The bias-variance tradeoff

STAT 4710

September 20, 2022

Where we are

Unit 1: R for data mining

Unit 2: Prediction fundamentals

Unit 3: Regression-based methods

Unit 4: Tree-based methods

Unit 5: Deep learning

Lecture 1: Model complexity

Lecture 2: Bias-variance trade-off

Lecture 3: Cross-validation

Lecture 4: Classification

Lecture 5: Unit review and quiz in class

What drives test error?

Problem parameters

- Sample size
- Noise level
- Fitted model complexity (number of parameters)
- True model complexity

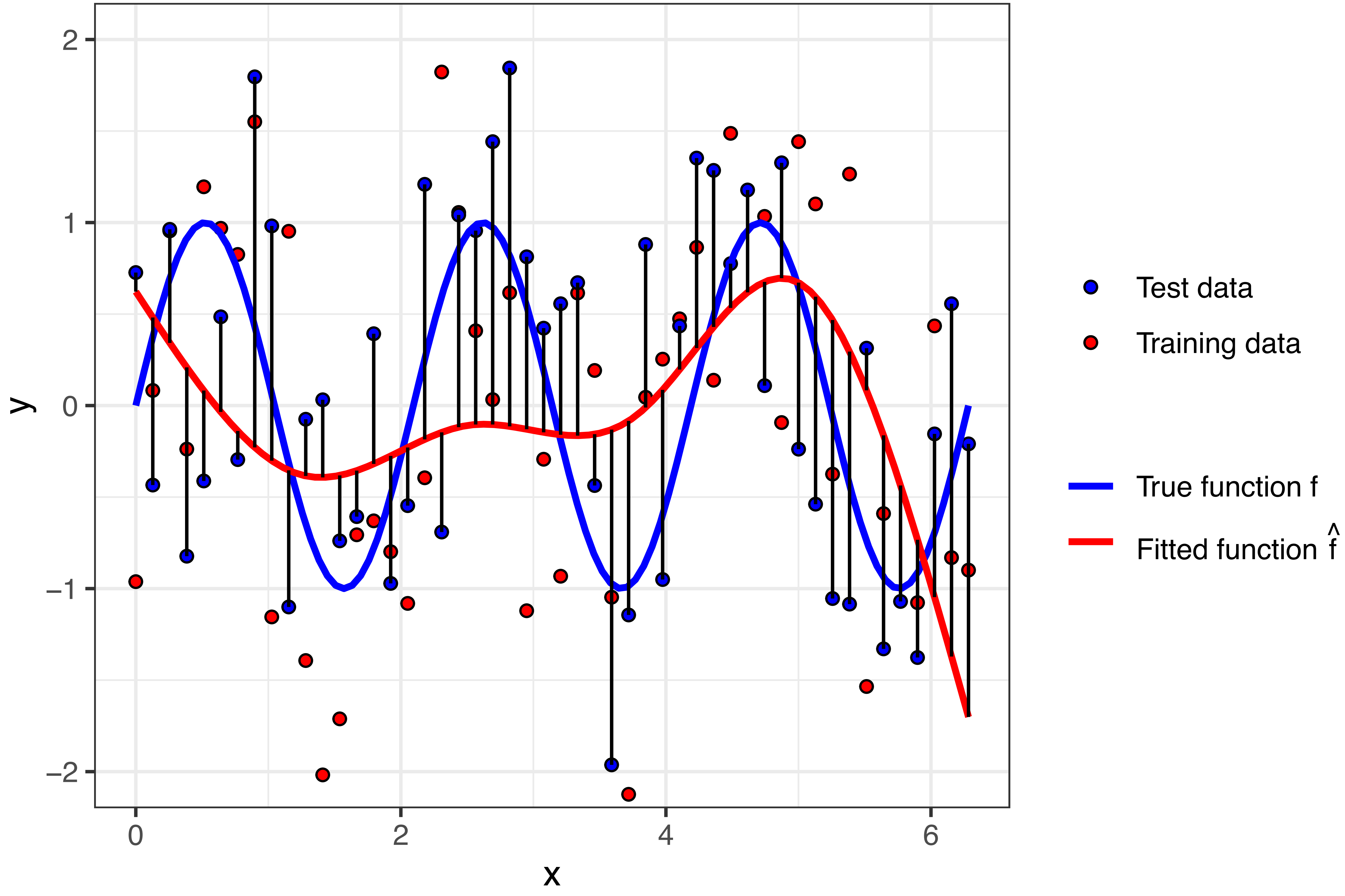
Phenomena

- Model bias: extent to which model unable to capture the truth
- Overfitting: extent to which the fit is sensitive to noise in training data
- Irreducible error: noise in test points that is impossible to predict

How do all these elements come together?

The expected test error

How to quantify performance of a prediction method (e.g. natural spline with df = 5)?



The expected test error

$$\text{Test error} = \frac{1}{N}\sum_{i=1}^{N}(Y_i^{\text{test}} - \hat{Y}_i^{\text{test}})^2$$
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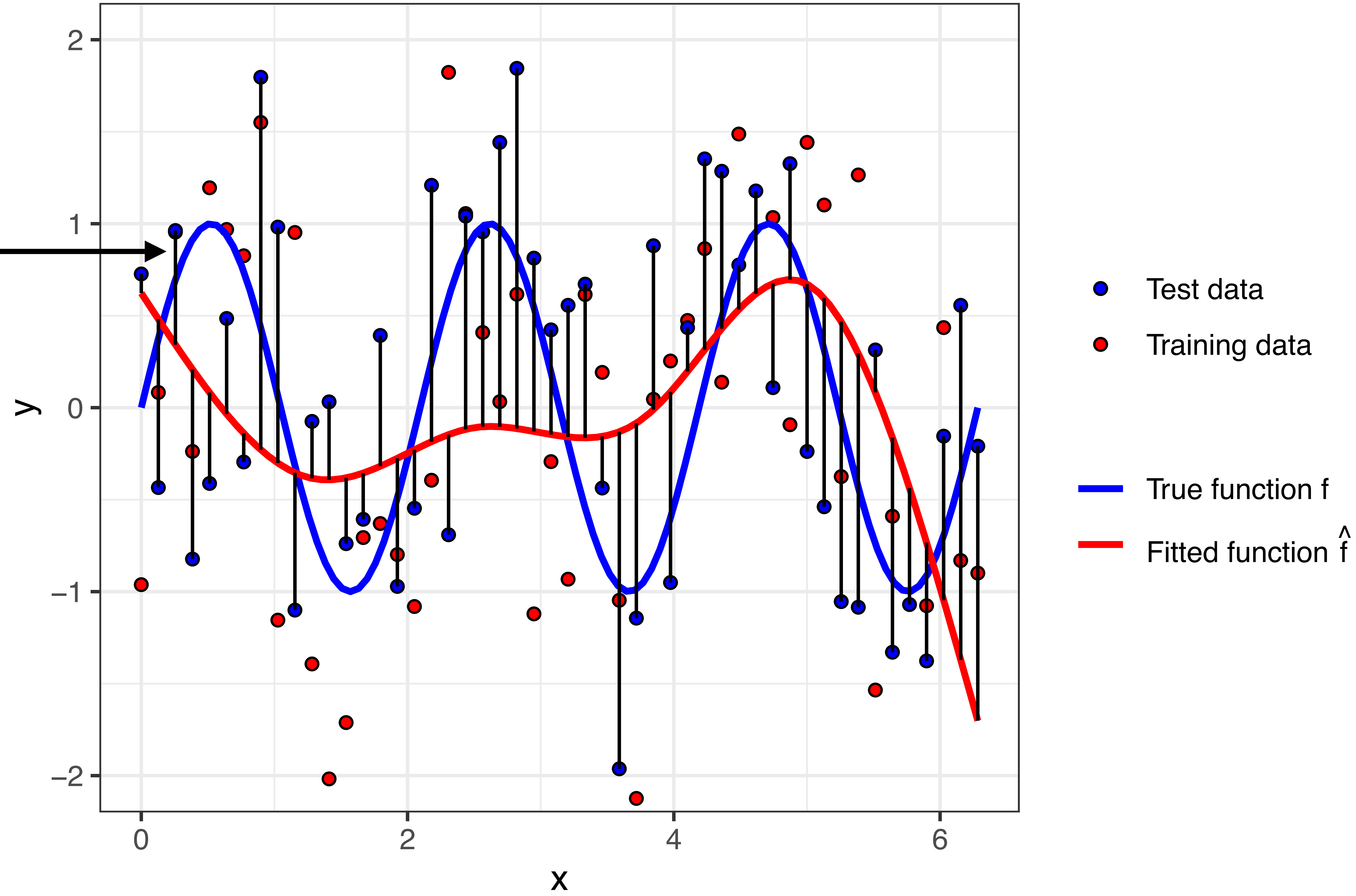

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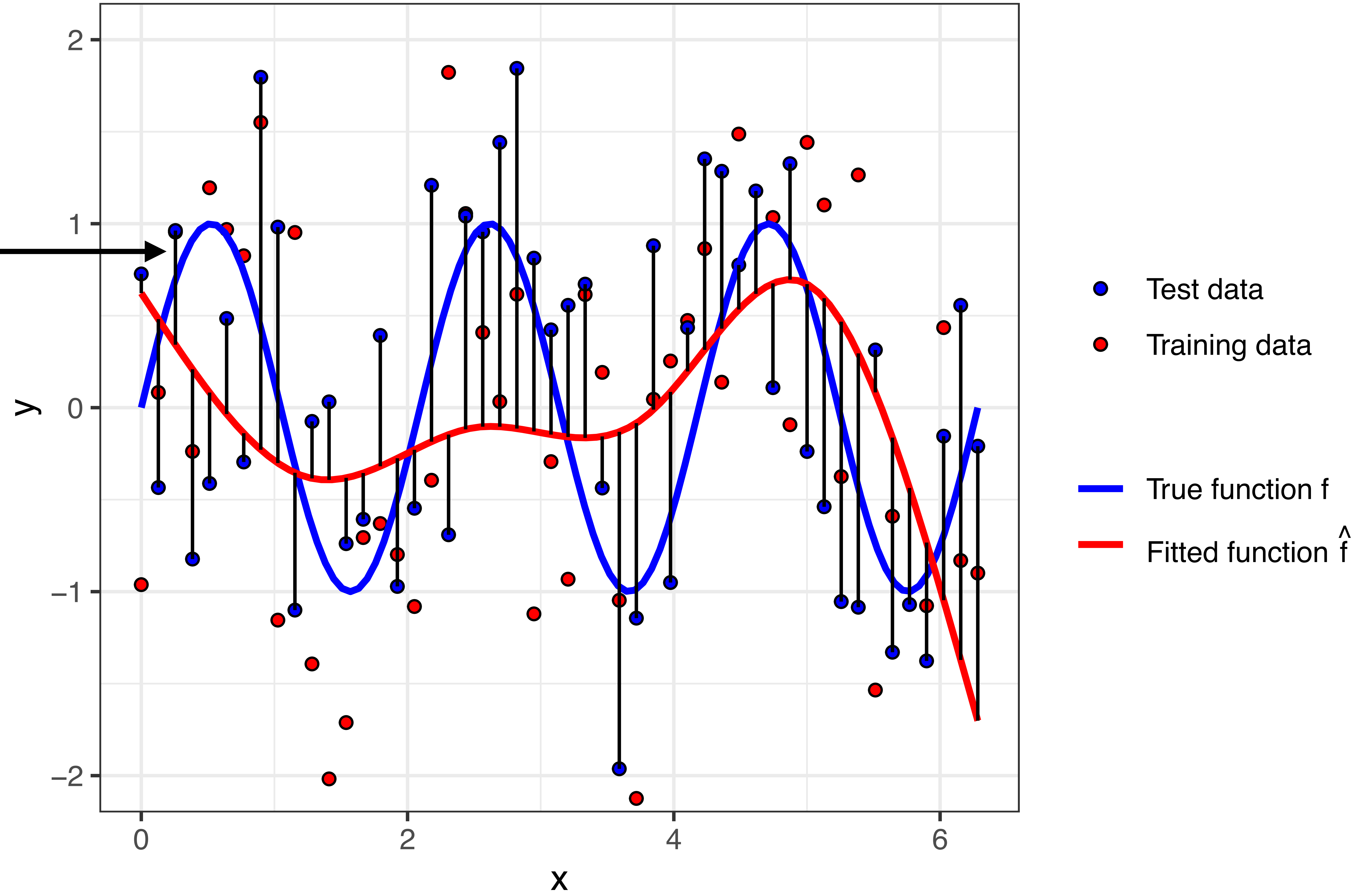

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$$\text{ETE} = \mathbb{E}[\text{Test error}]$$

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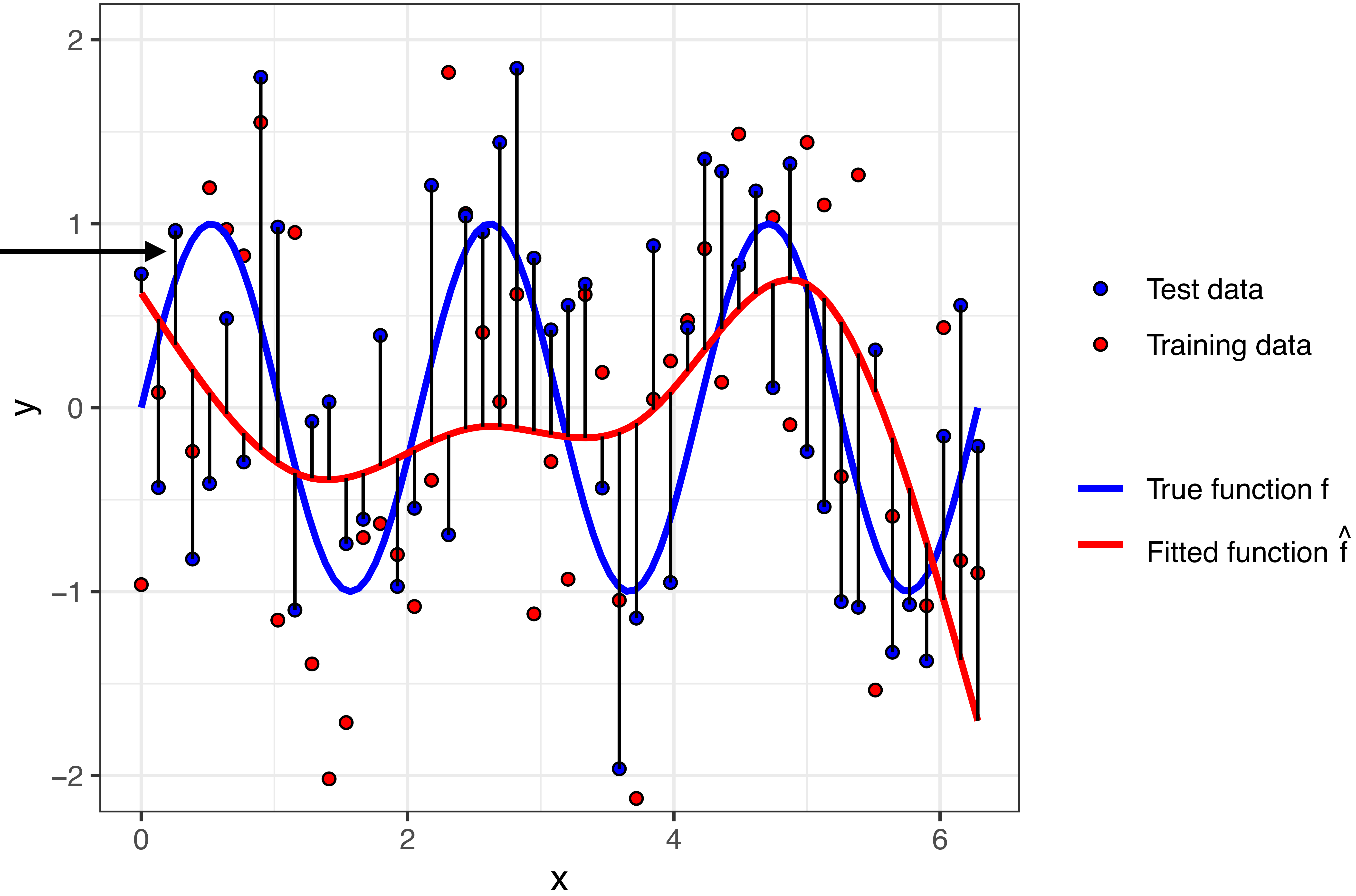

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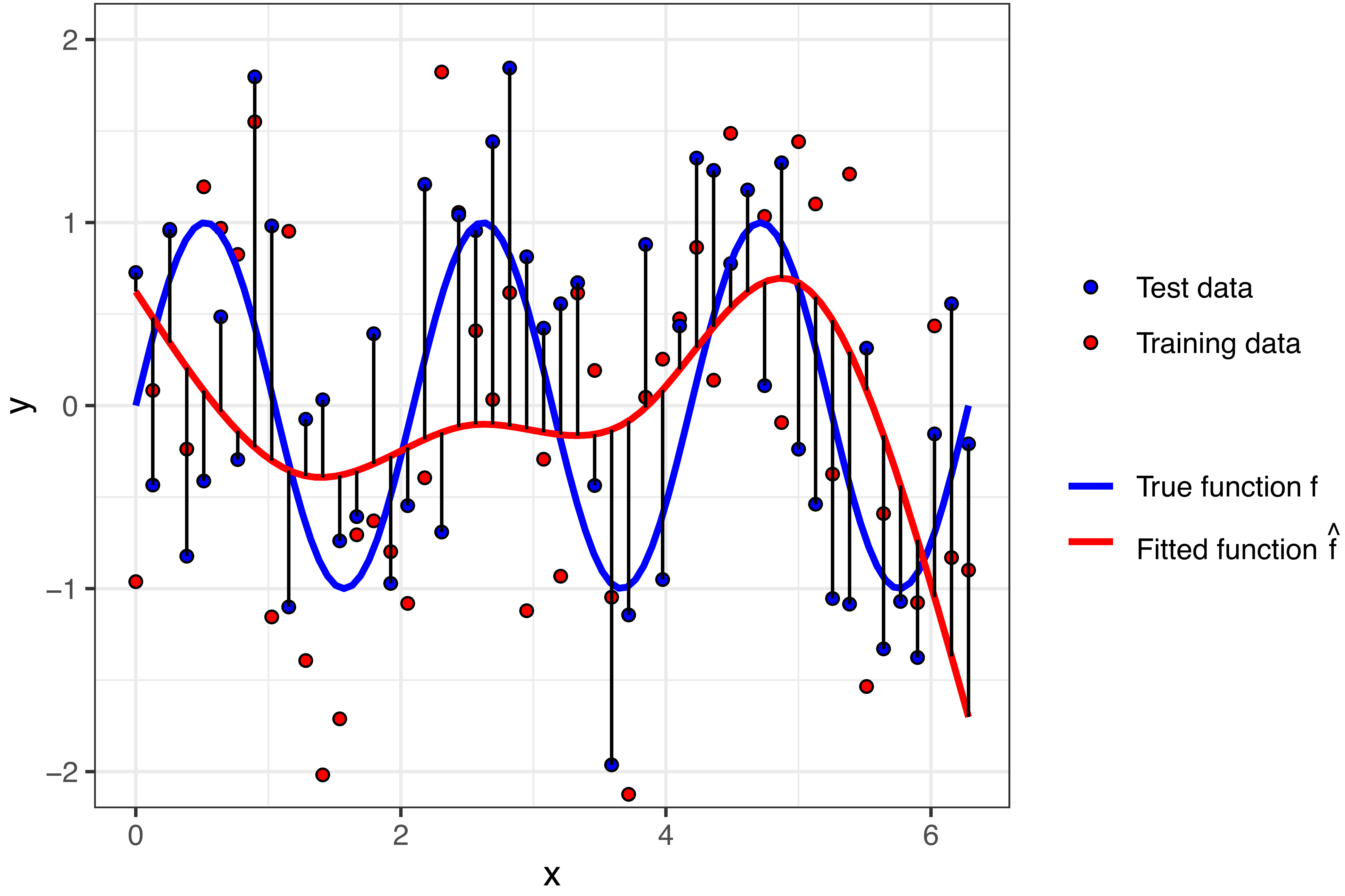
Averaging over randomness in Y^{train} and Y^{test} (think of X^{train} and X^{test} as fixed).

Contribution of randomness in test set



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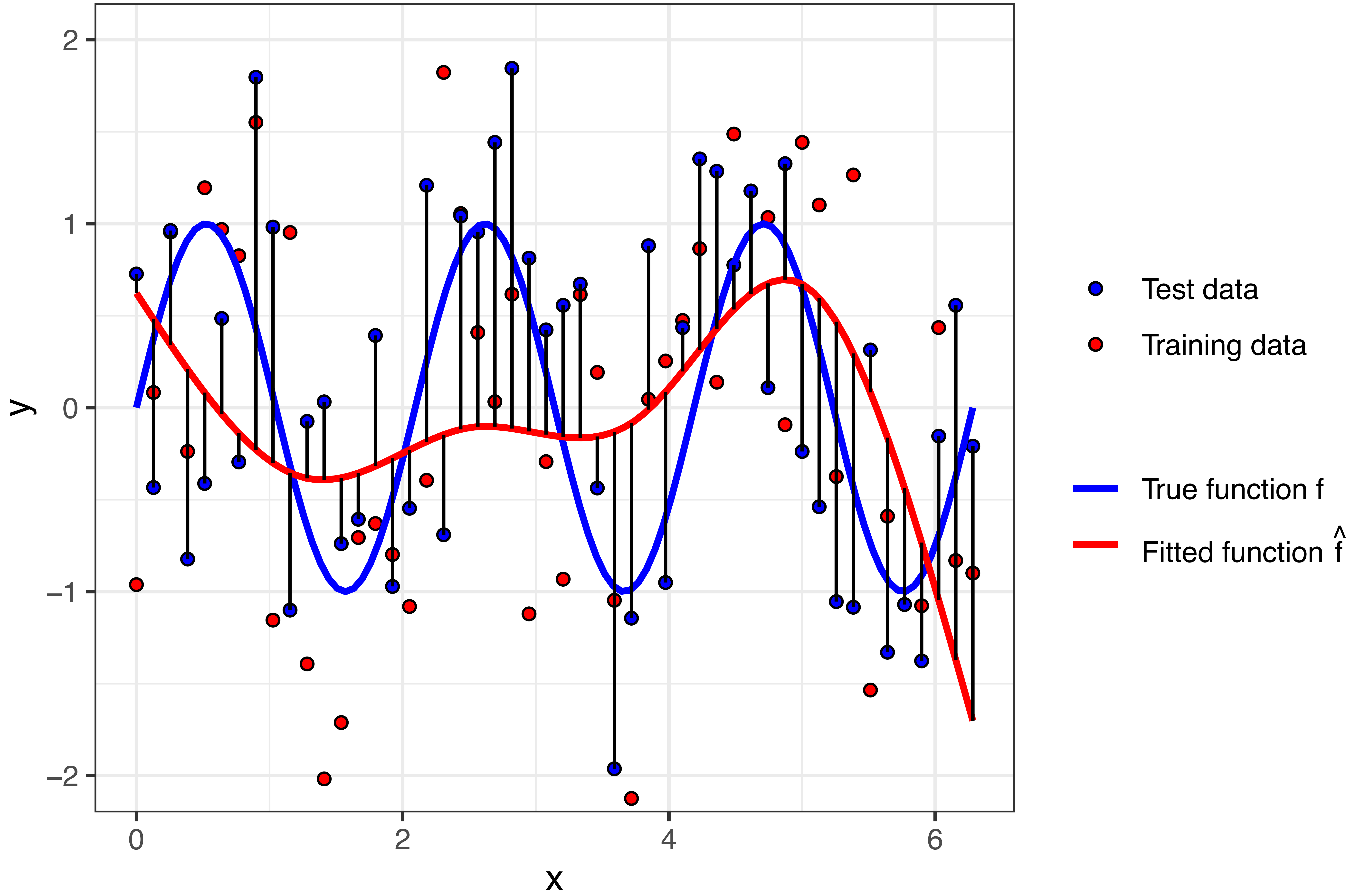

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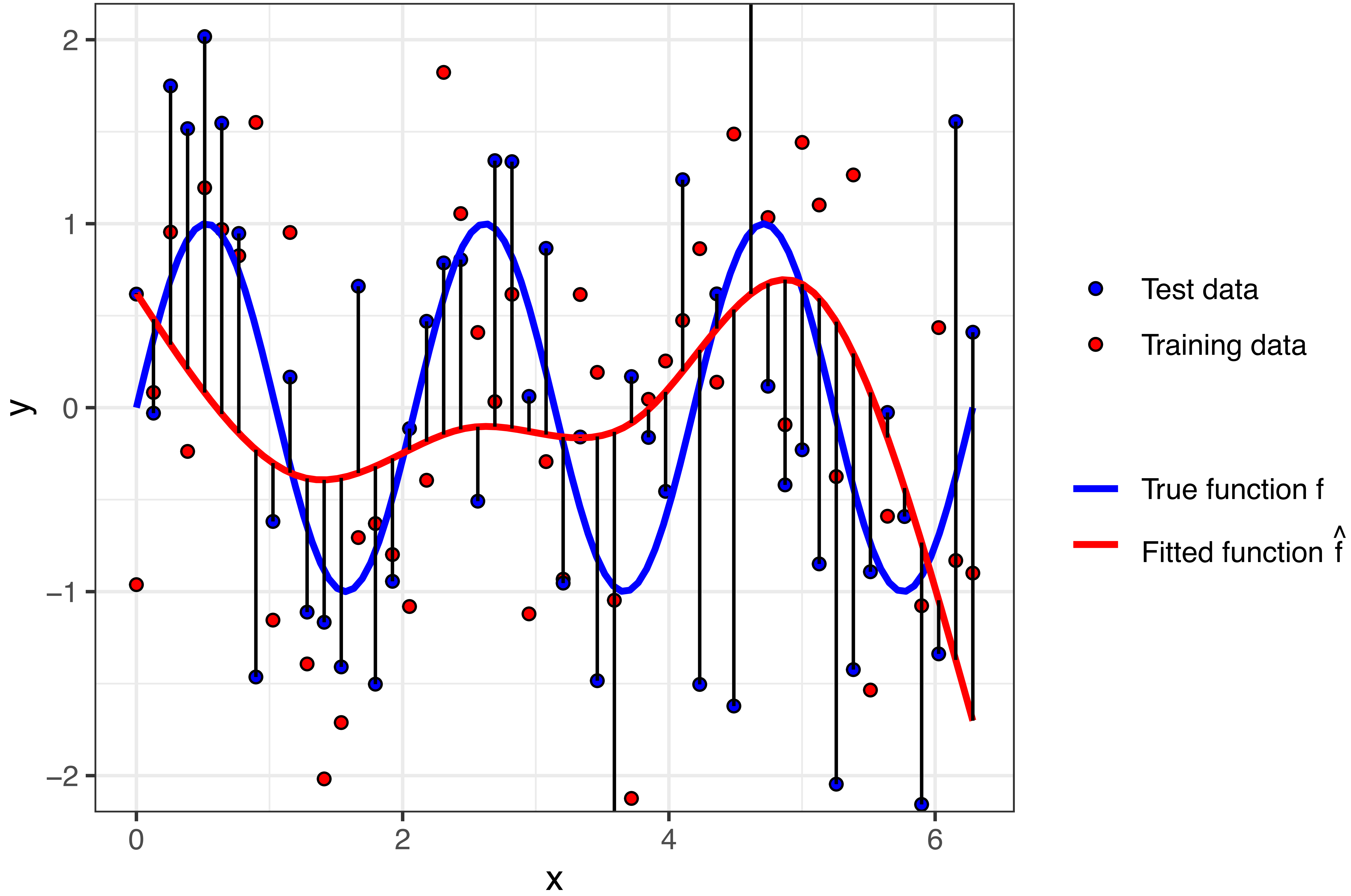

