsilon_i - y \right)^2 \right] \\ &= E \left[\left((\hat{y} - y) + \left(\sum_{i=1}^n w_i \varepsilon_i \right) \right)^2 \right] \end{aligned}$$



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

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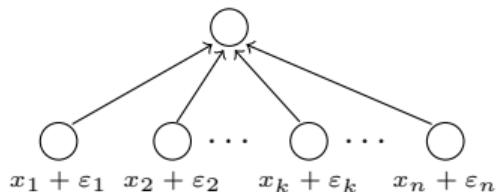
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$$= E[(\hat{y} - y)^2] + E \left[2(\hat{y} - y) \sum_{i=1}^n w_i \varepsilon_i \right] + E \left[\left(\sum_{i=1}^n w_i \varepsilon_i \right)^2 \right]$$



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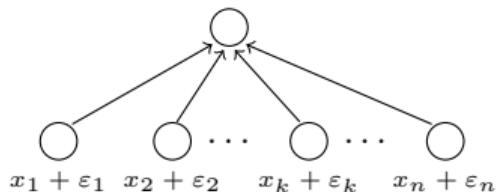
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$$= E[(\hat{y} - y)^2] + 0 + E \left[\sum_{i=1}^n w_i^2 \varepsilon_i^2 \right]$$

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



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

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

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

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

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



0	0	1	0	0	0	0	0	0	0
---	---	---	---	---	---	---	---	---	---

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

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estimated distribution : q



0	0	1	0	0	0	0	0	0	0
---	---	---	---	---	---	---	---	---	---

Hard targets

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

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estimated distribution : q

Intuition

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



0	0	1	0	0	0	0	0	0	0
---	---	---	---	---	---	---	---	---	---

Hard targets

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

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

estimated distribution : q

Intuition

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



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

Soft targets



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

Soft targets

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



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

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

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



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

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

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

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



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

Soft targets

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

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

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estimated distribution : q

Module 8.9 : Early stopping

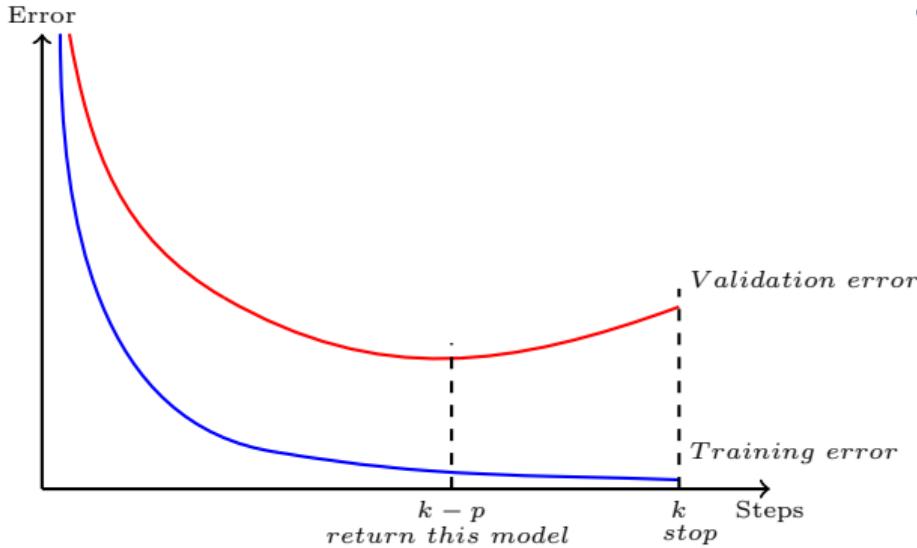
Other forms of regularization

- l_2 regularization
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- Adding Noise to the inputs
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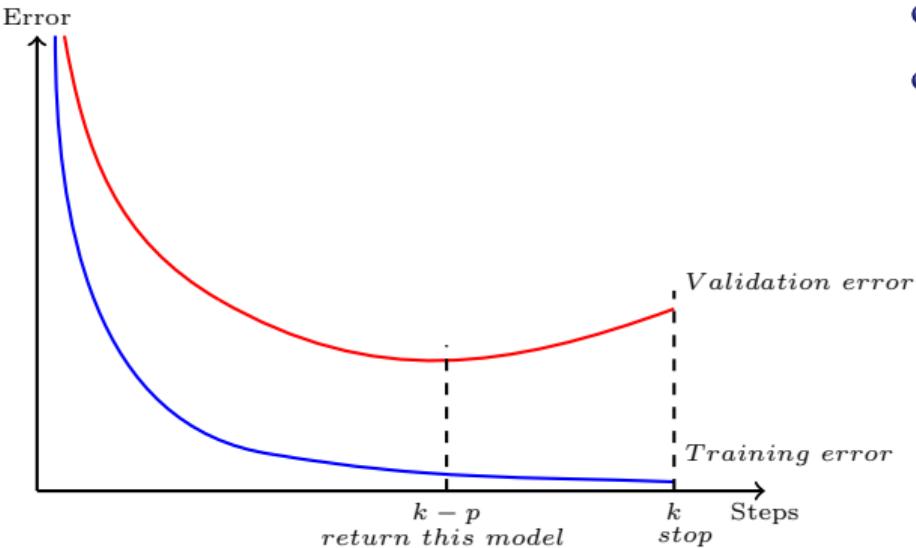
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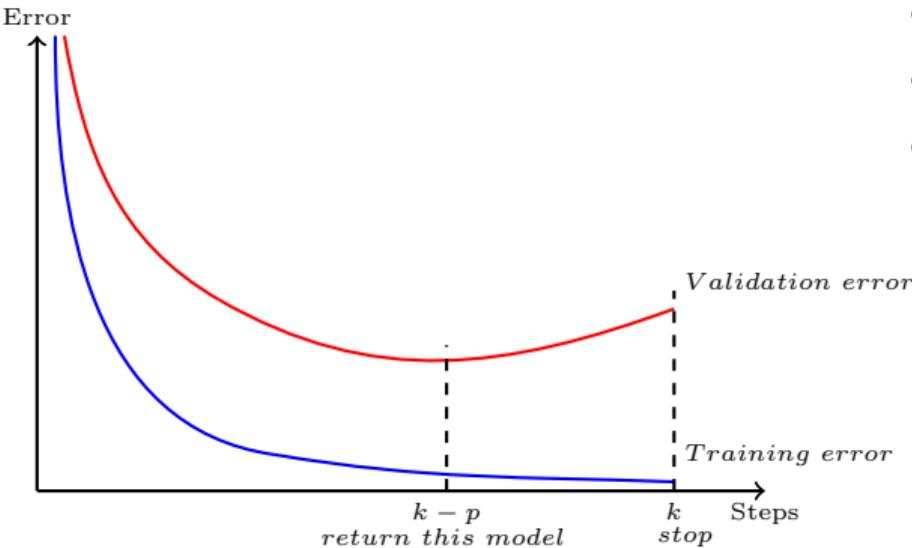
- l_2 regularization
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- Track the validation error

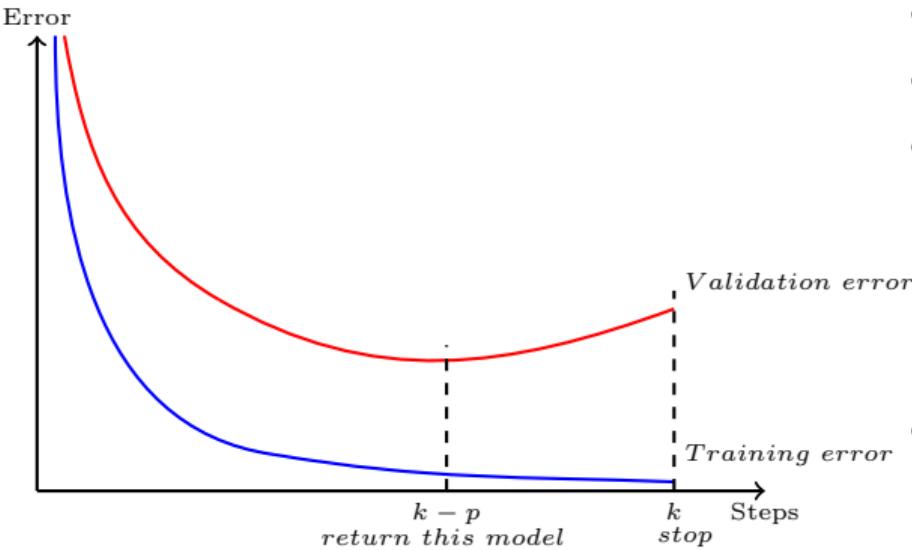


- Track the validation error
- Have a patience parameter p



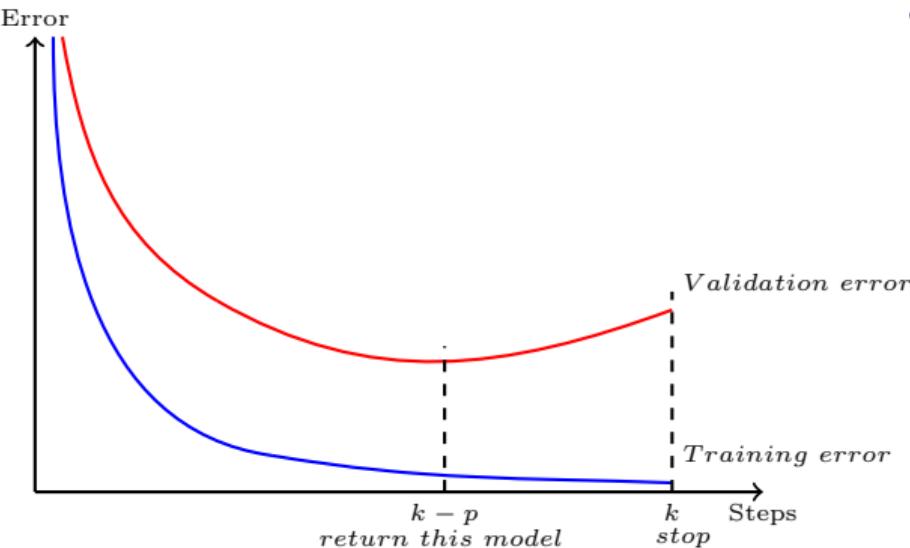


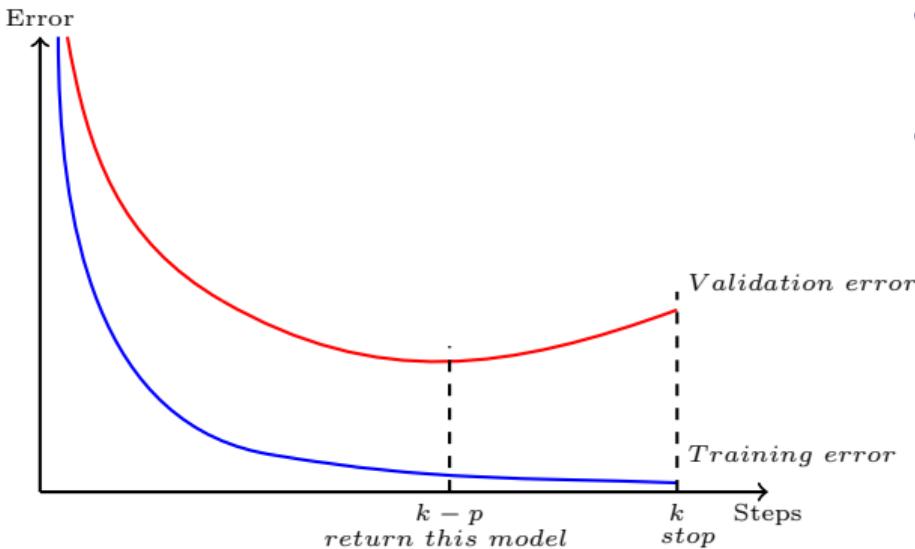
- Track the validation error
- Have a patience parameter p
- If you are at step k and there was no improvement in validation error in the previous p steps then stop training and return the model stored at step $k - p$



