Model Assessment & Selection

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Outline

- Bias, Variance and Model Complexity
- The Bias-Variance Decomposition
- Optimism of the Training Error Rate
- Estimates of In-Sample Prediction Error
- The Effective Number of Parameters
- The Bayesian Approach and BIC
- Minimum Description Length
- Vapnik-Chernovenkis Dimension
- Cross-Validation
- Bootstrap Methods

OBE of The Chapter

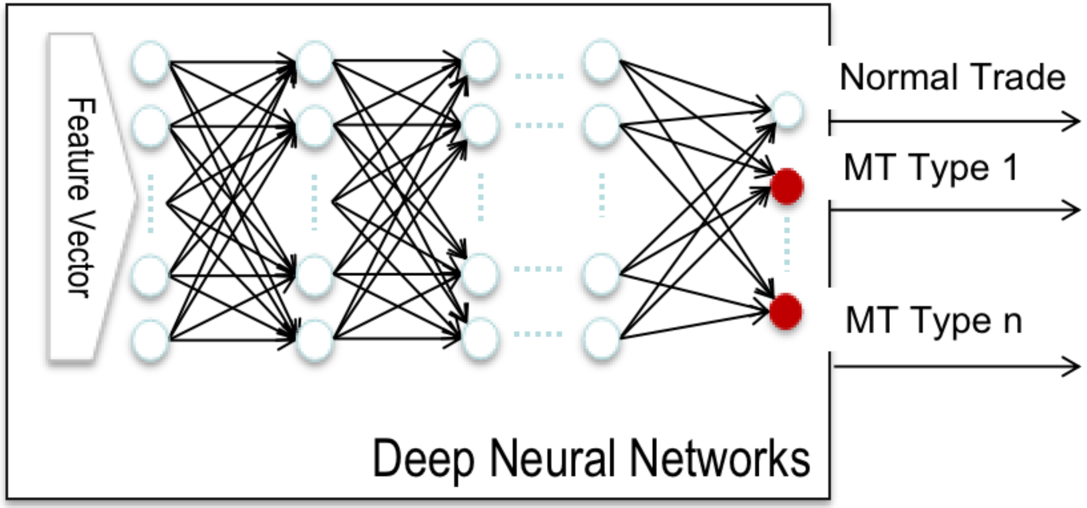
- To grasp the concept of model selection and assessment
- To derive criterions for model selection
  - In-sample error
- What are the most popular model selection criteria
  - AIC; BIC; MDL; VC
- CV for model selection

- Bootstrap method

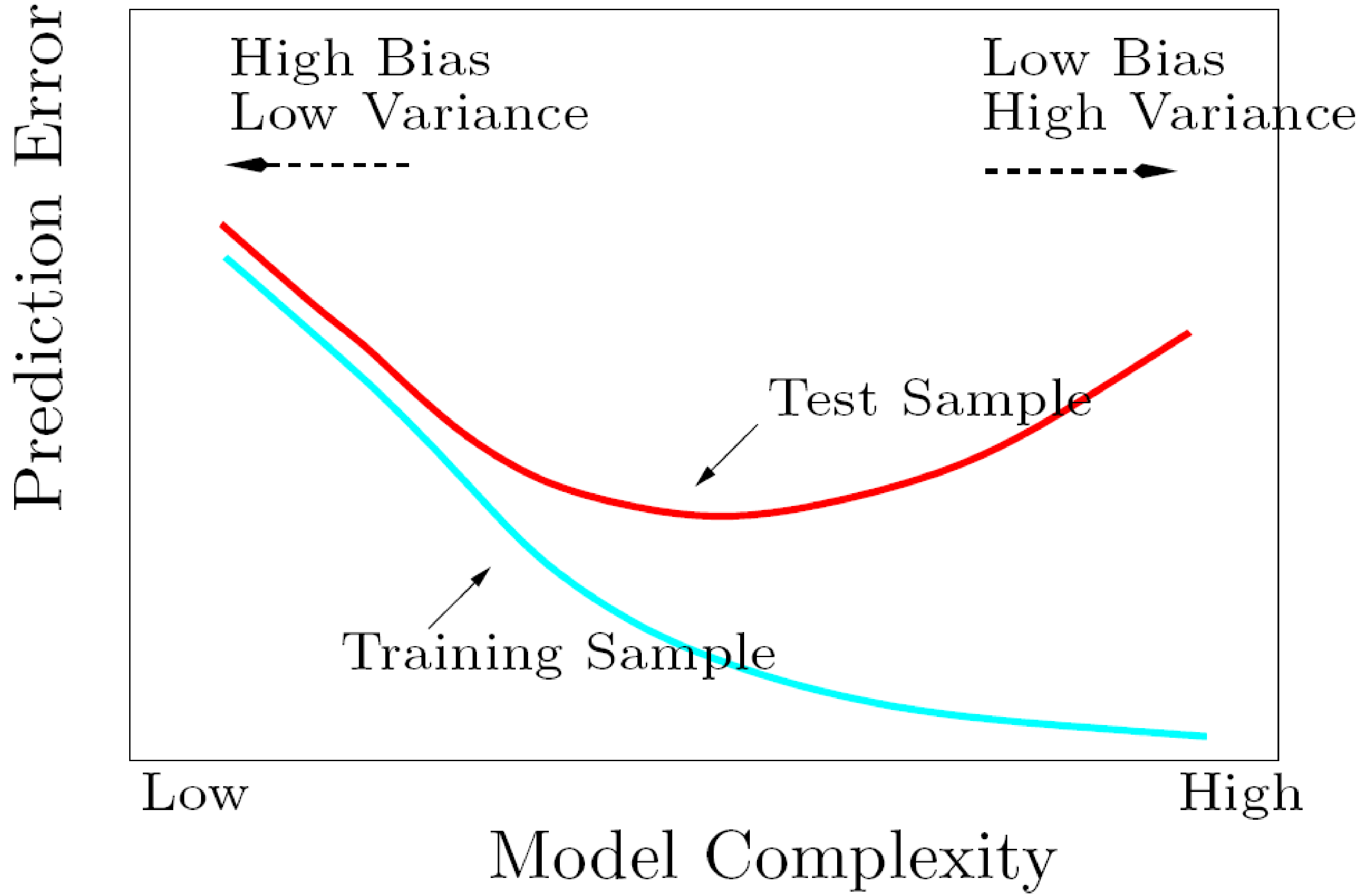
Model Selection

– To estimate the performance of different models in order to choose the best one.
– What is the parameters for model selection
– CNN – parameter for model selection

