CAP 4630 – Bias Vs Variance

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Introduction to Model Performance

- Understanding Model Performance:
  - When we talk about a Machine Learning model, we refer to how well it performs in terms of accuracy and prediction errors.
  - Our goal is to design a model that generalizes well to new, unseen data, not just to the data it was trained on.
- Key Concept: Generalization:
  - A model is said to be good if it can generalize to any new input data from the problem domain.
  - Generalization helps in making accurate predictions about future data that the model has never encountered.

Overfitting and Underfitting

- Evaluating Generalization:
  - To evaluate how well a model generalizes, we compare its performance on unseen test data.
- Challenges in Generalization:
  - Overfitting: When a model performs well on training data but poorly on unseen data.
  - Underfitting: When a model performs poorly on both training and unseen data.
- Impact: Both overfitting and underfitting are major causes of poor performance in machine learning algorithms.

Bias vs Variance

Bias in Machine Learning

- What is Bias?
  - Bias refers to the error introduced by overly simplistic assumptions made by the learning algorithm.
  - These assumptions make the model easier to understand but may prevent it from capturing the full complexity of the data.
- Impact of High Bias:
  - A model with high bias is too simplified, failing to represent the relationship between input and output accurately.
  - High bias typically leads to underfitting, where the model performs poorly on both training and test data.

Consequences of High Bias

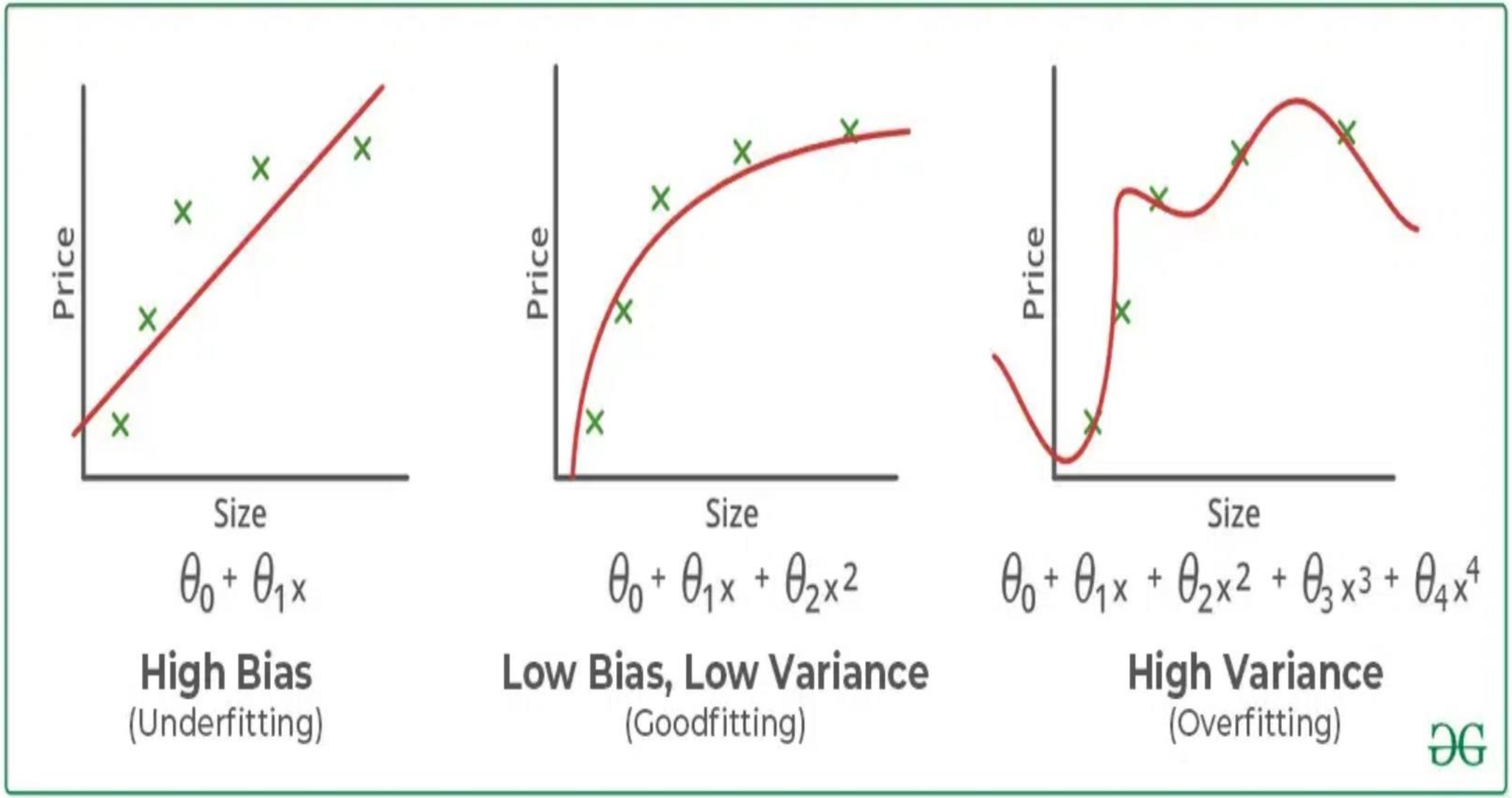
- Symptoms of High Bias:
  - Poor performance on both training and testing datasets.
  - The model is unable to capture the underlying patterns in the data.
- Example of High Bias:
  - A linear model applied to data that requires a more complex representation (e.g., nonlinear patterns).
- Real-World Implication:
  - High bias often indicates that the model needs to be more complex or have additional features to better represent the data.