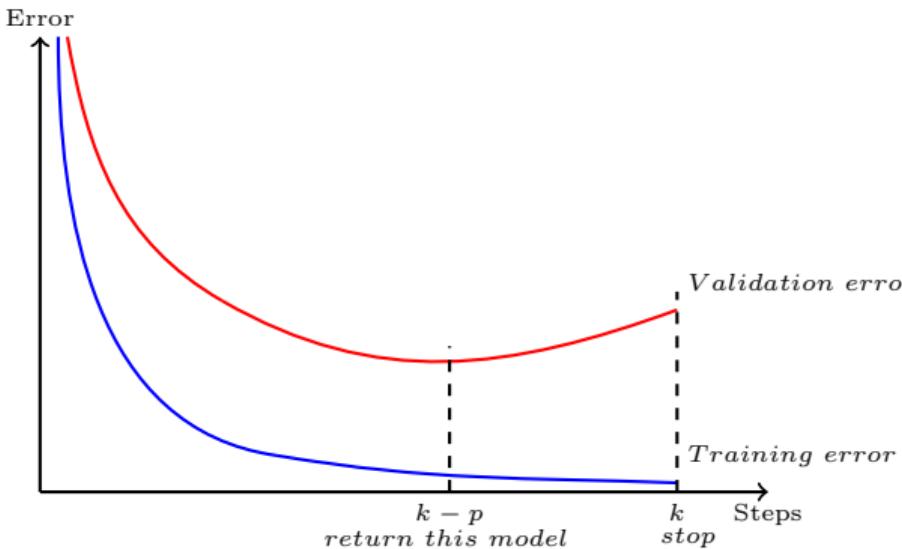
- Track the validation error
- Have a patience parameter p
- If you are at step k and there was no improvement in validation error in the previous p steps then stop training and return the model stored at step $k - p$
- Basically, stop the training early before it drives the training error to 0 and blows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

- Very effective and the mostly widely used form of regularization

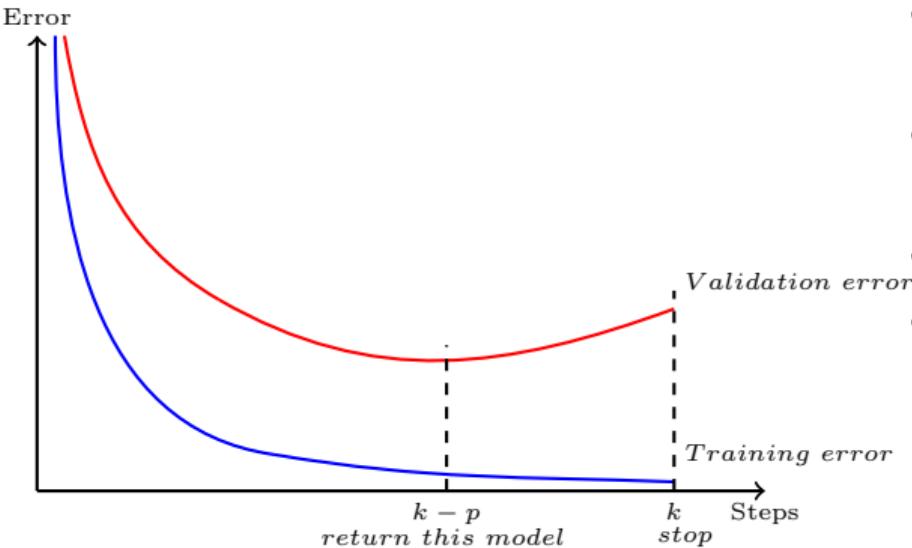




- Very effective and the mostly widely used form of regularization
- Can be used even with other regularizers (such as l_2)

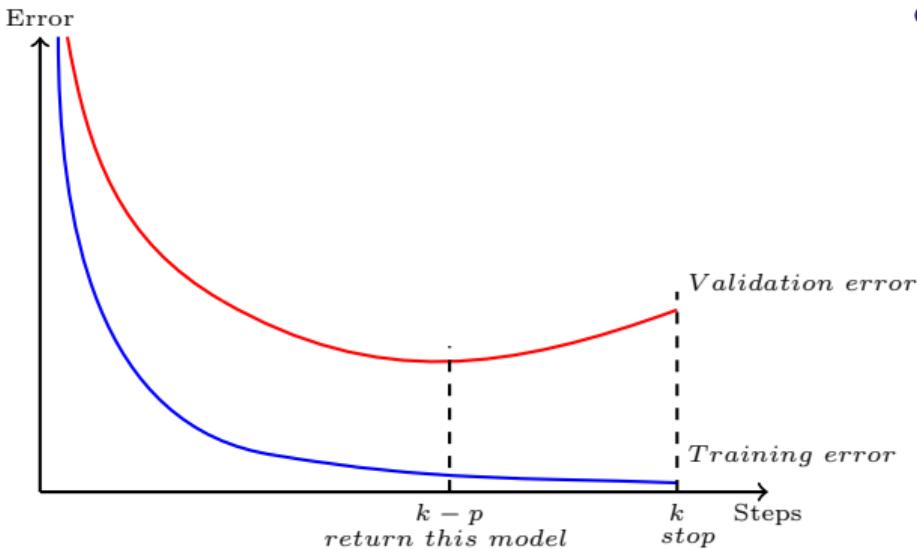


- Very effective and the mostly widely used form of regularization
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- How does it act as a regularizer ?



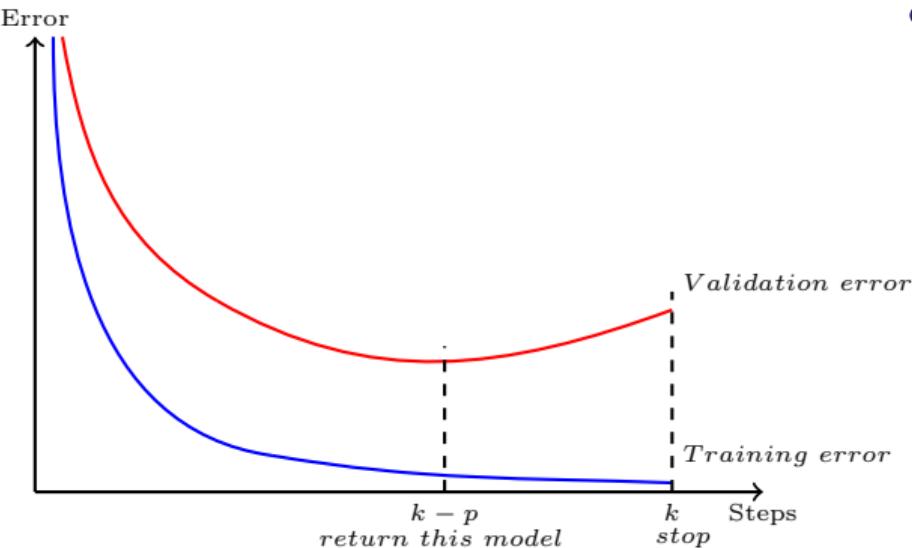
- Very effective and the mostly widely used form of regularization
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- How does it act as a regularizer ?
- We will first see an intuitive explanation and then a mathematical analysis

- Recall that the update rule in SGD is



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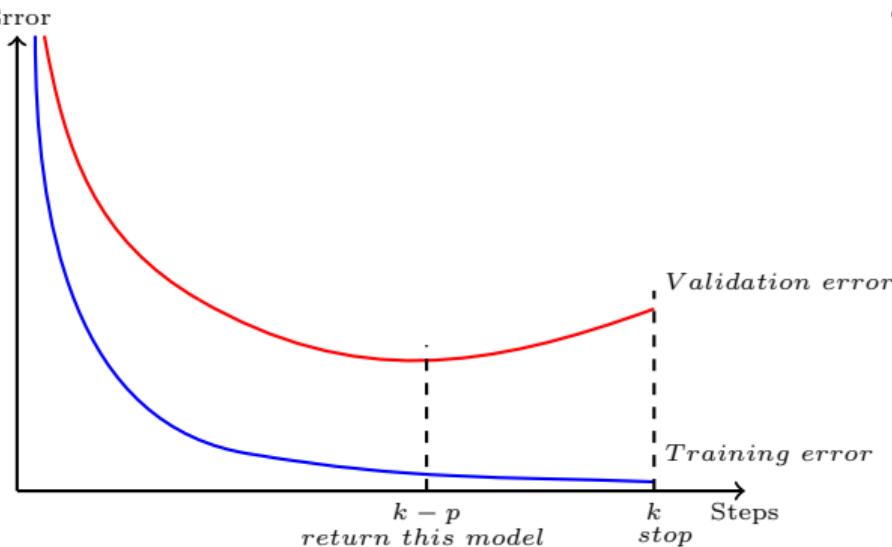
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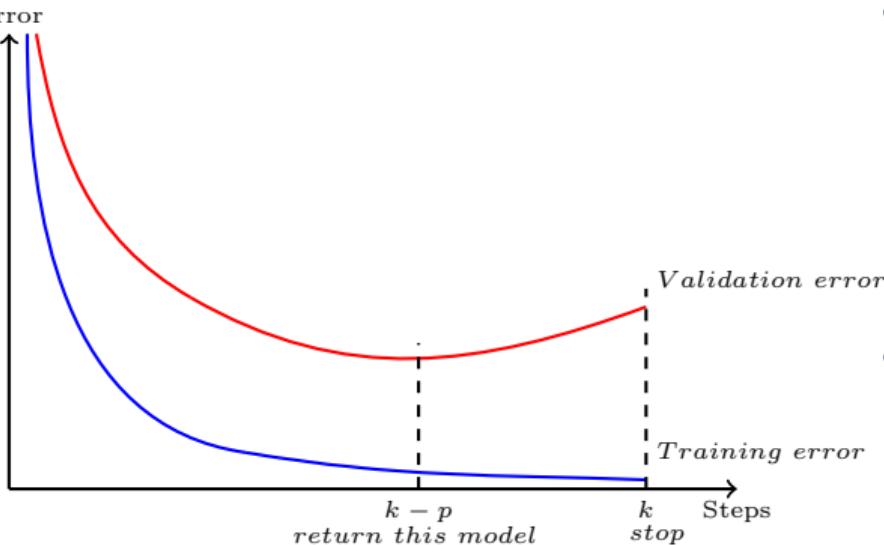
Error

