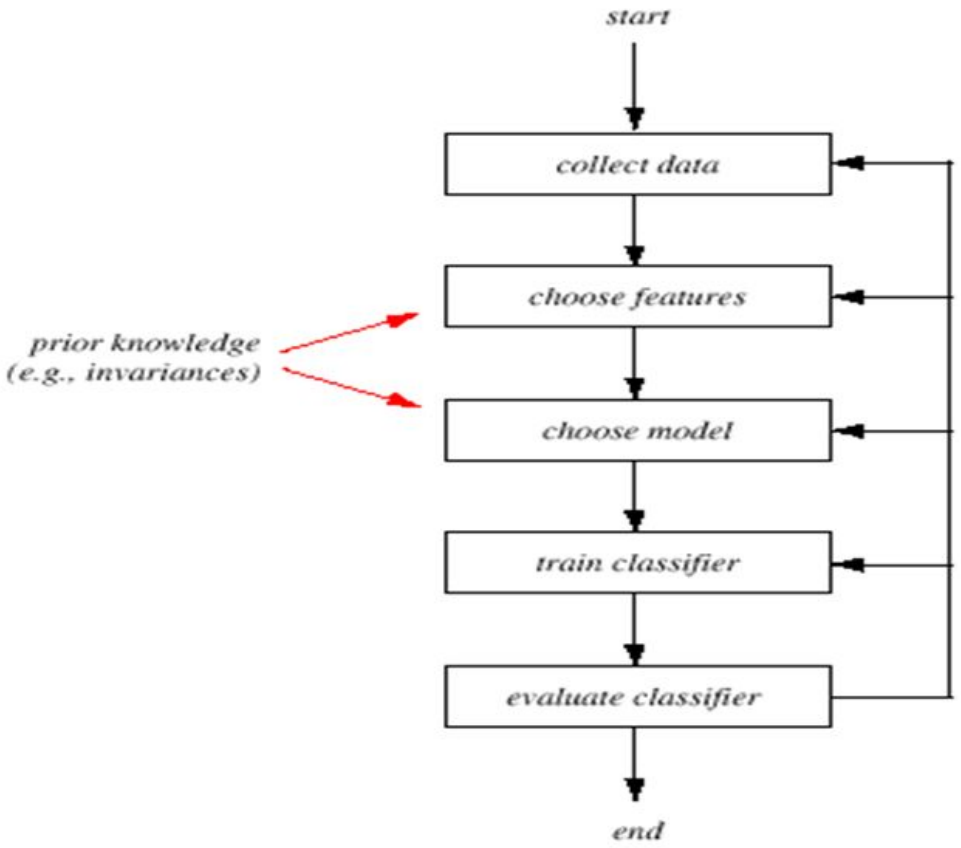
Machine Learning in Practise

INDRAPRASTHA INSTITUTE *of*
INFORMATION TECHNOLOGY
DELHI

The Design Cycle



Computational Complexity

- What is the trade-off between computational ease and performance?

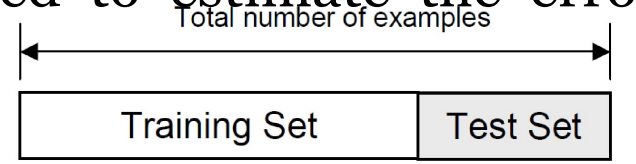
- How an algorithm scales as a function of the number of features, patterns or categories?

Performance Evaluation of Learning Tasks

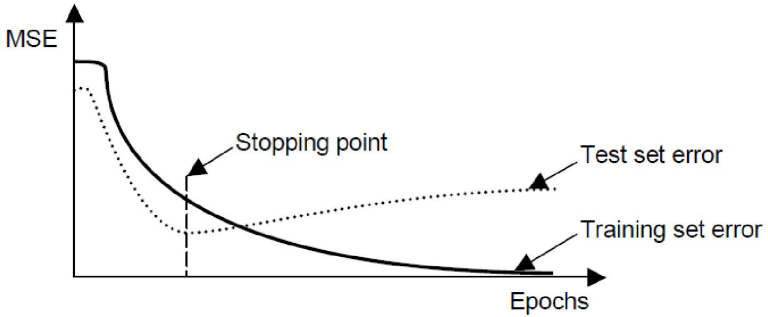
- Entire population is unavailable
- Finite set of training data, usually smaller than desired
- Naïve approach: use all available data
  - The final model will typically **overfit** the training data
    - More pronounced with high-capacity models (e.g., neural nets)
  - The true error rate is **underestimated**
    - Not uncommon to have 100% accuracy on training data

Validation Method: Holdout

- Split dataset into two groups:
  - Training set: used to train the model
  - Test set: used to estimate the error rate of the trained model



- Typical application: early stopping

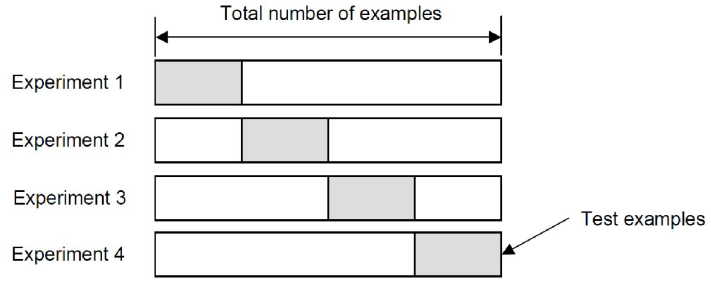


Holdout

- Drawbacks
  - For small training sets, setting aside a subset may be infeasible
    - Sample Size = 10 => Training set = 7, Testing set = 3
  - For a single train-and-test experiment, the holdout estimate of error rate will be misleading if we happen to get an '*unfortunate*' split
    - Training Set = 1,0,1,0,0,0,0, Testing set = 1,1,1
- Alternatives: a family of resampling methods: Cross Validation
  - Random Subsampling
  - Leave-one-out Cross-Validation
  - K-Fold Cross-Validation

Validation Method: K-Fold Cross-validation

- Create a K-fold partition of the dataset
  - For each of K experiments, use K-1 folds for training and the remaining one for testing



- True error is estimated as the average error rate

$$E = \frac{1}{K}\sum_{i=1}^{K} E_i$$

Validation Method: K-Fold Cross-validation

- Example: [0.1, 0.2, 0.3, 0.4, 0.5]
- K = 3

Fold	Training Set	Testing Set
1	[0.1, 0.2, 0.3]	[0.4, 0.5]
2	[0.1, 0.2, 0.5]	[0.3, 0.4]
3	[0.1, 0.4, 0.5]	[0.2, 0.3]

Validation Method: K-Fold Cross-validation

- Example: [0.1, 0.2, 0.3, 0.4, 0.5]
- K = 3

Fold	Training Set	Testing Set	Predictions
1	[0.1, 0.2, 0.3]	[0.4, 0.5]	[0.3, 0.5]
2	[0.1, 0.2, 0.5]	[0.3, 0.4]	[0.35, 0.35]
3	[0.1, 0.4, 0.5]	[0.2, 0.3]	[0.23, 0.33]

Calculate average error rate

Validation Method: K-Fold Cross-validation

Fold	Testing Set	Predictions	Error Rate
1	[0.4, 0.5]	[0.3, 0.5]	0.005
2	[0.3, 0.4]	[0.35, 0.35]	0.0025
3	[0.2, 0.3]	[0.23, 0.37]	0.0058

Average Error Rate= 0.0044

How many folds are needed?

- Large number of folds
  - + smaller bias of the true error rate estimator
  - - larger variance of the true error rate estimator
  - - higher computational time (many experiments)
- Small number of folds
  - + lower computation time
  - + smaller variance
  - - larger bias
- In practice, the choice of the number of folds depends on the size of the dataset
  - For large datasets, even 3-Fold Cross Validation is reasonable
  - For very sparse datasets, '*leave-one-out*' is beneficial
- A common choice for K-Fold Cross Validation is K=10

Bias and Variance

Two ways to measure the “match” or “alignment” of the learning algorithm.

- Bias measures accuracy of the match: high => poor match
  - Bias arises when the classifier cannot represent the true function – that is, the classifier underfits the data
- Variance measures precision of match: high => weak match
  - Variance arises when the classifier overfits the data.
- There is often a tradeoff between bias and variance.

