CS7015 (Deep Learning) : Lecture 8

Regularization: Bias Variance Tradeoff, L2 regularization, Early stopping, Dataset augmentation, Parameter sharing and tying, Injecting noise at input, Ensemble methods, Dropout

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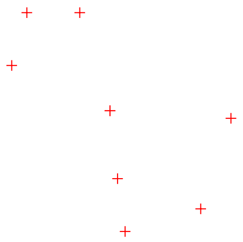
Acknowledgements

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

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

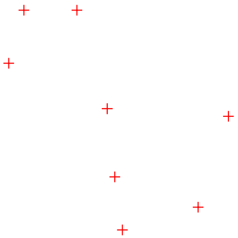
Module 8.1 : Bias and Variance

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



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

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



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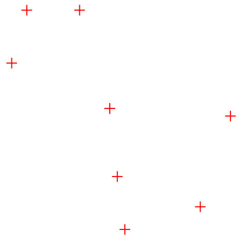
- Let us consider the problem of fitting a curve through a given set of points
- We consider two models :



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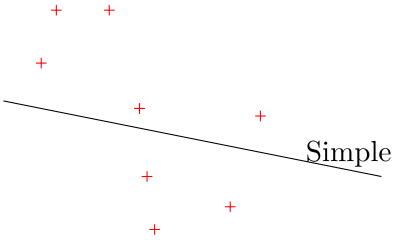
- Let us consider the problem of fitting a curve through a given set of points
- We consider two models :

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



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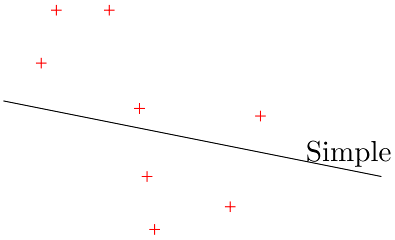

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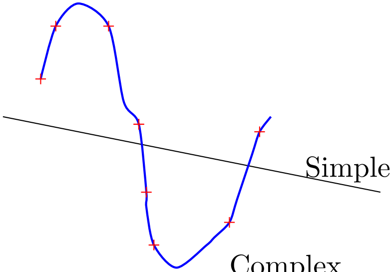
- Let us consider the problem of fitting a curve through a given set of points
- We consider two models :

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

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



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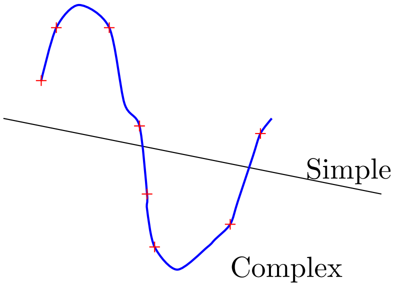

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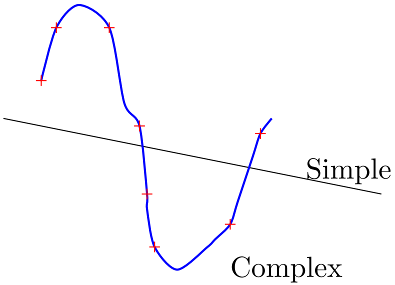
- Note that in both cases we are making an assumption about how y is related to x. We have no idea about the true relation $f(x)$



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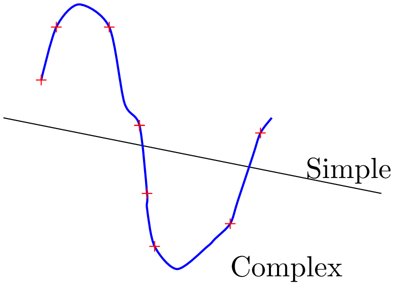
- Note that in both cases we are making an assumption about how y is related to x. We have no idea about the true relation $f(x)$
- The training data consists of 100 points



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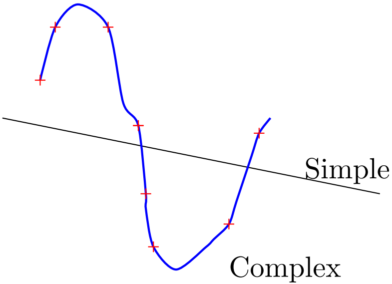
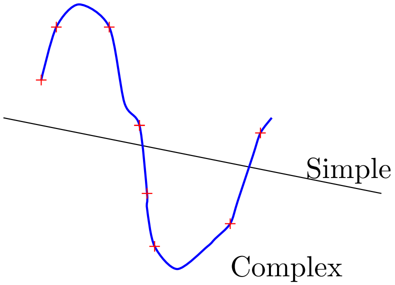
- We sample 25 points from the training data and train a simple and a complex model



