Hyperparameter Selection

- Every ML model has some hyperparameters that need to be tuned, e.g.,
  - K in KNN or ϵ in ϵ-NN
  - Choice of distance to use in LwP or nearest neighbors

- Would like to choose h.p. values that would give best performance on test data

Generalization

Training set (labels known)

Test set (labels unknown)

- How well does a learned model generalize from the data it was trained on to a new test set?

Slide credit: L. Lazebnik

Generalization

- Components of generalization error

- **Bias:** Assumptions made by a model to make a function easier to learn. It is actually the error rate of the training data. When the error rate has a high value, we call it High Bias and when the error rate has a low value, we call it low Bias.
- **Variance:** The error rate of the testing data is called variance. When the error rate has a high value, we call it High variance and when the error rate has a low value, we call it Low variance.

- **Underfitting:** model is too "simple" to represent all the relevant class characteristics
- **Overfitting:** model is too "complex" and fits irrelevant characteristics (noise) in the data

Slide credit: L. Lazebnik

Reasons for Underfitting:

- High bias and low variance
- The size of the training dataset used is not enough.
- The model is too simple.
- Training data is not cleaned and also contains noise in it.

Techniques to reduce underfitting:

- Increase model complexity
- Increase the number of features, performing feature engineering
- Remove noise from the data.
- Increase the number of epochs or increase the duration of training to get better results.

Slide credit: L. Lazebnik

Reasons for Overfitting are as follows:

- High variance and low bias
- The model is too complex
- The size of the training data

Techniques to reduce overfitting:

- Increase training data.
- Reduce model complexity.
- Early stopping during the training phase (have an eye over the loss over the training period as soon as loss begins to increase stop training).
- Ridge Regularization and Lasso Regularization
- Use dropout for neural networks to tackle overfitting.