Bias and Variance

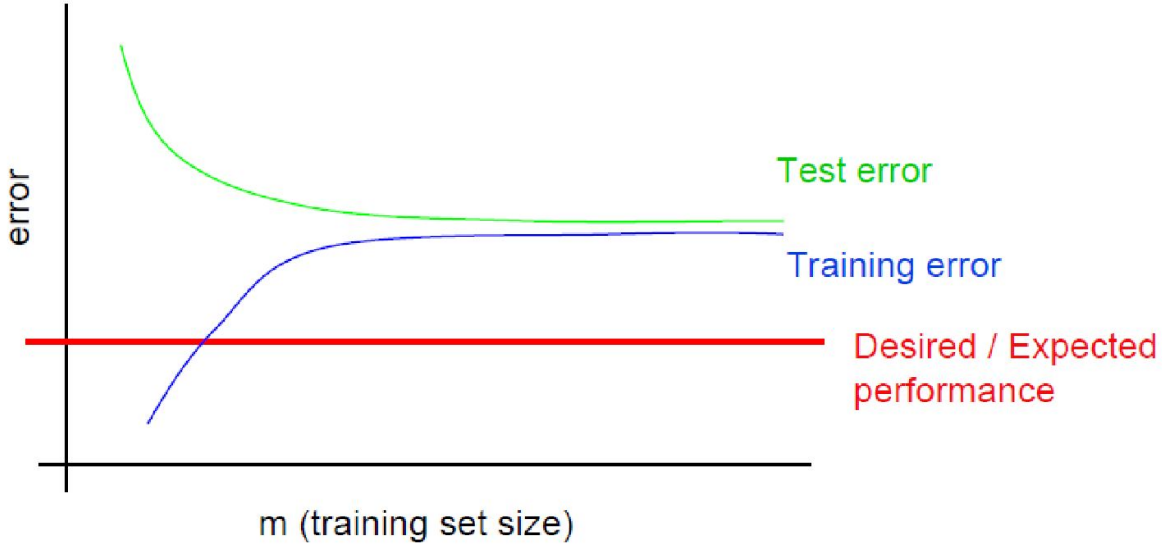
Calculate bias, variance and give conclusions.

Training error	Dev error	Bias	Variance	Conclusions
1%	11%			
15%	16%			
15%	30%			
0.5%	1%			

Bias and Variance

Training error	Dev error	Bias(Training error)	Variance(Dev error - Training error)	Conclusions
1%	11%	1%	10%	High variance, overfitting
15%	16%	15%	1%	High bias, underfitting
15%	30%	15%	15%	High bias and high variance, poor performance
0.5%	1%	0.5%	0.5%	Low bias and low variance, good performance

Bias vs. Variance Analysis: High Bias

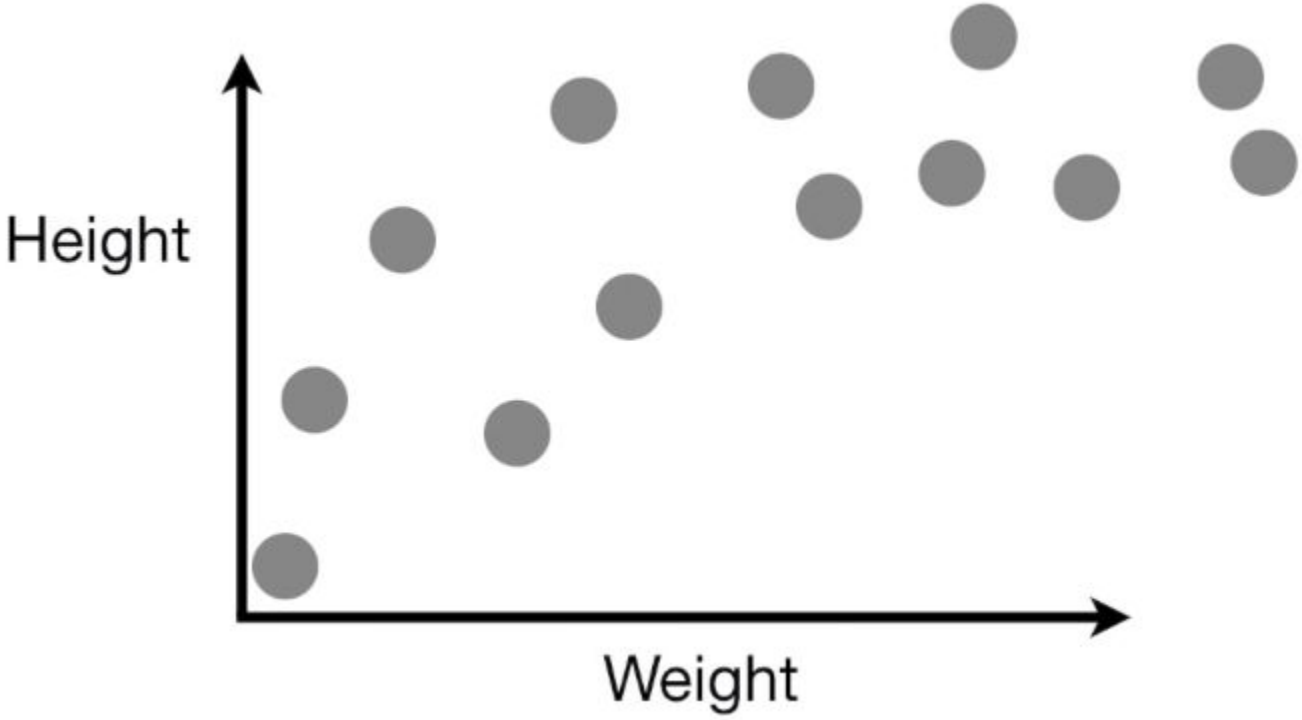


- Even training error is unacceptably high.
  - Features are not discriminative enough
- Small gap between training and test error.
  - Likely underfitting: a higher capacity model could be tried

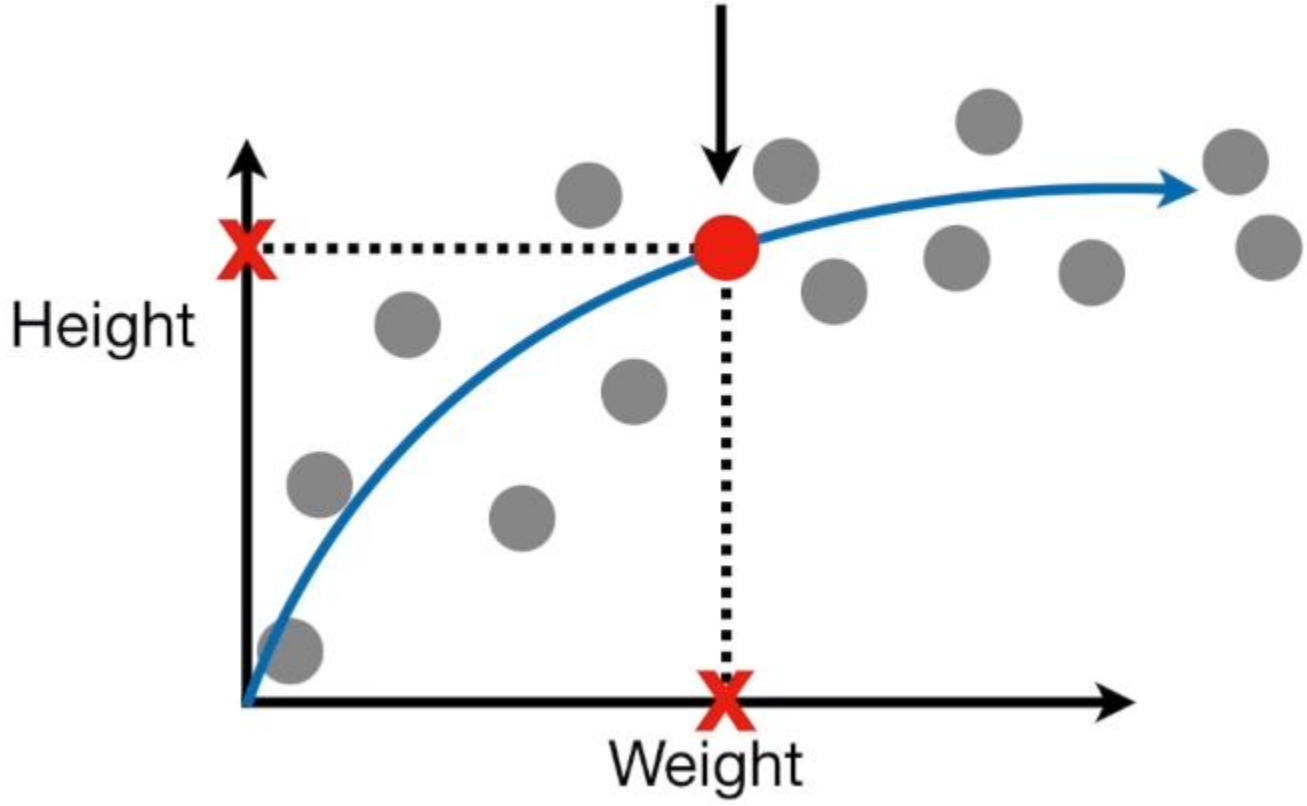
Bias vs. Variance Analysis: High Variance

- Test error still decreasing as training set size increases.
  - Suggests a larger training set will help.
- Large gap between training and test error
  - Likely overfitting

