Unit 2 Review: Tuning Predictive Models

STAT 471

Lecture 1: Model complexity

Lecture 2: Bias-variance trade-off

Lecture 3: Cross-validation

Lecture 4: Classification

September 30, 2021

Lecture 1: Model Complexity

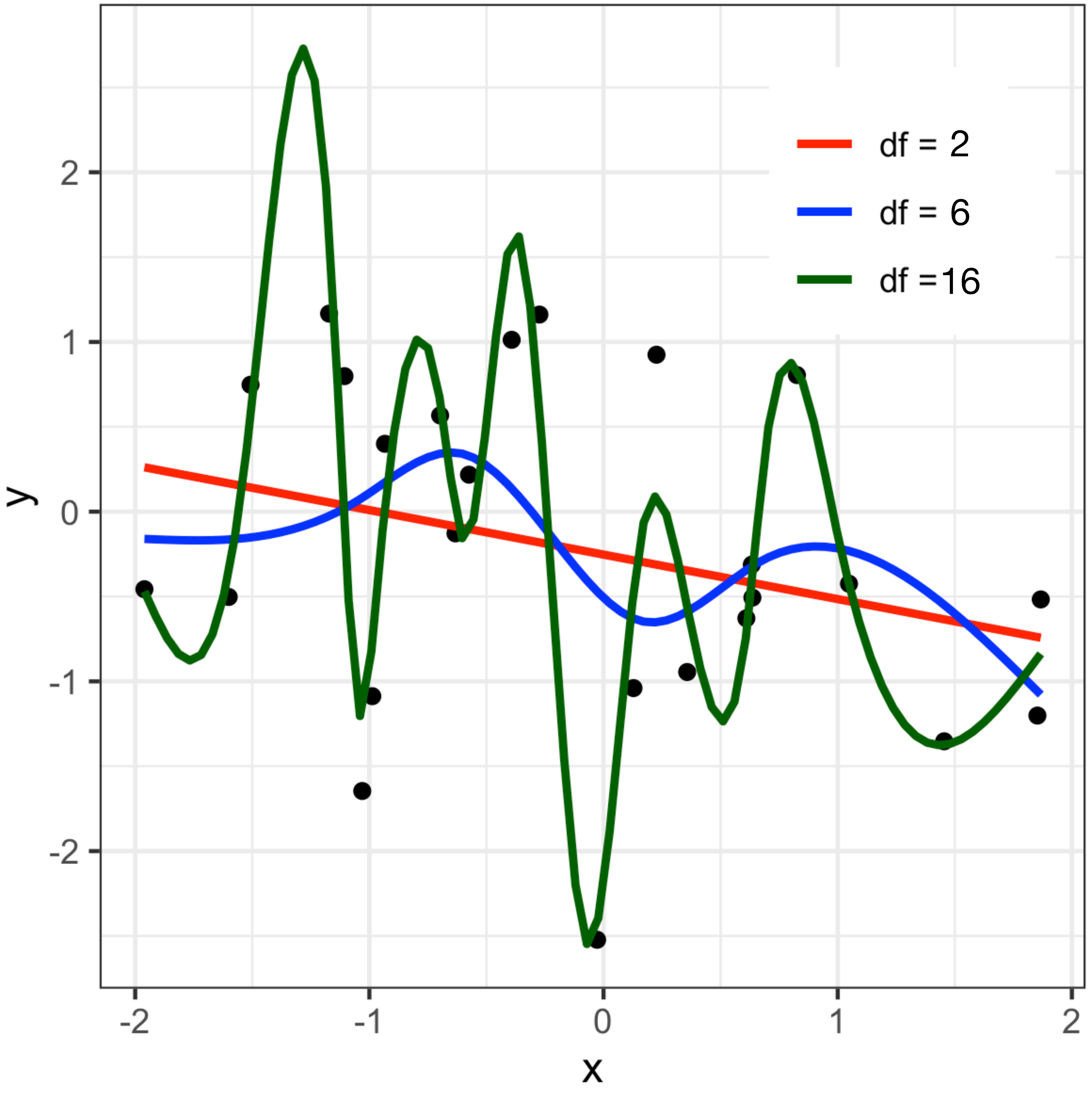
- The same data can be fit with models of varying degrees of *flexibility* or *complexity*.

- Example: Smooth curve fits to data (called *splines*) are more flexible if they are more wiggly.

- Model complexity has an important effect on predictive performance:

  - Too flexible → too sensitive to noise in training data

  - Not flexible enough → can't capture the underlying trend



Fitting curves to data

Not all relationships are linear…

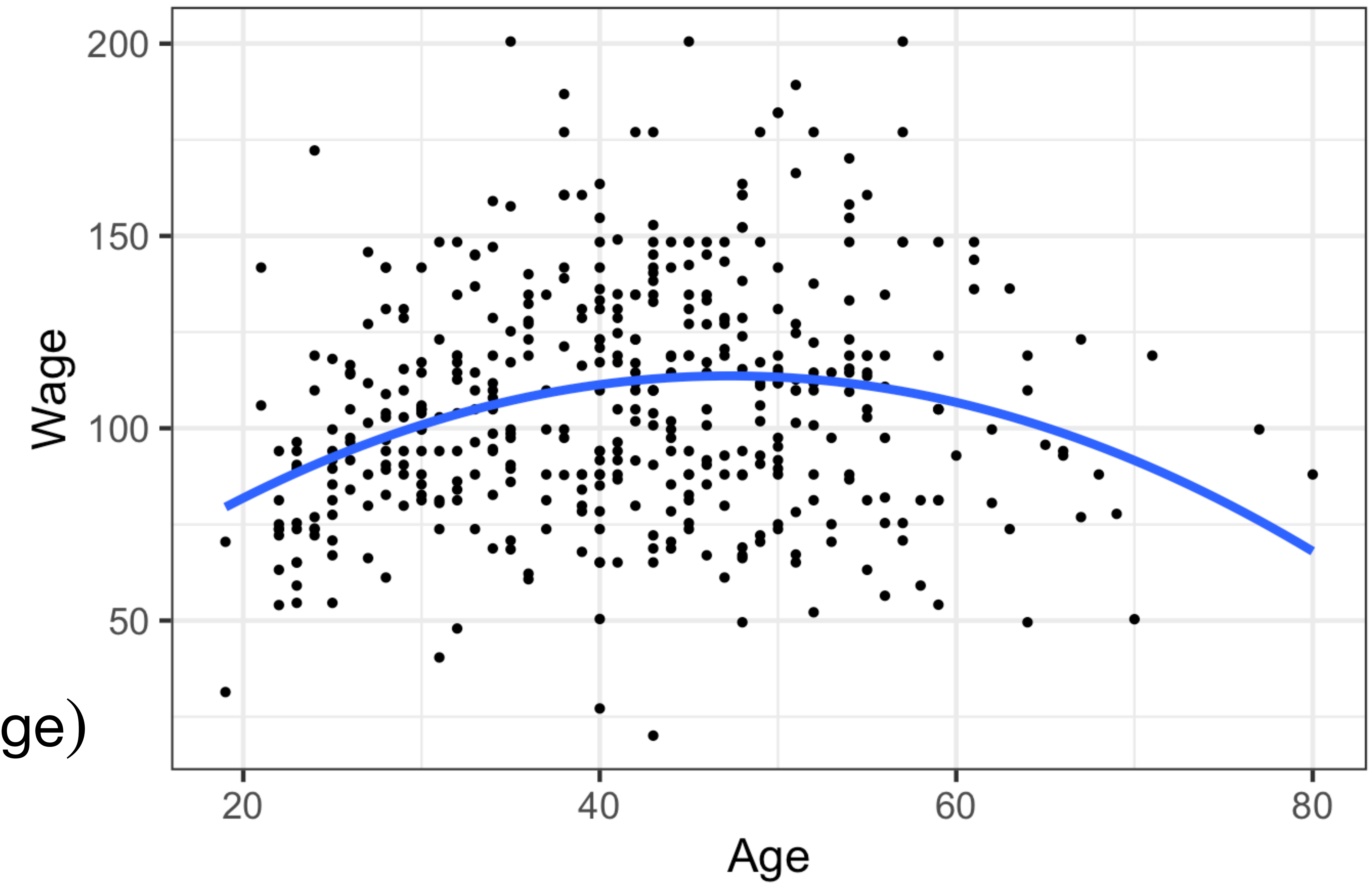
…at least in terms of the original variables.

Consider the *polynomial* model

$$\text{Wage} \approx \beta_0 + \beta_1 \text{Age} + \beta_2 \text{Age}^2.$$

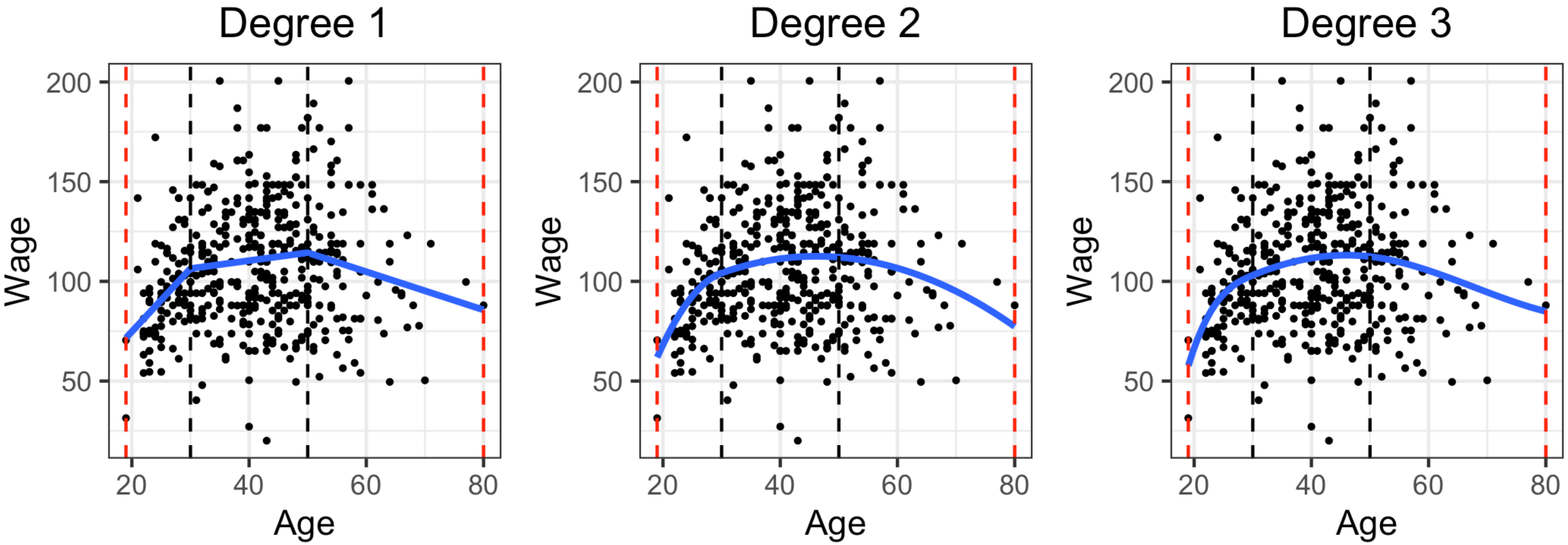
Or more generally:

$$\text{Wage} \approx \beta_1 f_1(\text{Age}) + \cdots + \beta_p f_p(\text{Age})$$



Splines: A fancier curve-fitting method

- Break range of Age into intervals separated by *internal knots* (in black below) and bounded by *boundary knots* (in red below).
- Fit a polynomial of degree d to the data in each interval.
- "Stitch" the polynomials together to smooth transitions at knots.

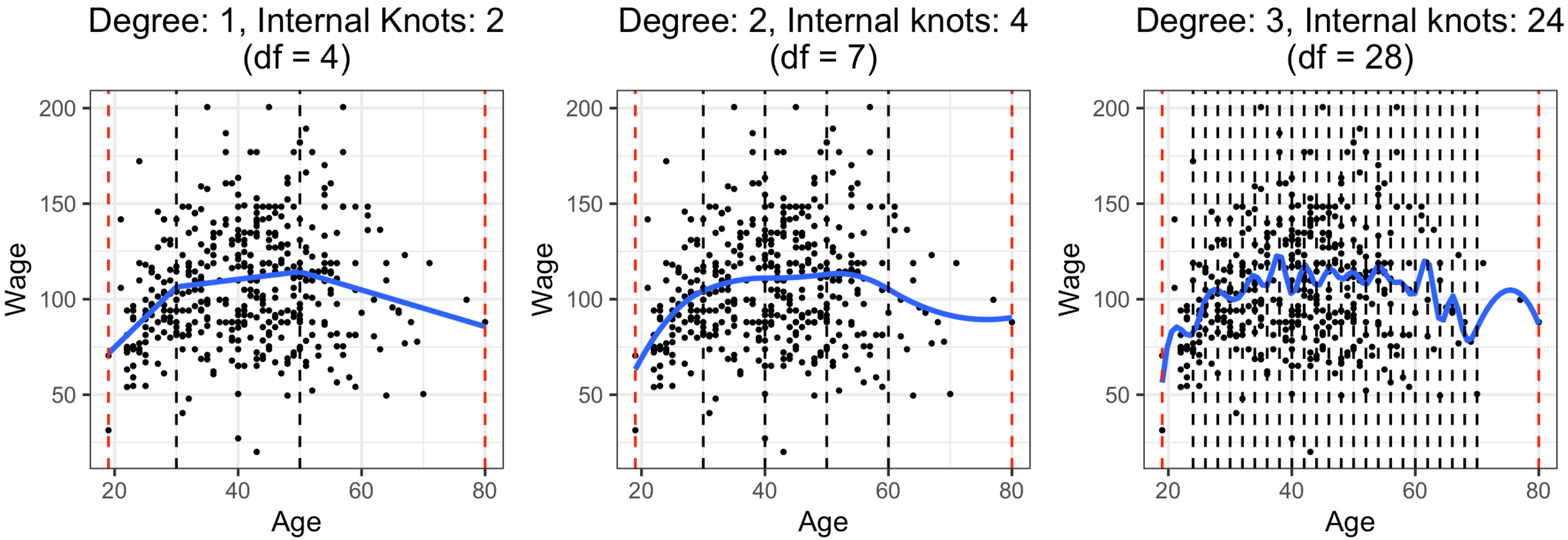


Degrees of freedom

Each spline fit can be represented in terms of a basis representation

$$\text{Wage} \approx \beta_1 f_1(\text{Age}) + \cdots + \beta_p f_p(\text{Age}).$$

The higher p is, the more freedom the curve has to fit the data. Hence, we define *degrees of freedom (df)* = p.



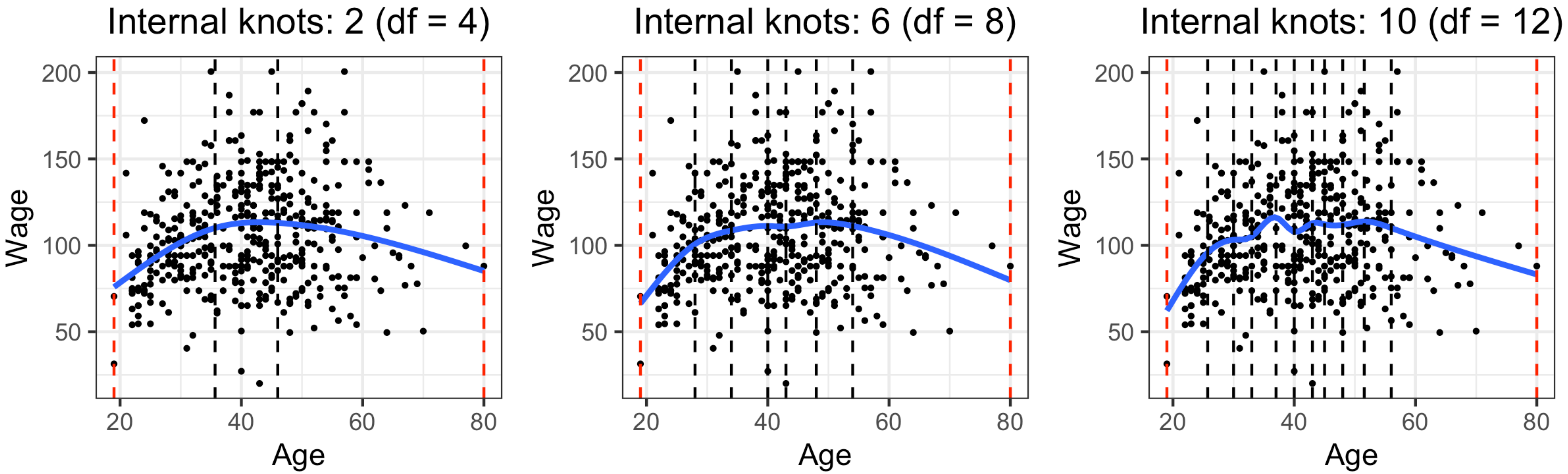
Natural cubic splines

Like regular splines, except:

df = intercepts (2) + number of knows

- Degree is always cubic
- Fit must be linear as you approach edges of the data
- Knots are chosen automatically at quantiles of the data

do not want behavior that is too wild at the edges



Recall: Prediction performance

You have training data $(X_1^{\text{train}}, Y_1^{\text{train}}), \ldots, (X_n^{\text{train}}, Y_n^{\text{train}})$, based on which you construct a predictive model $\hat{f}$ such that, hopefully, $Y \approx \hat{f}(X)$.

Will deploy $\hat{f}$ on test data $X_1^{\text{test}}, \ldots, X_N^{\text{test}}$ to guess $\hat{Y}_i^{\text{test}} = \hat{f}(X_i^{\text{test}})$ for each i.

Each X_i^{test} comes with a response Y_i^{test}, unknown to the predictive model.

