Machine Learning with Python

MTH786U/P 2022/23

Lecture 4: The model selection problem

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Model selection

Recall ridge regression:

Model selection

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$$\mathbf{w}_\alpha = \arg\min_{\mathbf{w}} \left\{ \frac{1}{2s} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \frac{\alpha}{2} \|\mathbf{w}\|^2 \right\}$$

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How do we choose hyperparameters?

Selection of hyperparameters is known as the *model selection* problem

Probabilistic setup

Assume underlying distribution $\mathscr{D}$

and that we sample from this distribution:

$$S := \left\{ (\mathbf{x}_i, \mathbf{y}_i) \text{ iid } \sim \mathscr{D} \right\}_{i=1}^{s}$$

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Based on these samples the ridge regression model computes the 'best' (linear) weight function for fixed regularisation parameter α

$$f_S(x) := \langle \mathbf{x}, \mathbf{w}_\alpha \rangle \quad \text{for} \quad \mathbf{w}_\alpha = \arg\min_{\mathbf{w}} \left\{ \frac{1}{2s} \sum_{i=1}^{s} \left| \langle \mathbf{x}_i, \mathbf{w} \rangle - \mathbf{y}_i \right|^2 + \frac{\alpha}{2} \|\mathbf{w}\|^2 \right\}$$

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and $$\mathbb{E}_{\mathbf{x},\mathbf{y}}\left[\ell(\mathbf{y}, f(\mathbf{x}))\right] = \int_{(\mathbf{x},\mathbf{y})\in\mathscr{D}} \ell(\mathbf{y}, f(\mathbf{x}))\,\rho(\mathbf{x}, \mathbf{y})\,dxdy$$

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Hence, we cannot compute $E(f_S)$!

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It is therefore natural to compute the empirical risk

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This quantity is also known as the *training error*

Training error vs. expected error

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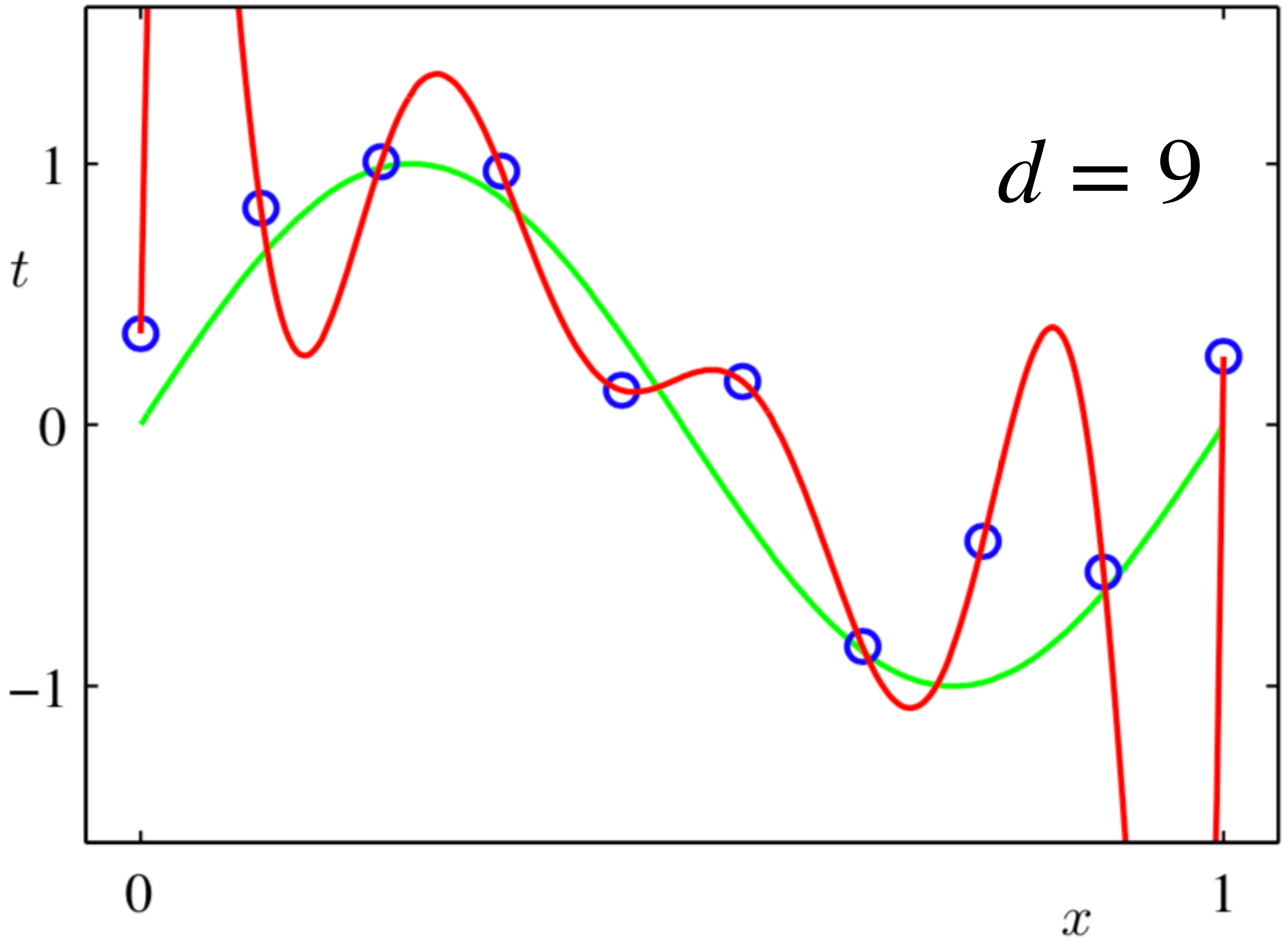
Training error is usually not representative for generalisation error, remember



From Bishop. Pattern Recognition & Machine Learning

Splitting the data

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Example: take original data and split into 80% training and 20 % validation data

Training error vs. validation error

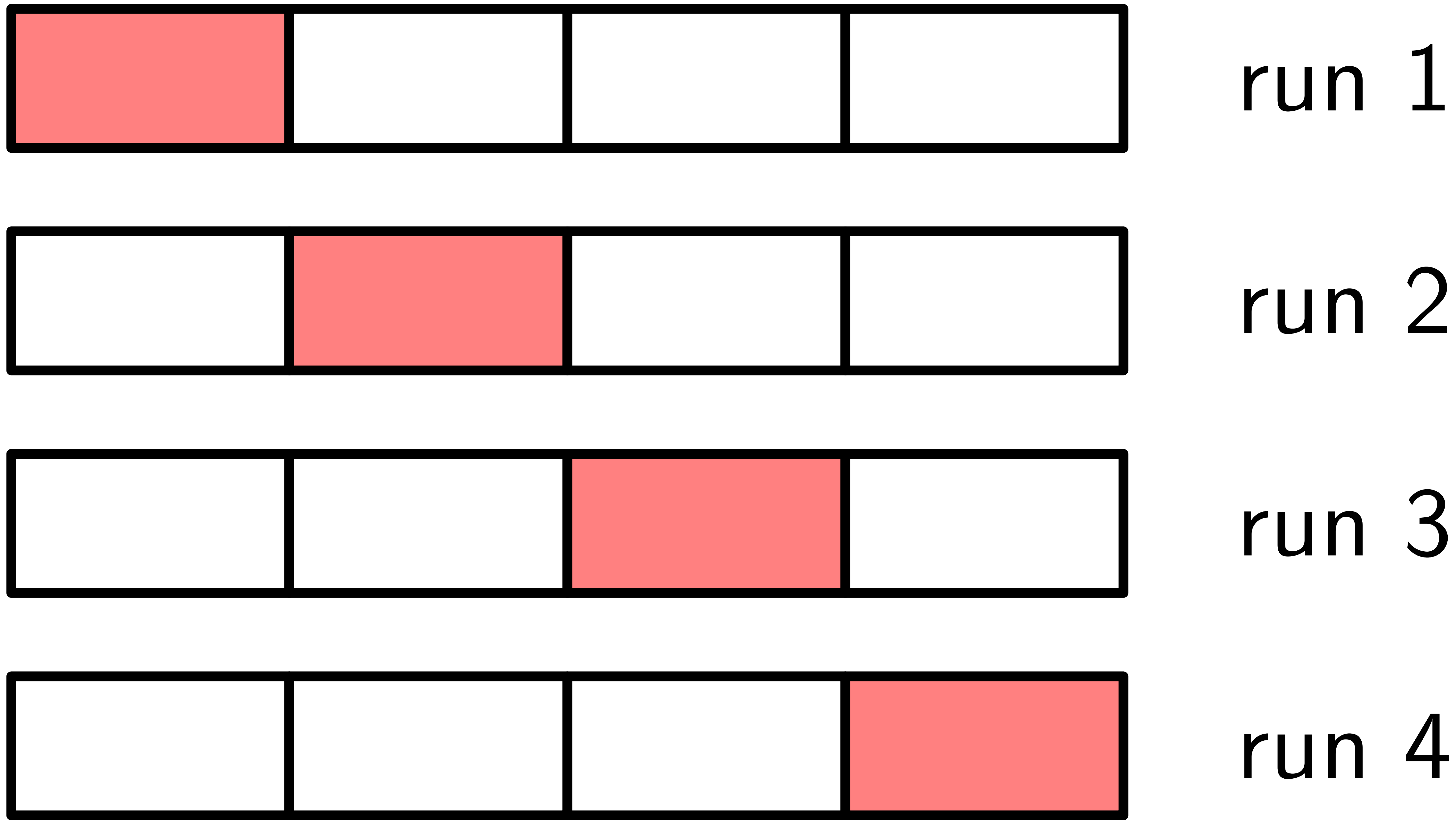
Training error: $$L_t(f_t) = \frac{1}{|S_t|} \sum_{(\mathbf{x}_i, \mathbf{y}_i) \in S_t} \ell(\mathbf{y}_i, f_t(\mathbf{x}_i))$$

Validation error: $$L_v(f_t) = \frac{1}{|S_v|} \sum_{(\mathbf{x}_i, \mathbf{y}_i) \in S_v} \ell(\mathbf{y}_i, f_t(\mathbf{x}_i))$$

where f_t is short-hand-notation for

$$f_t := f_{S_t}$$

Cross-validation



K-fold cross-validation

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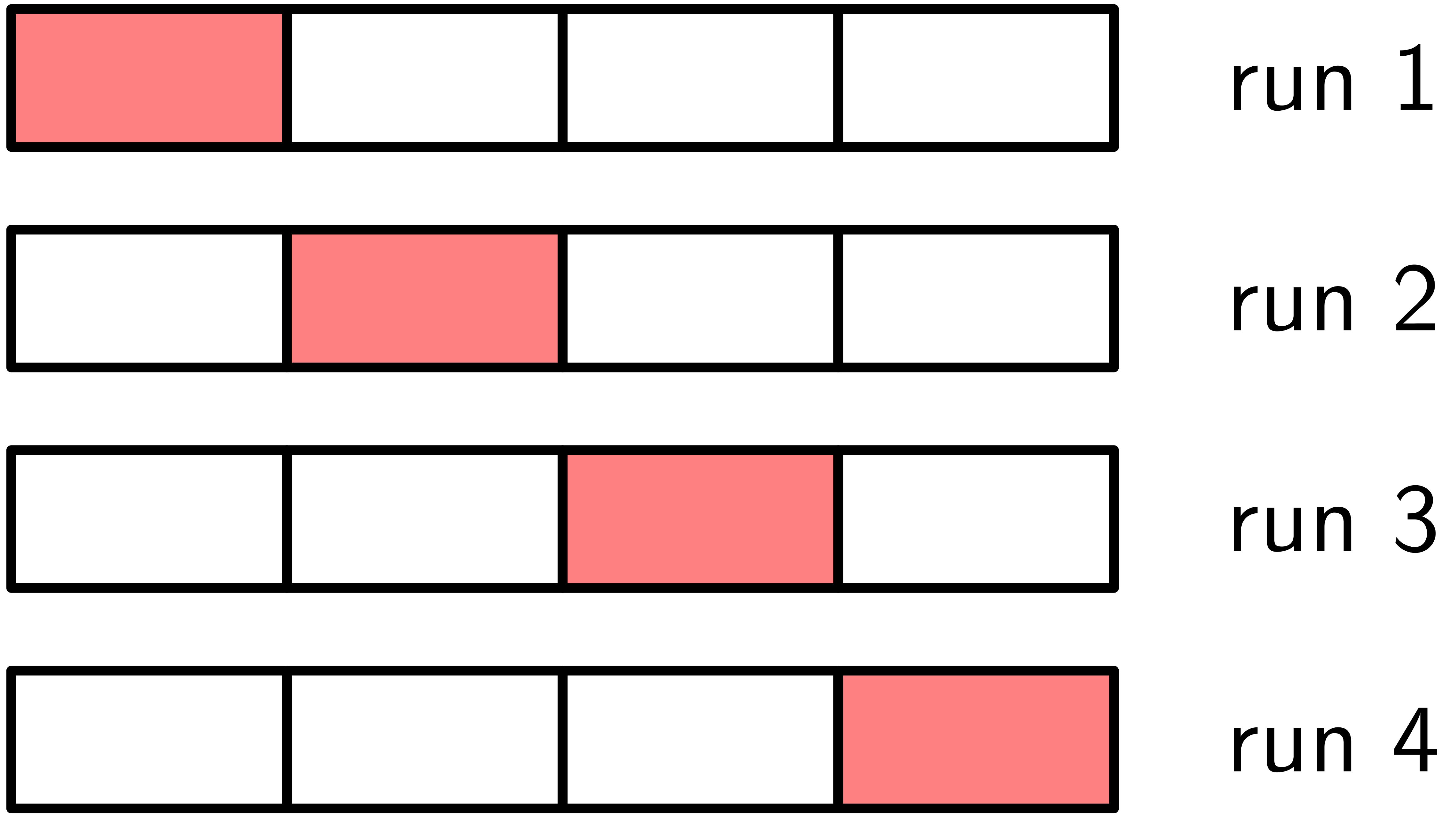