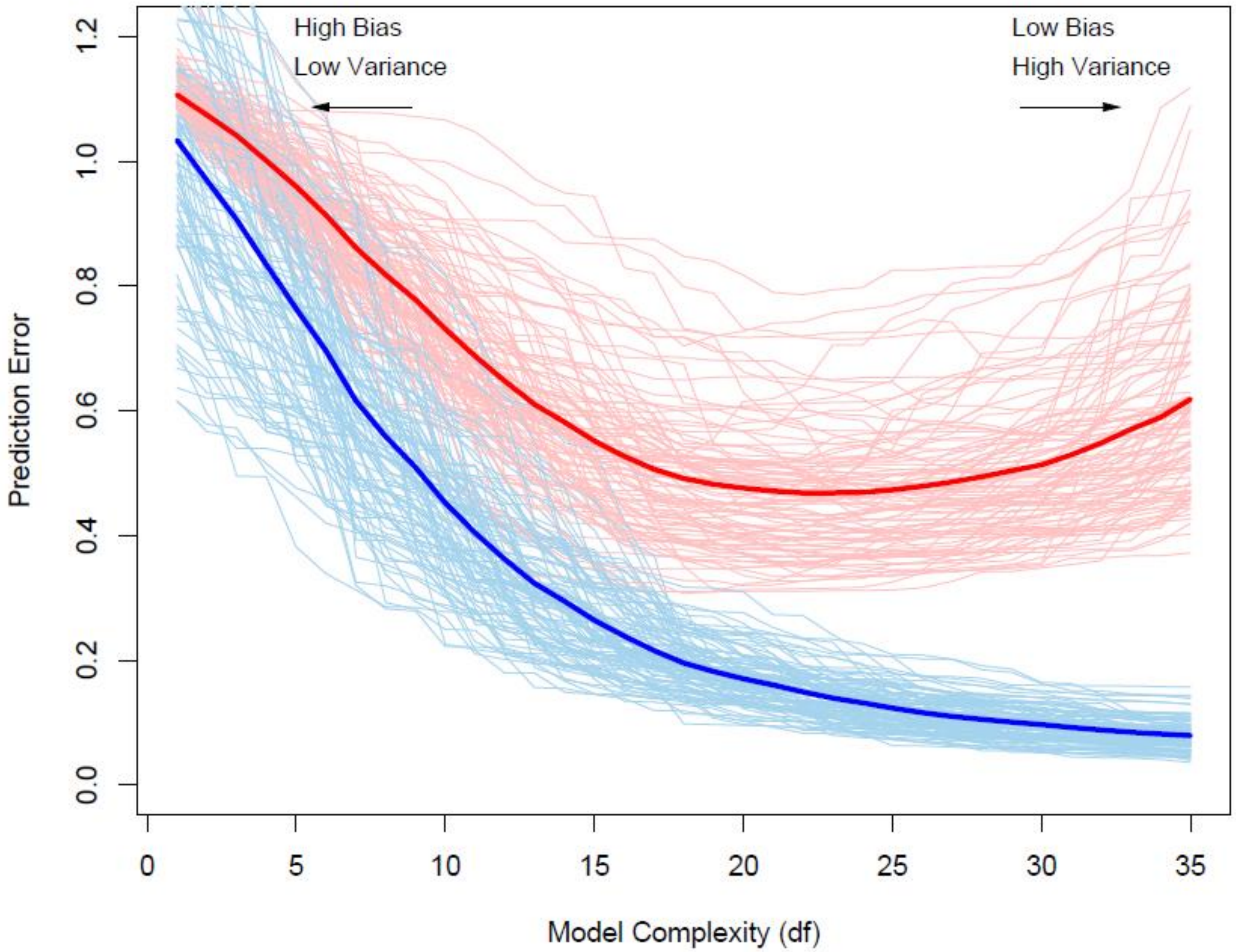
- The number of layers?
- The number of neurons in each layer?
- The activation function?
- The size of convolution kernels?
- …



Bias, Variance & Model Complexity



Bias, Variance & Model Complexity



Bias, Variance & Model Complexity

- The standard of model assessment : the generalization performance of a learning method
  - Model: $X \to Y;\ Y = f(X) + \varepsilon$
  - Prediction Model: $\hat{f}(X)$
  - Loss function:

$$L(Y, \hat{f}(X)) = \begin{cases} (Y - \hat{f}(X))^2 & \text{squared error} \\ |Y - \hat{f}(X)| & \text{absolute error} \end{cases}$$

Bias, Variance & Model Complexity

- Error: training error, generalization error

$$\text{Training error}: \overline{err} = \frac{1}{N}\sum_{i=1}^{N} L(y_i, \hat{f}(x_i))$$

$$\text{Generalization error}: Err = E\left[L(Y, \hat{f}(X))\right]$$

- Typical loss function:

$$\text{0-1 loss} \quad L(G, \hat{G}(X)) = I(G \neq \hat{G}(X))$$

$$\text{log-likelihood} \quad L(G, \hat{p}(X)) = -2\sum_{k=1}^{K} I(G = k)\log \hat{p}_k(X)$$
$$= -2\log \hat{p}_G(X)$$

Two Tasks in Model Selection

- **Model selection:**
  - estimating the performance of different models in order to choose the best one.
- **Model assessment:**
  - having chosen a final model, estimating its prediction error (generalization error) on new data.

