Bias-Variance Tradeoff and Generalization

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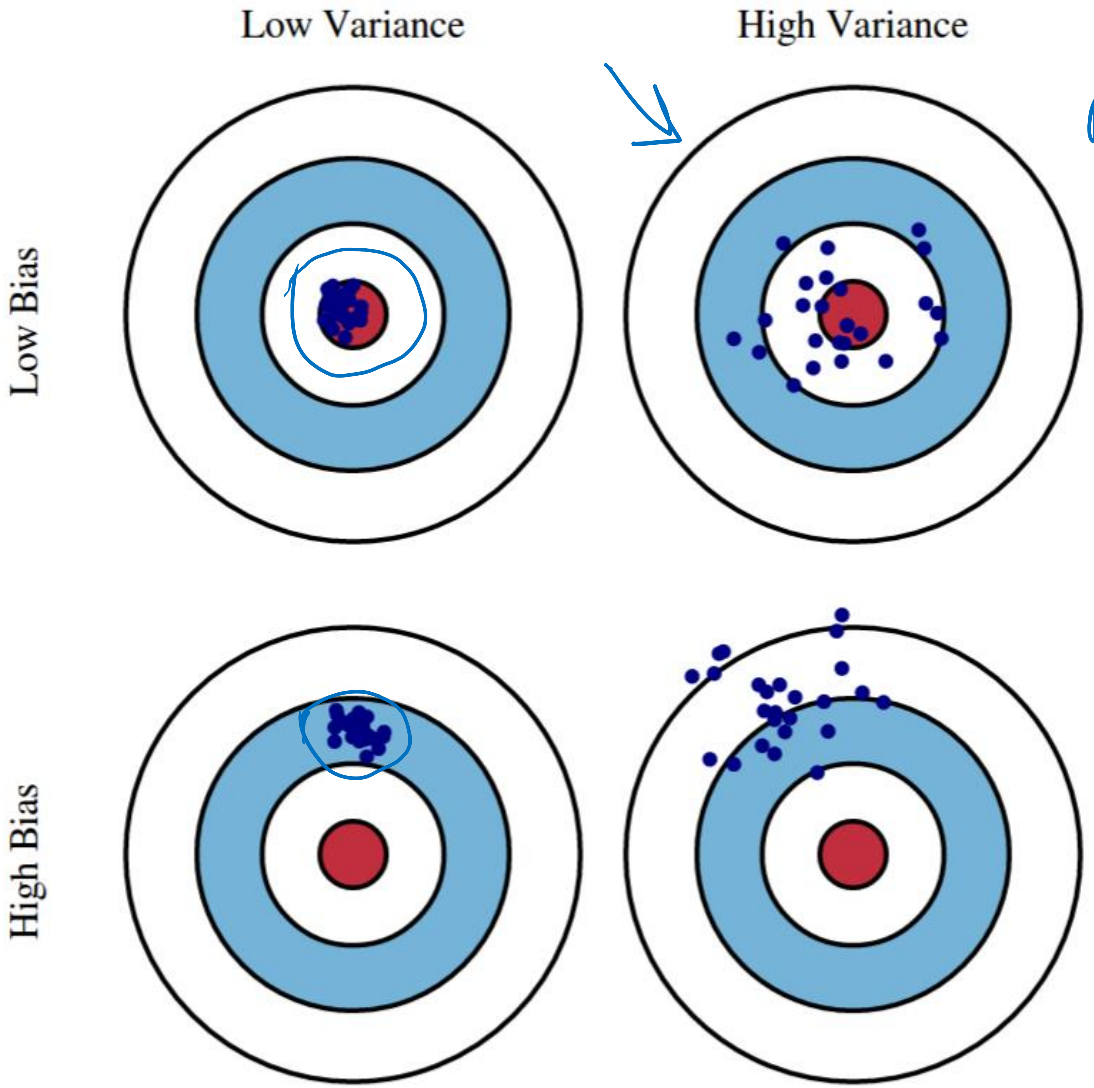
Bias-Variance Tradeoff