Understanding Variance in Machine Learning

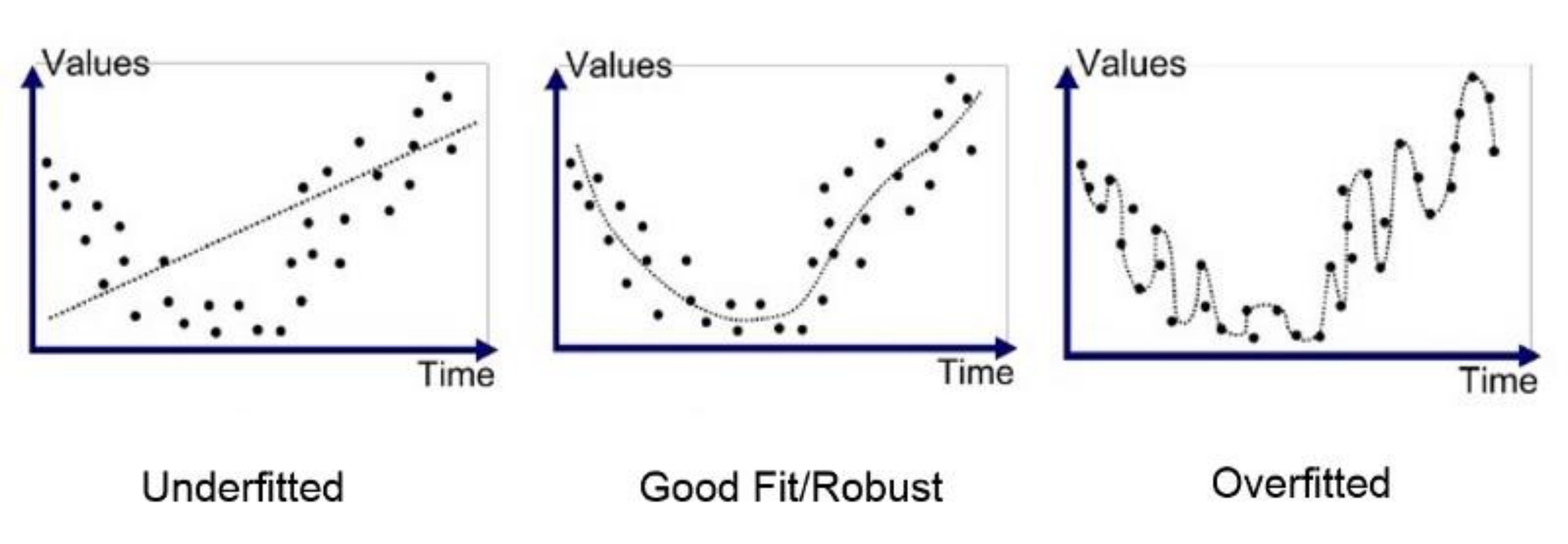
- What is Variance?
  - Variance refers to the model's sensitivity to small changes or fluctuations in the training data.
  - It is the variability in the model's predictions for different subsets or instances of the training data.
- Impact of High Variance:
  - High variance models are typically very complex and capture random noise in the training data.
  - Such models tend to perform well on the training data but fail to generalize to unseen data, leading to overfitting.