Prediction quality: extent to which $Y_i^{\text{test}} \approx \hat{f}(X_i^{\text{test}})$, e.g. mean squared test error:

$$\text{Test error of } \hat{f} = \frac{1}{N}\sum_{i=1}^{N}(Y_i^{\text{test}} - \hat{f}(X_i^{\text{test}}))^2.$$

f-hat is trained on the same data

Contrast test error with the training error:

$$\text{Training error of } \hat{f} = \frac{1}{n}\sum_{i=1}^{n}(Y_i^{\text{train}} - \hat{f}(X_i^{\text{train}}))^2.$$

if you are overfitting, training error will be small, but this does not mean test error will also be small

Model complexity impacts prediction performance

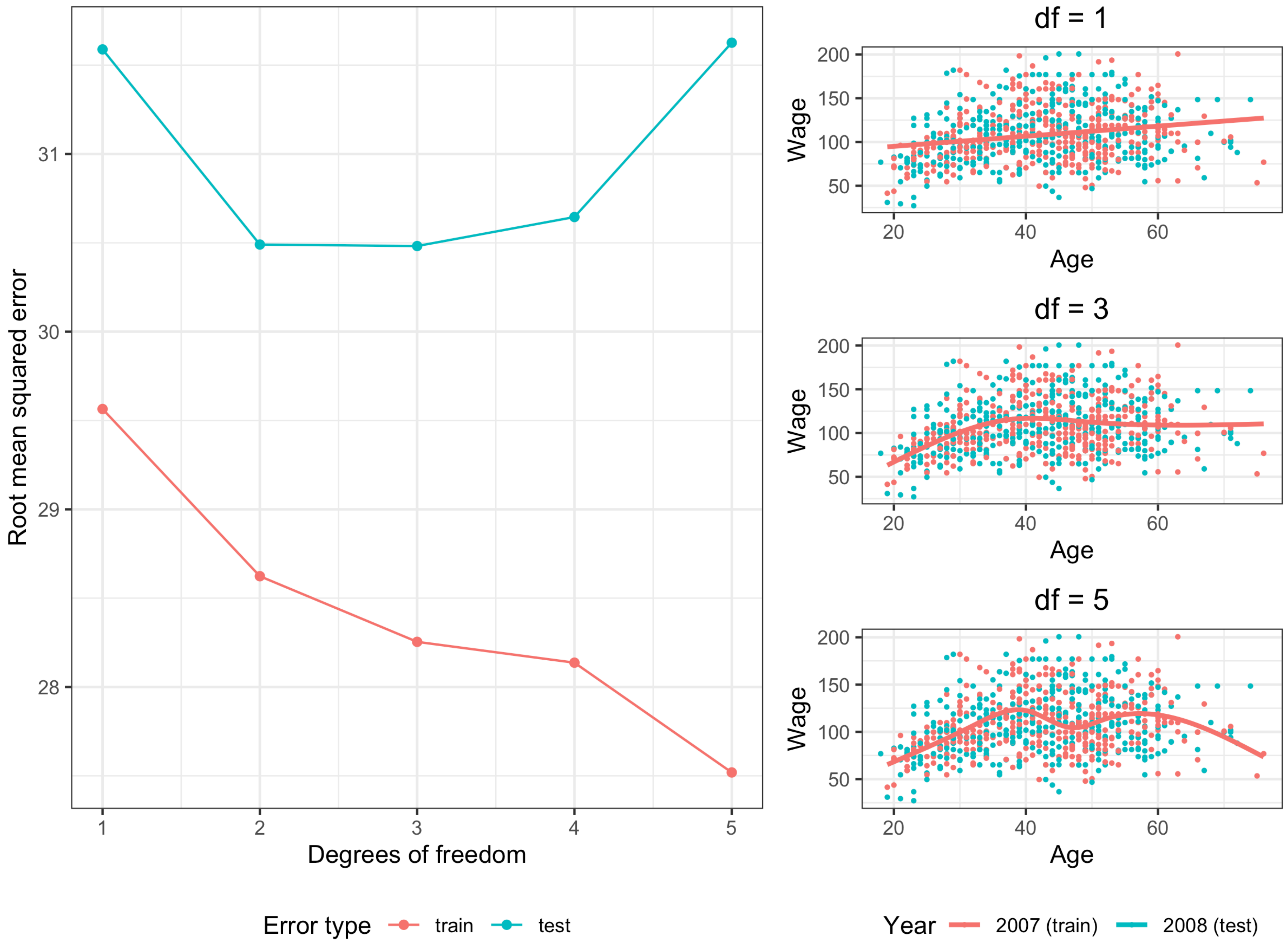
Model complexity: how closely the model $\hat{f}$ fits the training data:

$$Y_i^{\text{train}} = f(X_i^{\text{train}}) + \epsilon_i.$$

During training, $\hat{f}$ picks up on patterns in both f (the signal) and ϵ_i (the noise).

Training error of $\hat{f}$ decreases as we increase model complexity, but test error will be high if model complexity is too low or too high.

Training error is an underestimate of the test error, especially as the model complexity increases (overfitting).



Lecture 2: Bias-variance tradeoff

What drives model complexity?

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

Expected test error

Given a fitted $\hat{f}$ and a test set $(X_1^{\text{test}}, Y_1^{\text{test}}), \ldots, (X_N^{\text{test}}, Y_N^{\text{test}})$, recall that

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

The test error is a random function of the test set and the training set.

Define the **expected test error (ETE)** of a prediction rule as

$$\text{ETE} = \frac{1}{N}\sum_{i=1}^{N}\mathbb{E}[(Y_i^{\text{test}} - \hat{f}(X_i^{\text{test}}))^2].$$

The ETE is easier to understand theoretically.

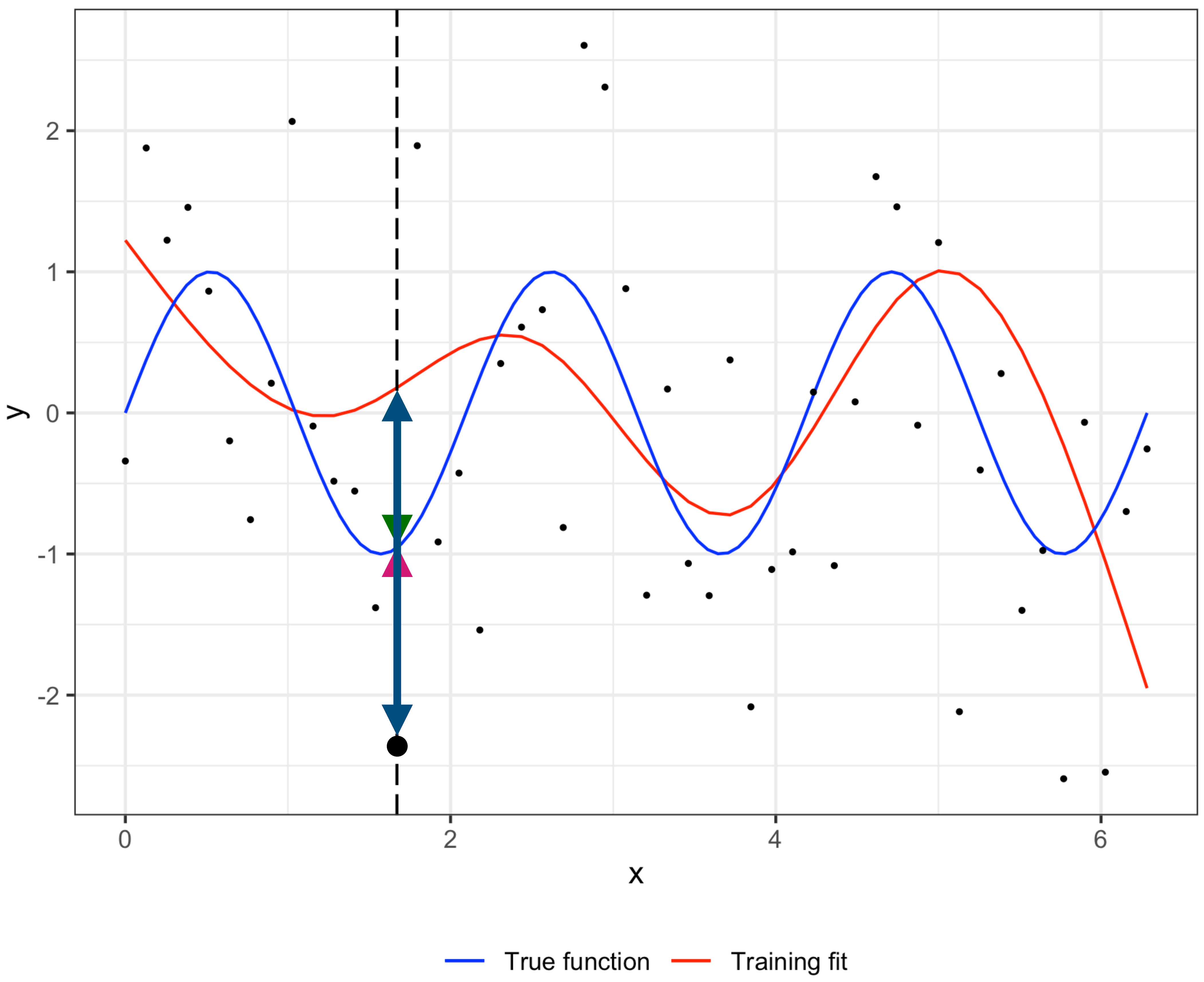
Dissecting the expected test error

Suppose $Y = f(X) + \epsilon, \quad \epsilon \sim N(0, \sigma^2)$.

Then,

$$\begin{aligned}
\text{ETE}_i &= \mathbb{E}[\underline{(Y_i^{\text{test}} - \hat{f}(X_i^{\text{test}})}\,)^2] \\
&= \mathbb{E}[(f(X_i^{\text{test}}) + \epsilon_i^{\text{test}} - \hat{f}(X_i^{\text{test}}))^2] \\
&= \underbrace{\mathbb{E}[(f(X_i^{\text{test}}) - \hat{f}(X_i^{\text{test}}))^2]}_{\text{difference between your function prediction and true function prediction}} + \underbrace{\sigma^2}_{\text{noise}}
\end{aligned}$$

focuses us on one test point



Dissecting the expected test error

If cannot fit many models on this data set, impossible to calc bias or variance or sd

$$\text{ETE}_i = \mathbb{E}[(f(X_i^{\text{test}}) - \hat{f}(X_i^{\text{test}}))^2] + \sigma^2$$

$$= (f(X_i^{\text{test}}) - \text{Ave}(\hat{f}(X_i^{\text{test}}))^2 + \text{Var}[\hat{f}(X_i^{\text{test}})] + \sigma^2$$

$$= \underline{\text{Bias}_i^2} + \underline{\text{Variance}_i} + \underline{\text{Irreducible error}_i}$$

Averaging over i, we get

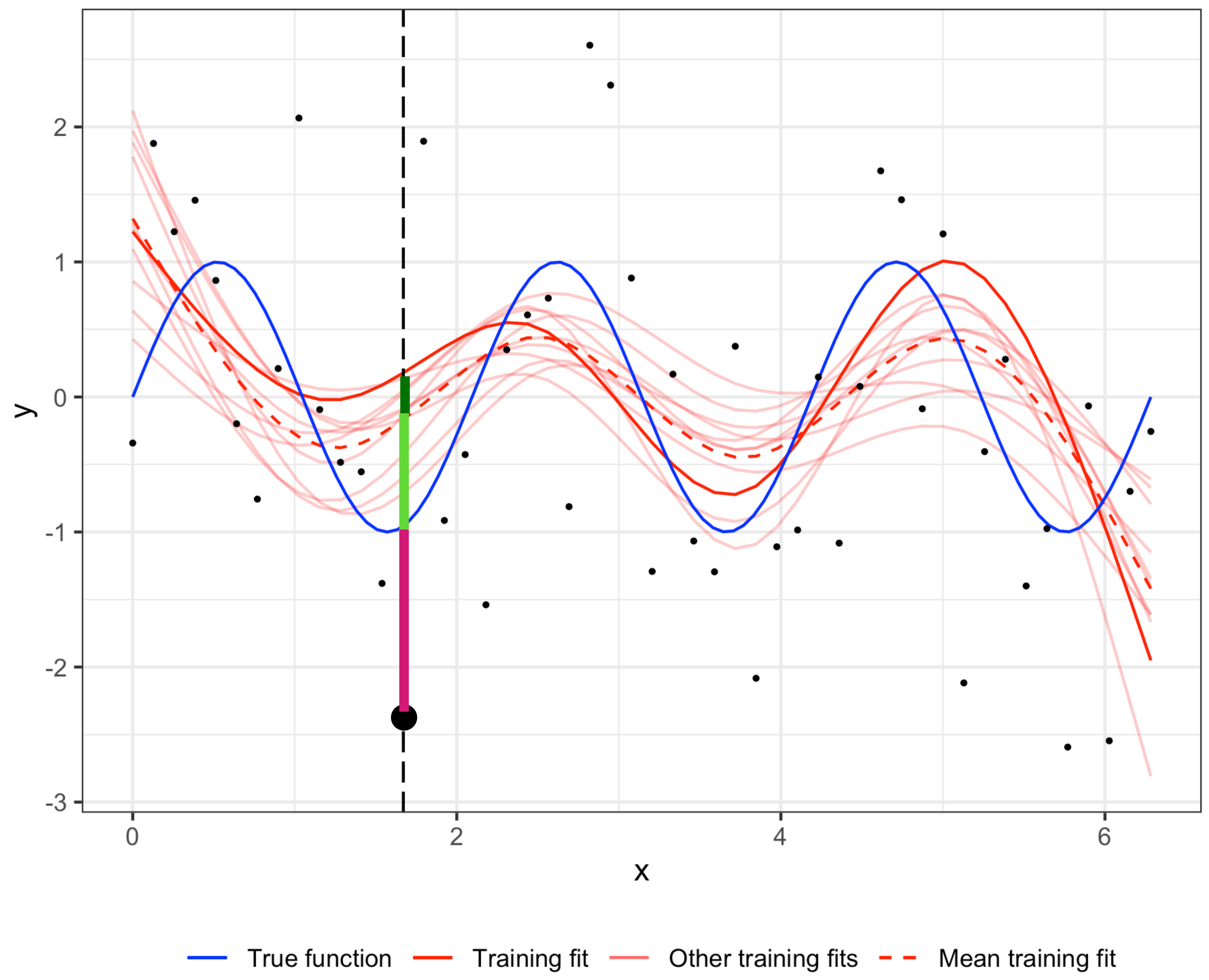
$$\text{ETE} = \frac{1}{N}\sum_{i=1}^{N} \mathbb{E}[(Y_i^{\text{test}} - \hat{f}(X_i^{\text{test}}))^2]$$

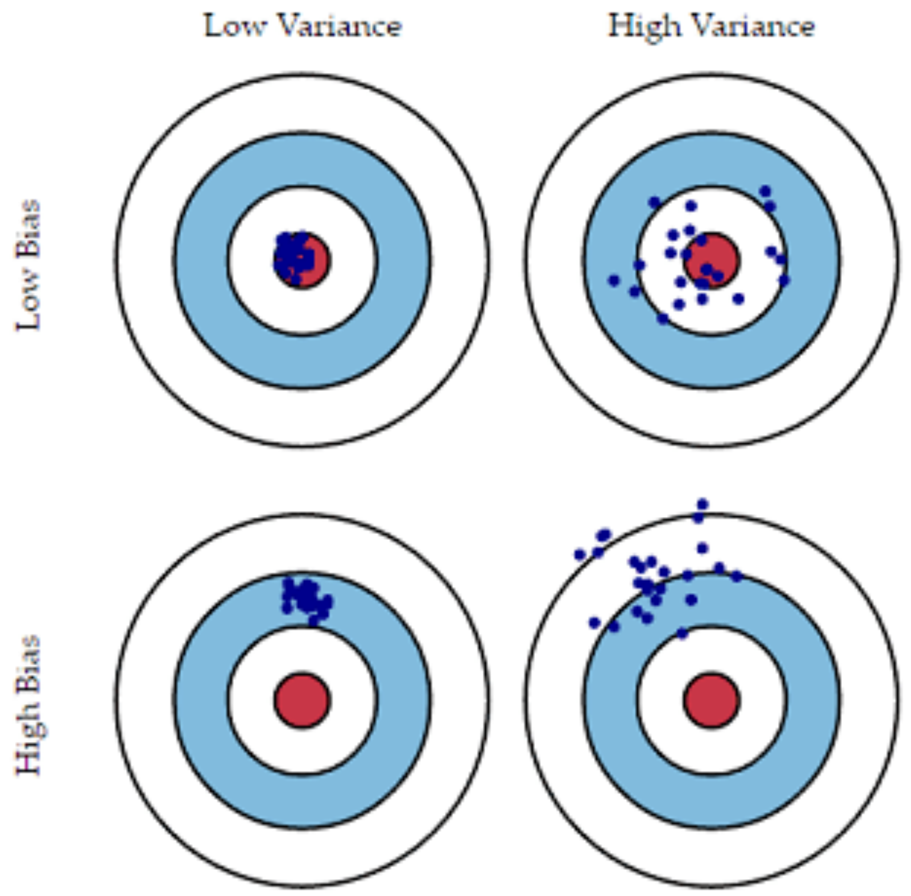
$$= \frac{1}{N}\sum_{i=1}^{N} \text{Bias}_i^2 + \frac{1}{N}\sum_{i=1}^{N} \text{Variance}_i^2 + \sigma^2$$

= “Bias” + “Variance” + “Irreducible error”

really talking about bias and variance averaged across all test points

This is the bias-variance decomposition.



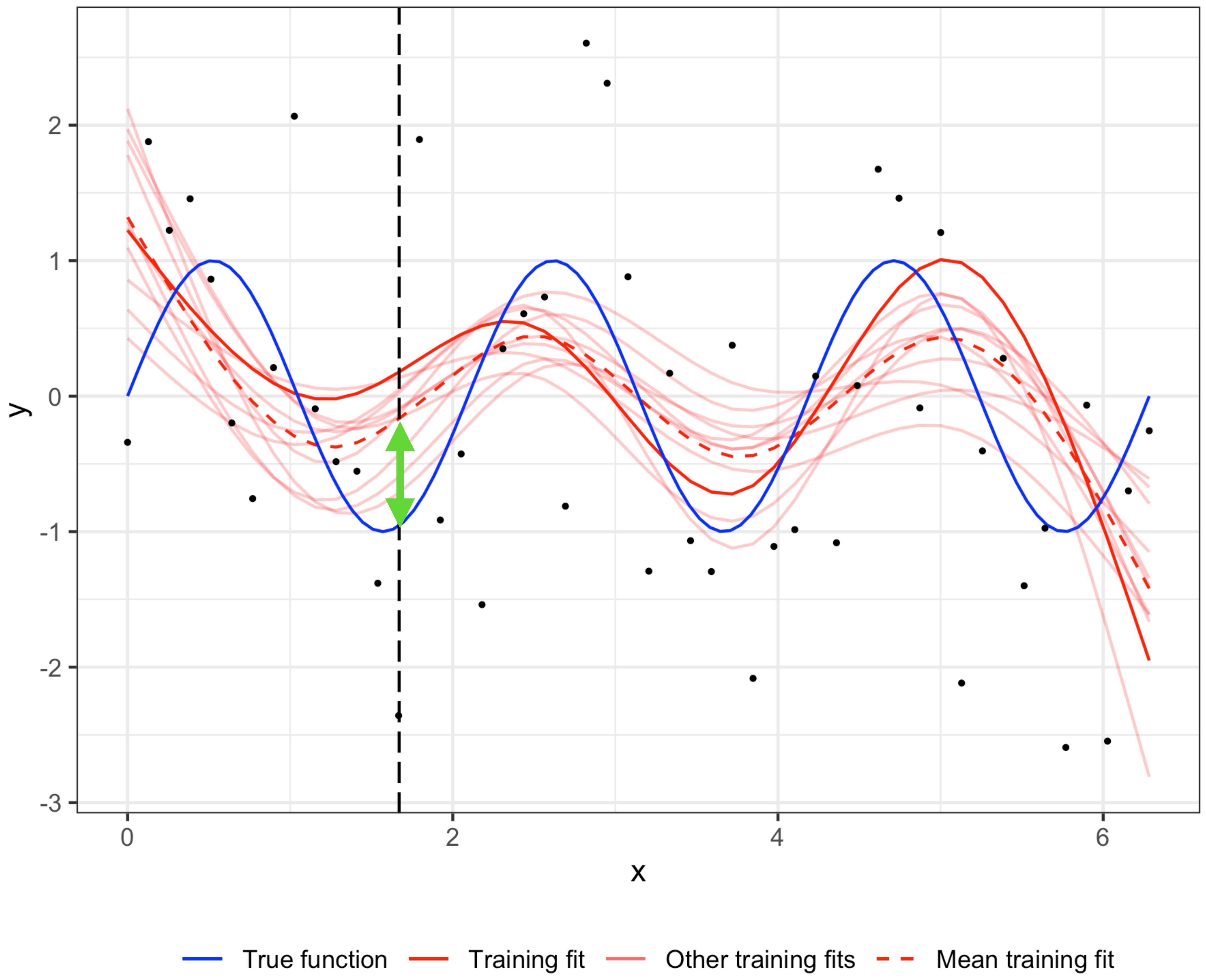


Understanding bias

$$\text{Bias}_i = \underline{\text{Ave}(\hat{f}(X_i^{\text{test}})) - f(X_i^{\text{test}})}$$

Bias reflects the distance from the average fitted model to the true trend.