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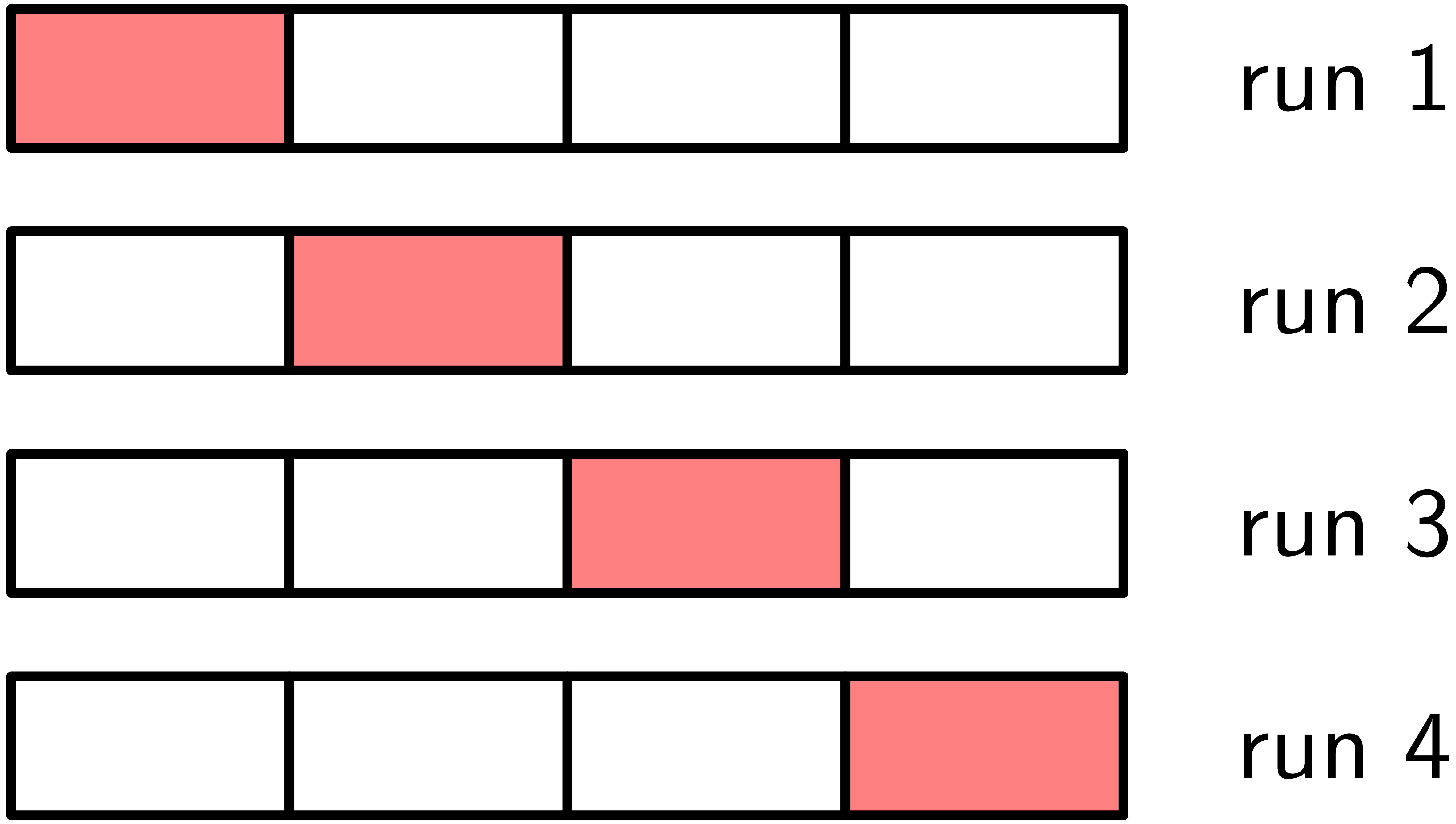

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K-fold cross-validation

- Randomly partition data into K groups
- Train K times, each time leaving 1 group for testing and $K-1$ for training

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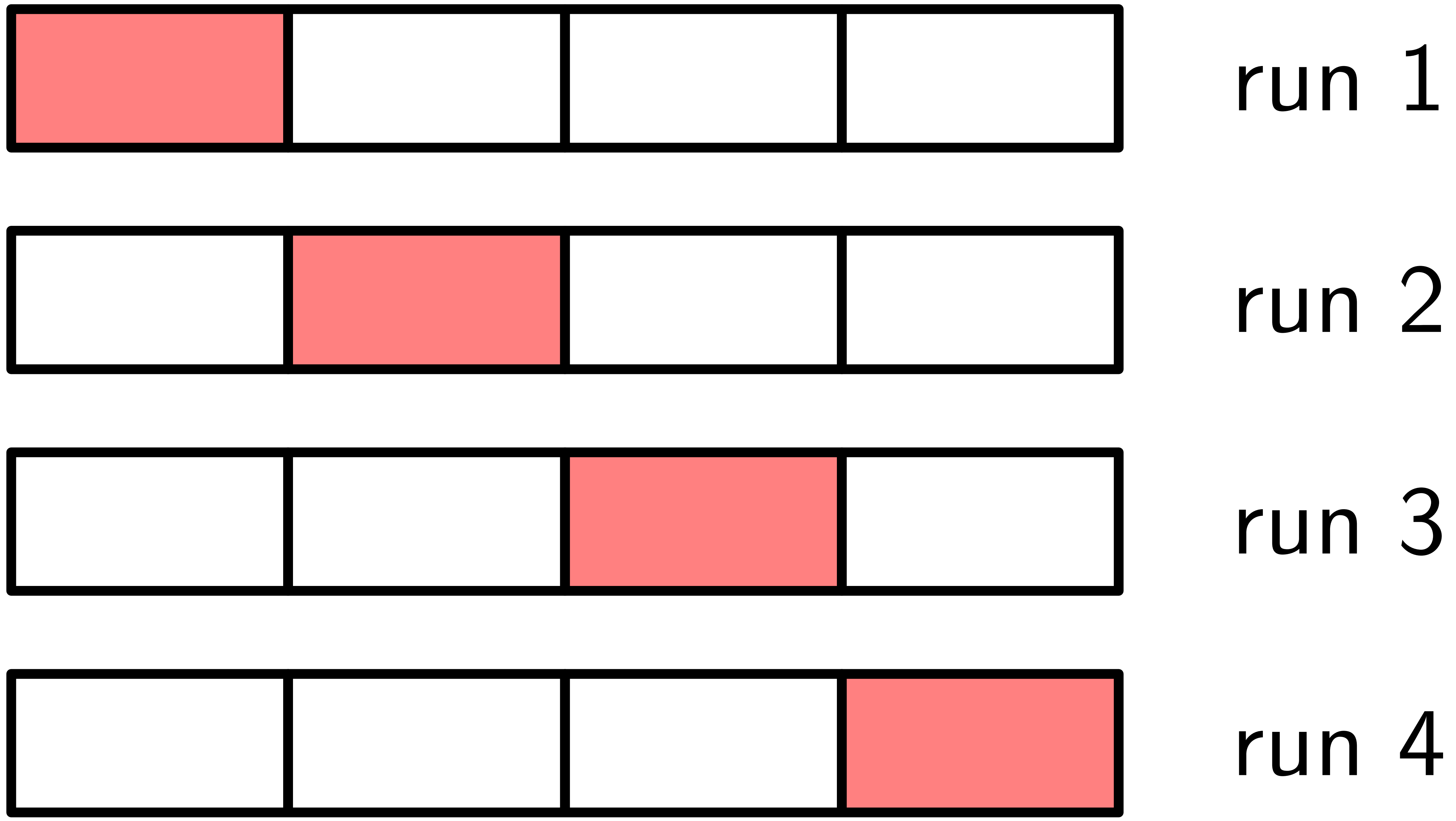

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K-fold cross-validation

- Randomly partition data into K groups
- Train K times, each time leaving 1 group for testing and $K-1$ for training
- Average the K results

The validation error

Central question that we need to address:

How do we choose hyper parameters in

$$f_t(\mathbf{x}) = \langle \phi(\mathbf{x}), \mathbf{w}_\alpha \rangle \text{ for } \mathbf{w}_\alpha = \arg\min_{\mathbf{w}} \left\{ \frac{1}{2s} \sum_{(\mathbf{x}_i, \mathbf{y}_i) \in S_t} \left| \langle \phi(\mathbf{x}_i), \mathbf{w} \rangle - \mathbf{y}_i \right|^2 + \frac{\alpha}{2} \|\mathbf{w}\|^2 \right\}$$

such that we minimise

$$L_v(f_t) = \frac{1}{|S_v|} \sum_{(\mathbf{x}_i, \mathbf{y}_i) \in S_v} \ell(\mathbf{y}_i, f_t(\mathbf{x}_i)) \qquad ?$$

The validation error

This is a bi-level optimisation problem:

$$(\hat{\alpha}, \hat{d}) = \arg\min_{\alpha,d} \left\{ L_v(f_t) = \frac{1}{|S_v|} \sum_{(\mathbf{x}_i, \mathbf{y}_i) \in S_v} \ell(\mathbf{y}_i, f_t(\mathbf{x}_i)) \right\}$$

subject to

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Lower-level problem

Important: given α and d we are guaranteed to find the best possible solution of the lower-level problem

How can we solve such a problem?

Grid search

The easiest of all optimisation algorithms is grid search:

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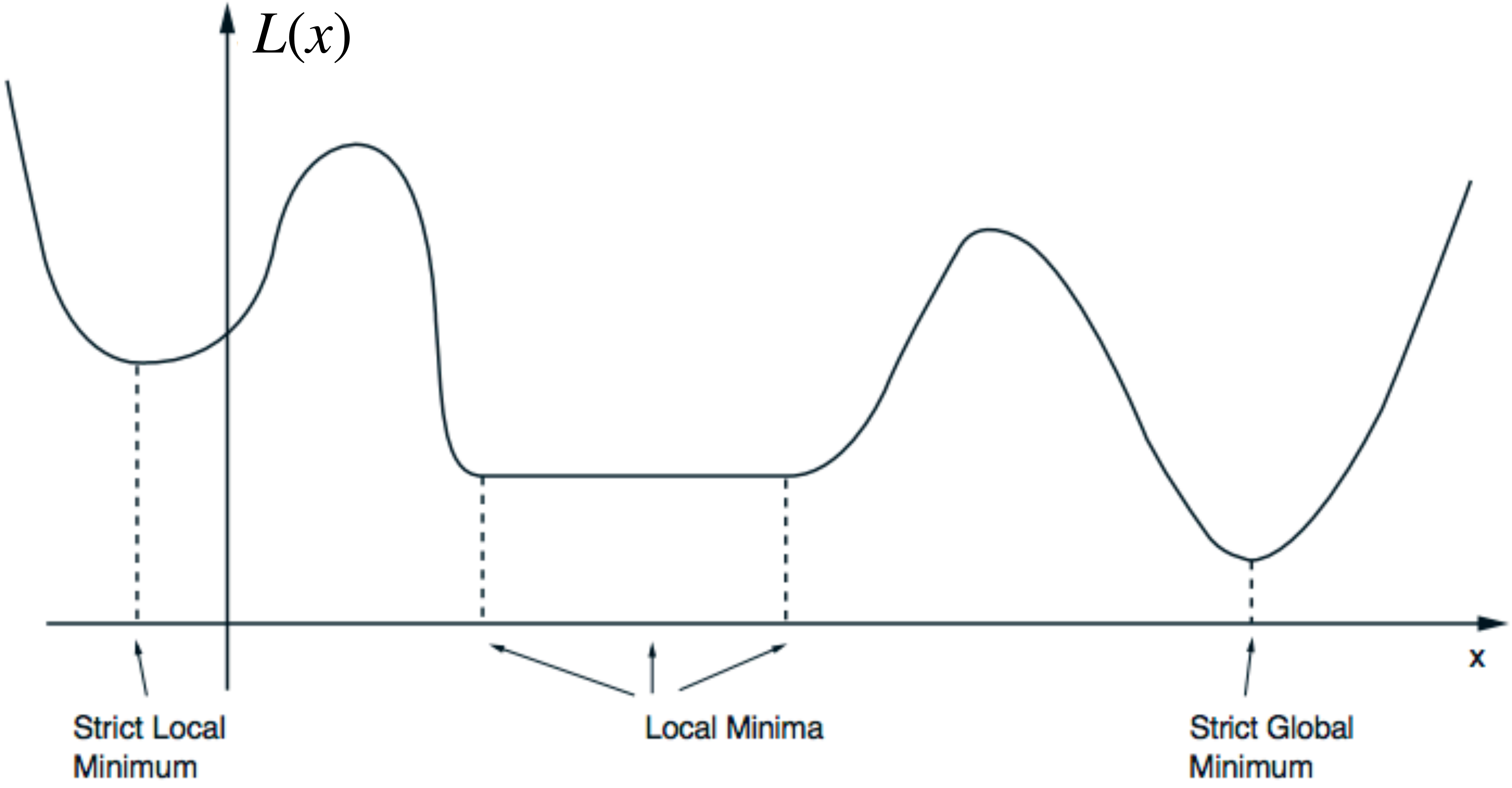
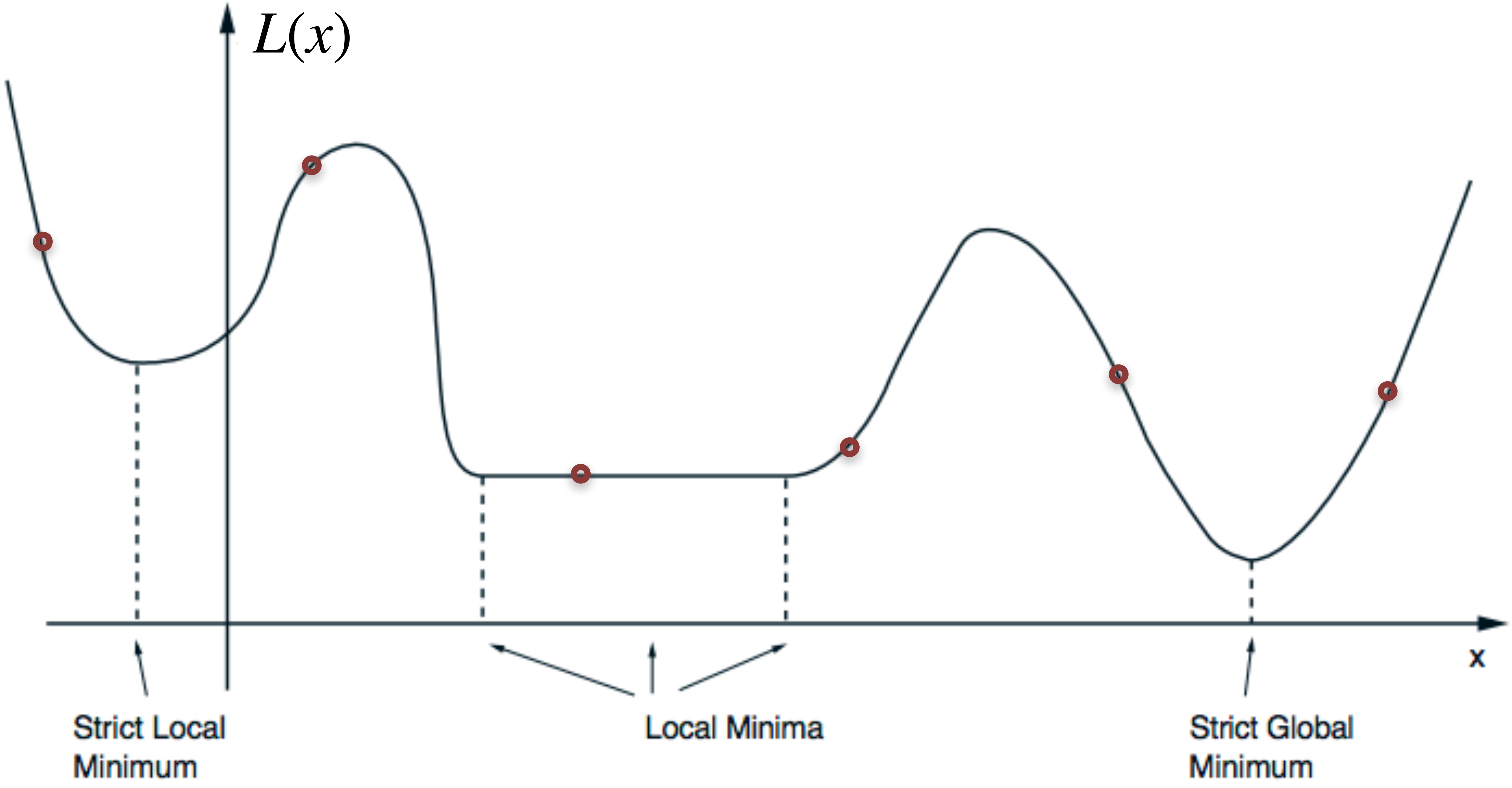
Evaluate a function L at points on a grid and record smallest value

Grid search



From Bertsekas, Nonlinear programming

Grid search



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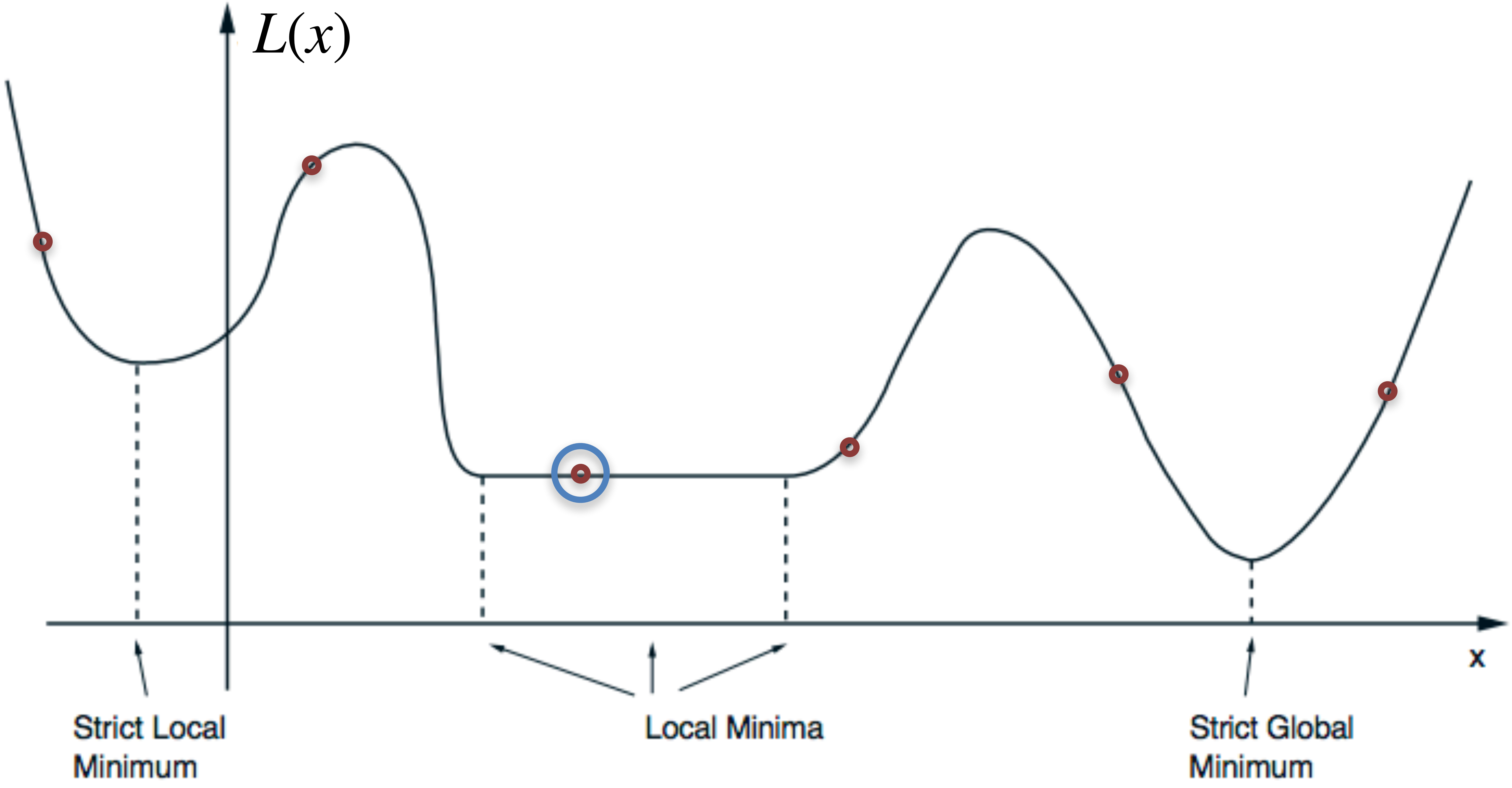

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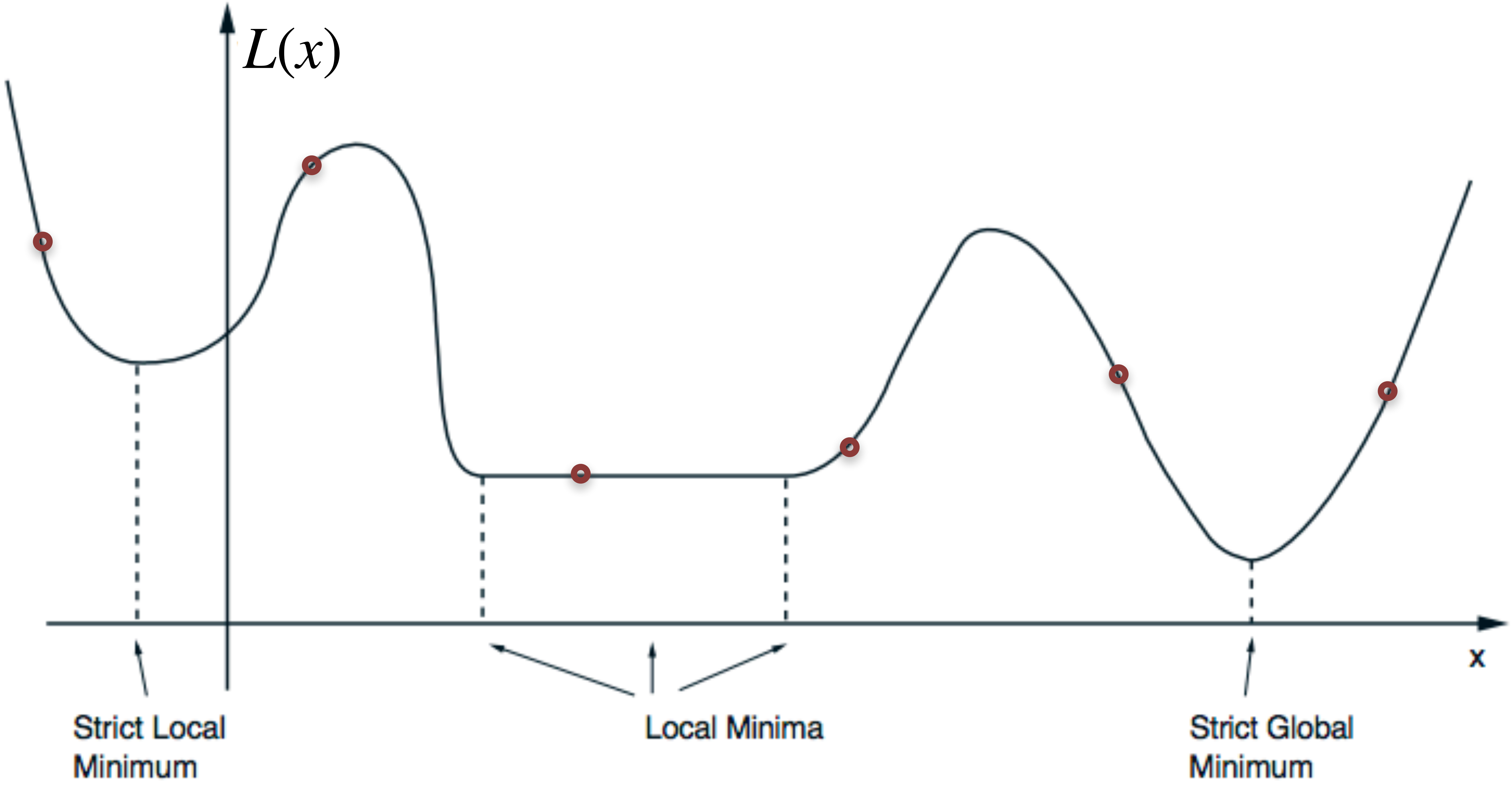
Sample L at n points $\mathbf{p} \in \mathbb{R}^m$ in each dimension $\implies$ m^n evaluations of L

Other disadvantage: no guarantee that we end up close to a minimum!