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

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



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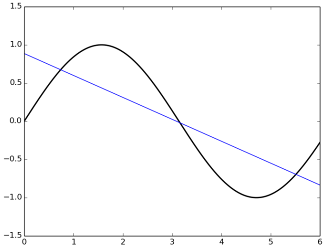
- We sample 25 points from the training data and train a simple and a complex model
- We repeat the process 'k' times to train multiple models (each model sees a different sample of the training data)
- We make a few observations from these plots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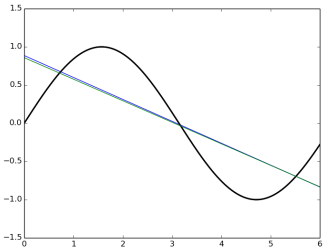
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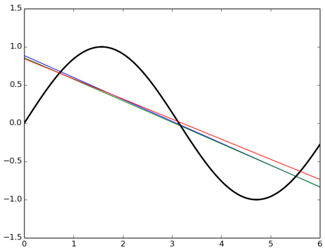
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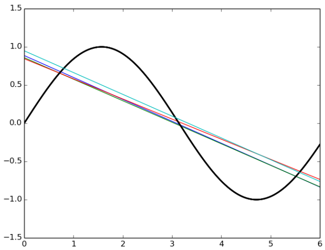
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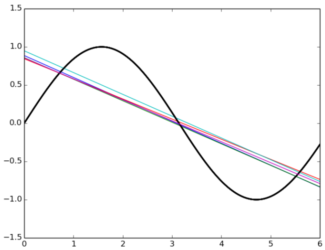
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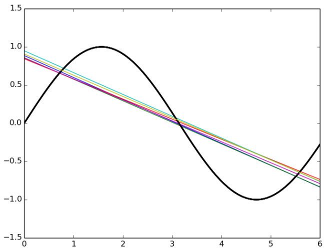
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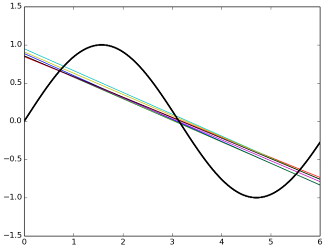

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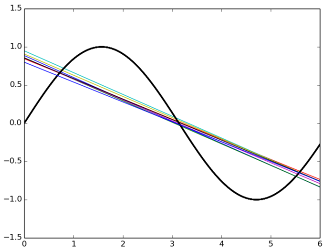
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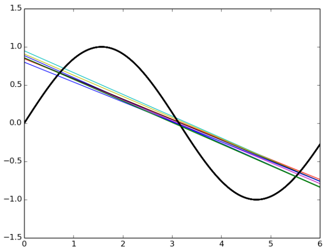
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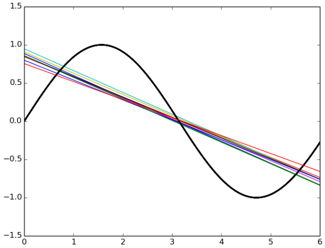

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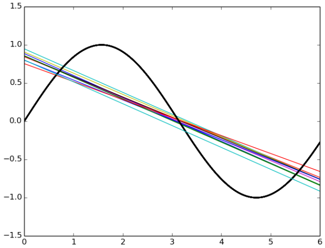
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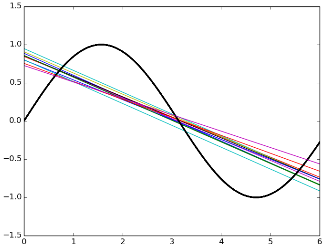
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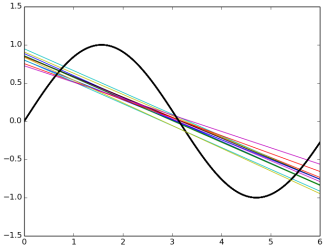
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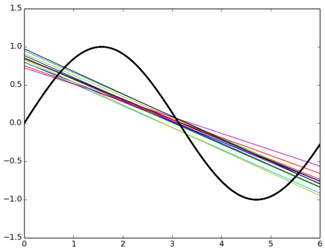
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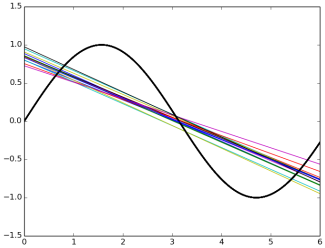
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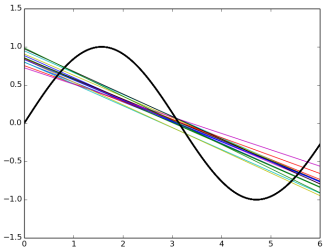
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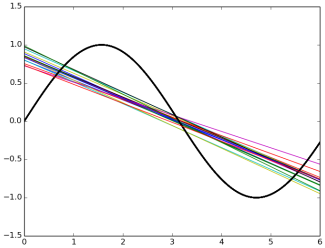
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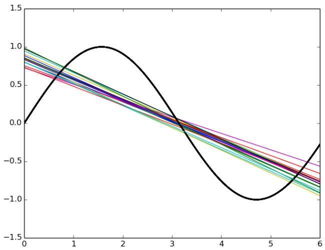
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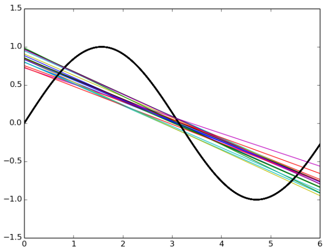
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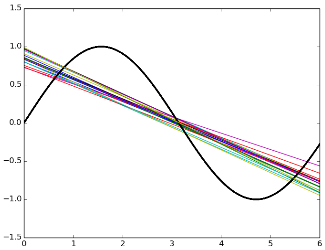
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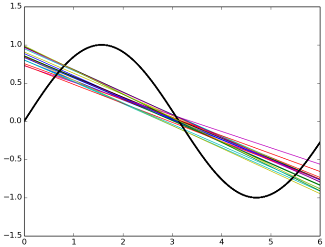