Adding model complexity reduces bias.



Understanding variance

$$\text{Variance}_i = \underline{\mathbb{E}[(\hat{f}(X_i^{\text{test}}) - \text{Ave}(\hat{f}(X_i^{\text{test}})))^2]}$$

Variance is the wobbling of the model fit due to the randomness in the training data.

Variance is a consequence of overfitting.

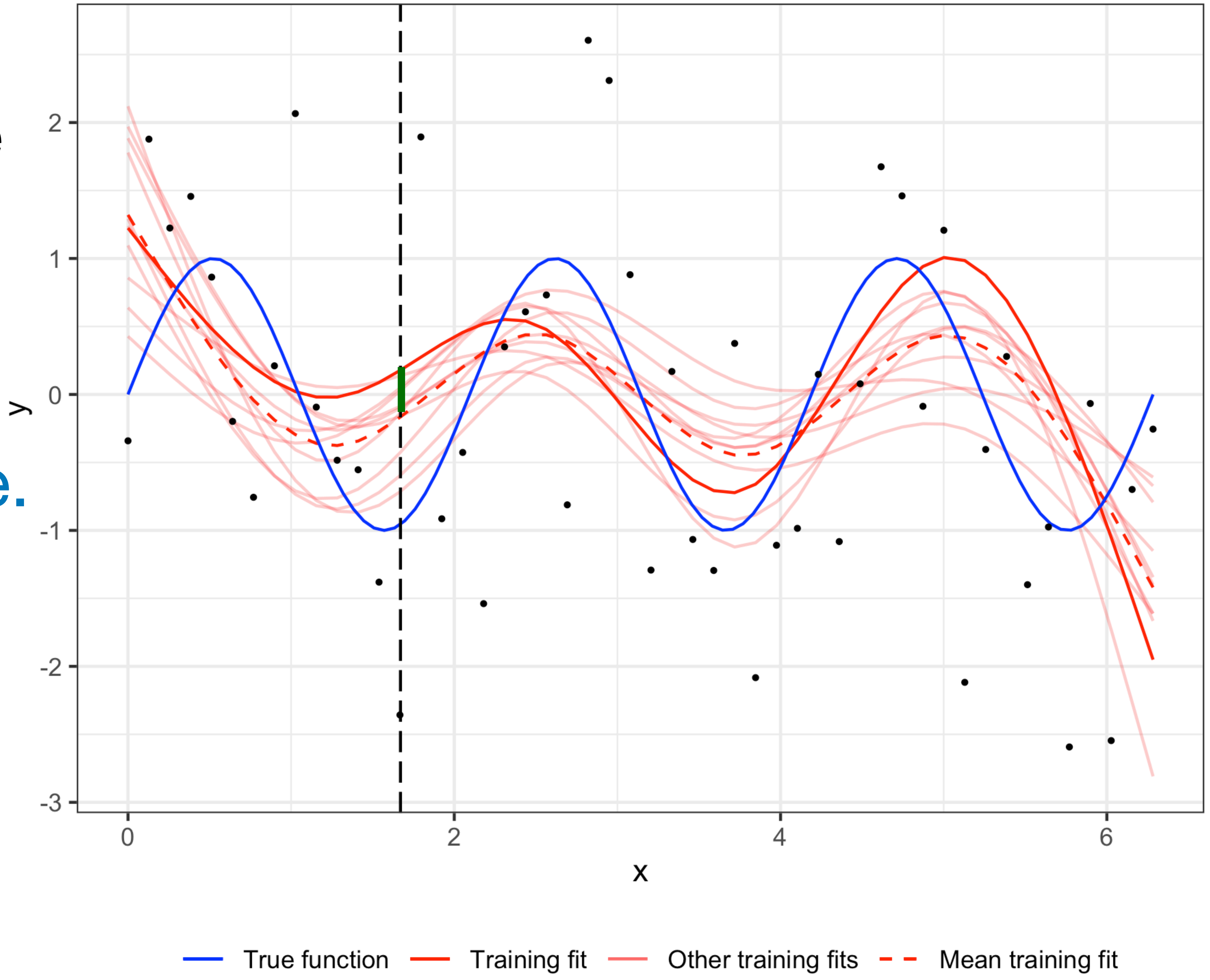
Adding model complexity increases variance.

In linear models,

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

p = df

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



The bias-variance tradeoff

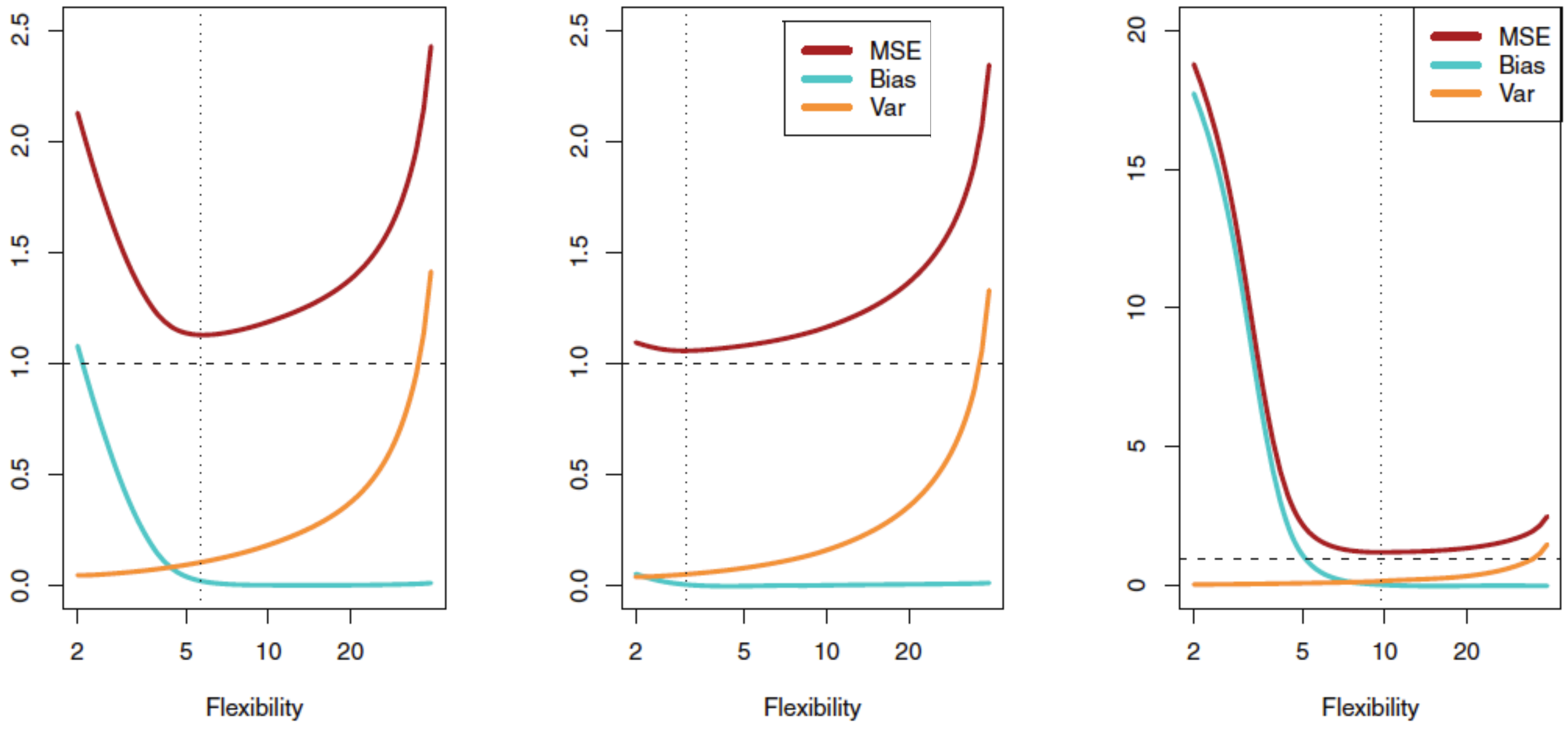
Recall that

ETE = “Bias” + “Variance” + “Irreducible error”

- Adding model complexity reduces bias
- Adding model complexity increases variance

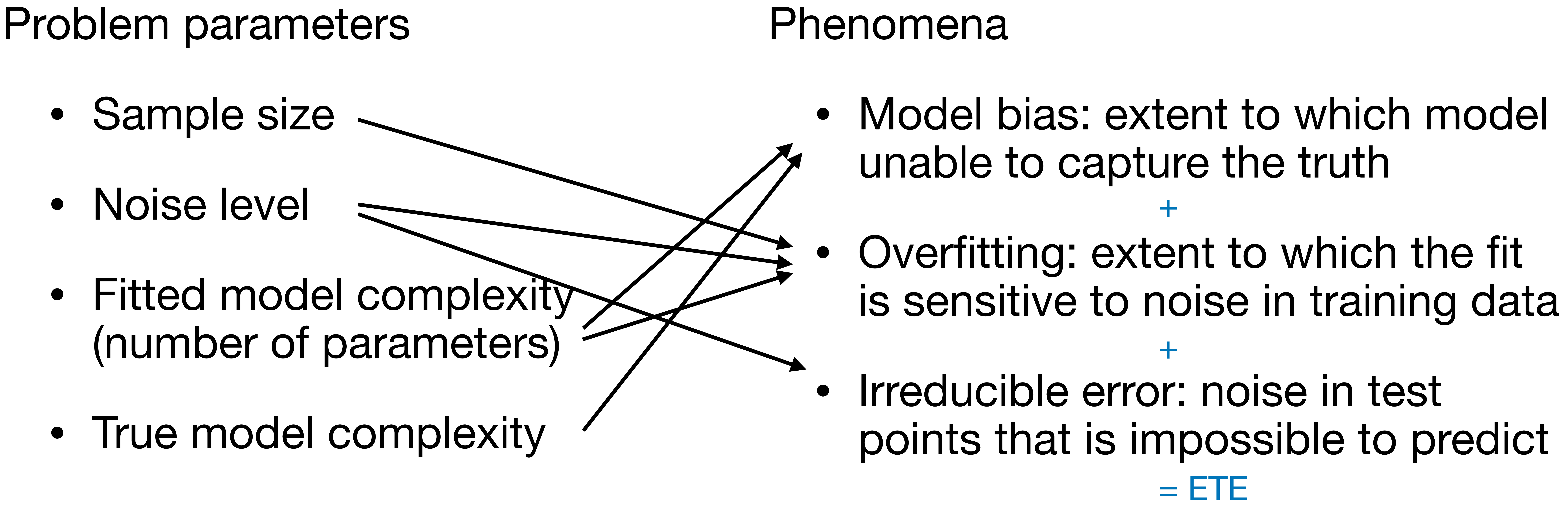
When varying model complexity, there is a tradeoff between bias and variance.

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

+

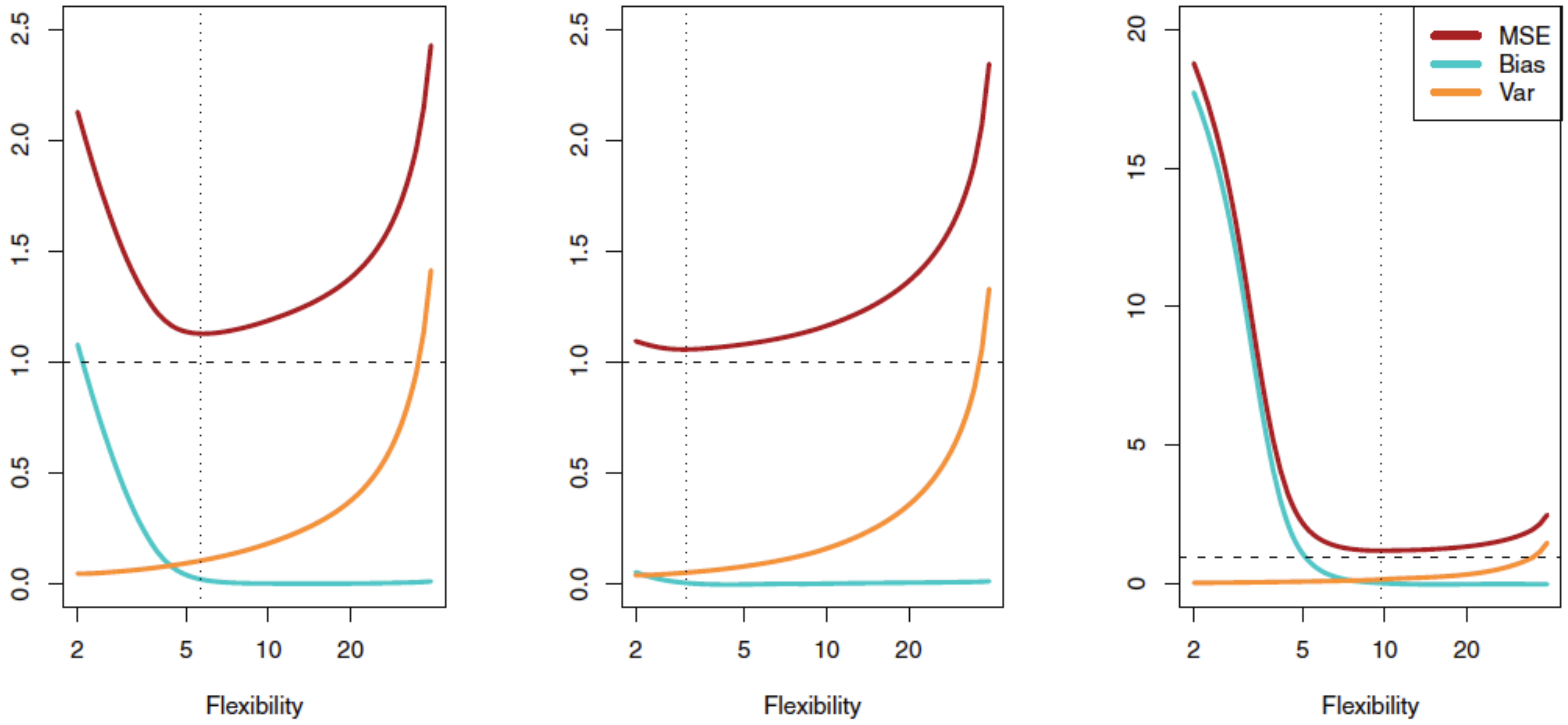
- Overfitting: extent to which the fit is sensitive to noise in training data

+

- Irreducible error: noise in test points that is impossible to predict

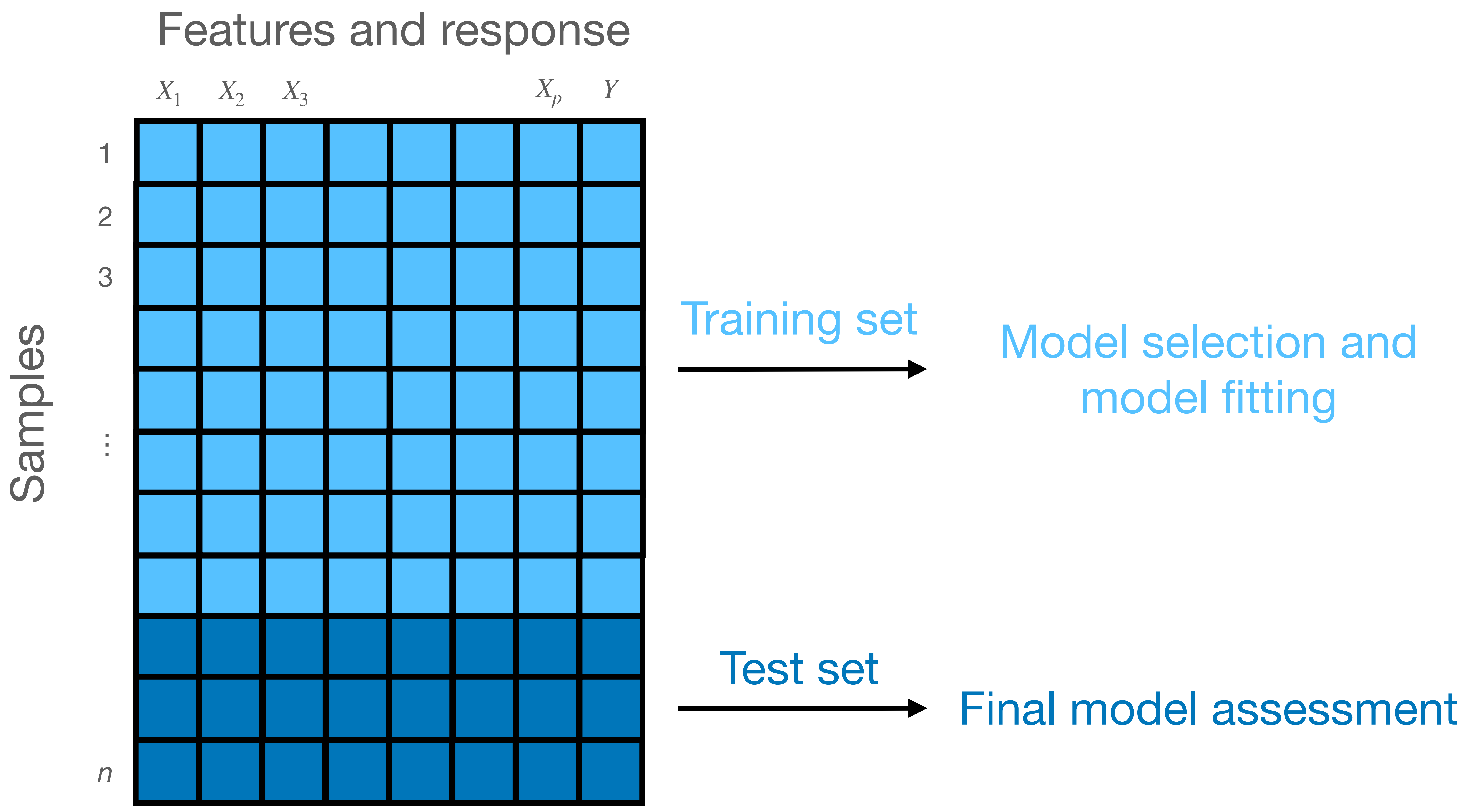
= ETE

Lecture 3: Cross-validation



- How do we estimate the test error for model selection?
- How do we estimate the test error for final model assessment?