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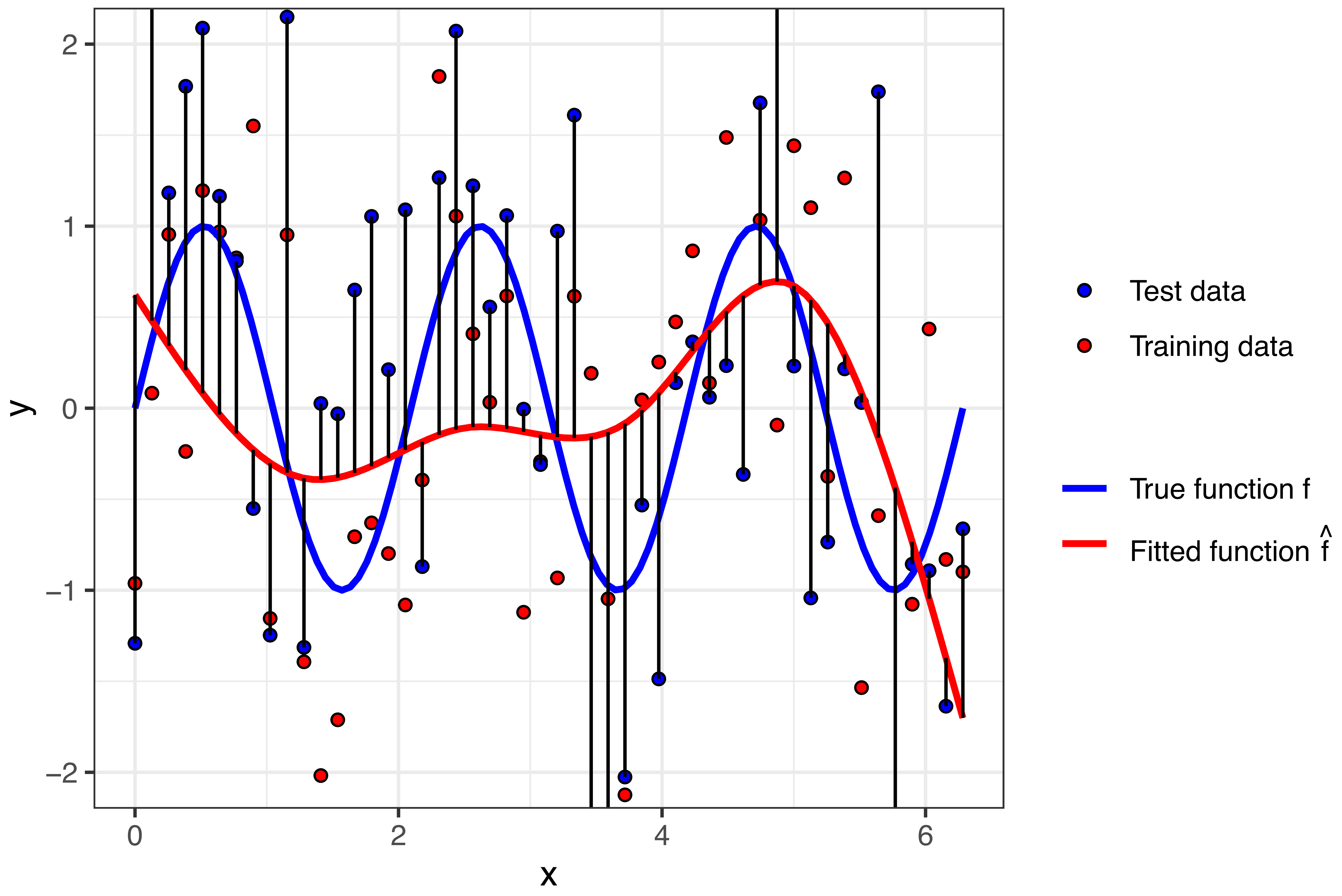

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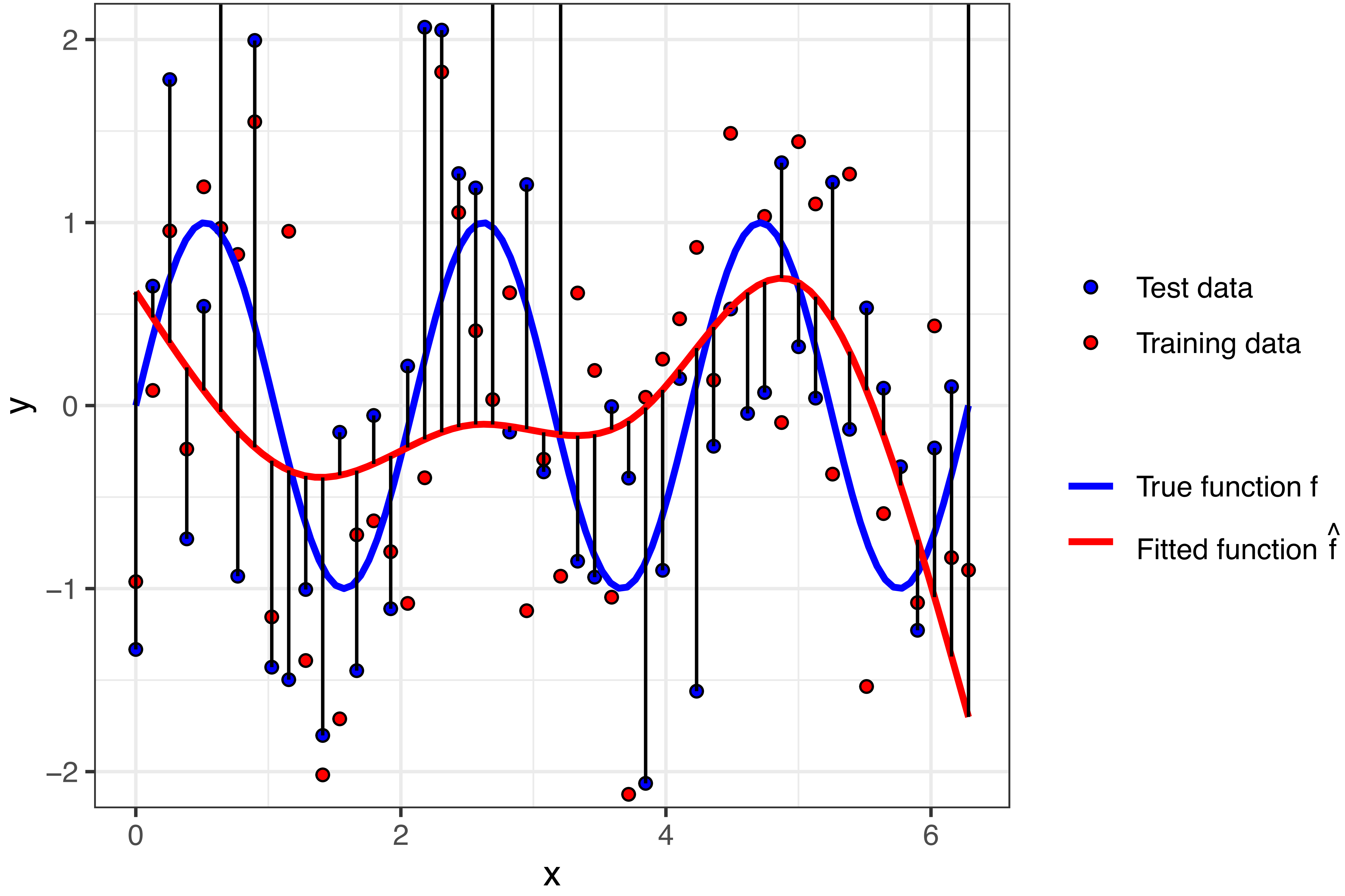
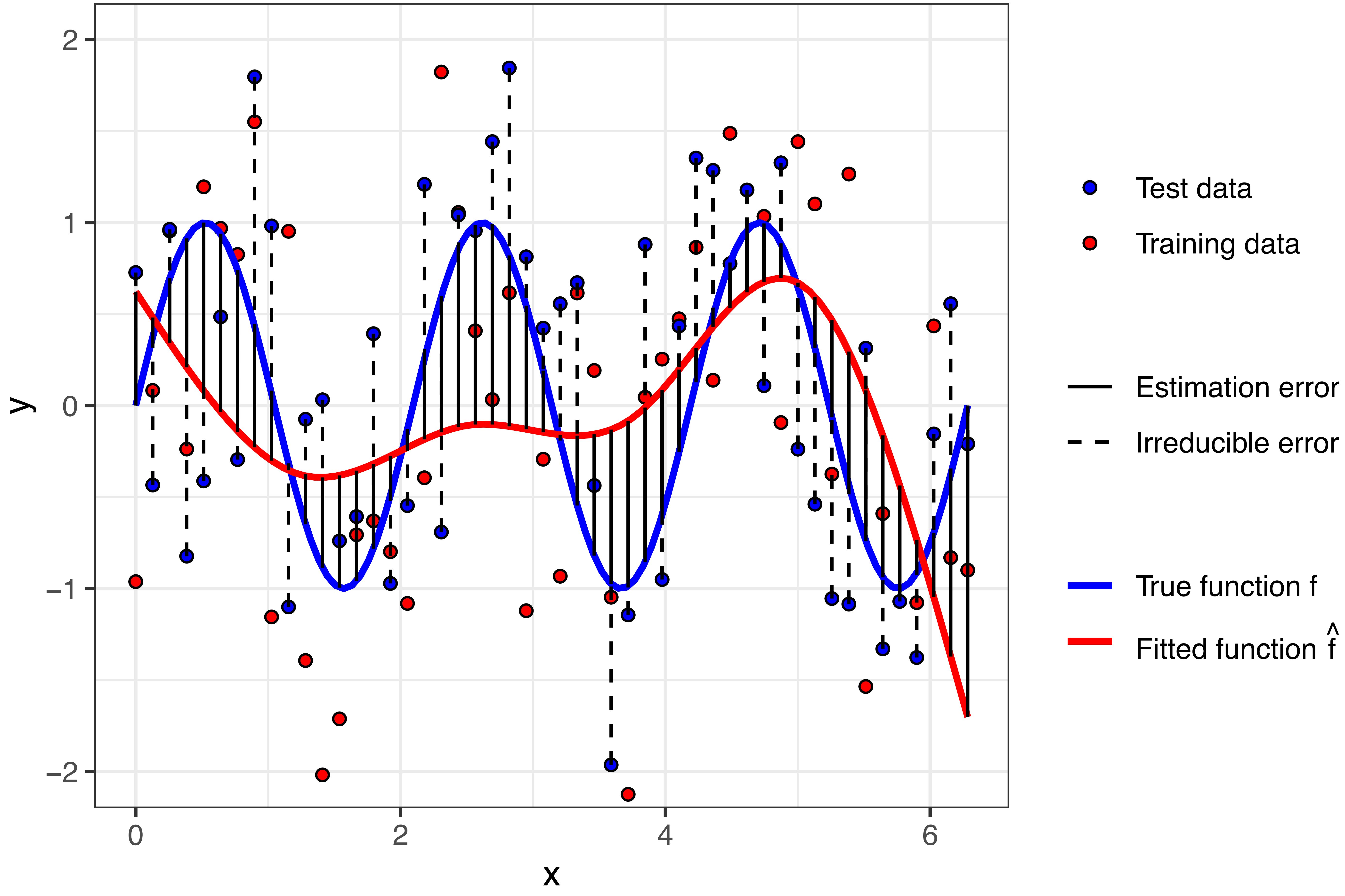


Prediction error = Estimation error + Irreducible error



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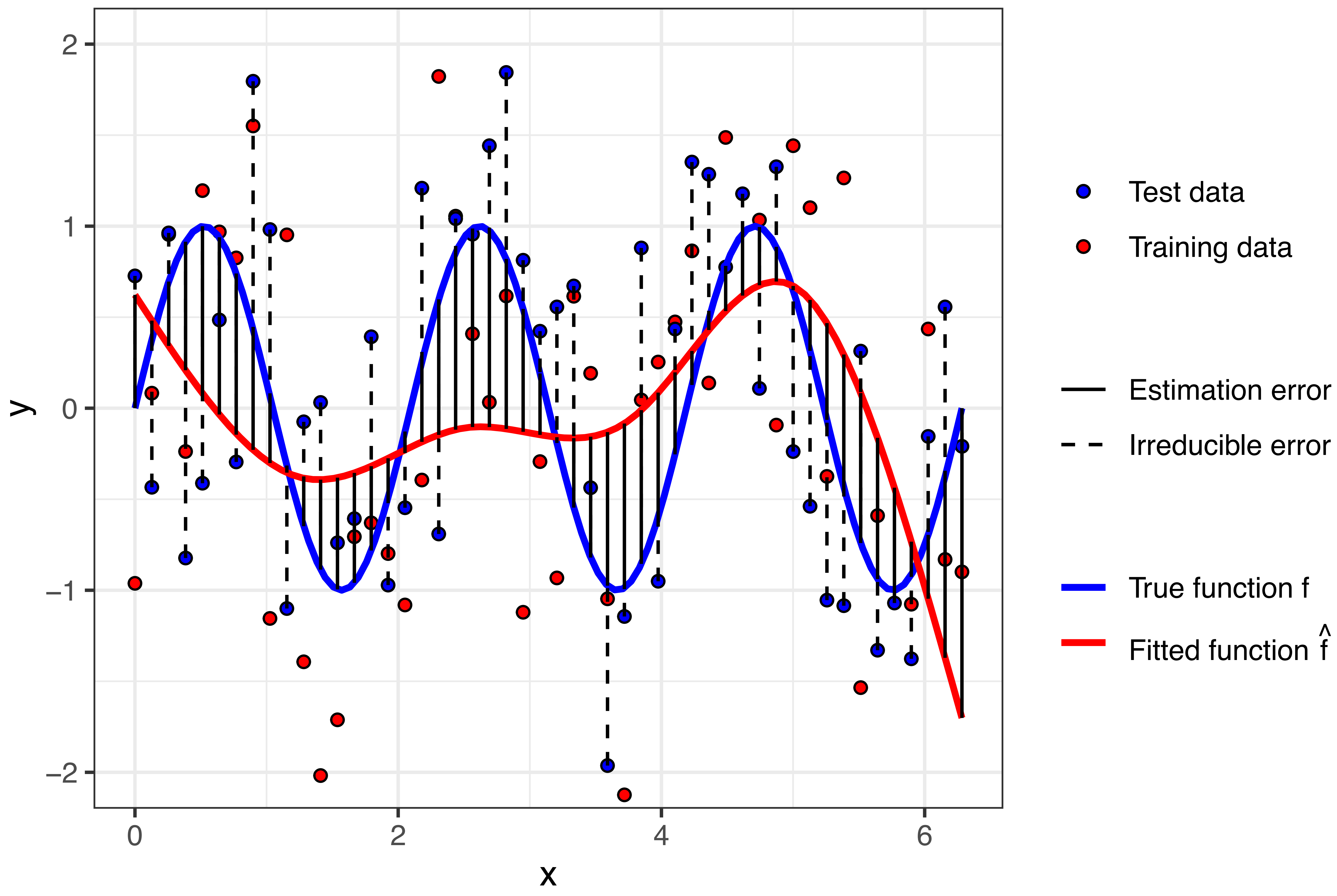

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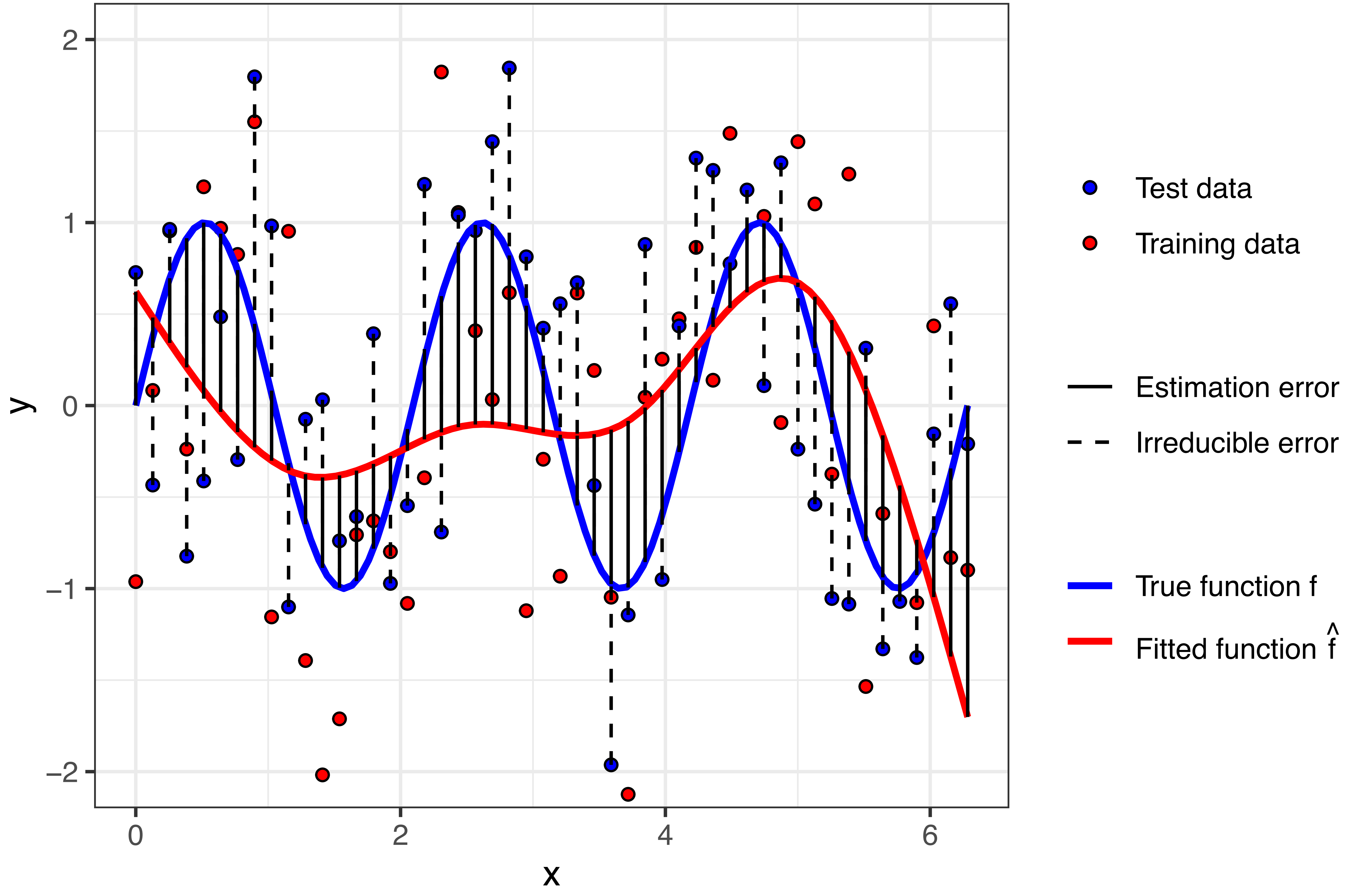

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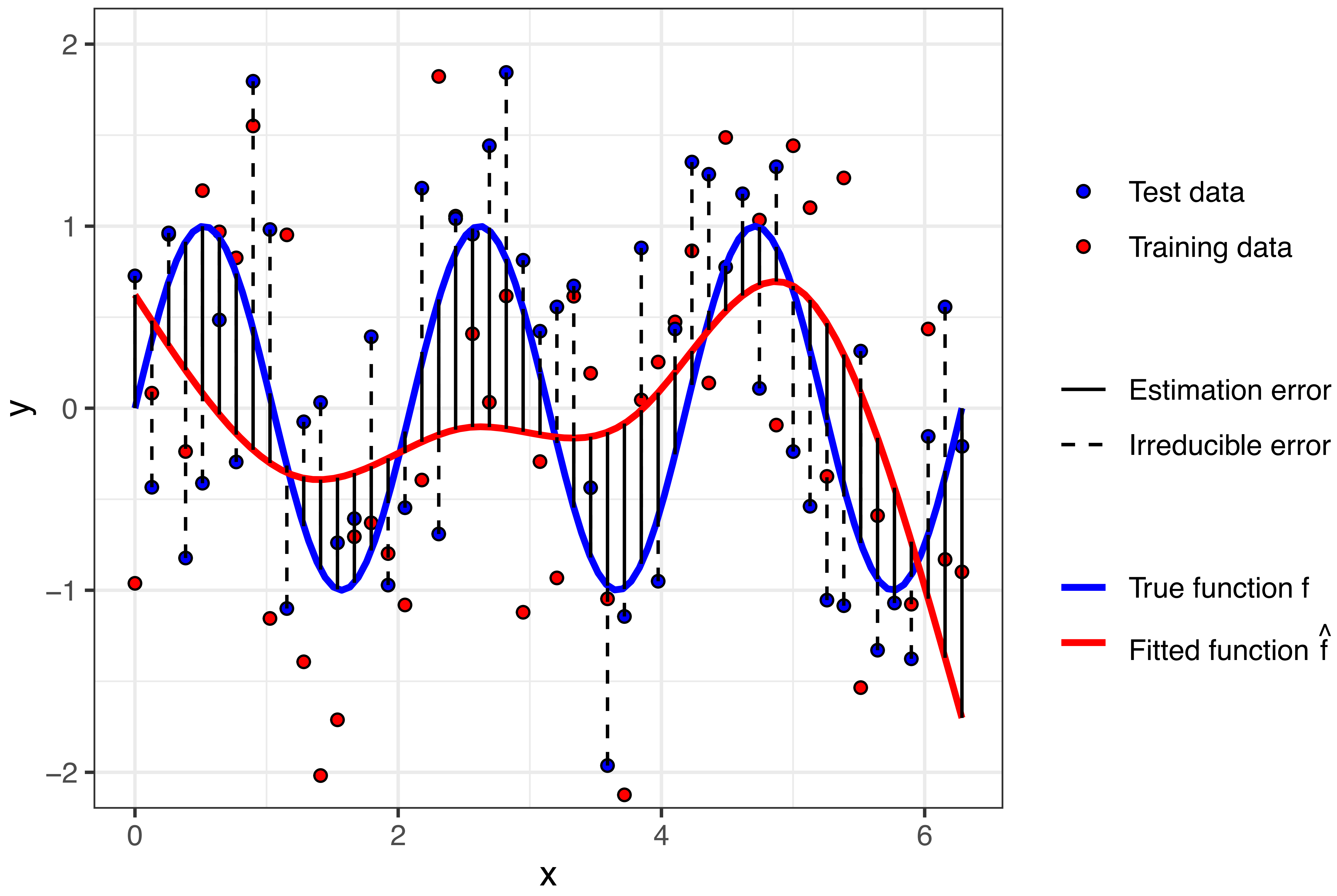

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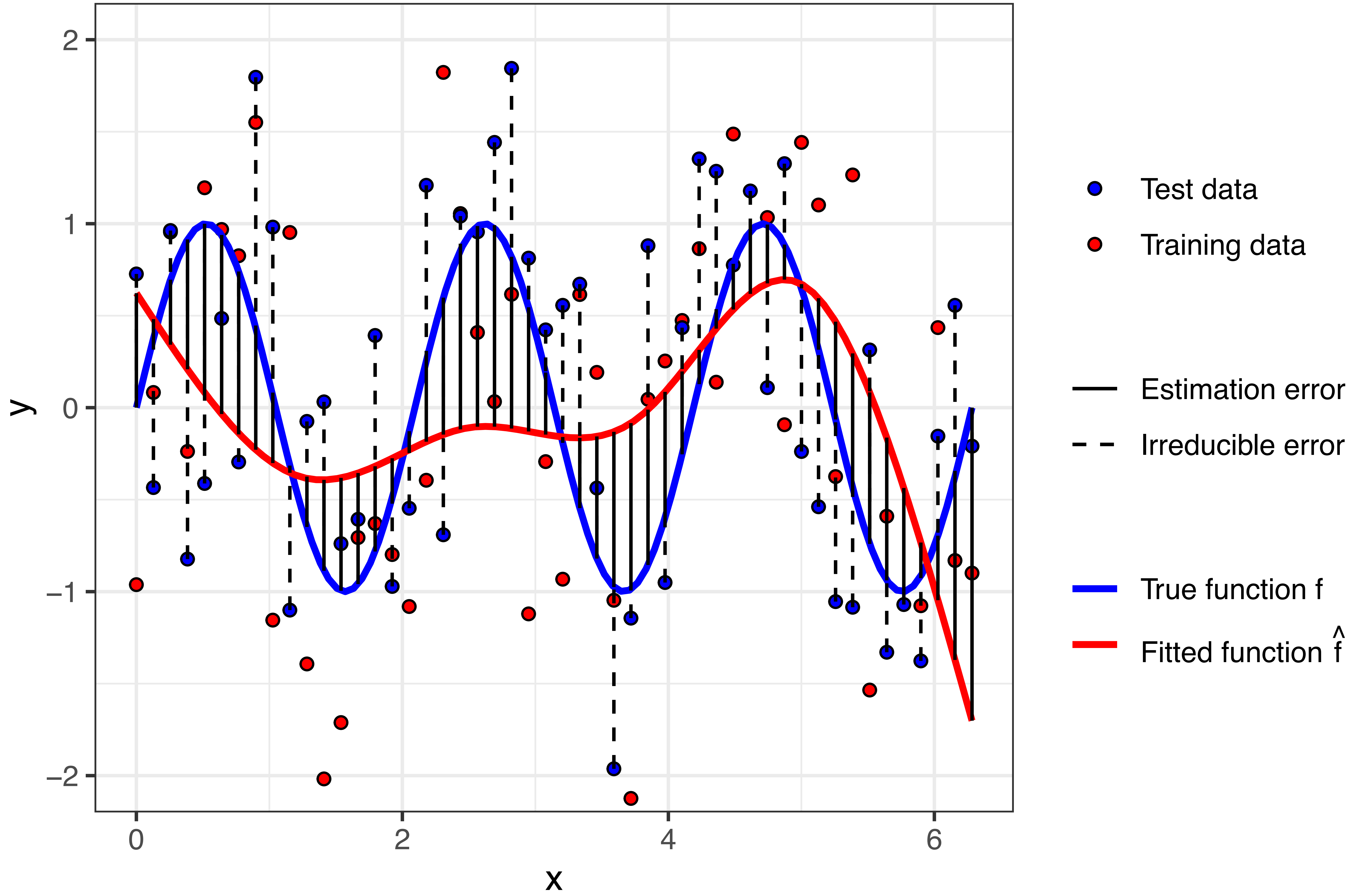

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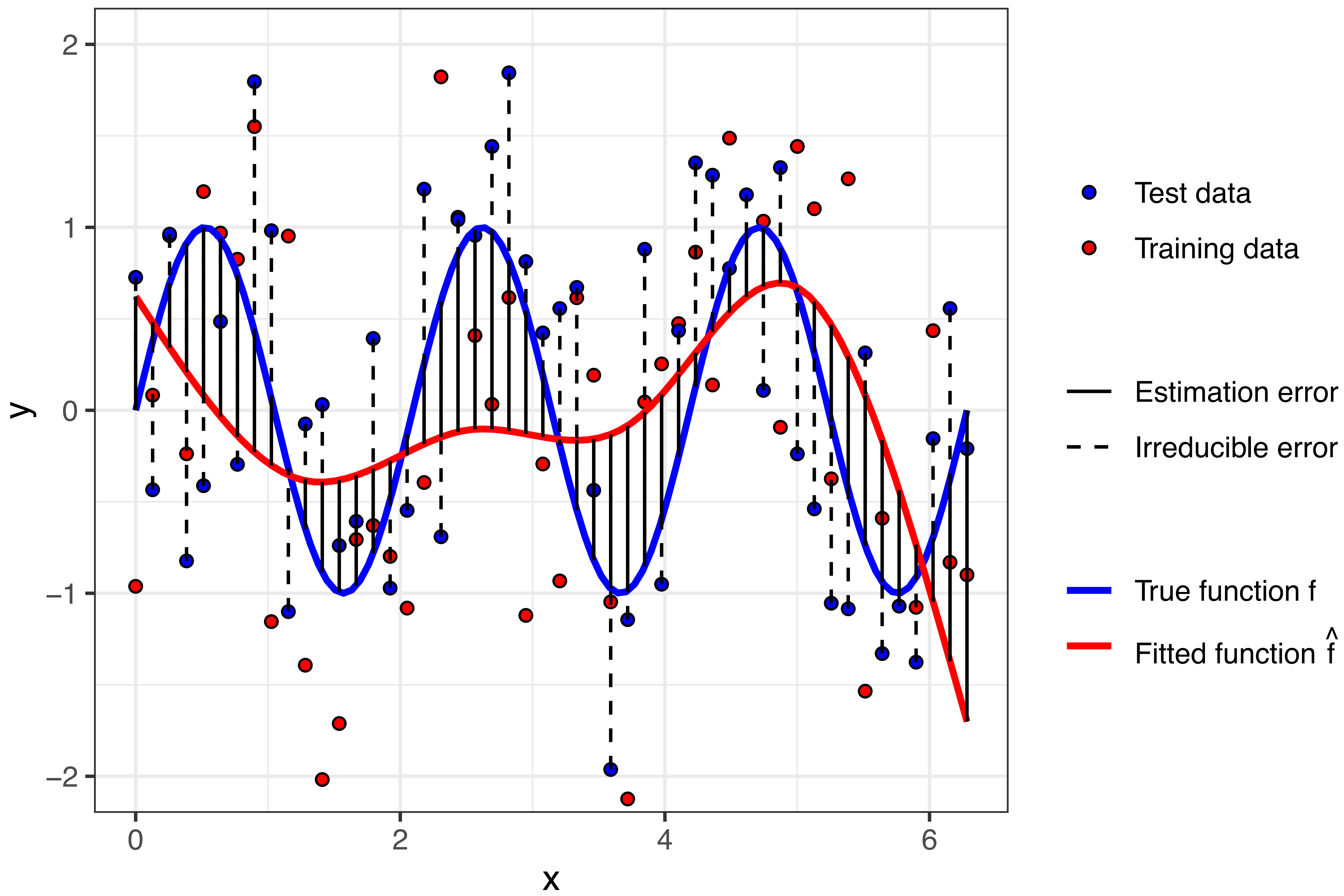