Error = Bias + Variance



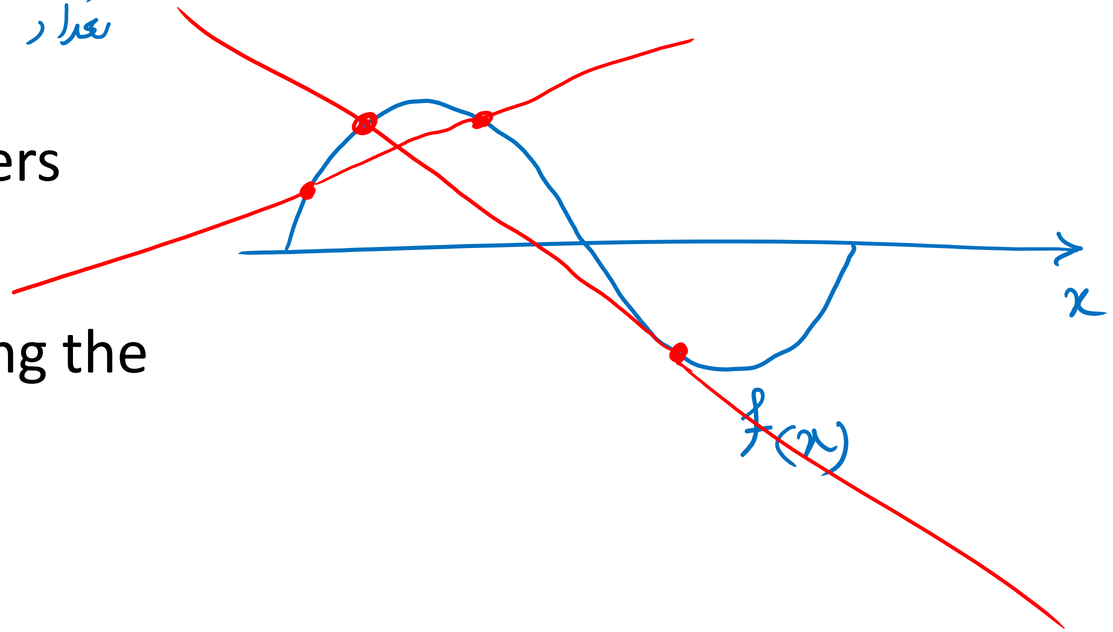
Bias = $f - E[\hat{f}]$

Sources of Error: Bias and Variance

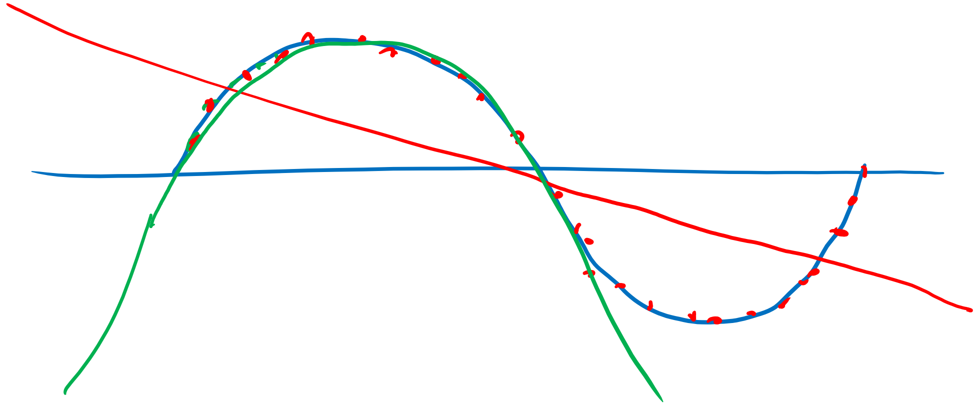
$$Error = Bias^2 + \underbrace{Variance}_{\text{تعداد داده‌های آموزشی}} + \text{Bayes Error}$$

ناشی از انتخاب مدل

- **Bias**: Error of the model
- **Variance**: Estimation error of the parameters



- The variance can be decreased by increasing the training samples.