Consequences of High Variance

- Symptoms of High Variance:
  - The model performs very well on the training data but poorly on the testing data.
  - High variance means the model is too sensitive to noise and fluctuations in the training set, rather than capturing the true underlying patterns.
- Example of High Variance:
  - A highly complex decision tree model that fits perfectly to the training data but fails on test data.
- Real-World Implication:
  - High variance indicates that the model may need to be simplified by pruning or regularizing to prevent overfitting and improve generalization.



Bias and Variance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Underfitting

What is Underfitting?

- Definition: Underfitting occurs when a machine learning model is too simple to capture the underlying patterns in the data.
  - This leads to poor performance both on the training and testing datasets, as the model fails to learn from the data.
- Characteristics:
  - The model exhibits high bias and low variance.
  - It performs poorly on both known (training) data and unseen (test) data, making inaccurate predictions.

Causes of Underfitting

- Model is too simple: The model lacks complexity to capture data relationships (e.g., using a linear model for nonlinear data).
- Inadequate features: Input features do not adequately represent the factors influencing the target variable.
- Small training dataset: Insufficient data may prevent the model from learning key patterns.
- Excessive regularization: Too much regularization restricts the model's ability to learn effectively.

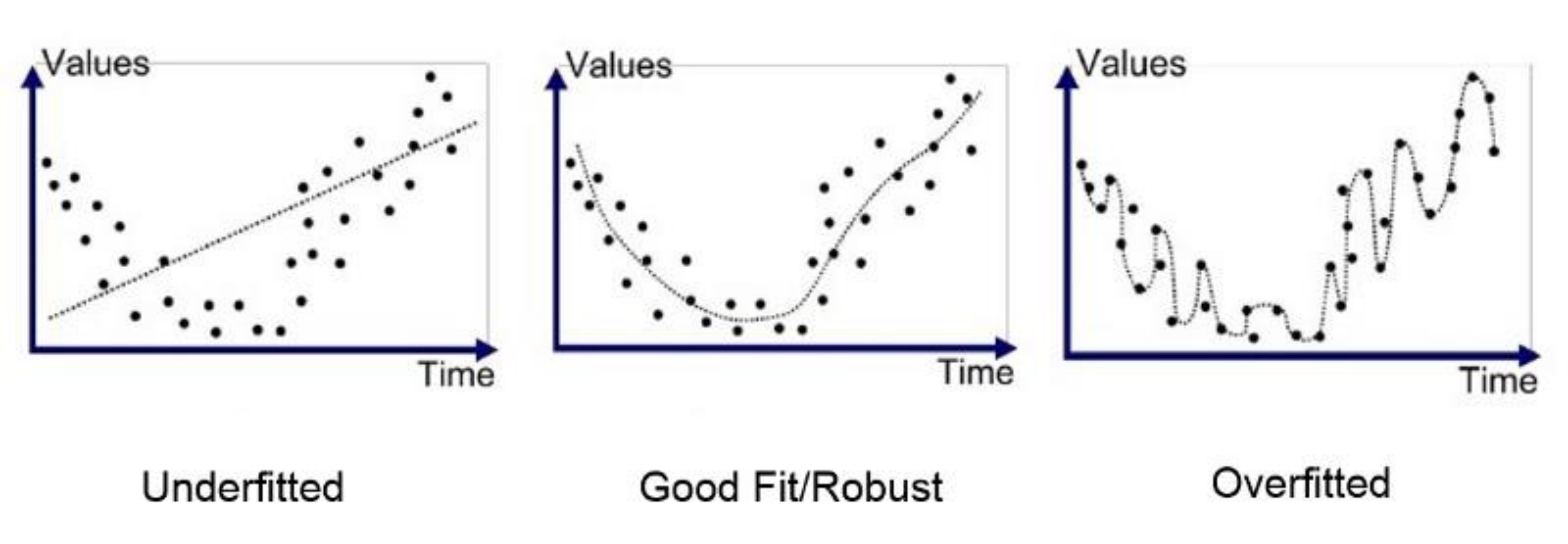
How to Address Underfitting

- Increase model complexity: Use more advanced algorithms to capture data complexities.
- Add more features: Perform feature engineering to improve representation.
- Remove noise: Clean the dataset to enhance model accuracy.
- Train longer: Increase the number of epochs or training time to allow the model to better learn from the data.

Overfitting

What is Overfitting?

- Definition: Overfitting occurs when a model learns not only the underlying patterns in the training data but also the noise and random fluctuations, causing poor generalization to unseen data.
- Key Symptoms:
  - Low bias, but high variance.
  - Excellent performance on training data, but poor performance on test data.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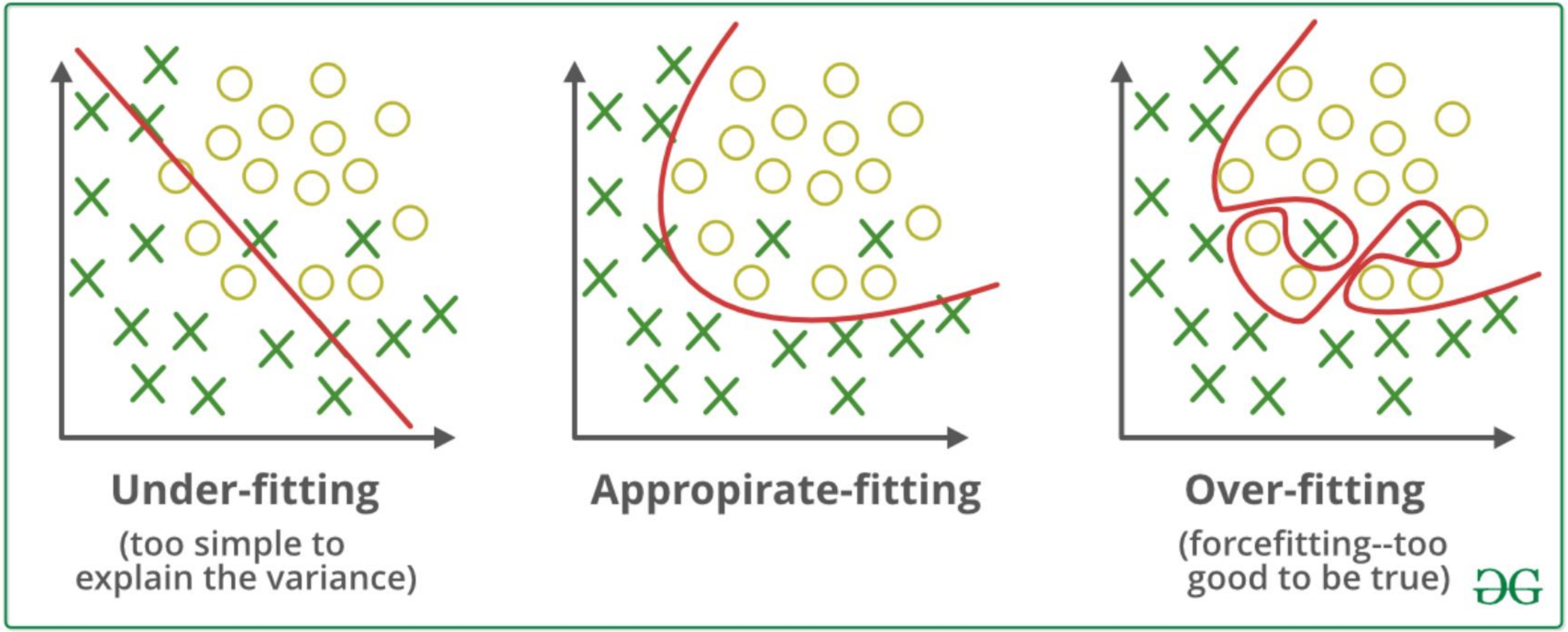
Causes of Overfitting