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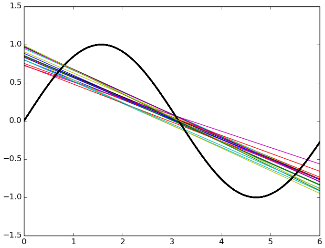

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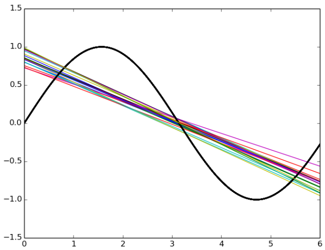
- However they are very far from the true sinusoidal curve (under fitting)



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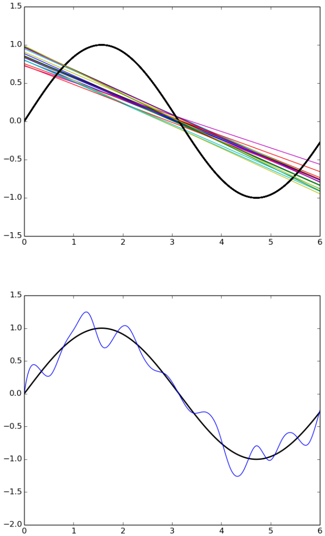

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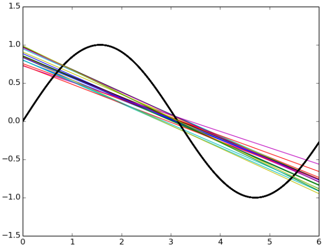

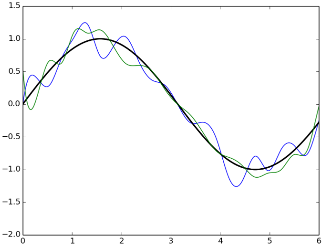

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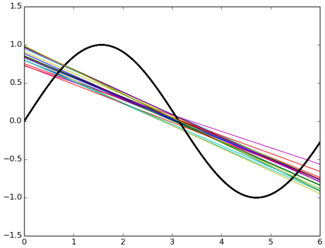

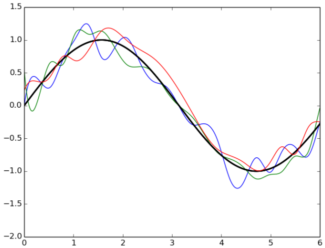

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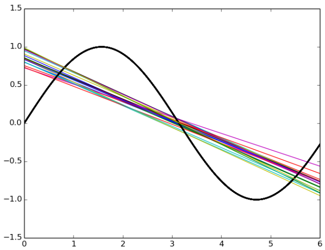

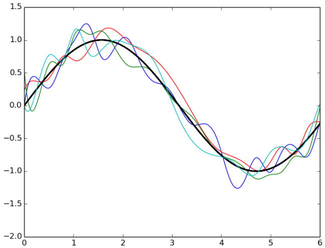

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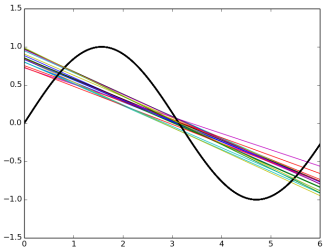

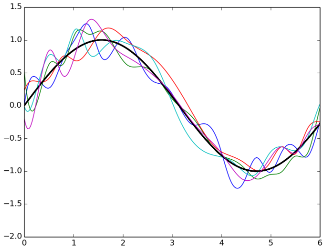

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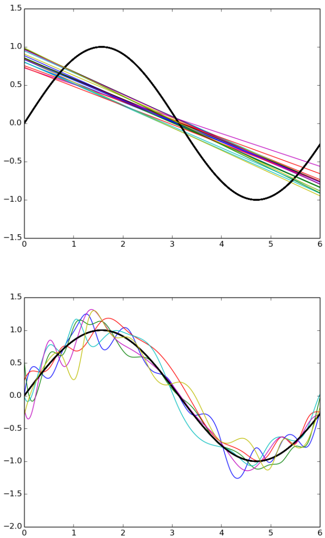