Bias-Variance Decomposition

- Basic Model: $Y = f(X) + \varepsilon, \quad \varepsilon \sim N(0, \sigma_\varepsilon^2)$

- The expected prediction error of a regression fit $\hat{f}(X)$

$$
\begin{aligned}
Err(x_0) &= E[(Y - \hat{f}(x_0))^2 \mid X = x_0] \\
&= \sigma_\varepsilon^2 + [E\hat{f}(x_0) - f(x_0)]^2 + E[E\hat{f}(x_0) - \hat{f}(x_0)]^2 \\
&= \sigma_\varepsilon^2 + Bias(\hat{f}(x_0))^2 + Var(\hat{f}(x_0)) \\
&= \text{Irreducible Error} + \text{Bias}^2 + \text{Variance}
\end{aligned}
$$

- The more complex the model, the lower the (squared) bias but the higher the variance.

Bias-Variance Decomposition

- For the k-NN regression fit the prediction error:

$$Err(x_0) = E[(Y - \hat{f}(x_0))^2 | X = x_0]$$
$$= \sigma_\varepsilon^2 + [f(x_0) - \frac{1}{k}\sum_{j=1}^{k} f(x_j)]^2 + \sigma_\varepsilon^2 / k$$

$$\hat{f}(x_0) = \frac{1}{k} \sum_{x_j \in N(x_0)} f(x_j),$$

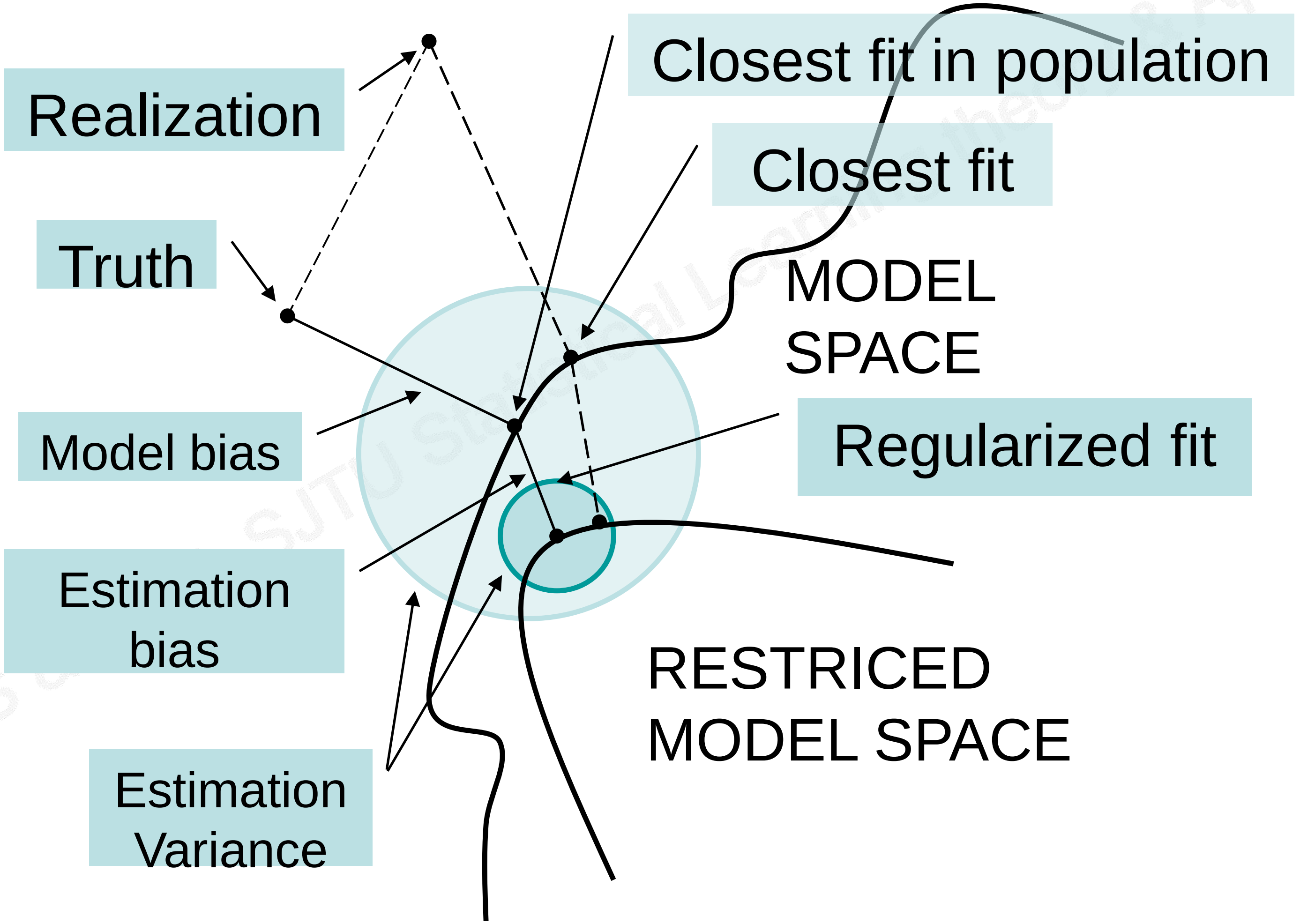
- The in-sample error of the Linear Model

$$\frac{1}{N}\sum_{i=1}^{N} Err(x_i) = \sigma_\varepsilon^2 + \frac{1}{N}\sum_{i=1}^{N}[f(x_i) - E\hat{f}(x_i)]^2 + \boxed{\frac{p}{N}\sigma_\varepsilon^2}$$

– The model complexity is directly related to the number of parameters p.