- Model complexity: The model is too complex, capturing noise and irrelevant patterns in the training data.
- Insufficient data: Small training datasets can lead to models that overfit due to learning irrelevant details.
- Excessive training: Training for too many epochs can cause the model to fit the data too closely

Techniques to Prevent Overfitting

- **Increase training data**: Provide more examples to help the model learn better generalizations.
- **Reduce model complexity:** Use simpler models or limit the parameters (e.g., pruning decision trees, reducing the number of layers in a neural network).
- **Regularization techniques:**
  - Lasso (L1) and Ridge (L2) regularization.
- **Early stopping:** Stop training when the performance on validation data begins to degrade.
- **Dropout (for neural networks):** Randomly drop neurons during training to avoid over-reliance on specific features.



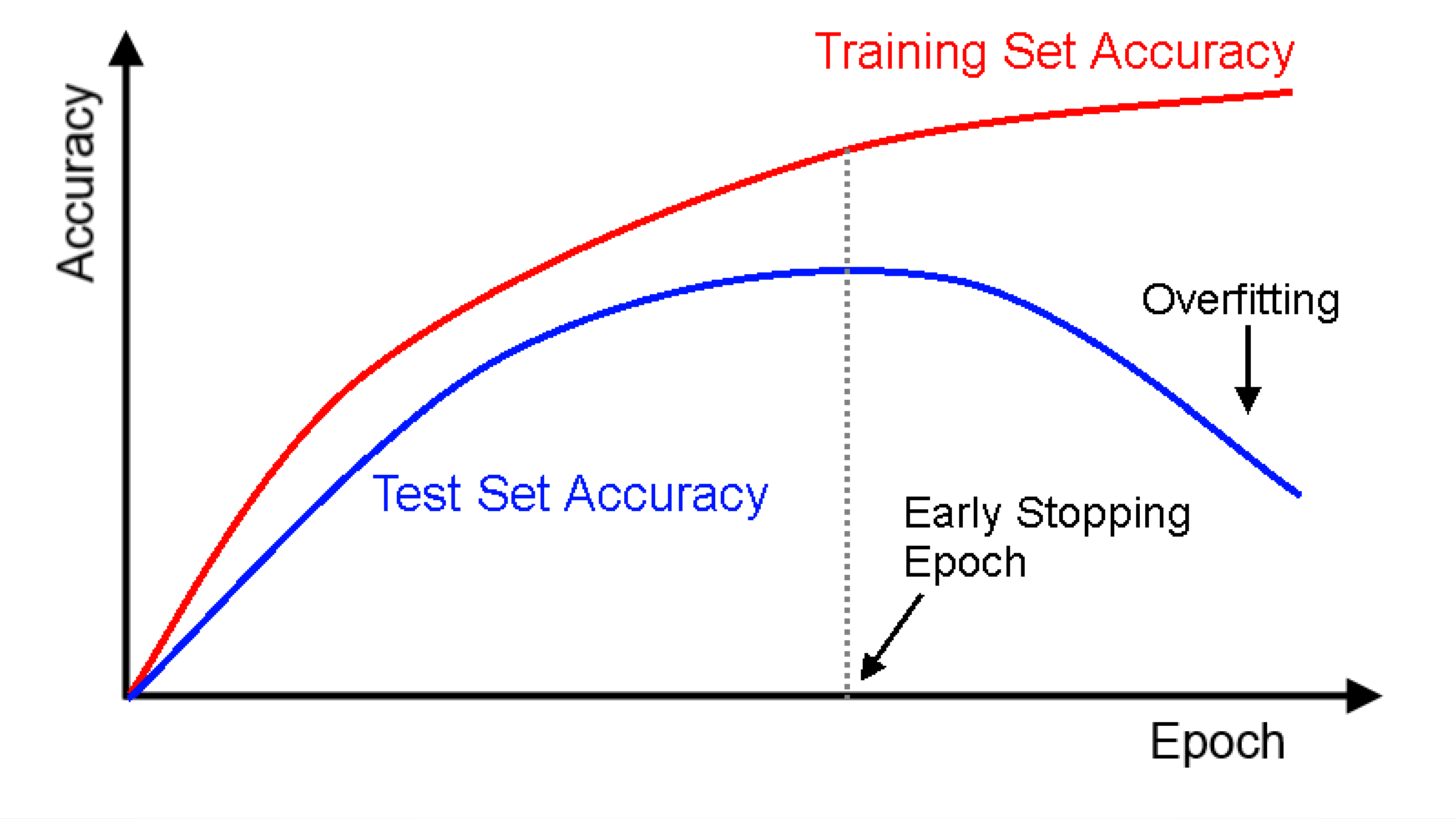
Underfitting and Overfitting

Early Stopping

Early Stopping - Concept

- What is Early Stopping?
  - During training, a model (especially a large neural network) can reach a point where it stops generalizing and begins overfitting, learning the noise in the training data.
  - Early Stopping helps to prevent this by halting training once performance on validation data starts to degrade.
- Solution:
  - Stop training as soon as the generalization error (validation error) starts increasing.
  - This prevents overfitting and ensures better performance on unseen data.

Early Stopping - Visualization



Early Stopping - Implementation and Benefits

- Why Use Early Stopping?
  - Prevents Overfitting: Stops training before the model begins to memorize noise in the training data, ensuring better generalization to new, unseen data.
  - Simplicity and Effectiveness: Easy to implement in most deep learning frameworks, yet highly effective in preventing model overfitting.
  - Efficient Use of Resources: Saves time and computational power by halting training when further progress will no longer improve performance on validation data.
- How to Implement in Practice:
  - Framework Support: Many libraries, such as Keras, provide an EarlyStopping callback. This can monitor validation loss and stop training when it starts increasing, saving the model with the best performance:
  - The callback can also be configured to **save the best weights** during training, not just when early stopping occurs.