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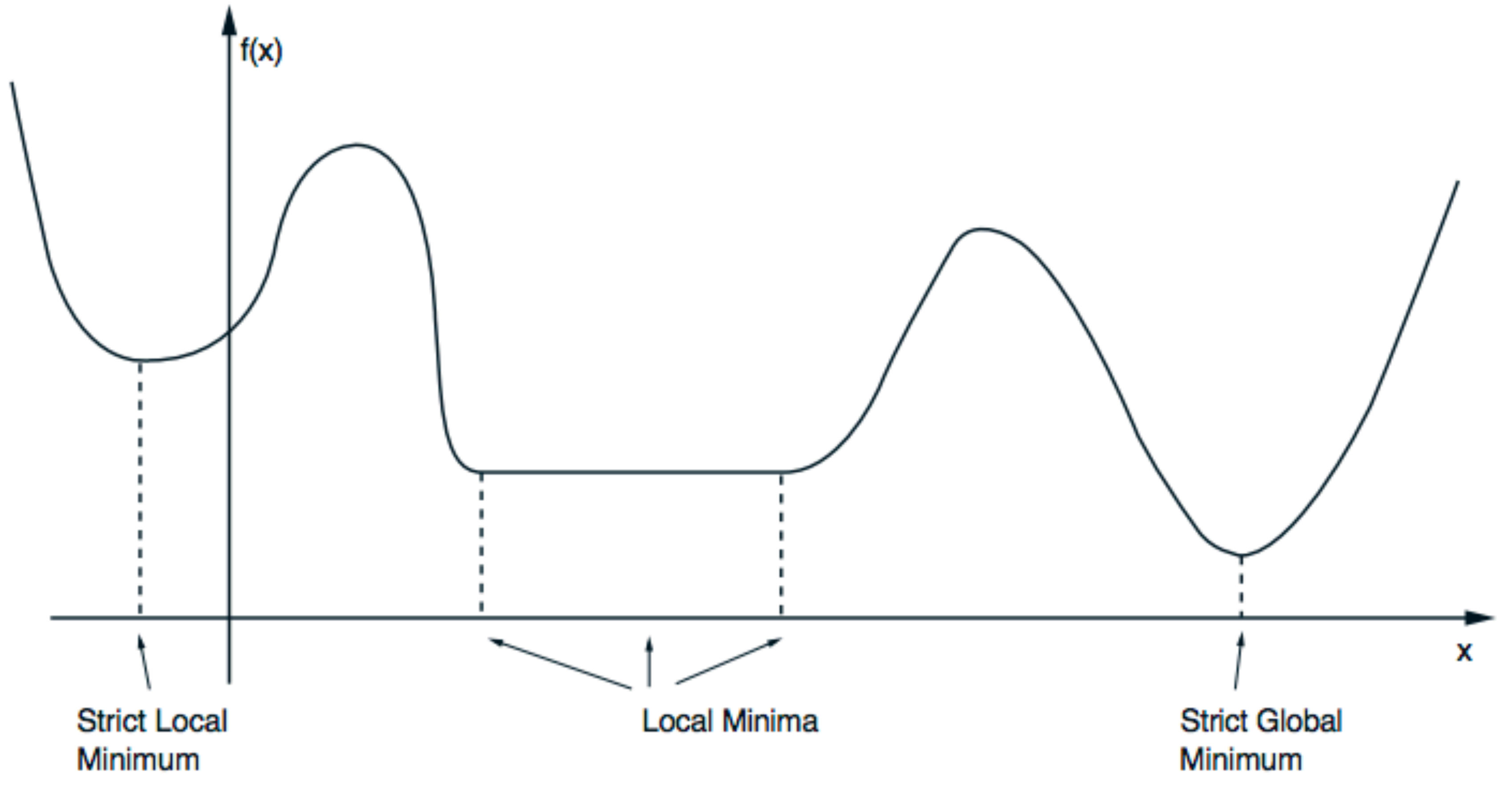

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An element is called a local minimum point if there exists $\hat{p}$ such that

$$L(\hat{\mathbf{p}}) \leq L(\mathbf{p}) \qquad \forall \mathbf{p} \text{ with } \|\mathbf{p} - \hat{\mathbf{p}}\| \leq \varepsilon$$

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Other noticeable approaches

Random search: grid search with random selection of parameter combinations

Gradient-based opt.: we will see in more details next

Bayesian opt.: builds a probabilistic model of function mapping hyperparameters to validation error

Evolutionary opt.: use evolutionary algorithms to search space of hyperparameters

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Bayesian opt.: builds a probabilistic model of function mapping hyperparameters to validation error

Evolutionary opt.: use evolutionary algorithms to search space of hyperparameters

In this module, grid search will usually be sufficient as we deal with relatively few hyperparameters

Bias-variance decomposition

Assume the following data generation model:

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

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Prediction function: f_t

Bias-variance decomposition

For fixed input $\tilde{x}$, look at error between model and prediction function:

$$\left(f(\tilde{x}) + \varepsilon - f_t(\tilde{x})\right)^2$$

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Imagine we do this for many different instances of S_t and ε

then we can look at the expected value of the error:

$$\mathbb{E}_{t,\varepsilon}\left[\left(f(\tilde{x}) + \varepsilon - f_t(\tilde{x})\right)^2\right]$$

Bias-variance decomposition

$$\mathbb{E}_{t,\varepsilon}\left[\left(f(\tilde{x}) + \varepsilon - f_t(\tilde{x})\right)^2\right]$$

$$= \sigma^2 \quad + \quad \left(f(\tilde{x}) - \mathbb{E}_t[f_t(\tilde{x})]\right)^2 \quad + \quad \mathbb{E}_t\left[\left(\mathbb{E}_t[f_t(\tilde{x})] - f_t(\tilde{x})\right)^2\right]$$

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Always there
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Systematic error/bias

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Always there in the data!

Systematic error/bias

Variance in the prediction function. How much one instance deviates from the average

Bias-variance decomposition

Example: polynomial regression

$$f(x) = \sin(2\pi x)\,, \quad x \in [0,1]$$

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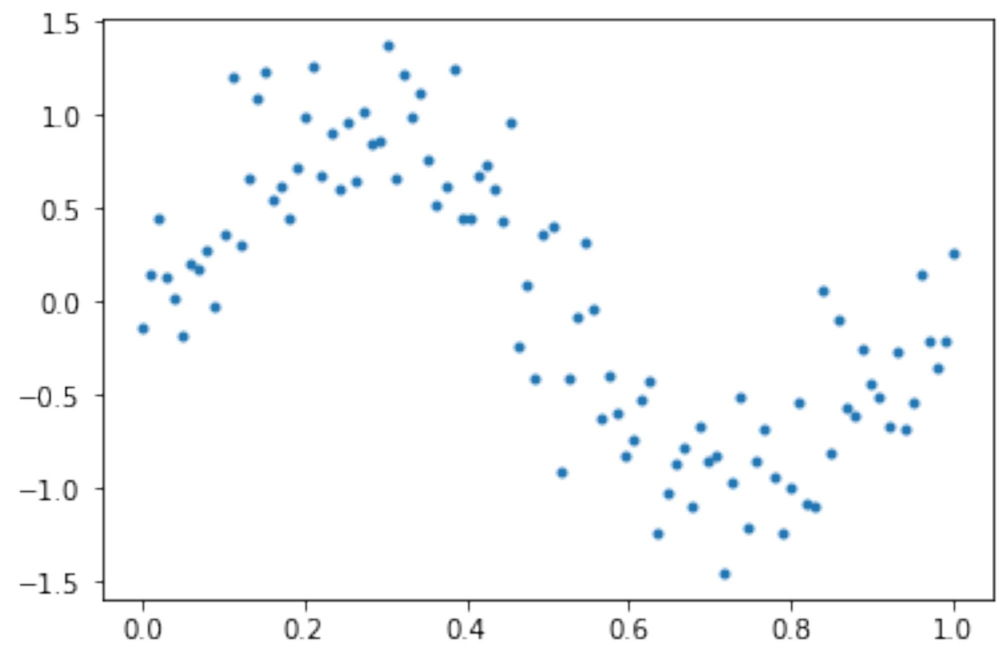
Different noisy instances for training & testing



Bias-variance decomposition

Example: polynomial regression

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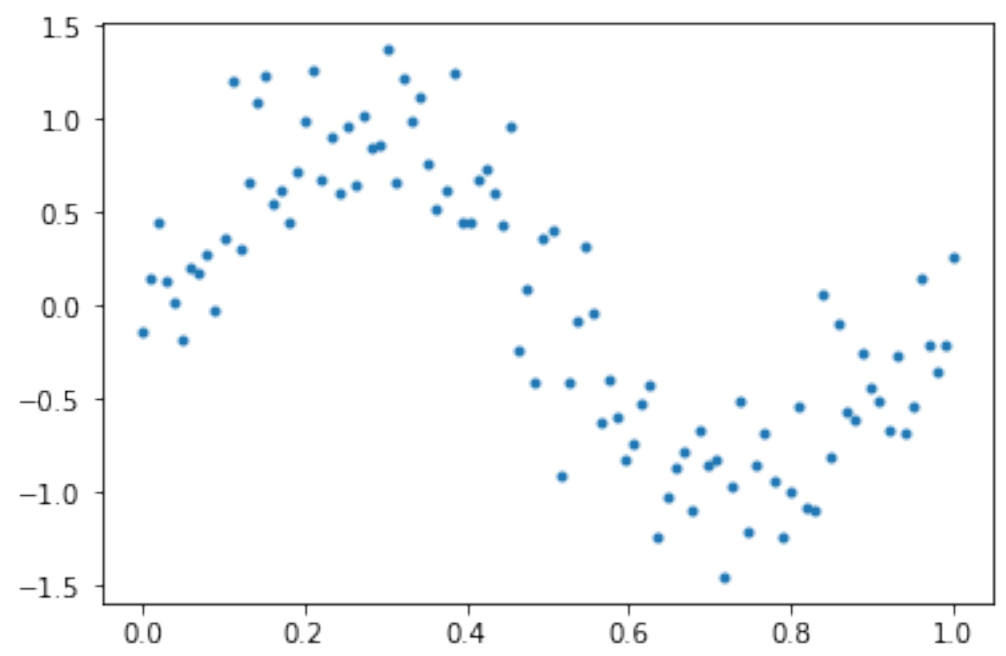
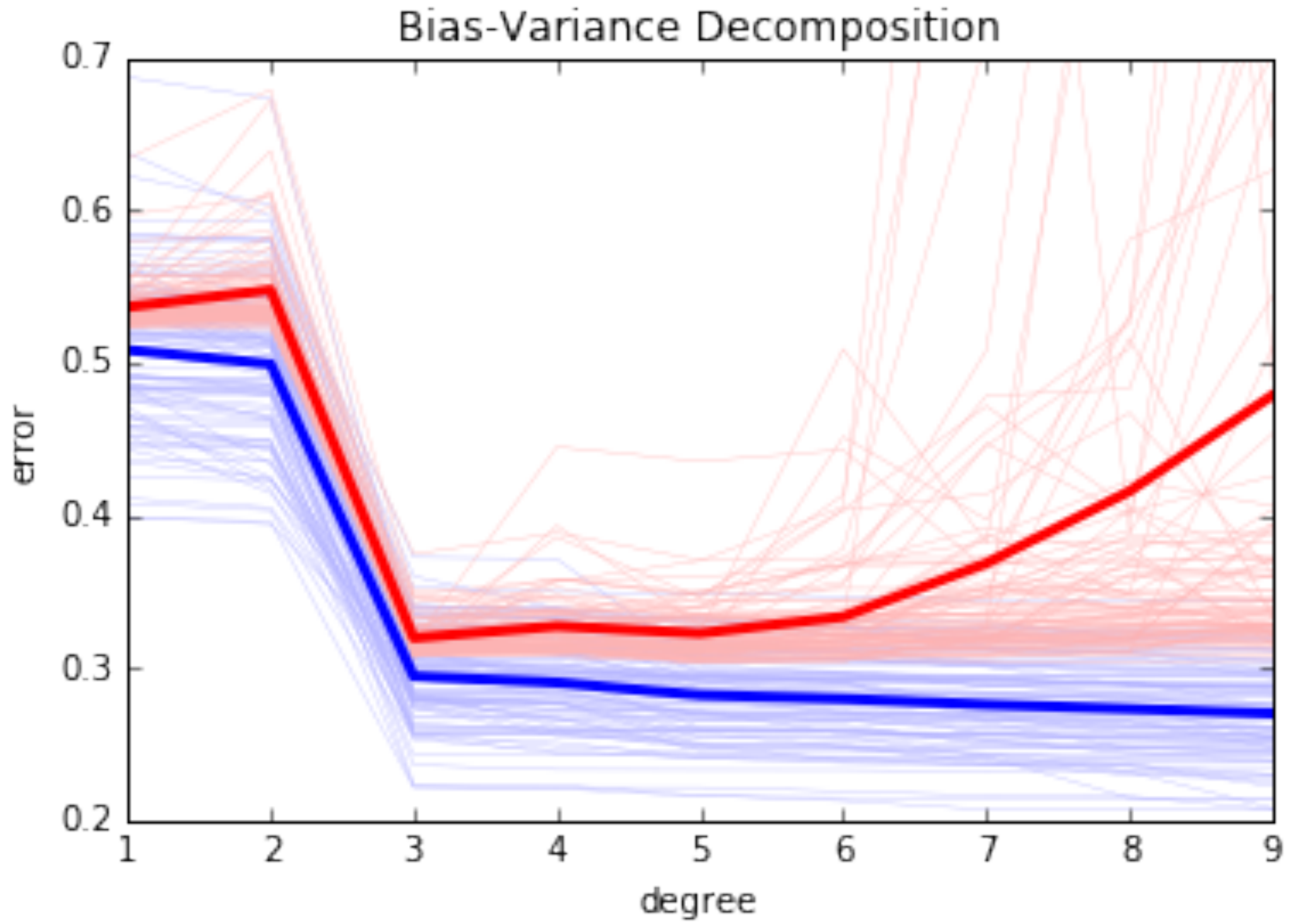
Different noisy instances for training & testing