Bias-Variance Decomposition

- Schematic of the behavior of bias and variance



Example: Bias–Variance Tradeoff

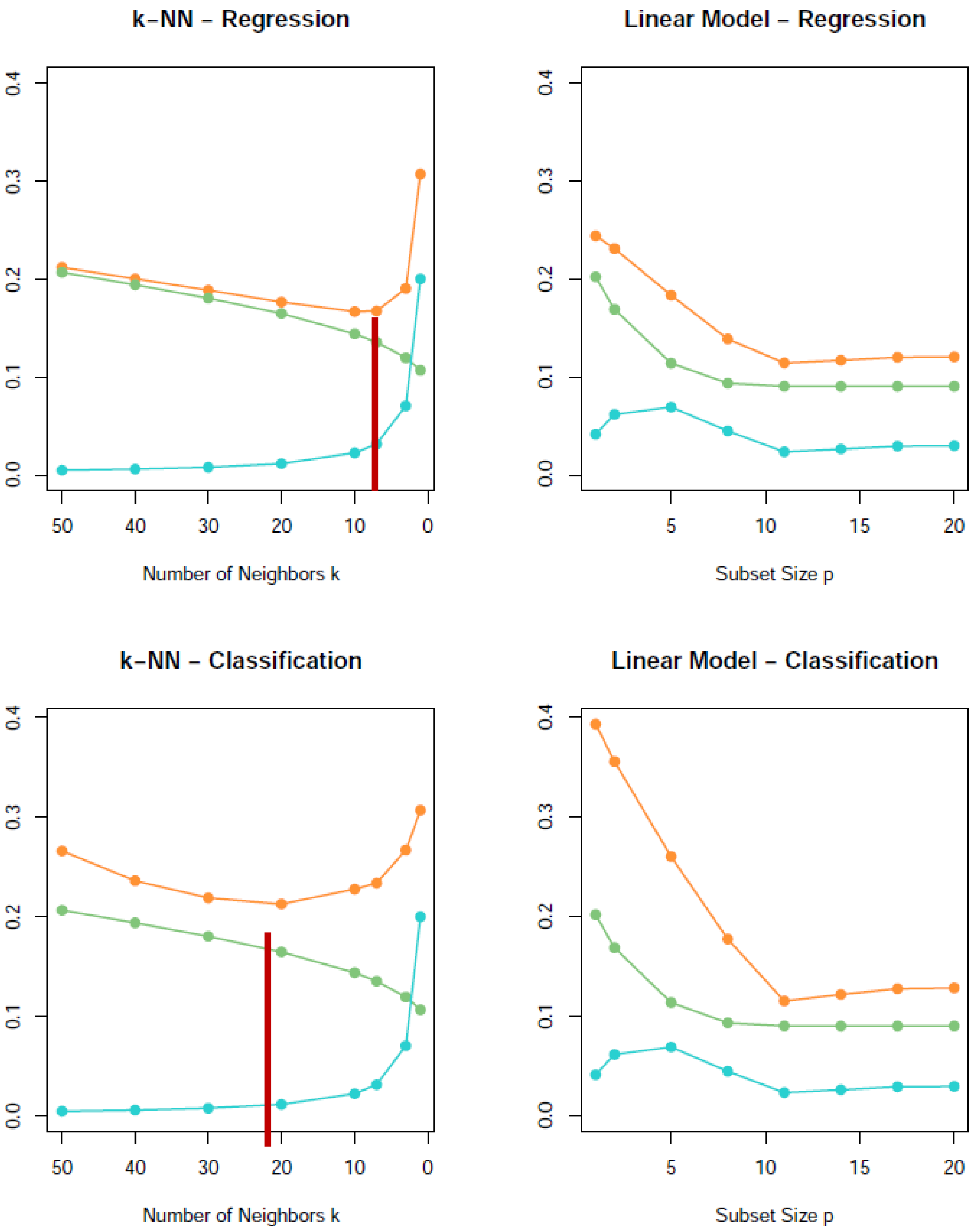
- There are 80 observations and 20 predictors, uniformly distributed in the hypercube $[0, 1]^{20}$.
- Left panels: Y is 0 if $X_1 \leq 1/2$, and 1 otherwise, and we apply k-nearest neighbors.
- Right panels: *Y is 1* if $\sum_{j=1}^{10} X_j \geq 5$, and *0* otherwise. We use best subset linear regression of size p.

- The bias–variance tradeoff **behaves differently** for 0–1 loss than it does for squared error loss.

- Assume
  - The true probability of class 1 is 0.9
  - The expected value of our estimate is 0.6.

- **The squared bias** $(0.6-0.9)^2$ which is considerable
- **The prediction error** is zero since we make the correct decision.

The prediction error (red), squared bias (green) and variance (blue)



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Question?

- How to describe the generalization performance of model?
  - Cross-validation
  - Resampling?

Optimism of the Training Error Rate

- Training Error < True Error

$$\text{Training Error} \quad \overline{err} = \frac{1}{N}\sum_{i=1}^{N} L(y_i, \hat{f}(x_i))$$

$$\text{True Error} \quad Err = E[L(Y, \hat{f}(X))]$$

- Err is extra-sample error
- The in-sample error

$$Err_{in} = \frac{1}{N}\sum_{i=1}^{N} E_{Y^{new}}\left[L(Y_i^{new}, \hat{f}(x_i)) | \mathcal{T}\right]$$

- Optimism:

$$\boxed{op \equiv Err_{in} - \overline{err}}$$

Optimism of the Training Error Rate

- The average optimism is the expectation of the optimism over training sets

$$\boxed{\omega \equiv \mathrm{E}_{y}(op) \equiv \mathrm{E}_{y}(Err_{in} - \overline{err})}$$

$$\text{Training Error} \quad \overline{err} = \frac{1}{N}\sum_{i=1}^{N} L(y_i, \hat{f}(x_i))$$

$$\text{In sample error:} \quad Err_{in} = \frac{1}{N}\sum_{i=1}^{N} E_{Y^{new}}\left[L(Y_i^{new}, \hat{f}(x_i)) | \mathcal{T} \right]$$

$$\omega = E_y(op) = E_y\left[Err_{in} - \overline{err}\right]$$

$$= \frac{1}{N}\sum_{i=1}^{N} E_{Y^{new}} E_y\left[(Y_i^{new} - \hat{f}(x_i))^2 - (y_i - \hat{f}(x_i))^2\right]$$