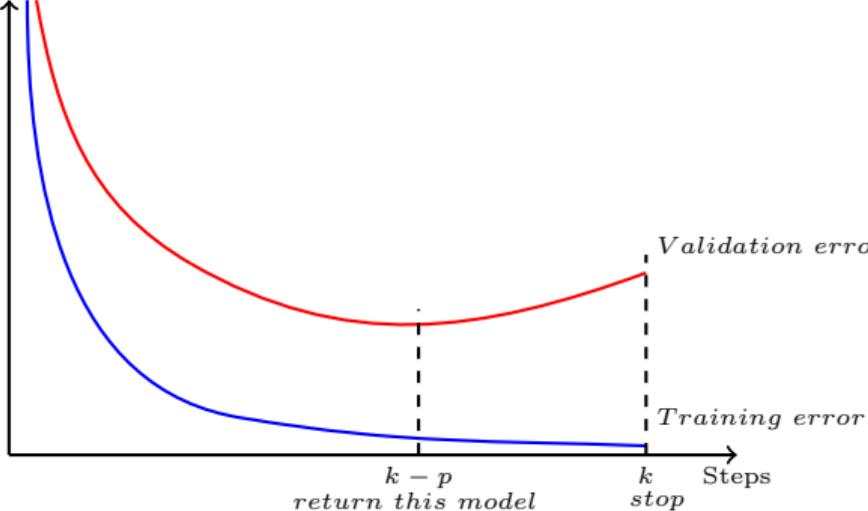
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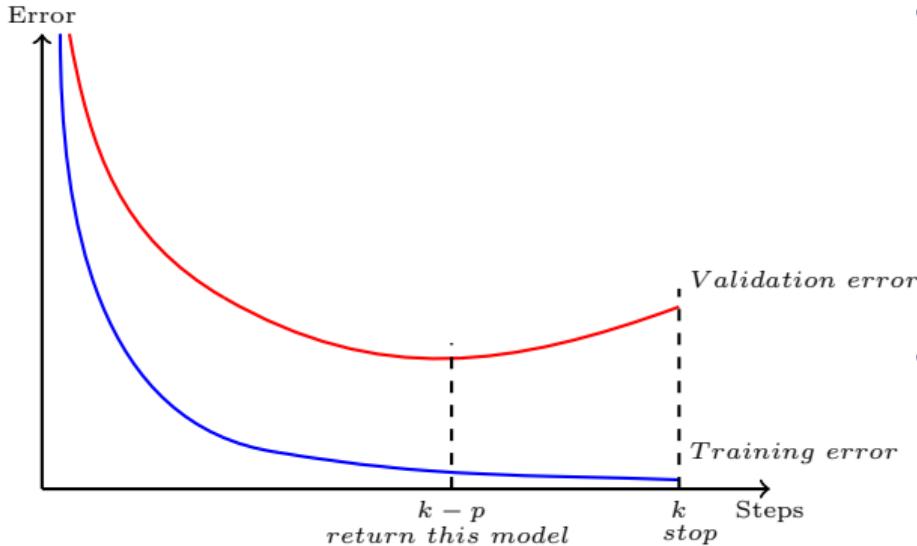
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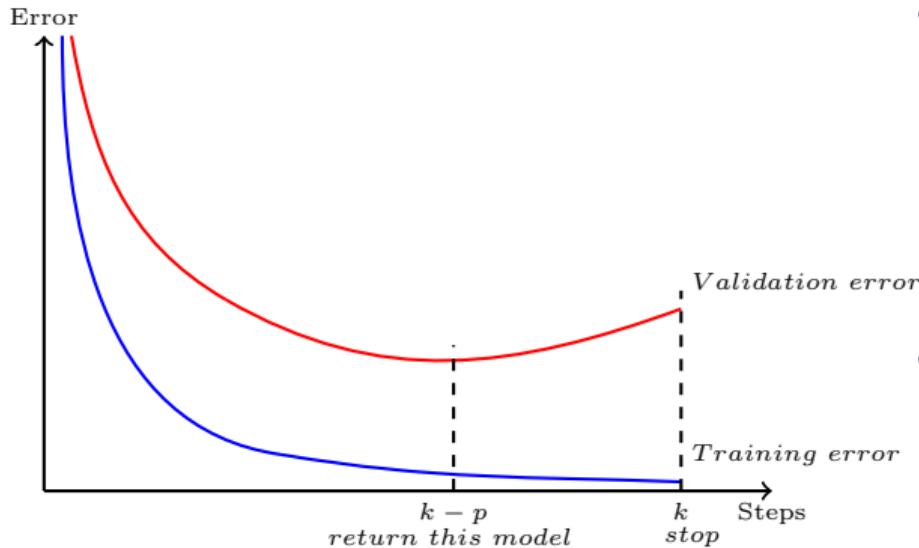
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- Let τ be the maximum value of $\nabla \omega_i$ then

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

- 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 $L(\omega)$ is

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

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

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

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

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$$\begin{aligned}\omega_t &= \omega_{t-1} + \eta \nabla L(\omega_{t-1}) \\ &= \omega_{t-1} + \eta H(\omega_{t-1} - \omega^*)\end{aligned}$$

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

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

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- If we start with $\omega_0 = 0$ then we can show that (See Appendix)

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

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

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

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

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

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- If we start with $\omega_0 = 0$ then we can show that (See Appendix)

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

- 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

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

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

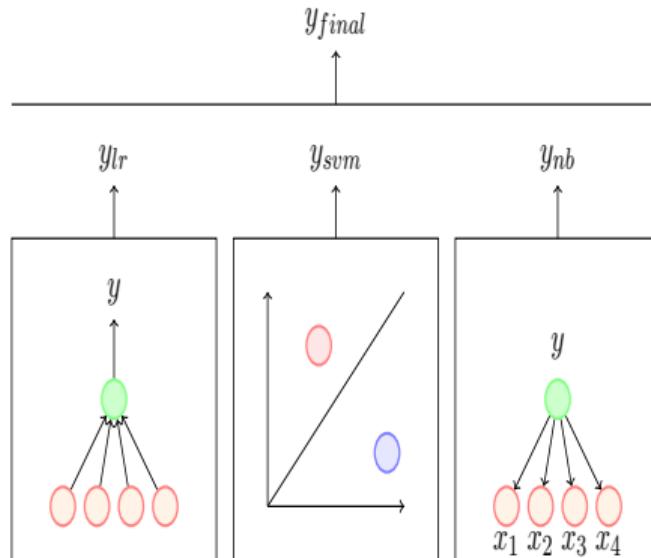
Module 8.10 : Ensemble methods

Other forms of regularization

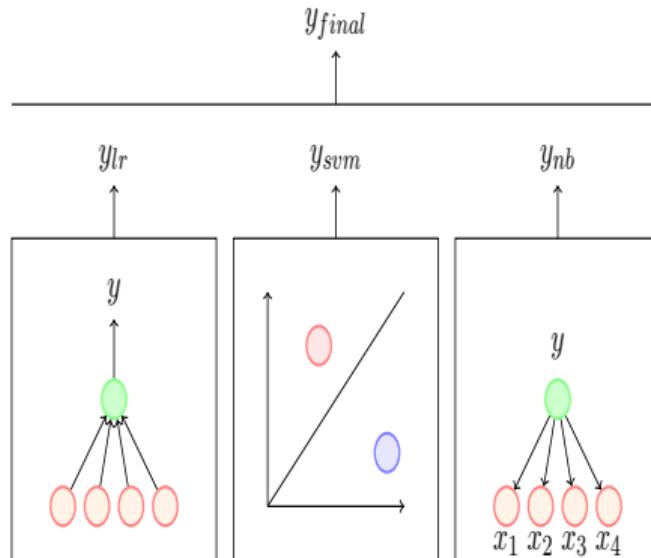
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- Ensemble methods
- Dropout

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- **Ensemble methods**
- Dropout



- Combine the output of different models to reduce generalization error

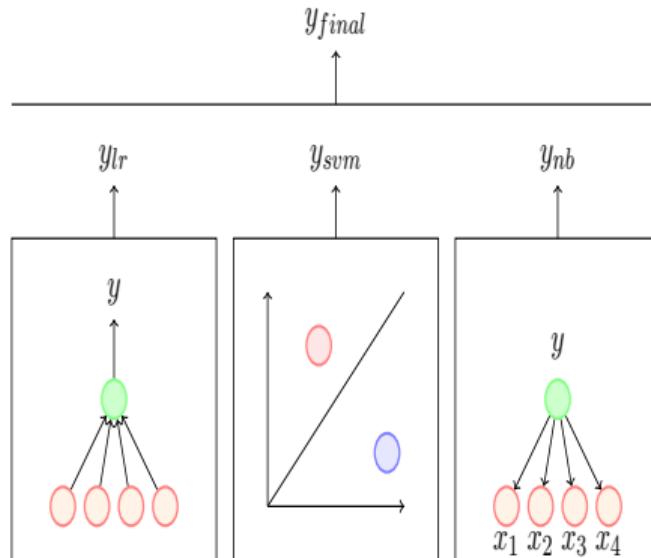


Logistic Regression

SVM

Naive Bayes

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

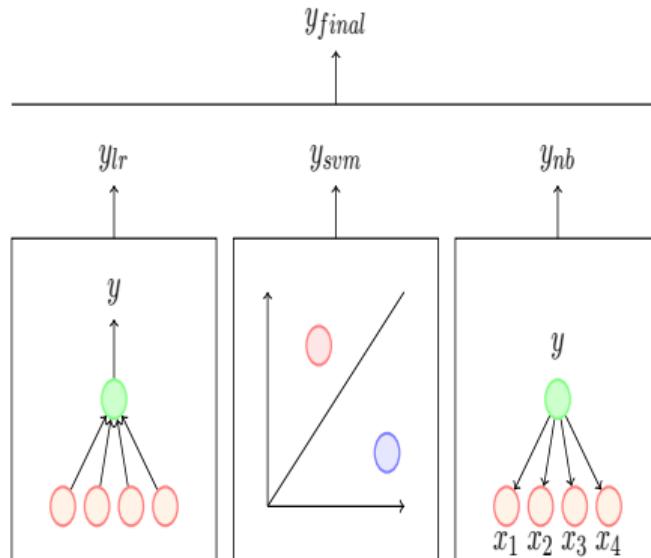


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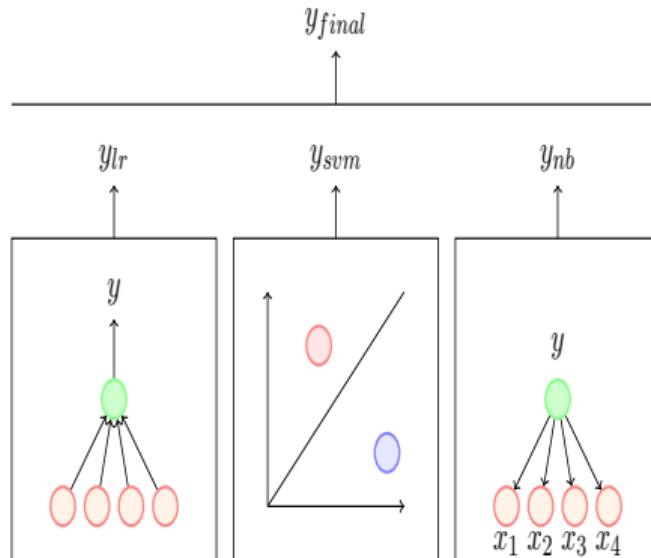


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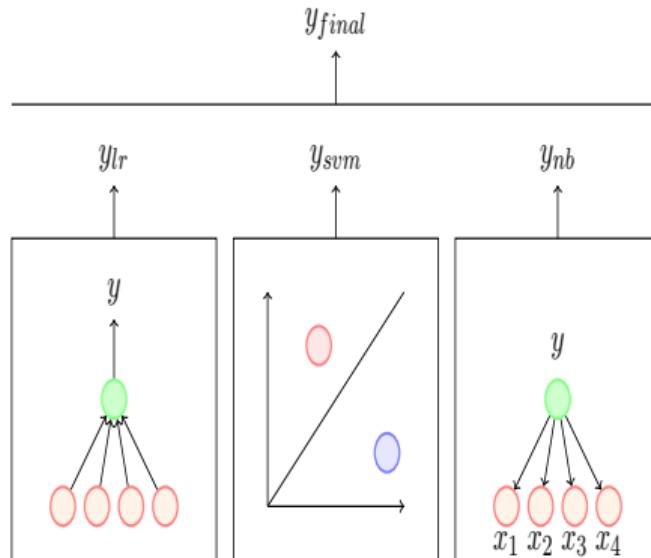