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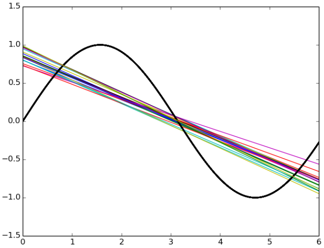

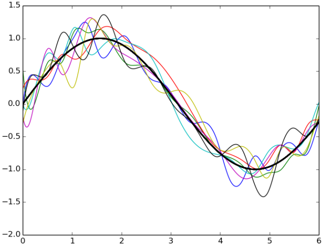

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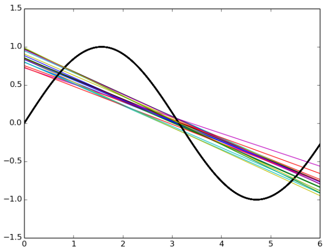

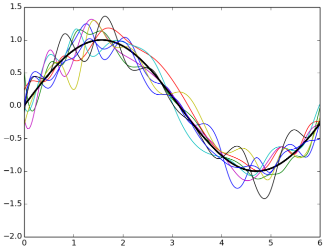

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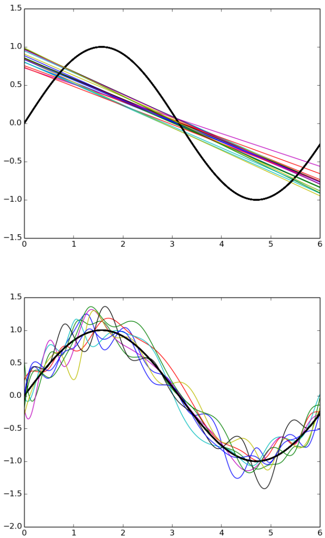

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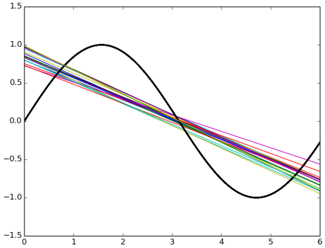

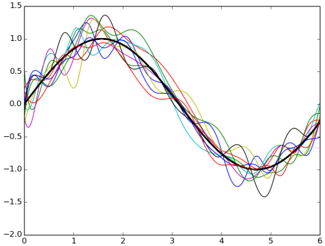

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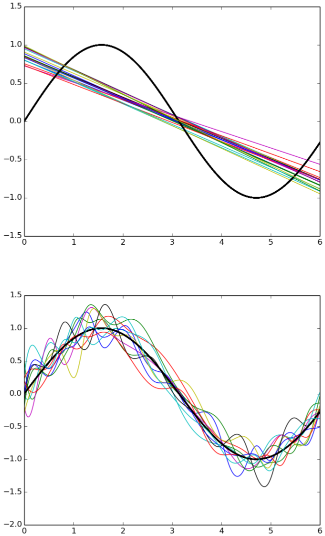

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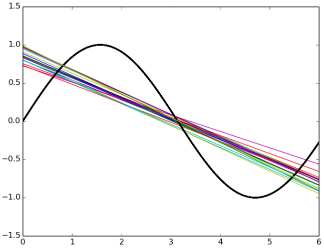

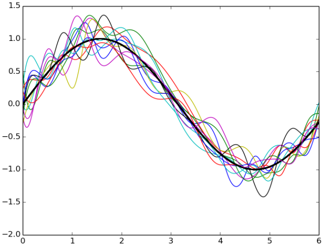

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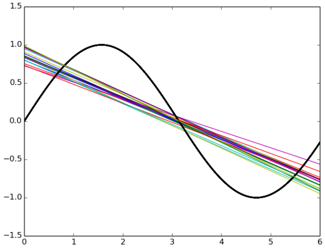

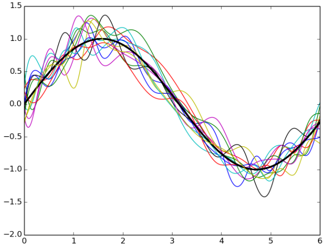

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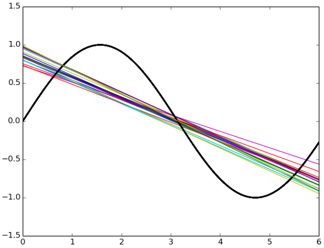