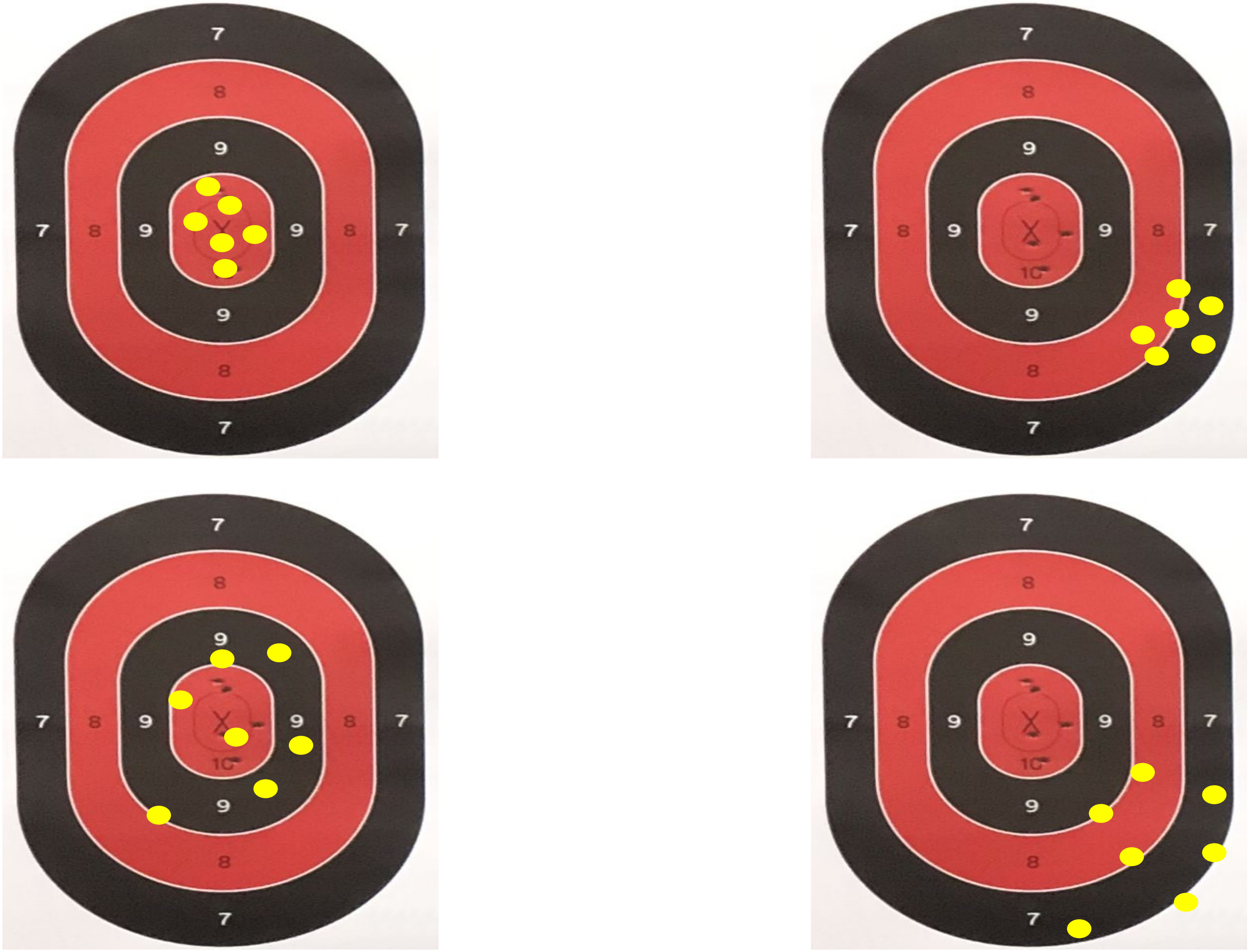
Bias-Variance Trade-off

Low Bias

High Bias

Low Variance

High Variance



Bias-Variance Trade-off

$$E(MSE) = noise^2 + bias^2 + variance$$