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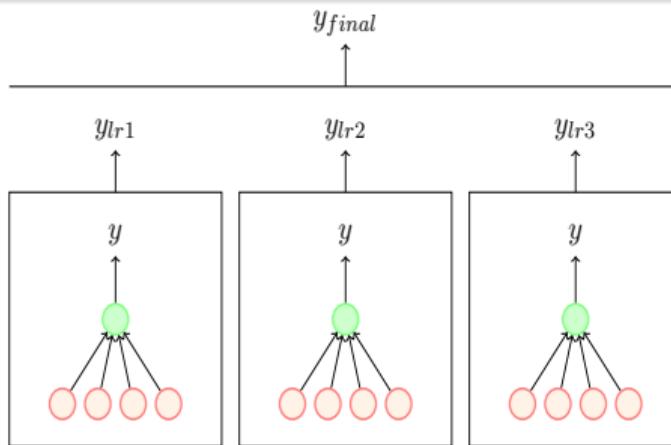


Logistic Regression

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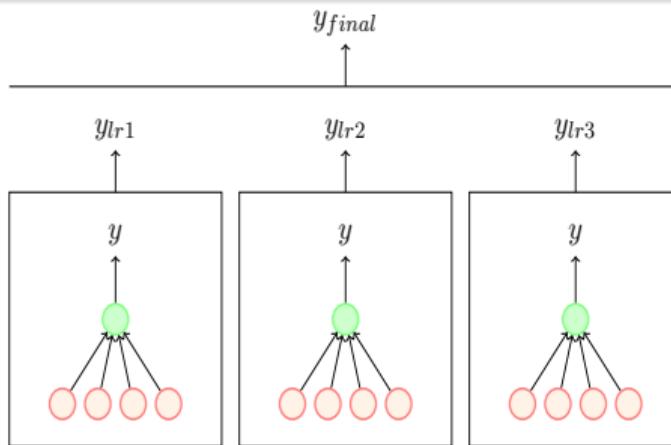
- Combine the output of different models to reduce generalization error
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 - different features
 - different samples of the training data



*Logistic
Regression*

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Regression*

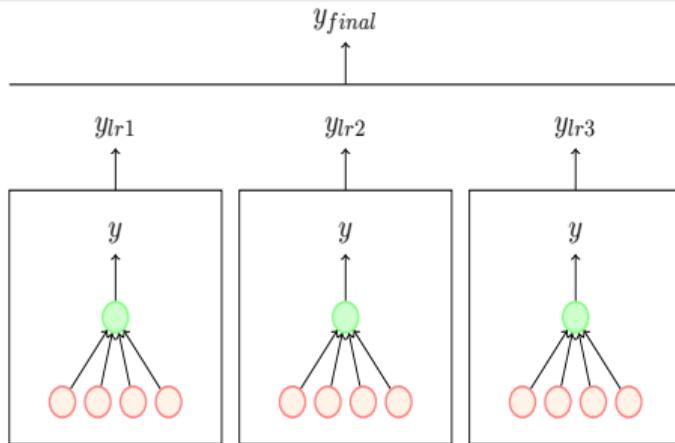
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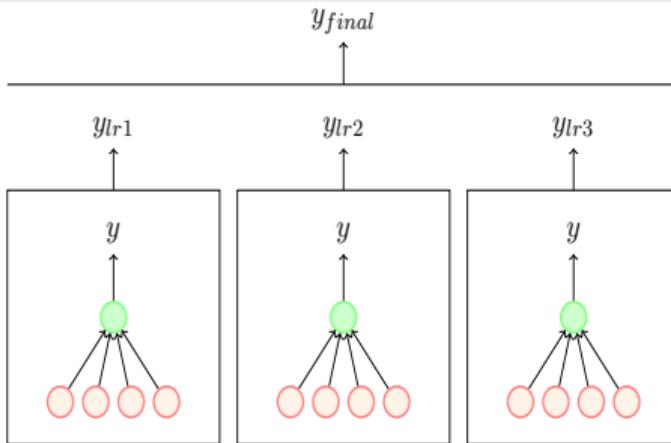


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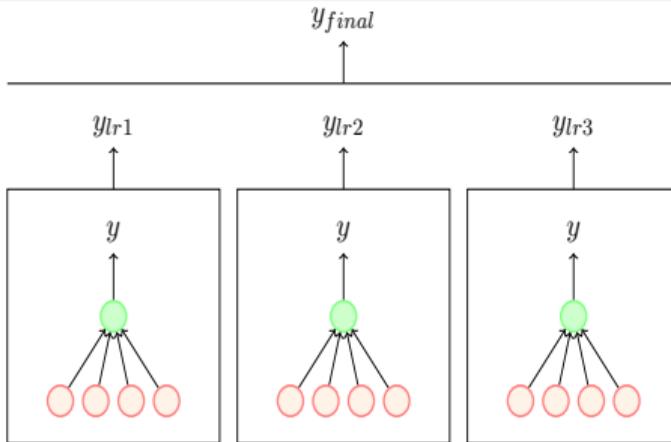
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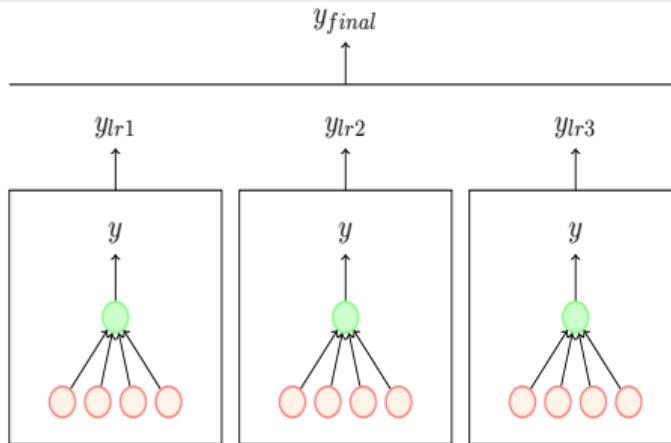
- Bagging: form an ensemble using different instances of the same classifier



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*Logistic
Regression*

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

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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 $\frac{1}{k}V$

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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

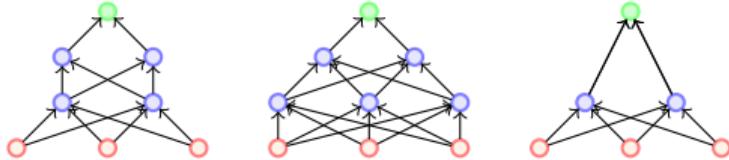
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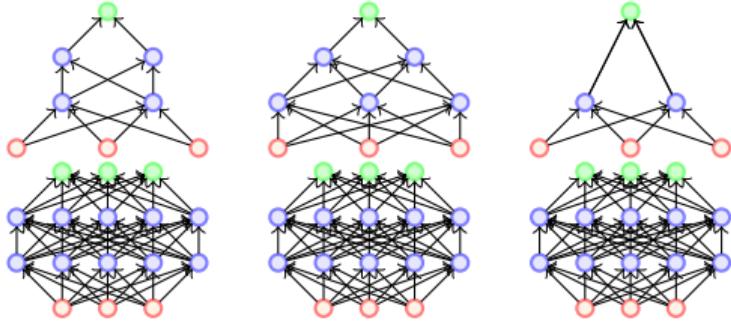
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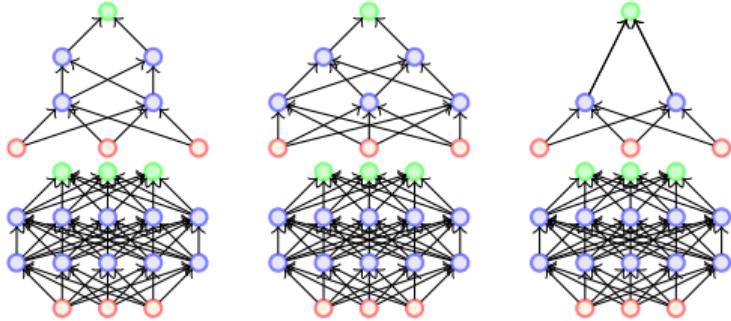
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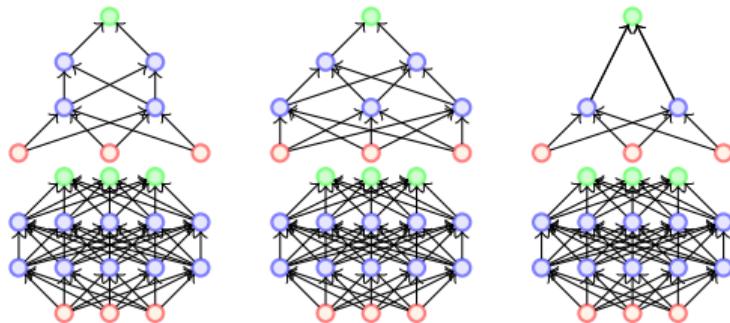


- Typically model averaging(bagging ensemble) always helps
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- Option 1: Train several neural networks having different architectures(obviously expensive)
- Option 2: Train multiple instances of the same network using different training samples (again expensive)

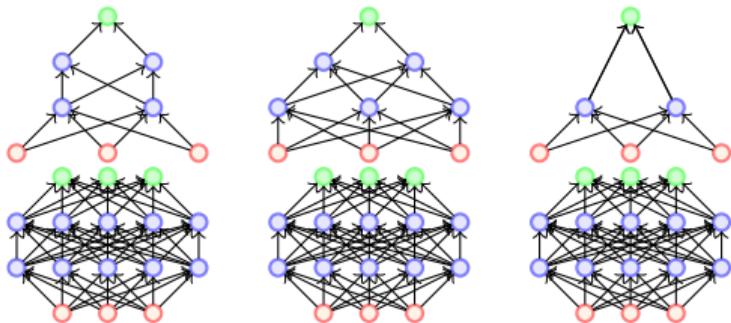


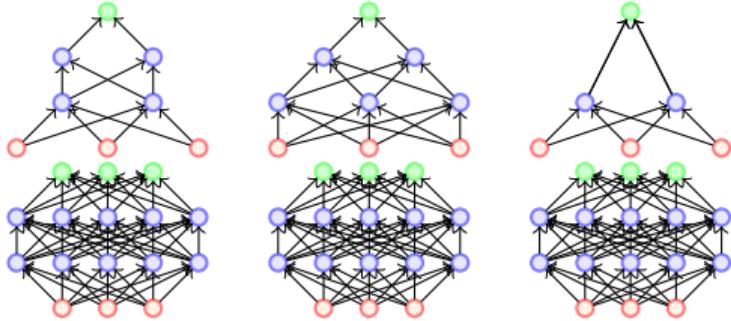
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- Training several large neural networks for making an ensemble is prohibitively expensive
- Option 1: Train several neural networks having different architectures(obviously expensive)
- Option 2: Train multiple instances of the same network using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

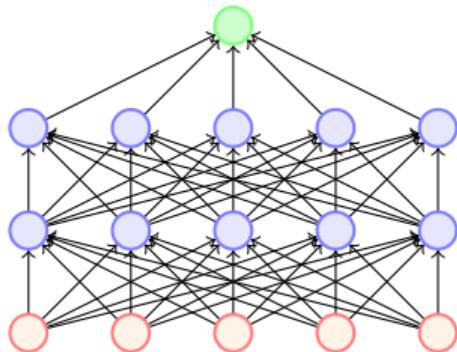


- Dropout is a technique which addresses both these issues.
- Effectively it allows training several neural networks without any significant computational overhead.