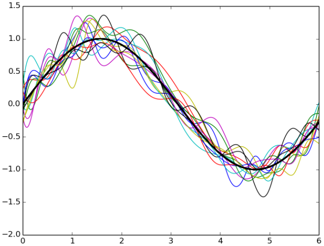

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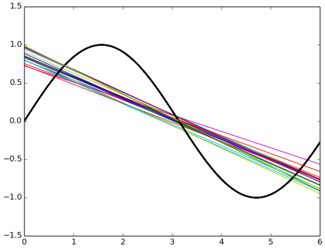

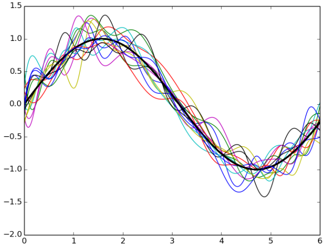

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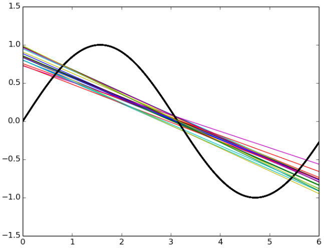

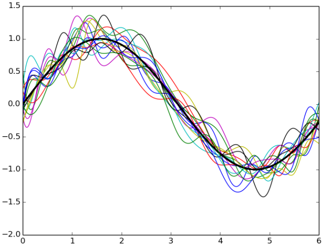

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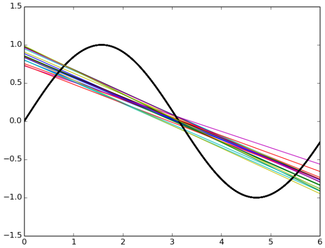

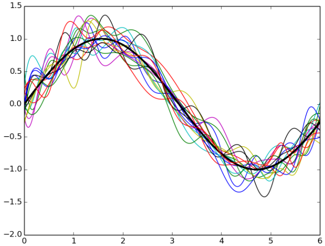

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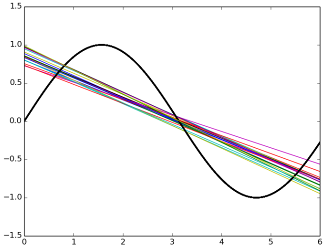

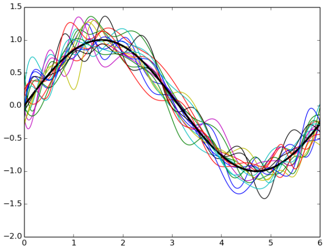

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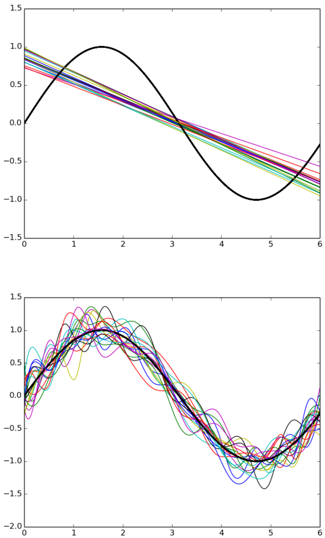

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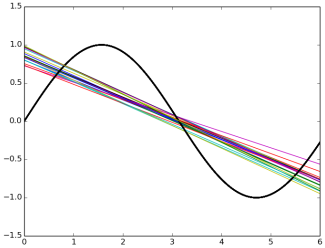

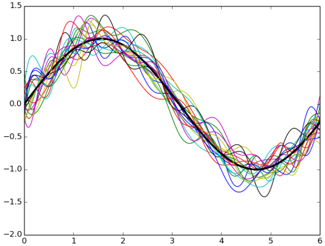

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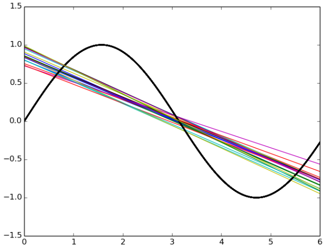
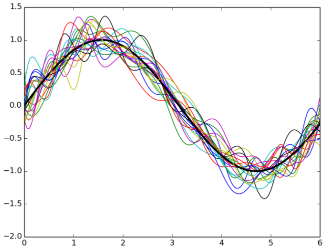
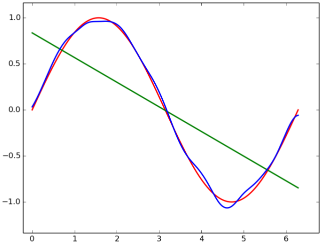




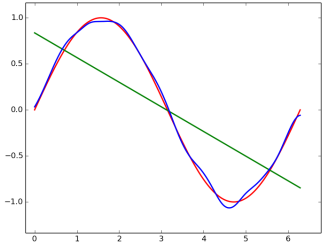
- Simple models trained on different samples of the data do not differ much from each other
- However they are very far from the true sinusoidal curve (under fitting)
- On the other hand, complex models trained on different samples of the data are very different from each other (high variance)