Unavoidable error

Error due to incorrect assumptions

Error due to variance of training samples

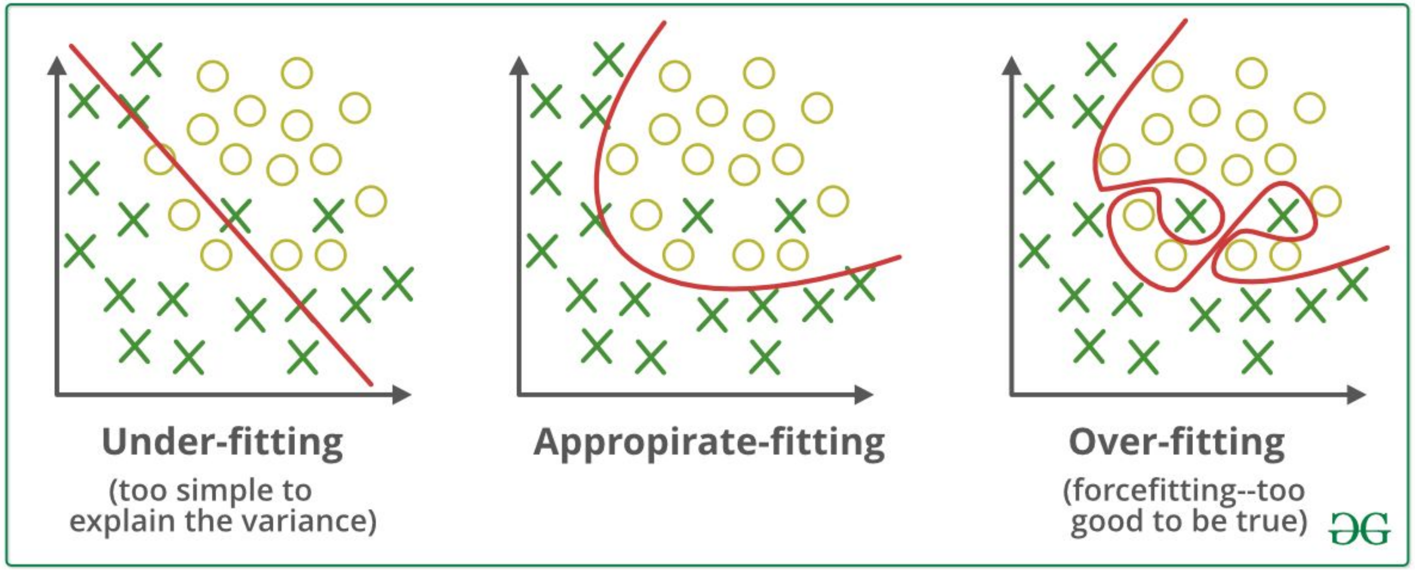
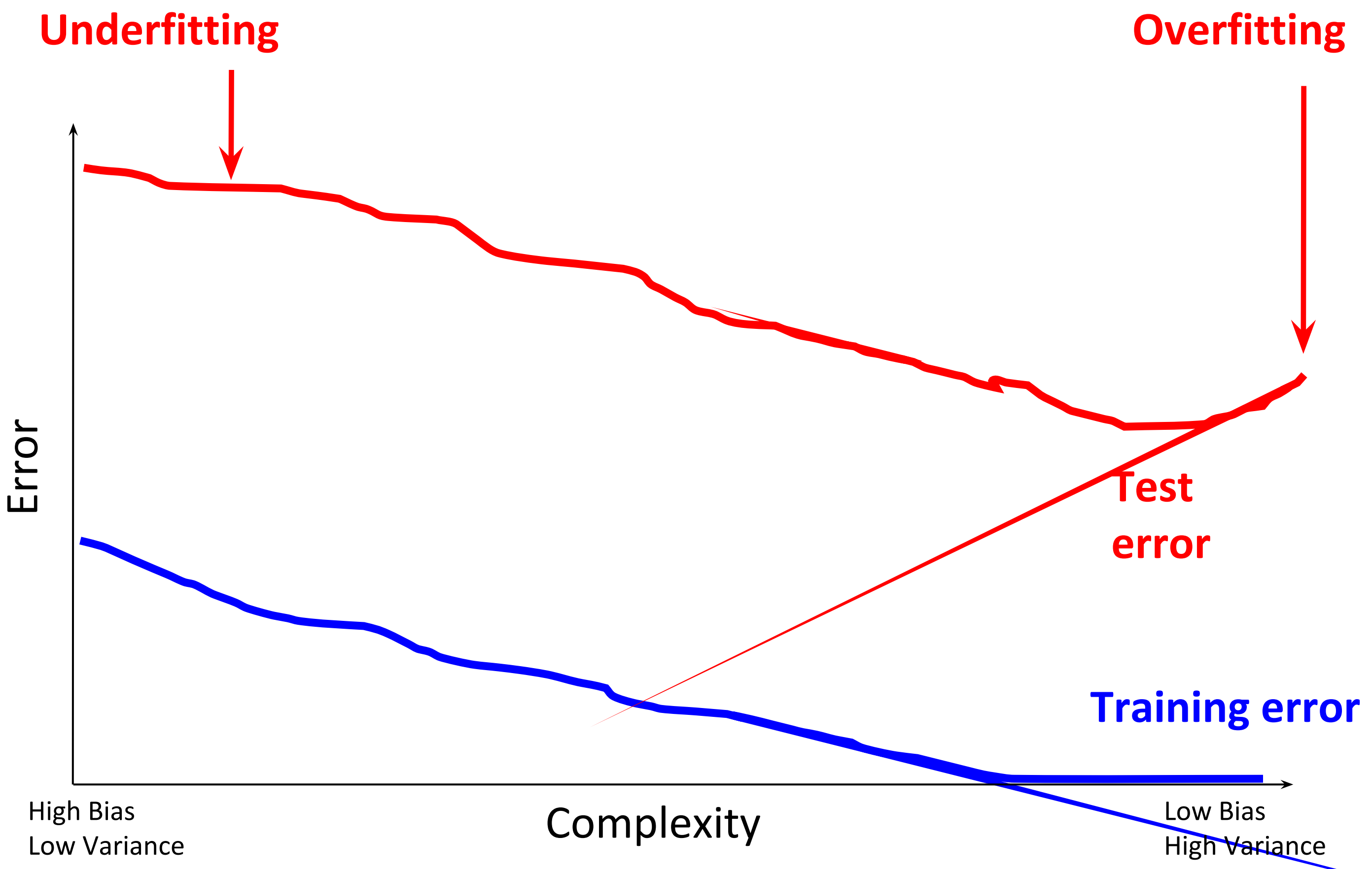