Model: $f_t(x) = \sum_{k=0}^{d} x^k w_k$ for $\hat{w} = \arg\min_w \left\{ \frac{1}{2} \sum_{i=1}^{s} \left| \sum_{k=0}^{d} x_{ij}^k w_k - y_i \right|^2 \right\}$ and $S_t := \{(x_i, y_i) \text{ iid } \sim \mathscr{D}\}_{i=1}^{s}$

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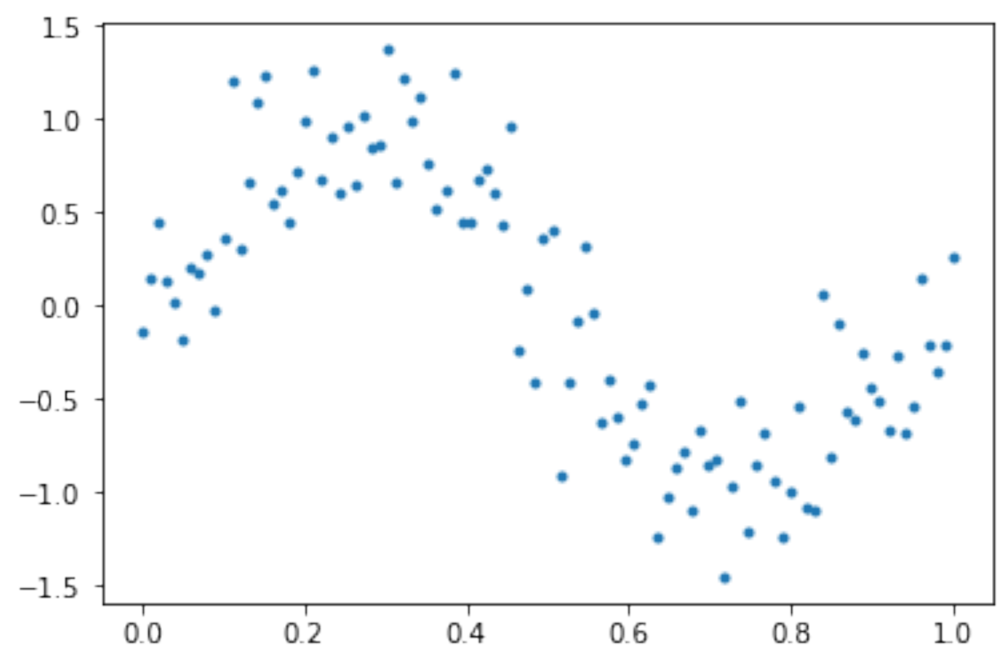

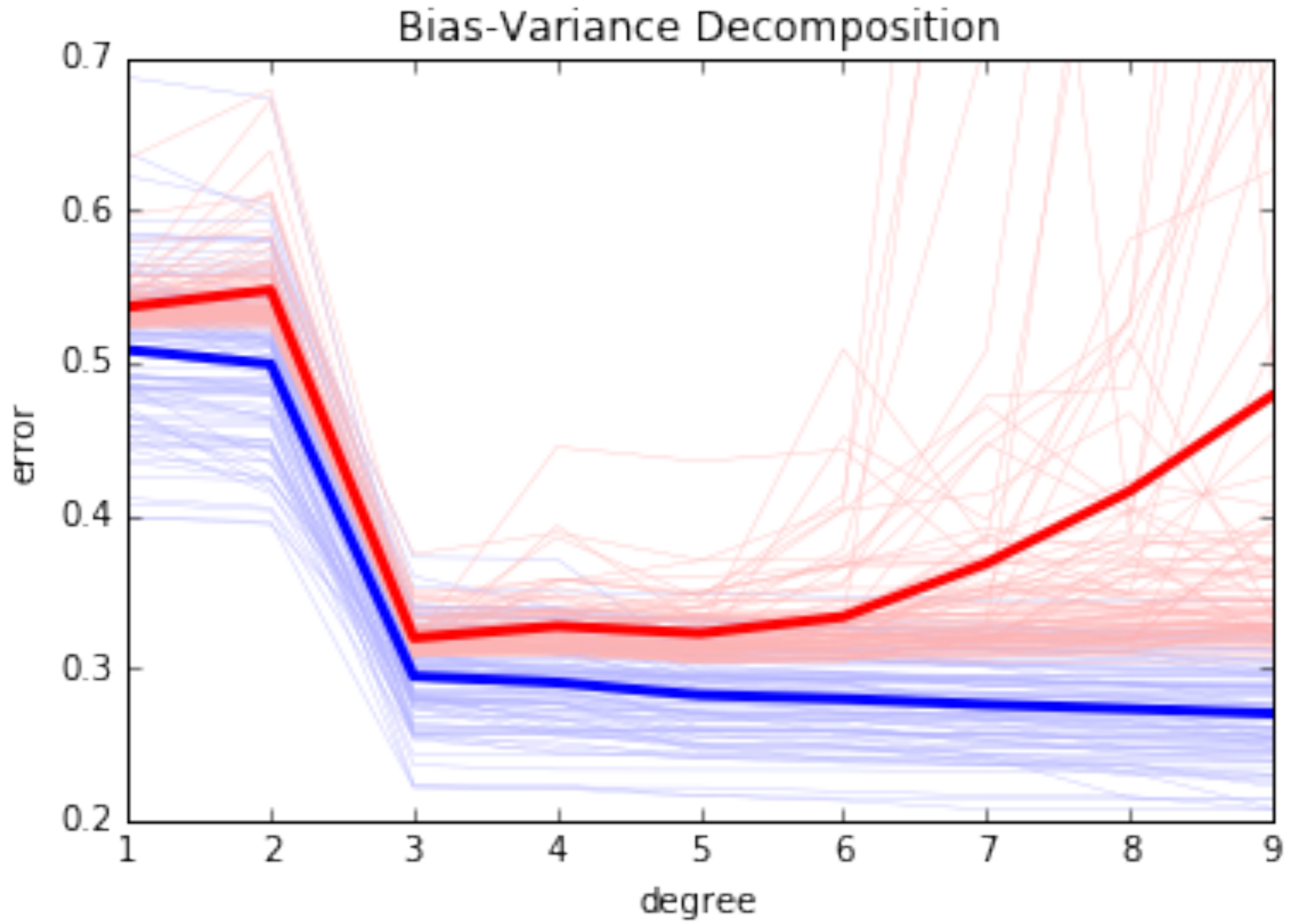

Training error

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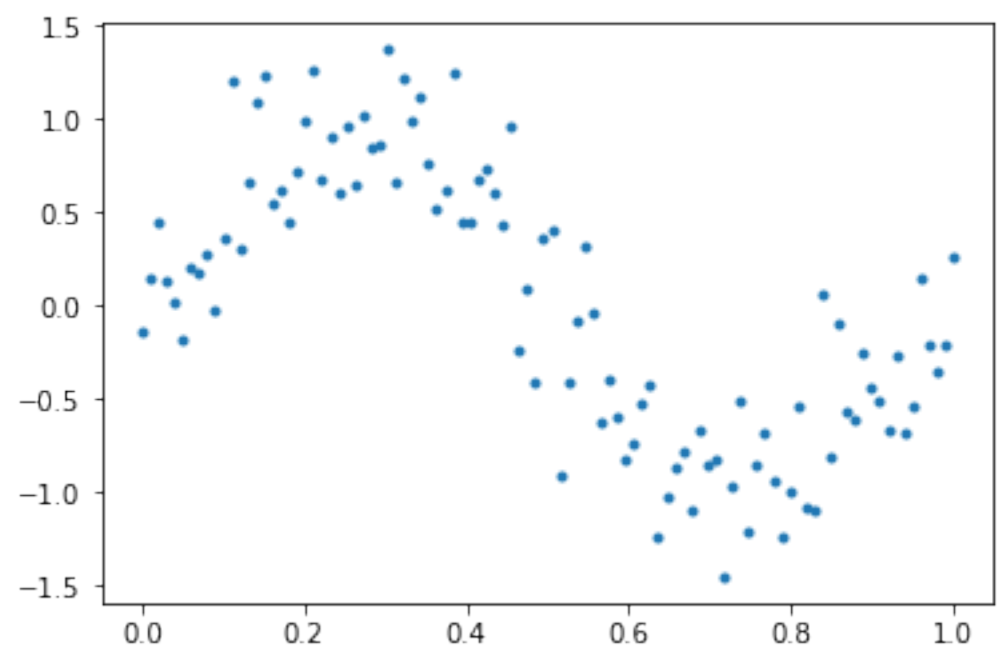