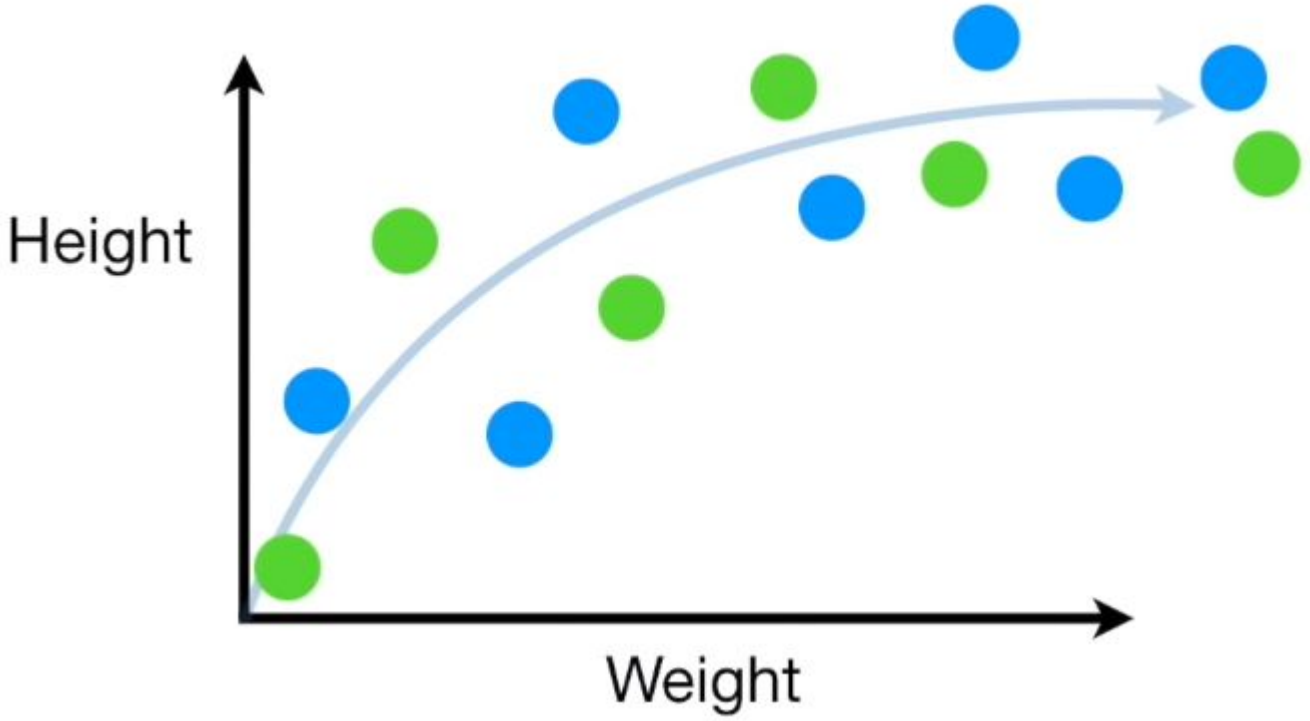
A sample data [Regression]



