Week 7: Model Training and Evaluation

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Which model is the best choice?

$$h_\theta(x) = \theta_0 + \theta_1 x_1$$

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2^2$$

...

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2^2 + ... + \theta_9 x_9^9$$

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2^2 + ... + \theta_9 x_9^9 + \theta_{10} x_{10}^{10}$$

Two Methods in Training process (1/2)

- **Hold-out Method**
  - 80% Train set
  - 20% Test set
- Pros:
  - Simple
  - Fast
- Cons:
  - Overfitting

Two Methods in Training process (2/2)

- **Cross validation Method**
  - Training set: 60%
  - Validation set: 20%
  - Test set: 20%
- Pros:
  - Variance (Overfitting) is reduced
- Cons:
  - Slow

Which one reduces the error caused by overfit or underfit?

- Get more training data
- Try smaller sets of features
- Try getting additional features
- Try adding polynomial features
- Try decreasing λ (Ridge penalty)
- Try increasing λ (Ridge penalty)

Bias vs Variance

- **Underfit:** High Bias (Linear Model: $\theta_0 + \theta_1 x$)
- **Good Fit:** Proper Balance (Quadratic Model: $\theta_0 + \theta_1 x + \theta_2 x^2$)
- **Overfit:** High Variance (Higher-order Polynomial Model: $\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$)

Diagnosis: Bias vs Variance (Polynomial Degree)

- Plot error (MSE) against polynomial degree
- Low-degree polynomial: Underfitting
- Moderate-degree polynomial: Good Fit
- High-degree polynomial: Overfitting

Diagnosis: Bias vs Variance (Regularization Parameter)

- Regularization function:

$$J(\theta) = \frac{1}{2N}\sum_{i=1}^{N}(h_\theta(x_i) - y_i)^2 + \frac{\lambda}{2}\sum_{j=1}^{d}\theta_j^2 \tag{1}$$

- Increasing λ reduces variance but increases bias
- Decreasing λ reduces bias but increases variance

Effect of Training Data Size

- Increasing training data reduces variance but not bias
- Underfit: Not enough complexity to capture patterns
- Overfit: Too complex, memorizing data instead of generalizing

Error Metrics

- Confusion Matrix
- Precision, Recall, Accuracy
- F1-Score
- ROC, AUC

Confusion Matrix for Classification

	Actual Positive	**Actual Negative**
Predicted Positive	TP (True Positive)	FP (False Positive)
Predicted Negative	FN (False Negative)	TN (True Negative)

Key Metrics:

- Sensitivity (TPR): $\frac{TP}{TP+FN}$
- Specificity (TNR): $\frac{TN}{TN+FP}$
- False Positive Rate (FPR): $\frac{FP}{FP+TN}$

Accuracy, Recall, and Precision

- Accuracy: $\frac{TP+TN}{TotalPopulation}$
- Recall: $\frac{TP}{TP+FN}$
- Precision: $\frac{TP}{TP+FP}$

Imbalanced Dataset Challenges

- Accuracy alone is misleading for imbalanced datasets
- Need to consider Precision and Recall
- Example of different models and their performance metrics

Reference

- Raschka,S.(2018).Modelevaluation,modelselection, andalgorithmselectioninmachinelearning.arXivpreprint arXiv:1811.12808.