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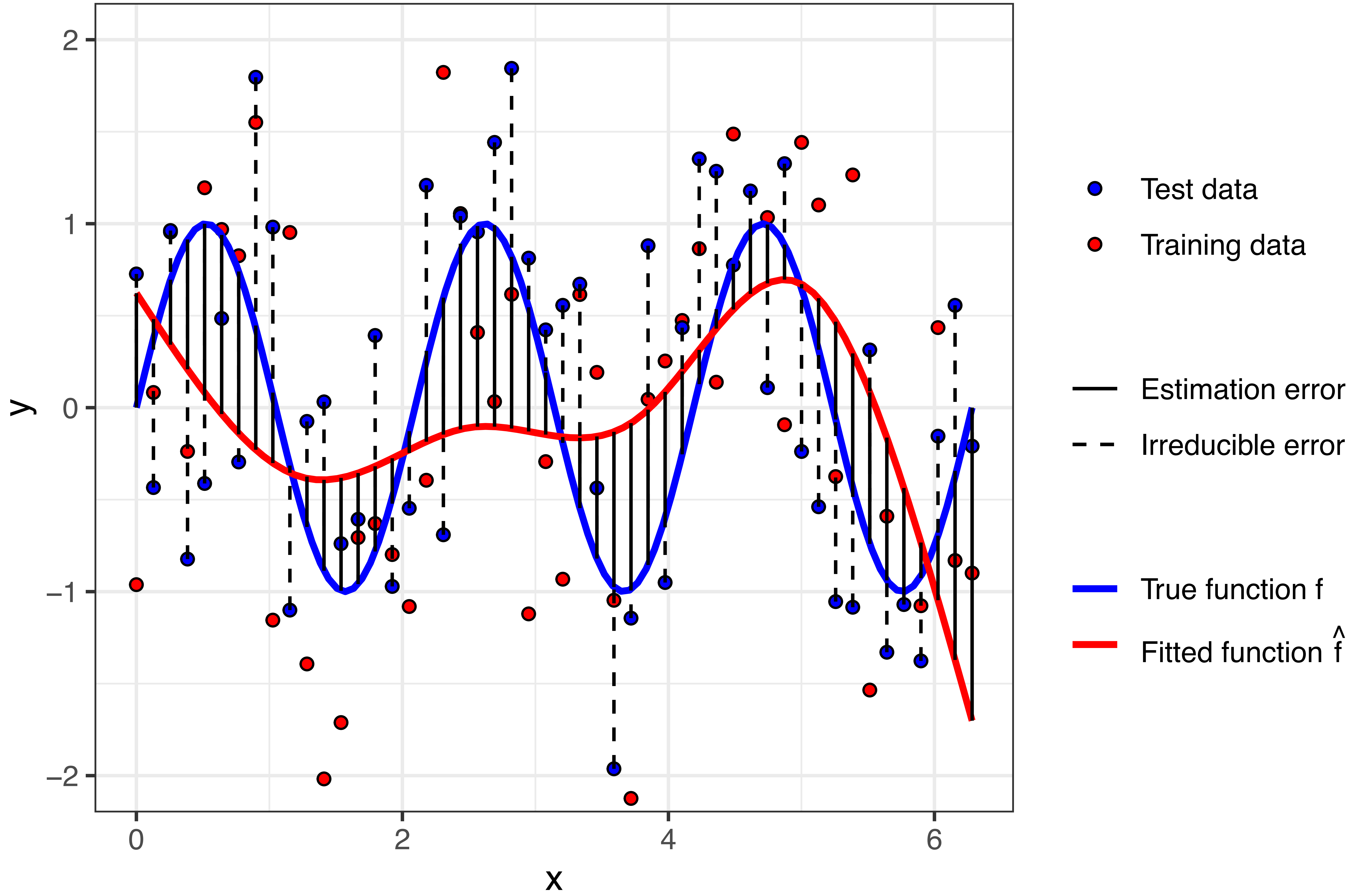
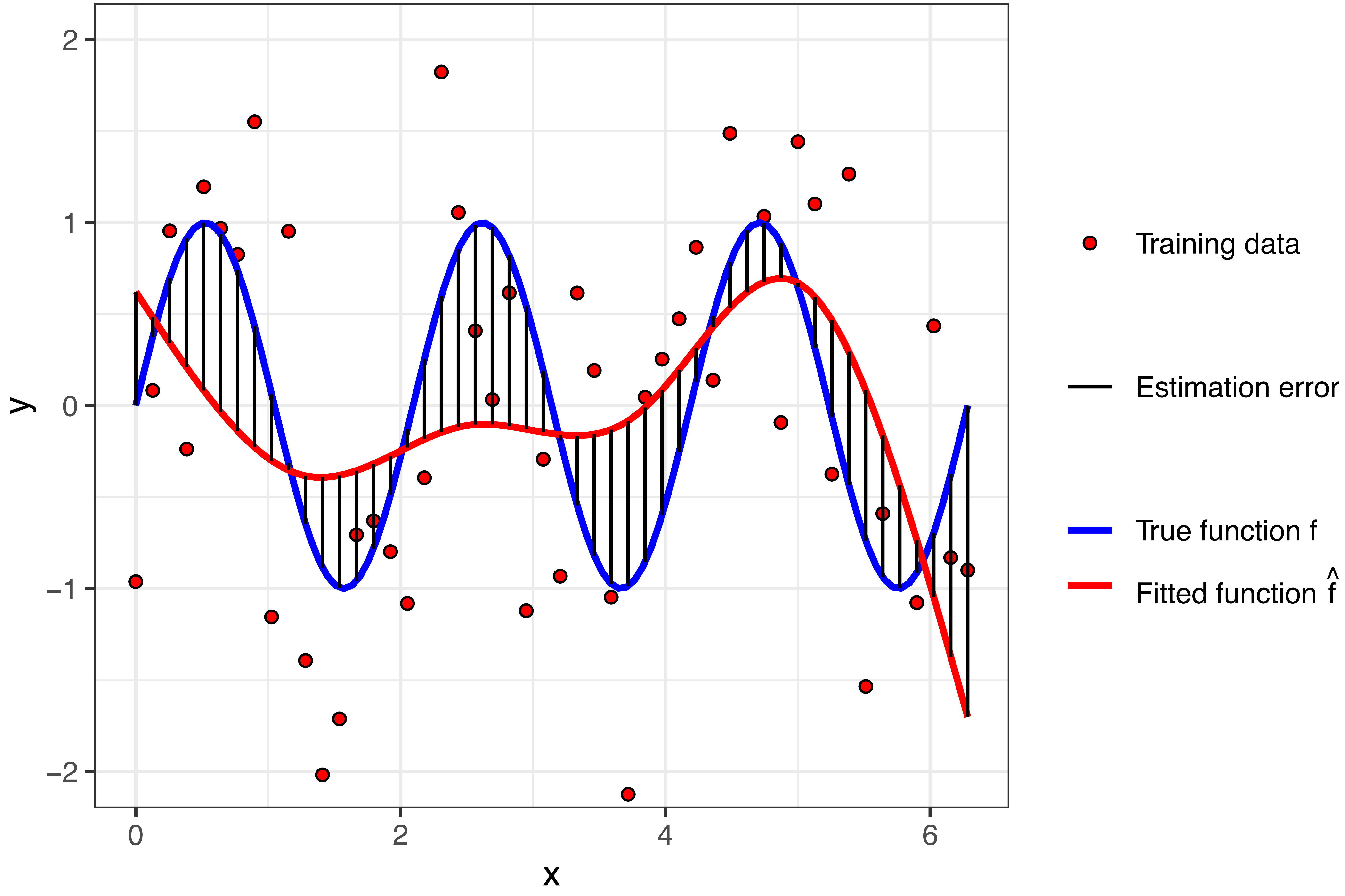


Contribution of randomness in training set

How estimation error $f(X_i^{\text{test}}) - \hat{f}(X_i^{\text{test}})$ varies as function of the training set.



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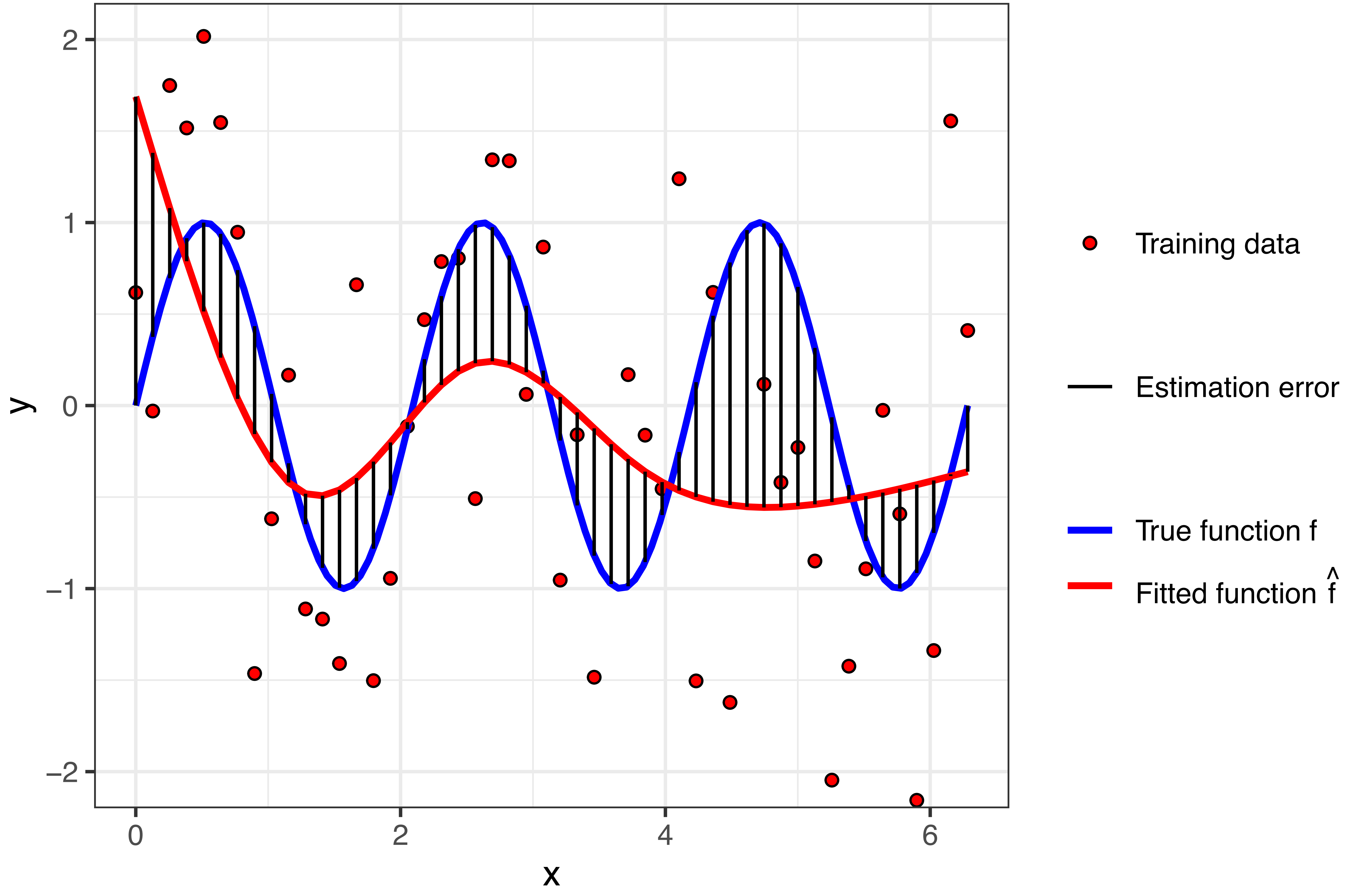

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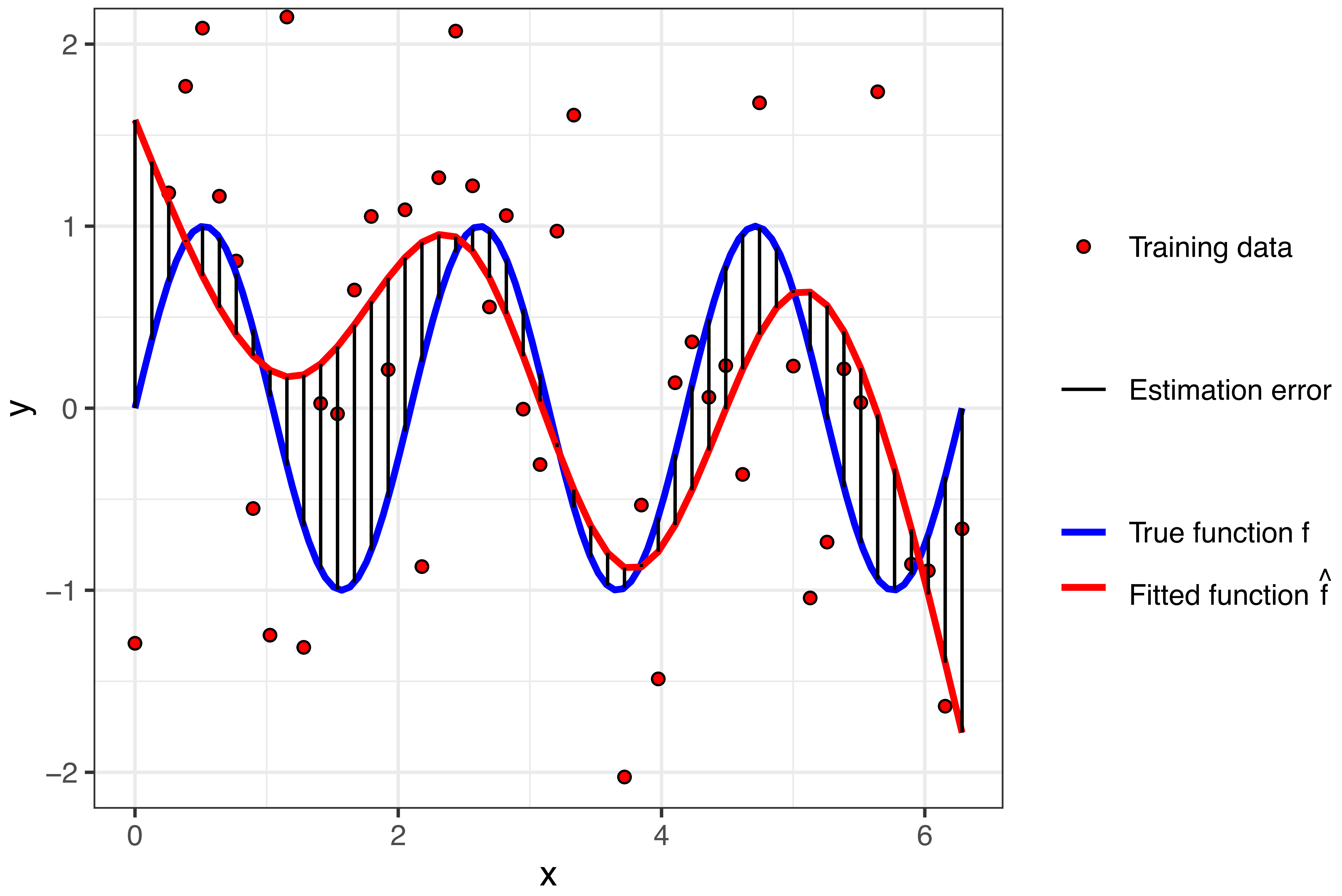

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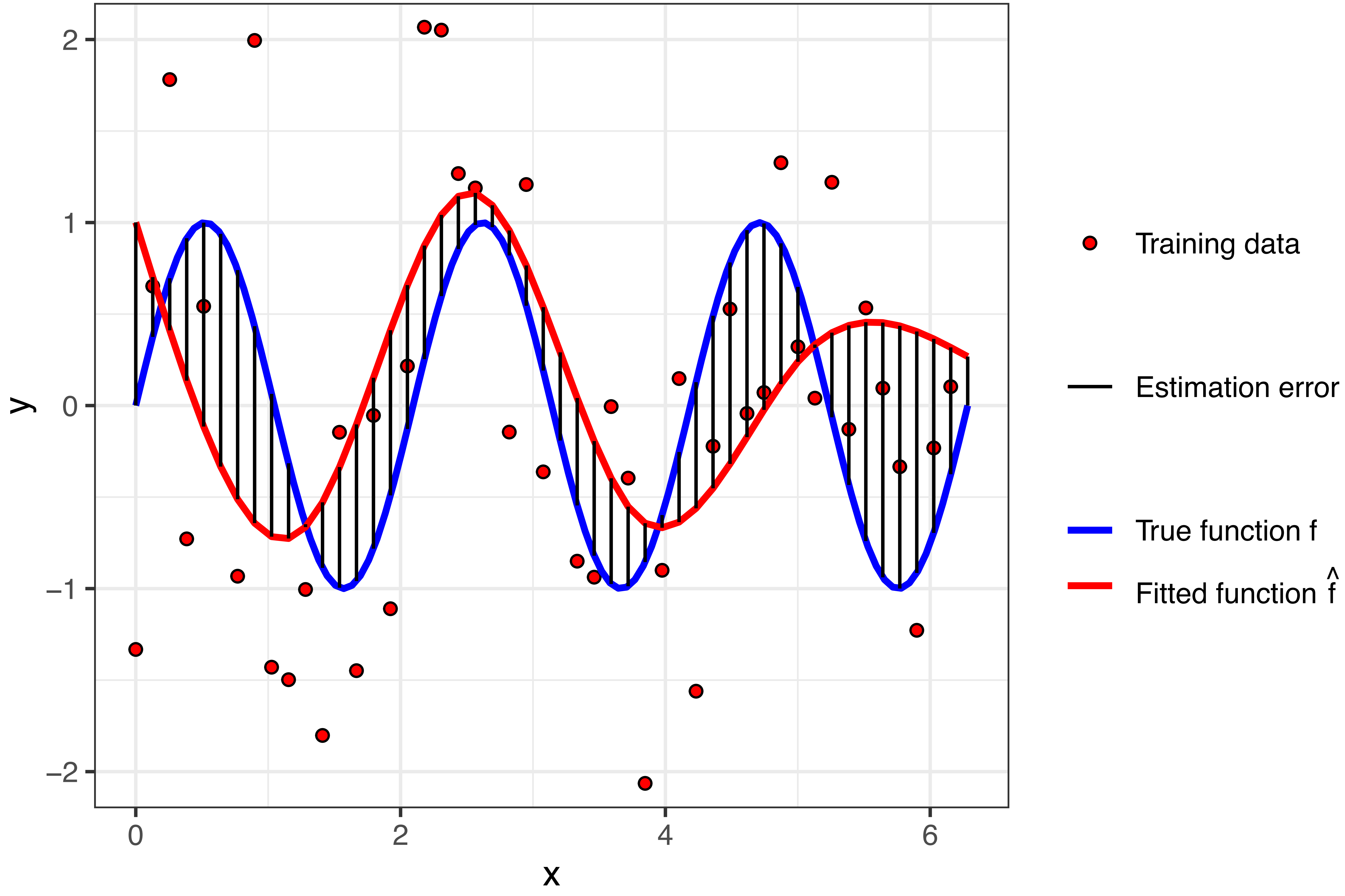
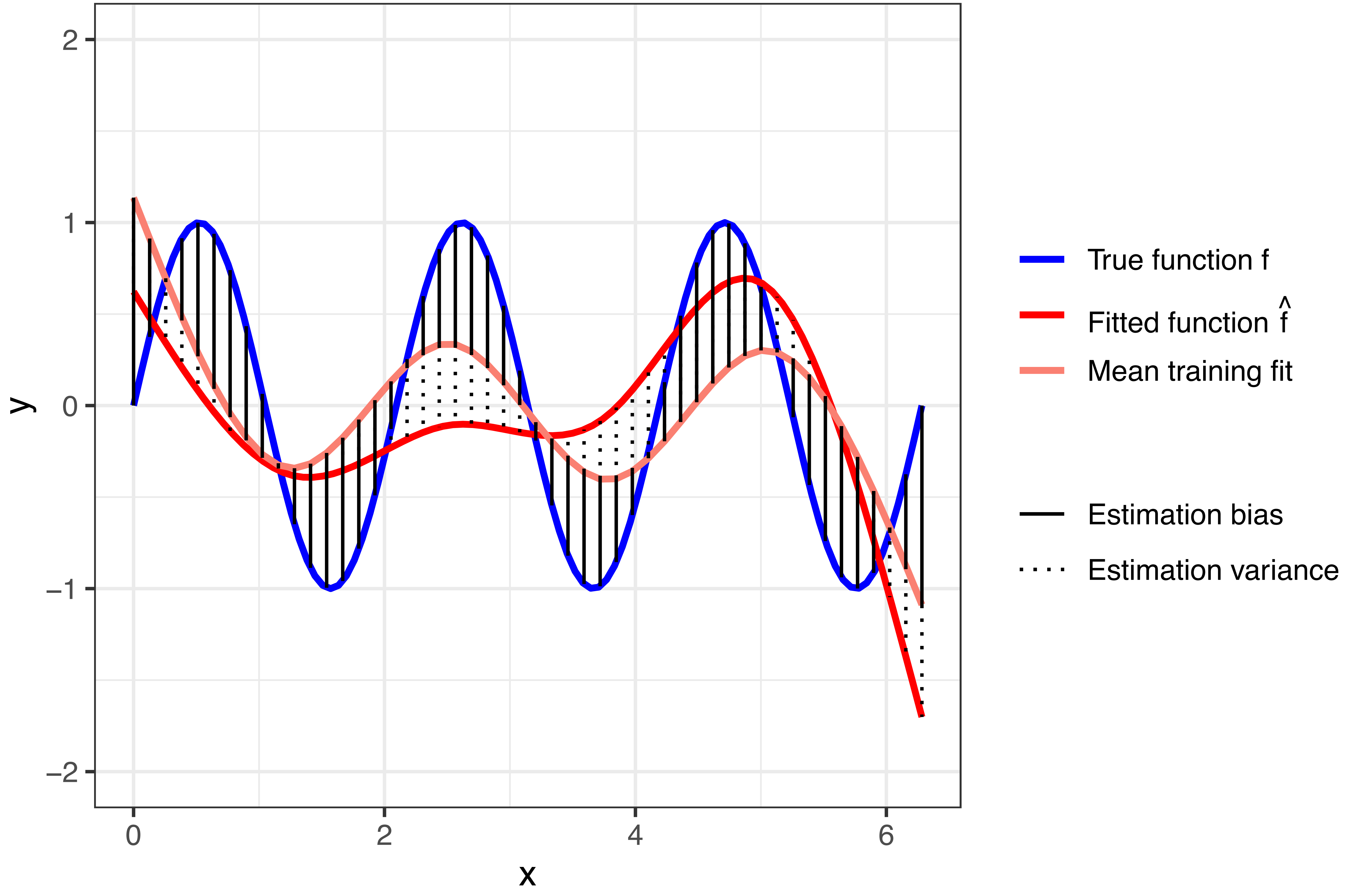


Estimation error = Bias^2 + Variance



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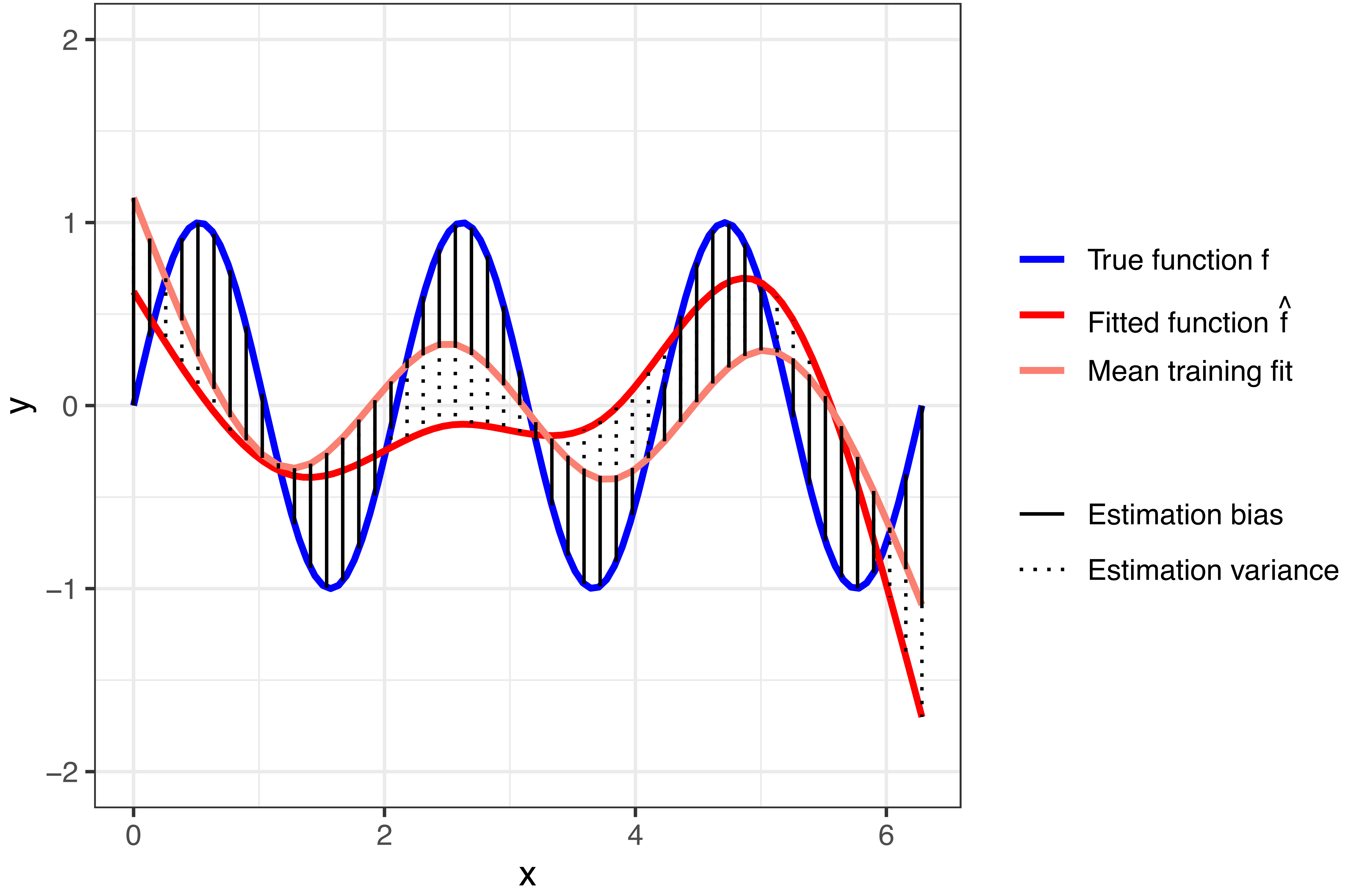

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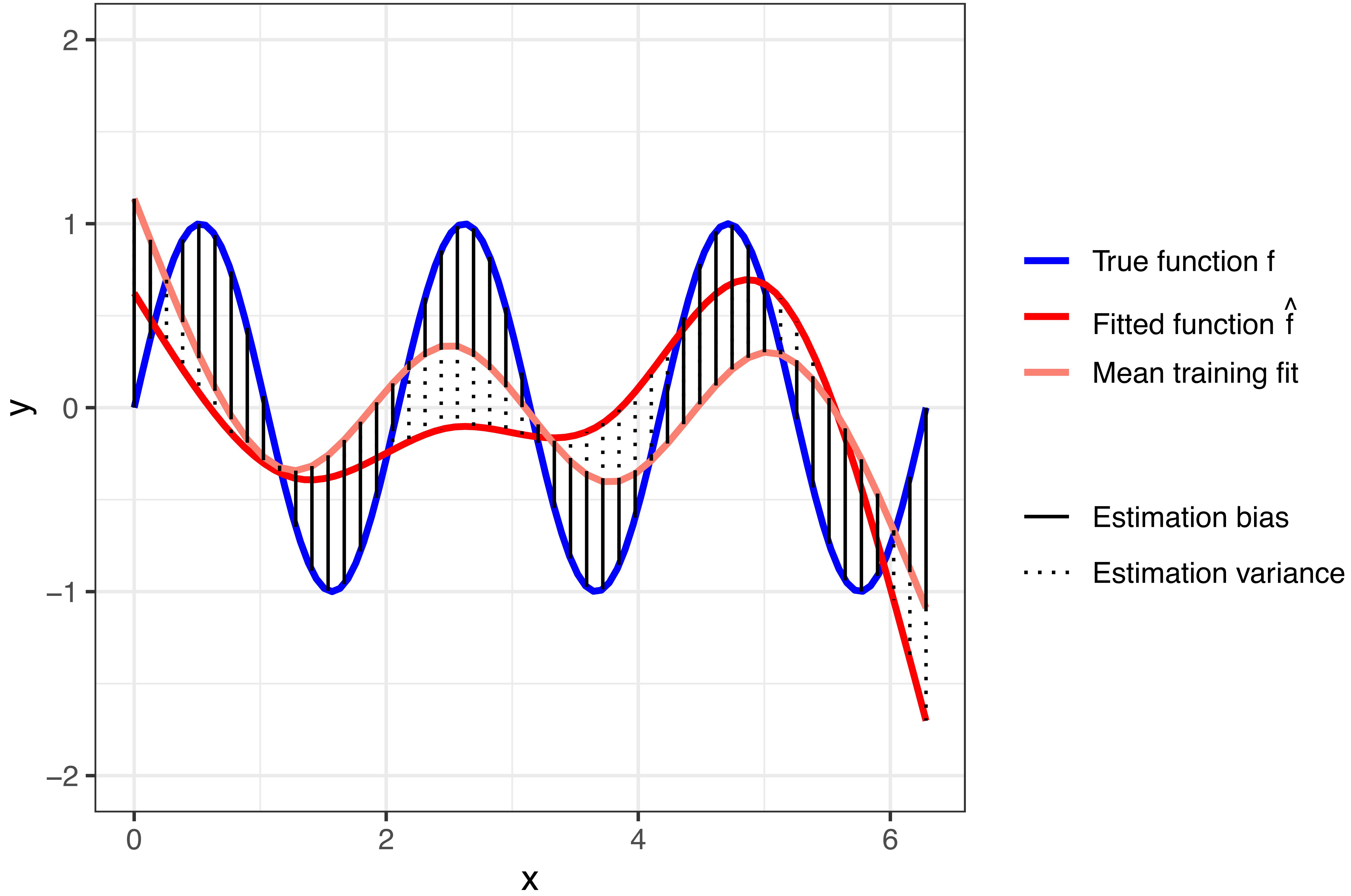