Estimating test error for final model assessment



Features and response

Samples

Training set

Model selection and model fitting

Test set

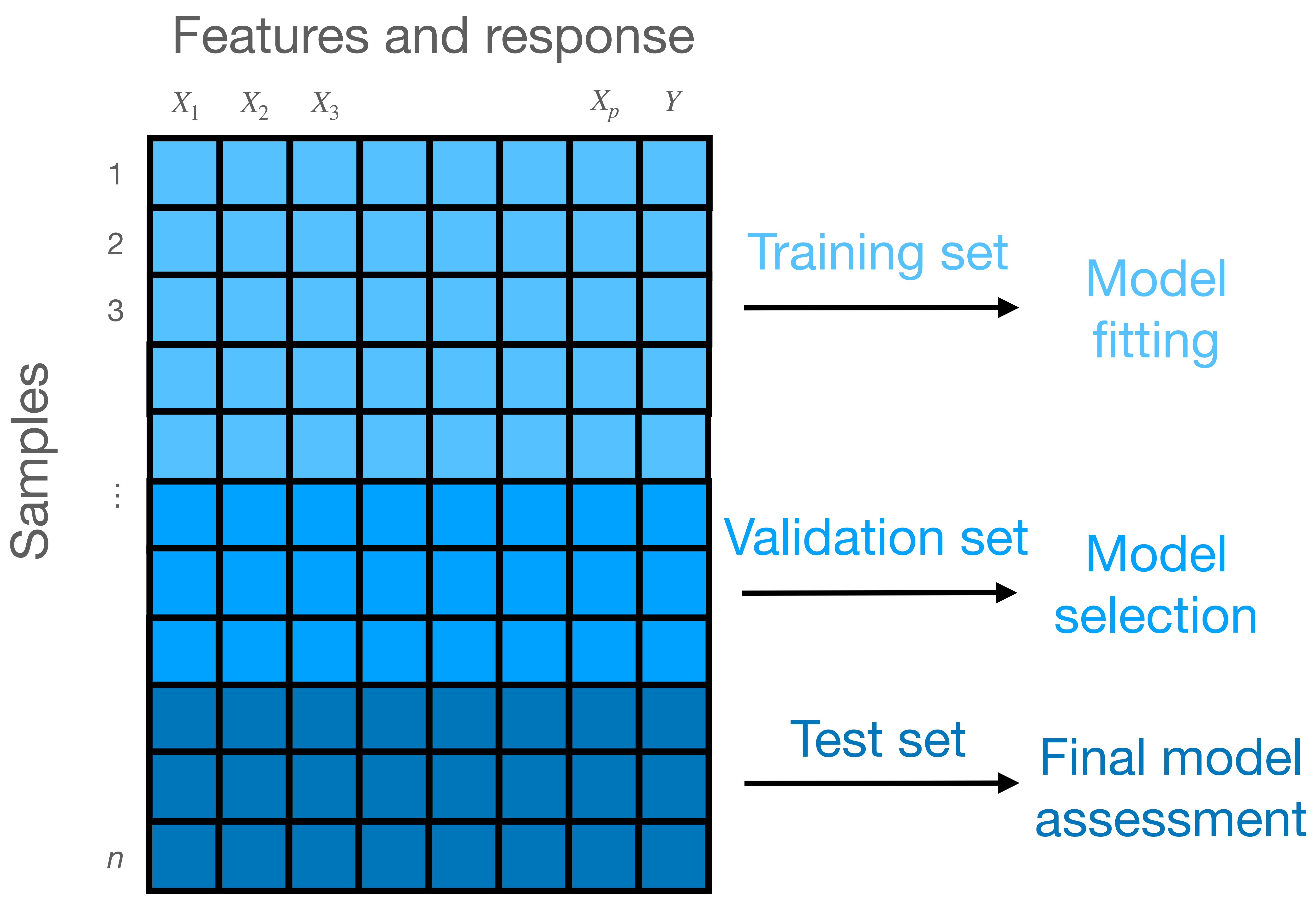
Final model assessment

More samples for training: better fitted model.

More samples for testing: better estimate of test error.

Common splits range from
50% training / 50% testing
to
80% training / 20% testing.

Validation set approach for model selection



Training set → Model fitting

Validation set → Model selection

Test set → Final model assessment

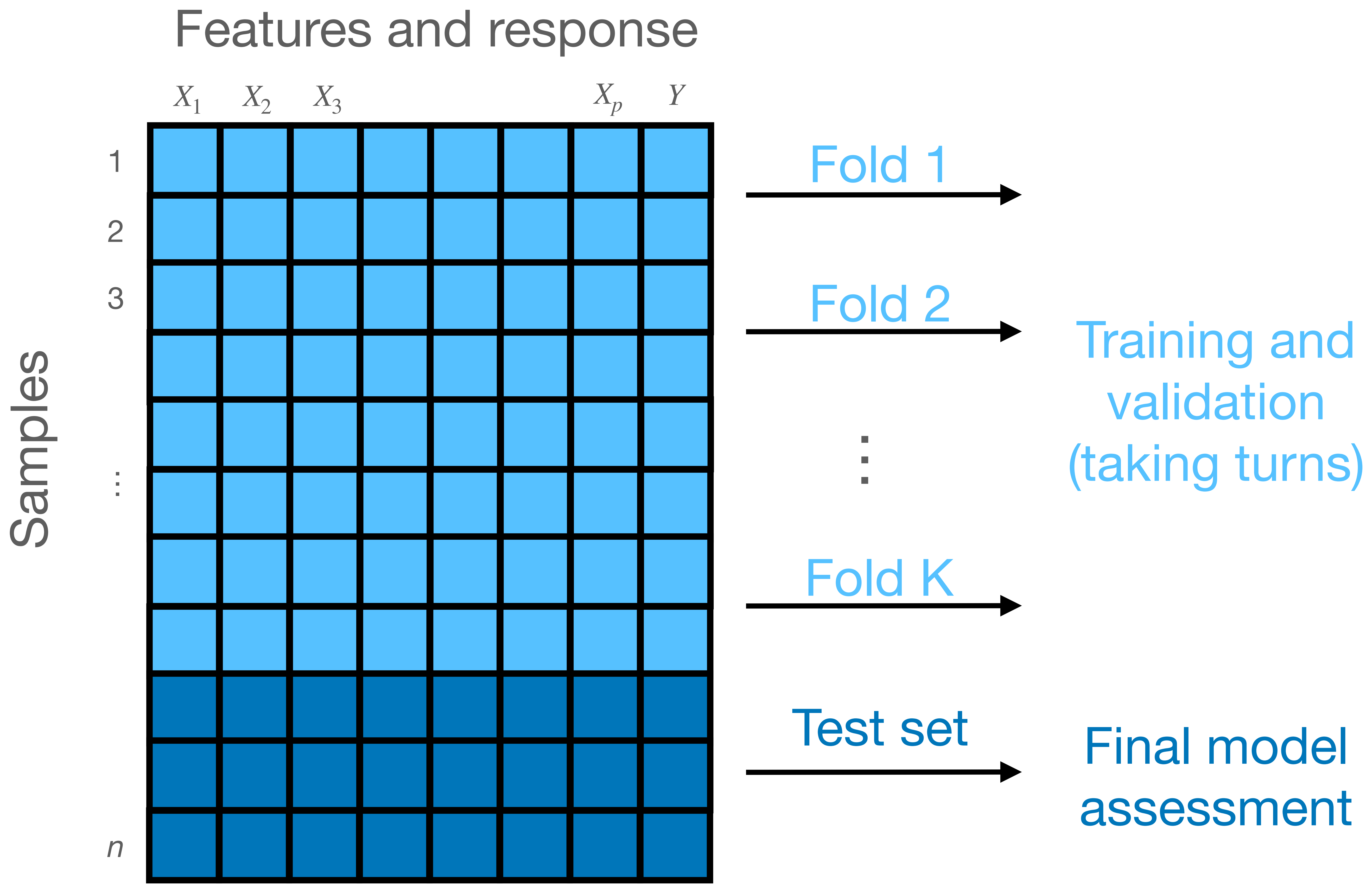
1. Fit models of varying complexity to training set
2. Estimate test error for each model on validation set
3. Choose model complexity to minimize validation error
4. Refit this model on combined training and validation sets
5. Evaluate the final model on the test set

Drawback of validation set approach

The validation set approach does not make efficient use of samples.

Using a small validation set can lead to a suboptimal model complexity choice.

Cross-validation for model selection



Features and response

X_1 X_2 X_3 X_p Y

Samples

1

2

3

⋮

n

Fold 1

Fold 2

⋮

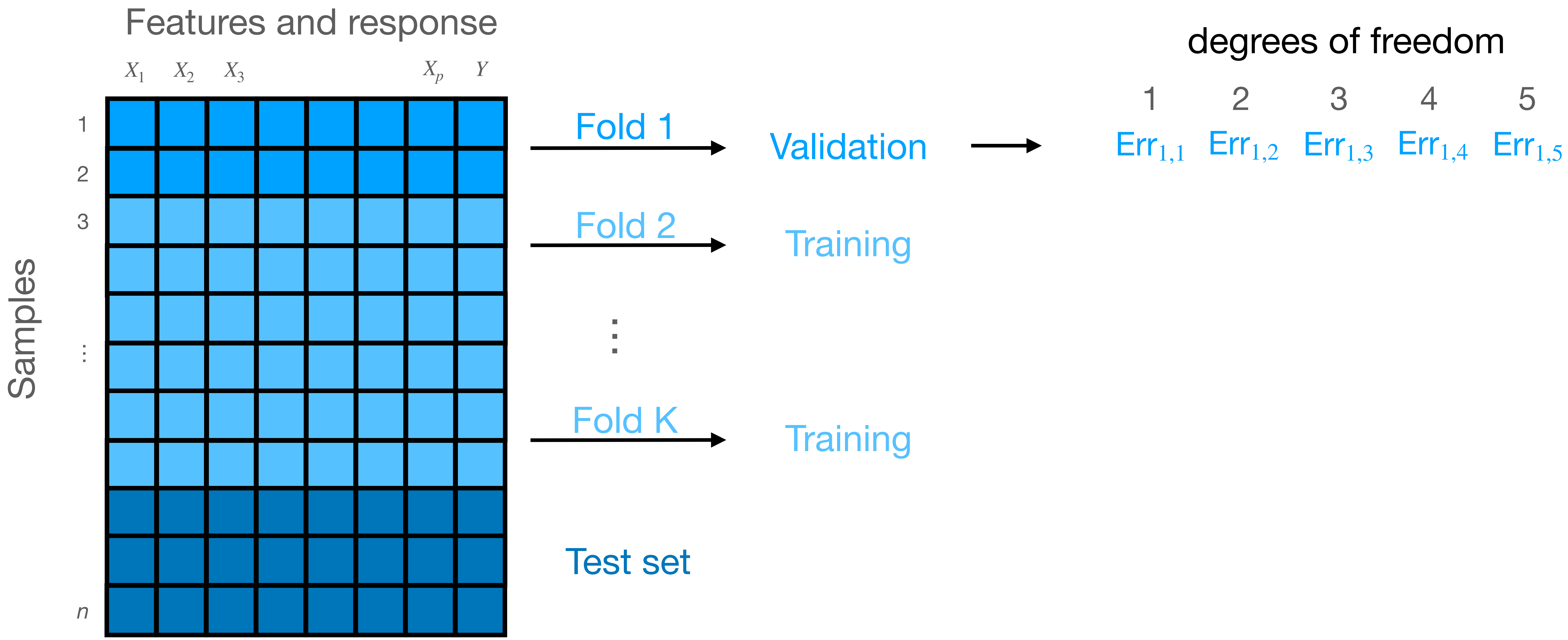
Fold K

Training and validation (taking turns)

Test set

Final model assessment

Cross-validation for model selection



Features and response

X_1 X_2 X_3 X_p Y

Samples

1

2

3

⋮

n

Fold 1 → Validation →

Fold 2 → Training

⋮

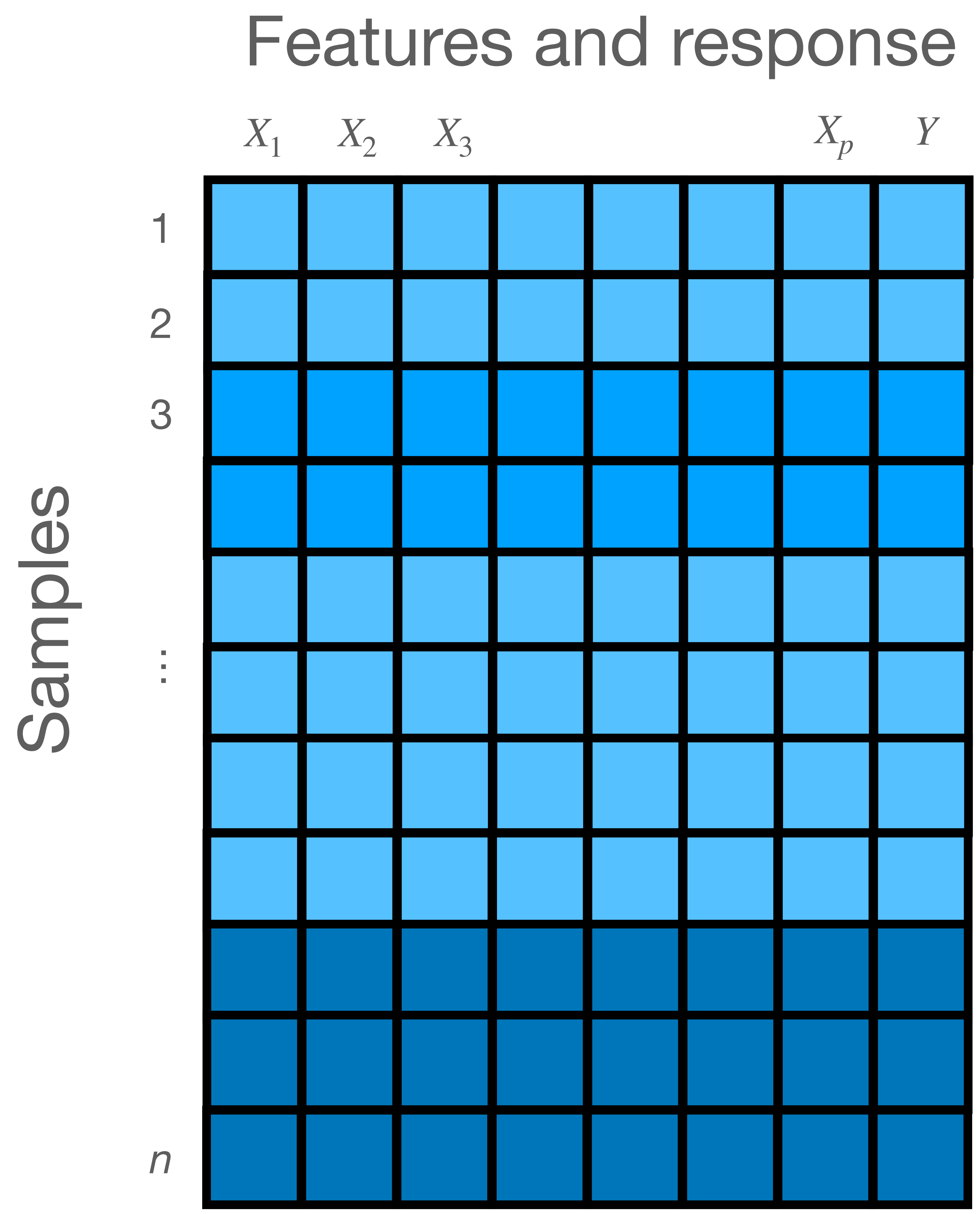
Fold K → Training

Test set

degrees of freedom

1	2	3	4	5
$\mathrm{Err}_{1,1}$	$\mathrm{Err}_{1,2}$	$\mathrm{Err}_{1,3}$	$\mathrm{Err}_{1,4}$	$\mathrm{Err}_{1,5}$