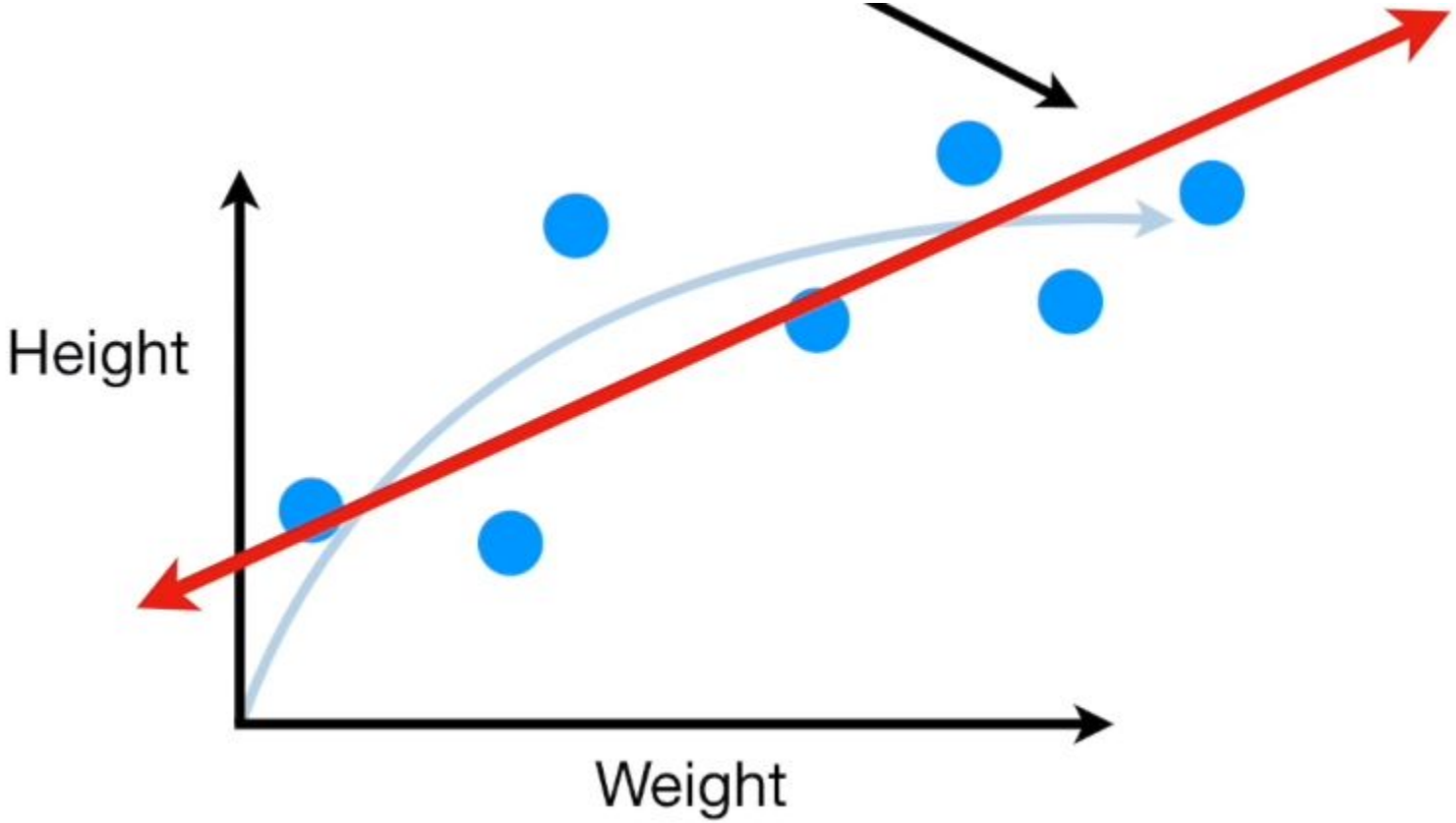
True Relationship



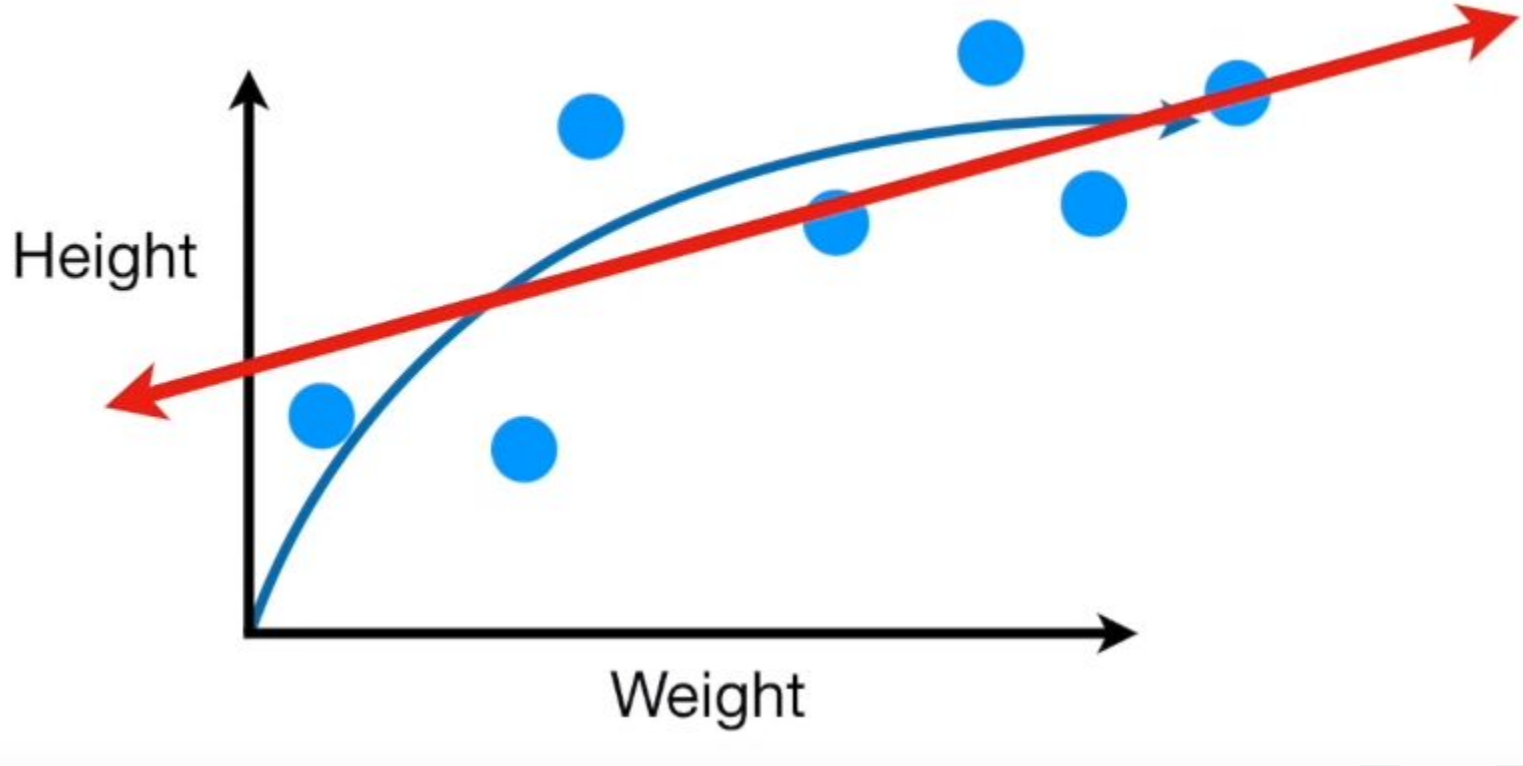
Training and Testing Data



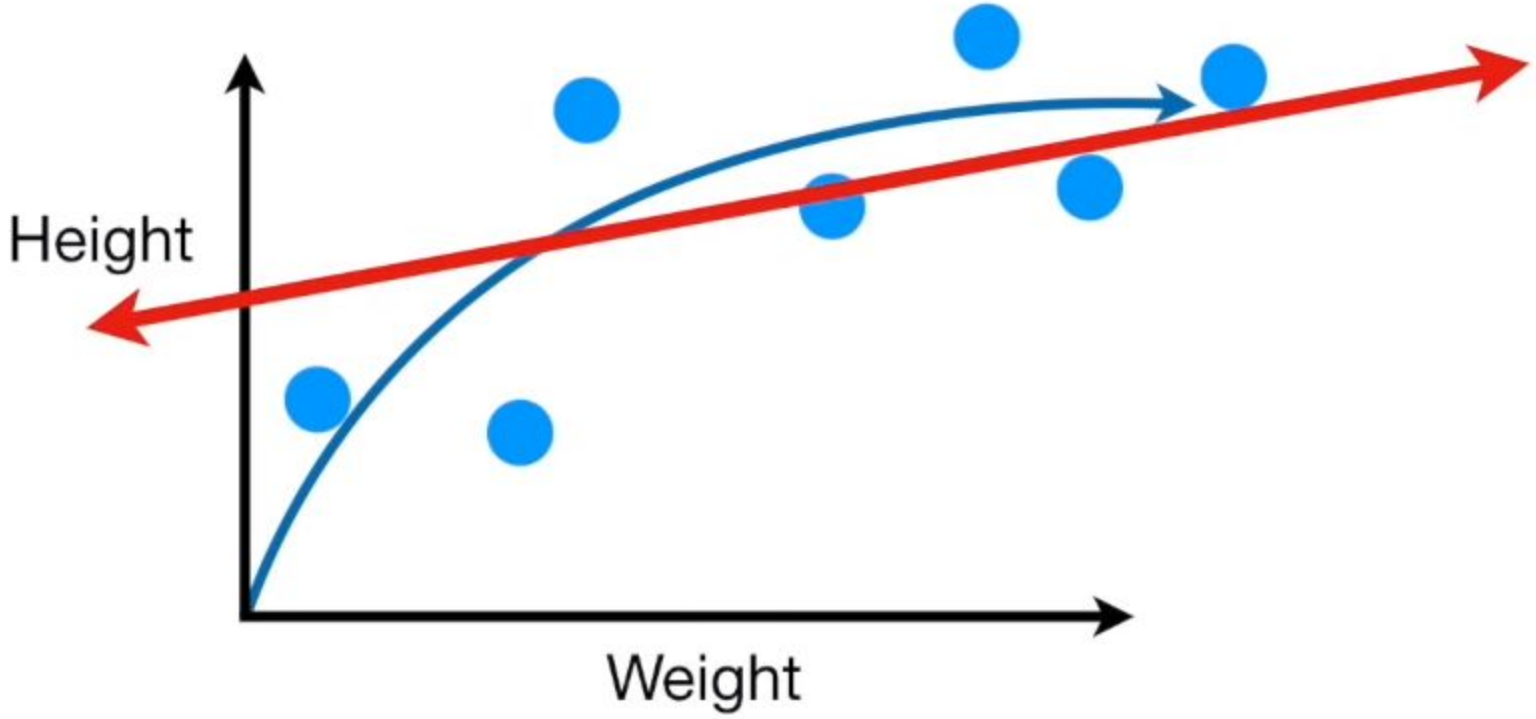
Linear Regression Fit - I



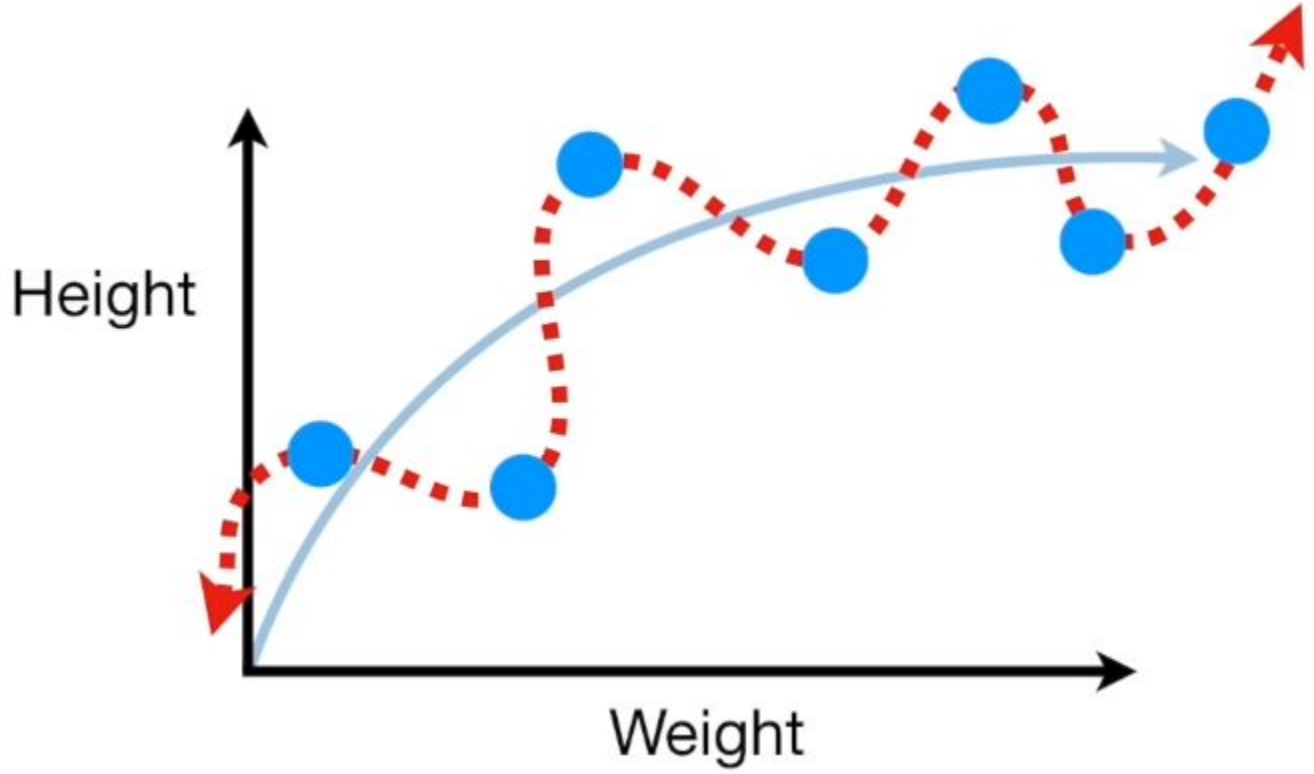
Linear Regression Fit - II



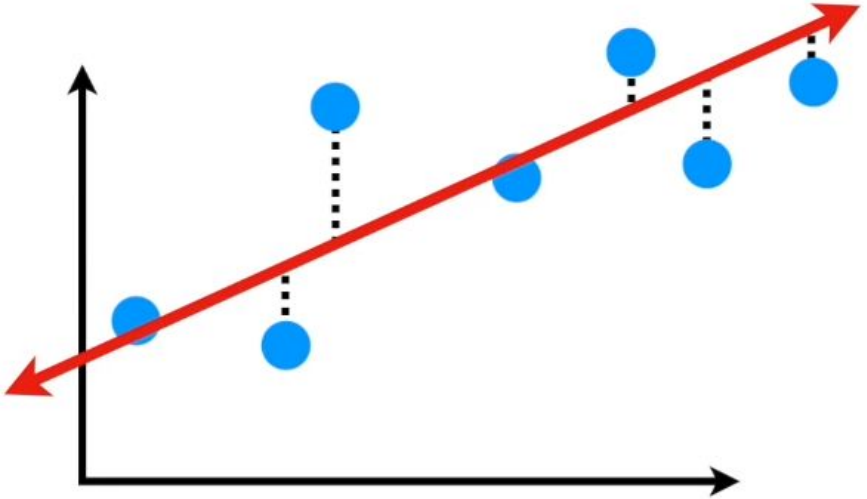
Linear Regression Fit - III

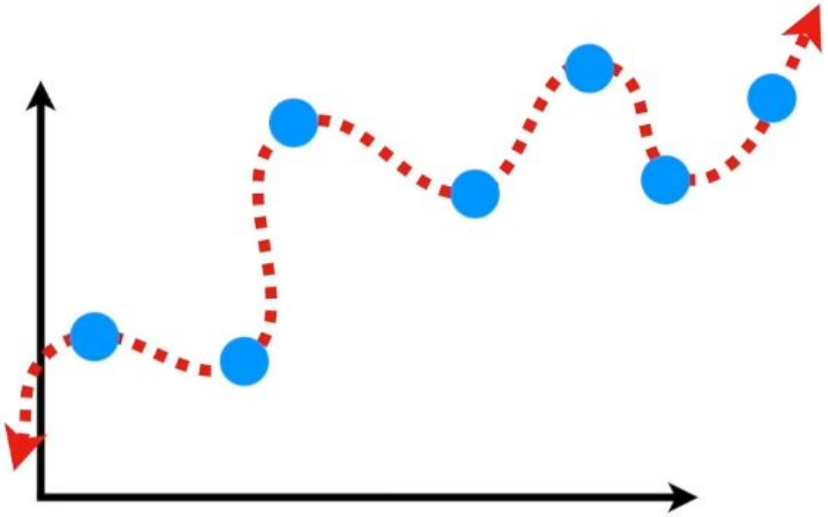


Polynomial Fit

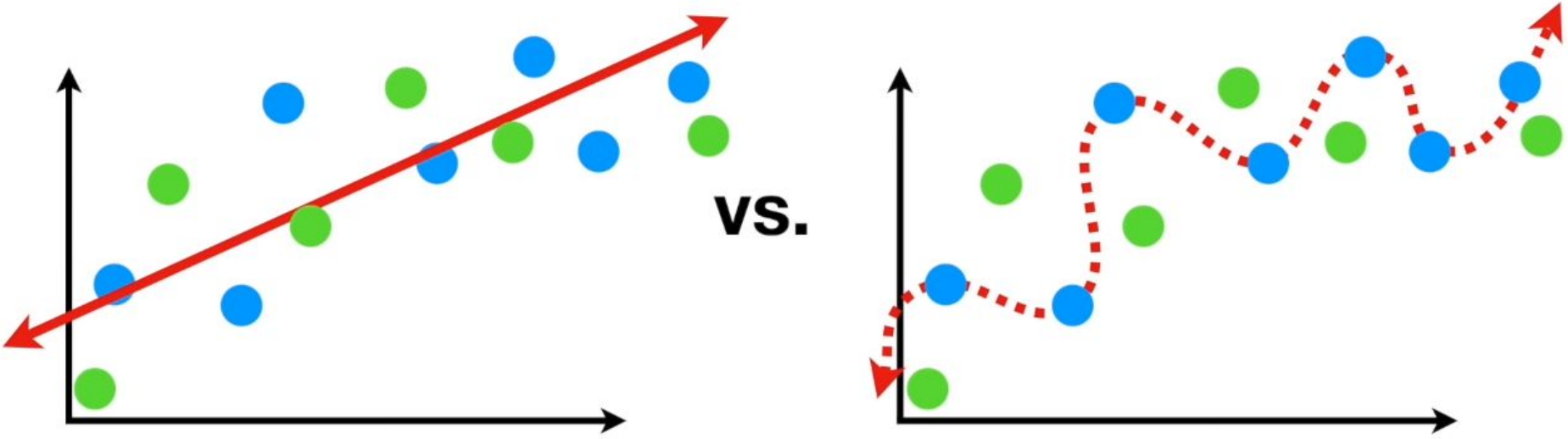


Bias

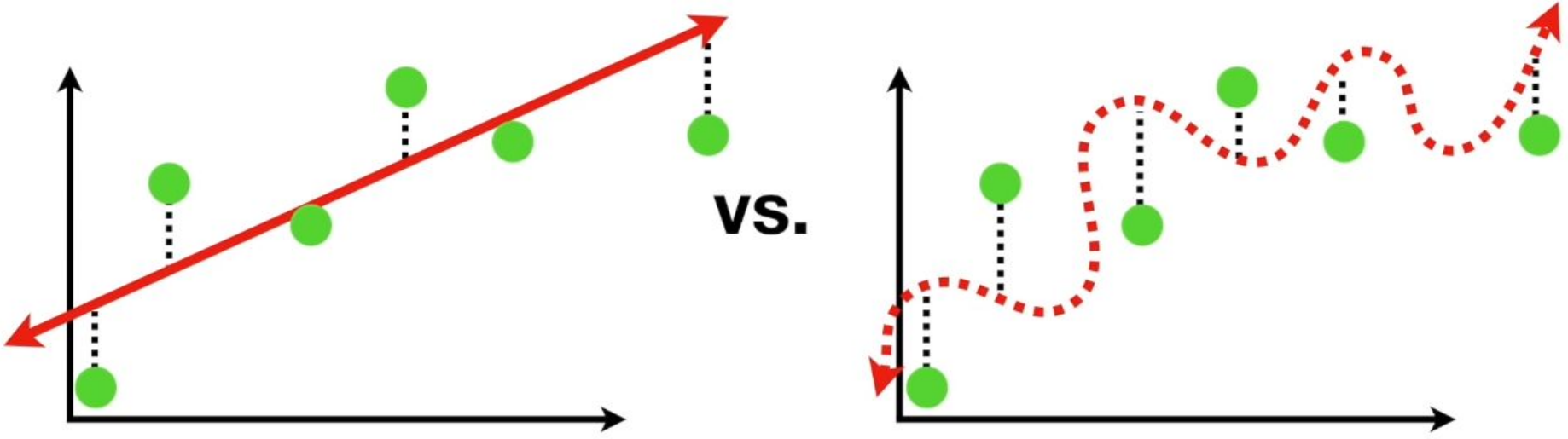




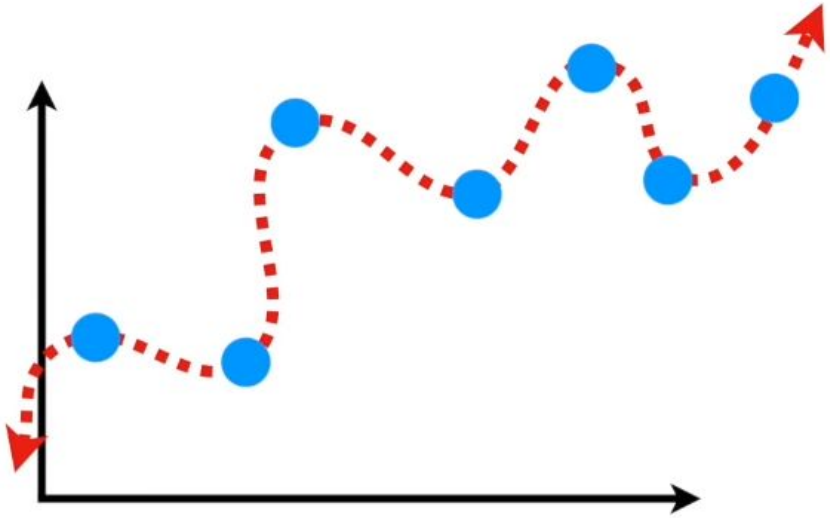
Performance on Testing Data

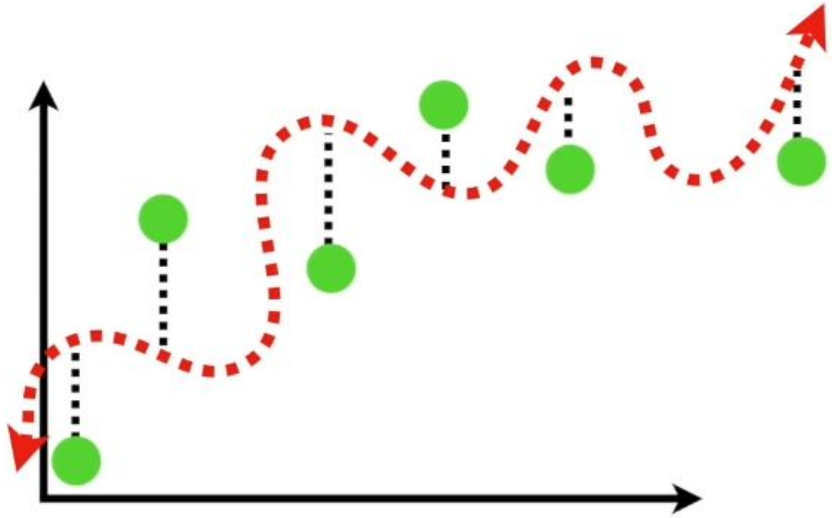


Performance on Testing Data

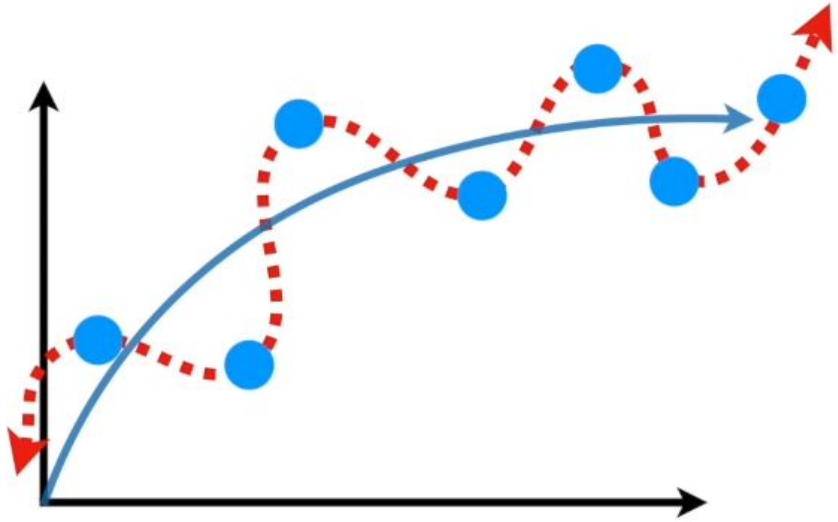


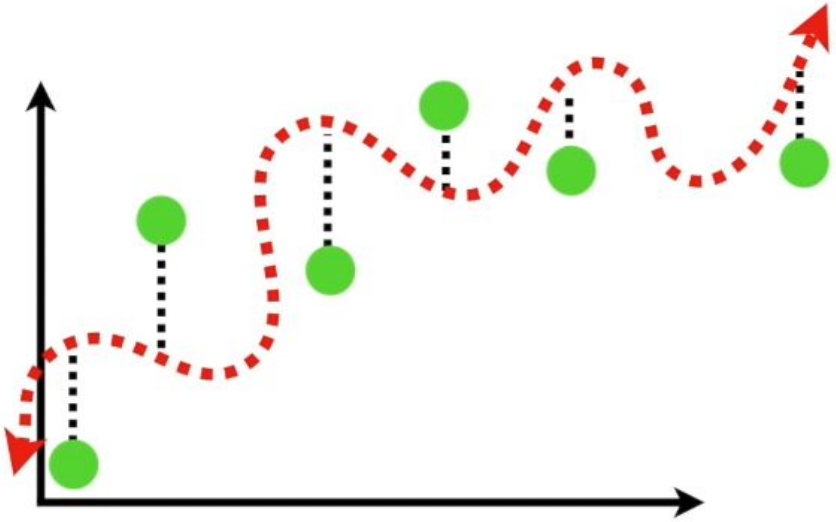
Variance



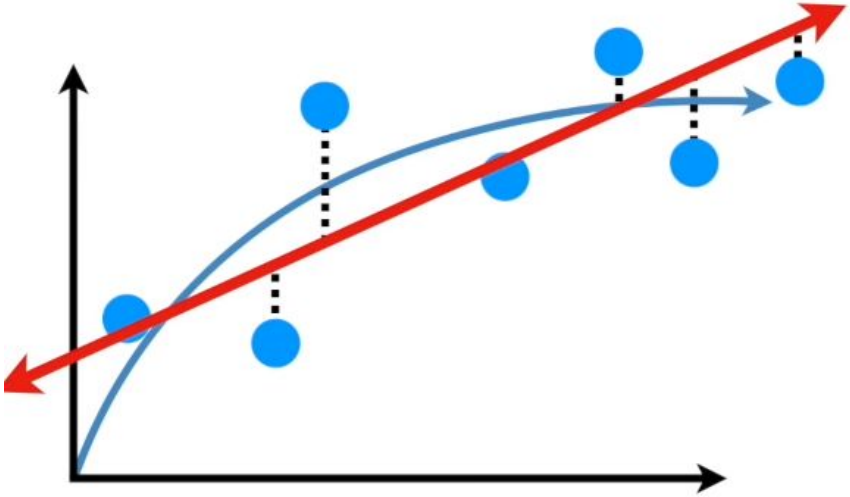


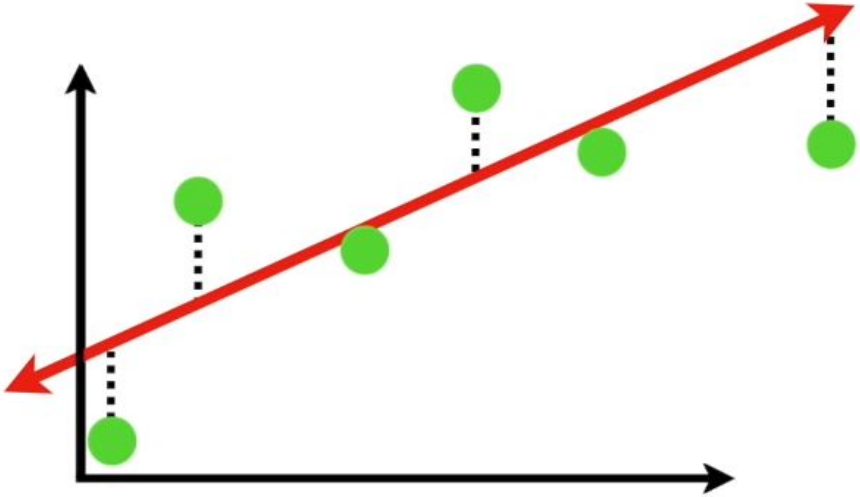
Low Bias and High Variance: Overfit



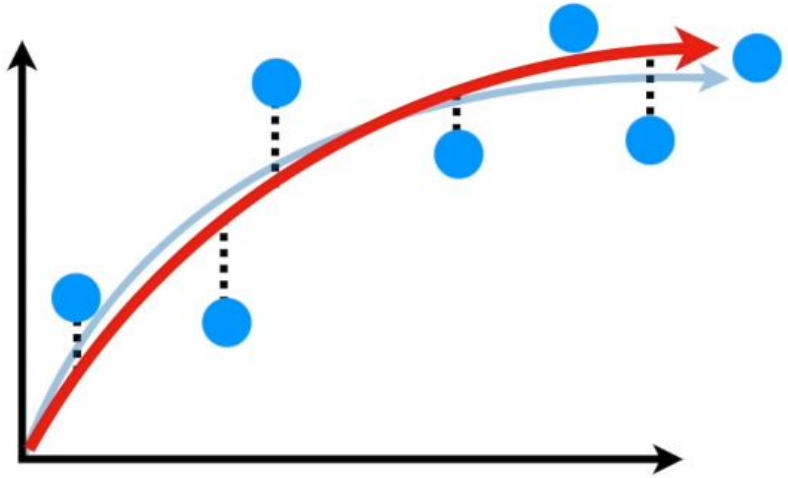


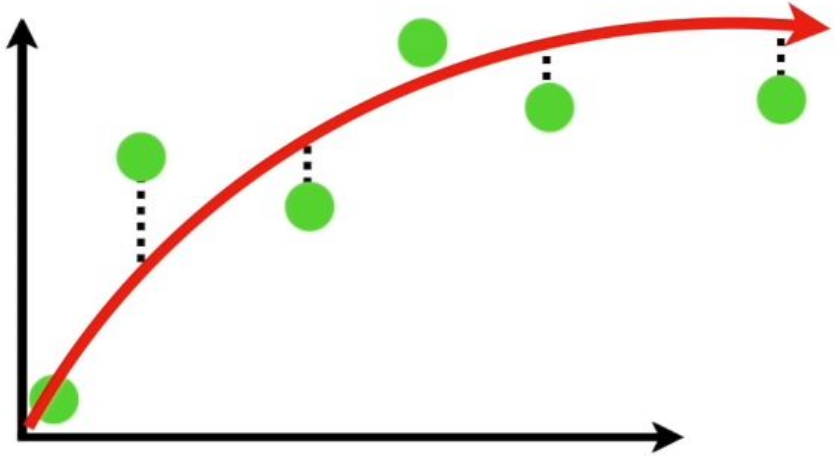