Error Decomposition

x: input

y: output

f: true function

$\hat{f}$: ML model

$$\boxed{y = f(x) + \epsilon}$$

$$x \rightarrow \boxed{f} \rightarrow y$$

$$y = f(x) + \varepsilon$$

$$E[\epsilon] = 0 \quad , \quad var(\epsilon) = \sigma^2$$

$$MSE = E\left[(y - \hat{f}(x))^2\right] = E\left[y^2 - 2y\hat{f} + \hat{f}^2\right] = E[y^2] - 2E[y\hat{f}] + E[\hat{f}^2]$$

$$E[y^2] = E\left[(f+\epsilon)^2\right] = E\left[f^2 + 2f\epsilon + \epsilon^2\right] = E[f^2] + 2f\underbrace{E[\epsilon]}_{0} + E[\epsilon^2] = \boxed{f^2 + \sigma^2}$$

$$E[y\hat{f}] = E\left[(f+\epsilon)\hat{f}\right] = f\,E[\hat{f}] + \underbrace{E[\epsilon\hat{f}]}_{0} = \boxed{f\,E[\hat{f}]}$$

$$var(X) = E[X^2] - E[X]^2 \Longrightarrow E[X^2] = var(X) + E[X]^2$$

$$E[\hat{f}^2] = \boxed{var(\hat{f}) + E[\hat{f}]^2}$$

$$\text{Error} = \underbrace{\left(f - E[\hat{f}]\right)^2}_{\text{Bias}^2} + \underbrace{\text{var}(\hat{f})}_{\text{variance}} + \sigma^2$$

$\sigma^2 \rightarrow$ Bayes Error

$$\text{Error} = \left(f(x) - \underset{\text{train data}}{E}\left[\hat{f}(x)\right]\right)^2 + \cdots$$

$$E_x\left[\hat{f}(x)\right]$$

$$\hat{f}\left(E[x]\right)$$

Example: Mean estimation

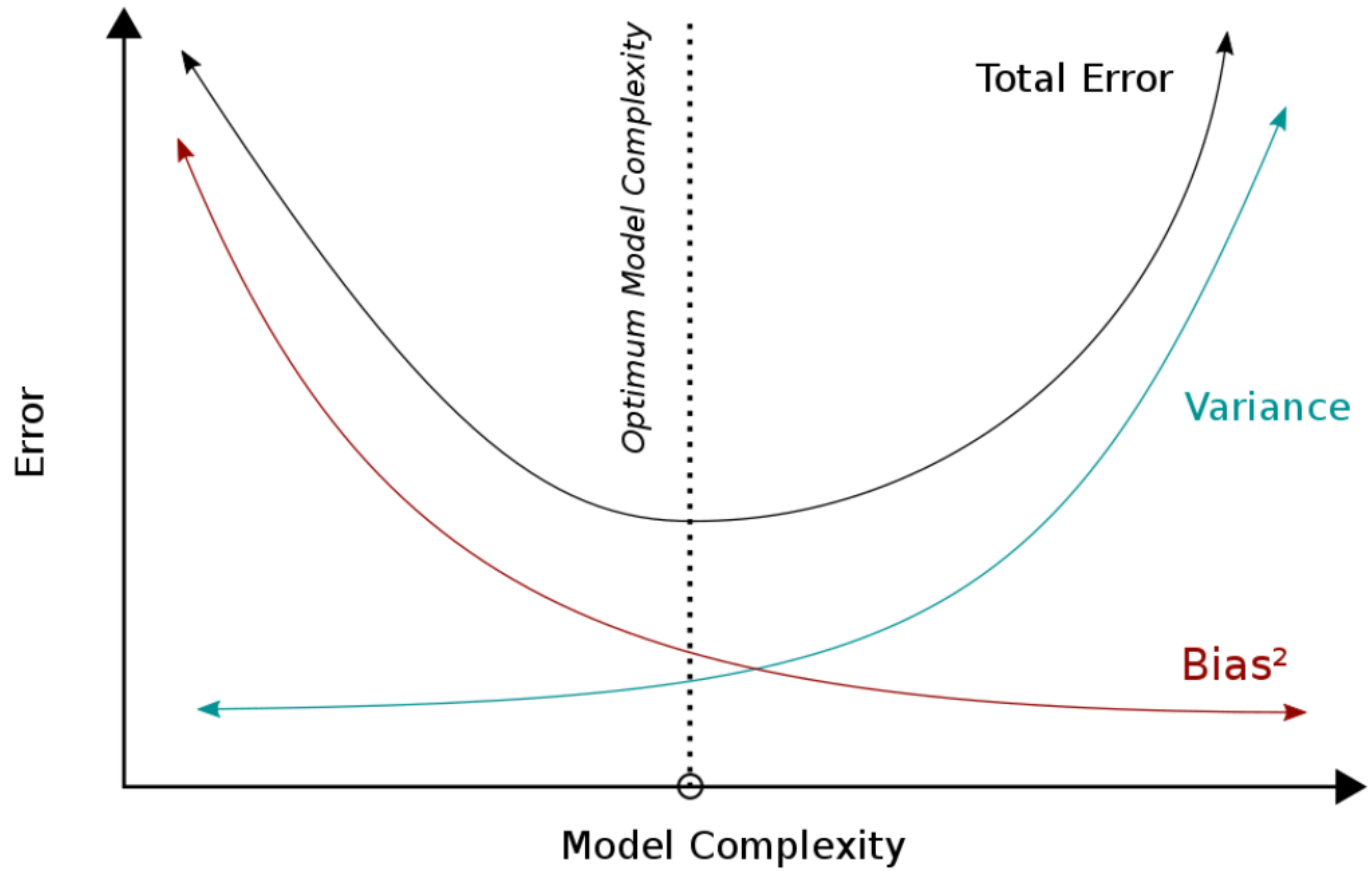
$\mu \longrightarrow \hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} x_i$ $\{x_1, \ldots, x_n\}$ i.i.d.