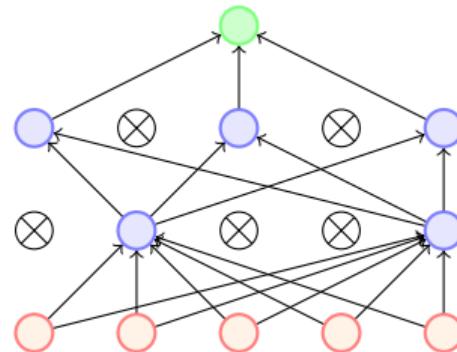
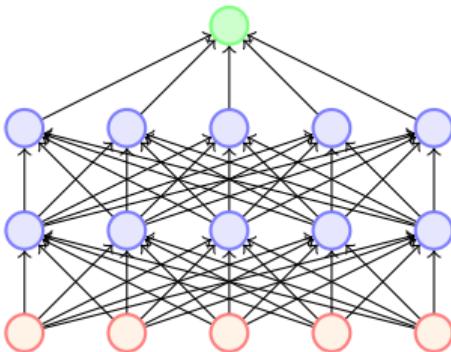




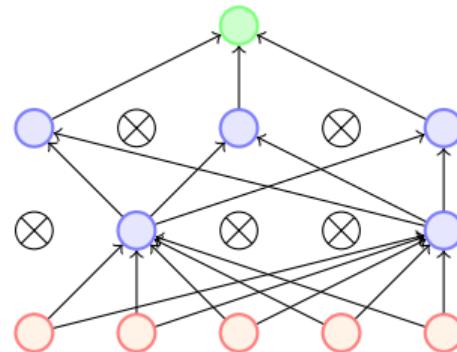
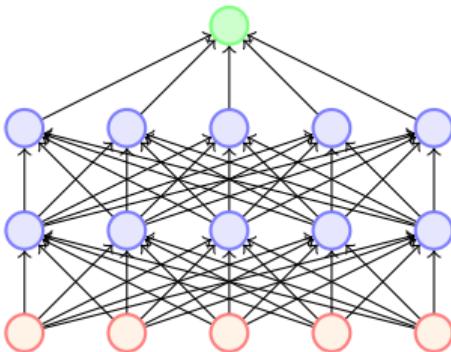
- Dropout is a technique which addresses both these issues.
- Effectively it allows training several neural networks without any significant computational overhead.
- Also gives an efficient approximate way of combining exponentially many different neural networks.



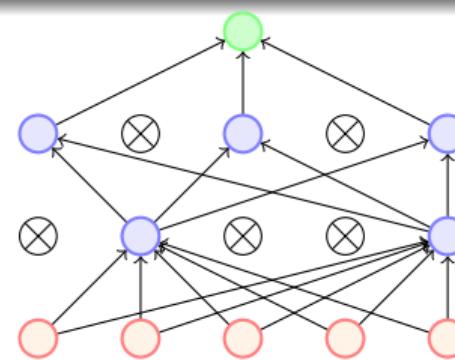
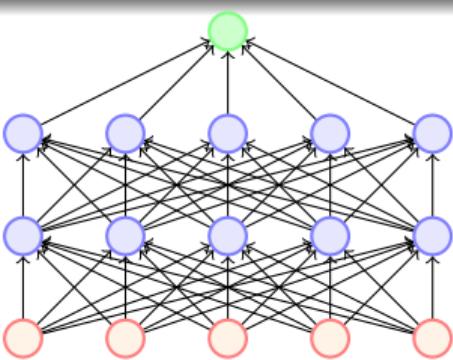
- Dropout refers to dropping out units

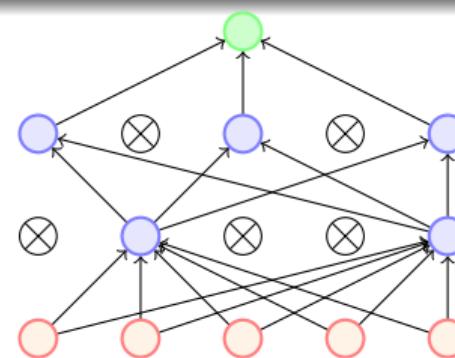
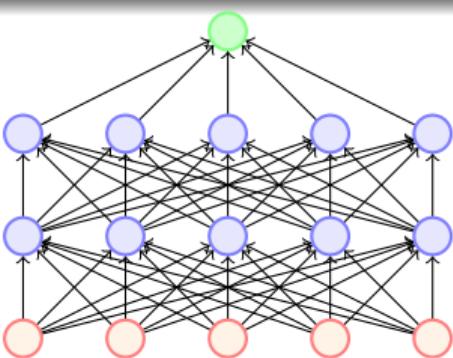


- Dropout refers to dropping out units
- Temporarily remove a node and all its incoming/outgoing connections resulting in a thinned network

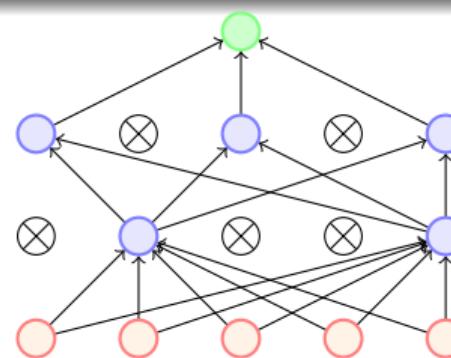
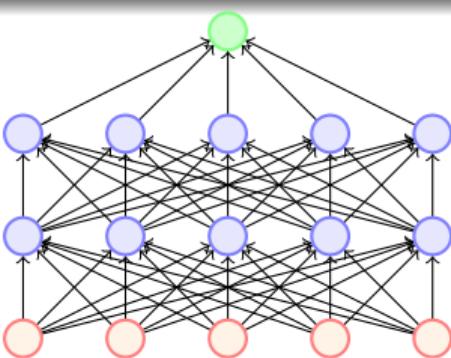


- Dropout refers to dropping out units
- Temporarily remove a node and all its incoming/outgoing connections resulting in a thinned network
- Each node is retained with a fixed probability (typically $p = 0.5$) for hidden nodes and $p = 0.8$ for visible nodes

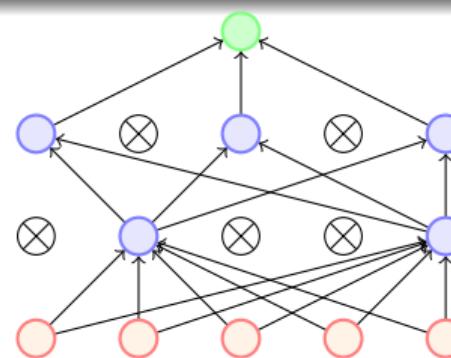
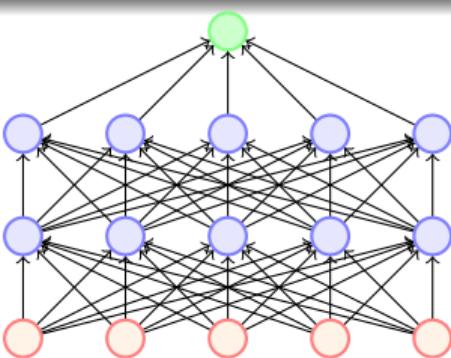




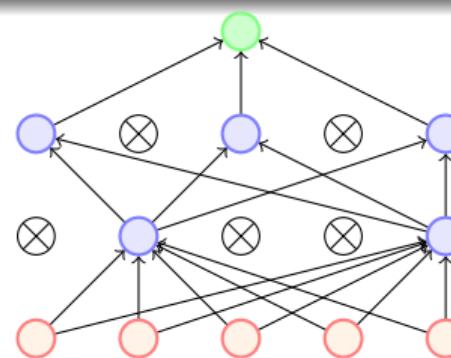
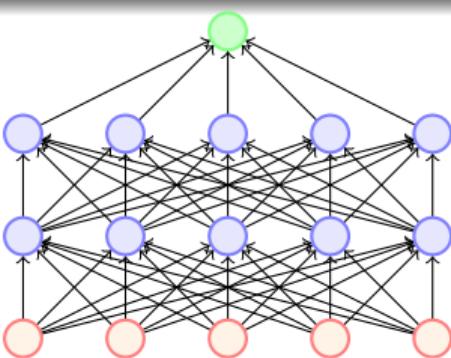
- Suppose a neural network has n nodes



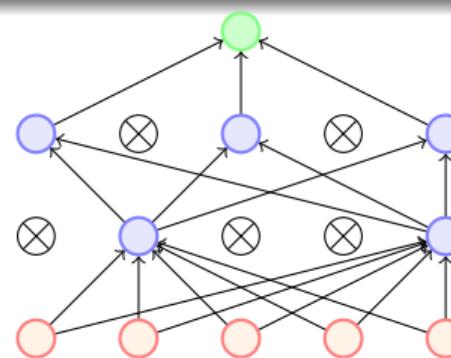
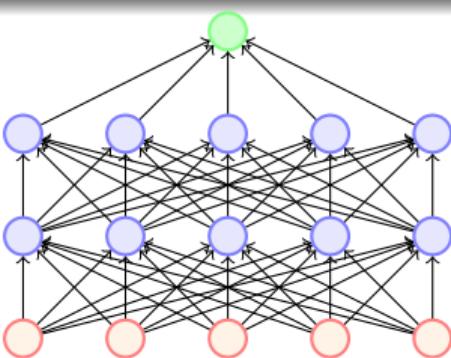
- Suppose a neural network has n nodes
- Using the dropout idea, each node can be retained or dropped



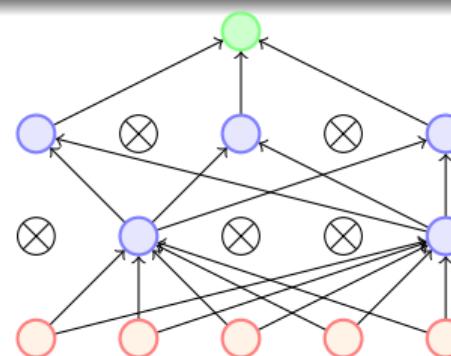
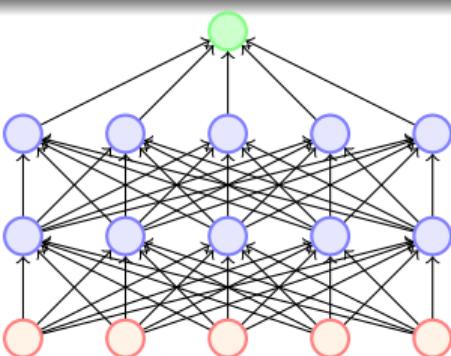
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- For example, in the above case we drop 5 nodes to get a thinned network



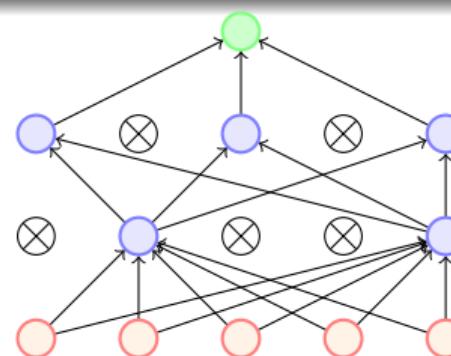
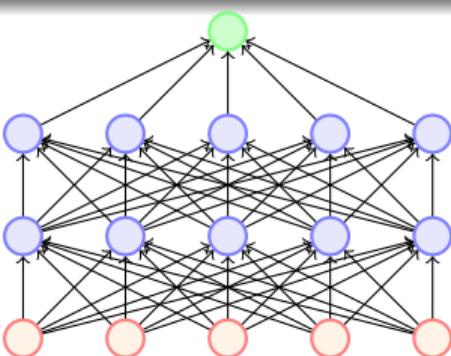
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- For example, in the above case we drop 5 nodes to get a thinned network
- Given a total of n nodes, what are the total number of thinned networks that can be formed?