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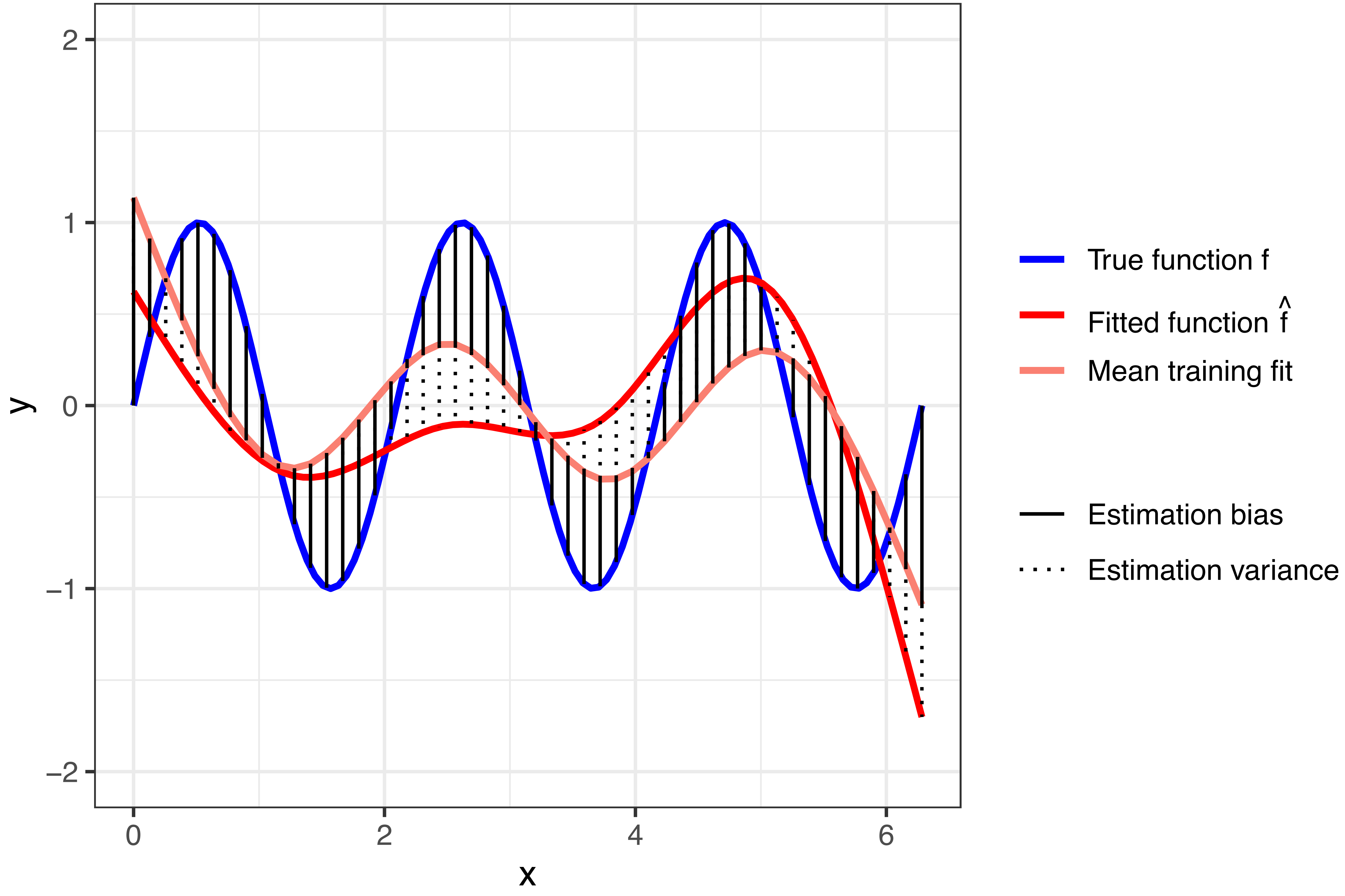

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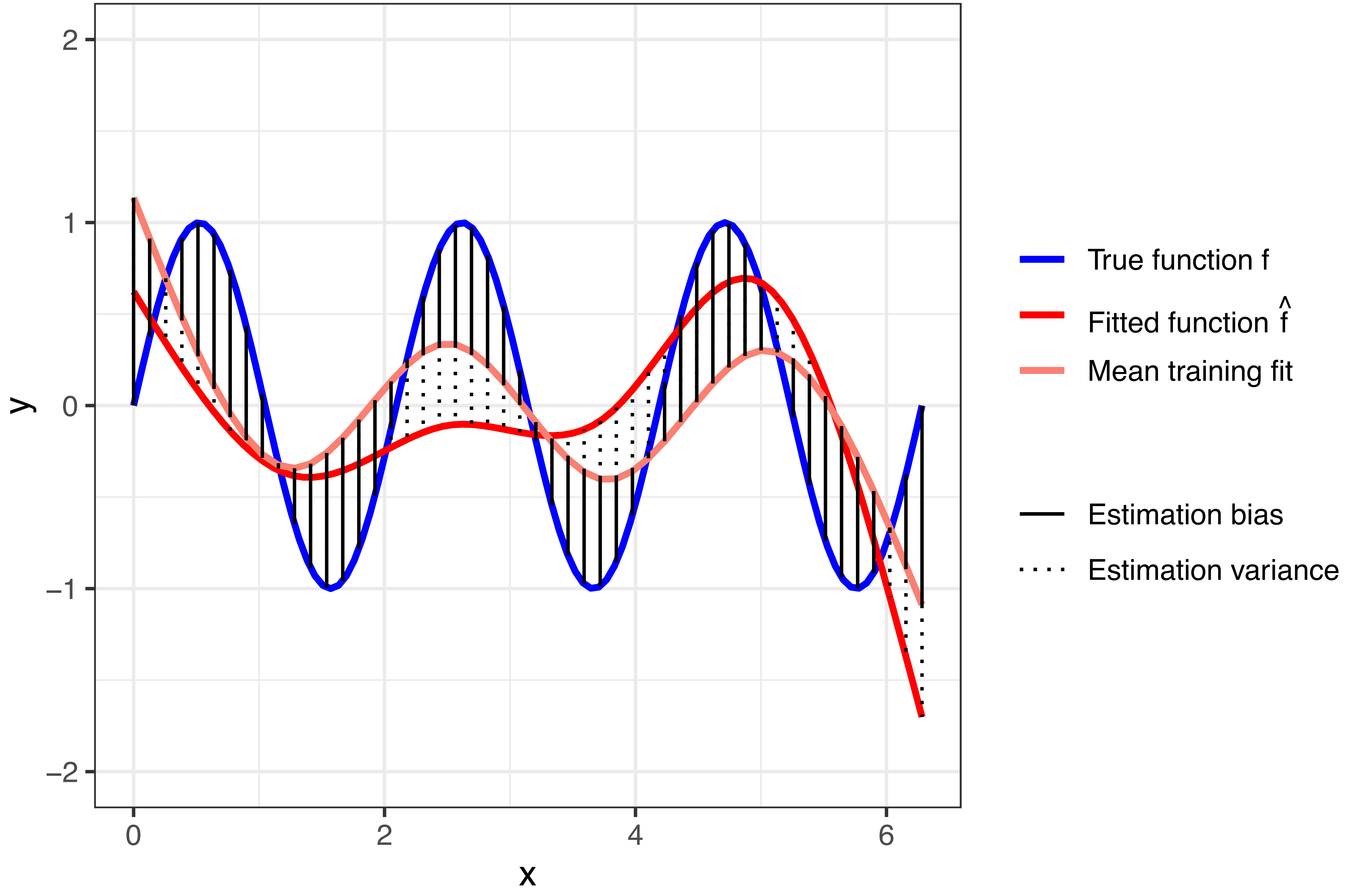

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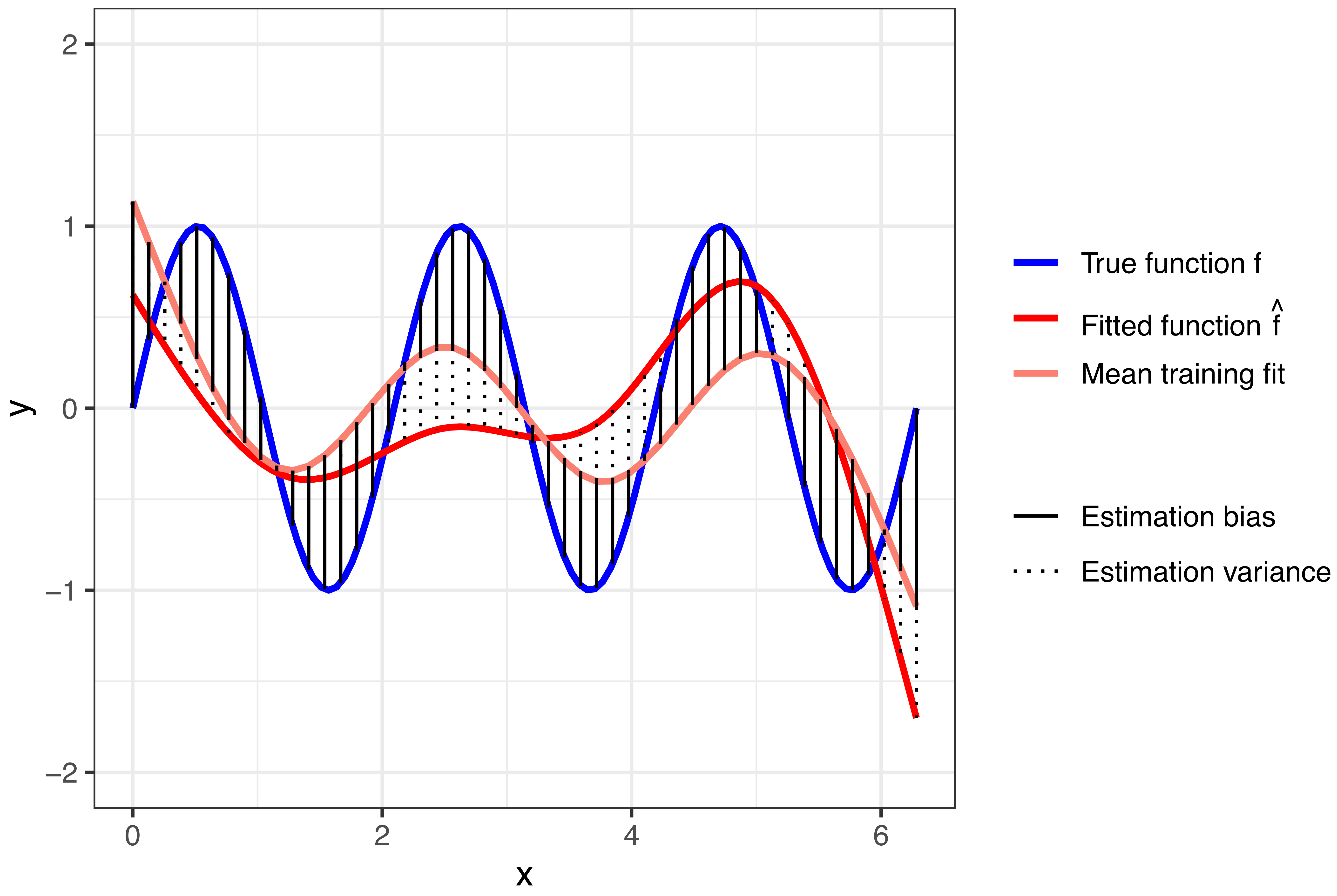
This is the bias-variance decomposition.



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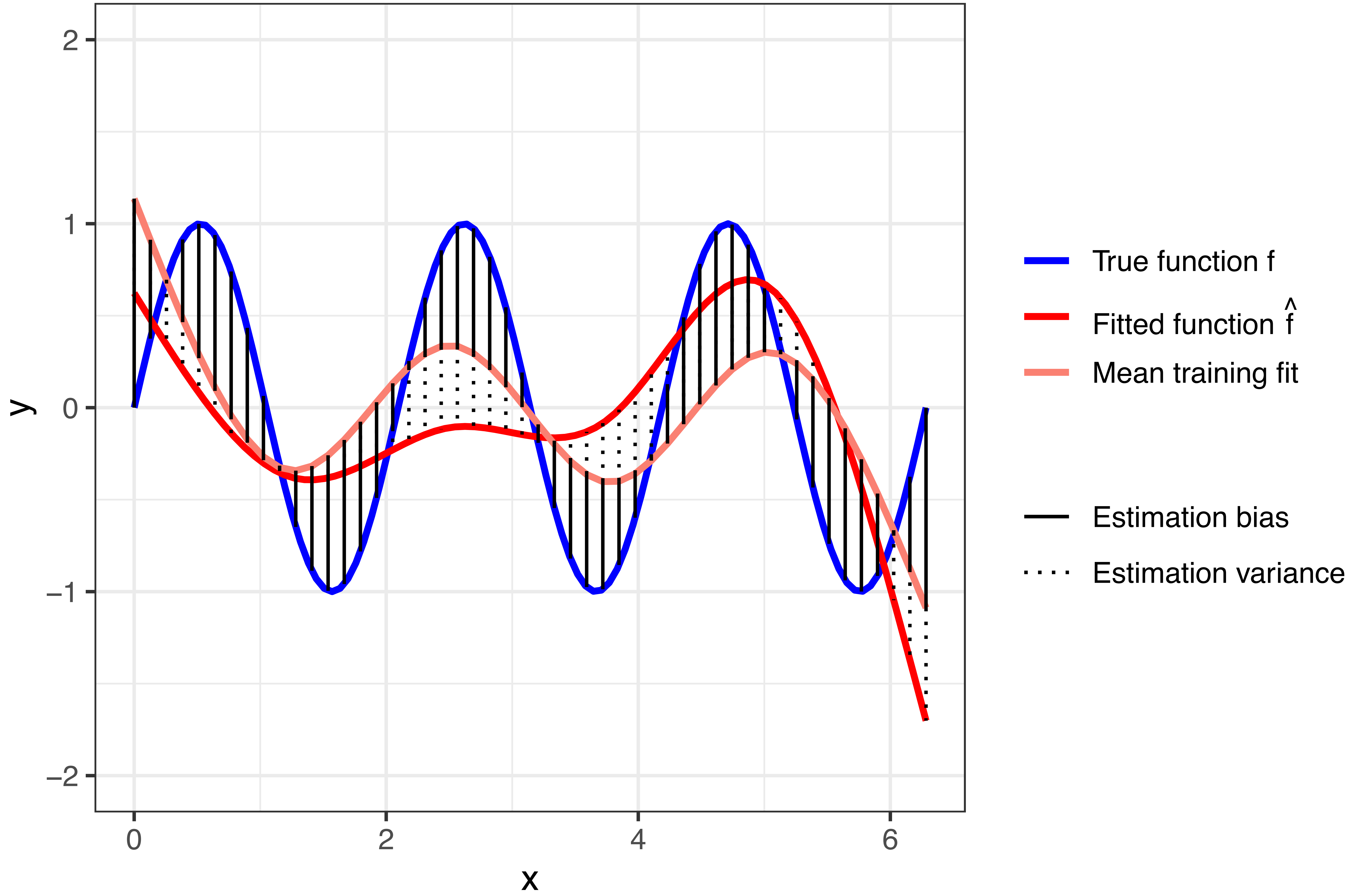

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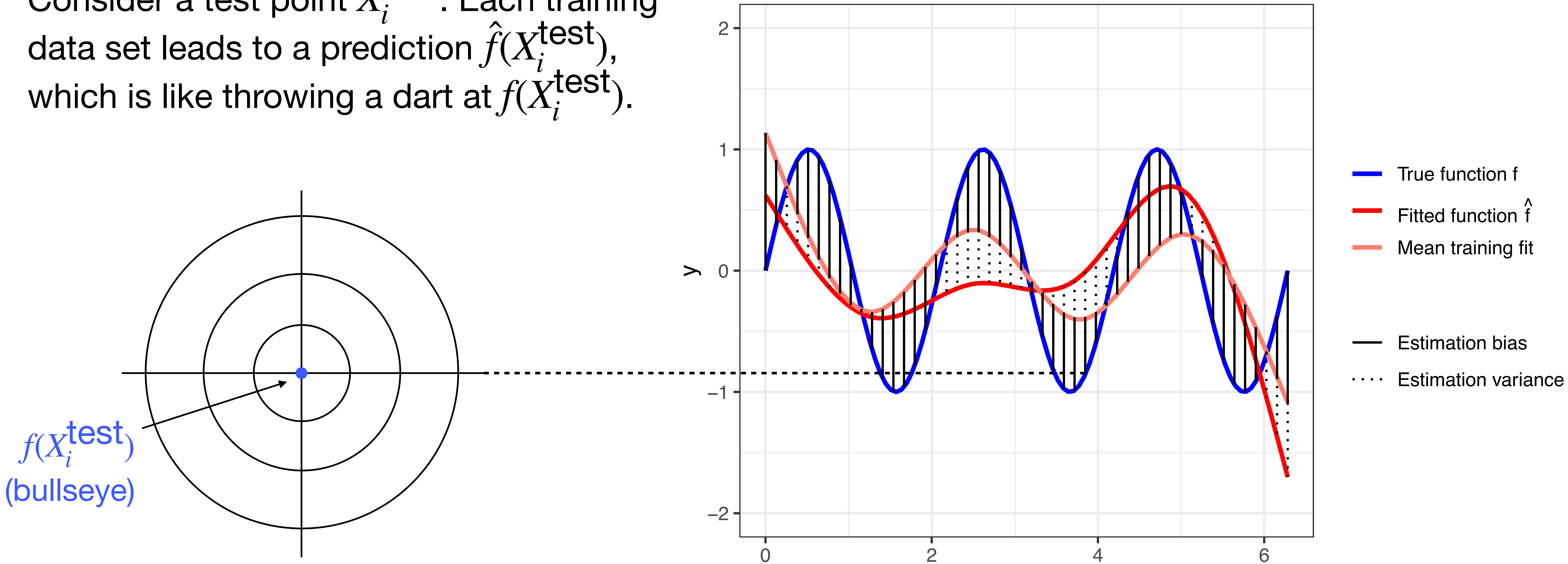

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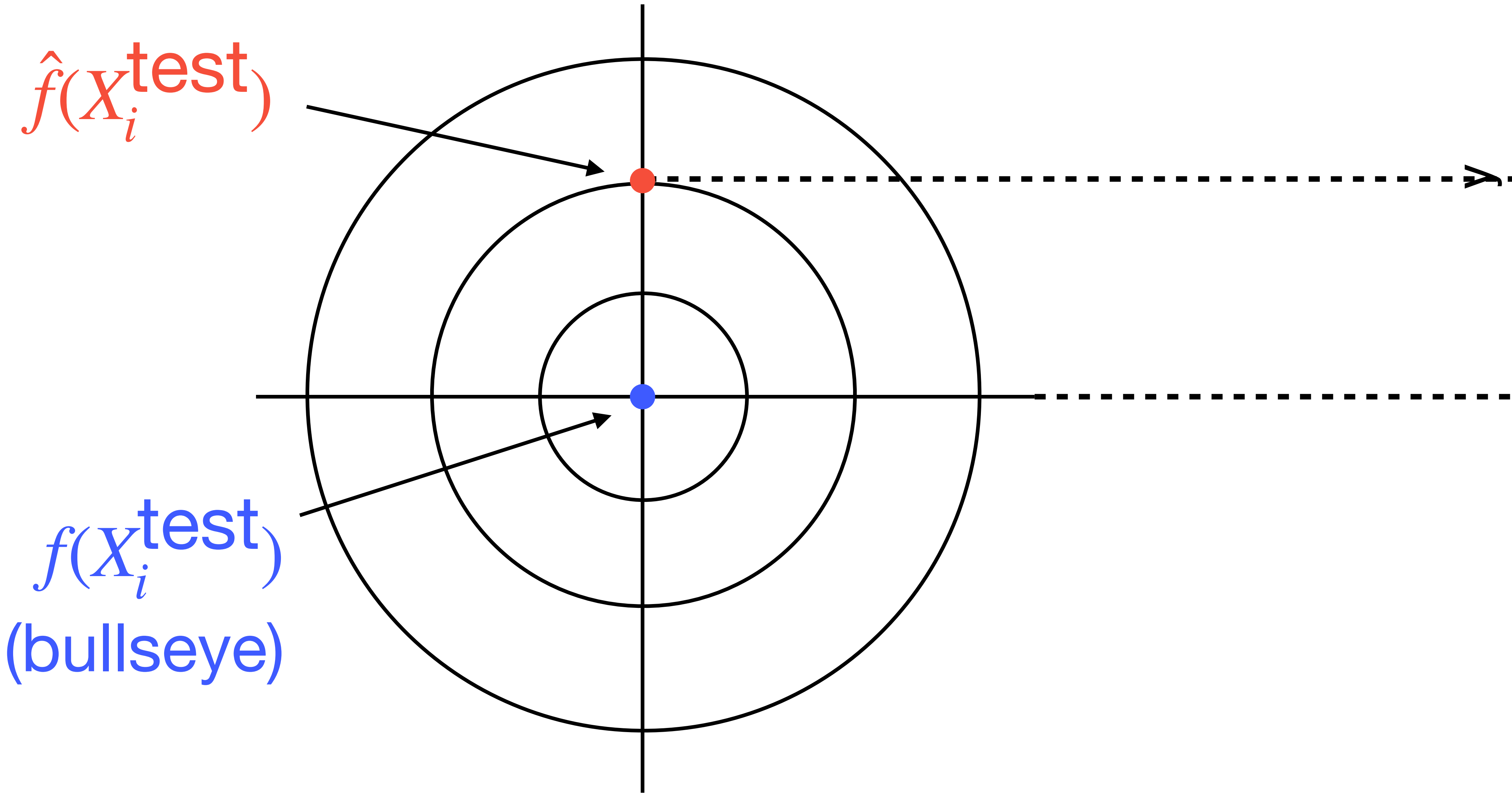

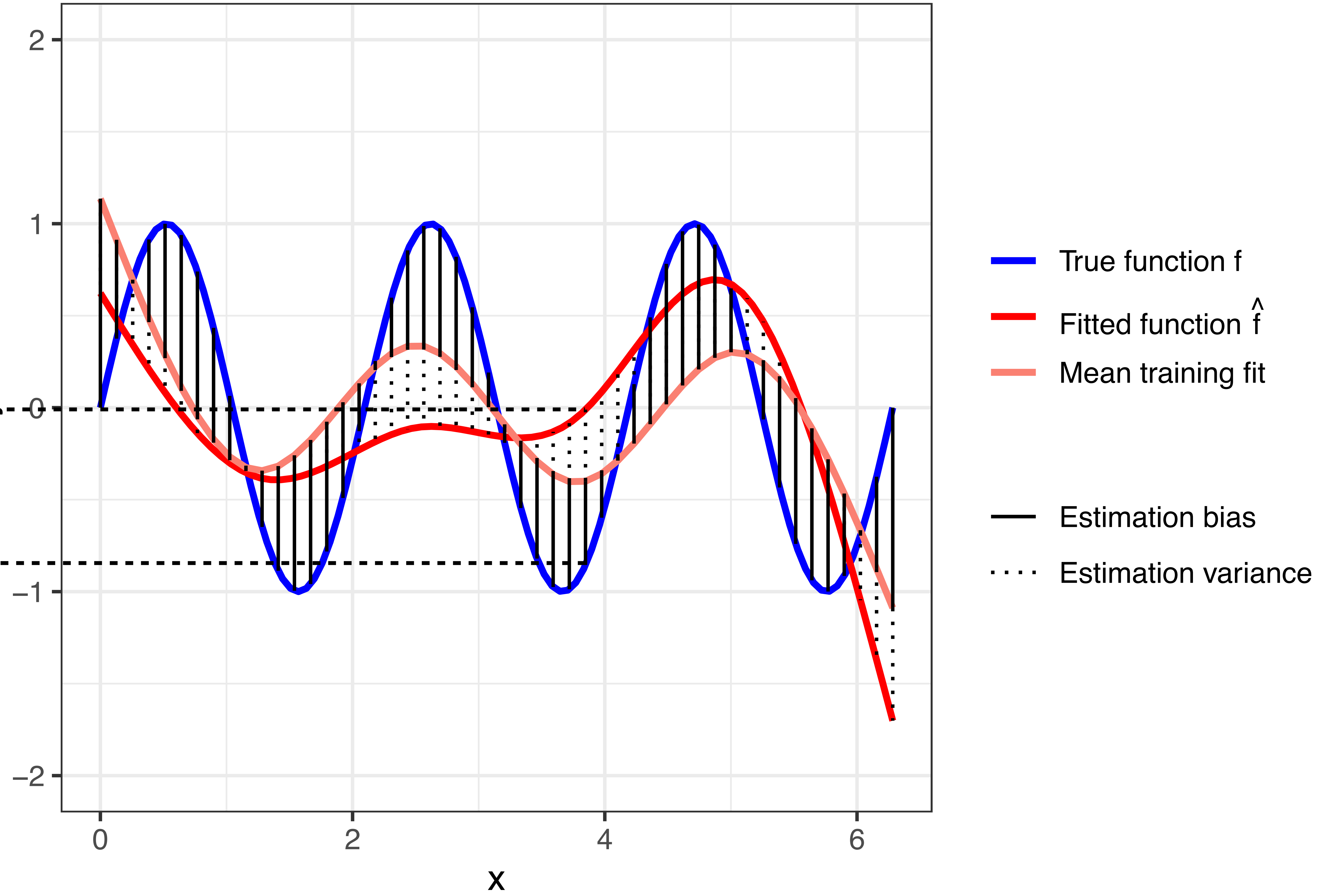

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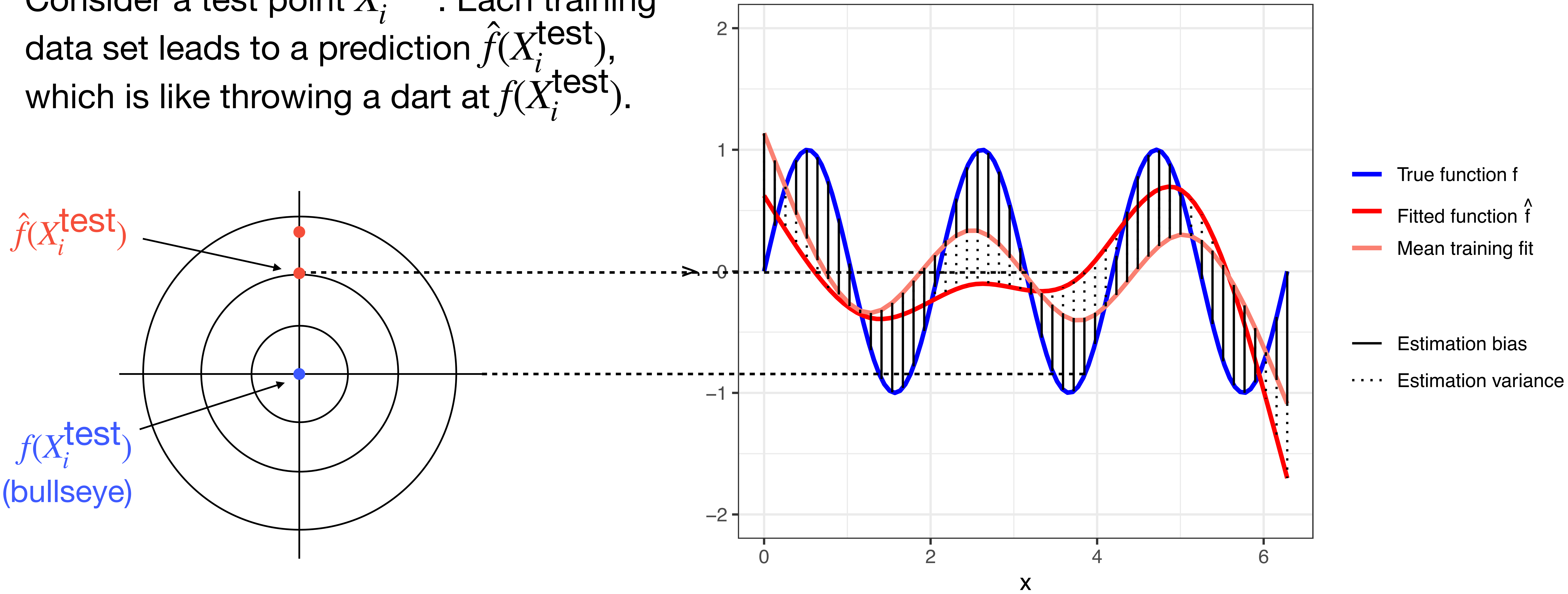