High Bias and Low Variance: Underfit



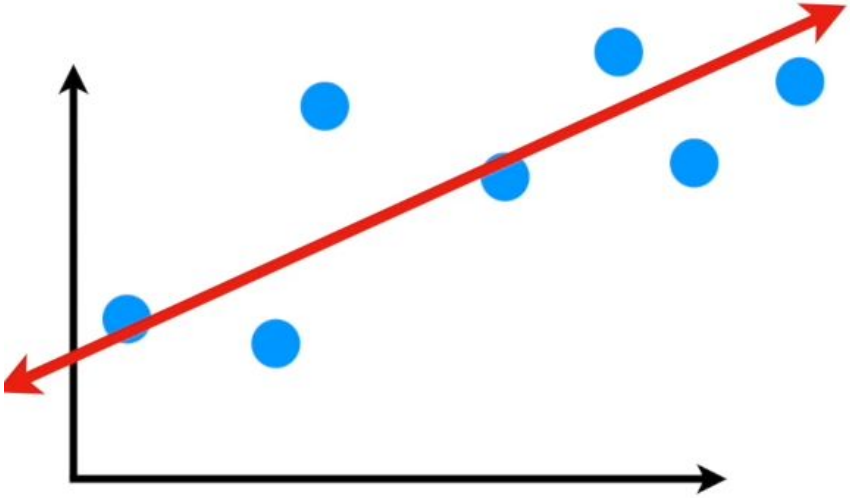


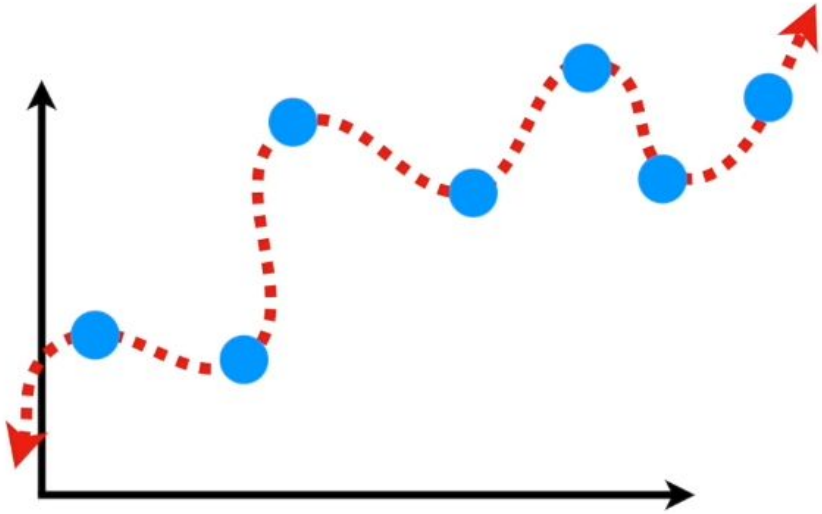
Ideal: Low Bias and Low Variance



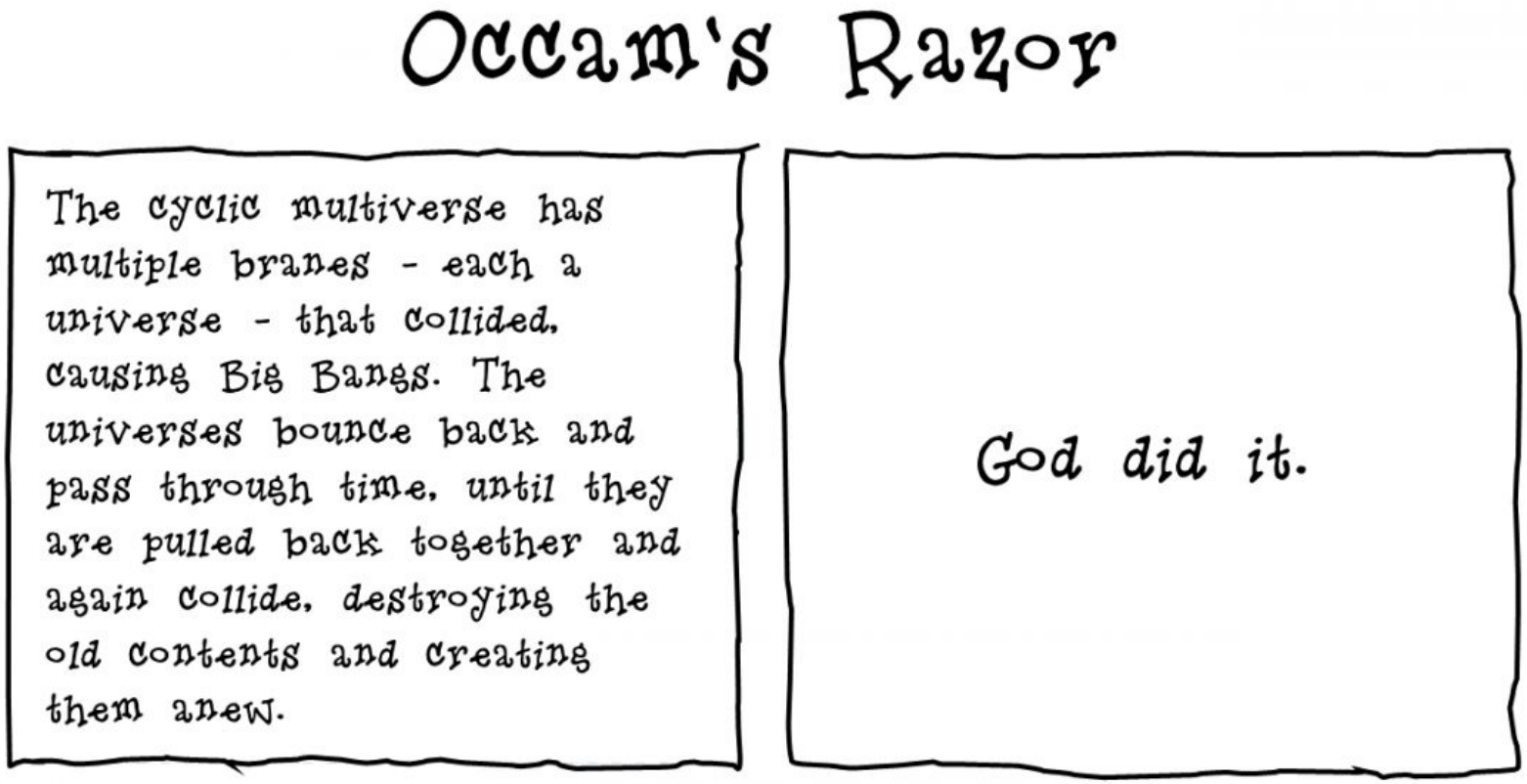


Optimal Solution in between





Occam's Razor



Practice Question – I

Question: Suppose your model is demonstrating high variance across different training sets. Which of the following is NOT a valid way to try and reduce the variance?

A. Increase amount of training data in each training set

B. Change the loss function for error minimisation

C. Decrease model complexity

D. Reduce noise in the training dataset

Practice Question – I

Answer: B

- High variance across different sets implies that it is a case of overfitting in the model.
  - Due to this, we can do all of the options A, C and D to reduce the overfitting constraint.