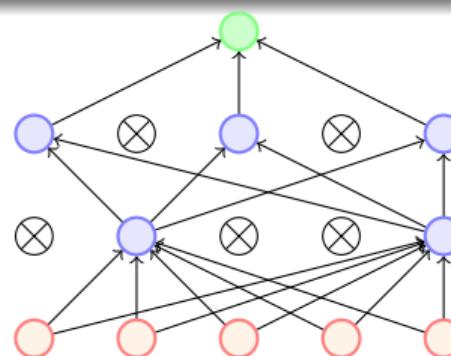
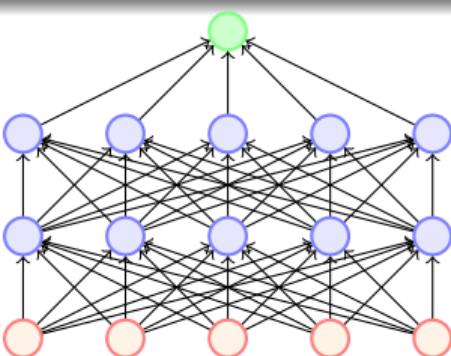
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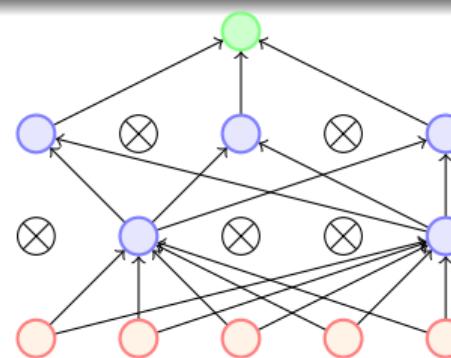
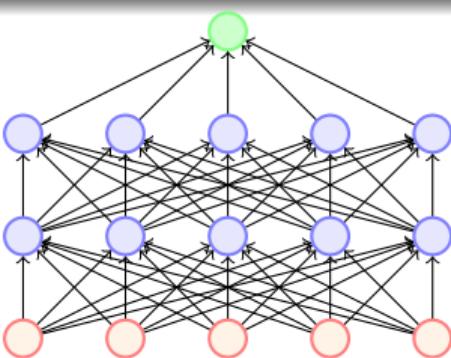
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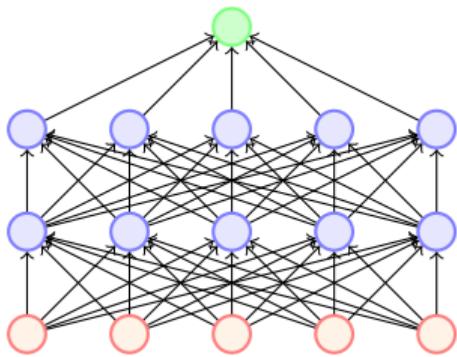
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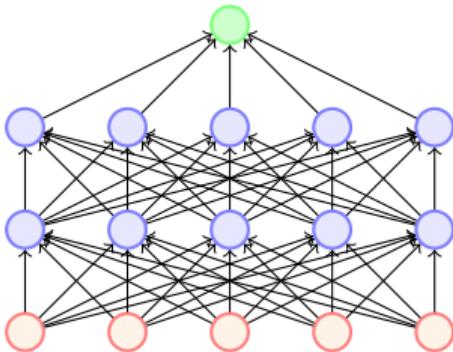


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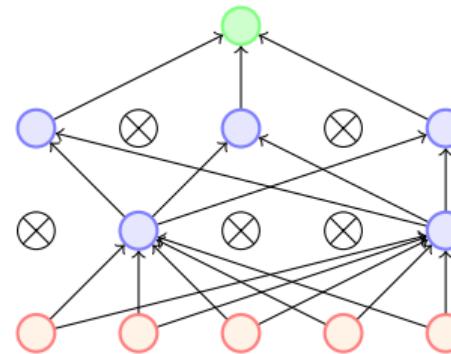
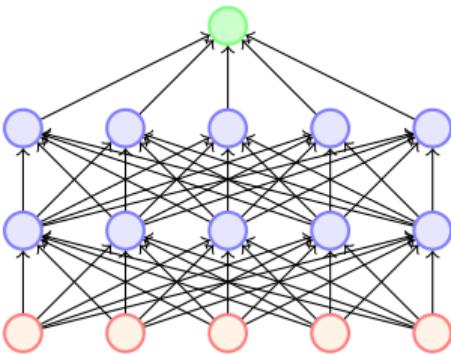


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- Let us see how?

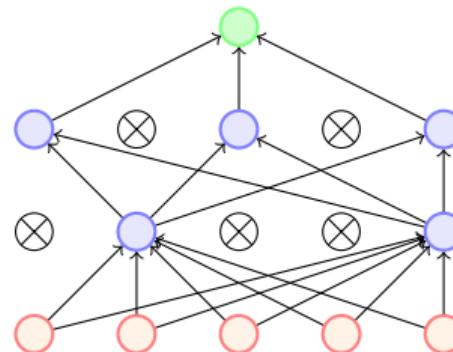
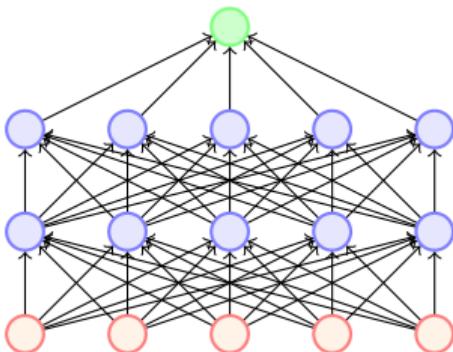




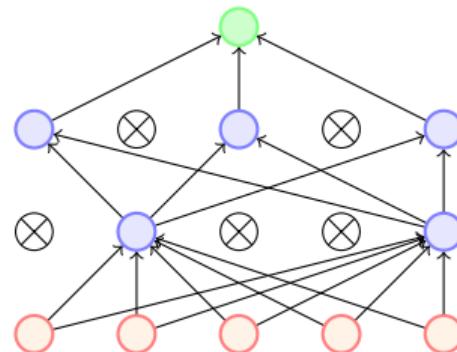
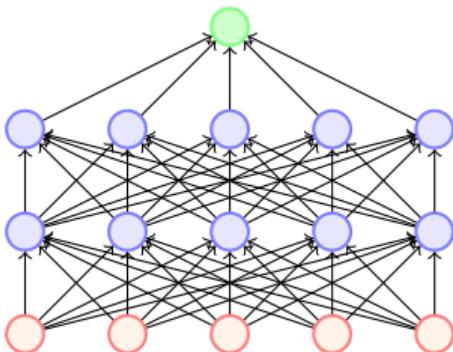
- We initialize all the parameters (weights) of the network and start training