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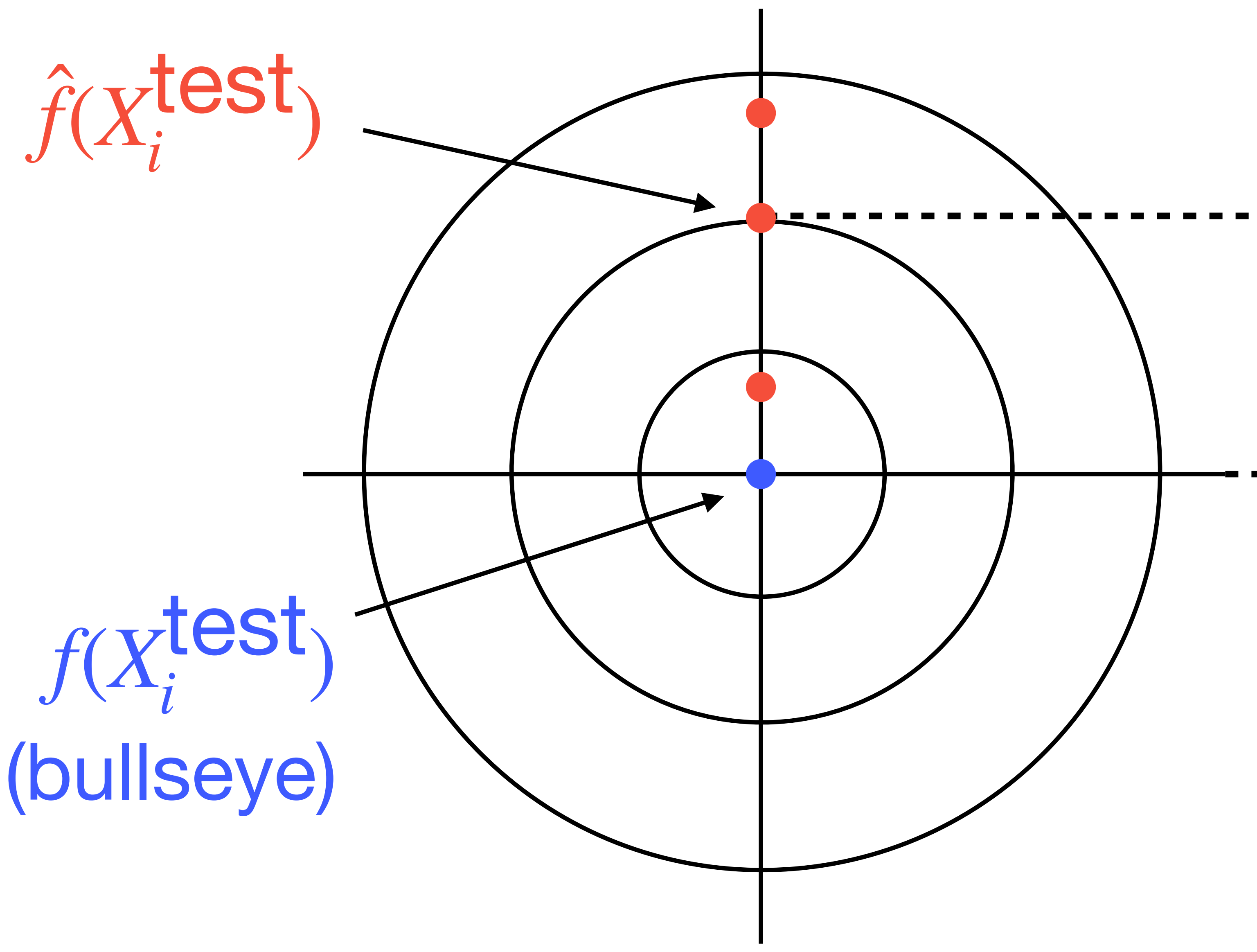

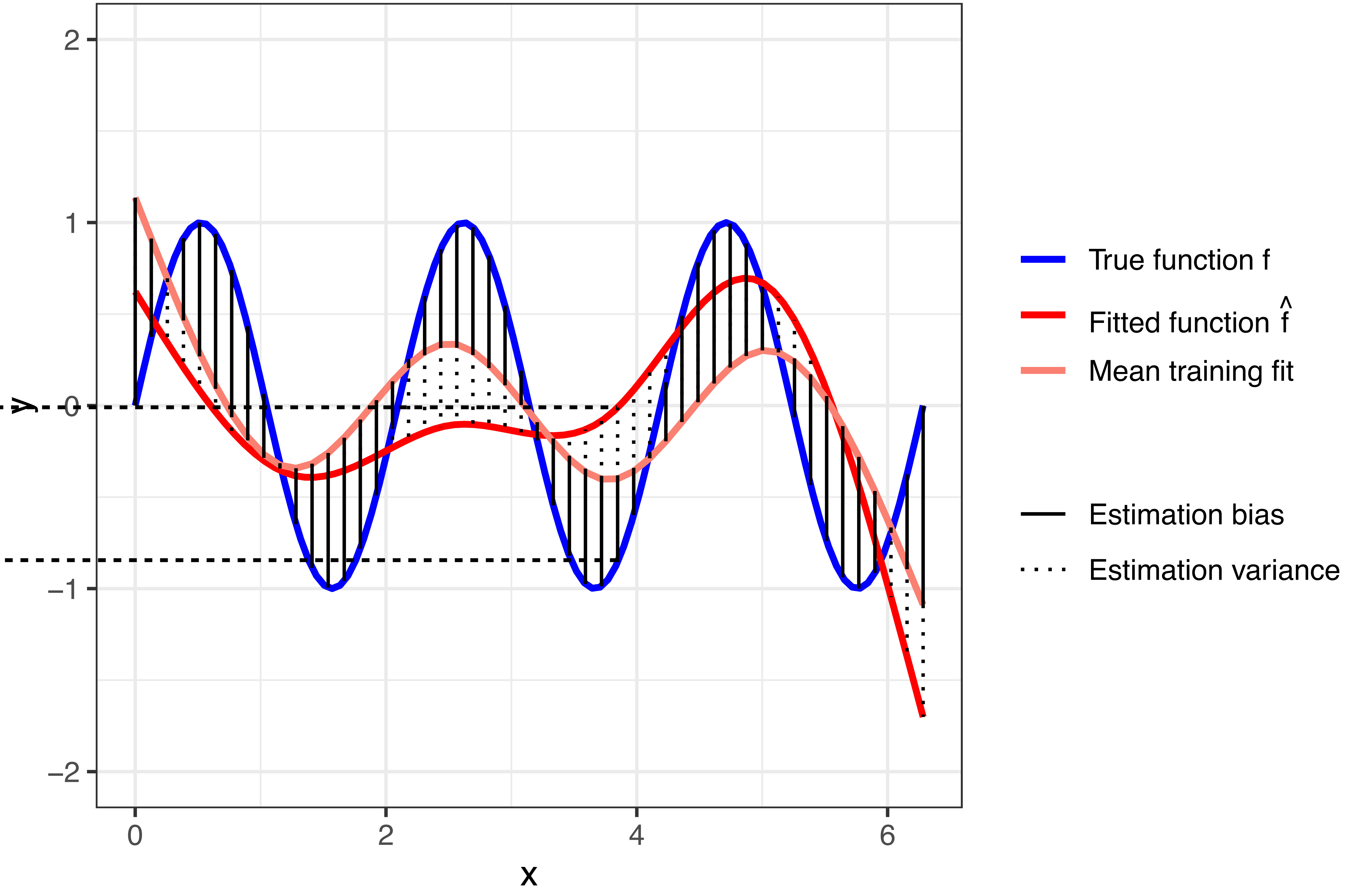

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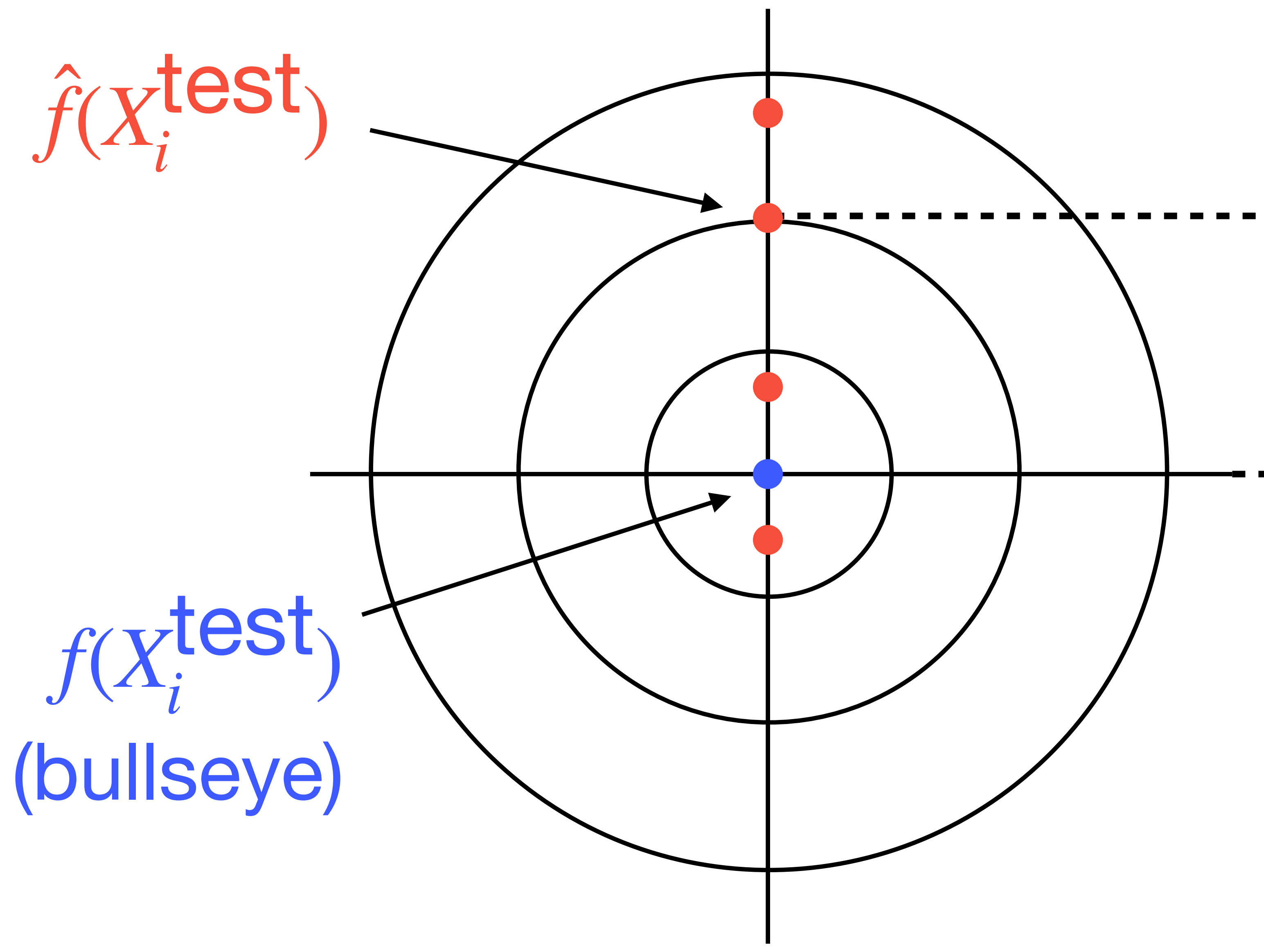

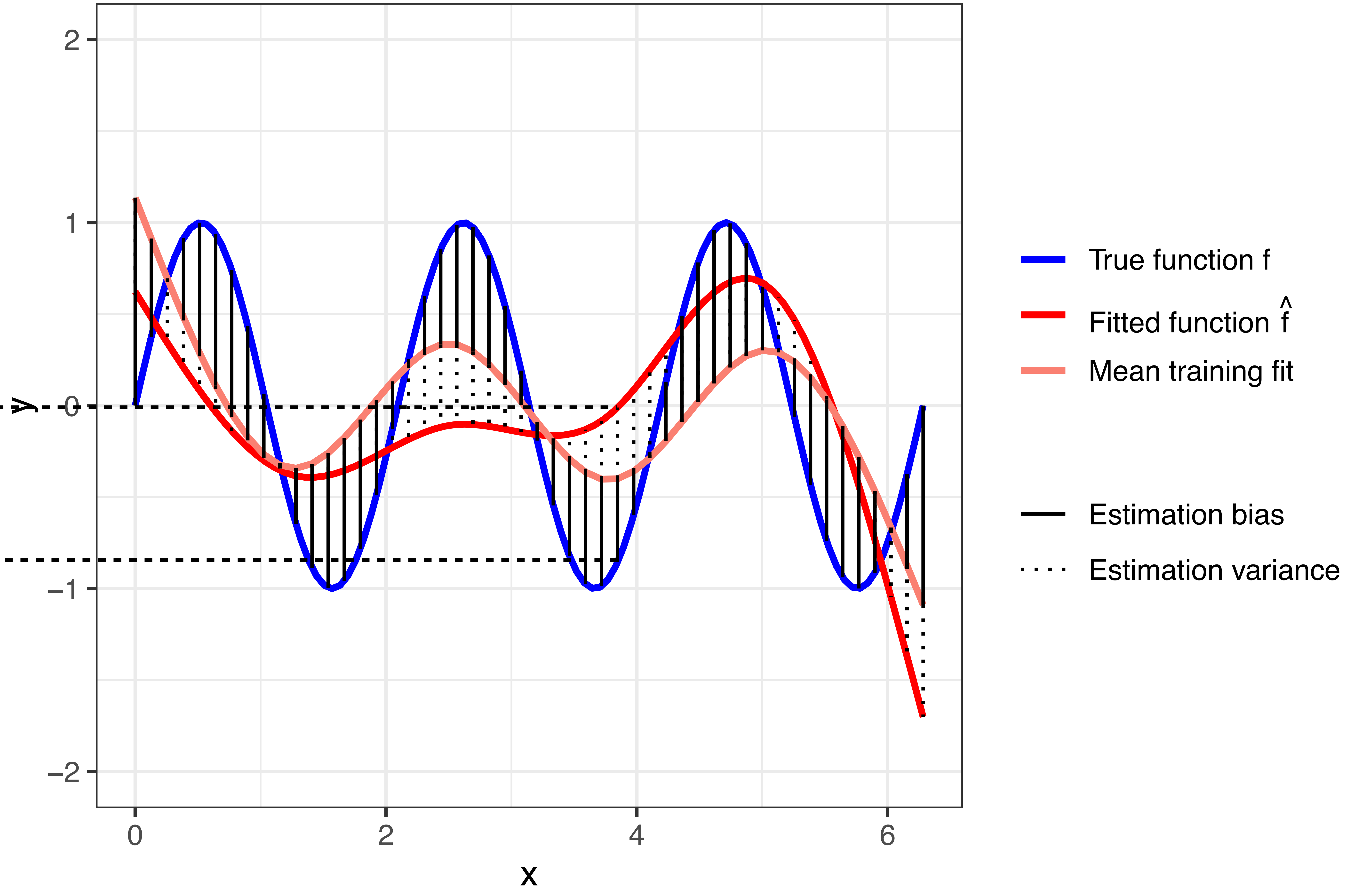

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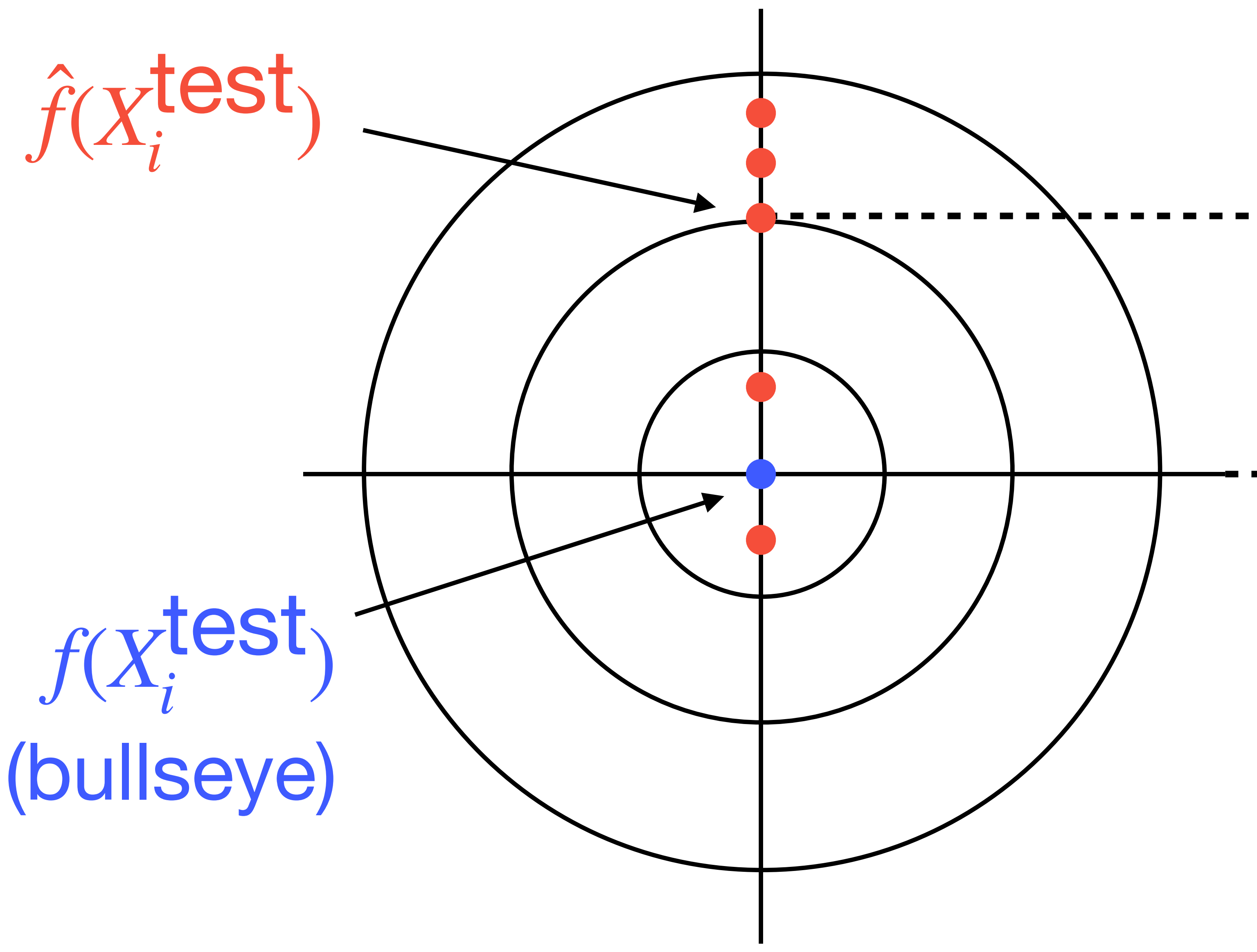

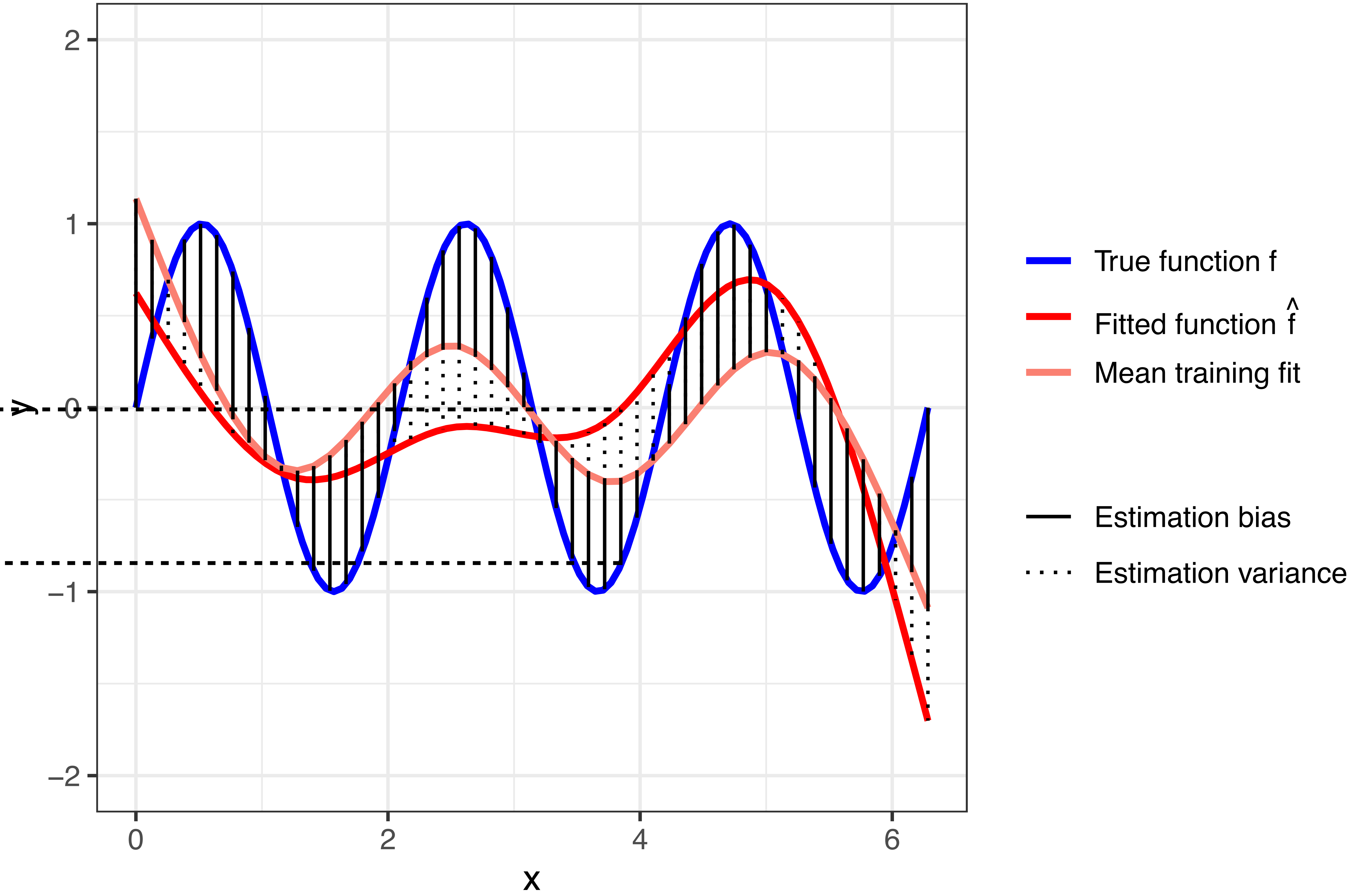

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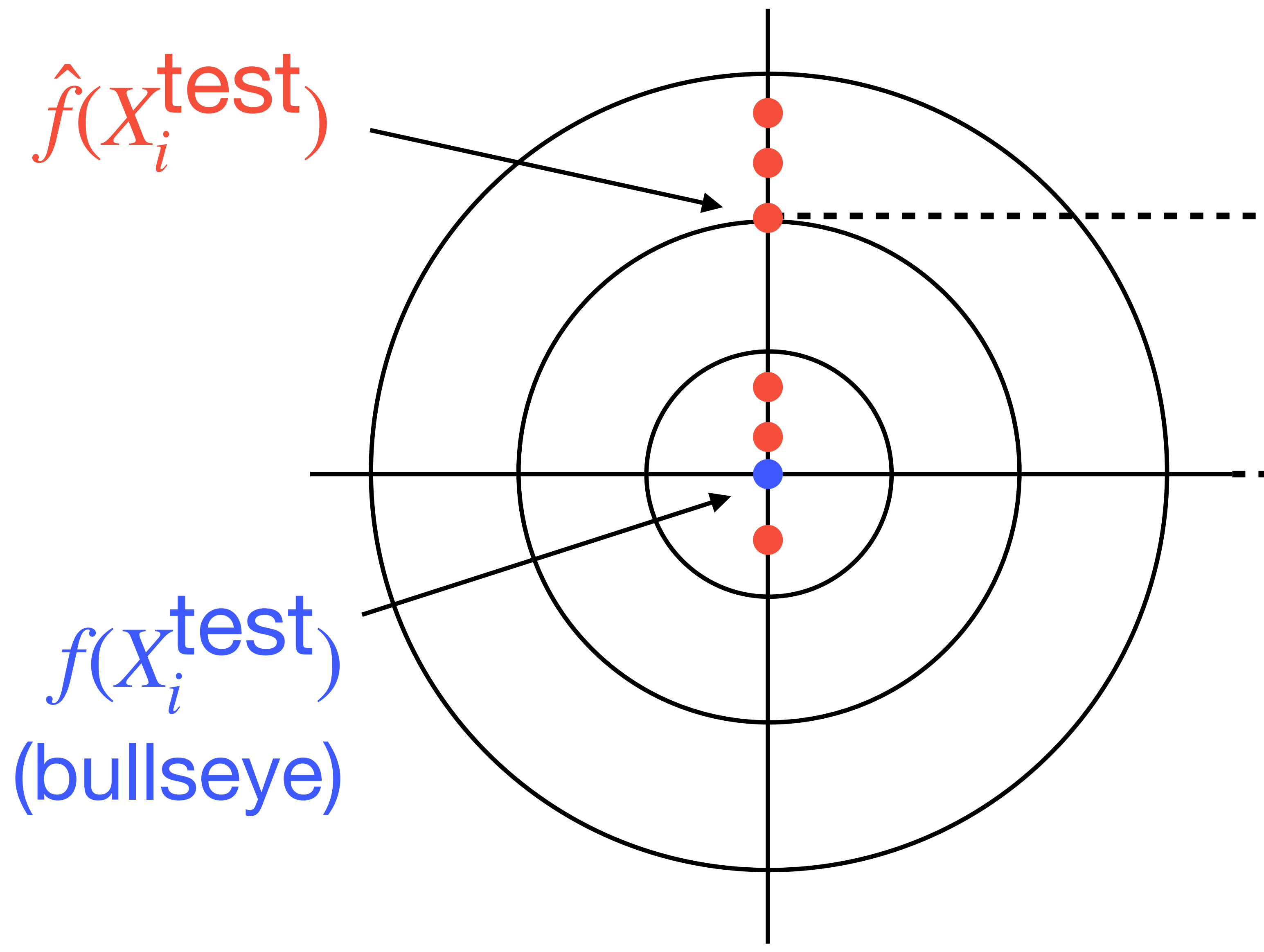

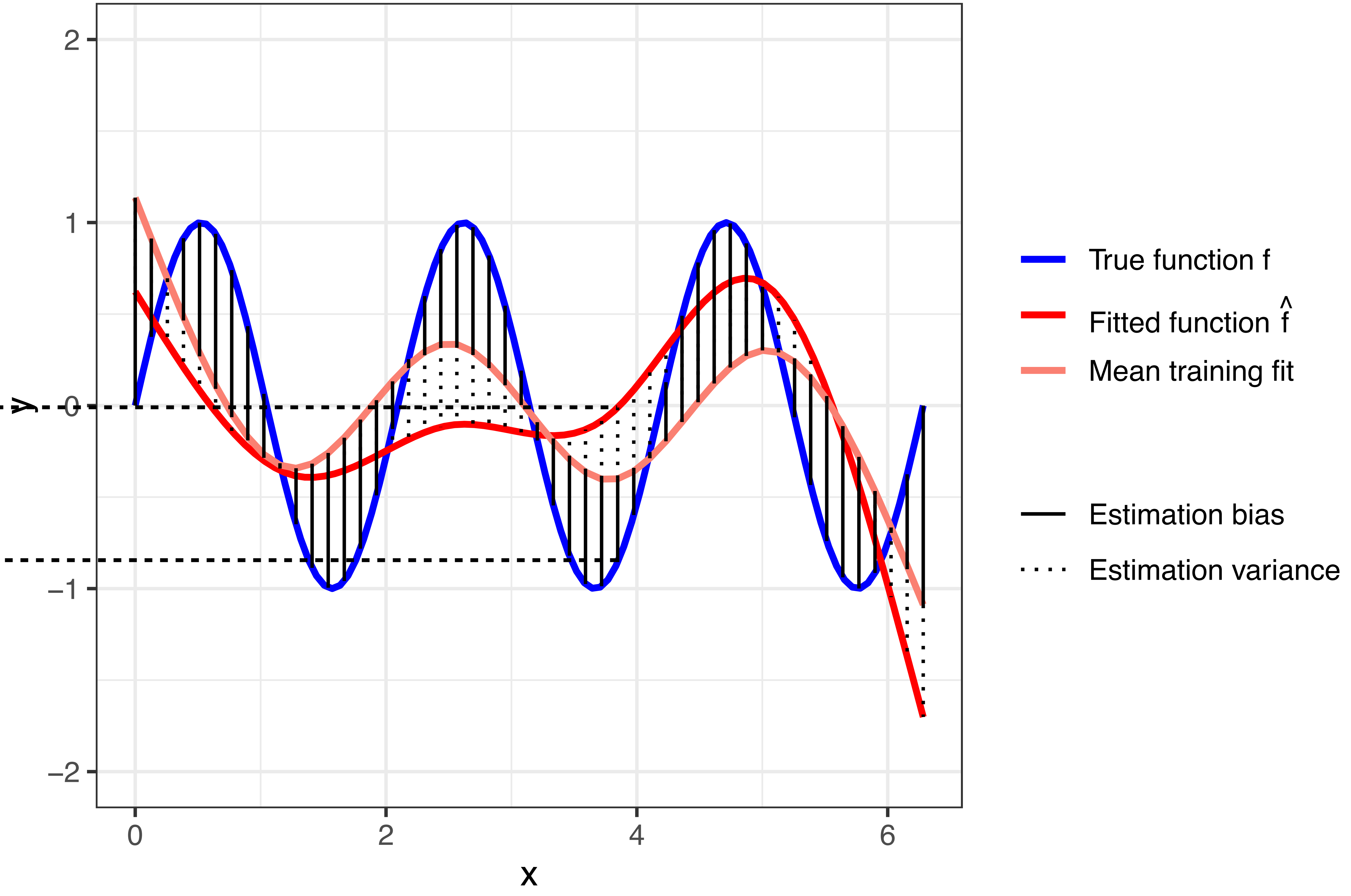

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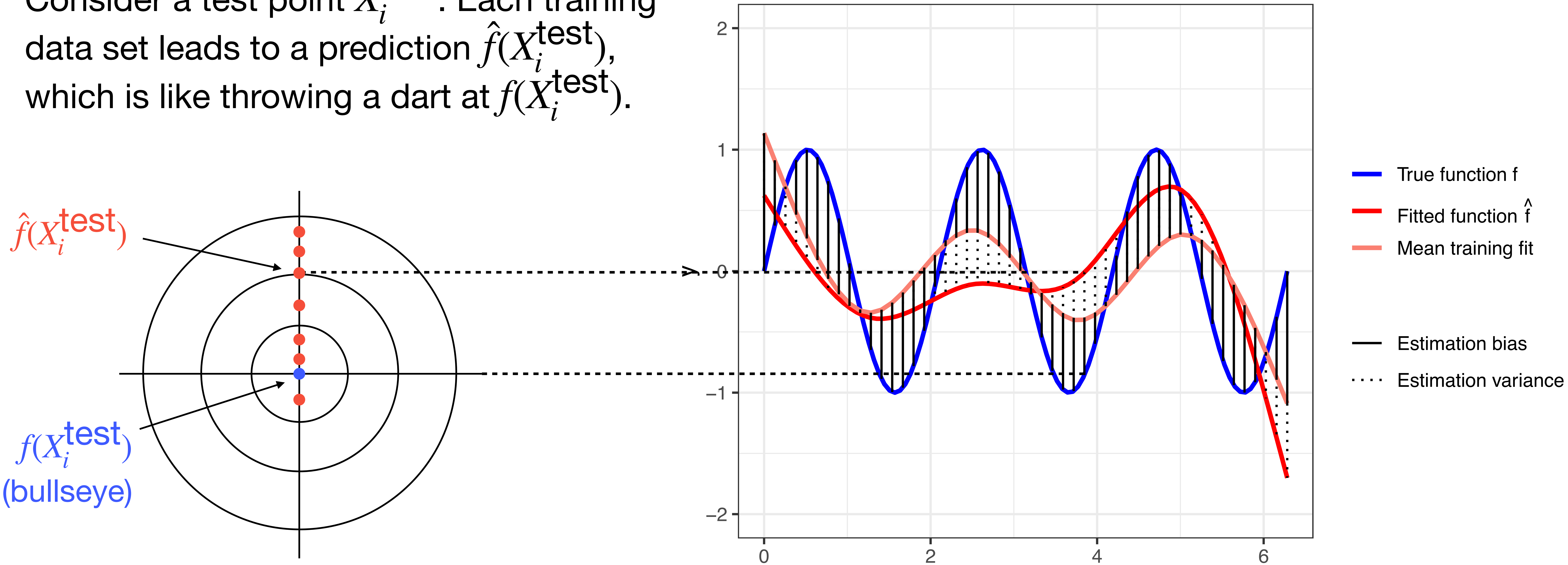