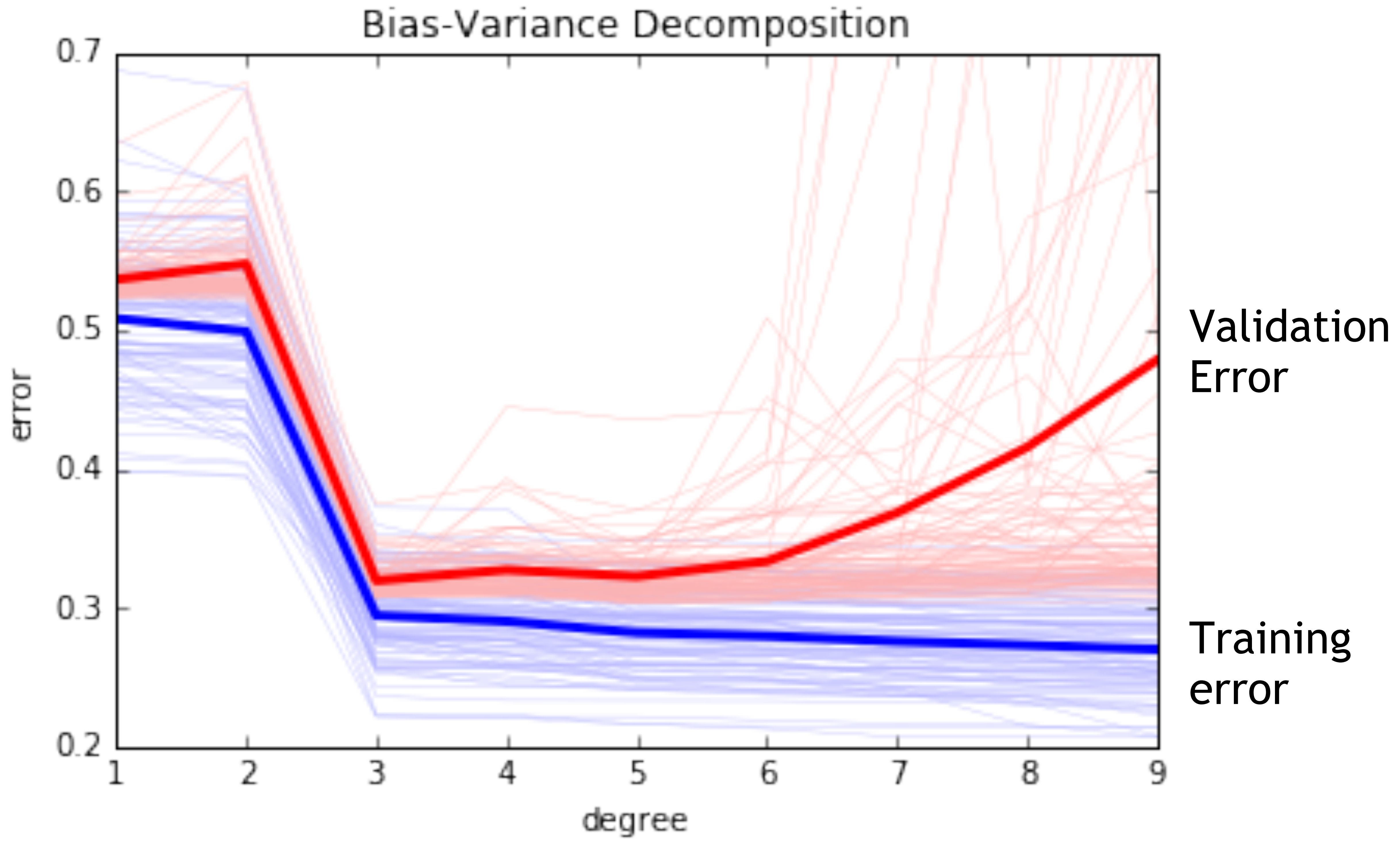

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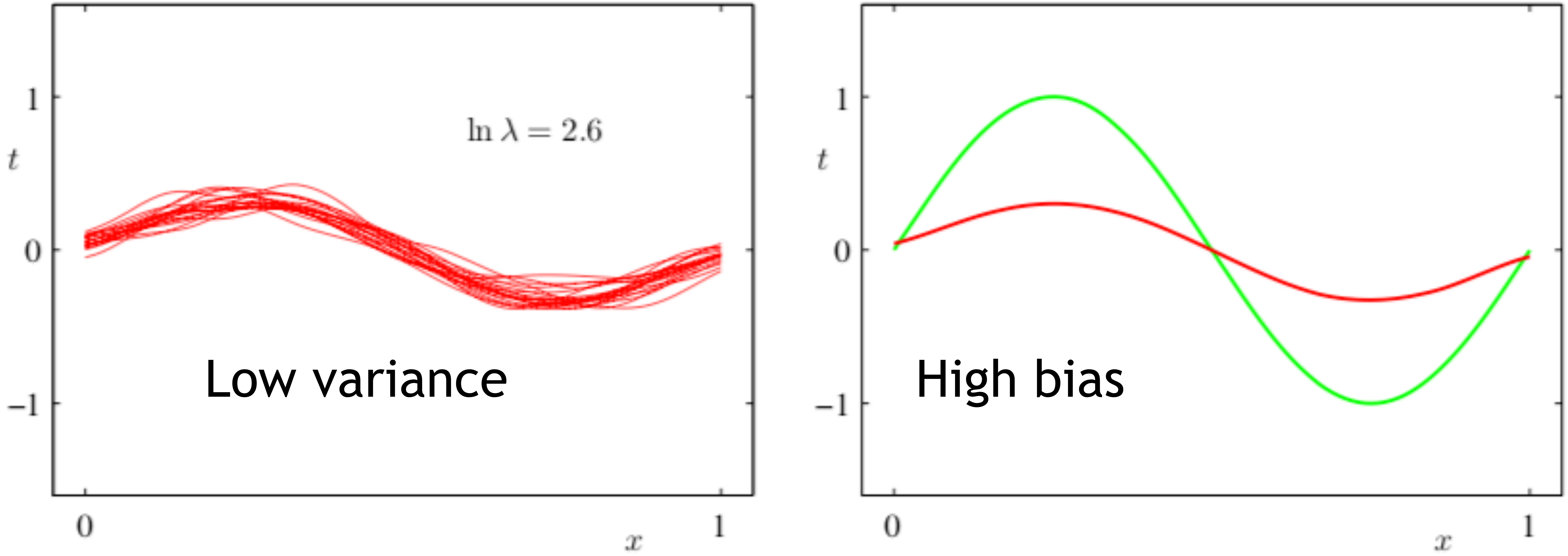
Bias-variance decomposition

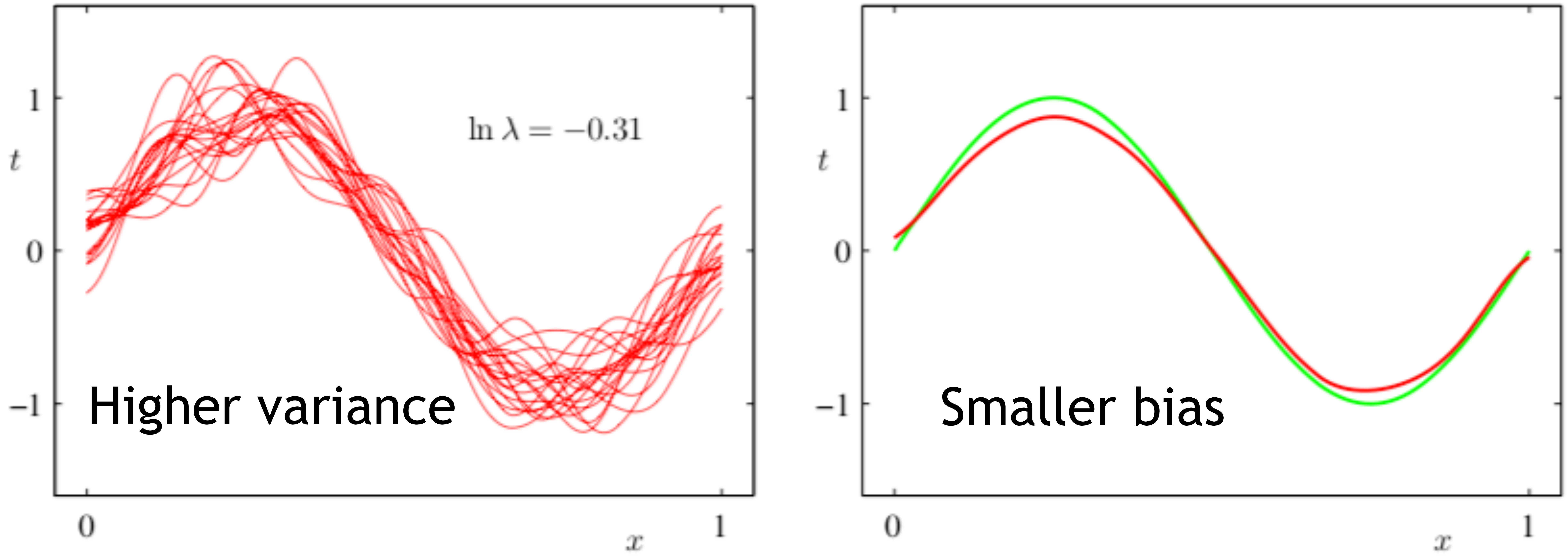
Example: ridge regression $$\hat{\mathbf{w}} = \arg\min_{w} \left\{ \frac{1}{2} \|\boldsymbol{\Phi}(\mathbf{X})\mathbf{w} - \mathbf{y}\|^2 + \frac{\lambda}{2} \|\mathbf{w}\|^2 \right\}$$



From Bishop. Pattern Recognition & Machine Learning

Bias-variance decomposition

Example: ridge regression $$\mathbf{w} = \arg\min_{\mathbf{w}} \left\{ \frac{1}{2}\|\Phi(\mathbf{X})\mathbf{w} - \mathbf{y}\|^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2 \right\}$$



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Bias-variance decomposition

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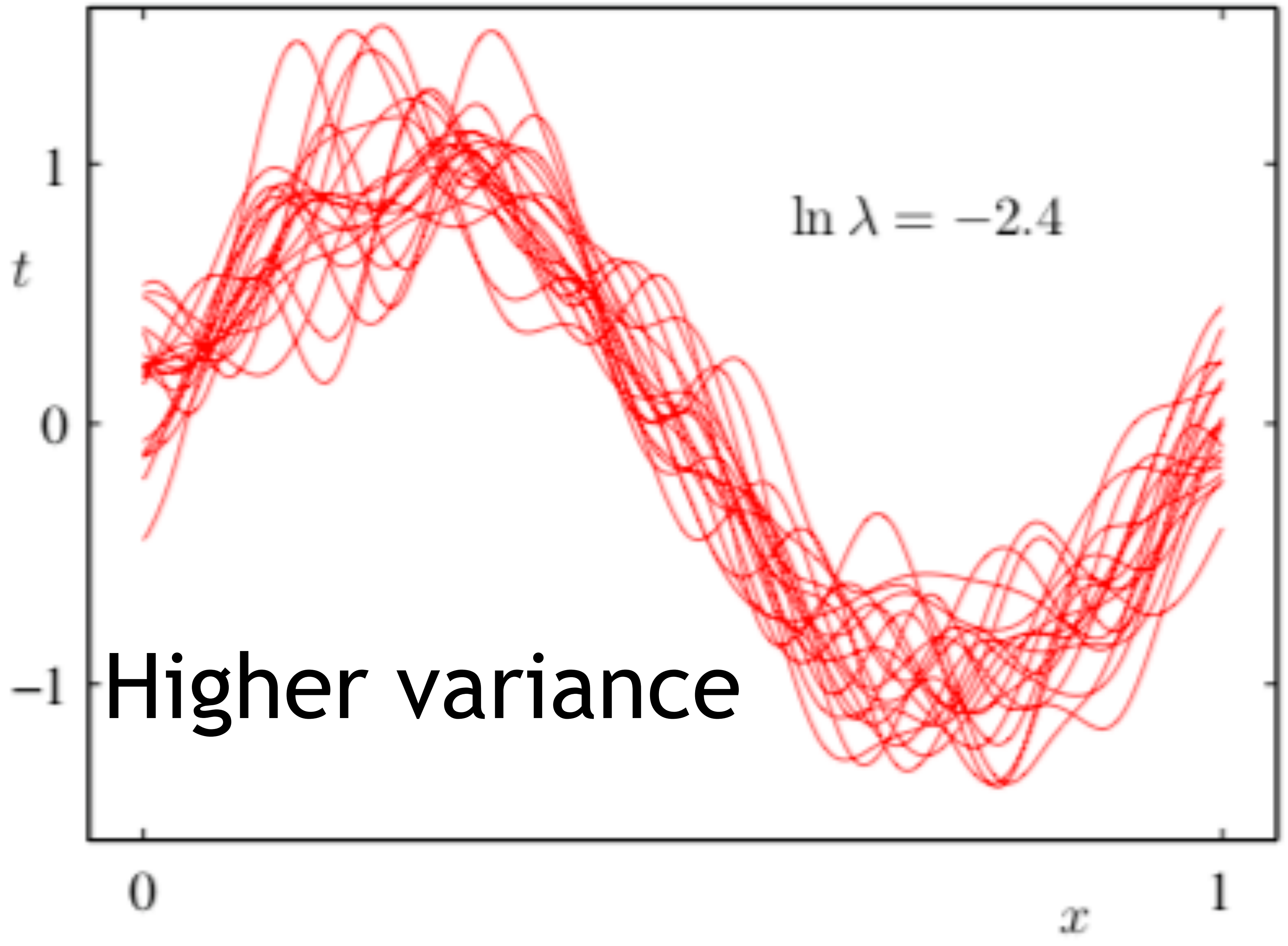