- 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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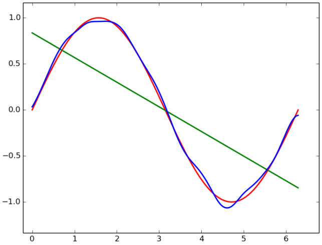
- $E[\hat{f}(x)]$ is the average (or expected) value of the model



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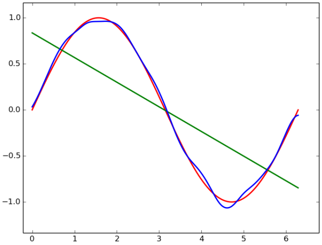
- We can see that for the simple model the average value (blue line) is very far from the true value $f(x)$ (sinusoidal function)



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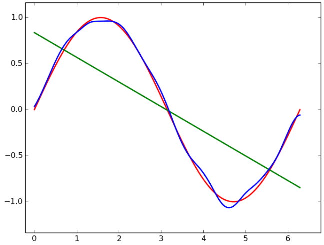
- $E[\hat{f}(x)]$ is the average (or expected) value of the model
- We can see that for the simple model the average value (blue line) is very far from the true value $f(x)$ (sinusoidal function)
- Mathematically, this means that the simple model has a high bias



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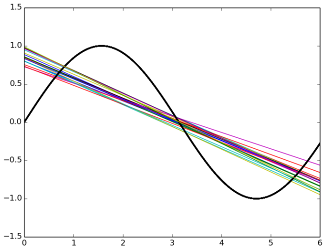
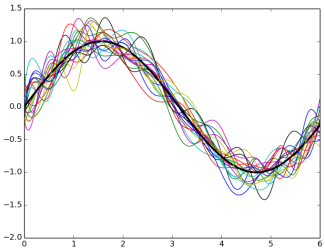
- $E[\hat{f}(x)]$ is the average (or expected) value of the model
- We can see that for the simple model the average value (blue line) is very far from the true value $f(x)$ (sinusoidal function)
- Mathematically, this means that the simple model has a high bias
- On the other hand, the complex model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

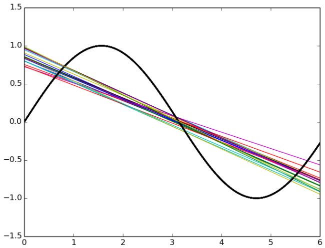


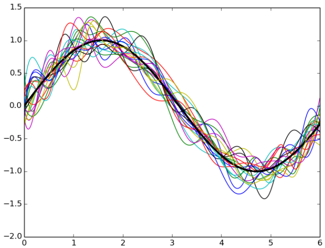


- We now define,

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

(Standard definition from statistics)





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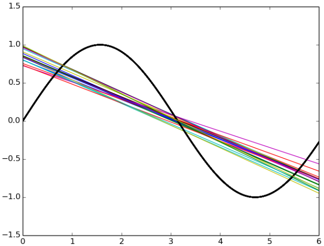

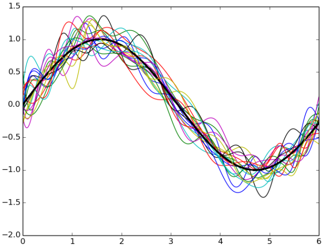

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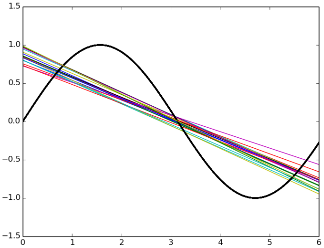
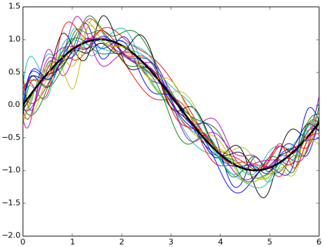
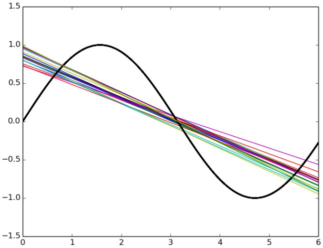
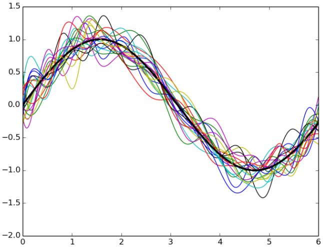
- It is clear that the simple model has a low variance whereas the complex model has a high variance





- In summary (informally)





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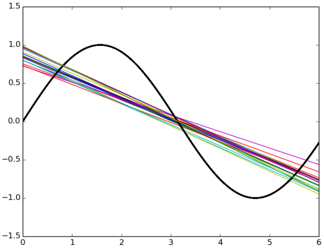
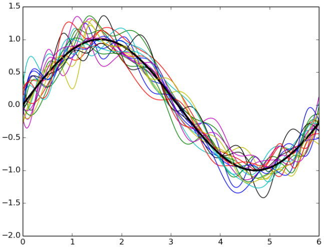
- Simple model: high bias, low variance