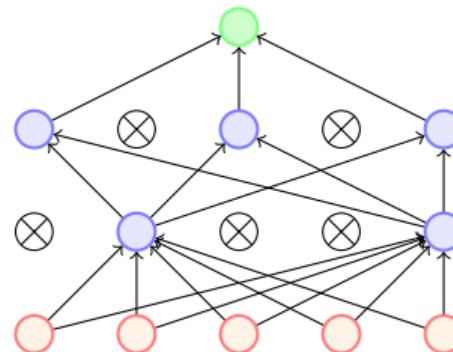
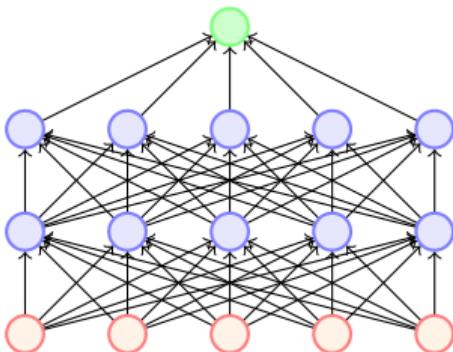
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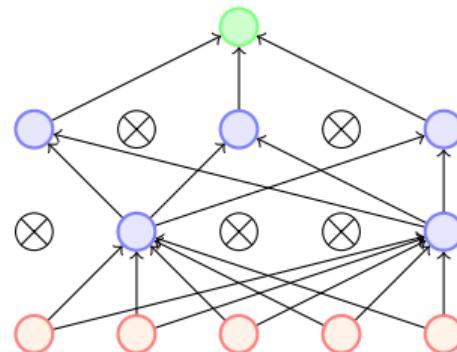
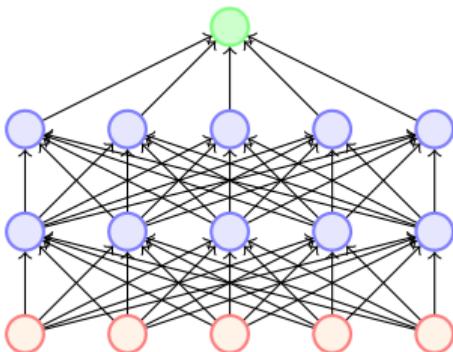
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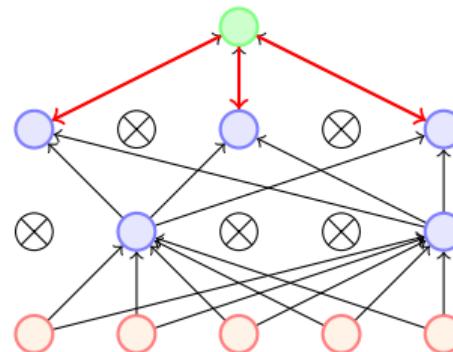
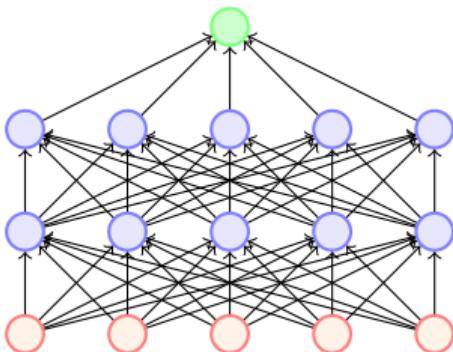
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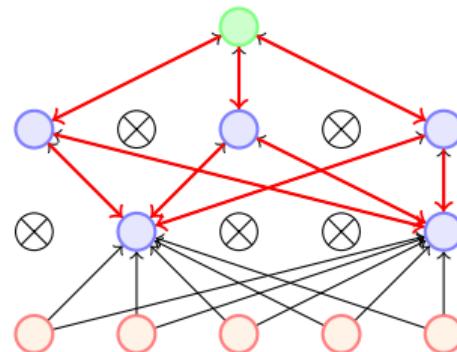
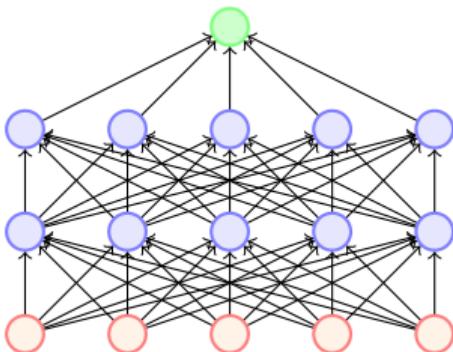
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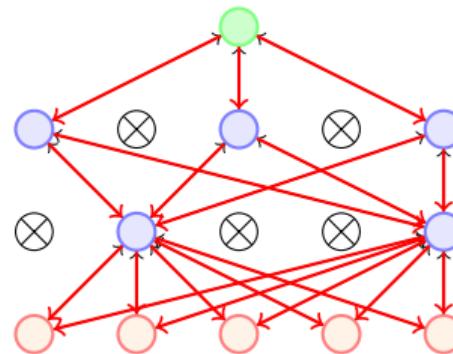
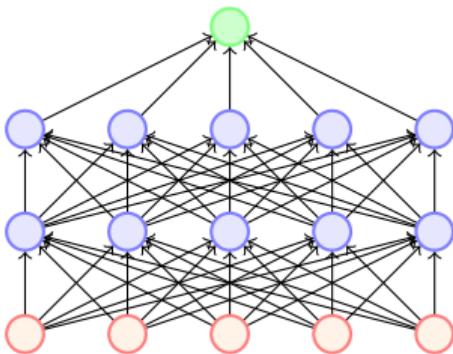
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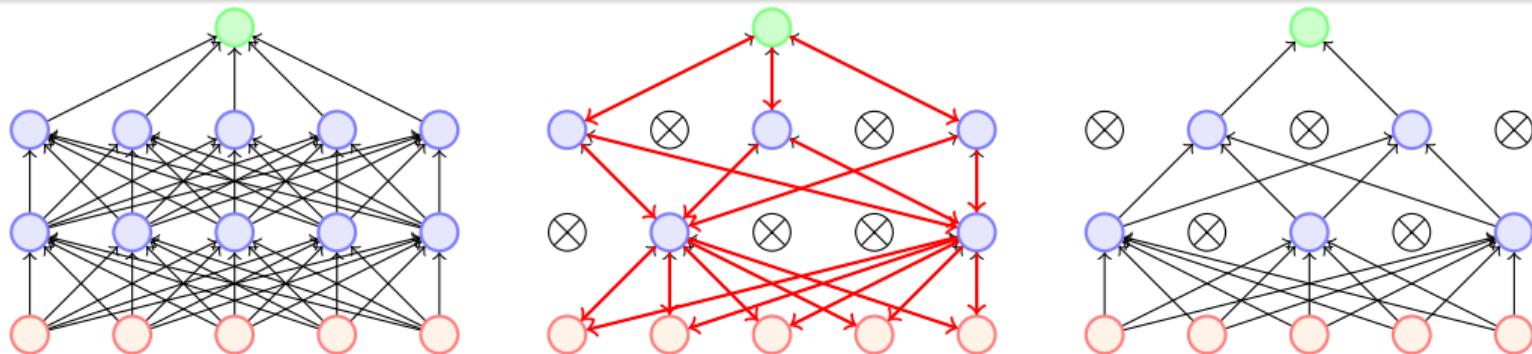
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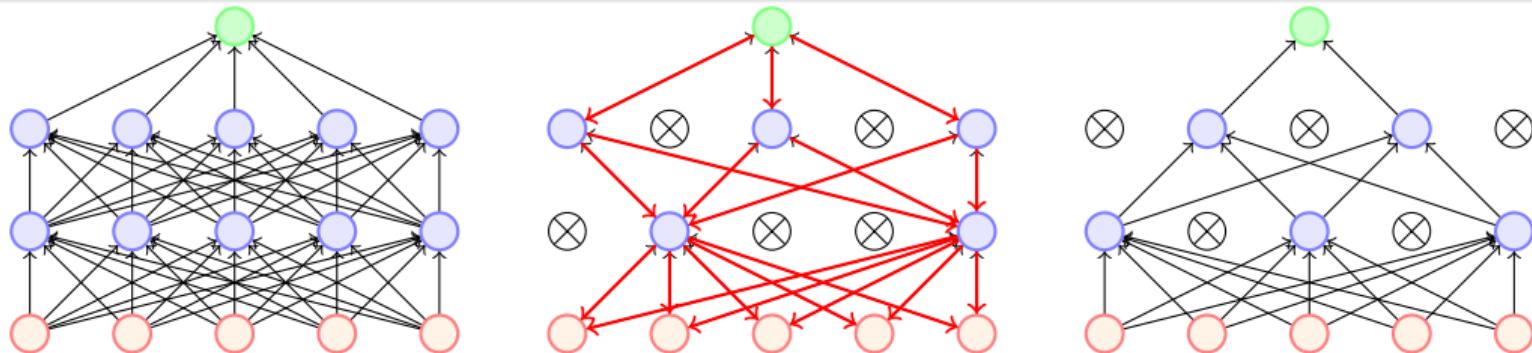
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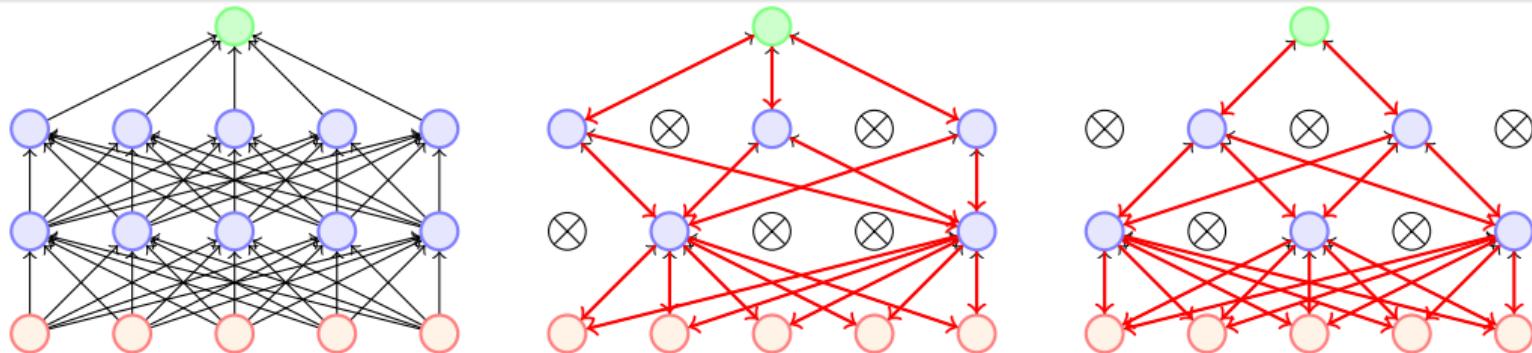
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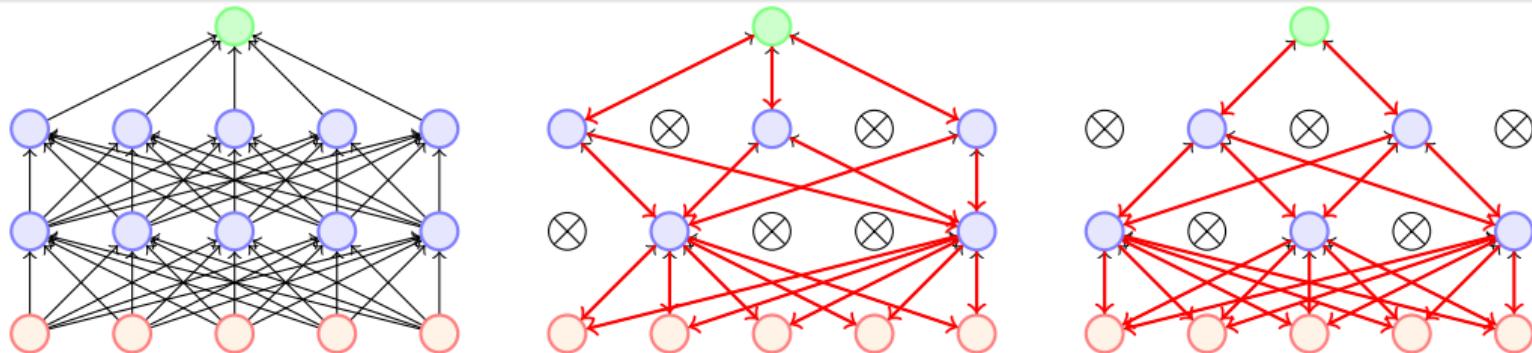
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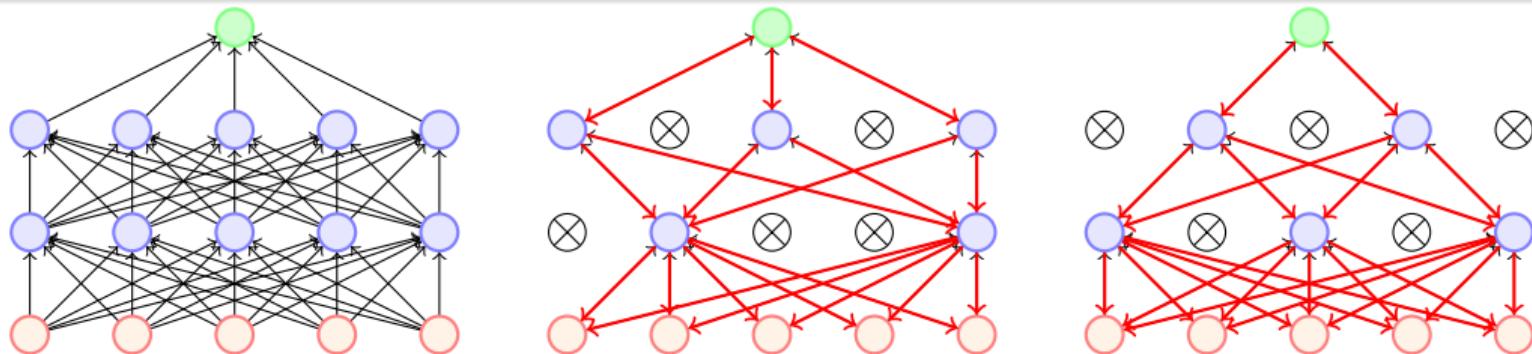
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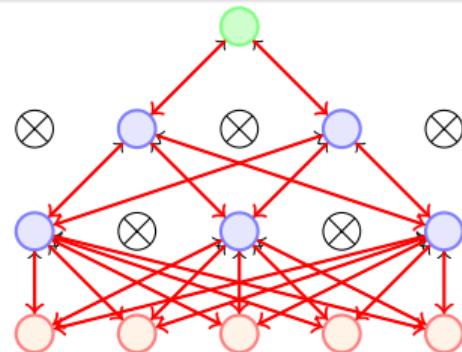
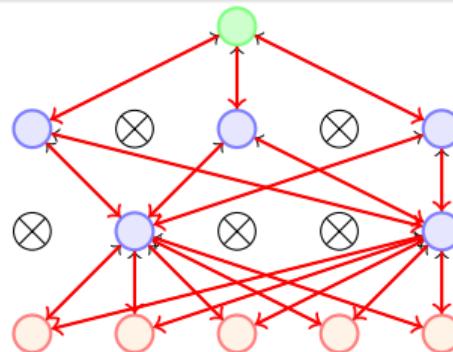
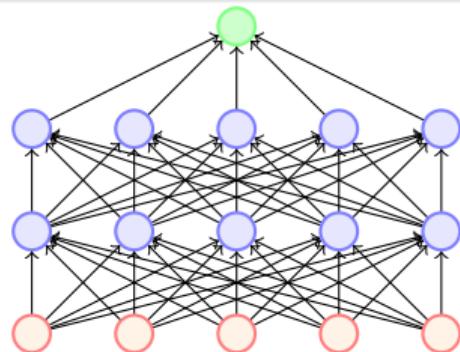
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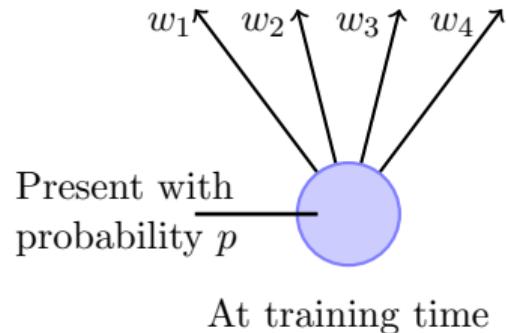
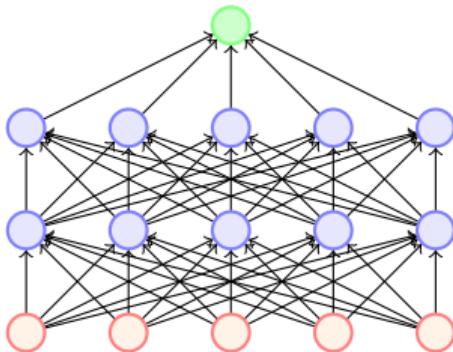
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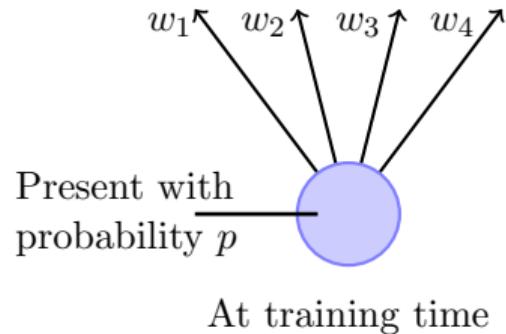
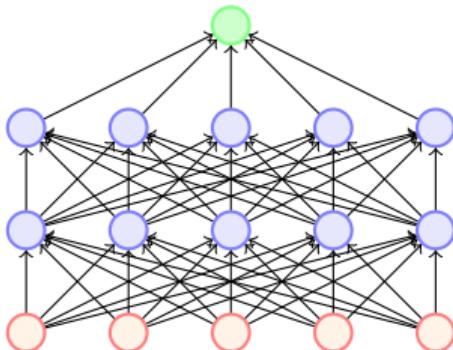