bias $= 0$

$\mathrm{var}(\hat{\mu}) = \frac{1}{n} \mathrm{var}(x)$

Bias-Variance Tradeoff

- Dimensionality reduction decreases the model complexity.
- Adding feature increases the model complexity.
- The **more complex** model, the **larger sample size** is needed.



Generalization Error

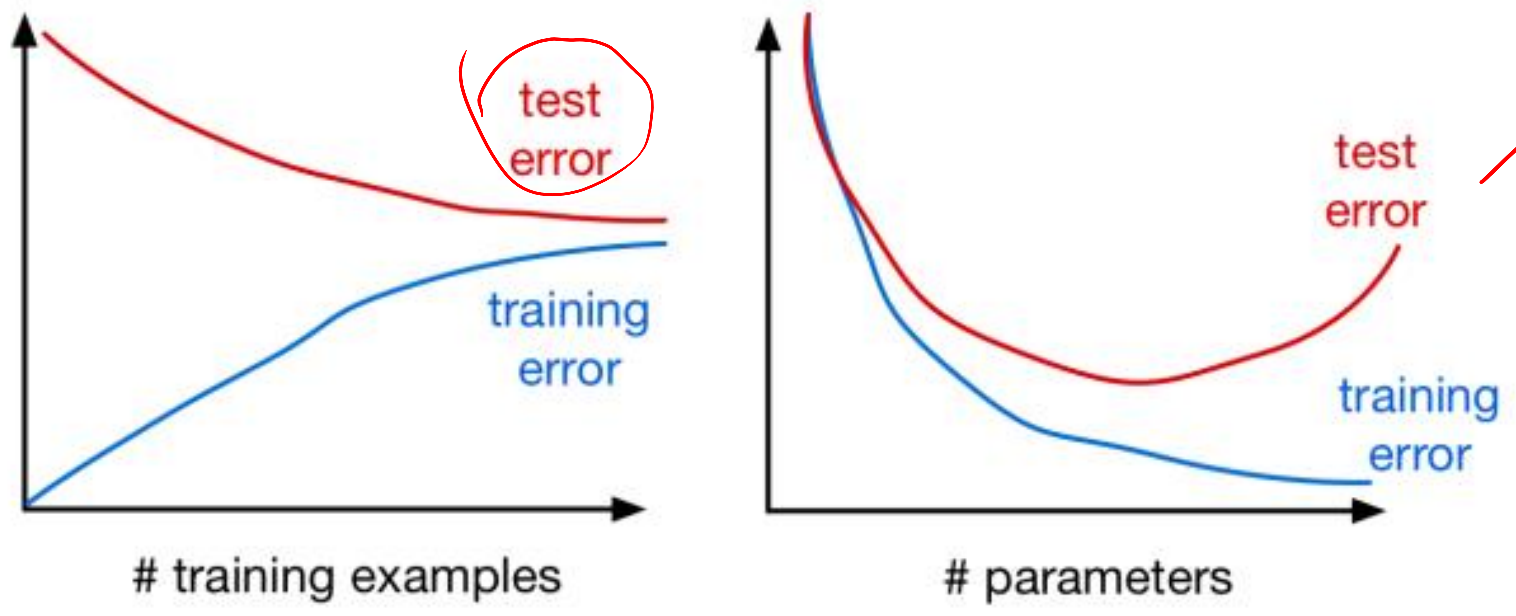


Figure 1: **(left)** Qualitative relationship between the number of training examples and training and test error. **(right)** Qualitative relationship between the number of parameters (or model capacity) and training and test error.