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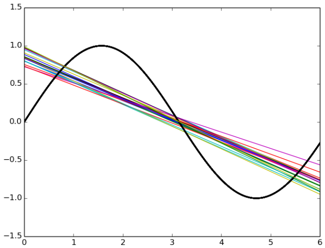
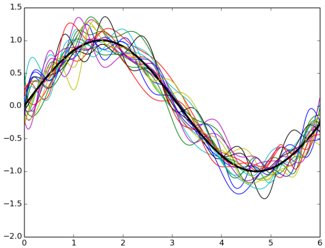
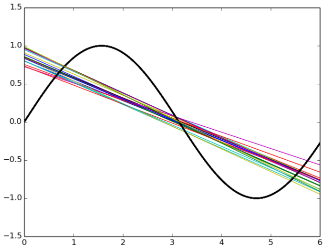
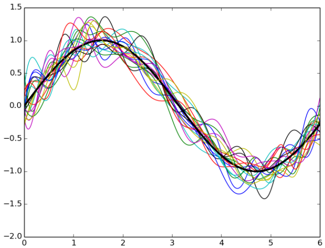




- In summary (informally)
- Simple model: high bias, low variance
- Complex model: low bias, high variance
- There is always a trade-off between the bias and variance





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

Module 8.2 : Train error vs Test error

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

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- See proof here

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  $train_{err}$ (say, mean square error)
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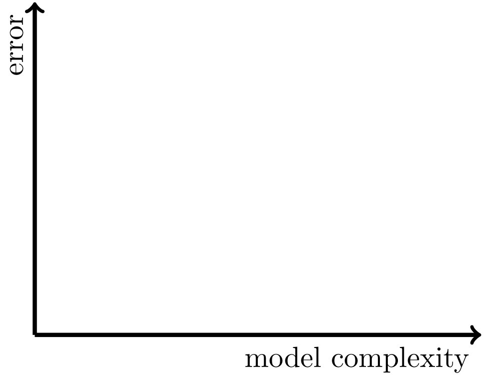

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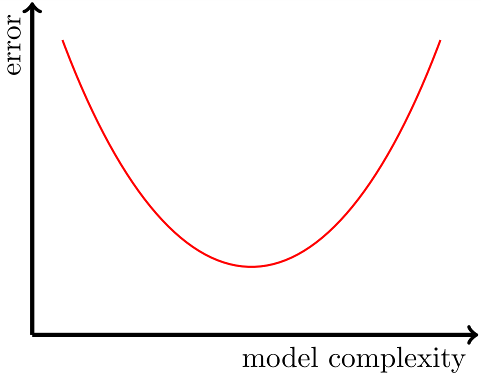

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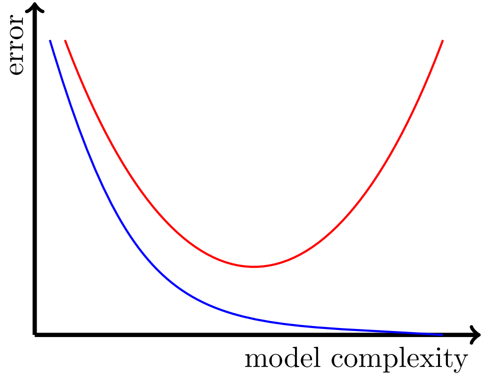

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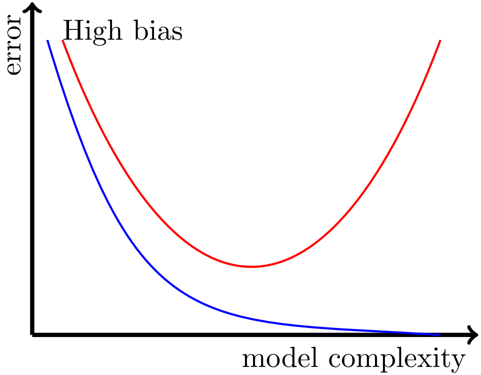

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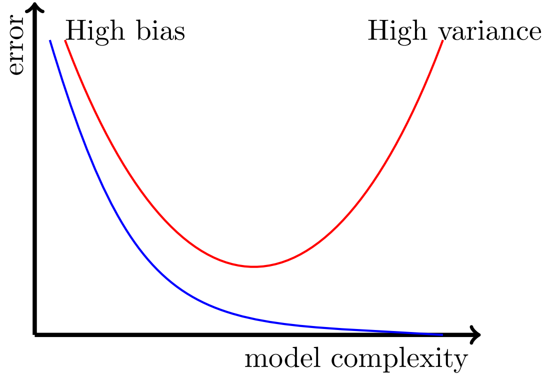