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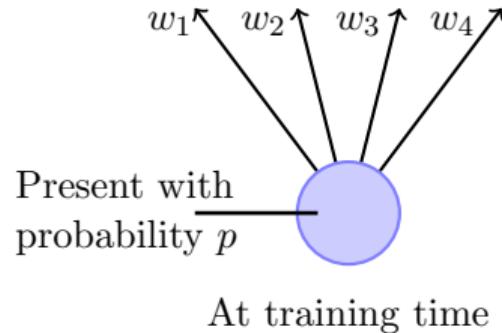
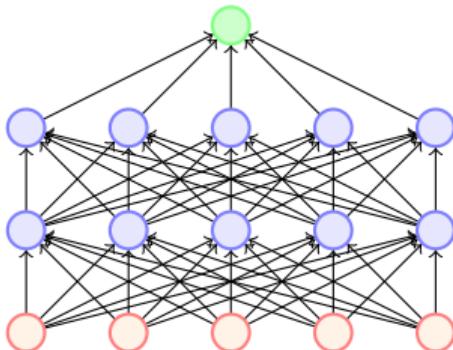


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 - Each thinned network gets trained rarely (or even never) but the parameter sharing ensures that no model has untrained or poorly trained parameters

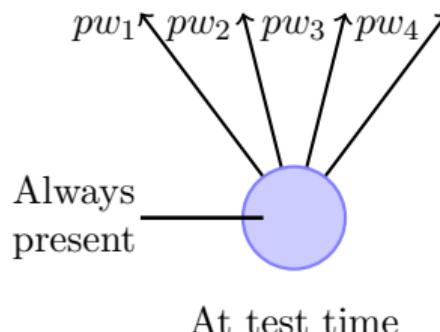
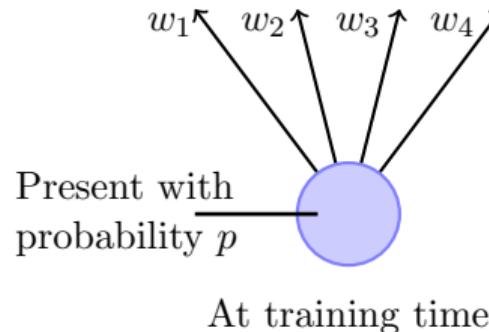
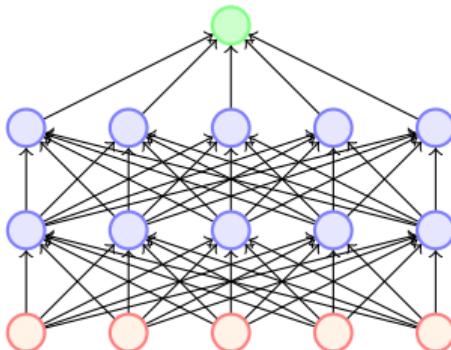




- What happens at test time?

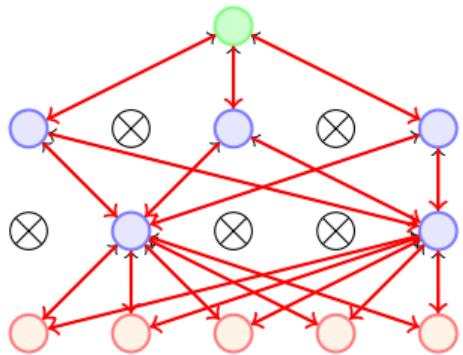


- What happens at test time?
- Impossible to aggregate the outputs of 2^n thinned networks

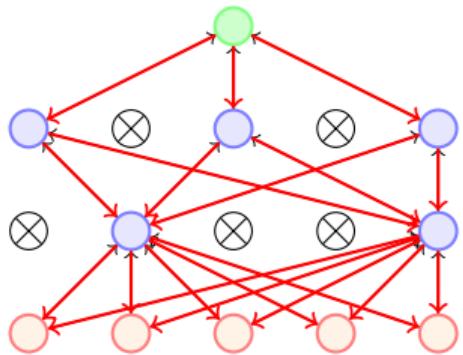


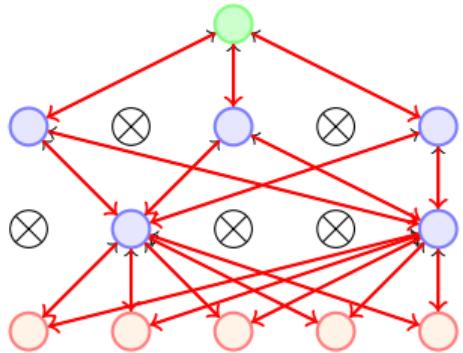
- What happens at test time?
- Impossible to aggregate the outputs of 2^n thinned networks
- Instead we use the full Neural Network and scale the output of each node by the fraction of times it was on during training

- Dropout essentially applies a masking noise to the hidden units

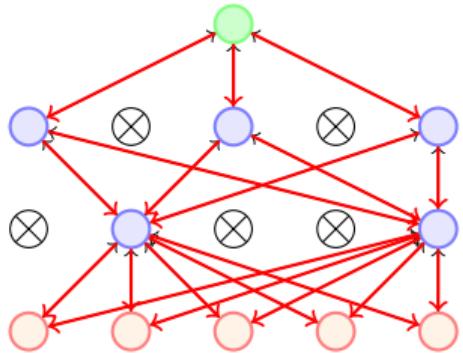


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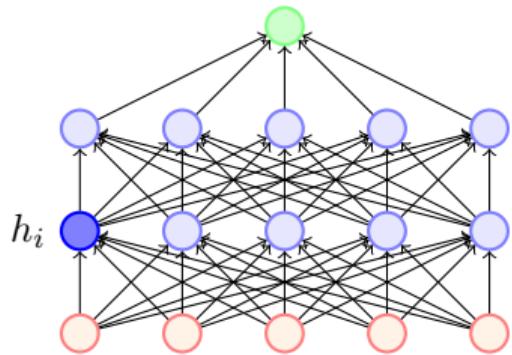




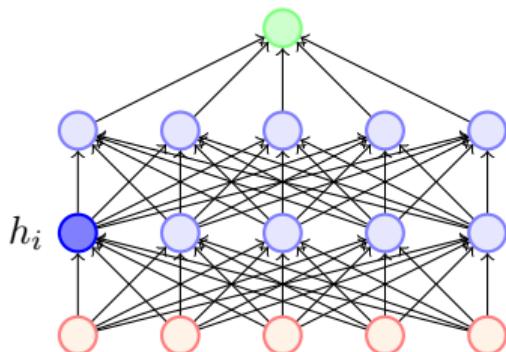
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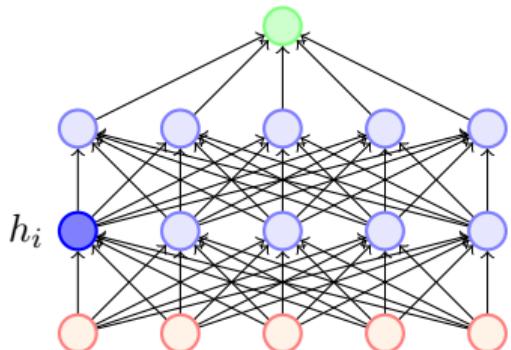
- Dropout essentially applies a masking noise to the hidden units
- Prevents hidden units from co-adapting
- Essentially a hidden unit cannot rely too much on other units as they may get dropped out any time
- Each hidden unit has to learn to be more robust to these random dropouts

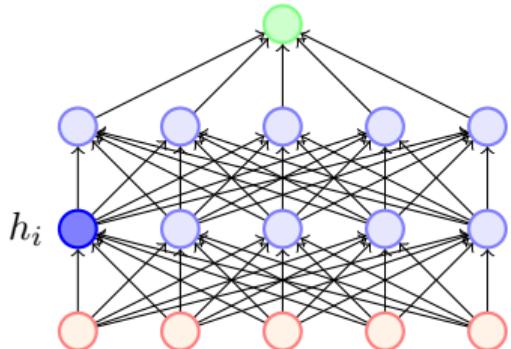


- Here is an example of how dropout helps in ensuring redundancy and robustness

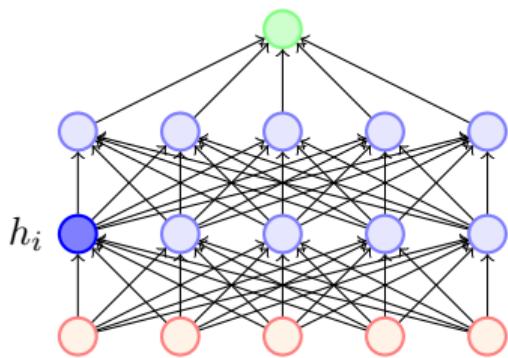


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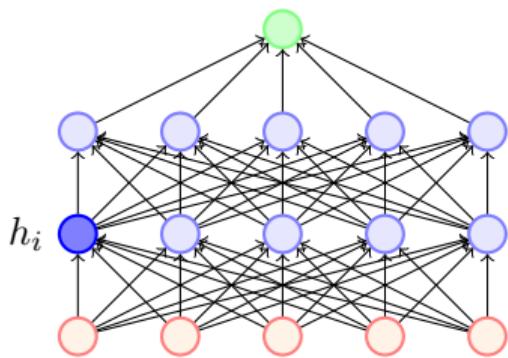




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- Suppose h_i learns to detect a face by firing on detecting a nose
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- The model should then learn another h_i which redundantly encodes the presence of a nose
- Or the model should learn to detect the face using other features

Recap

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

Appendix

- To prove: The below two equations are equivalent

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

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

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- Base case: $t = 1$ and $\omega_0 = 0$:

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- Base case: $t = 1$ and $\omega_0 = 0$:
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- ω_1 according to the second equation:

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

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

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

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

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

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

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

- Continuing

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

- Continuing

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

- Continuing

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

- Continuing

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

- Continuing

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

- Continuing

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

- Continuing

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

Hence, proved!