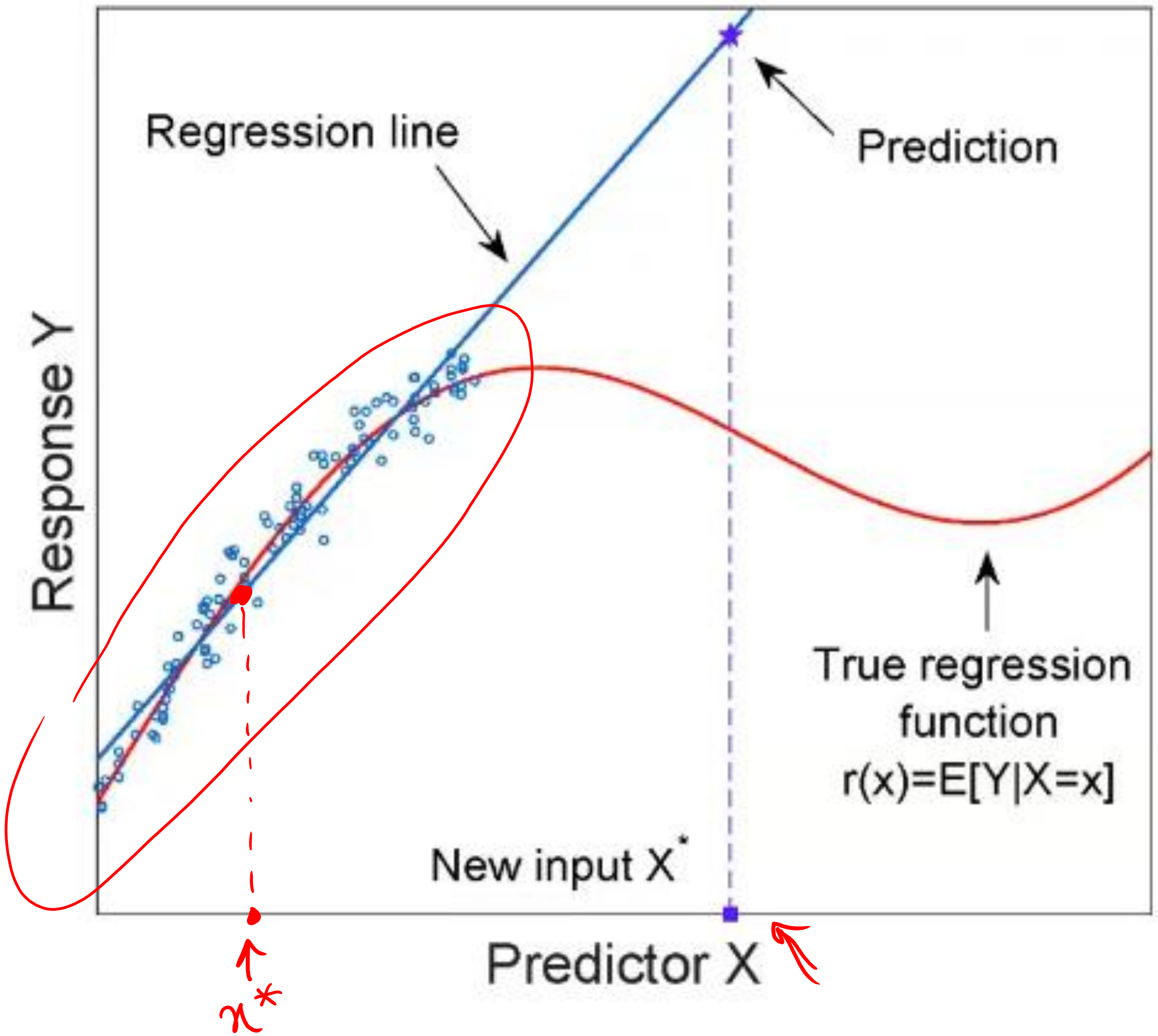
Interpolation vs Extraplation

درون‌یابی

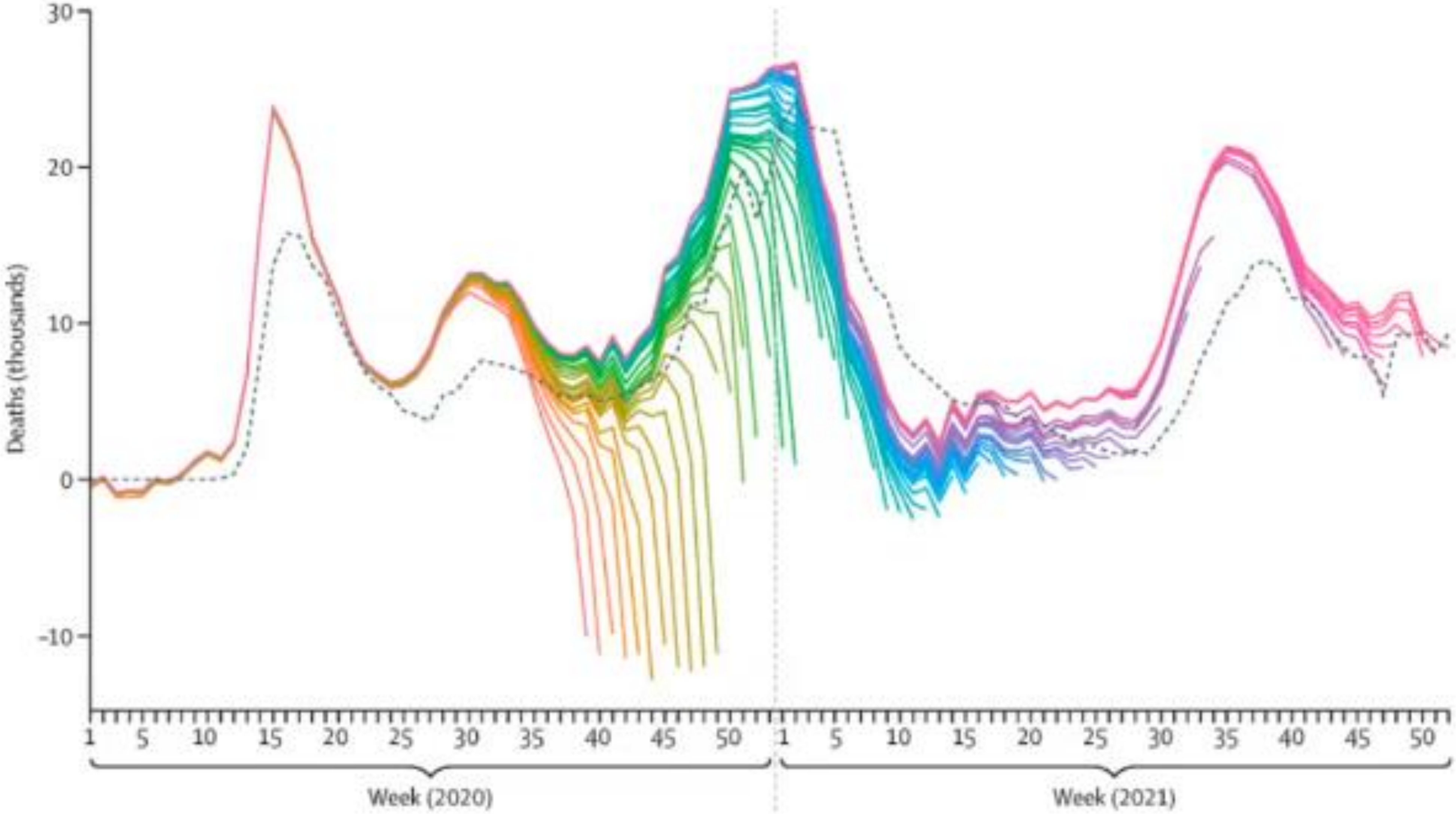
برون‌یابی

Robastness

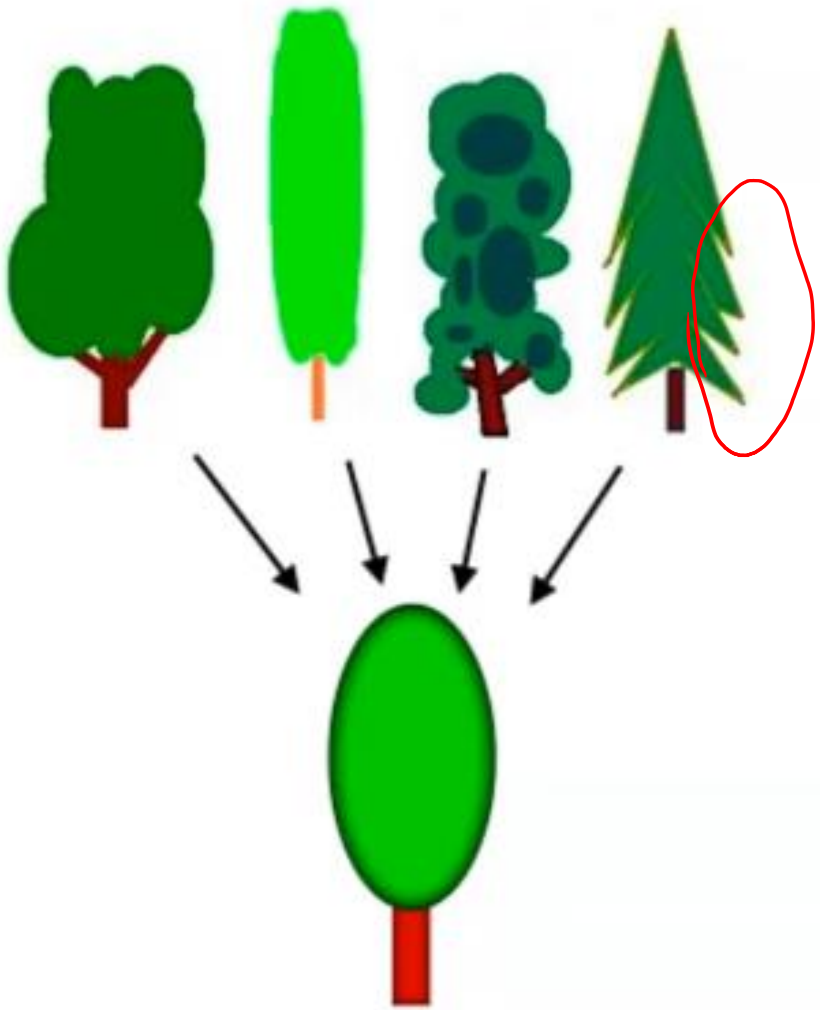
Generalization



Covid prediction



Generalization



Inductive Bias

- The set of assumptions that a learning algorithm uses to predict outputs.

- These biases shape how the model generalized from the training data to unseen data.

- Models:
  - Linear models
  - Decision tree
  - Neural network

Inductive Bias