Cross-validation for model selection



Fold 1 → Training

Fold 2 → Validation →

⋮

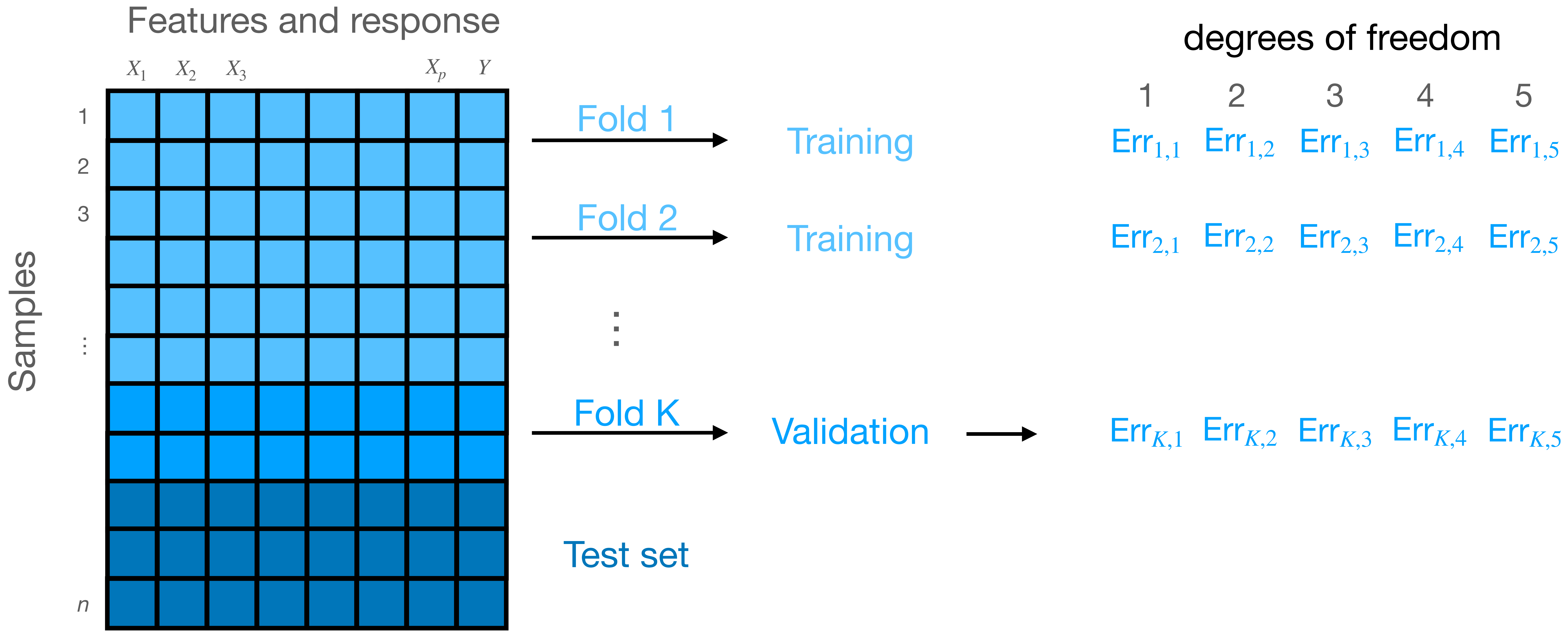
Fold K → Training

Test set

degrees of freedom

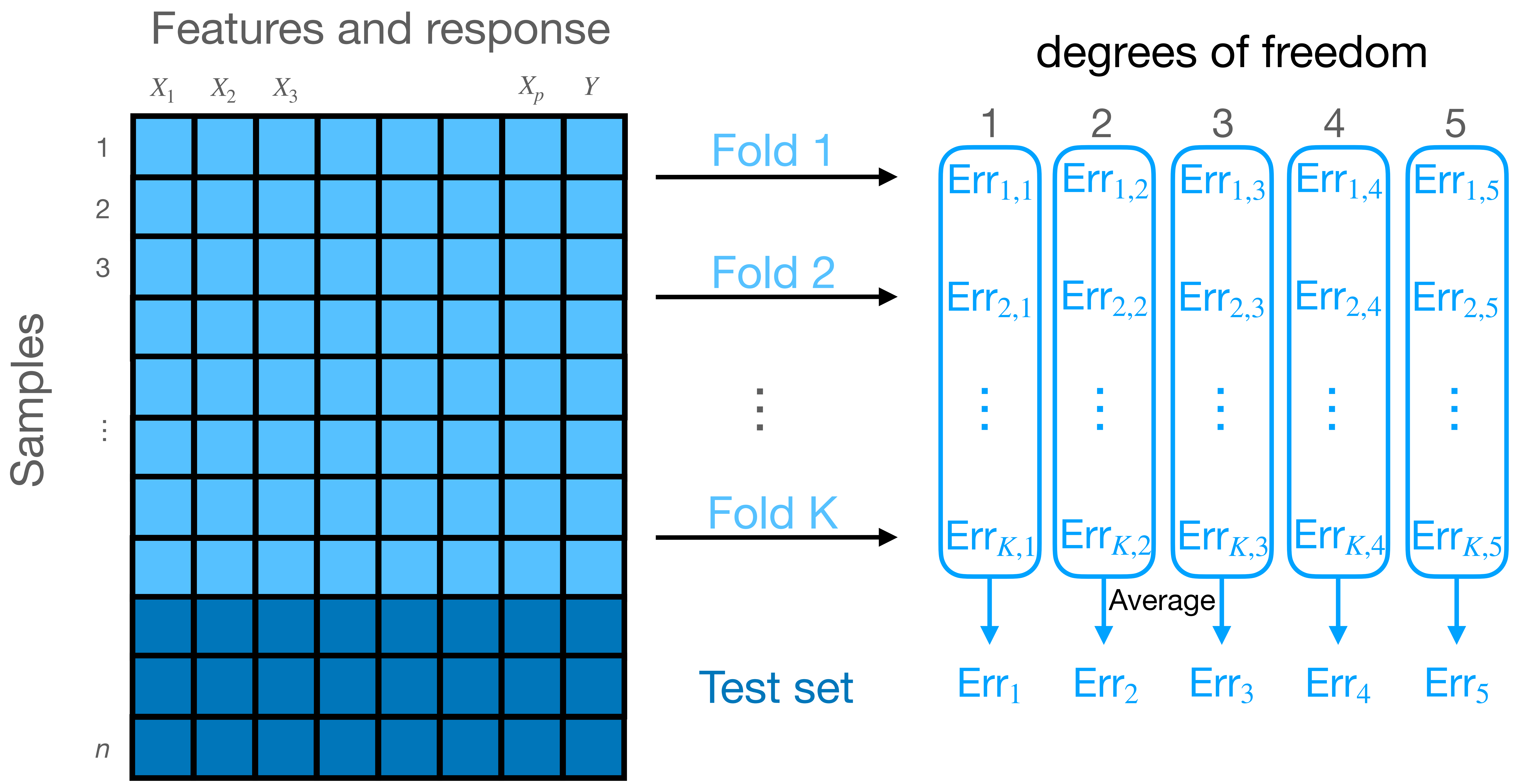
1	2	3	4	5
$\text{Err}_{1,1}$	$\text{Err}_{1,2}$	$\text{Err}_{1,3}$	$\text{Err}_{1,4}$	$\text{Err}_{1,5}$
$\text{Err}_{2,1}$	$\text{Err}_{2,2}$	$\text{Err}_{2,3}$	$\text{Err}_{2,4}$	$\text{Err}_{2,5}$

Cross-validation for model selection



degrees of freedom				
1	2	3	4	5
$\mathrm{Err}_{1,1}$	$\mathrm{Err}_{1,2}$	$\mathrm{Err}_{1,3}$	$\mathrm{Err}_{1,4}$	$\mathrm{Err}_{1,5}$
$\mathrm{Err}_{2,1}$	$\mathrm{Err}_{2,2}$	$\mathrm{Err}_{2,3}$	$\mathrm{Err}_{2,4}$	$\mathrm{Err}_{2,5}$
$\mathrm{Err}_{K,1}$	$\mathrm{Err}_{K,2}$	$\mathrm{Err}_{K,3}$	$\mathrm{Err}_{K,4}$	$\mathrm{Err}_{K,5}$

Cross-validation for model selection



Features and response

X_1 X_2 X_3 X_p Y

Samples

1
2
3
⋮
n

Fold 1

Fold 2

⋮

Fold K

Test set

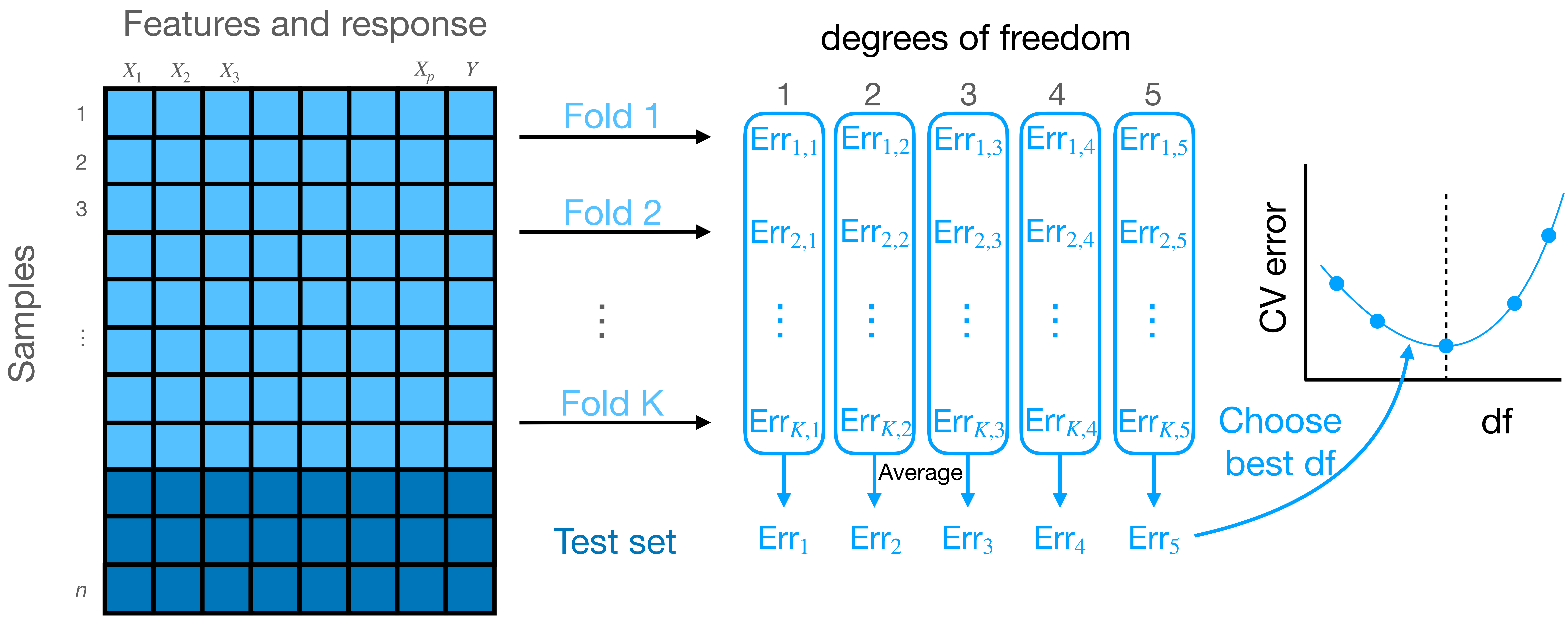
degrees of freedom

1	2	3	4	5
$\mathrm{Err}_{1,1}$	$\mathrm{Err}_{1,2}$	$\mathrm{Err}_{1,3}$	$\mathrm{Err}_{1,4}$	$\mathrm{Err}_{1,5}$
$\mathrm{Err}_{2,1}$	$\mathrm{Err}_{2,2}$	$\mathrm{Err}_{2,3}$	$\mathrm{Err}_{2,4}$	$\mathrm{Err}_{2,5}$
⋮	⋮	⋮	⋮	⋮
$\mathrm{Err}_{K,1}$	$\mathrm{Err}_{K,2}$	$\mathrm{Err}_{K,3}$	$\mathrm{Err}_{K,4}$	$\mathrm{Err}_{K,5}$

Average

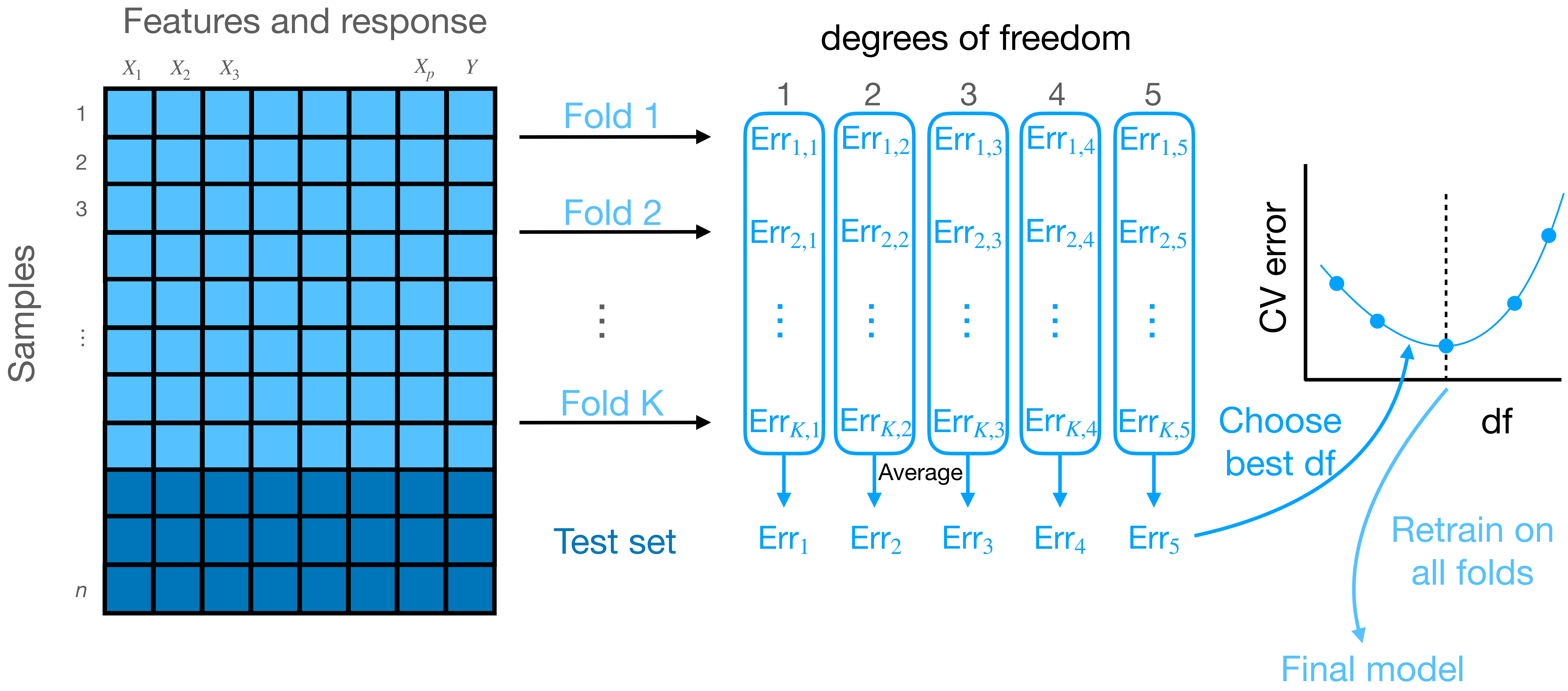
Err_1 Err_2 Err_3 Err_4 Err_5

Cross-validation for model selection



	1	2	3	4	5
Fold 1	$\text{Err}_{1,1}$	$\text{Err}_{1,2}$	$\text{Err}_{1,3}$	$\text{Err}_{1,4}$	$\text{Err}_{1,5}$
Fold 2	$\text{Err}_{2,1}$	$\text{Err}_{2,2}$	$\text{Err}_{2,3}$	$\text{Err}_{2,4}$	$\text{Err}_{2,5}$
⋮	⋮	⋮	⋮	⋮	⋮
Fold K	$\text{Err}_{K,1}$	$\text{Err}_{K,2}$	$\text{Err}_{K,3}$	$\text{Err}_{K,4}$	$\text{Err}_{K,5}$
	Err_1	Err_2	Err_3	Err_4	Err_5

Cross-validation for model selection



Features and response

Test set

degrees of freedom

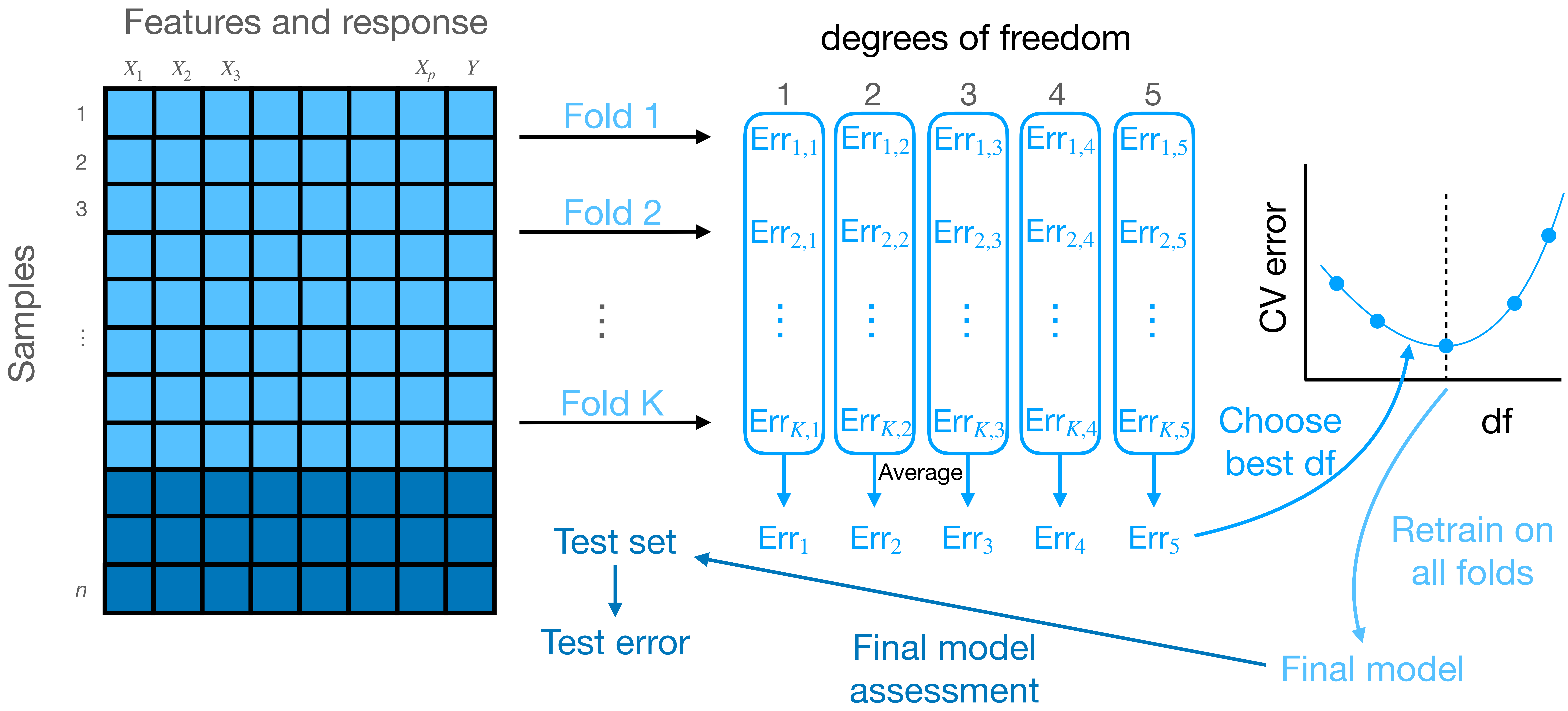
	1	2	3	4	5
Fold 1	$\text{Err}_{1,1}$	$\text{Err}_{1,2}$	$\text{Err}_{1,3}$	$\text{Err}_{1,4}$	$\text{Err}_{1,5}$
Fold 2	$\text{Err}_{2,1}$	$\text{Err}_{2,2}$	$\text{Err}_{2,3}$	$\text{Err}_{2,4}$	$\text{Err}_{2,5}$
⋮	⋮	⋮	⋮	⋮	⋮
Fold K	$\text{Err}_{K,1}$	$\text{Err}_{K,2}$	$\text{Err}_{K,3}$	$\text{Err}_{K,4}$	$\text{Err}_{K,5}$
Average	Err_1	Err_2	Err_3	Err_4	Err_5