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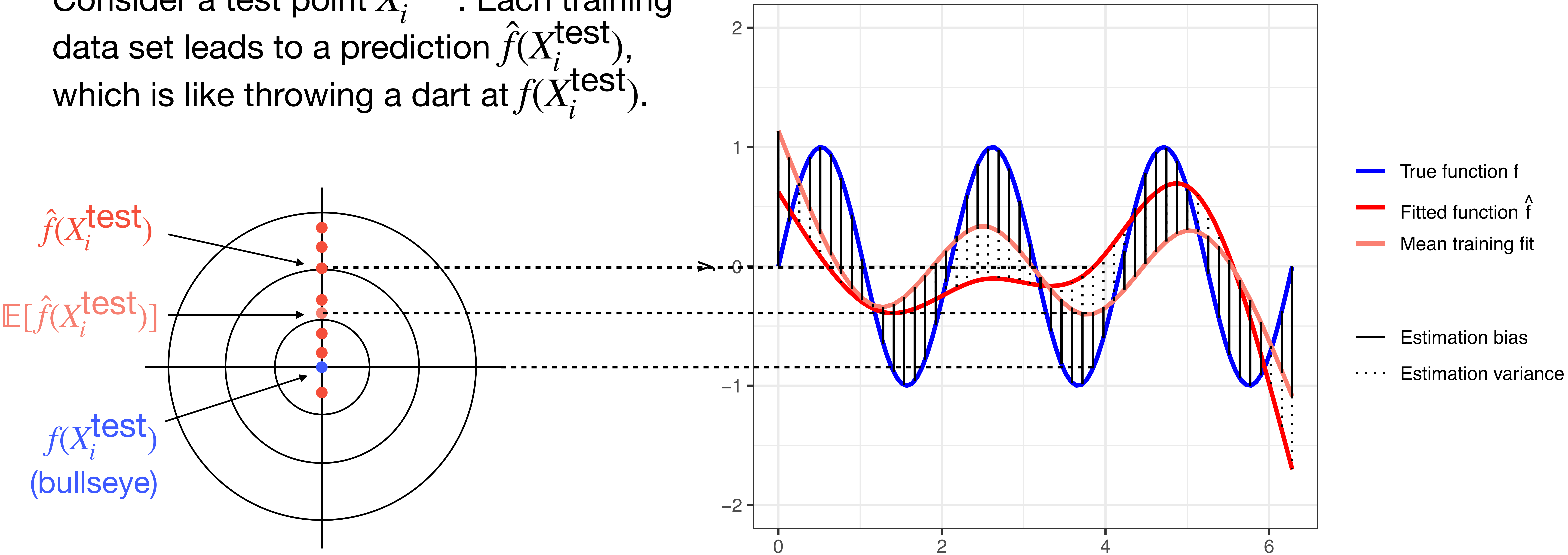

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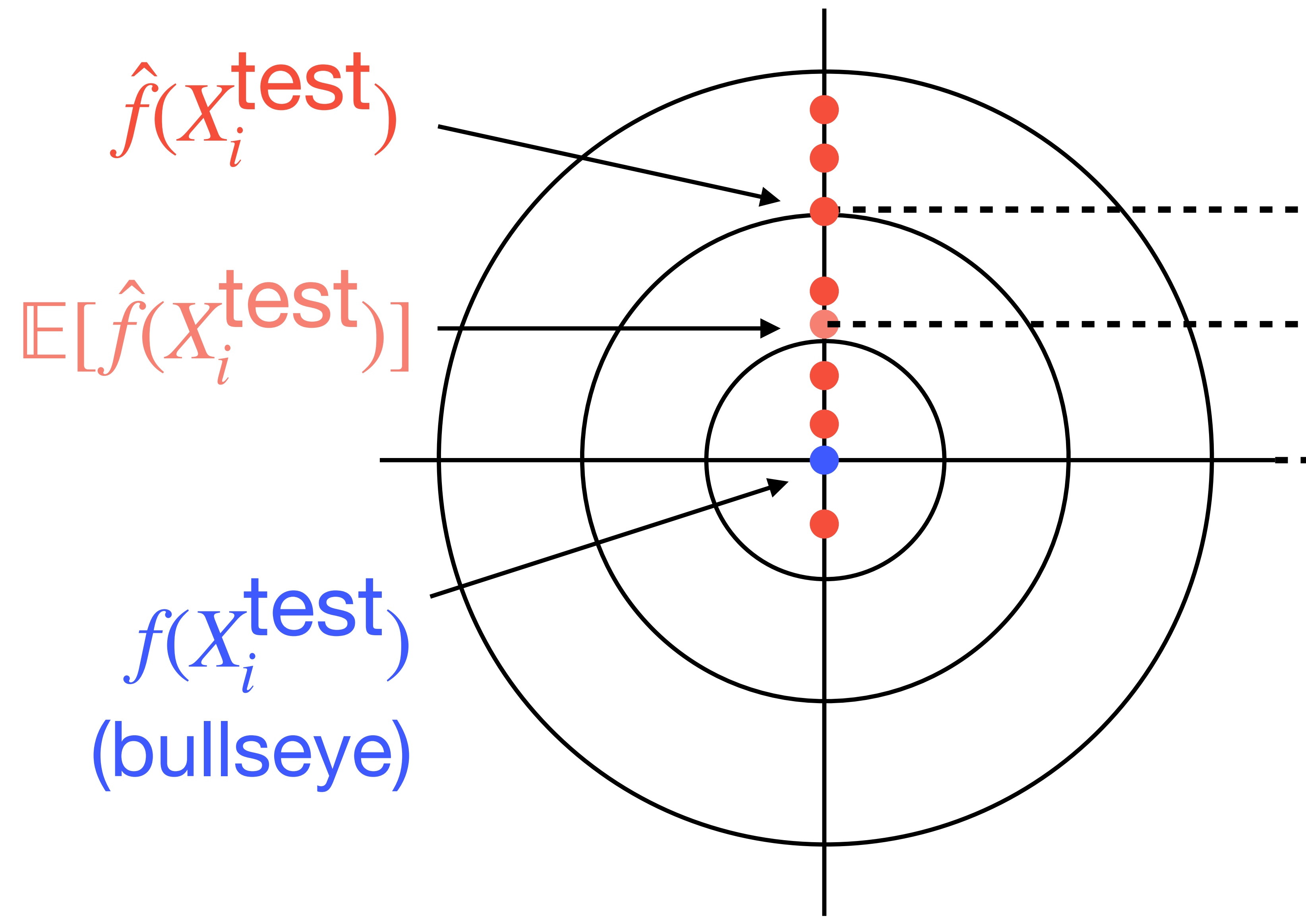

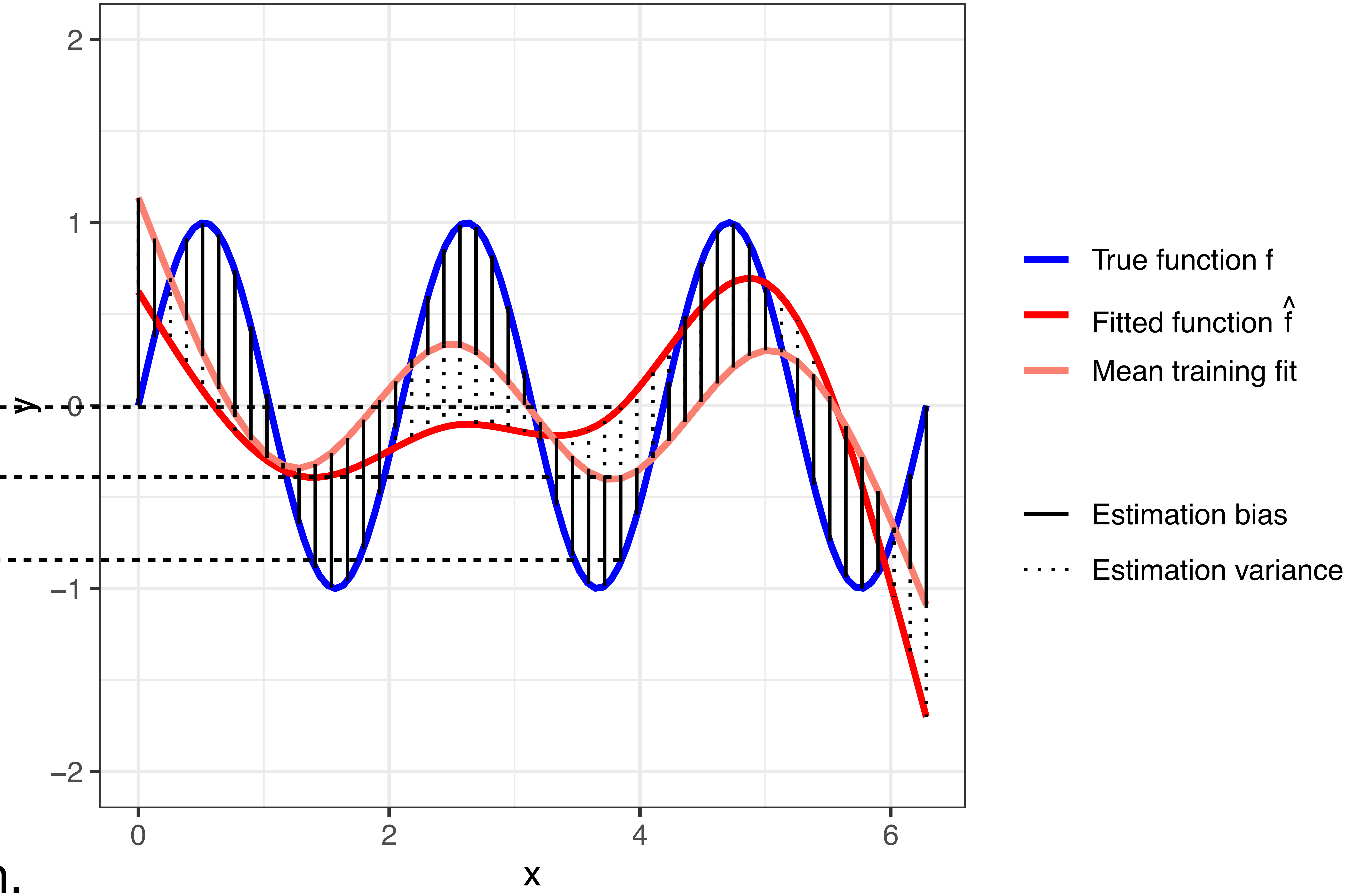

Bias: Aim systematically off in one direction.

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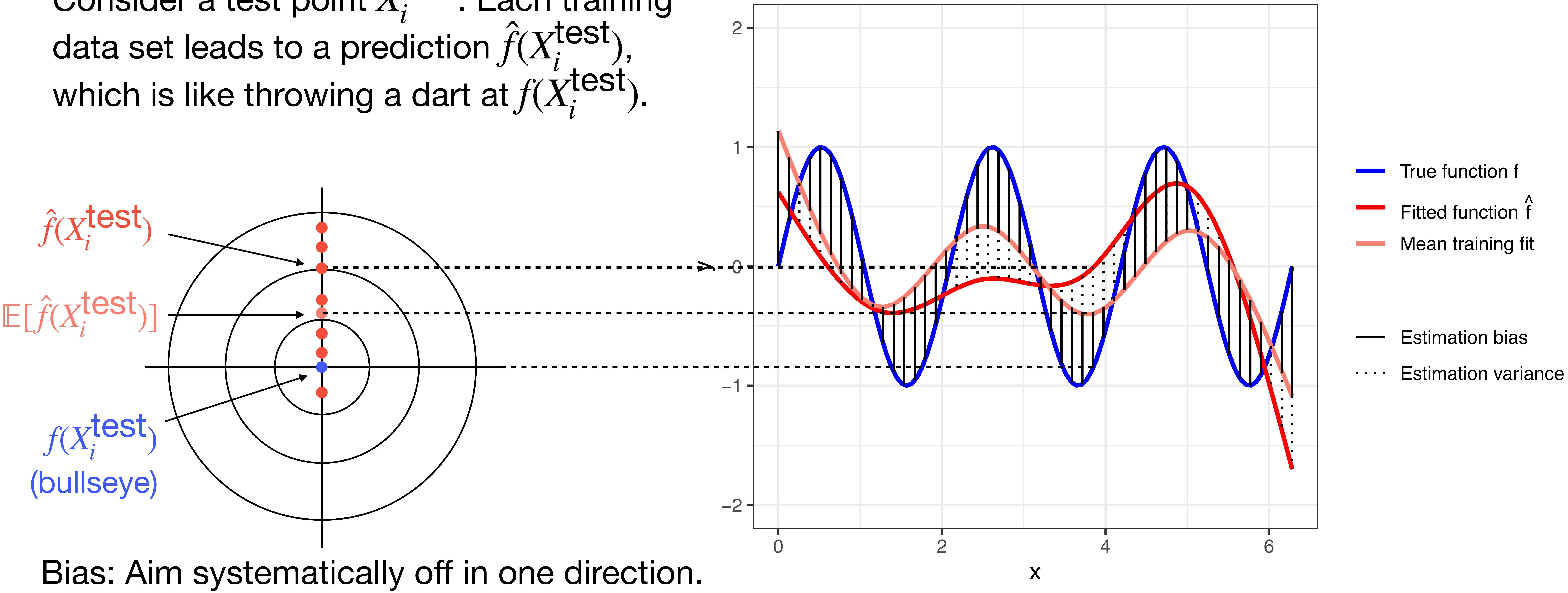
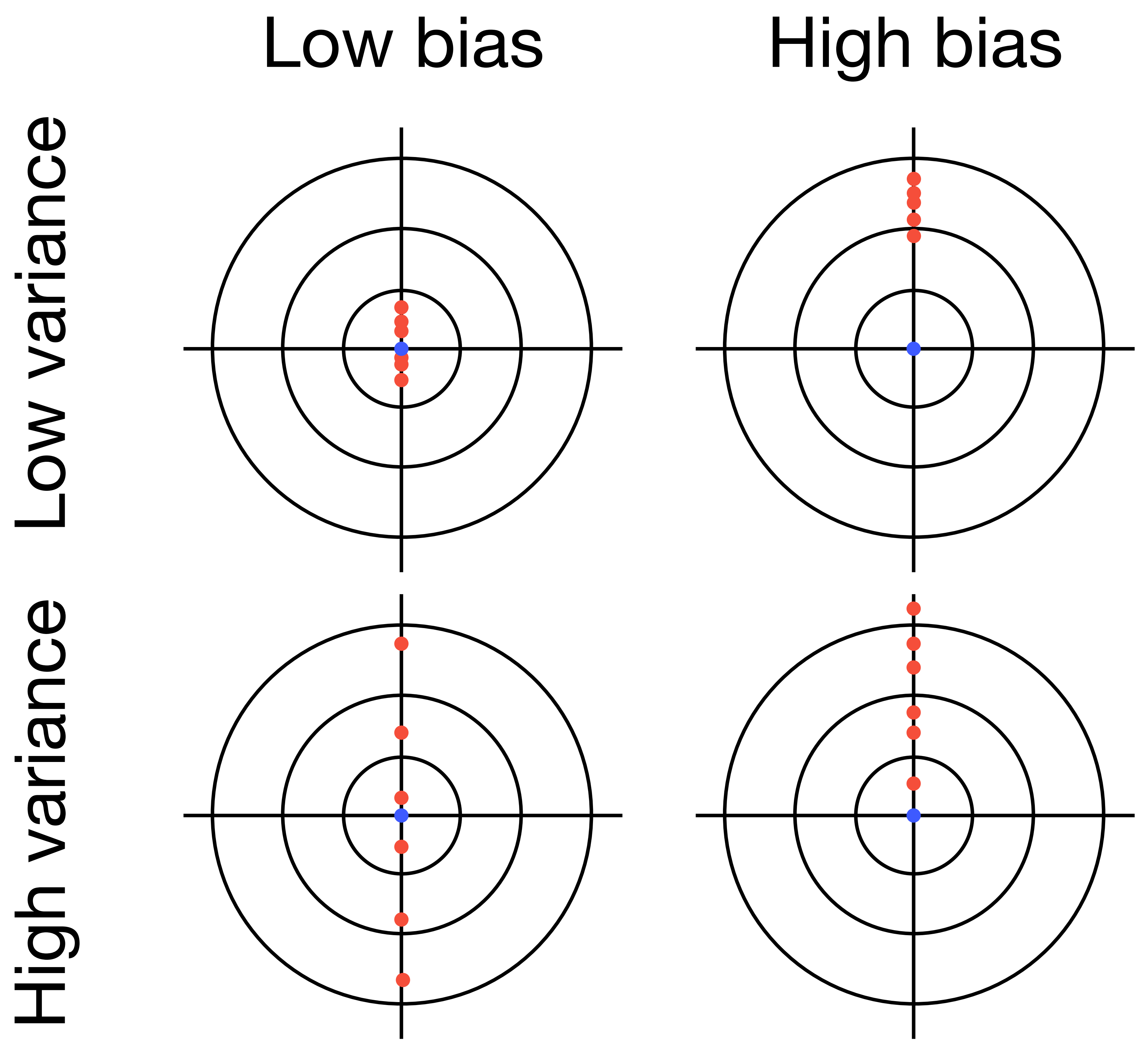


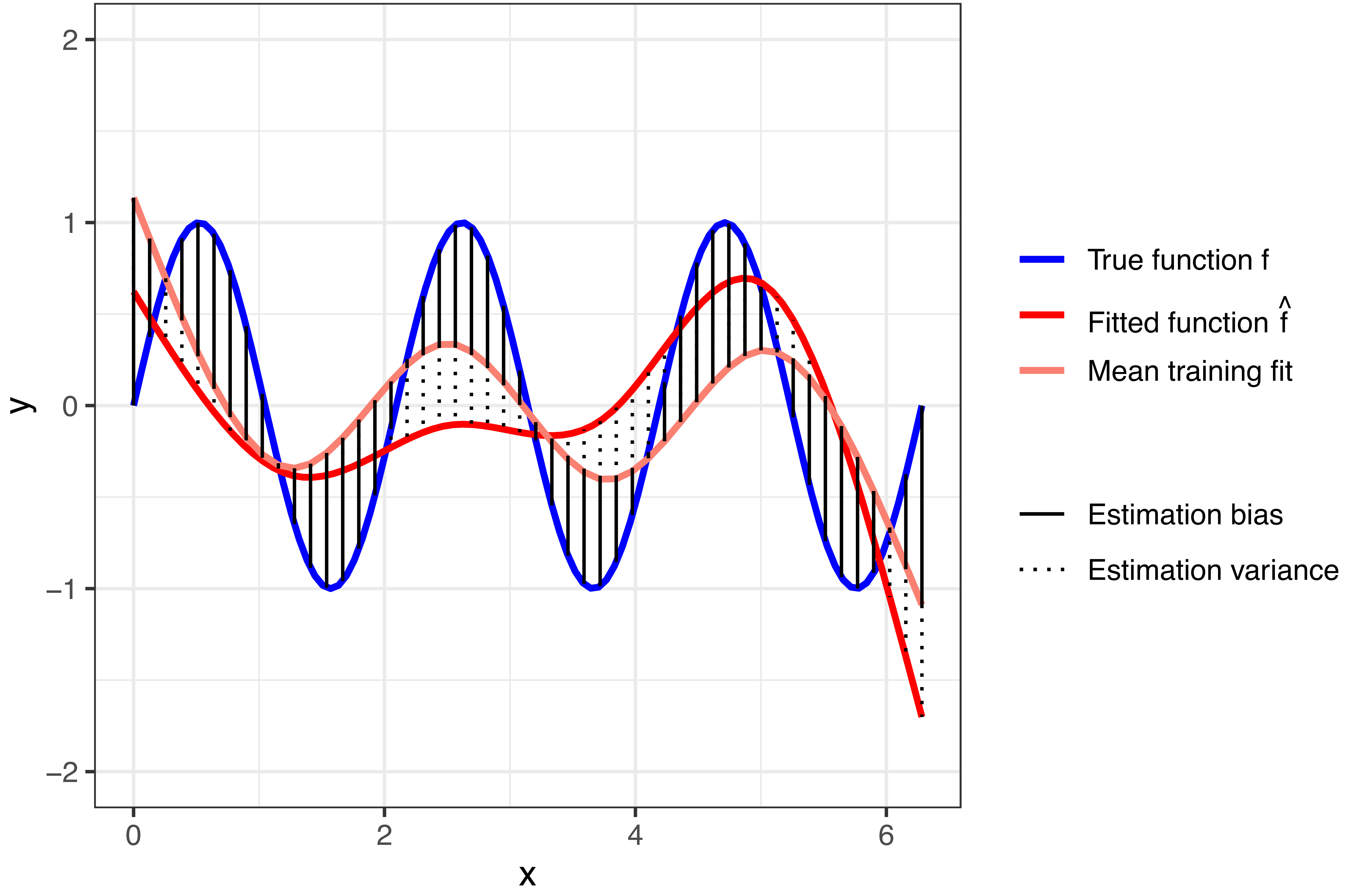
Bias: Aim systematically off in one direction.

Variance: Aim wobbling between throws.

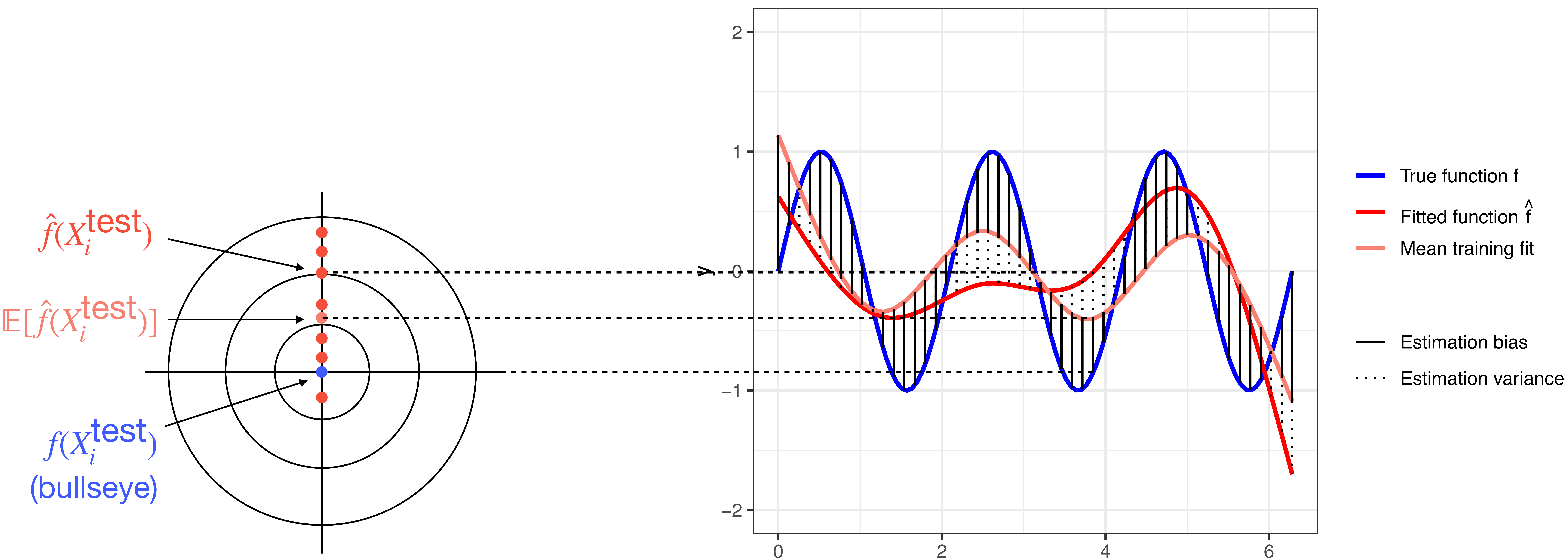
Estimation error = Bias² + Variance

Consider a test point X_i^{test}. Each training data set leads to a prediction $\hat{f}(X_i^{\text{test}})$, which is like throwing a dart at $f(X_i^{\text{test}})$.





Understanding bias



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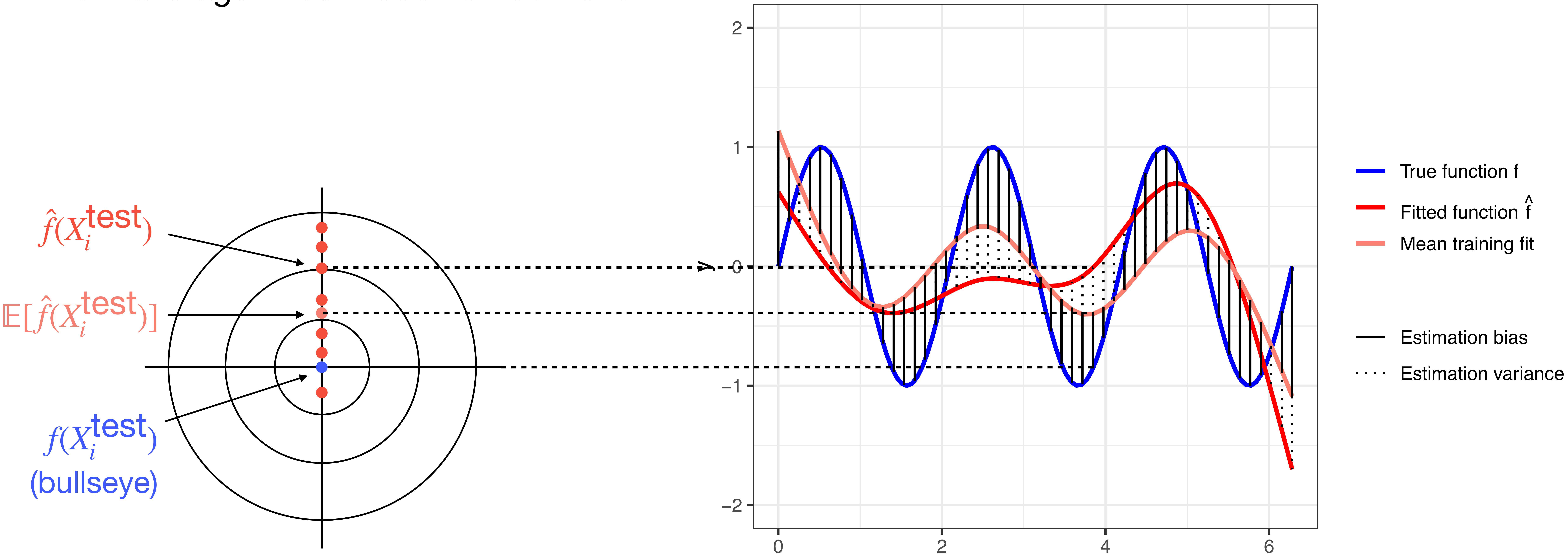
$\text{Bias}_i = \mathbb{E}[\hat{f}(X_i^{\text{test}})] - f(X_i^{\text{test}})$, distance from average fitted model to true trend.