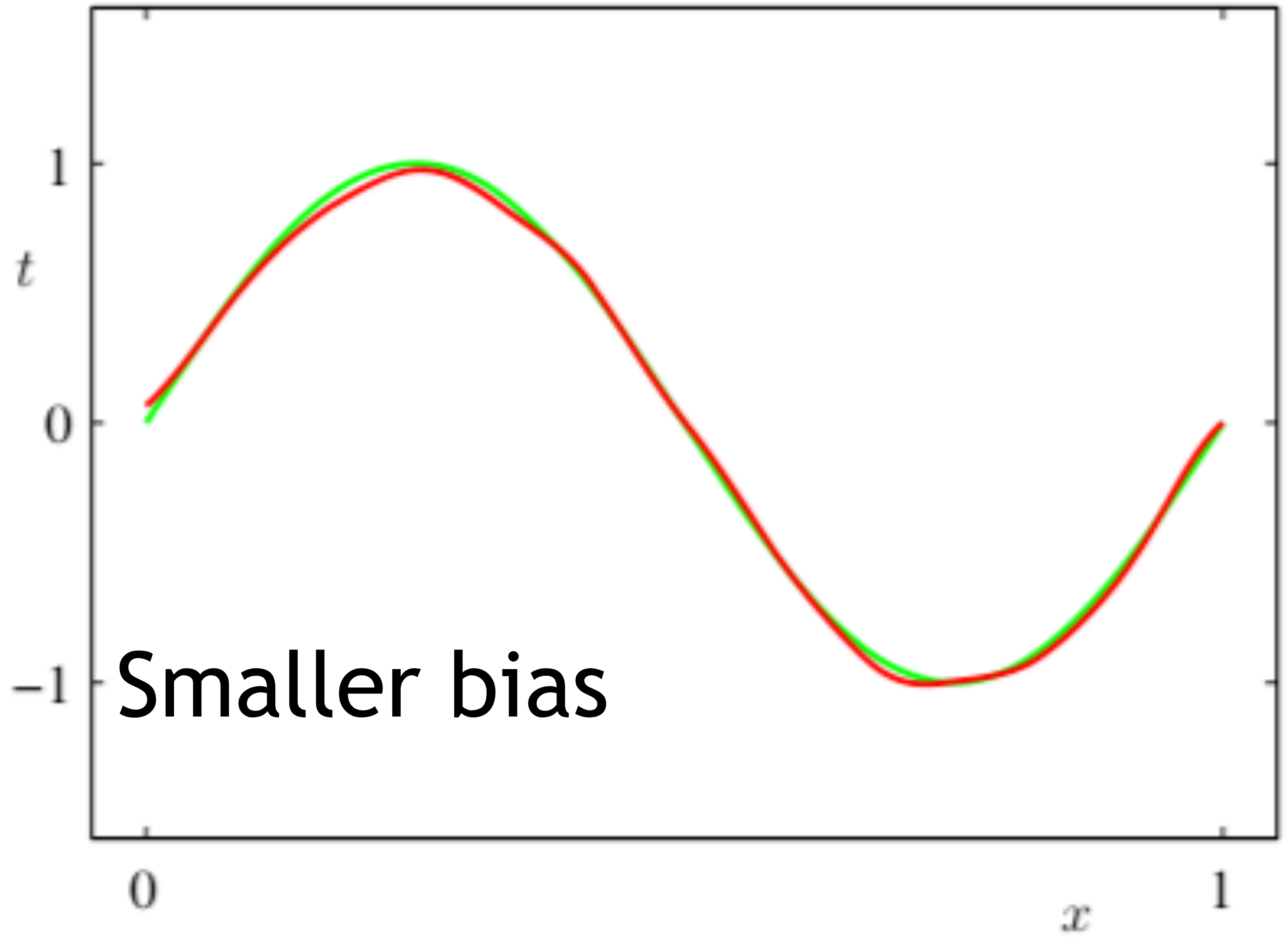

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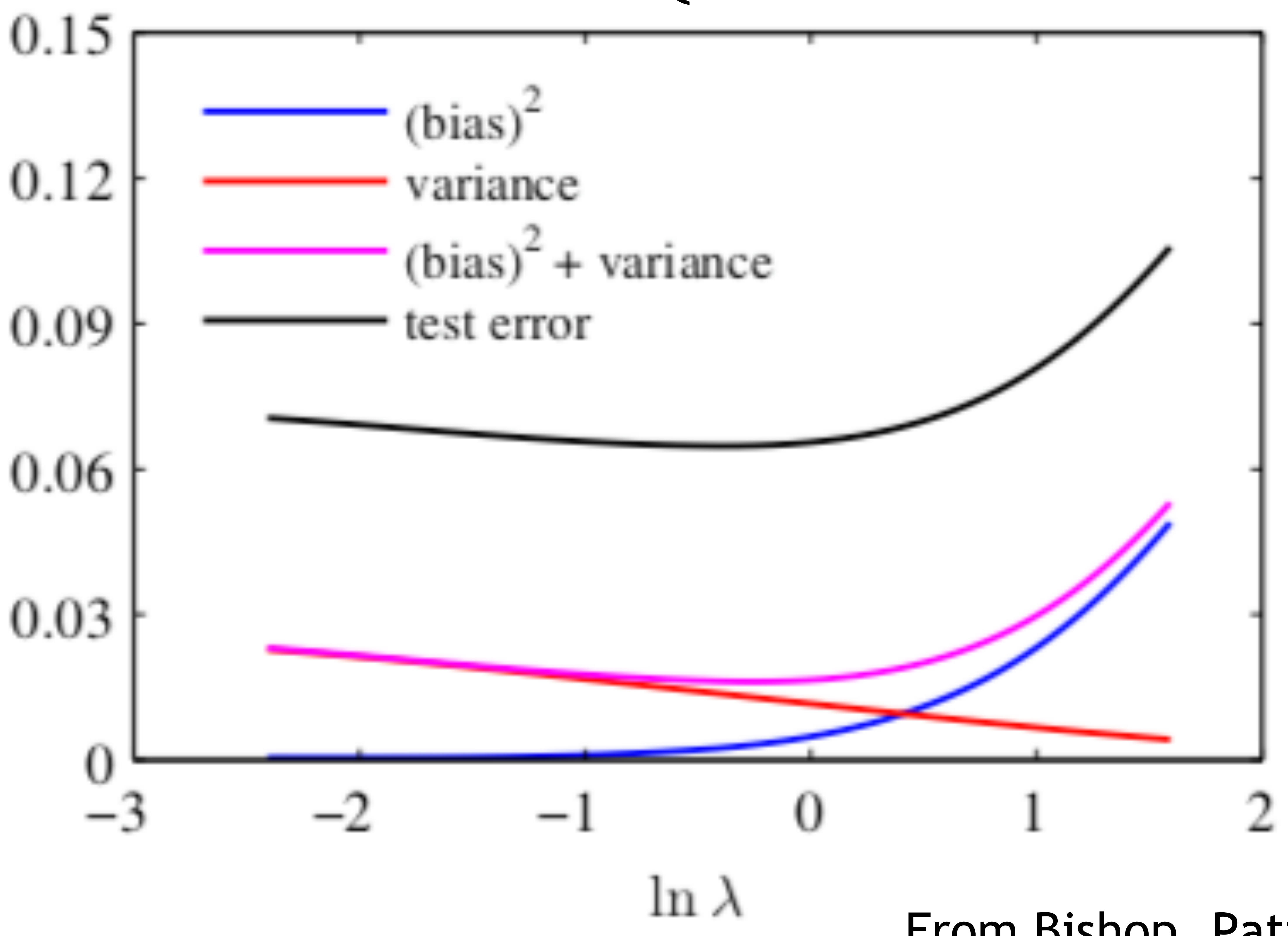

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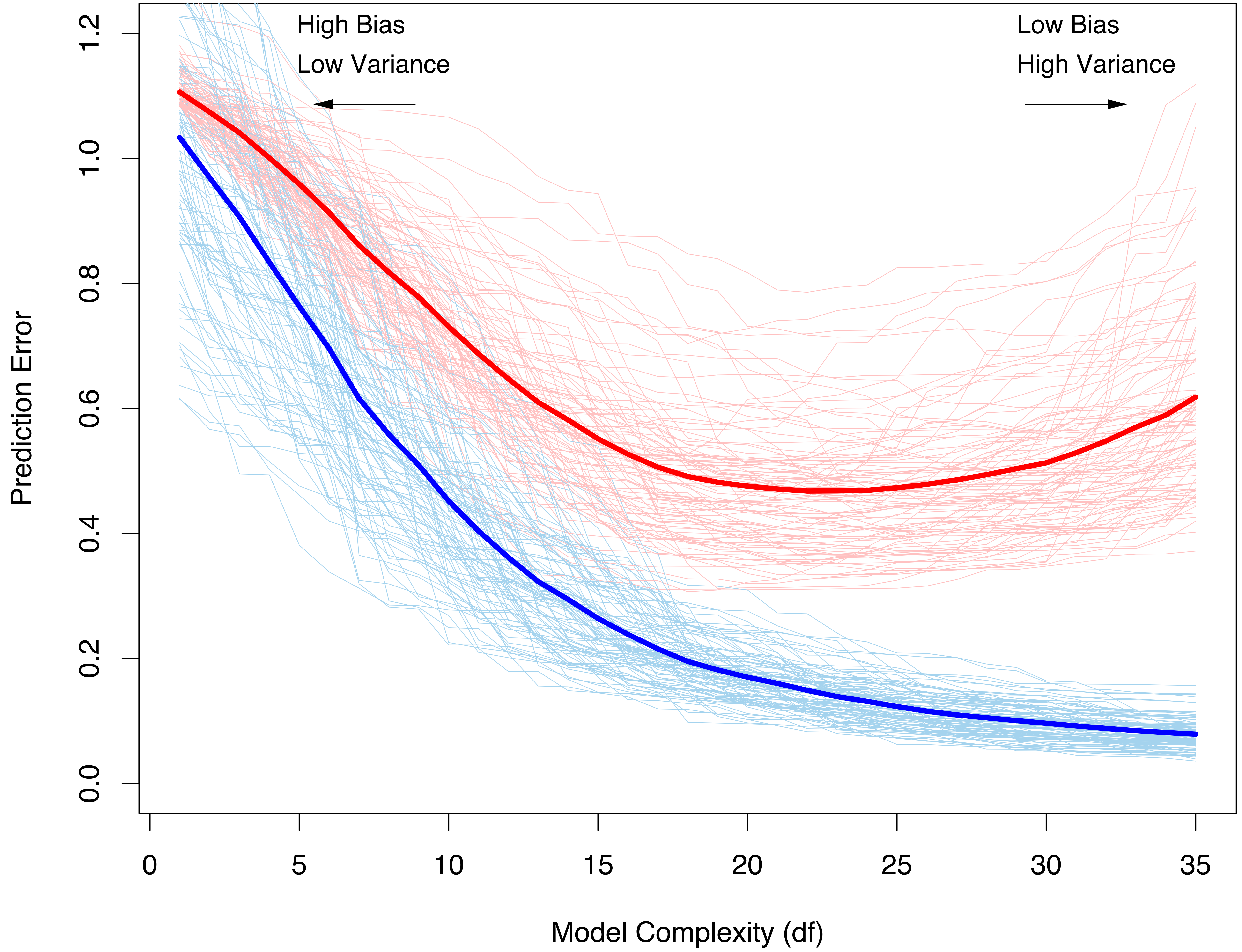
Bias-variance decomposition