$$(Y_i^{new} - \hat{f}(x_i))^2 - (y_i - \hat{f}(x_i))^2$$

$$= (Y_i^{new})^2 - 2Y_i^{new}\hat{f}(x_i) - y_i^2 + 2y_i\hat{f}(x_i)$$

$$\hat{y}_i = \hat{f}(x_i)$$

$$E_{Y^{new}}(Y_i^{new})^2 = E_y y_i^2$$

$$E_{Y^{new}} E_y\left[(Y_i^{new} - \hat{f}(x_i))^2 - (y_i - \hat{f}(x_i))^2\right]$$

$$= 2E[y_i, \hat{y}_i] - 2E\hat{y}_i E y_i = \boxed{2Cov(\hat{y}_i, y_i)}$$

Optimism of the Training Error Rate

- For squared error, 0-1, other loss function：

$$\omega = \mathrm{E}_y(op) = \frac{2}{N}\sum_{i=1}^{N} Cov(\hat{y}_i, y_i)$$

$$Err_{in} = E_y\left(\overline{err}\right) + \frac{2}{N}\sum_{i=1}^{N} Cov(\hat{y}_i, y_i)$$

- $\hat{y}_i$ is obtained by a linear fit with d inputs or basis function, a simplification is:

$$Err_{in} = E_y\left(\overline{err}\right) + 2\frac{d}{N}\sigma_\varepsilon^2, \qquad \sum_{i=1}^{N} \mathrm{cov}(\hat{y}_i, y_i) = d\sigma_\varepsilon^2$$

- If the dimension / the number of Basis Functions increases, Optimism will increase too.
- If the number of training samples, Optimism will decrease

In-sample Prediction Error

- The general form of the in-sample estimates is

$$\hat{Err}_{in} = E_y[\overline{err}] + \hat{op}$$

- d parameters are fit under Squared error loss

$$C_p \text{ statistic : } C_p = \overline{err} + 2\frac{d}{N}\hat{\sigma}_\varepsilon^2$$

- Use a log-likelihood function to estimate Err_{in}

$$N \to \infty, \quad -2E\left[\log \Pr_\theta(Y)\right] \approx -\frac{2}{N}E\left[loglik\right] + 2\frac{d}{N}$$

$$loglik = \sum_{i=1}^{N} \log \Pr_\theta(y_i)$$

  – This relationship introduces the Akaike Information Criterion

Akaike Information Criterion

- Akaike Information Criterion is more generally applicable estimate of Err_{in}

- A set of models $f_{\alpha}(x)$ with a turning parameter α :

$$\mathrm{AIC}(\alpha)=\overline{err}(\alpha)+2\frac{d(\alpha)}{N}\hat{\sigma}_{\varepsilon}^{2}$$

$\overline{err}(\alpha)$:the training error; $d(\alpha)$: number of parameters

- $\mathrm{AIC}(\alpha)$ provides an estimate of the test error curve, and we find the turning parameter $\hat{\alpha}$ that minimizes it.

$$\{f_{\hat{\alpha}}(x)\,|\,\hat{\alpha}:\min\mathrm{AIC}(\hat{\alpha})\}$$

Akaike Information Criterion

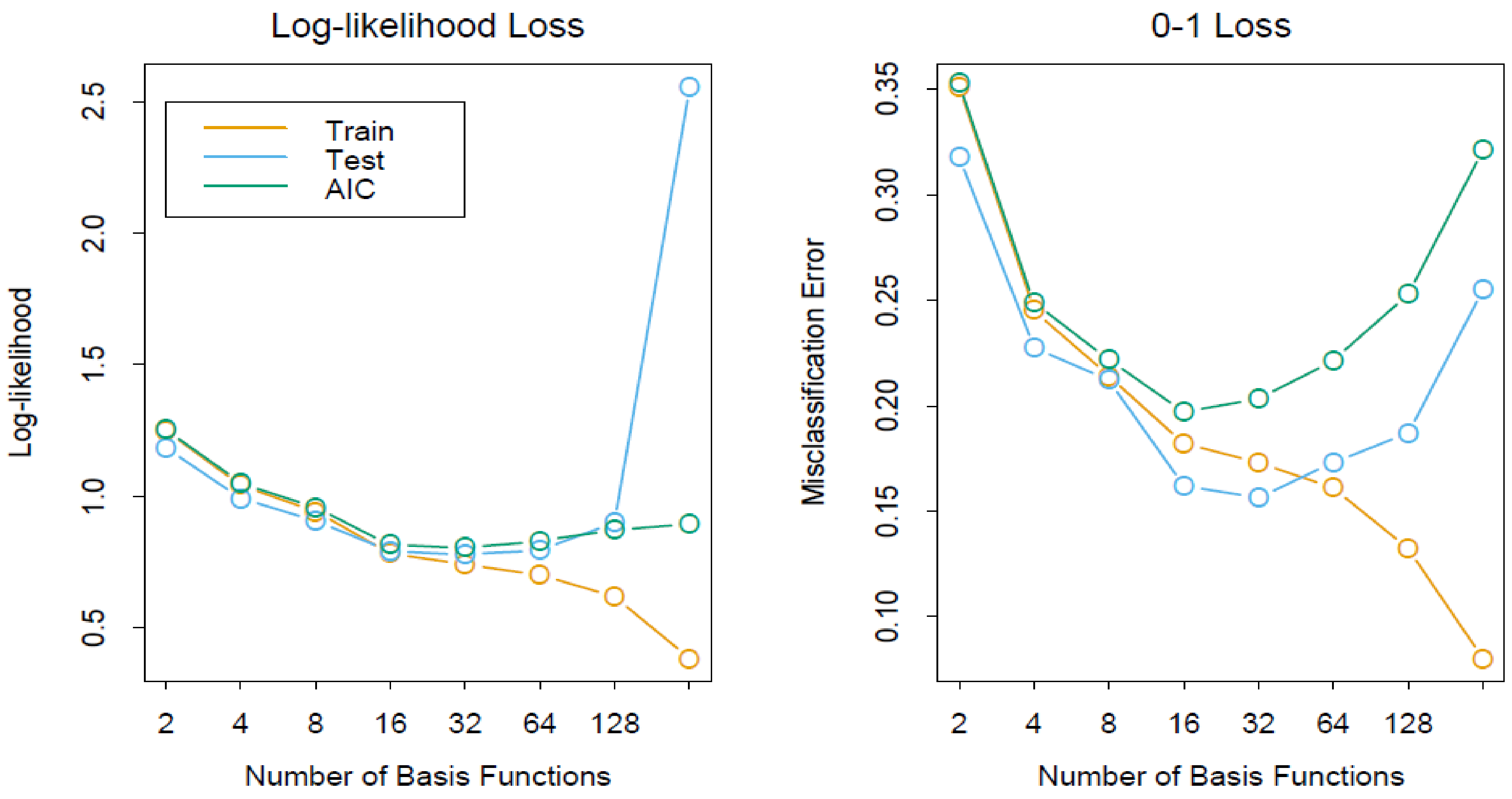
- For the logistic regression model, using the binomial **log-likelihood.**