Regularizing Techniques

Regularization in Machine Learning

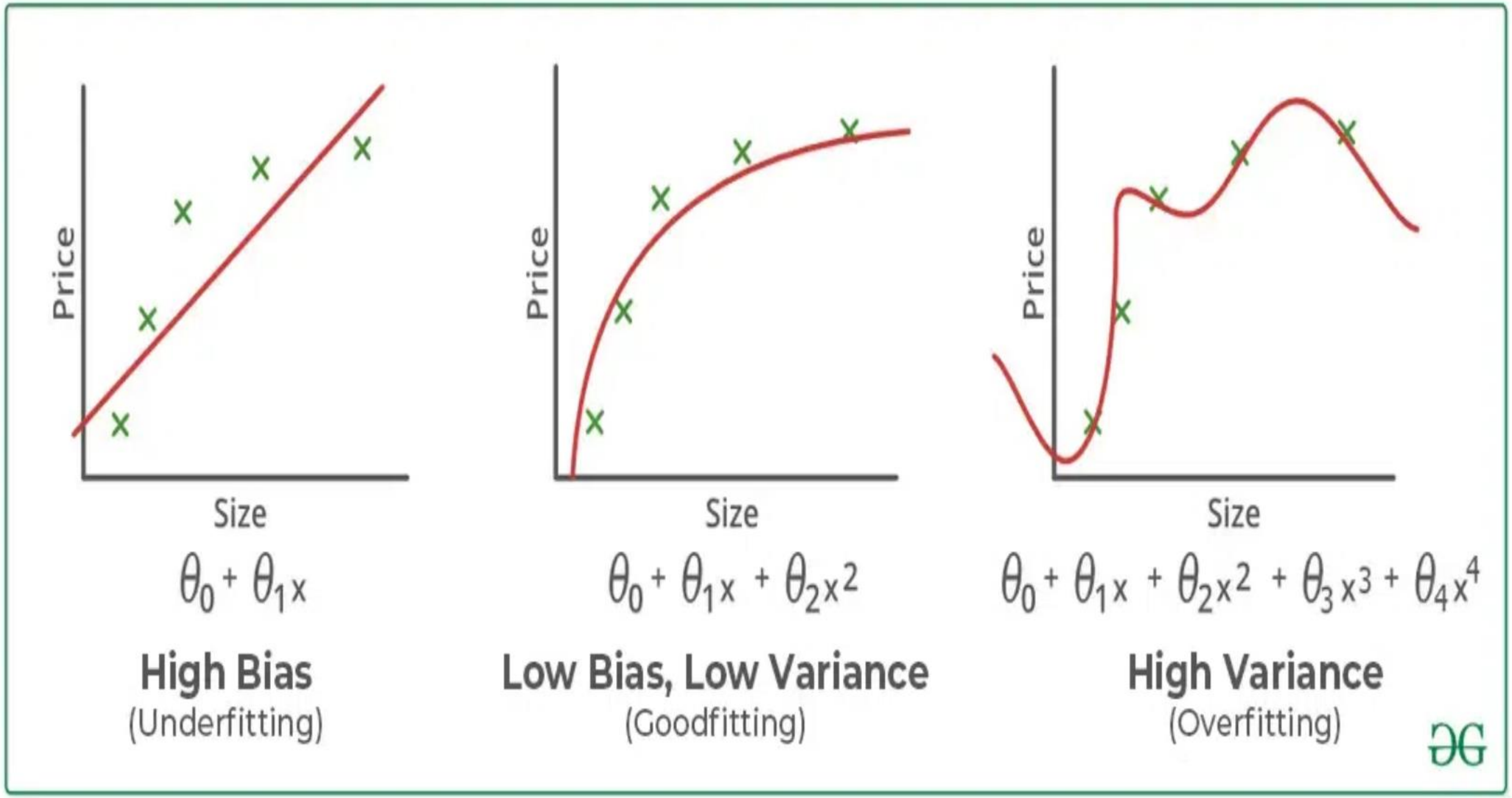
- Purpose of Regularization:
  - Regularization is used to reduce overfitting by penalizing overly complex models and encouraging simpler, more generalizable patterns.
  - It helps in striking a balance between bias and variance, ensuring that the model performs well on both the training and test datasets.

Common Regularization Techniques

- Lasso Regularization (L1): Adds a penalty proportional to the absolute value of coefficients, encouraging sparsity (i.e., many features may have zero weights).
- Ridge Regularization (L2): Adds a penalty proportional to the square of the coefficients, shrinking them, but all features are included.
- Elastic Net Regularization (L1 + L2): Combines both Lasso and Ridge regularization, balancing between shrinking and sparsity.

Introduction to Lasso Regression

- What is Lasso Regression?:
  - Lasso stands for Least Absolute Shrinkage and Selection Operator.
  - It is a type of linear regression that uses L1 regularization.
  - The goal of Lasso is not only to minimize the errors but also to shrink the coefficients of less important features to zero, effectively performing feature selection.
- When to Use Lasso Regression?:
  - Lasso is useful when we want a simple, interpretable model that selects only the most important features.



Bias and Variance

Key Idea Behind Lasso Regression

- L1 Regularization:
  - Lasso Regression adds a penalty term to the cost function, which is proportional to the absolute value of the coefficients.
- The objective function (cost function) becomes:

$$\text{Cost} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + \lambda\sum_{i=1}^{m}|\theta_i|$$

How Does Lasso Perform Feature Selection?

- Feature Selection with Lasso:
  - As the regularization parameter (λ) increases, the coefficients for less important features shrink towards zero.
  - If λ is large enough, many coefficients become zero, effectively eliminating features.
  - This is why Lasso is used not just for prediction but also for selecting the most relevant features.