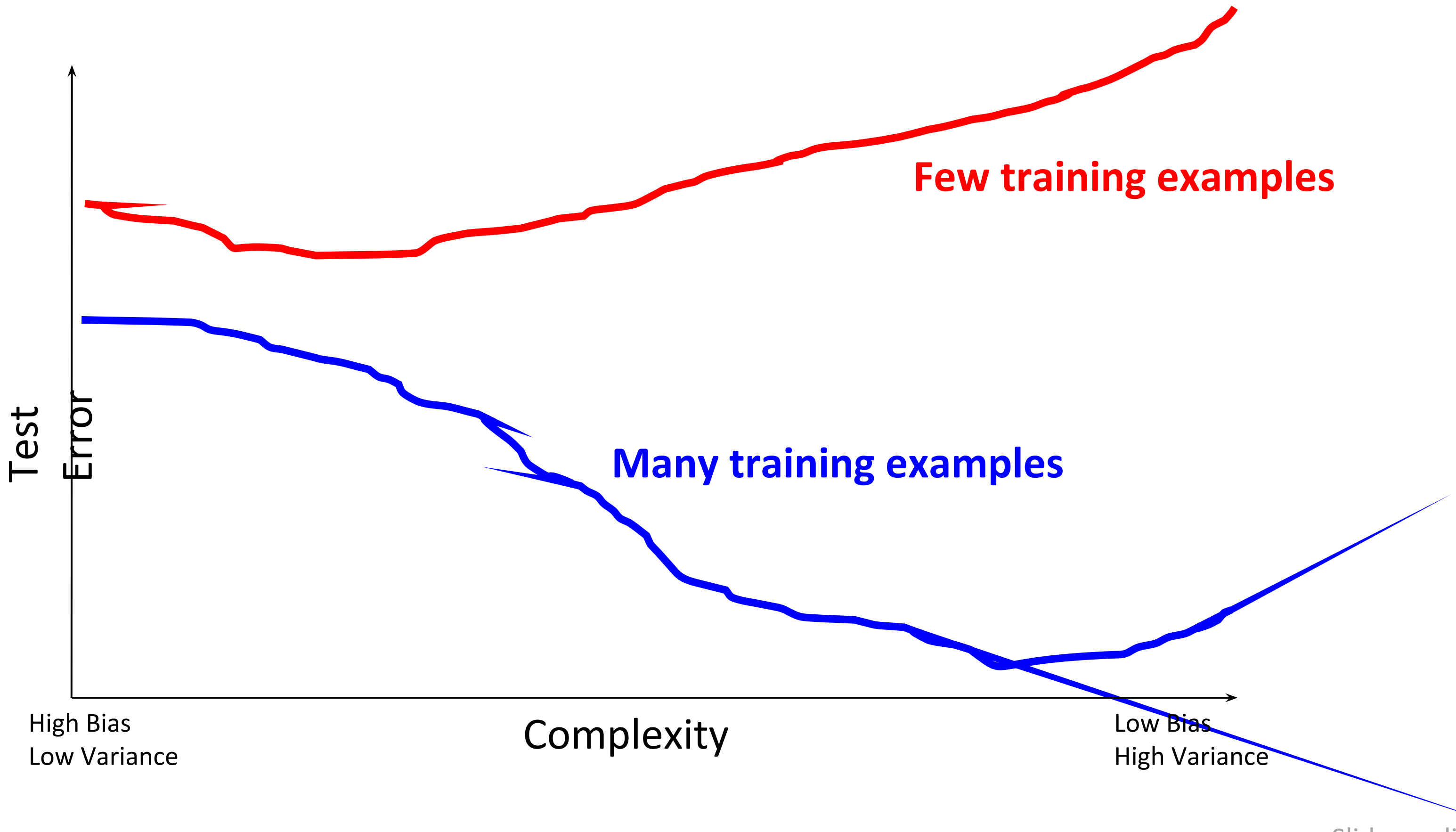
Image credit: geeksforgeeks.com
Slide credit: D. Hoiem