$$\text{AIC} = -\frac{2}{N} E[\log lik] + 2\frac{d}{N}$$

- For Gaussian model the **AIC** statistic equals to the $\mathbf{C_p}$ statistic.

$$\text{AIC} = C_p = \overline{err} + 2\frac{d}{N}\hat{\sigma}_\varepsilon^2$$

Phoneme Recognition (AIC)



- Data: Spoken Vowels

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Effective number of parameters

- A linear fitting method:

$$\hat{y} = Sy, \quad S \text{ is } N \times N \text{ matrix, depending on } x_i$$

- Effective number of parameters:

$$d(S) = \mathrm{trace}(S)$$

  – If S is an orthogonal projection matrix onto a basis set spanned by M features, then:

$$\mathrm{trace}(S) = M$$

  – $\mathrm{trace}(S) = M$ is the correct quantity to replace d in the $\mathbf{C_p}$ statistic

Bayesian Approach & BIC

- The Bayesian Information Criterion (BIC)

$$\mathrm{BIC} = -2loglik + (\log N)d$$

- Gaussian model:
  - Variance σ_ε^2

$$-2loglik = C\sum_{i=1}^{N}(y_i - \hat{f}(x_i))^2/\sigma_\varepsilon^2 = N\cdot\overline{err}/\sigma_\varepsilon^2$$

$$\mathrm{BIC} = \frac{N}{\sigma_\varepsilon^2}[\overline{err} + \boxed{(\log N)\frac{d}{N}\sigma_\varepsilon^2}]$$

  - BIC is proportional to $\mathrm{AIC}(\mathrm{C_p})$, 2 replaced by $\log N$
  - $N > e^2 \approx 7.4$, BIC tends to choose simple model

Bayesian Model Selection

- BIC derived from Bayesian Model Selection
- Candidate models $\mathcal{M}_m$, model parameter θ_m and a prior distribution $\Pr(\theta_m \mid M_m)$
- Posterior probability:

$$\Pr(M_m \mid \mathrm{Z}) \propto \Pr(M_m)\Pr(\mathrm{Z} \mid M_m)$$
$$\propto \Pr(M_m)\int \Pr(\mathrm{Z} \mid \theta_m, M_m)\Pr(\theta_m \mid M_m)d\theta_m$$

- Z represents the training data $\{x_i, y_i\}_1^N$

Bayesian Model Selection

- Compare two models M_m and M_ℓ

$$\frac{\Pr(M_m \mid \mathrm{Z})}{\Pr(M_\ell \mid \mathrm{Z})} = \frac{\Pr(M_m)}{\Pr(M_\ell)} \frac{\Pr(\mathrm{Z} \mid M_m)}{\Pr(\mathrm{Z} \mid M_\ell)}$$

- If the odds(胜率) are greater than 1, model m will be chosen, otherwise choose model ℓ
- Bayes Factor:

$$\mathrm{BF}(\mathrm{Z}) = \frac{\Pr(\mathrm{Z} \mid M_m)}{\Pr(\mathrm{Z} \mid M_\ell)}$$

  – The contribution of the data to the posterior odds

Bayesian Model Selection

- If the model prior Pr(M) is uniformly distributed，

$$\log \Pr(Z \mid M_m) = \log \Pr(Z \,\|\, \hat{\theta}_m, M_m\ ) - \frac{d_m}{2} \log N + O(1)$$

where $\hat{\theta}_m$ is maximum likelihood estimator,

d_m is the model dimension.

The Loss Function:

$$-2 \log \Pr(Z \,\|\, \hat{\theta}_m, M_m\ )$$

Minimizing BIC is equivalent to maximizing posterior

Advantage：When the true model is included in the model family, the number of samples tends to infinite, BIC selects the true model with probability one

Minimum Description Length(MDL)

- Problem：Optimal Coding
  - Message: a b c d
  - Coding： 0 10 110 111
  - Coding2： 110 10 111 0
- **Criterion：** Using the shortest coding length for the most frequent message.
- The probability of zi ： $\Pr(z_i)$
- The coding length ： $l_i = -\log \Pr(z_i)$

Minimum Description Length(MDL)

The Expected Description Lendth

$$E(\text{Length}) \geq -\sum \Pr(z_i) \log \Pr(z_i)$$

The equality holds if and only if $p_i = A^{-l_i}$。

$$Example: \quad \Pr(z_i) = 1/2;\ \ 1/4;\ \ 1/8;\ \ 1/8$$

Minimum Description Length(MDL)

Model： M; Parameter： θ; Input Output $Z = (X, y)$

Suppose the Conditional Probabilty function of y

$$p(y \mid \theta, M, X)$$

$$\text{length} = -\log Pr(y \mid \theta, M, X) - \log Pr(\theta \mid M)$$

$-\log Pr(y \mid \theta, M, X)$： the average code length for transmitting the discrepancy between the model and actual target values

$-\log Pr(\theta \mid M)$： the average code length for transmitting the model parameters

Minimum Description Length(MDL)

$Assume\ \ y \sim N(\theta, \sigma^2)$, and parameter $\theta \sim N(0,1)$

$$\text{Length} = \text{Const.} + \log \sigma + \frac{(y-\theta)^2}{\sigma^2} + \frac{\theta^2}{2}$$

=> the smaller σ is, the shorter on average is the message length, since y is more concentrated around θ.