Choose best df

Retrain on all folds

Final model

Cross-validation for model selection



Features and response

Fold 1

Fold 2

⋮

Fold K

degrees of freedom

Choose best df

Retrain on all folds

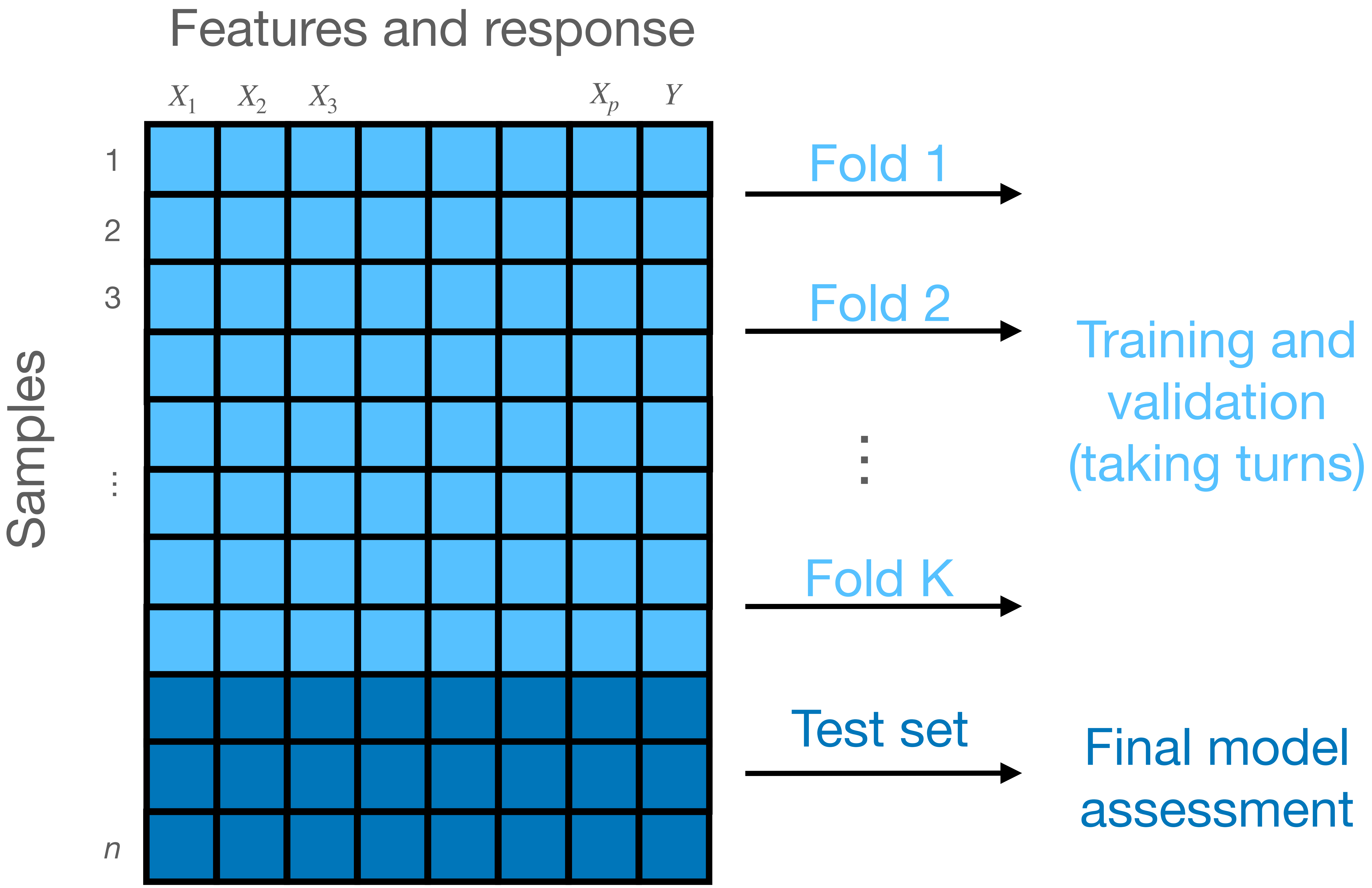
Final model

Final model assessment

Test set

Test error

Cross-validation (summary)



1. Split data into *K* folds
2. For each fold *k*,
   - Fit models of varying complexity to training data, holding out fold *k*
   - Evaluate validation error for each model on fold *k*
3. Average across folds to get CV error for each model complexity
4. Choose model complexity to minimize CV error
5. Refit this model on all folds
6. Evaluate final model on the test set

Different kinds of test error

Cross-validation is compatible with any definition of test error (e.g. mean squared error or misclassification error).

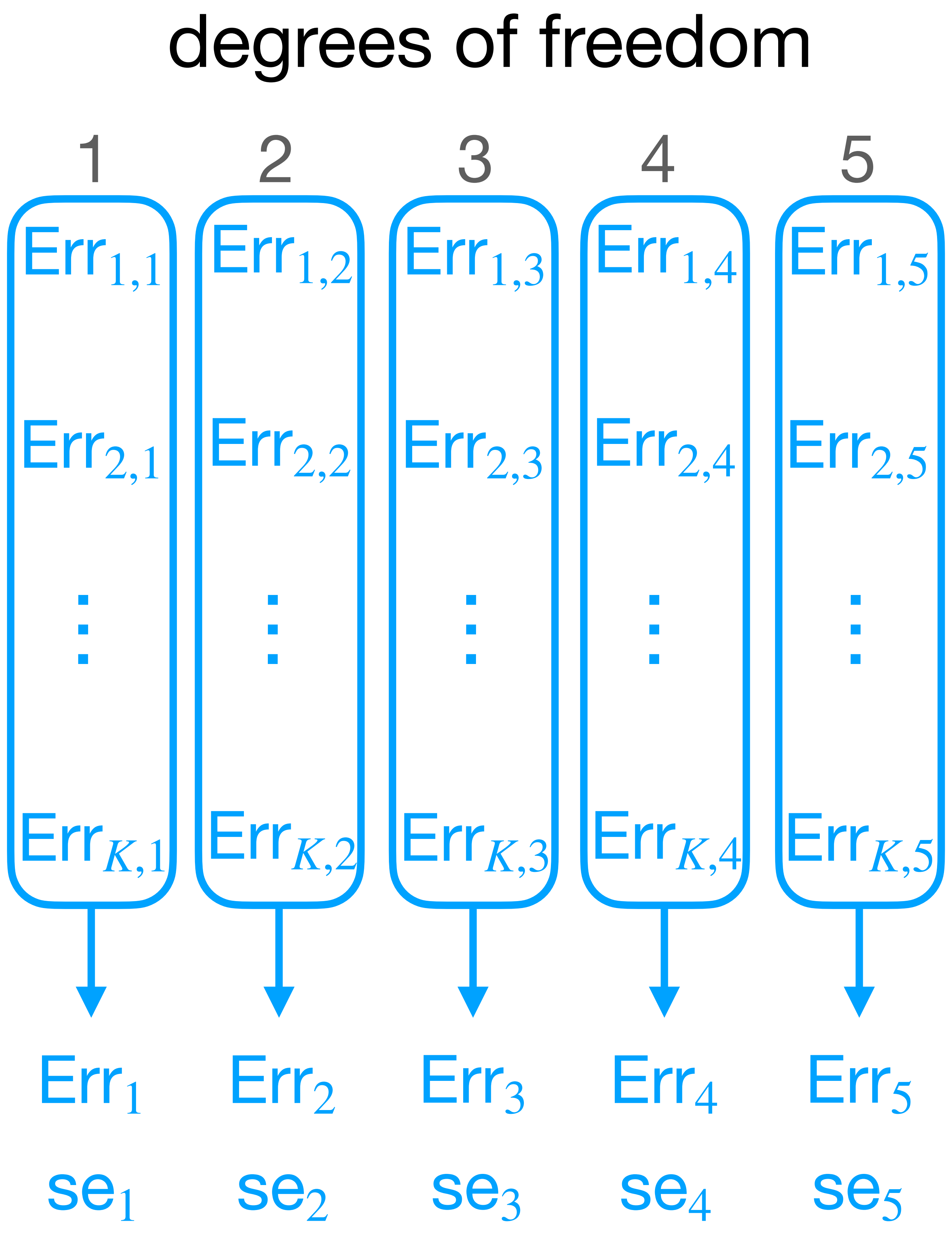
Cross-validation should be used with the same error metric as will be used in the final model evaluation.

Choosing the number of folds

- More folds means more computation
- Fewer folds means the training sets used for model selection are much smaller than the actual training set
- In practice, $K = 5$ or $K = 10$ are common choices

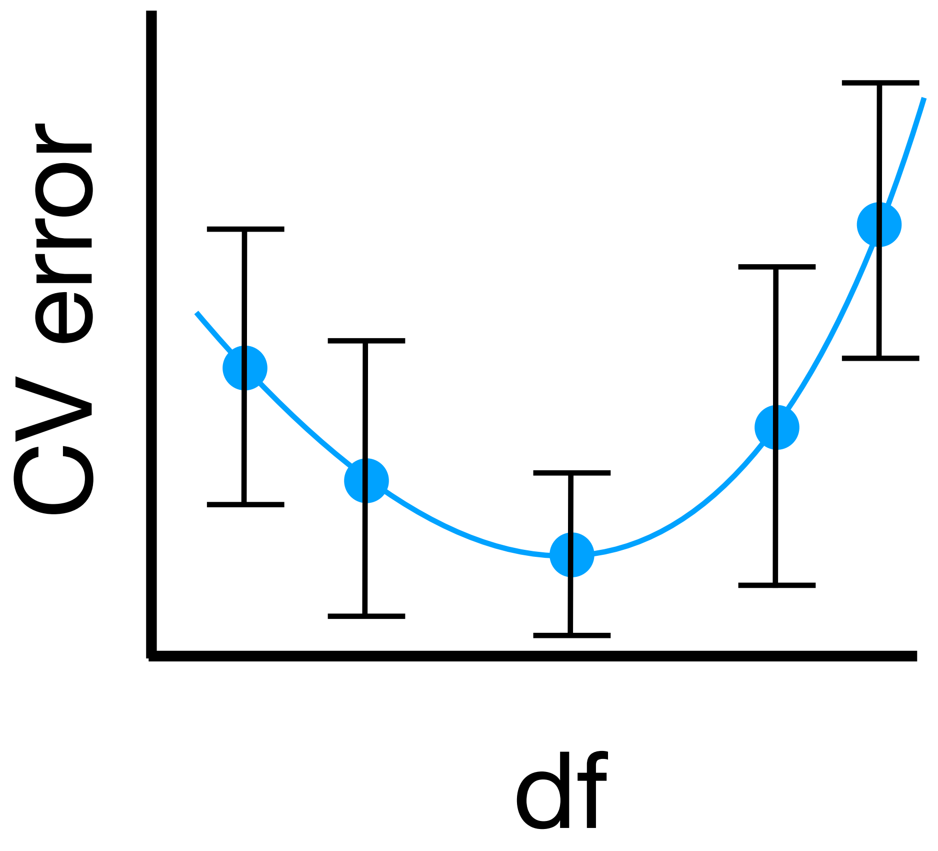
Really never use anything besides 5 or 10

Cross-validation standard error



degrees of freedom

1	2	3	4	5
$\text{Err}_{1,1}$	$\text{Err}_{1,2}$	$\text{Err}_{1,3}$	$\text{Err}_{1,4}$	$\text{Err}_{1,5}$
$\text{Err}_{2,1}$	$\text{Err}_{2,2}$	$\text{Err}_{2,3}$	$\text{Err}_{2,4}$	$\text{Err}_{2,5}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\text{Err}_{K,1}$	$\text{Err}_{K,2}$	$\text{Err}_{K,3}$	$\text{Err}_{K,4}$	$\text{Err}_{K,5}$
$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$
Err_1	Err_2	Err_3	Err_4	Err_5
se_1	se_2	se_3	se_4	se_5

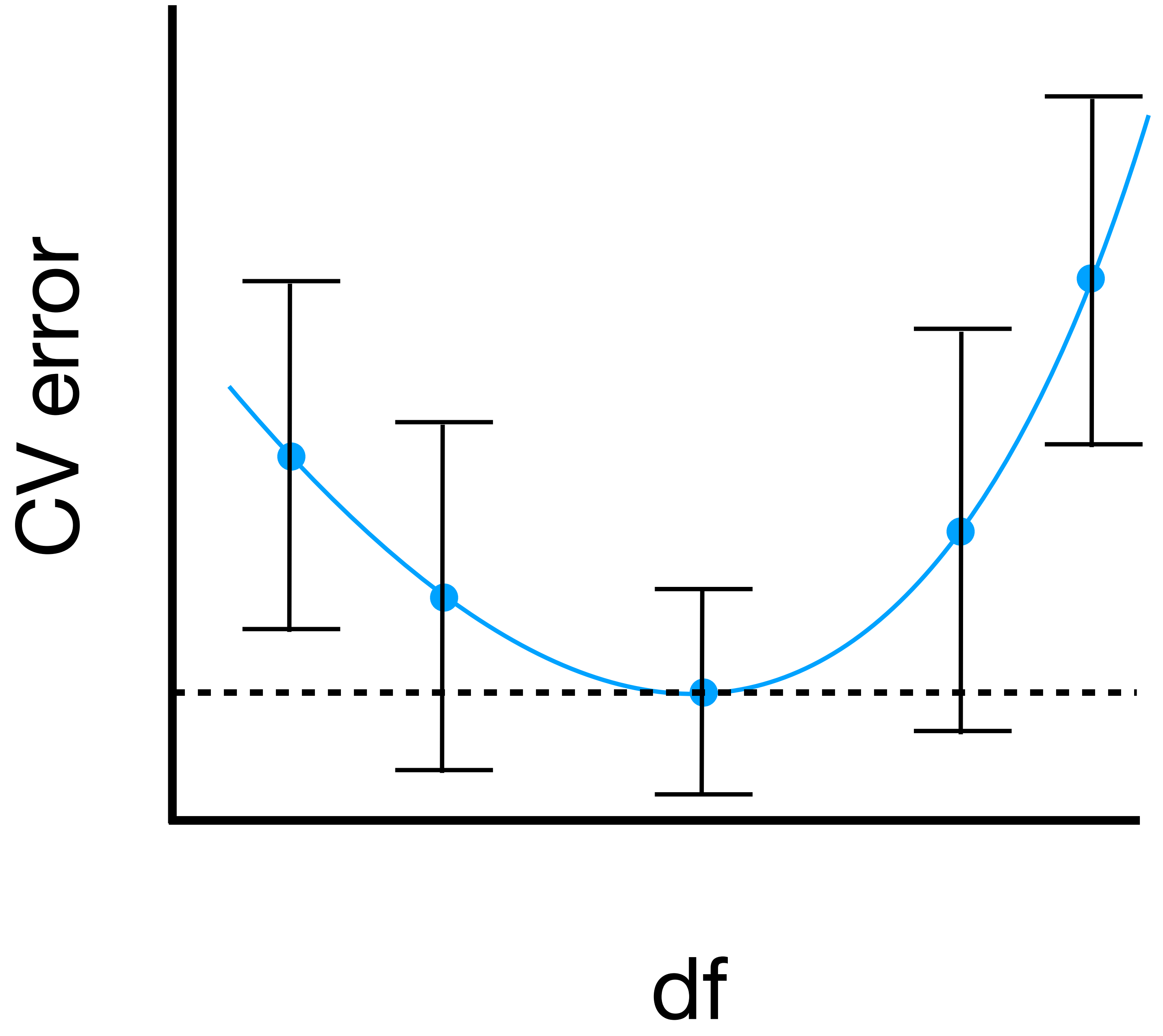


$$\text{se}_{\text{df}} = \frac{1}{\sqrt{K}} \times \text{s.d.}(\text{Err}_{1,\text{df}}, \ldots, \text{Err}_{K,\text{df}})$$

One standard error rule

Occam's razor:

Select the smallest model for which the CV error is within one standard error of the lowest point on the curve.



Lecture 4: Classification

A patient comes into the emergency room with stroke symptoms. Based on her CT scan, is the stroke ischemic or hemorrhagic?

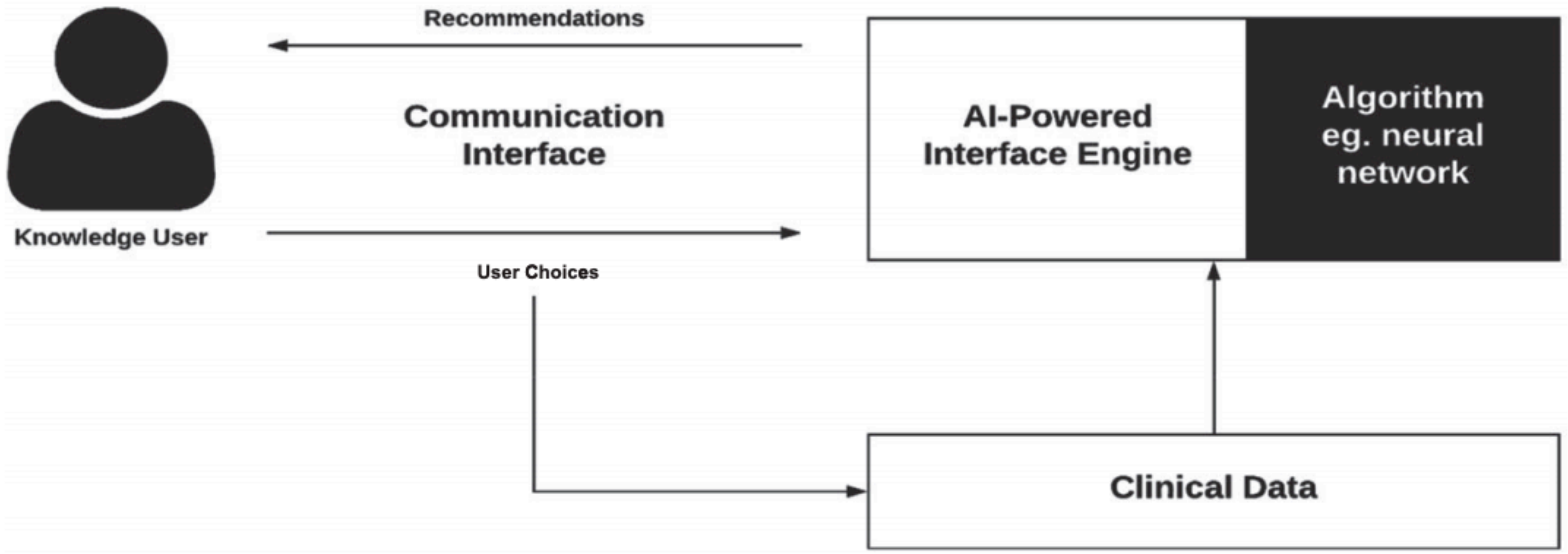


Image source: Sutton et al. 2020 (npj Digit. Med.)

This is a binary classification problem: $Y \in \{0,1\}$.