Bias-variance tradeoff



Slide credit: D. Hoiem

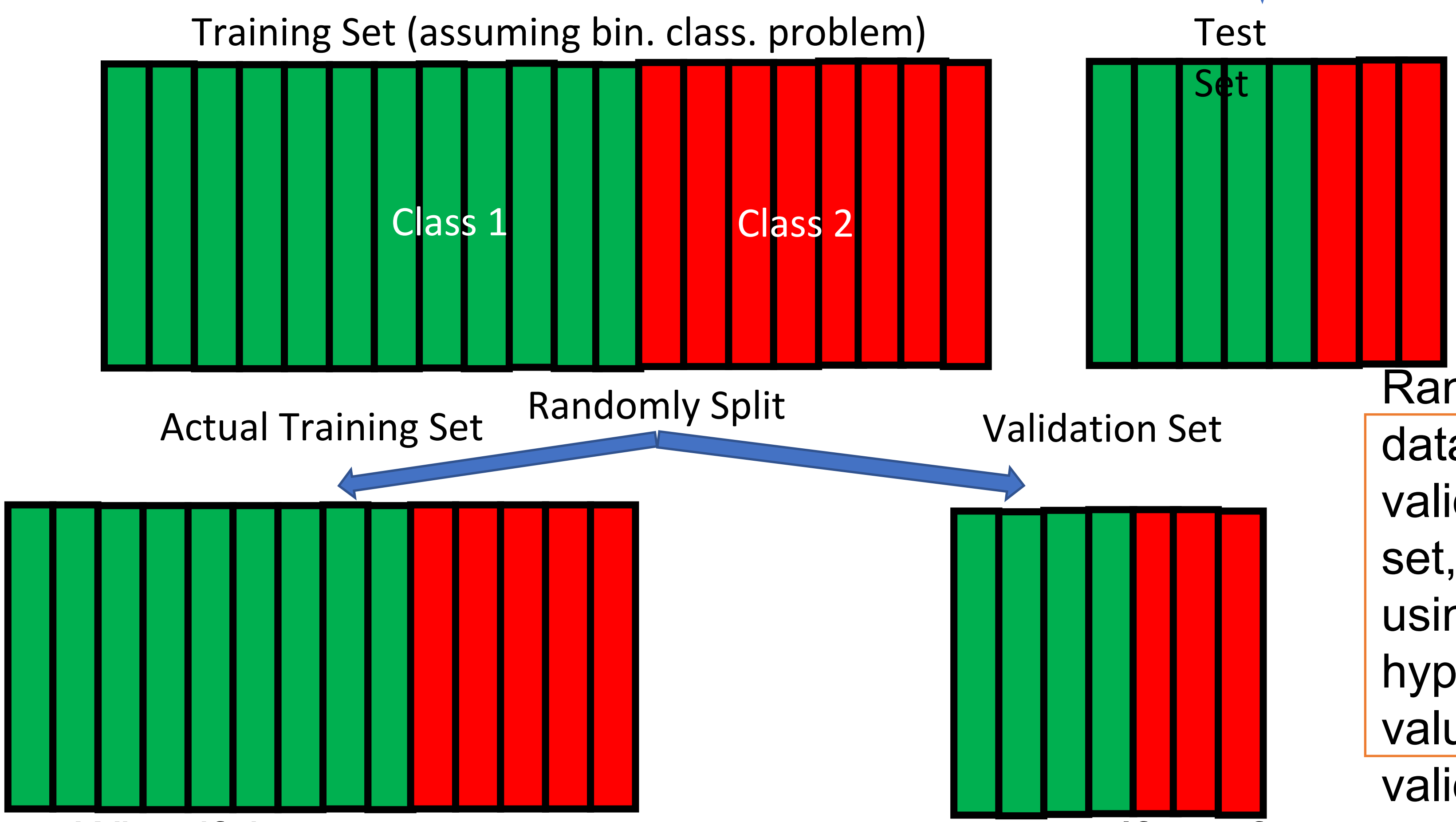
Bias-variance tradeoff



Slide credit: D. Hoiem

Cross-Validation

No peeking while building the model



Note: Not just h.p. selection; we can also use CV to pick the best ML model from a set of different ML models (e.g., say we have to pick between two models we may have trained - LwP and nearest neighbors. Can use CV to choose the better one.

Randomly split the original training data into actual training set and validation set. Using the actual training set, train several times, each time using a different value of the hyperparam. Pick the hyperparam value that gives best accuracy on the validation set

What if the random split is unlucky (i.e., validation data is not like test data)?

If you fear an unlucky split, try multiple splits. Pick the hyperparam value that gives the best average CV accuracy across all such splits. If you are using N splits, this is called N–fold cross validation