- However, we cannot change the loss function used for error minimisation since it does not have a direct effect on variance encountered by the model across different training sets.

Practice Question – II

Question: We are given a small dataset. The performance on this data after training a linear model is not satisfactory. Is switching to a polynomial model a reasonable option to try?

Practice Question – II

Question: We are given a small dataset. The performance on this data after training a linear model is not satisfactory. Is switching to a polynomial model a reasonable option to try?

Answer: No, it is not a reasonable option to try.

- Polynomial model is likely to overfit on the small dataset, will not generalize.
- Might be a high variance problem. Polynomial model will increase the variance.
- Try to collect more data, if possible.
- Try to use a smaller set of features, if possible.
- We can try K-Fold cross validation.

Revisiting MSE

- Known (Observed) function is $y = f(x) + \varepsilon$, where
  - Observed value = y; actual value = f(x)
  - ε is normally distributed with zero mean and standard deviation σ

- Given a set of training examples, $\{(x_i, y_i)\}$,
  - we fit an hypothesis $h(x) = w^T x + b$ to the data to minimize the squared error; $MSE = \Sigma_i [y_i - h(x_i)]^2$

- Given a new data point x^* (with observed value $y^* = f(x^*) + \varepsilon$), we would like to understand the expected prediction error $E[(h(x^*) - y^*)^2]$

Bias-Variance-Noise Decomposition: Lemma

- Let Z be a random variable with probability distribution P(Z)
- Let $\underline{Z} = E_P[\, Z \,]$ be the average value of Z
- Lemma: $E[(Z - \underline{Z})^2] = E[Z^2] - \underline{Z}^2$

- $E[(Z - \underline{Z})^2] = E[Z^2 - 2\, Z\underline{Z} + \underline{Z}^2]$
  $= E[Z^2] - 2E[Z]\underline{Z} + \underline{Z}^2$
  $= E[Z^2] - 2\underline{Z}^2 + \underline{Z}^2$
  $= E[Z^2] - \underline{Z}^2$