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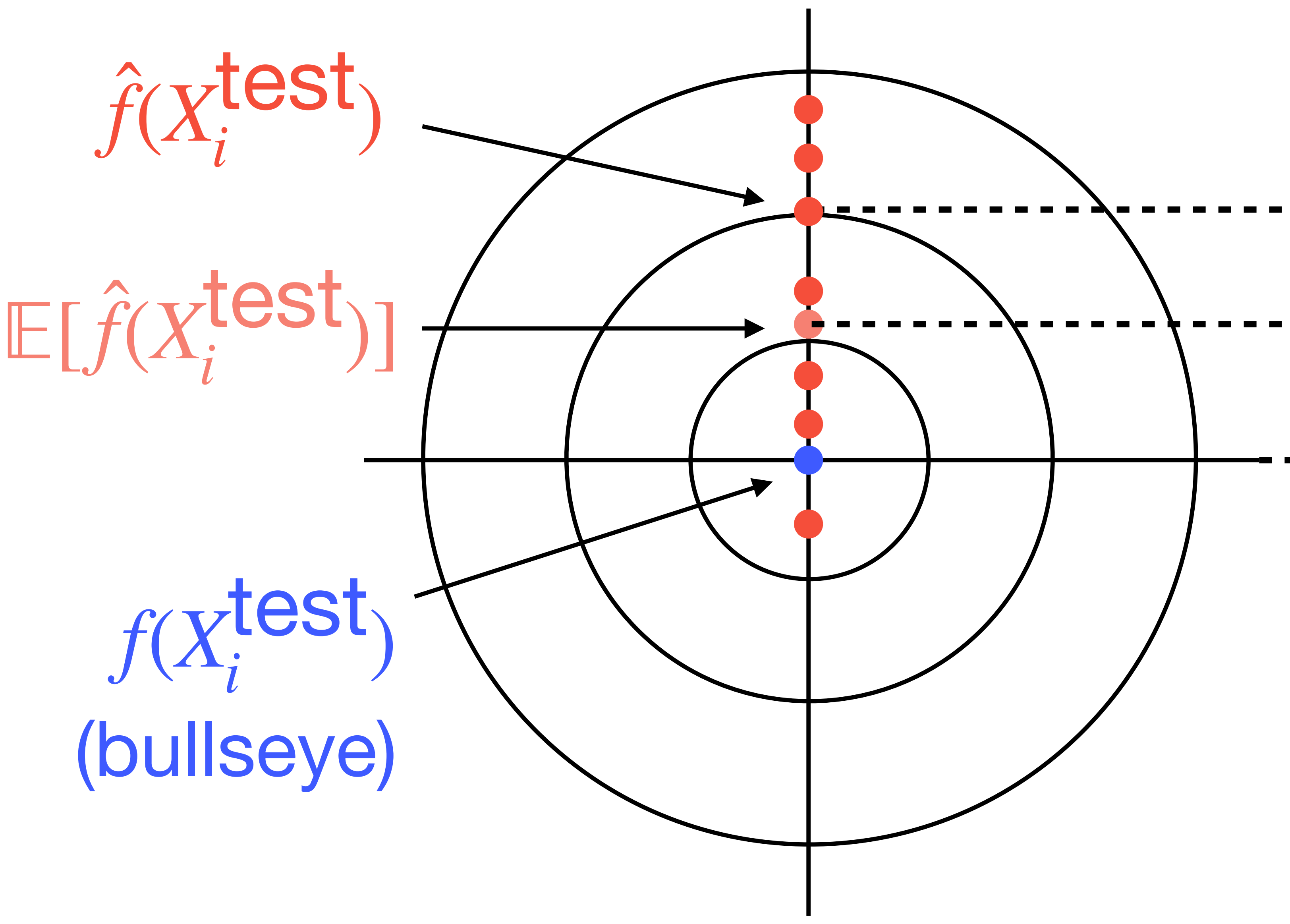

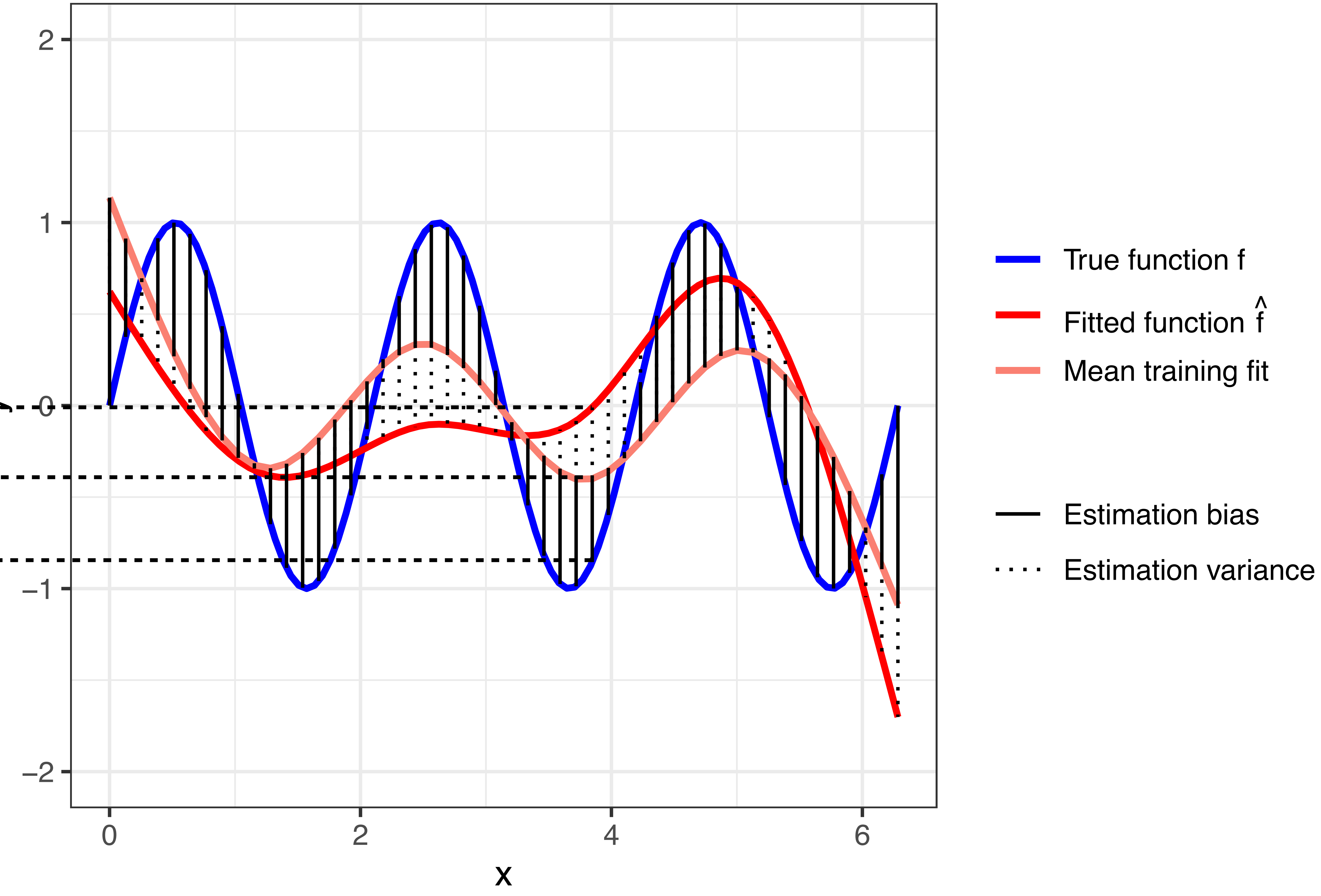

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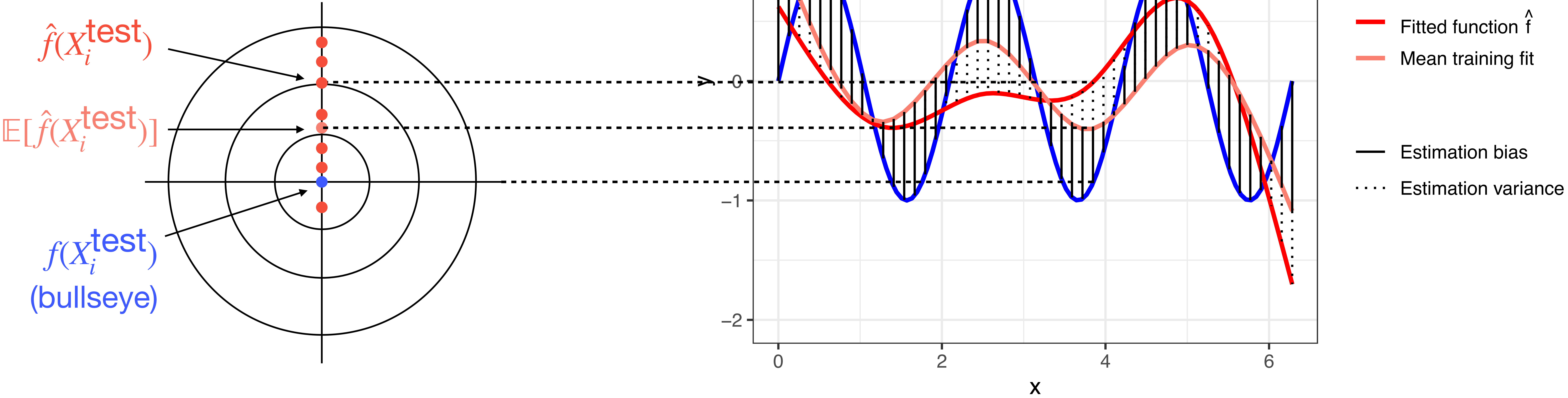

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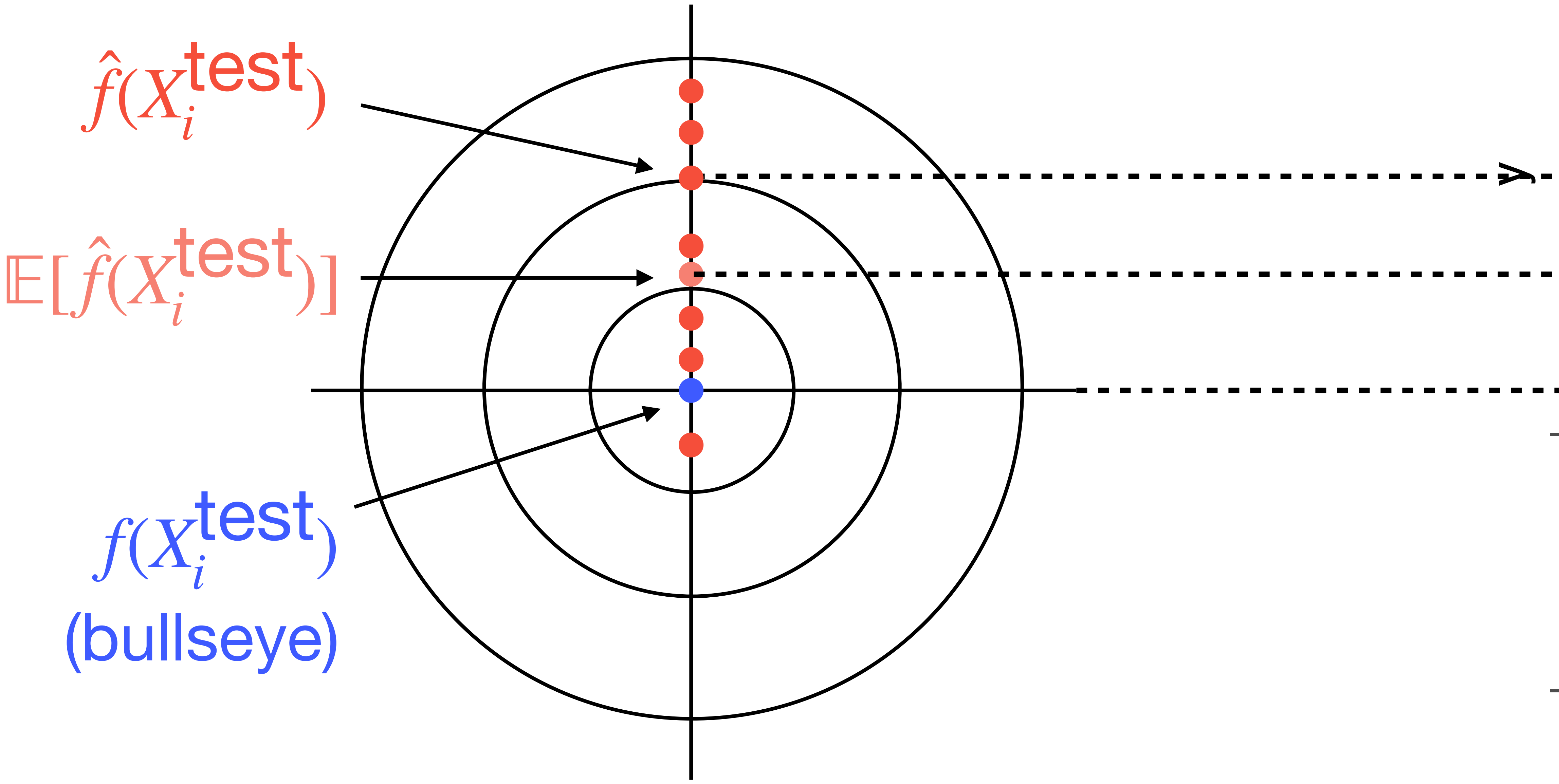
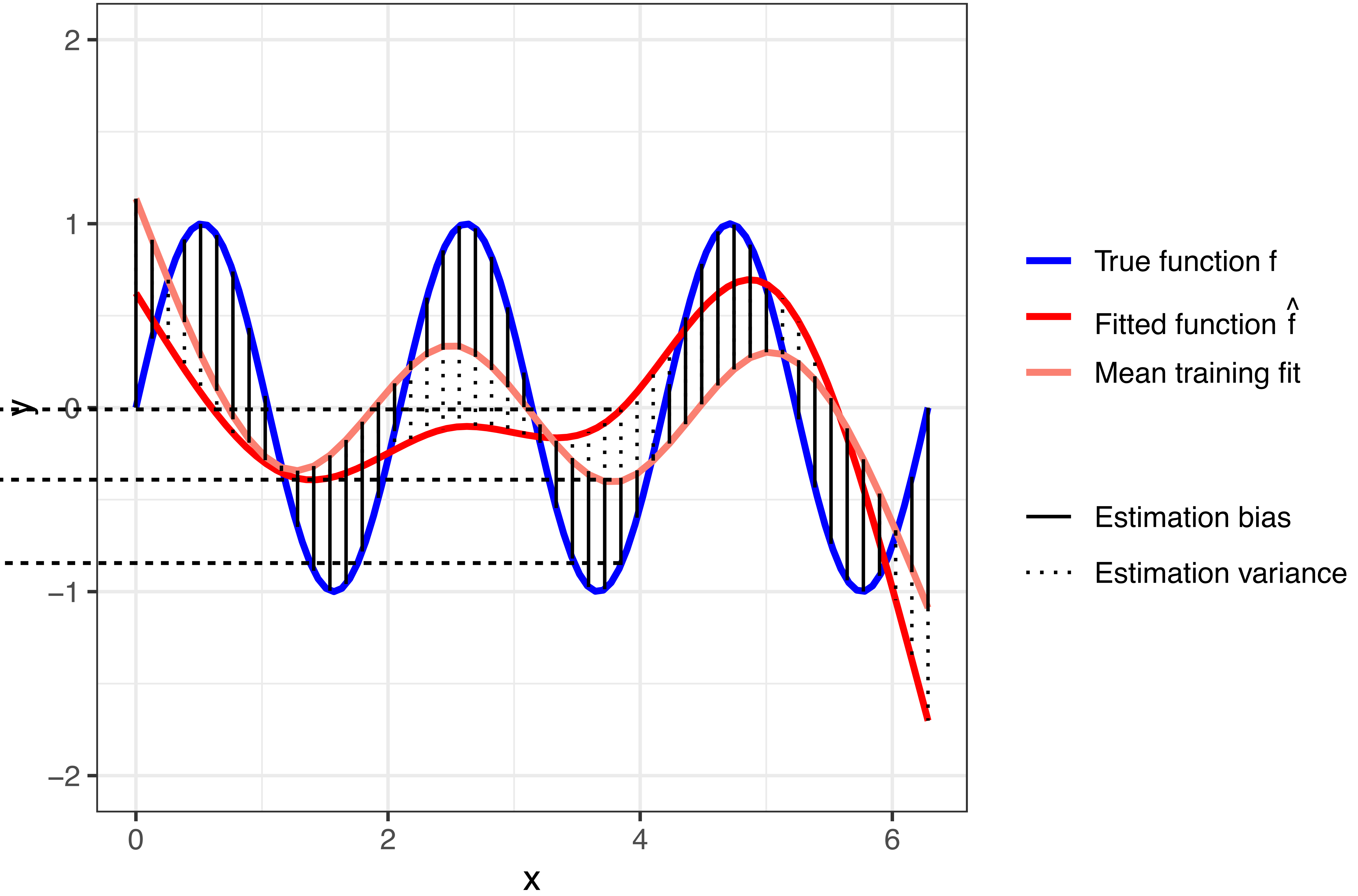
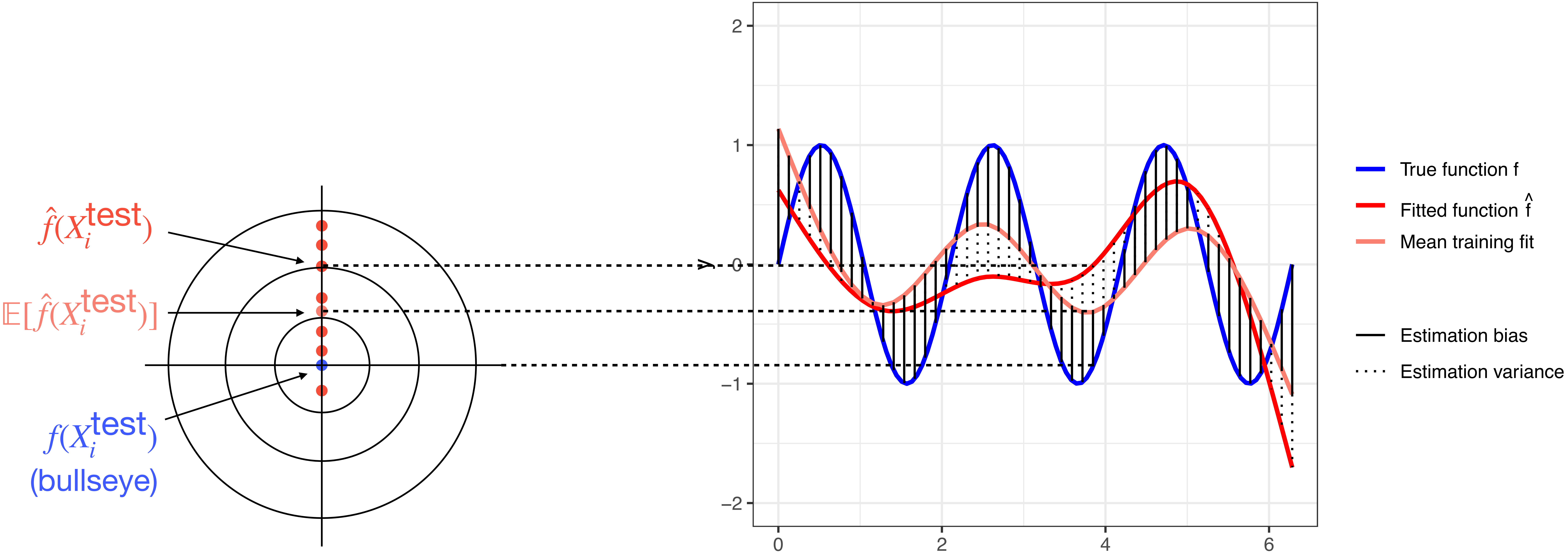




Note: Noise variance does not impact bias.

Understanding variance



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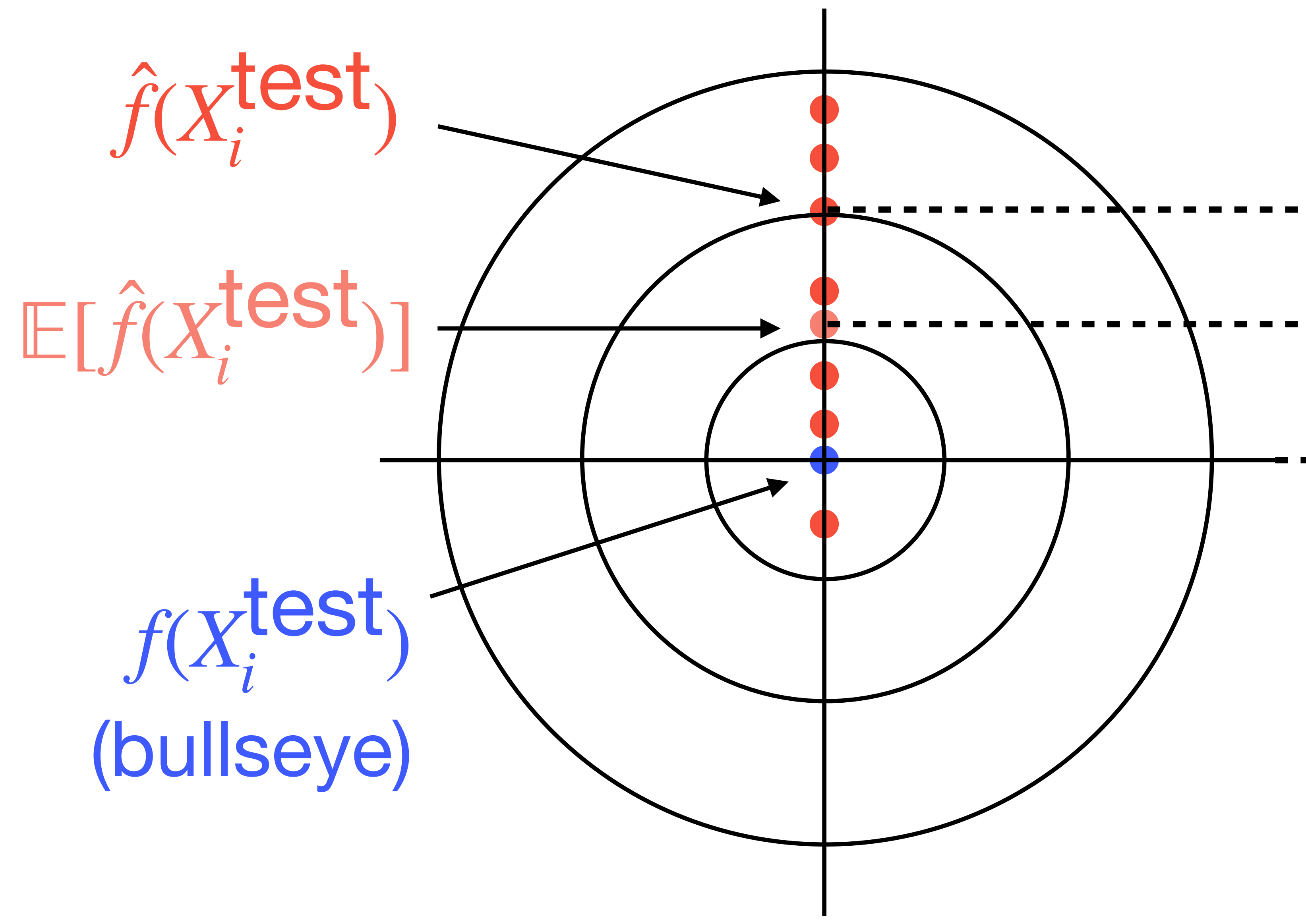
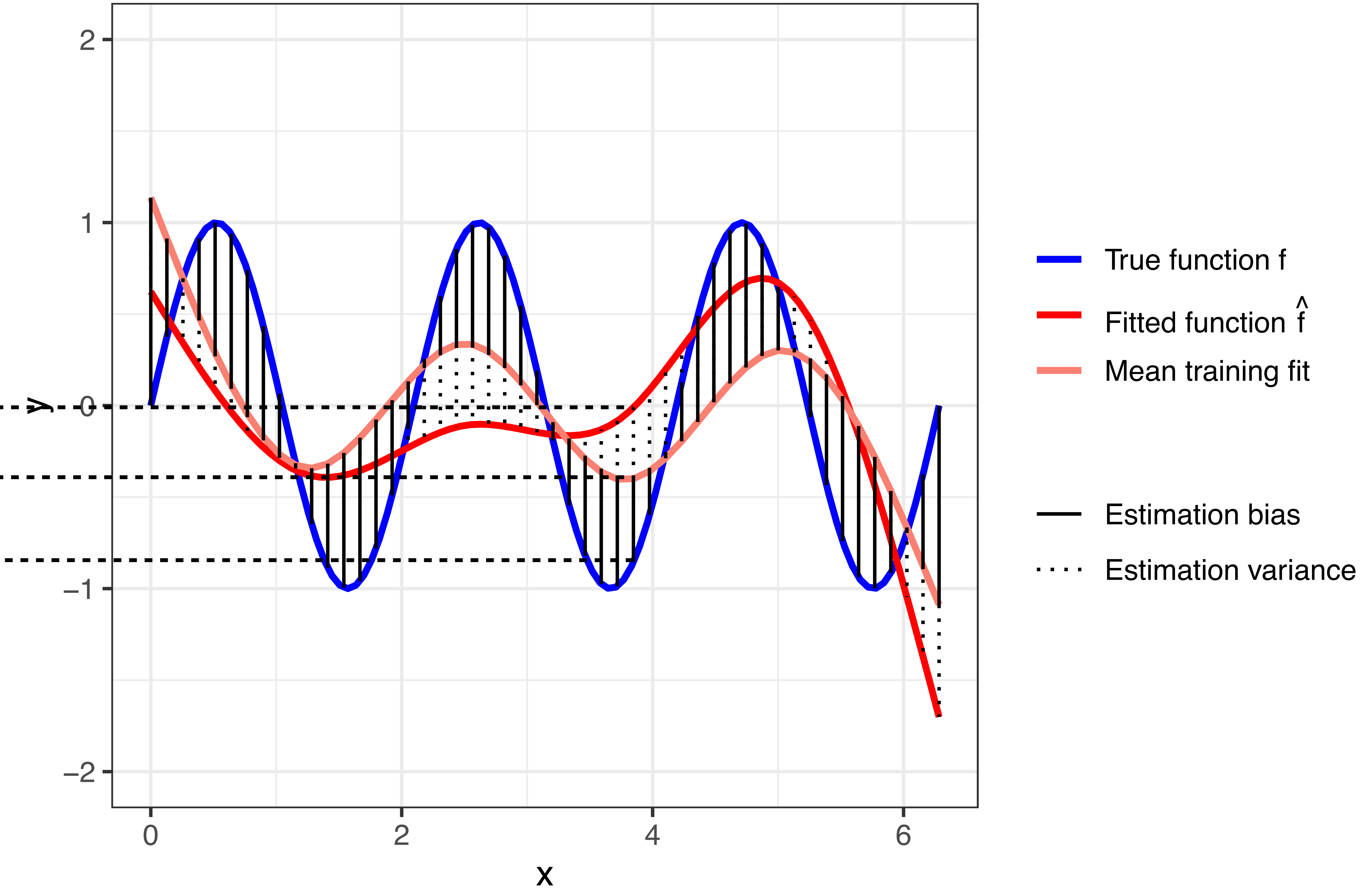
Variance$_i$ $= \mathbb{E}[(\hat{f}(X_i^{\text{test}}) - \mathbb{E}[\hat{f}(X_i^{\text{test}})])^2]$, the wobbling of the model fit due to the randomness in the training data.