Bias-variance decomposition

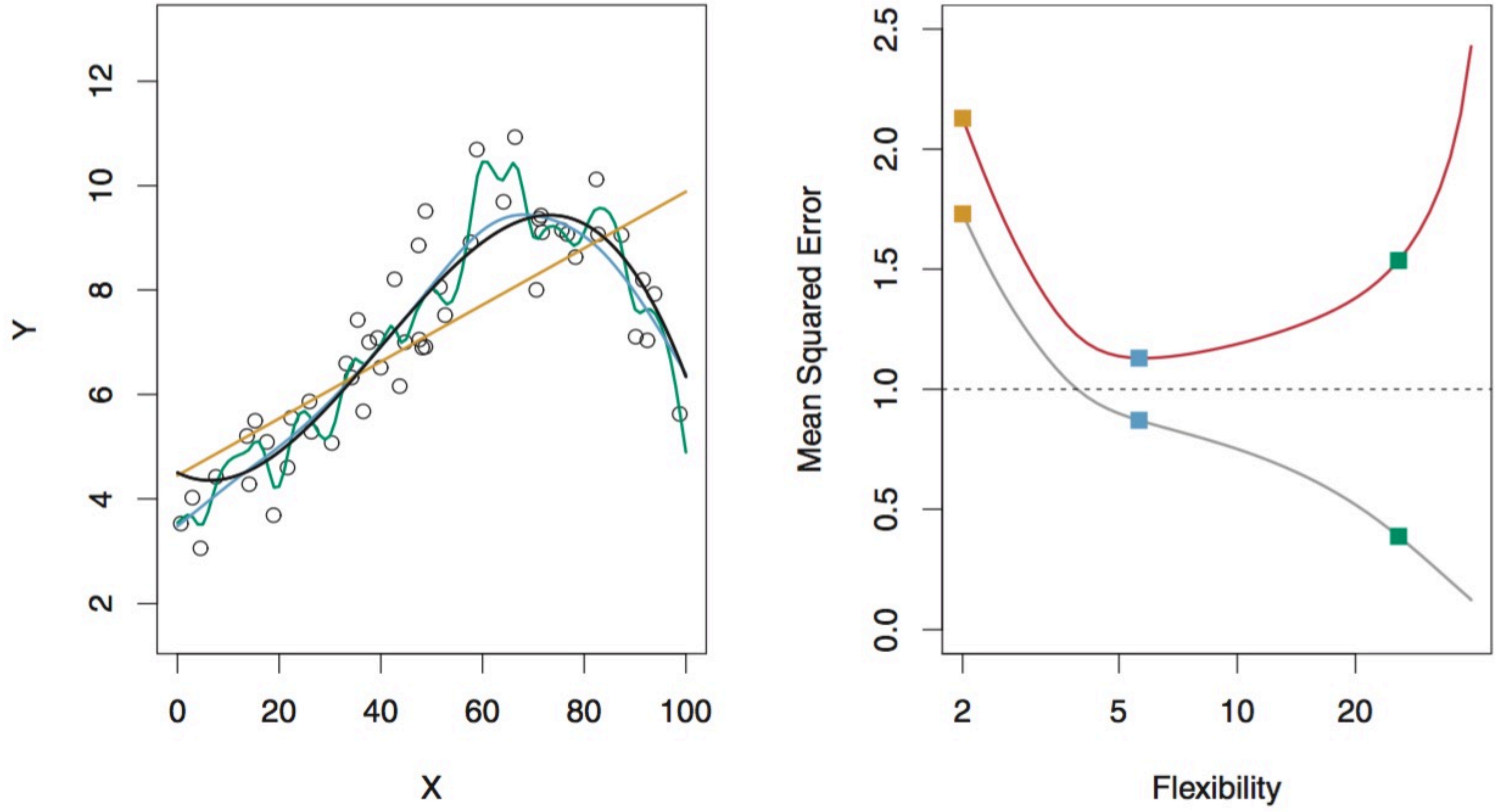
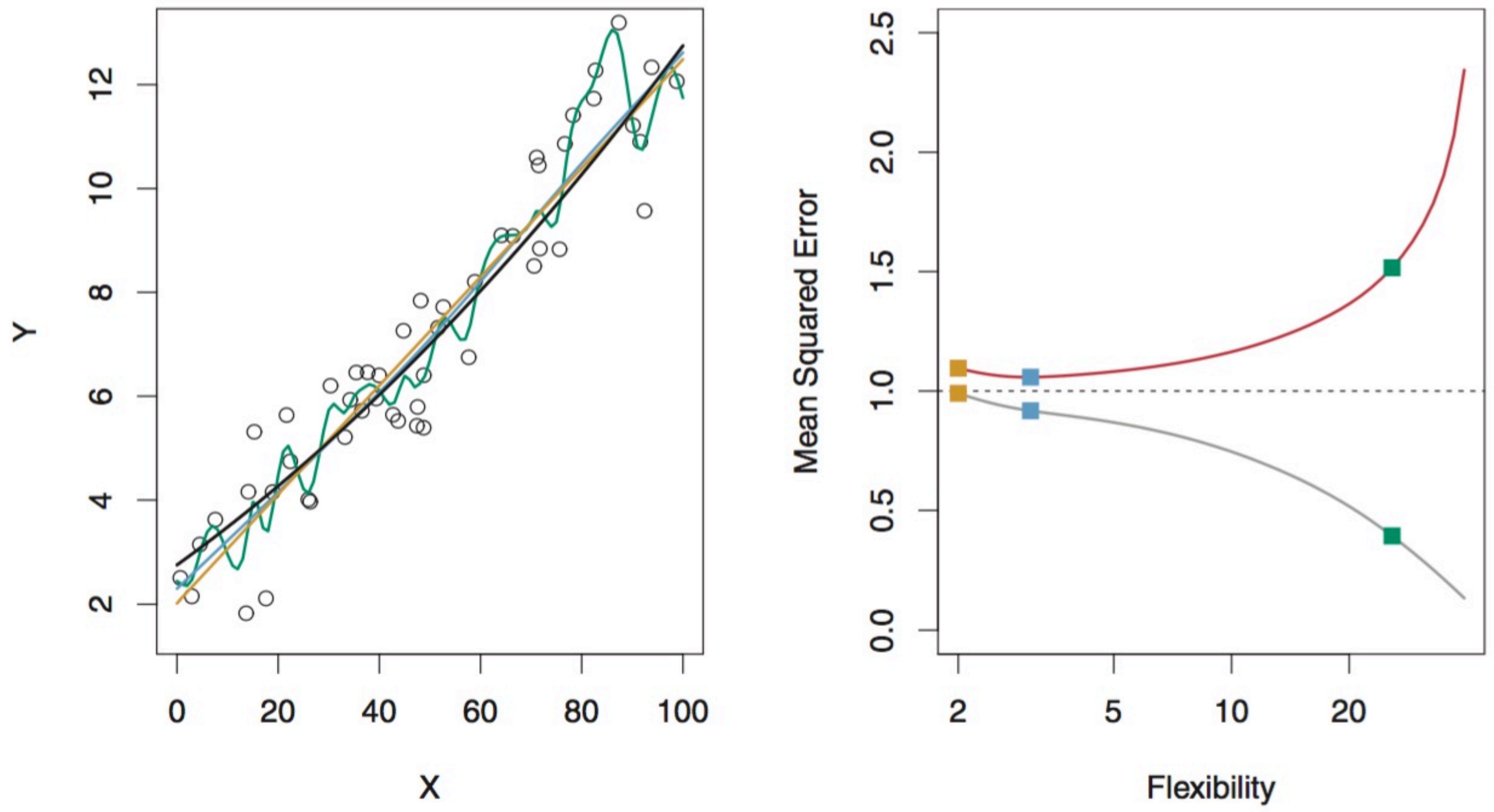


FIGURE 2.9. Left: *Data simulated from f, shown in black. Three estimates of f are shown: the linear regression line (orange curve), and two smoothing spline fits (blue and green curves).* Right: *Training MSE (grey curve), test MSE (red curve), and minimum possible test MSE over all methods (dashed line). Squares represent the training and test MSEs for the three fits shown in the left-hand panel.*

From Hastie, Tibshirani & Friedman, The Elements of Statistical Learning

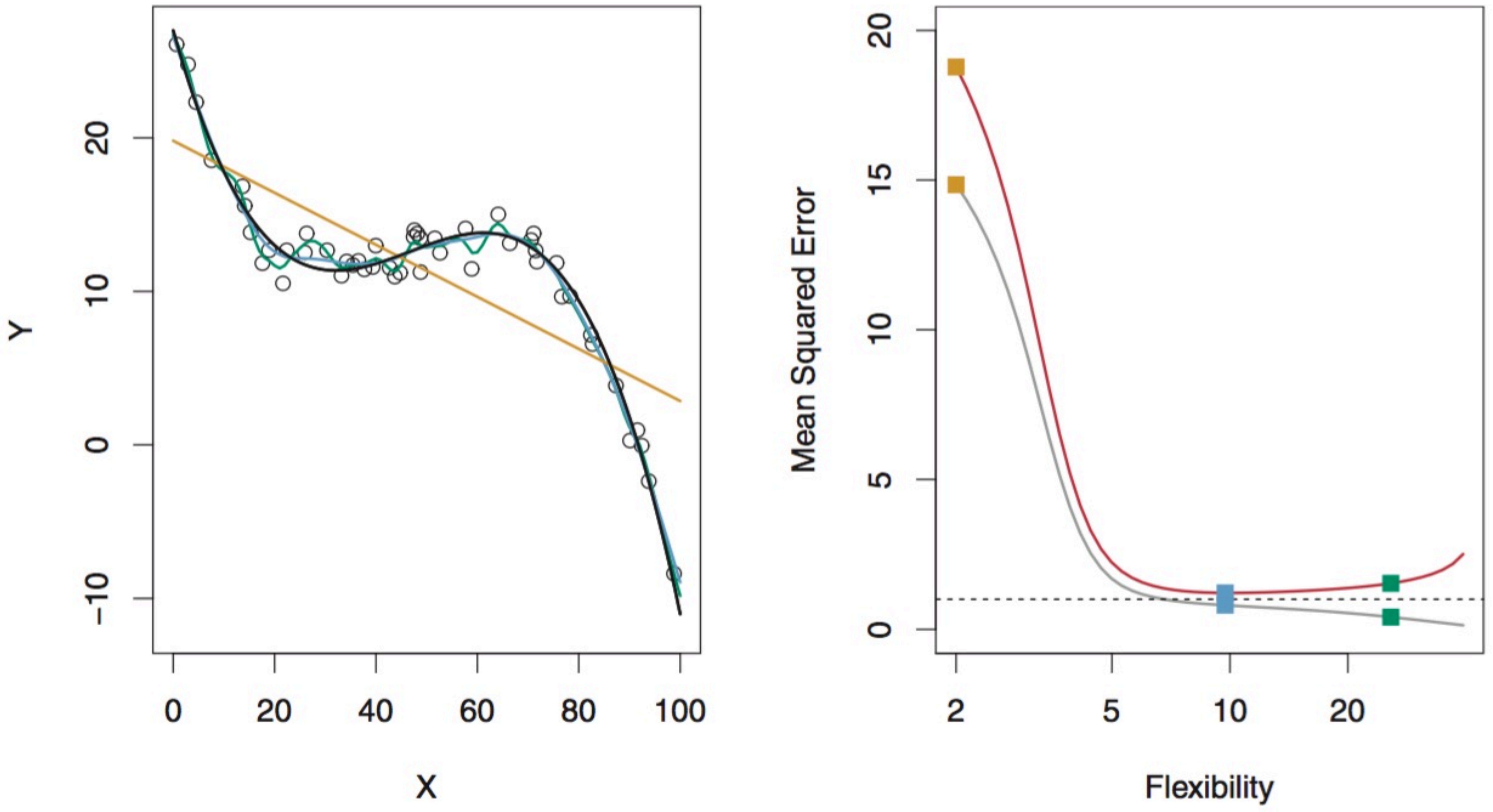
Bias-variance decomposition



From Hastie, Tibshirani & Friedman, The Elements of Statistical Learning

FIGURE 2.10. *Details are as in Figure 2.9, using a different true f that is much closer to linear. In this setting, linear regression provides a very good fit to the data.*

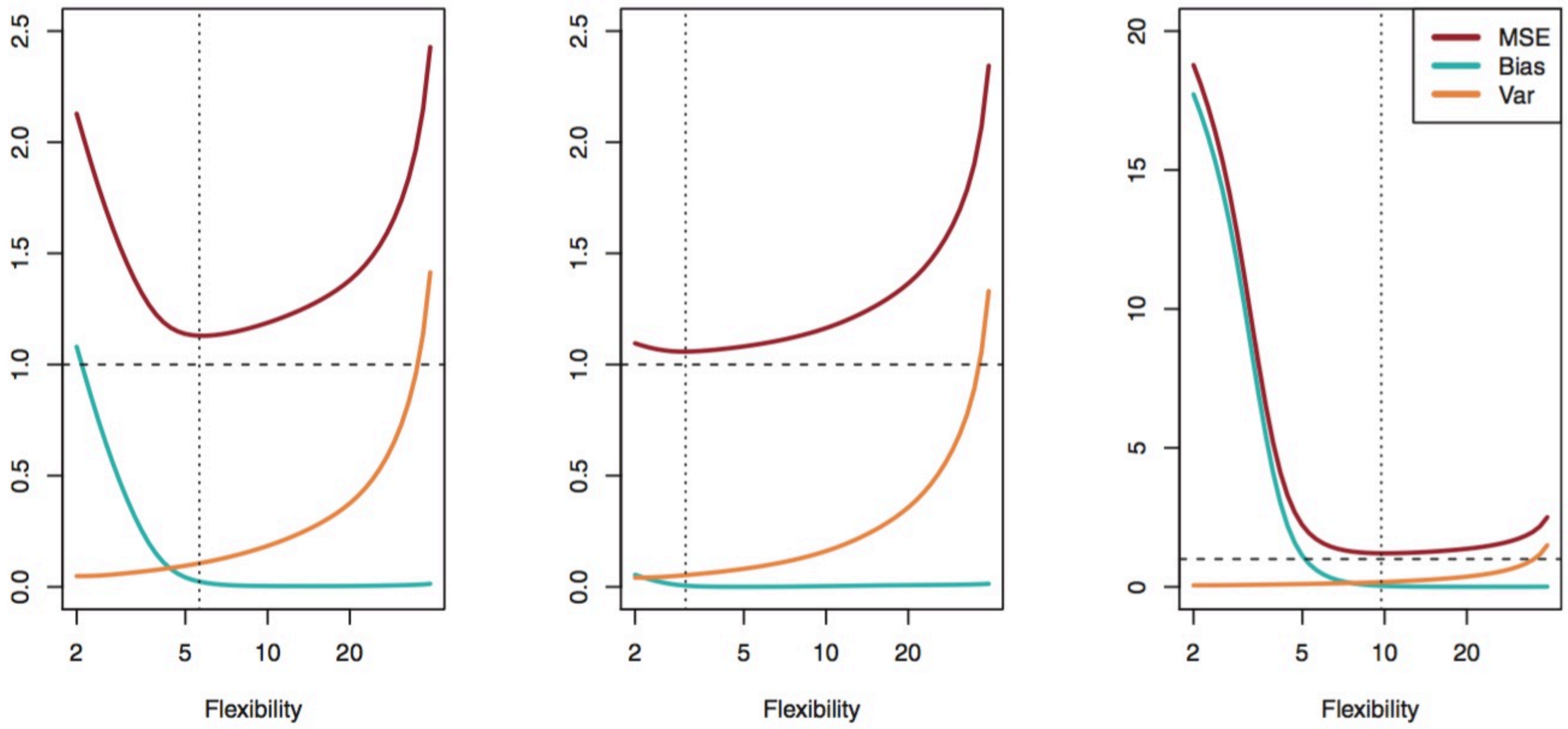
Bias-variance decomposition



From Hastie, Tibshirani & Friedman, The Elements of Statistical Learning

FIGURE 2.11. *Details are as in Figure 2.9, using a different f that is far from linear. In this setting, linear regression provides a very poor fit to the data.*

Bias-variance decomposition



From Hastie, Tibshirani & Friedman, The Elements of Statistical Learning

FIGURE 2.12. *Squared bias (blue curve), variance (orange curve), Var(ϵ) (dashed line), and test MSE (red curve) for the three data sets in Figures 2.9–2.11. The vertical dotted line indicates the flexibility level corresponding to the smallest test MSE.*