Impact of the Regularization Parameter λ

- Tuning the Regularization Parameter:
  - Small λ: The penalty term has little impact, leading to a model similar to ordinary least squares regression.
  - Large λ: Stronger penalty, resulting in fewer features being used in the model as more coefficients shrink to zero.
- How to Choose λ?:
  - Use cross-validation to find the optimal λ that balances bias and variance, and avoids overfitting or underfitting.

Advantages and Disadvantages of Lasso Regression

- Advantages:
  - Feature Selection: Automatically selects important features by shrinking the irrelevant ones to zero.
  - Interpretability: Results in simpler, interpretable models with only the most relevant features.
  - Avoids Overfitting: Helps to prevent overfitting by penalizing large coefficients.
- Disadvantages:
  - Bias Introduced: The model may introduce bias as coefficients are shrunk.

Introduction to Ridge Regression

- What is Ridge Regression?
  - Ridge regression is a type of linear regression that incorporates L2 regularization to prevent overfitting.
  - It is designed to improve the generalization of the model by adding a penalty for large coefficients.
- Key Feature of Ridge Regression:
  - Unlike ordinary least squares (OLS) regression, Ridge shrinks the regression coefficients by applying a penalty proportional to the squared magnitude of the coefficients.

Ridge Regression - Objective Function

- Cost Function in Ridge Regression:
  - The objective function (or cost function) in Ridge regression is modified as follows

$$\text{Cost} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + \lambda\sum_{i=1}^{m}\theta_i^2$$

y_i is the actual target value.

$\hat{y}_i$ is the predicted target value.

θ_i are the coefficients (weights) of the features.

λ is the **regularization parameter** that controls the strength of the penalty.

$\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$ represents the residual sum of squares (RSS).

How Ridge Regression Works

- Effect of the Regularization Parameter λ:
- When λ=0:
  - Ridge regression reduces to ordinary least squares (OLS) regression, meaning there's no penalty for large coefficients.
- As λ increases:
  - The penalty for larger coefficients becomes stronger, and the coefficients shrink, preventing overfitting by reducing the influence of irrelevant or noisy features.
- Key Concept: Ridge regression trades off bias and variance to improve the model's generalization ability. A larger λ will increase bias but reduce variance, leading to better generalization on unseen data.

Advantages and Disadvantages of Ridge Regression

- Advantages:
  - Prevents Overfitting: By shrinking coefficients, Ridge helps the model generalize better, especially when there are many features or noisy data.
  - Works Well in Multicollinearity: In cases where there are high correlations among features, Ridge regression helps stabilize the model.
  - Retains All Features: Unlike Lasso, Ridge regression keeps all the features in the model, which is beneficial when all features contribute to the prediction.
- Disadvantages:
  - Less Interpretability: Since Ridge does not perform feature selection (i.e., it doesn't set coefficients to zero), it can be harder to interpret the final model.
  - Bias-Variance Tradeoff: As λ increases, the model becomes biased, and choosing an optimal λ is crucial.

Comparison of Lasso (L1) vs. Ridge (L2) Regularization

- L1 Regularization (Lasso):
  - Feature Selection: L1 regularization drives some coefficients to exactly zero, which results in a sparse model. This makes it ideal for feature selection.
  - Unimportant features get zero coefficients, effectively removing them from the model.
  - Sparsity: Leads to models with fewer non-zero coefficients, which can simplify model interpretation.
  - Example: After applying L1 regularization on a layer with 4 weights, the coefficients might look like:
  - $\theta_1 = 0.8$, $\theta_2 = 0$, $\theta_3 = 1$, $\theta 4 = 0$

Comparison of Lasso (L1) vs. Ridge (L2) Regularization

- L2 Regularization (Ridge):
  - Coefficient Shrinking: L2 regularization shrinks all coefficients towards zero, but none of the coefficients become zero.
  - This means all features remain in the model, but their influence is reduced.
  - Small Coefficients for All Features: Useful when you believe that all features contribute somewhat to the prediction, but their impact needs to be controlled.
  - Example: After applying L2 regularization on the same layer, the coefficients might look like:
  - $\theta_1=0.3,\ \theta_2=0.1,\ \theta_3=0.3,\ \theta_4=0.2$

References

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