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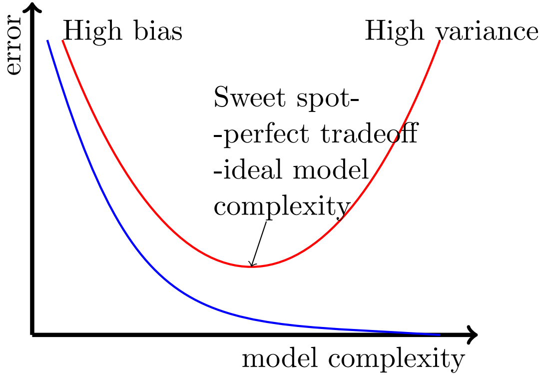

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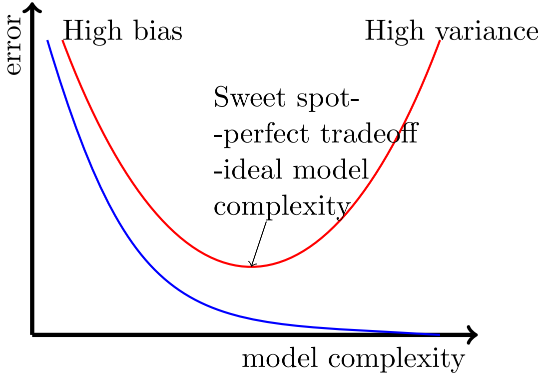

$$E[(y - \hat{f}(x))^2] = Bias^2 \\ + Variance \\ + \sigma^2 \text{ (irreducible error)}$$

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

Intuitions developed so far

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

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

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- The validation error gives the real picture of how close $\hat{f}$ is to f
- We will concretize this intuition mathematically now and eventually show how to account for the optimism in the training error

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

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

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

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

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

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... returning back to our derivation

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

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

Case 1: Using test observations

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

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$\because$ covariance(X, Y)

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

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

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

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

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

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

Case 2: Using training observations

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

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

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

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

Module 8.3 : True error and Model complexity

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

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

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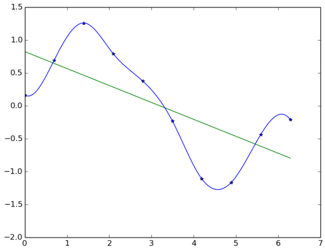
- Can you link this to model complexity?
- Yes, indeed a complex model will be more sensitive to changes in observations whereas a simple model will be less sensitive to changes in observations
- Hence, we can say that
  true error = empirical train error + small constant + Ω(model complexity)

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



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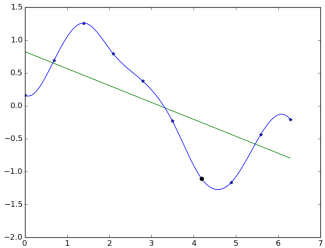

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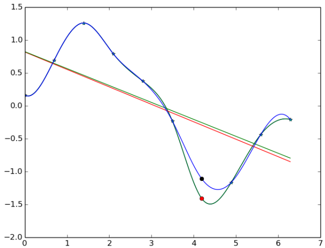

- Let us verify that indeed a complex model is more sensitive to minor changes in the data
- We have fitted a simple and complex model for some given data
- We now change one of these data points
- The simple model does not change much as compared to the complex model

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

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

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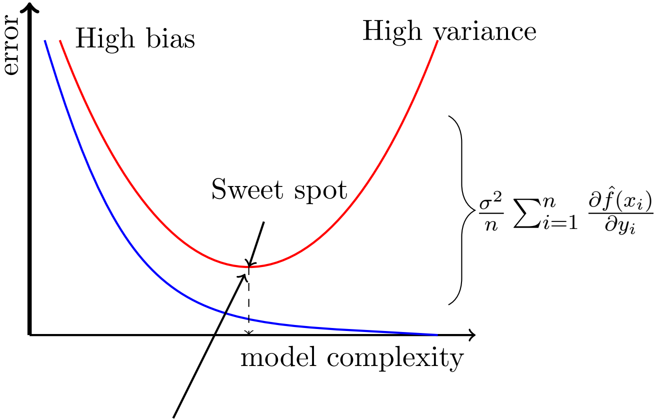
- $\Omega(\theta)$ acts as an approximate for $\frac{\sigma^2}{n}\sum_{i=1}^{n}\frac{\partial \hat{f}(x_i)}{\partial y_i}$
- This is the basis for all regularization methods
- We can show that L_1 regularization, L_2 regularization, early stopping and injecting noise in input are all instances of this form of regularization.



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

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

Different forms of regularization

- L_2 regularization

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- Dataset augmentation

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- Parameter Sharing and tying

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- Dropout