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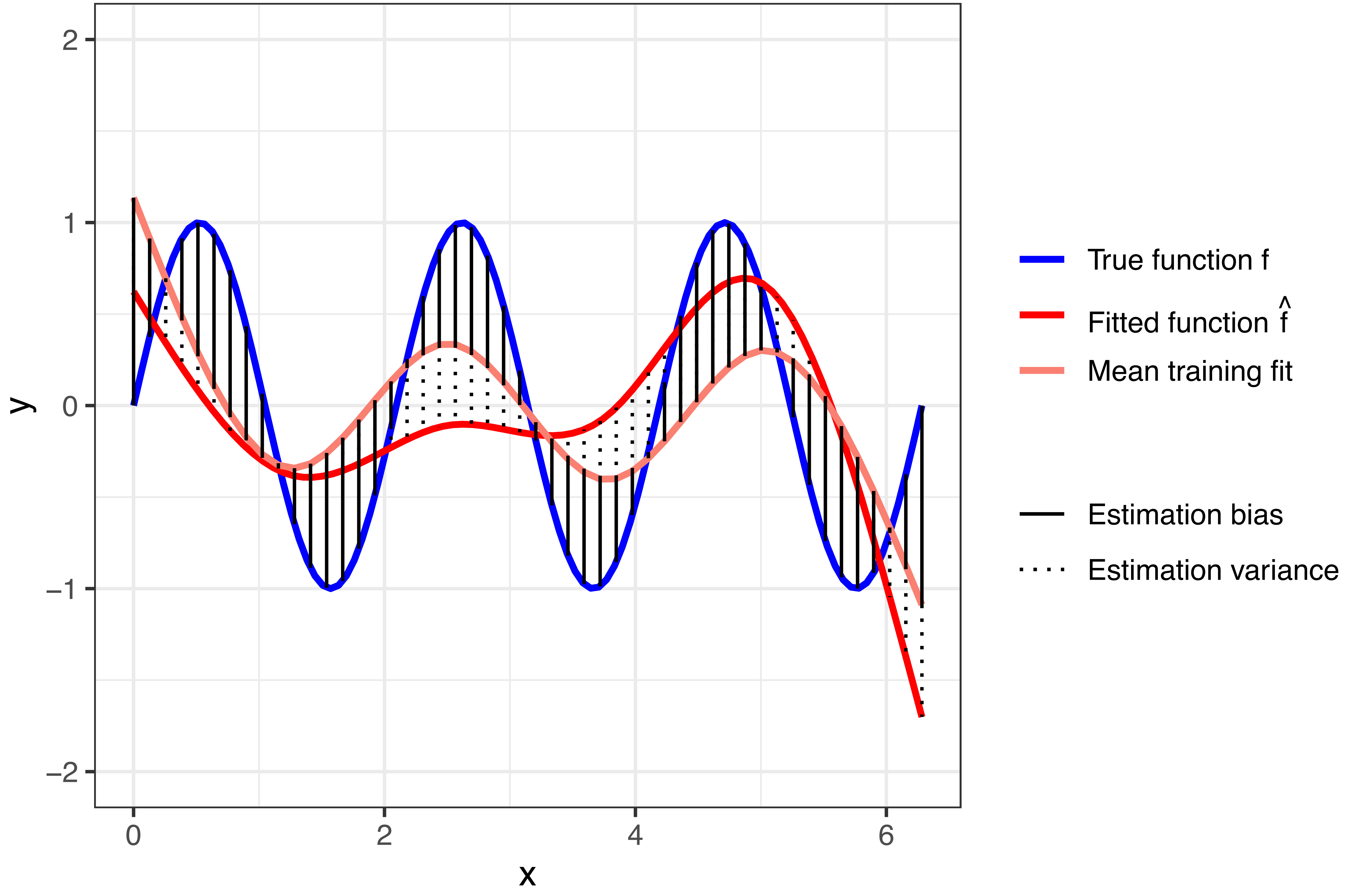

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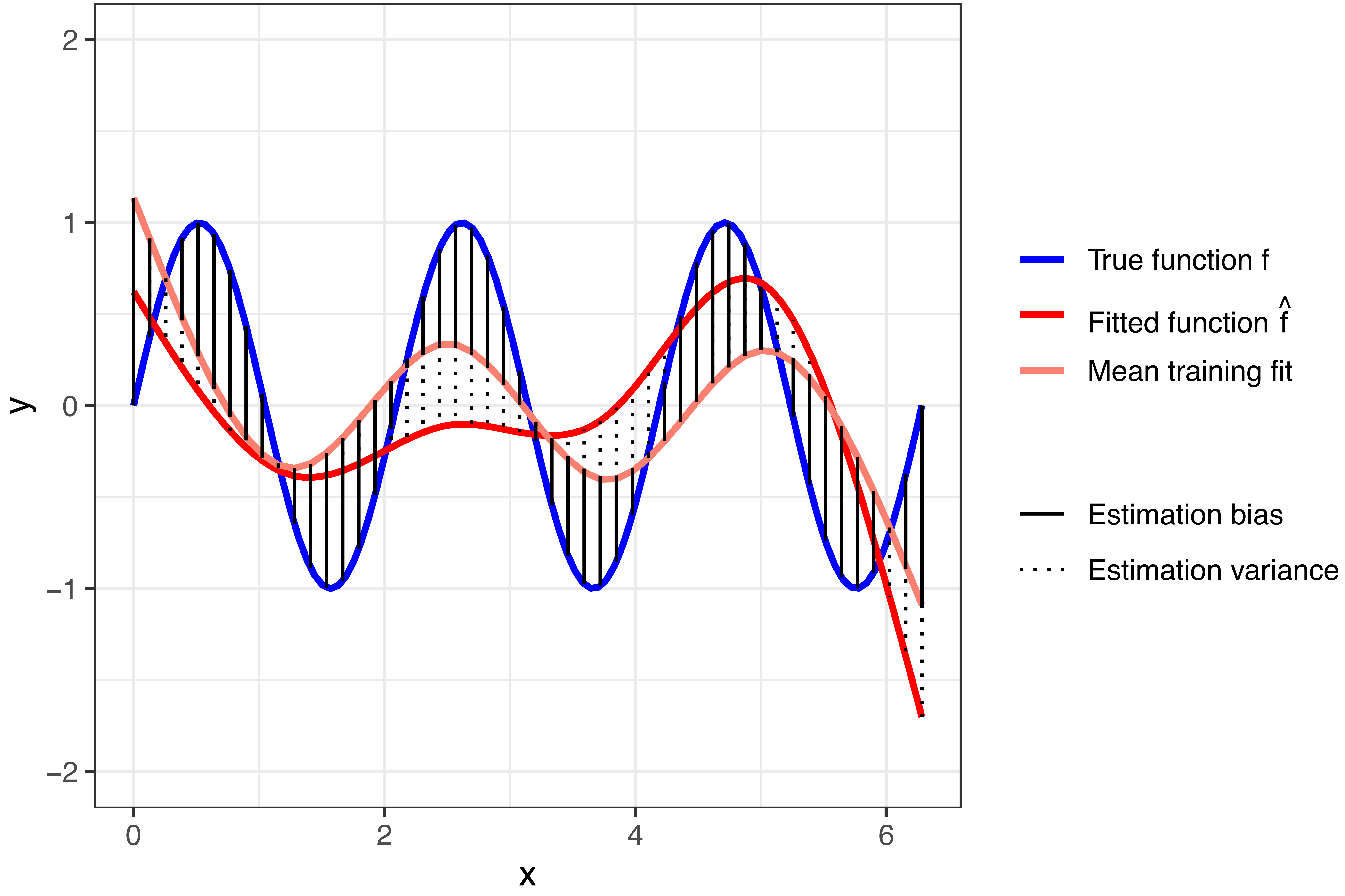

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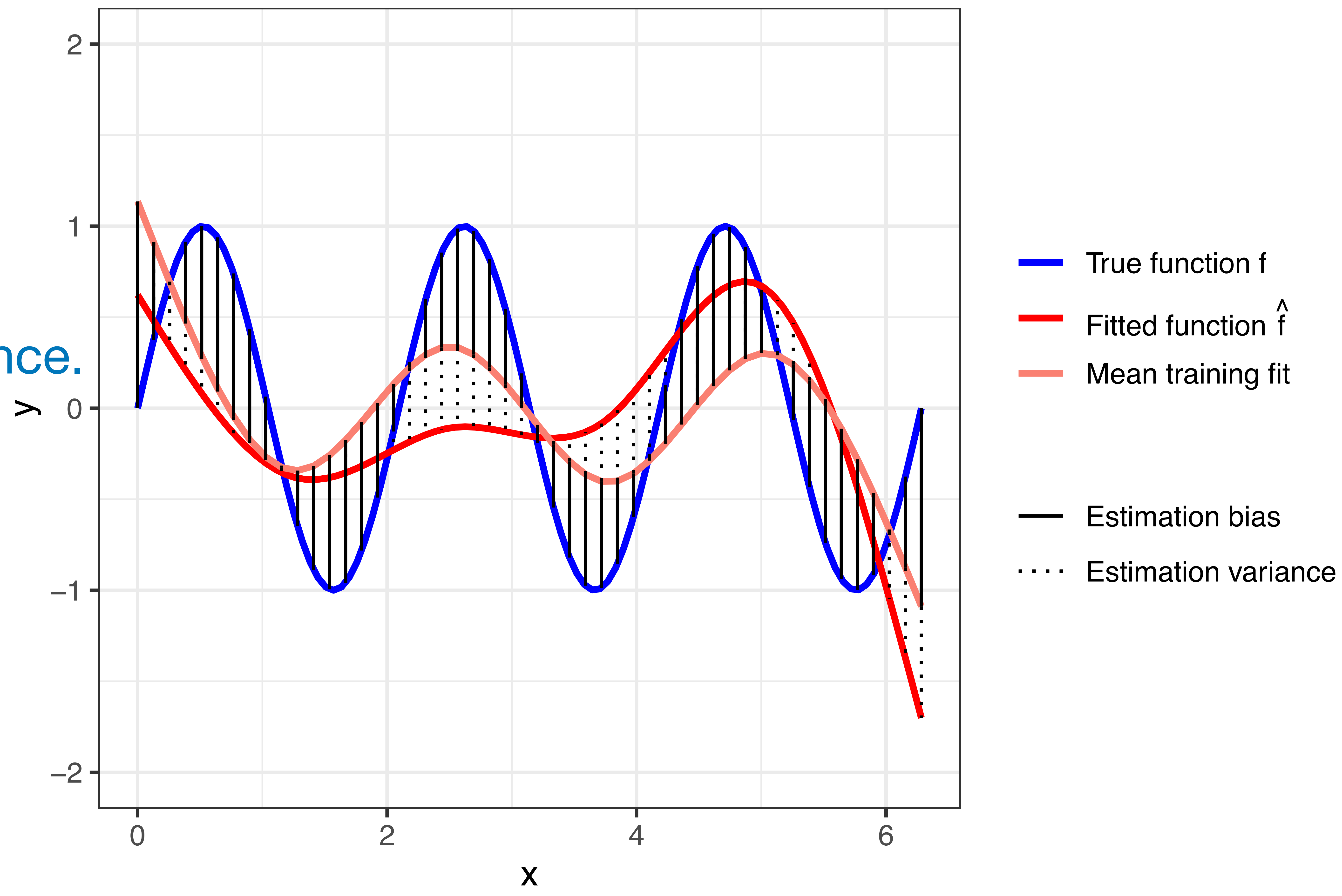

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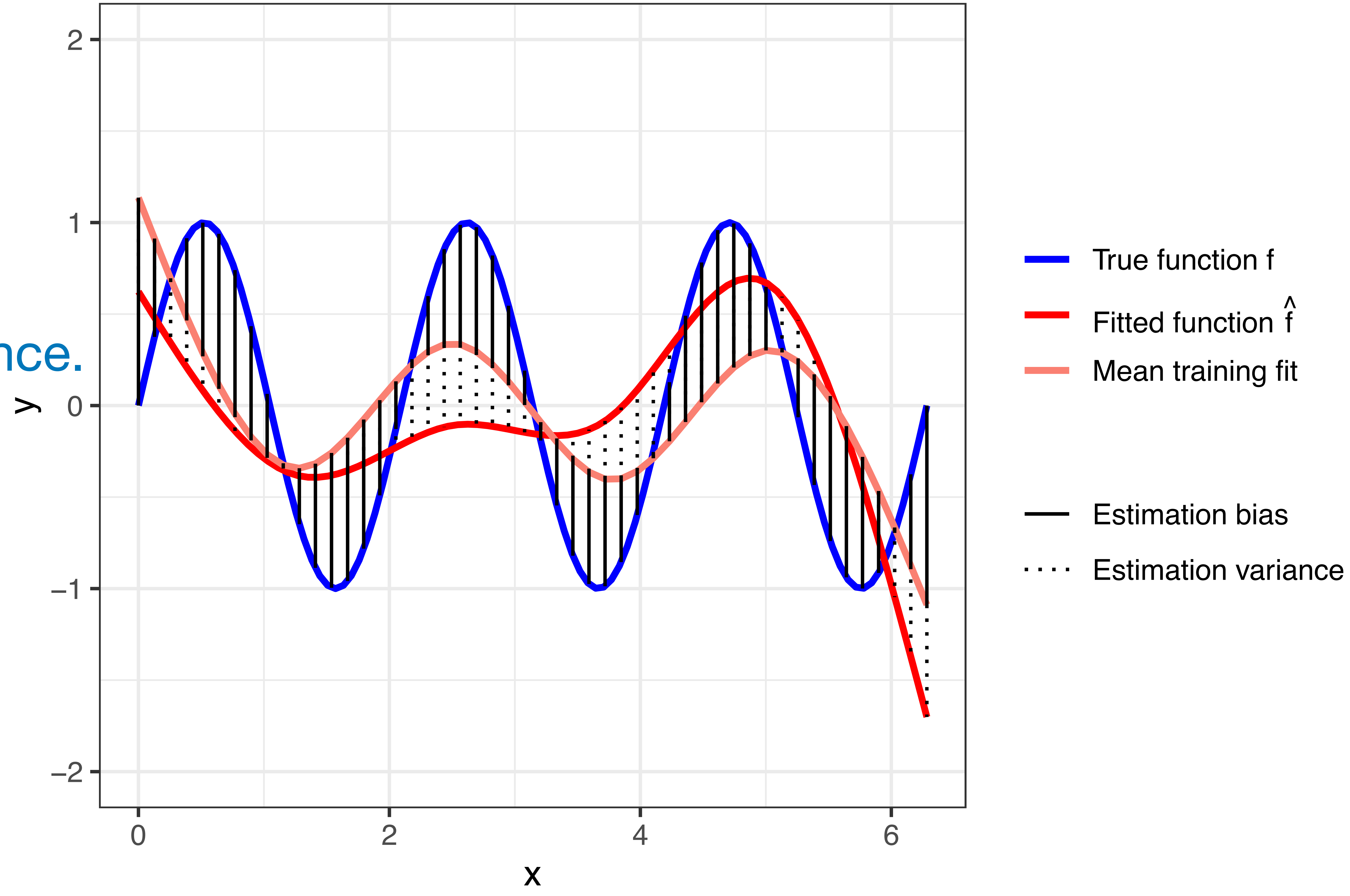
$$\text{Mean variance} = \frac{1}{n}\sum_{i=1}^{n} \text{Variance}_i = \frac{\sigma^2 p}{n}$$

(assuming $n = N$ and $X^{\text{test}} = X^{\text{train}}$).



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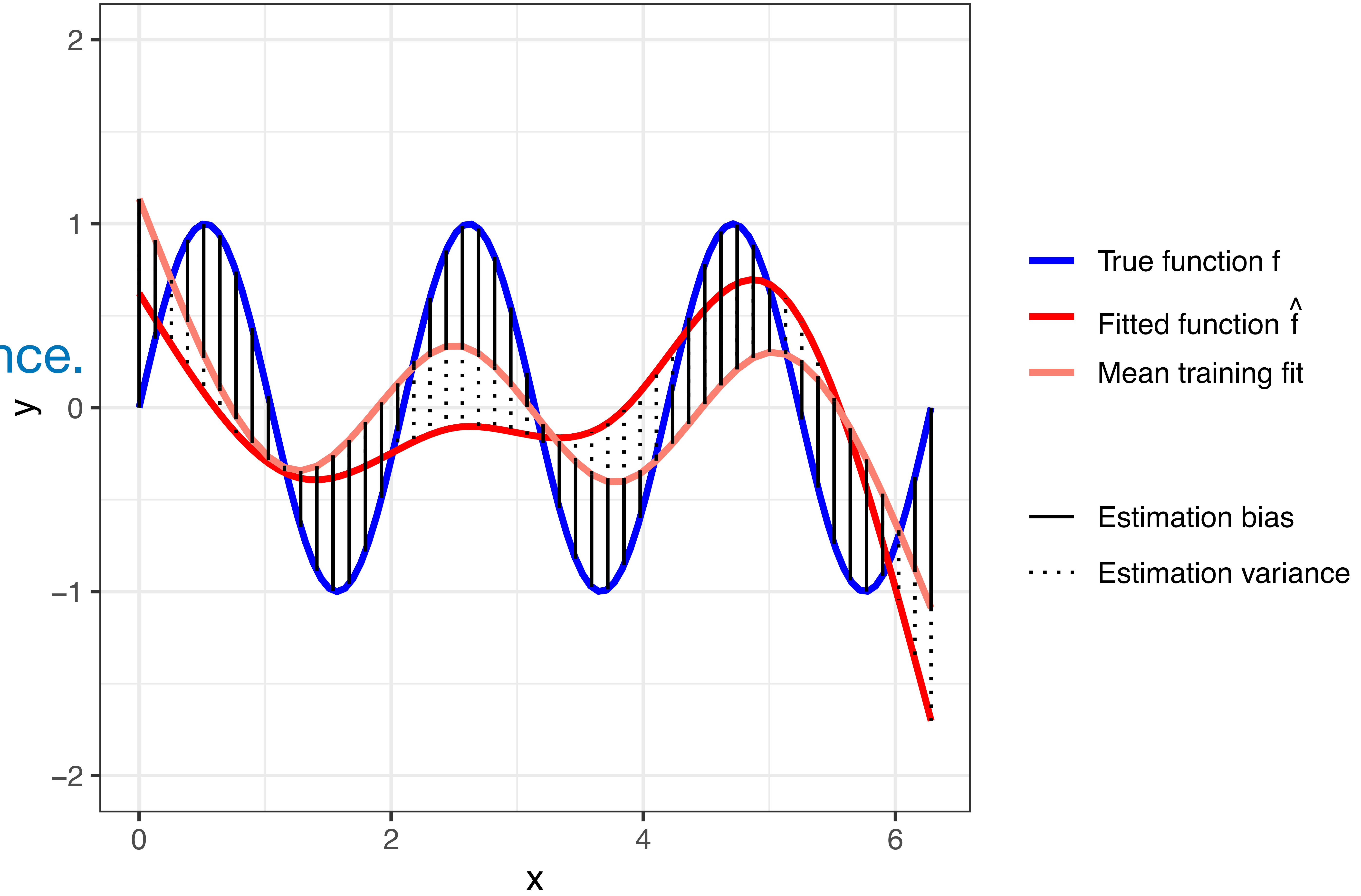

Note: Complexity of true model does not impact variance.

Putting it all together: The bias-variance tradeoff

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Averaging over i, we get

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When varying model complexity, there is a tradeoff between bias and variance.

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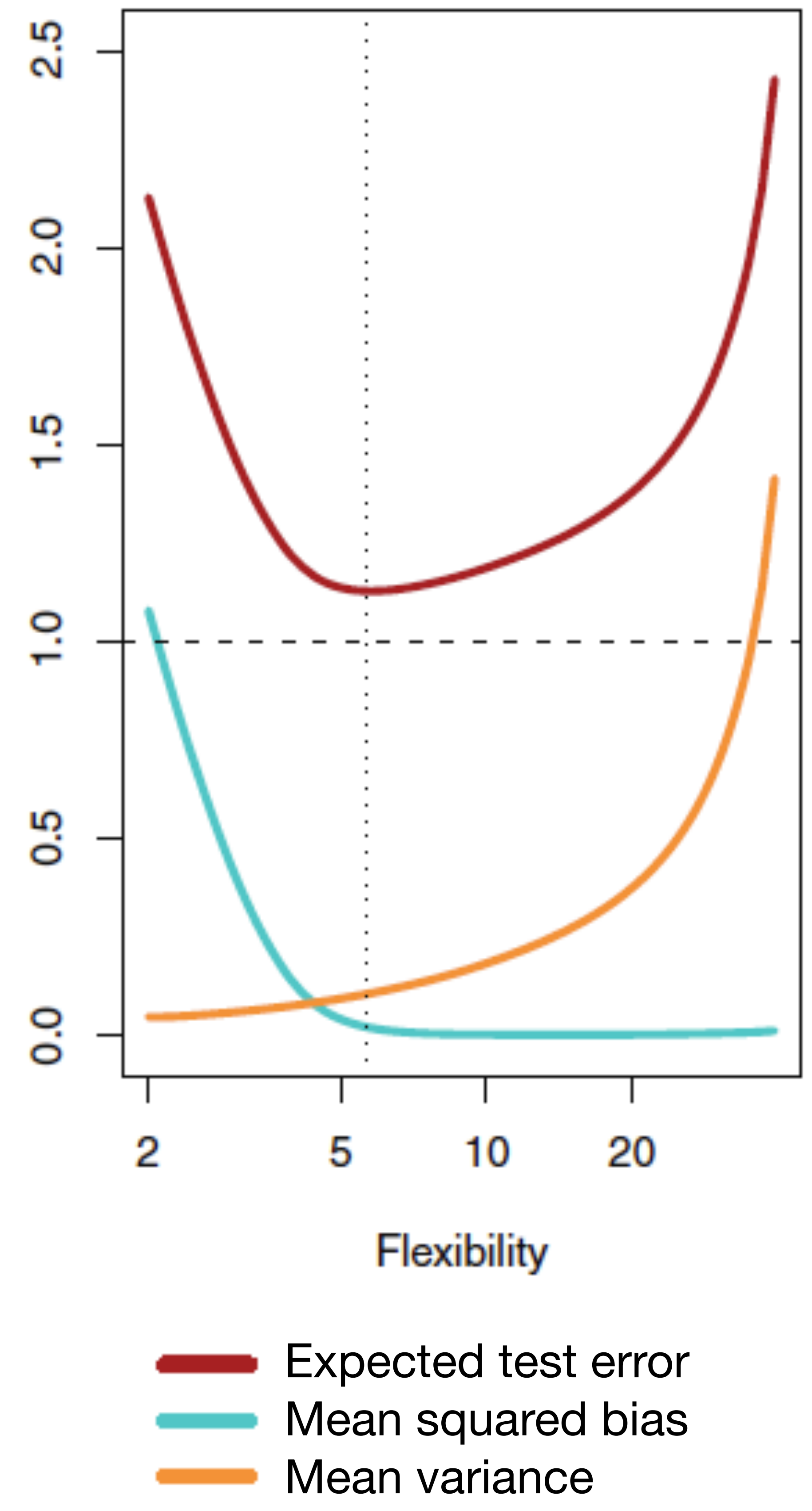

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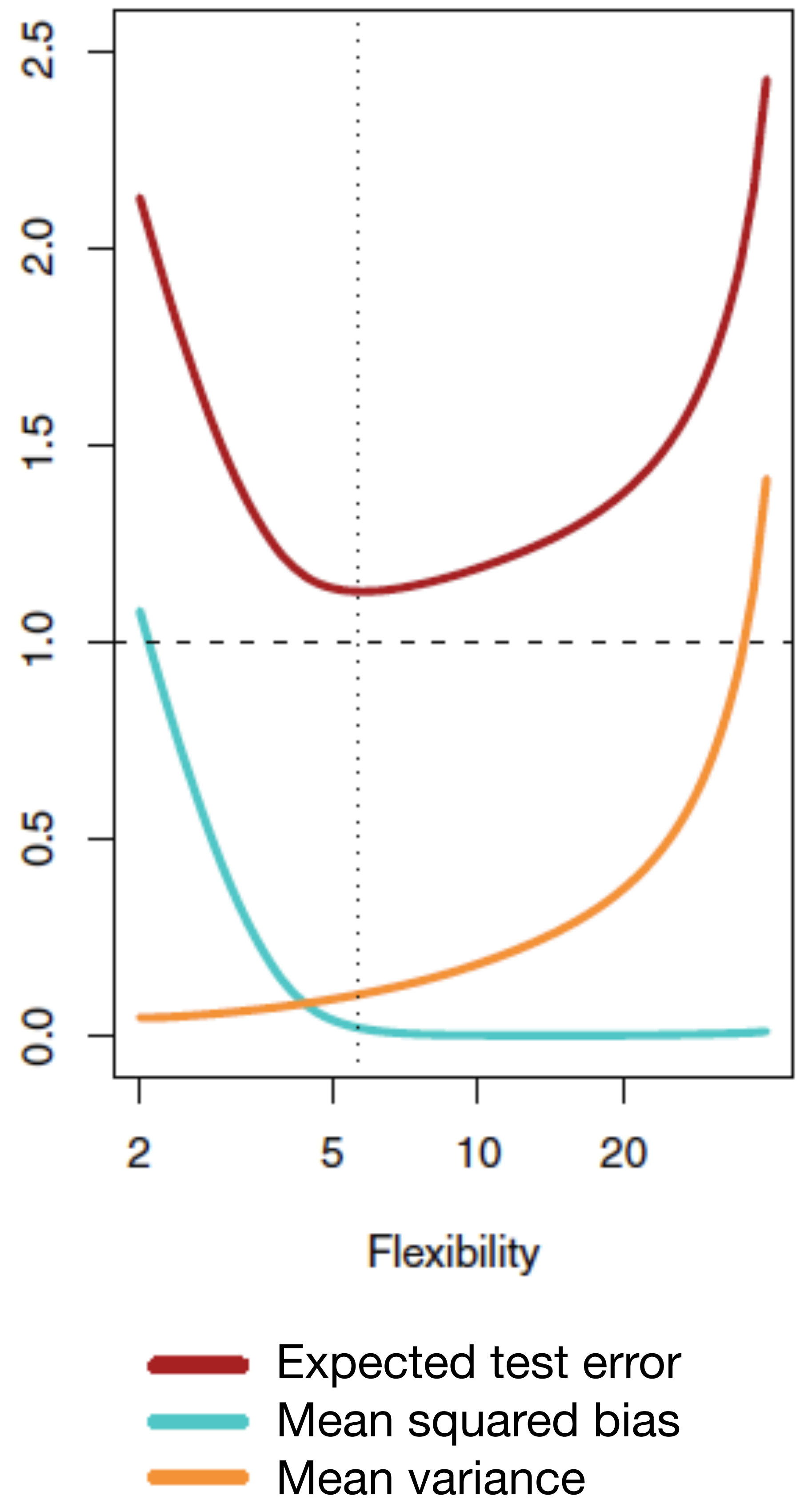

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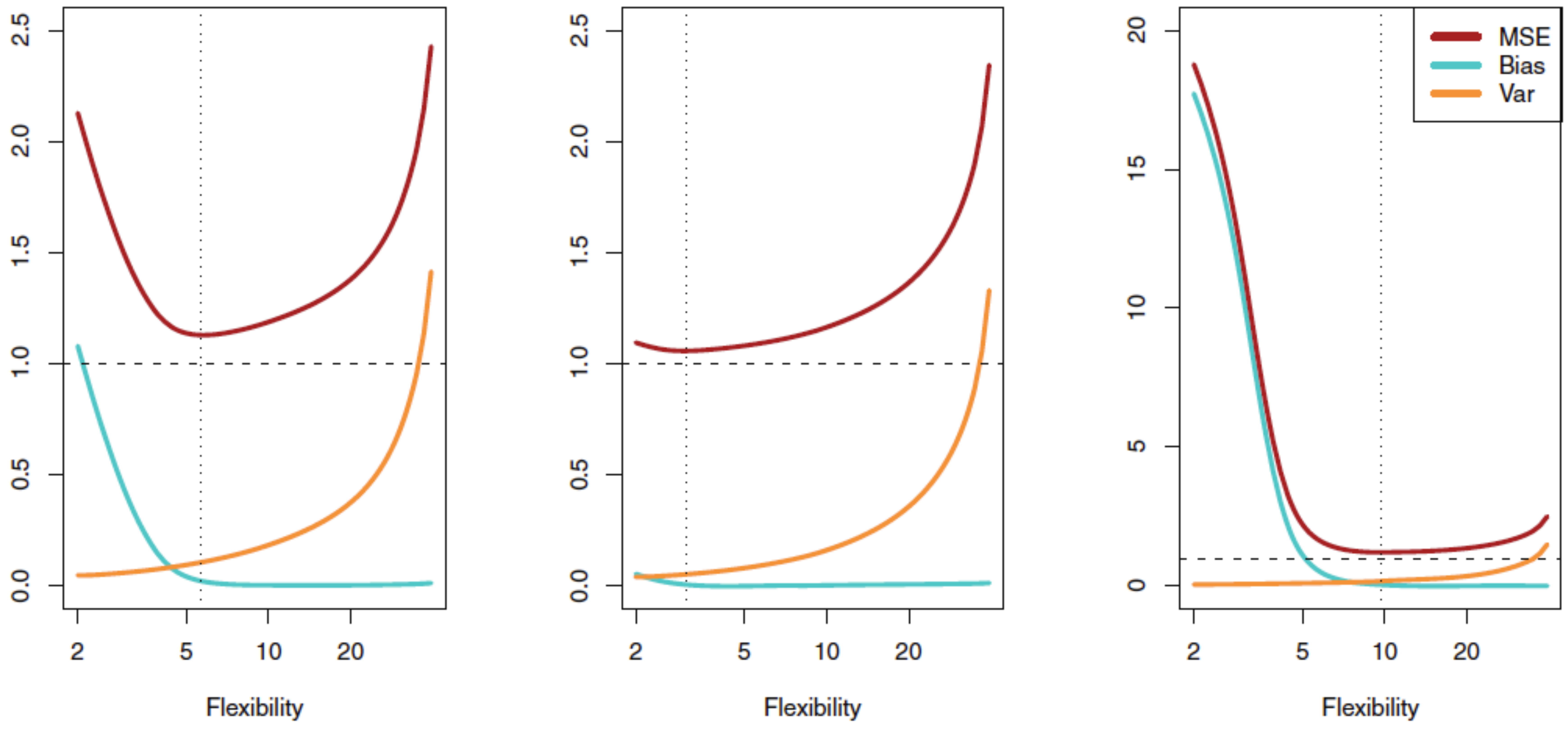
Choosing the best predictive model requires balancing the two (Goldilocks principle).

Navigating the bias-variance tradeoff



The shapes of these curves differ based on the problem parameters.

What drives test error?

Problem parameters

- Sample size
- Noise level
- Fitted model complexity (number of parameters)
- True model complexity

Phenomena

- Model bias: extent to which model unable to capture the truth
- Overfitting: extent to which the fit is sensitive to noise in training data
- Irreducible error: noise in test points that is impossible to predict

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