MDL Principle： Select a model, minimizing

$$\text{length} = -log\,Pr(y \mid \theta, M, x) - log\,Pr(\theta \mid M).$$

where model M is described by the parameter θ

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Vapnik-Chernovenkis Dimension

- Problem：How to select the model dimension d? which describes the model complexity
- VC dimension is a critical index describing the model complexity

$$\text{Function family:}\quad \{f(x,\alpha)\}, x \in IR^p$$

$$\alpha \text{ -- } parameter,\ f \text{ -- } index \text{ function}$$

$$Example:\ \alpha = (\alpha_0,\ \alpha_1),\ \text{linear function family}$$

$$f = I(\alpha_0 + \alpha^T{}_1 x > 0);\qquad f \text{ complexity: } p+1$$

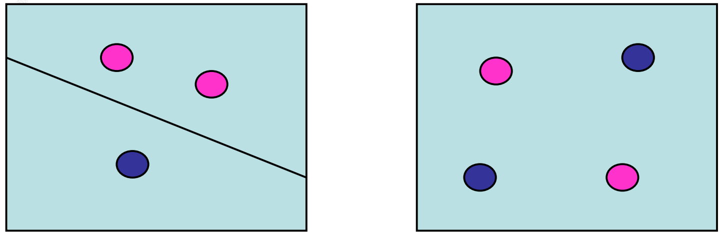
$$\text{Another example}\quad x \in IR, f(x,\alpha) = I(\sin\alpha \cdot x)?$$

f has only one parameter。

VC dimension

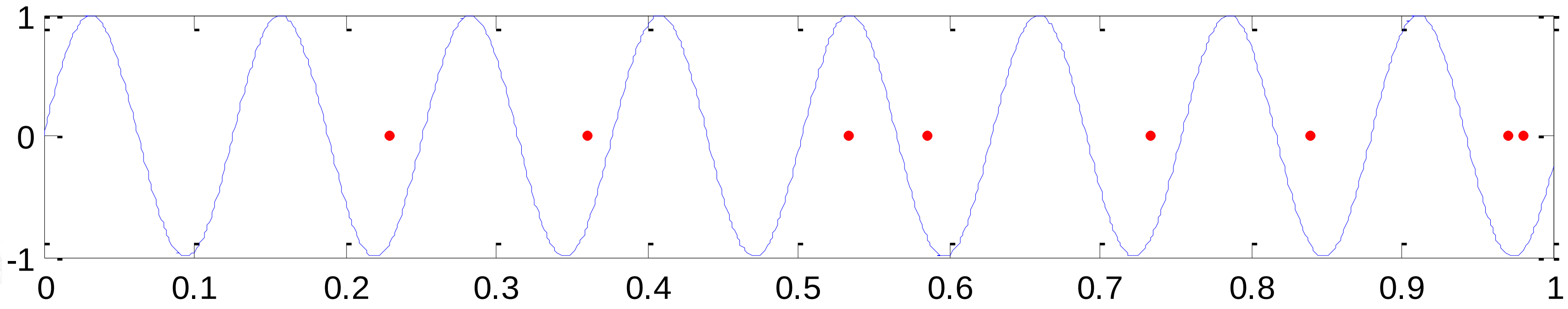
- The VC dimension of function family $\{f(x,\alpha)\}$ is defined to be the largest number *of points that can be* shattered *by members of*

$$\{f(x,\alpha)\}$$



- The VC dimension of 2d linear function family is 3.

- $\{\sin(\alpha x)\}$ its VC dimension is infinite.



VC Dimension

- The VC dimension of a class of real-valued functions $\{g(x,\alpha)\}$ is defined to be the VC dimension of the indicator class $\{I(g(x,\alpha)-\beta>0)\}$ where β takes values over the range of g.

- Assume has VC dimension h, the sample number *N*.

$$Err \le \overline{err} + \frac{\varepsilon}{2}\left(1+\sqrt{1+\frac{4\overline{err}}{\varepsilon}}\right) \quad 二类分类$$

$$Err \le \frac{\overline{err}}{(1-c\sqrt{\varepsilon})_+}; 回归 \quad \varepsilon = a_1 \frac{h[\log(a_2 N/h+1)-\log(\eta/4)]}{N}$$

$$0 < a_1 \le 4,\ 0 < a_2 \le 2$$

. Cherkassky and Mulier (2007, pages 116–118)

Cross Validation

1	2	3	4	5
Training	Training	Testing Set	Training	Training

Cross Validation

- Denote the fitted function by $\hat{f}^{-k}(x)$ with removing k-th fold data. Then the cross-validation estimate of prediction error is

$$\mathrm{CV}(\hat{f}) = \frac{1}{N}\sum_{i=1}^{N} L(y_i, \hat{f}^{-k}(x_i))$$

- The case K = N, *leave-one-out* cross-validation.

- Given model family $f(x,\alpha)$ indexed by a tuning parameter α.
- $\hat{f}^{-k}(x,\alpha)$: fited with the *k*th part of the data removed.

$$\mathrm{CV}(\hat{f},\alpha) = \frac{1}{N}\sum_{i=1}^{N} L(y_i, \hat{f}^{-k}(x_i,\alpha))$$

- Here it looks like a model with about p = 9predictors would be chosen, while the true model uses p = 10.