Given features $X = (X_1, \ldots, X_p)$, the goal is to guess a response $\widehat{Y} = \hat{f}(X)$ that is close to the true response, i.e. $\widehat{Y} \approx Y$. Measure of success is usually the

$$\text{test misclassification error} = \frac{1}{N}\sum_{i=1}^{N} I(Y_i^{\text{test}} \neq \hat{f}(X_i^{\text{test}})).$$

Classification via probability estimation

Suppose that the true relationship between Y and X is

$$\mathbb{P}[Y = 1 \,|\, X] = p(X), \quad \text{for some function } p.$$

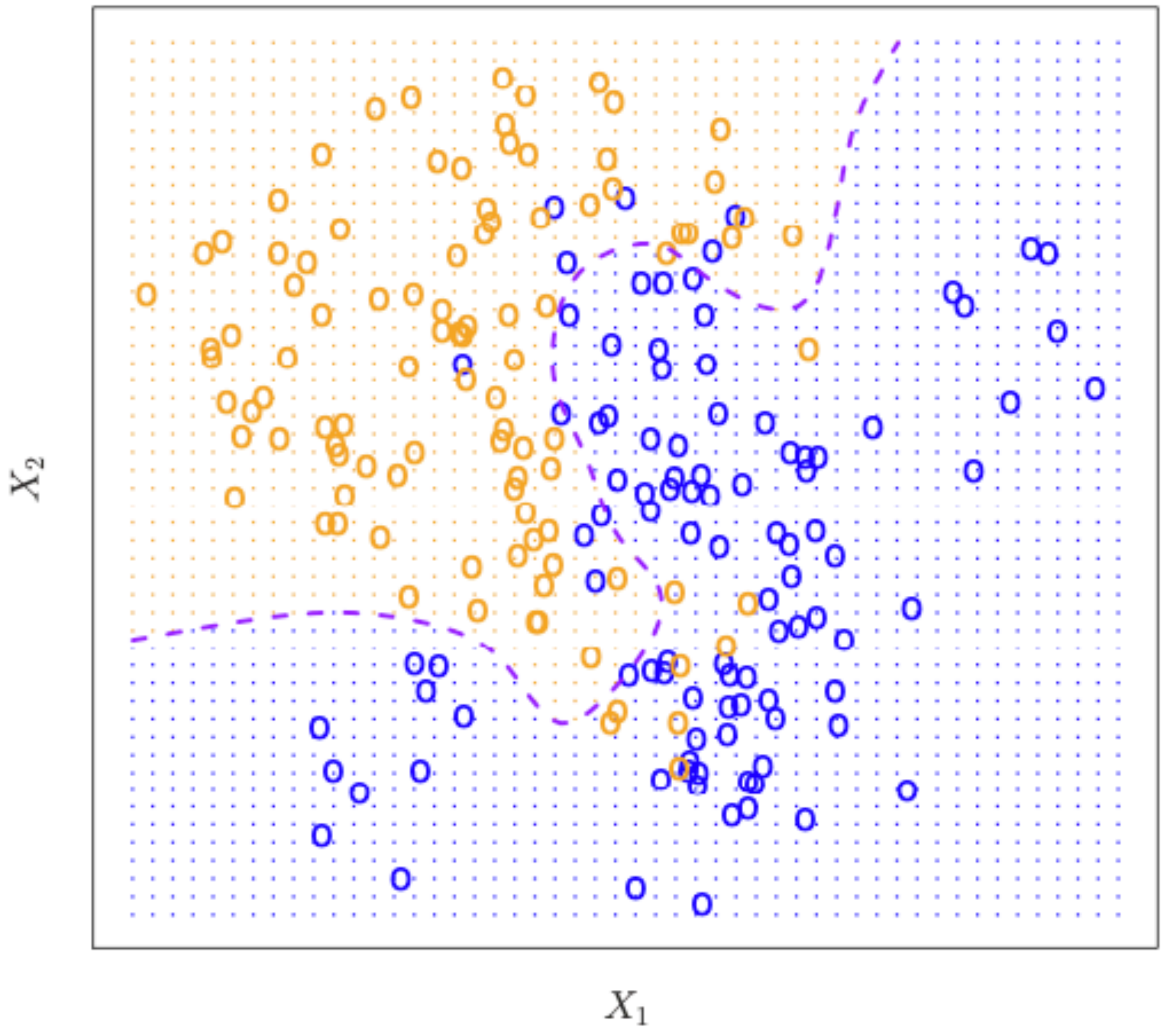
Then, the optimal classifier (called the Bayes classifier) is

$$\hat{f}^{\text{Bayes}}(X) = \begin{cases} 1, & \text{if } p(X) \geq 0.5; \\ 0 & \text{if } p(X) < 0.5. \end{cases}$$

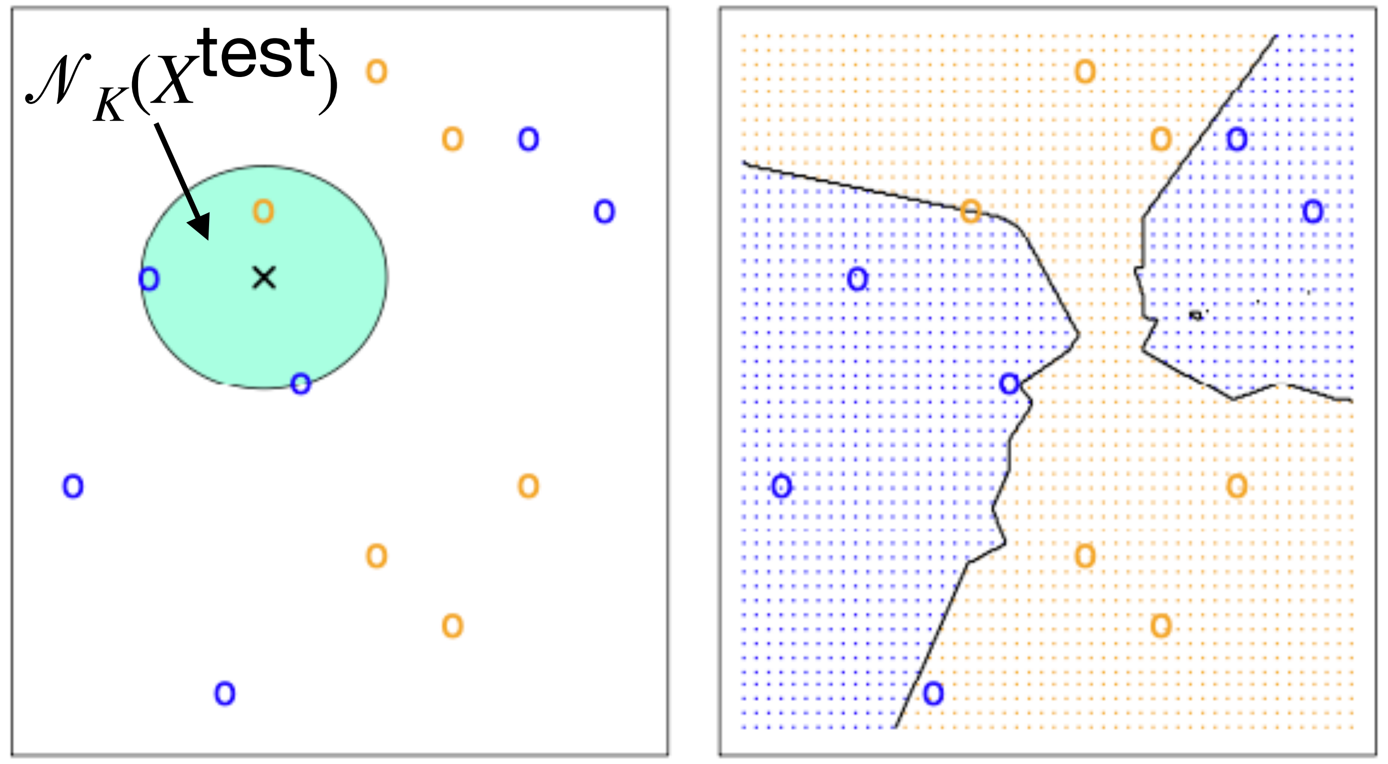
Classifiers usually build an approximation $\widehat{p}(X) \approx \mathbb{P}[Y = 1 \,|\, X]$, and define

$$\hat{f}(X) = \begin{cases} 1, & \text{if } \widehat{p}(X) \geq 0.5; \\ 0 & \text{if } \widehat{p}(X) < 0.5. \end{cases}$$

Example: K-nearest neighbors

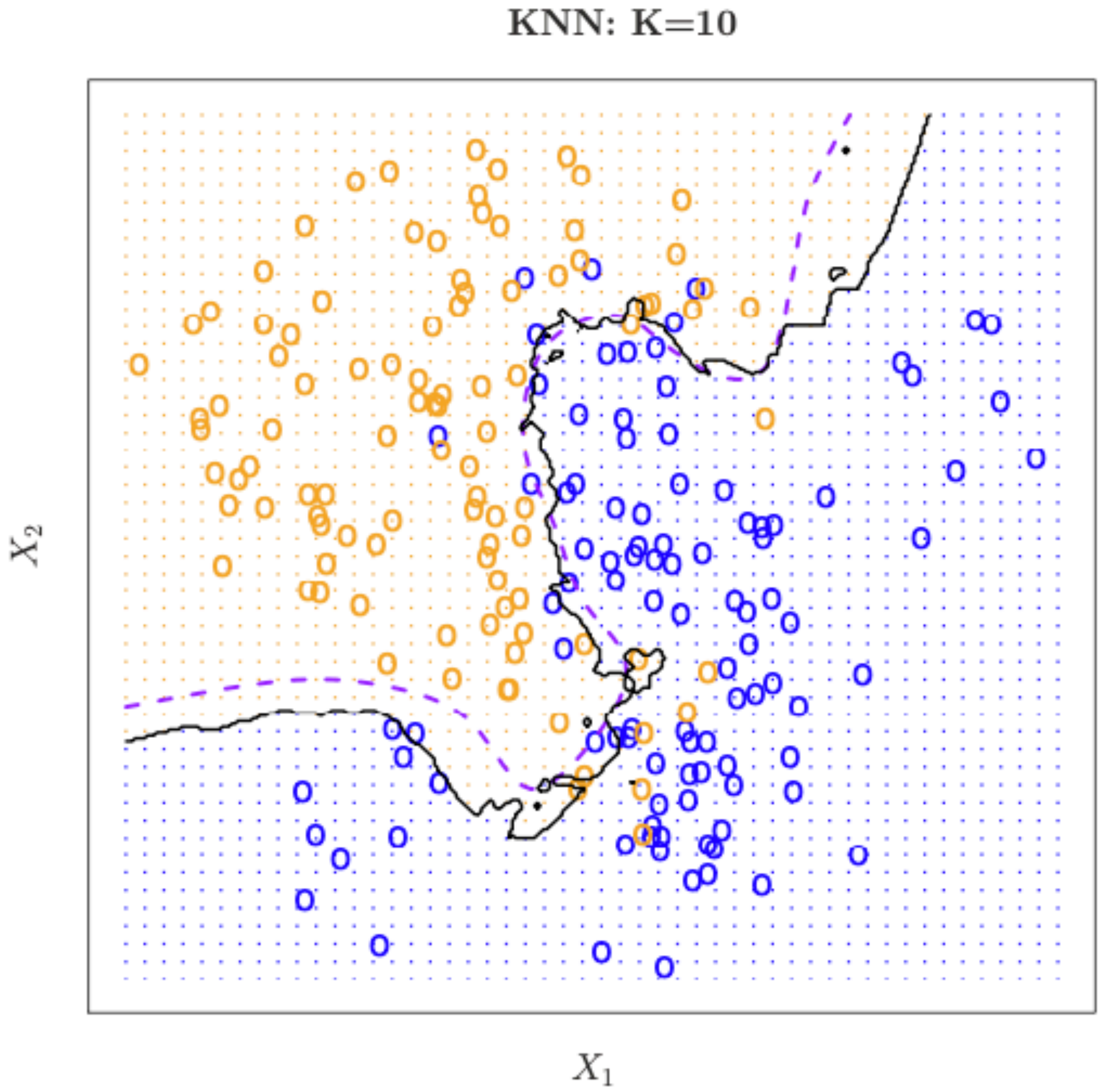


Simulated binary classification data.
Bayes classifier in purple.
E.g., color = stroke type, (X_1, X_2) = CT image.



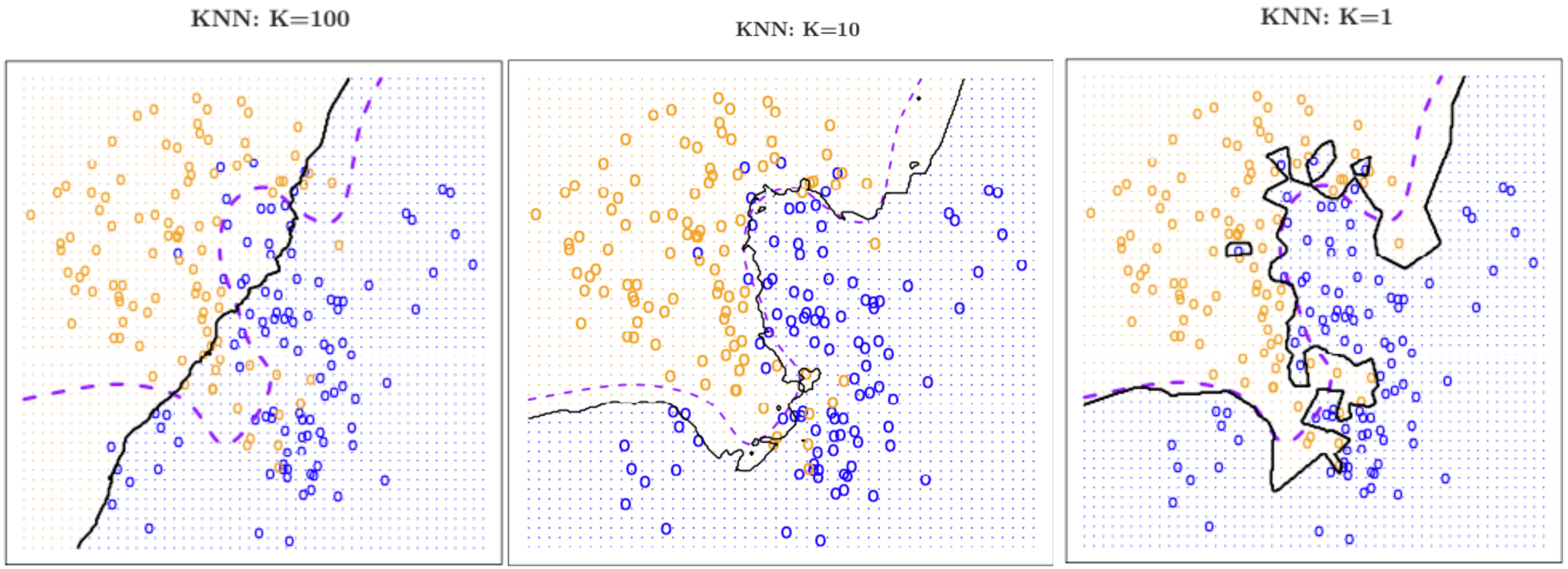
KNN illustration: Classify a test point based on majority vote among 3 nearest neighbors.

$$\hat{p}(X^{\text{test}}) = \frac{1}{K} \sum_{i \in \mathcal{N}_K} I(X_i^{\text{train}} = 1)\,.$$



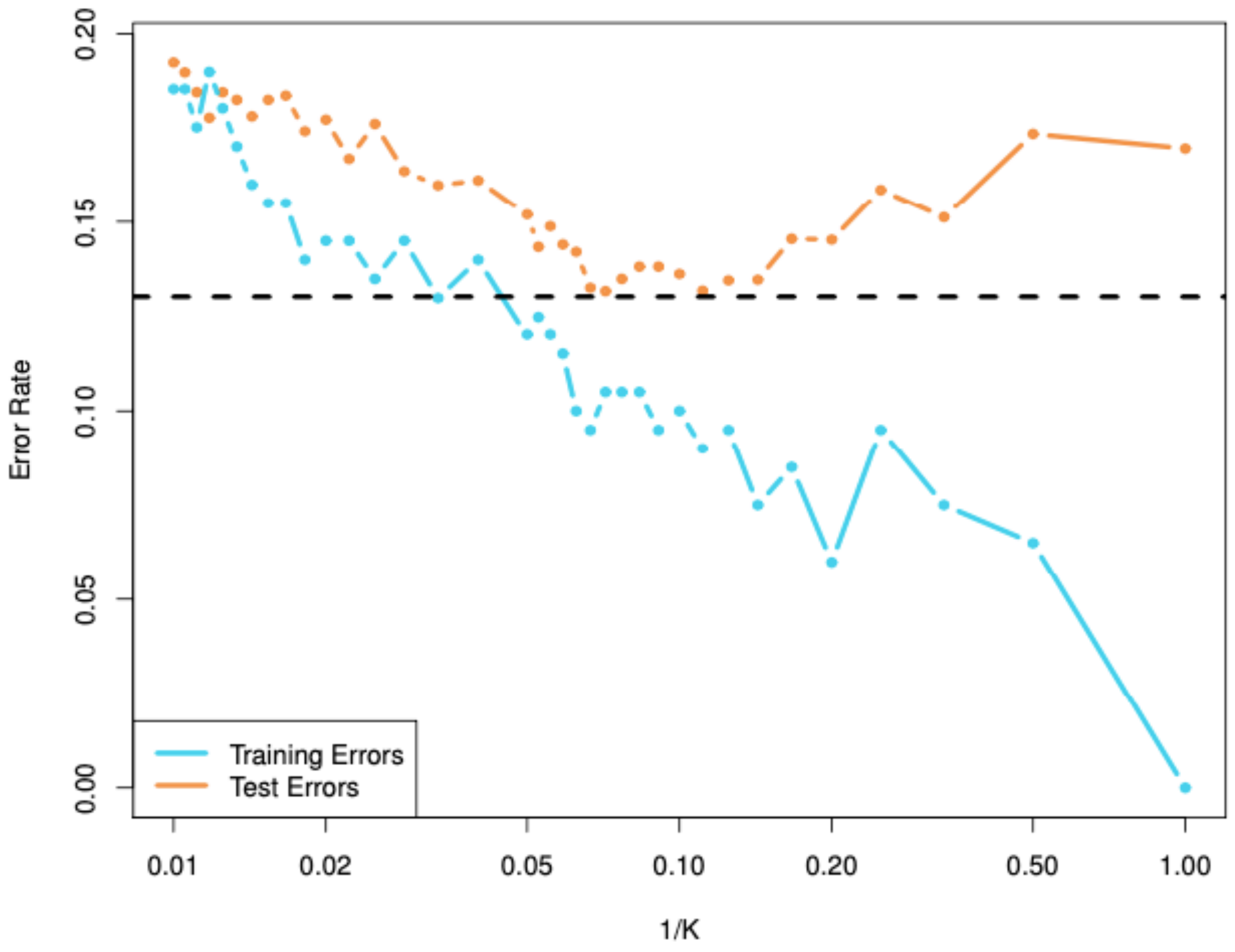
Applying KNN with K = 10 to simulated data.