- Corollary: $E[Z^2] = E[\, (Z - \underline{Z})^2 \,] + \underline{Z}^2$

Bias-Variance-Noise Decomposition: Derivation

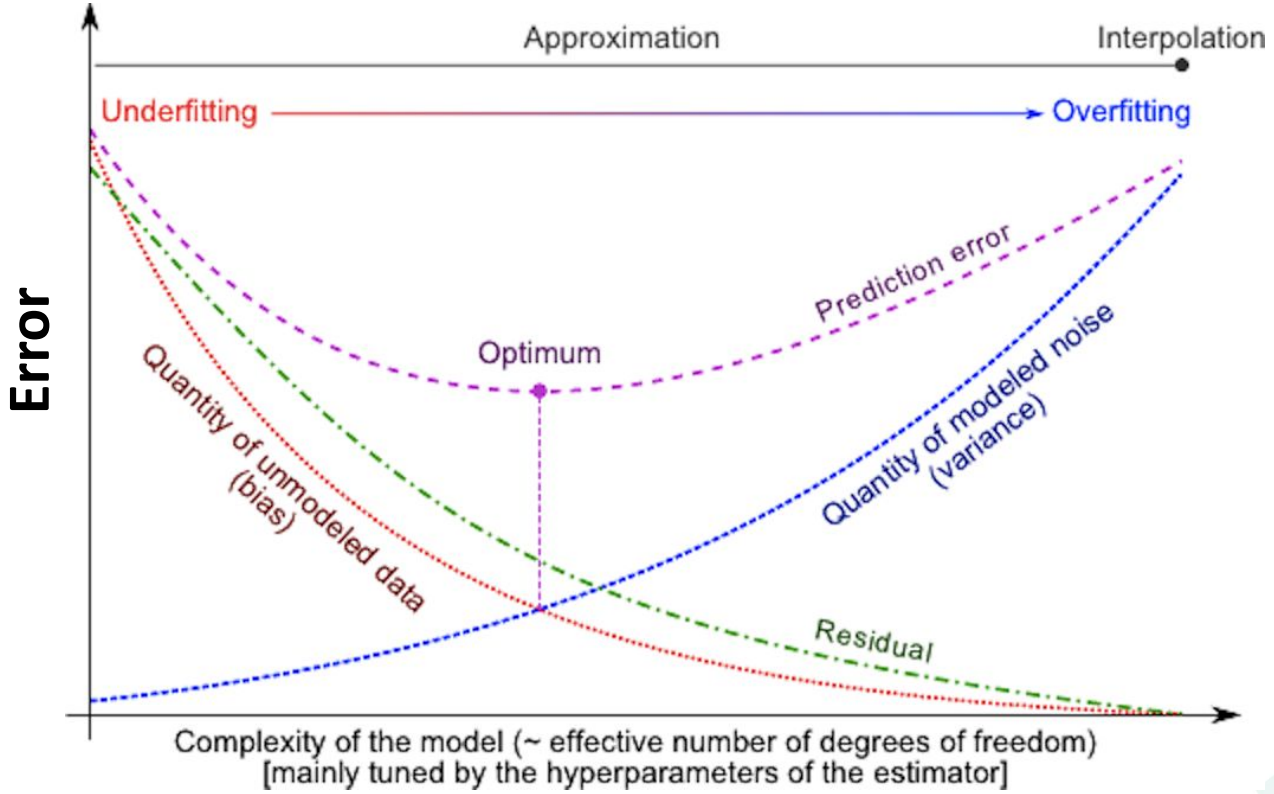
- $E[(h(x^*) - y^*)^2] = E[h(x^*)^2 - 2h(x^*)\, y^* + y^{*2}]$
  $= E[\, h(x^*)^2] - 2E[h(x^*)]E[y^*] + E[y^{*2}]$
  $= E[(h(x^*) - \underline{h(x^*)})^2] + \underline{h(x^*)}^2$ (lemma)
  $- 2\, \underline{h(x^*)} f(x^*)$ ($E(y^*) = E[f(x^*) + \varepsilon] = f(x^*)$)
  $+ E[(y^* - f(x^*))^2] + f(x^*)^2$ (lemma)
  $= E[\, (h(x^*) - \underline{h(x^*)})^2] + [\text{variance}]$
  $(\underline{h(x^*)} - f(x^*))^2 + [\text{bias}^2]$
  $E[\, (y^* - f(x^*))^2]$ [noise]

Bias-Variance-Noise Decomposition

- $E[(h(x^*) - y^*)^2] = E[(h(x^*) - \underline{h(x^*)})^2] + (\underline{h(x^*)} - f(x^*))^2 + E[(y^* - f(x^*))^2]$, where
  $\underline{h(x^*)} = E_p[h(x^*)]$ be the average value of $h(x^*)$
  $= Var(h(x^*)) + Bias(h(x^*))^2 + E[\varepsilon^2]$
  $= Var(h(x^*)) + Bias(h(x^*))^2 + \sigma^2$
- Expected prediction error = Variance + $Bias^2$ + $Noise^2$

- Variance = Describes how much the model varies from one training set to another training set.
- $Bias^2$ = Describes the <u>average-error</u> of the model.
- $Noise^2$ = Describes how much *actual value* varies from *known value*

Bias vs. Variance Analysis

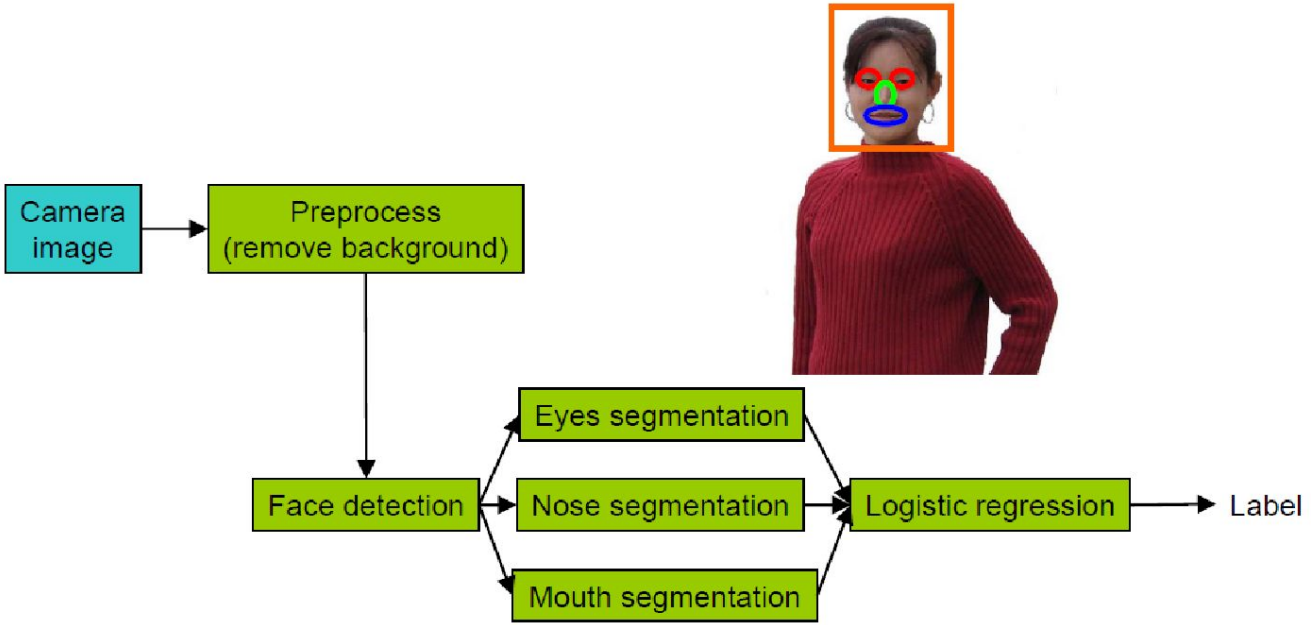


Diagnostics for ML Algorithms

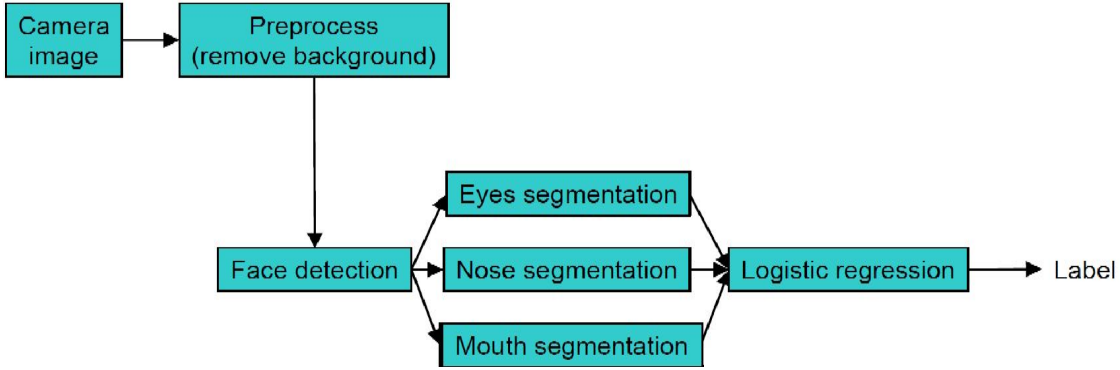
• Try getting more training examples.	• Fixes high variance.
• Try a smaller set of features.	• Fixes high variance.
• Try a larger set of features.	• Fixes high bias.
• Try changing the features.	• Fixes high bias.
• Run gradient descent for more iterations.	• Fixes optimization algorithm.
• Try Newton's method instead of gradient descent.	• Fixes optimization algorithm.
• Use a different value for reg. parameter λ.	• Fixes optimization objective.
• Try using a different model (e.g., SVM).	• Fixes optimization objective

Debugging ML Systems

- Many applications combine many different learning components into a “pipeline”, e.g., Face recognition from images [toy example].



Error Analysis



How much error is attributable to each of the components?

Plug in ground-truth for each component, and see how accuracy changes.

Conclusion: Most room for improvement in face detection and eyes segmentation.

Component	Accuracy
Overall system	85%
Preprocess (remove background)	85.1%
Face detection	91%
Eyes segmentation	95%
Nose segmentation	96%
Mouth segmentation	97%
Logistic regression	100%