Model complexity and misclassification error


KNN: K=100

KNN: K=10

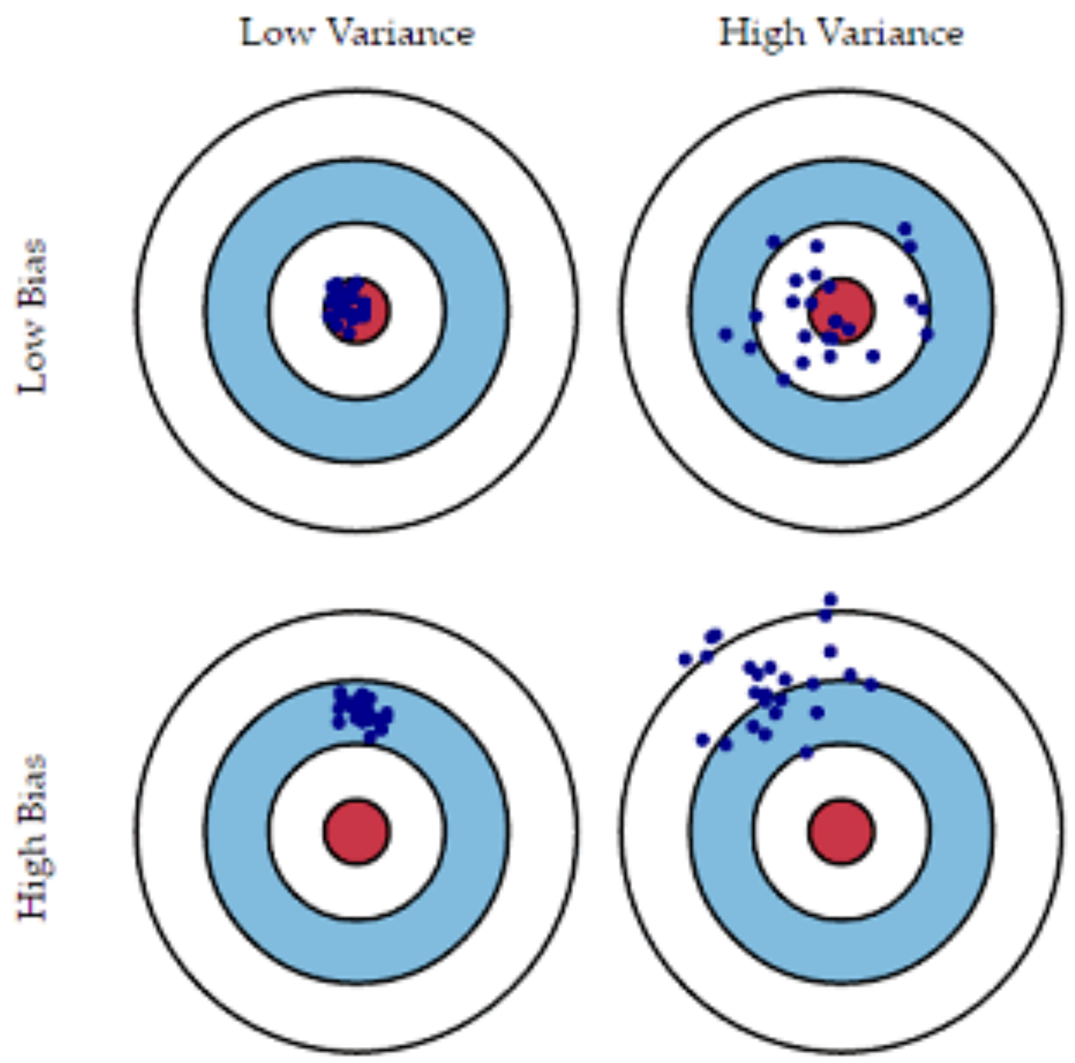
KNN: K=1



Same Goldilocks principle as in regression case:

- Too little complexity: Can’t capture the true trend in the data.
- Too much complexity: Too sensitive to noise in the training data (overfitting).

Bias-variance tradeoff



Mathematically: Applies only to continuous response variables and MSE.

Intuitively: Applies to any prediction problem, including classification.

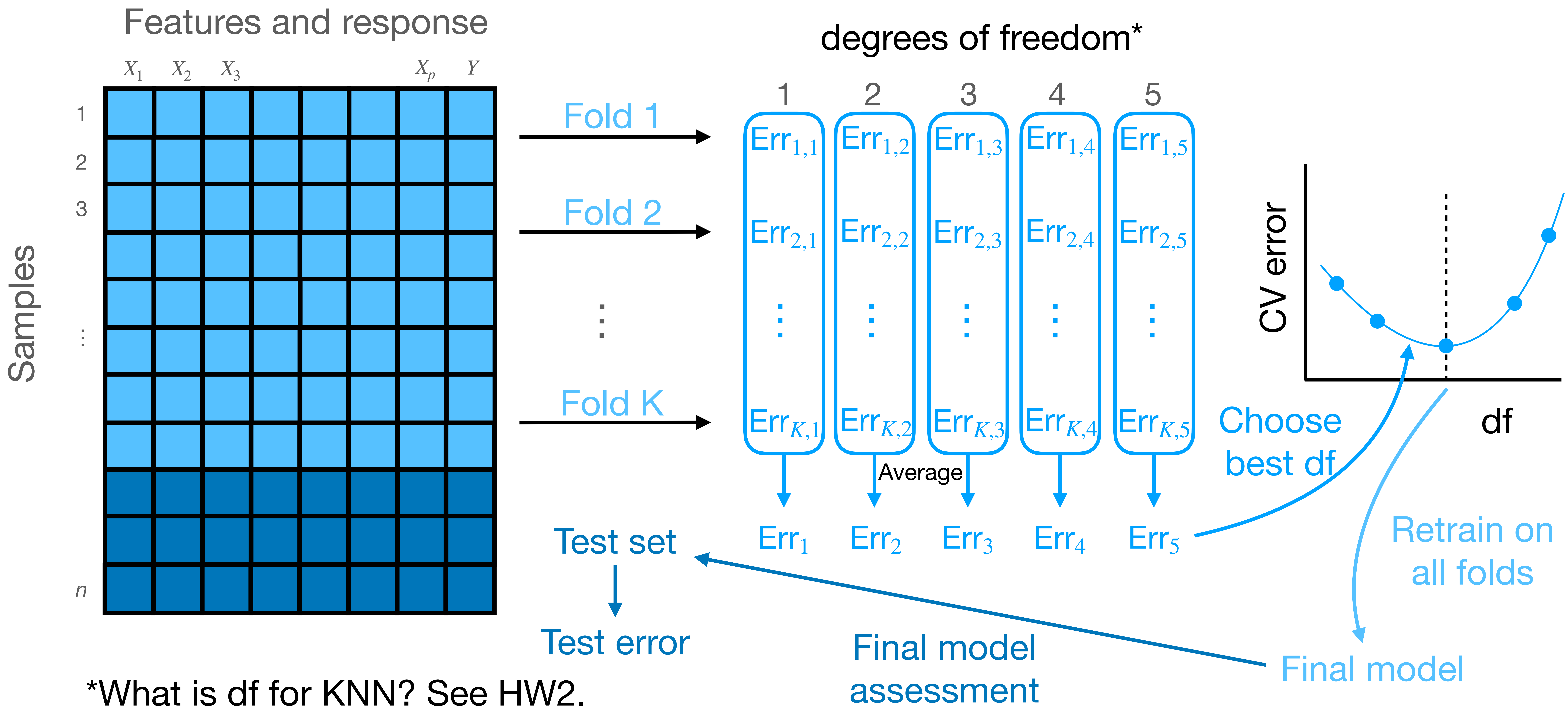
For the estimate $\widehat{p}(X)$

- Bias: $\mathbb{E}[\widehat{p}(X)] - p(X)$ ⟶
- Variance: $\text{Var}[\widehat{p}(X)]$ ⟶

For classifying $\widehat{Y} = I(p(X) \geq 0.5)$

- Bias: Predict wrong class on average, to the extent $\widehat{p}$ on wrong side of 0.5
- Variance: Prediction varies with training set, to the extent $\widehat{p}$ fluctuates above or below 0.5
- Irreducible error (AKA Bayes error): Error incurred by Bayes classifier because $0 < \mathbb{P}[Y = 1 \,|\, X] < 1$.

Cross-validation based on misclassification error
(otherwise same as before)



Features and response

X_1 X_2 X_3 X_p Y

Samples

1 2 3 ⋮ n

Fold 1

Fold 2

⋮

Fold K

degrees of freedom*

1	2	3	4	5
$\text{Err}_{1,1}$	$\text{Err}_{1,2}$	$\text{Err}_{1,3}$	$\text{Err}_{1,4}$	$\text{Err}_{1,5}$
$\text{Err}_{2,1}$	$\text{Err}_{2,2}$	$\text{Err}_{2,3}$	$\text{Err}_{2,4}$	$\text{Err}_{2,5}$
⋮	⋮	⋮	⋮	⋮
$\text{Err}_{K,1}$	$\text{Err}_{K,2}$	$\text{Err}_{K,3}$	$\text{Err}_{K,4}$	$\text{Err}_{K,5}$

Average

Err_1 Err_2 Err_3 Err_4 Err_5

Choose best df

Retrain on all folds

Final model

Final model assessment

Test set

Test error

*What is df for KNN? See HW2.

Class imbalance

In many real-world classification problems, one class (say $Y = 1$) is significantly less frequent than the other. For example:

- Credit card transaction classification: normal versus fraudulent
- COVID testing: negative versus positive

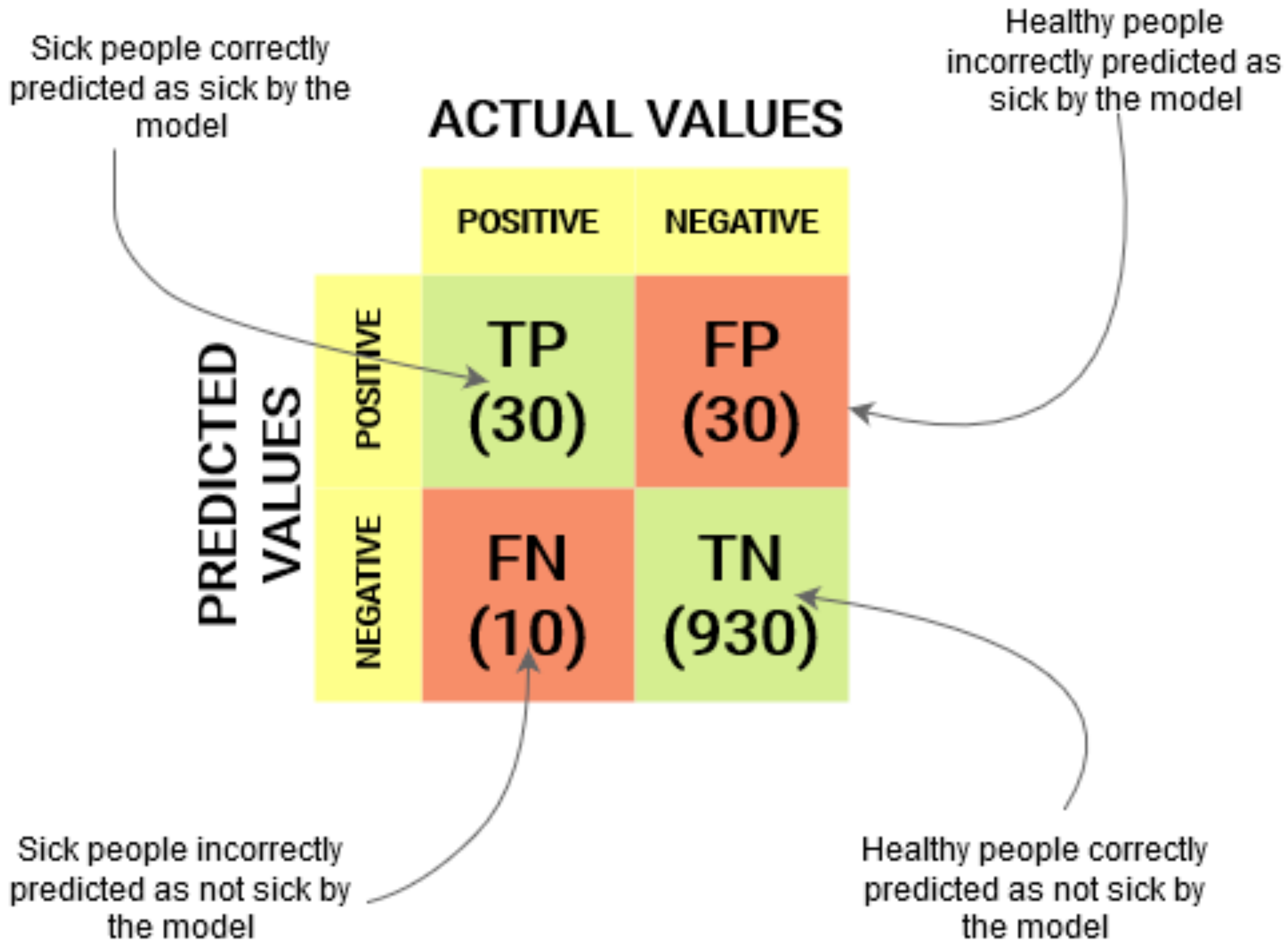
Often in these cases, the costs of misclassification are also asymmetric, i.e. the misclassification error is not the right metric.

Let’s say 1% of credit card transactions are fraudulent. Then, the classifier that always predicts “not fraudulent” will have a misclassification error of only 1%.

Cross-validation based on misclassification error leads to overly simple models that ignore the minority class.

A more wholistic picture of a classifier

Confusion matrix



Sick people correctly predicted as sick by the model

Healthy people incorrectly predicted as sick by the model

		ACTUAL VALUES	
		POSITIVE	NEGATIVE
PREDICTED VALUES	POSITIVE	TP (30)	FP (30)
	NEGATIVE	FN (10)	TN (930)

Sick people incorrectly predicted as not sick by the model

Healthy people correctly predicted as not sick by the model

Image source: https://www.analyticsvidhya.com/blog/2020/04/confusion-matrix-machine-learning/

Summaries of confusion matrix

$$\text{False positive rate} = \frac{\text{number false positives}}{\text{total actual negatives}}$$

$$\text{False negative rate} = \frac{\text{number false negatives}}{\text{total actual positives}}$$

Thinking about misclassification costs

The cost of a false negative might be much greater than a false positive:

- Undetected fraudulent credit card transaction (false negative)
  → drained bank account. Cost: C_{FN} = $10,000.
- False alarm of fraud (false positive)
  → annoying text message and/or replaced credit card. Cost: C_{FP} = $10.

Weighted misclassification error:

$$\frac{1}{N}\sum_{i=1}^{N} C_{\mathsf{FP}} \cdot I(\widehat{Y}_i^{\mathsf{test}} = 1, Y_i^{\mathsf{test}} = 0) + C_{\mathsf{FN}} \cdot I(\widehat{Y}_i^{\mathsf{test}} = 0, Y_i^{\mathsf{test}} = 1).$$

Building misclassification costs into training

There may be two issues with

$$\hat{f}(X) = \begin{cases} 1, & \text{if } \widehat{p}(X) \geq 0.5; \\ 0 & \text{if } \widehat{p}(X) < 0.5. \end{cases}$$

1. The minority class is poorly captured by the probability model $\widehat{p}(X)$.
2. The probability threshold of 0.5 is suboptimal.

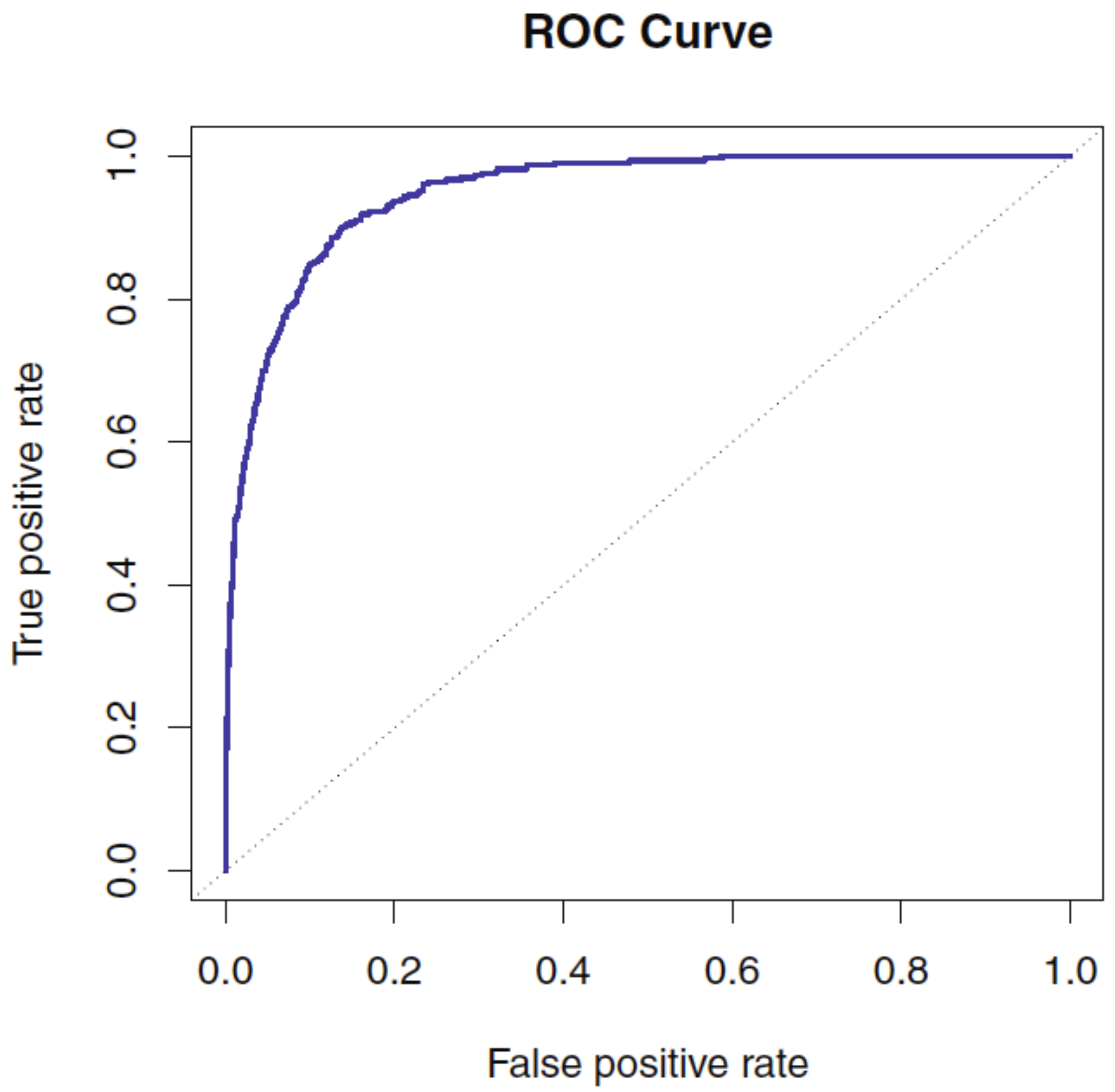
To fix these, a variety of strategies can be employed:

- Downsample the majority class by a factor $C_{\text{FP}}/C_{\text{FN}}$.
- Choose the probability threshold $C_{\text{FP}}/(C_{\text{FN}} + C_{\text{FP}})$ instead of 0.5.
- Build cost directly into the objective function when training.

Can geta better sample by accounting for actual costs in probability threshold

ROC curve

- The ROC curve plots the true positive rate (one minus the false negative rate) versus the false positive rate, as the threshold is varied from 0 to 1.
- We want the curve to get as close to the upper left-hand corner as possible.
- Area under the curve (AUC) is another measure of the quality of a classifier.



Unit 2 Summary

- Predictive models are evaluated based on their test error, which can be decomposed into bias, variance, and irreducible error (bias-variance tradeoff).

- Model complexity plays a crucial role in test error; models that are not complex enough suffer due to bias, models that are too complex suffer due to variance.

- For splines (and linear regression in general), model complexity captured by the number of parameters being fit.

- Cross-validation is the standard way of tuning model complexity; the trick is to always separate the data used for training from that used for validation/testing.

- Many of these phenomena carry over from regression to classification, but classification brings a few new challenges, like class imbalance.