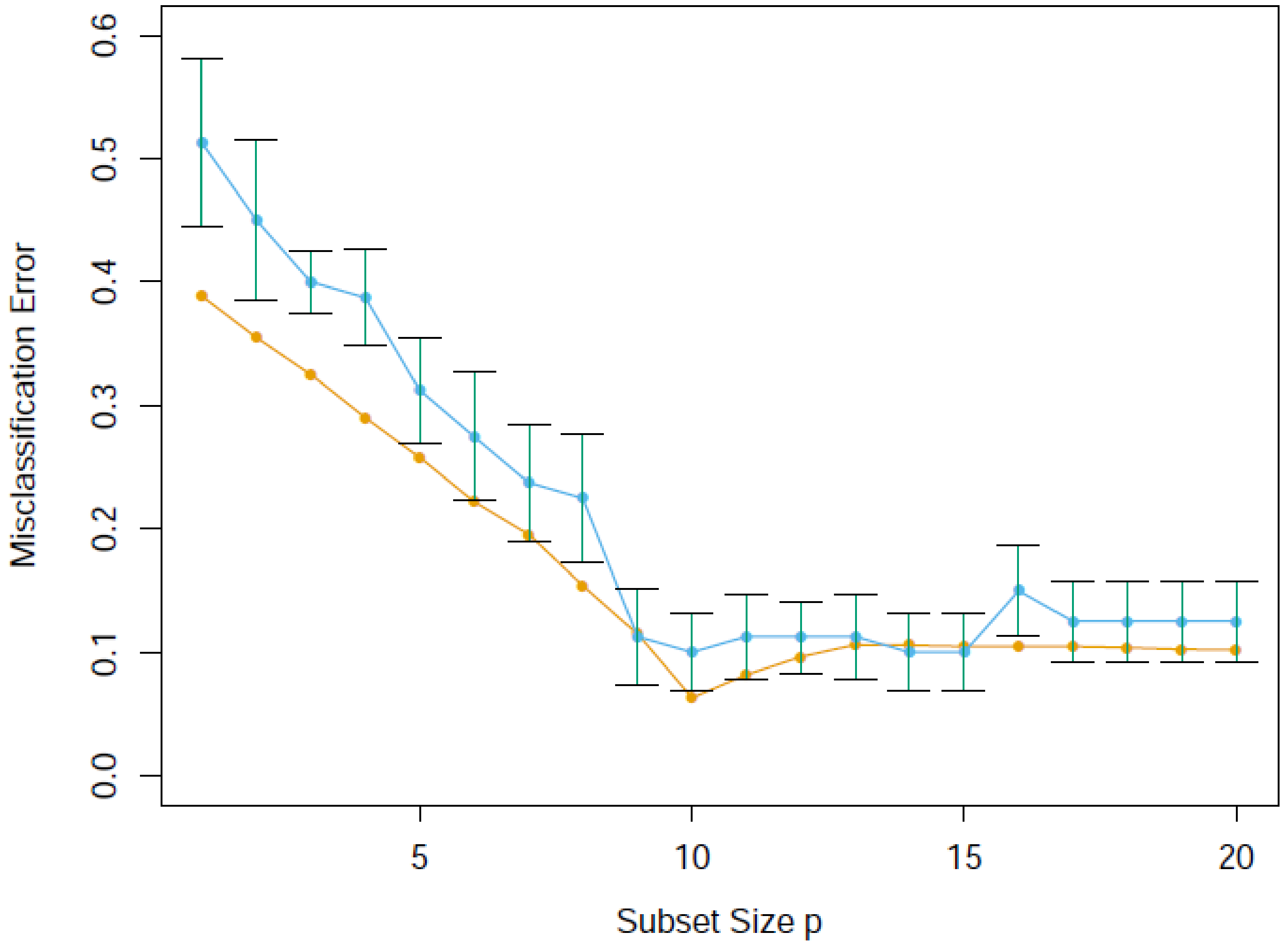


FIGURE 7.9. *Prediction error (orange) and tenfold cross-validation curve (blue) estimated from a single training set, from the scenario in the bottom right panel of Figure 7.3.*

Generalized cross-validation

- Linear fitting method：

$$\hat{y} = Sy$$

- For linear fitting methods,

$$\mathrm{CV}(\hat{f}) = \frac{1}{N}\sum_{i=1}^{N}\left[y_i - \hat{f}^{-k}(x_i)\right]^2 = \frac{1}{N}\sum_{i=1}^{N}\left[\frac{y_i - \hat{f}(x_i)}{1 - S_{ii}}\right]^2,$$

- where Sii is the ith diagonal element of S

$$\mathrm{GCV}(\hat{f}) = \frac{1}{N}\sum_{i=1}^{N}\left[\frac{y_i - \hat{f}(x_i)}{1 - trace(S)/N}\right]^2.$$

Right Way to Do CV?

- A typical strategy for CV might be as follows:
  - Screen the predictors: find a subset of “good” predictors that show fairly strong (univariate) correlation with the class labels
  - Using just this subset of predictors, build a multivariate classifier.
  - Use cross-validation to estimate the unknown tuning parameters and to estimate the prediction error of the final model.
- Is this a correct application of cross-validation?

A Toy Model

- Consider a scenario with $N = 50$ samples in two equal-sized classes, and $p = 5000$ quantitative predictors (standard Gaussian) that are independent of the class labels.
- The true (test) error rate of any classifier is 50%.
- Step (1): the 100 predictors having highest correlation with the class labels, and then using a 1-nearest neighbor classifier, based on just these 100 predictors.
- Step (2): Over 50 simulations from this setting, the average CV error rate was 3%, far lower than the true error rate of 50%.

Right Way to Do CV?

- A typical strategy for CV might be as follows:
  - X Screen the predictors: find a subset of “good” predictors that show fairly strong (univariate) correlation with the class labels
  - Using just this subset of predictors, build a multivariate classifier.
  - Use cross-validation to estimate the unknown tuning parameters and to estimate the prediction error of the final model.

The Correct Way to Do CV

- A typical strategy for CV might be as follows:
  - Divide the samples into K cross-validation folds (groups) at random.
  - For each fold k = 1, 2, . . . ,K
    - Find a subset of “good” predictors that show fairly strong (univariate) correlation with the class labels, using all of the samples except those in fold k.
    - Using just this subset of predictors, build a multivariate classifier, using all of the samples except those in fold k.
    - Use the trained classifier to predict the class labels for the samples in fold k.

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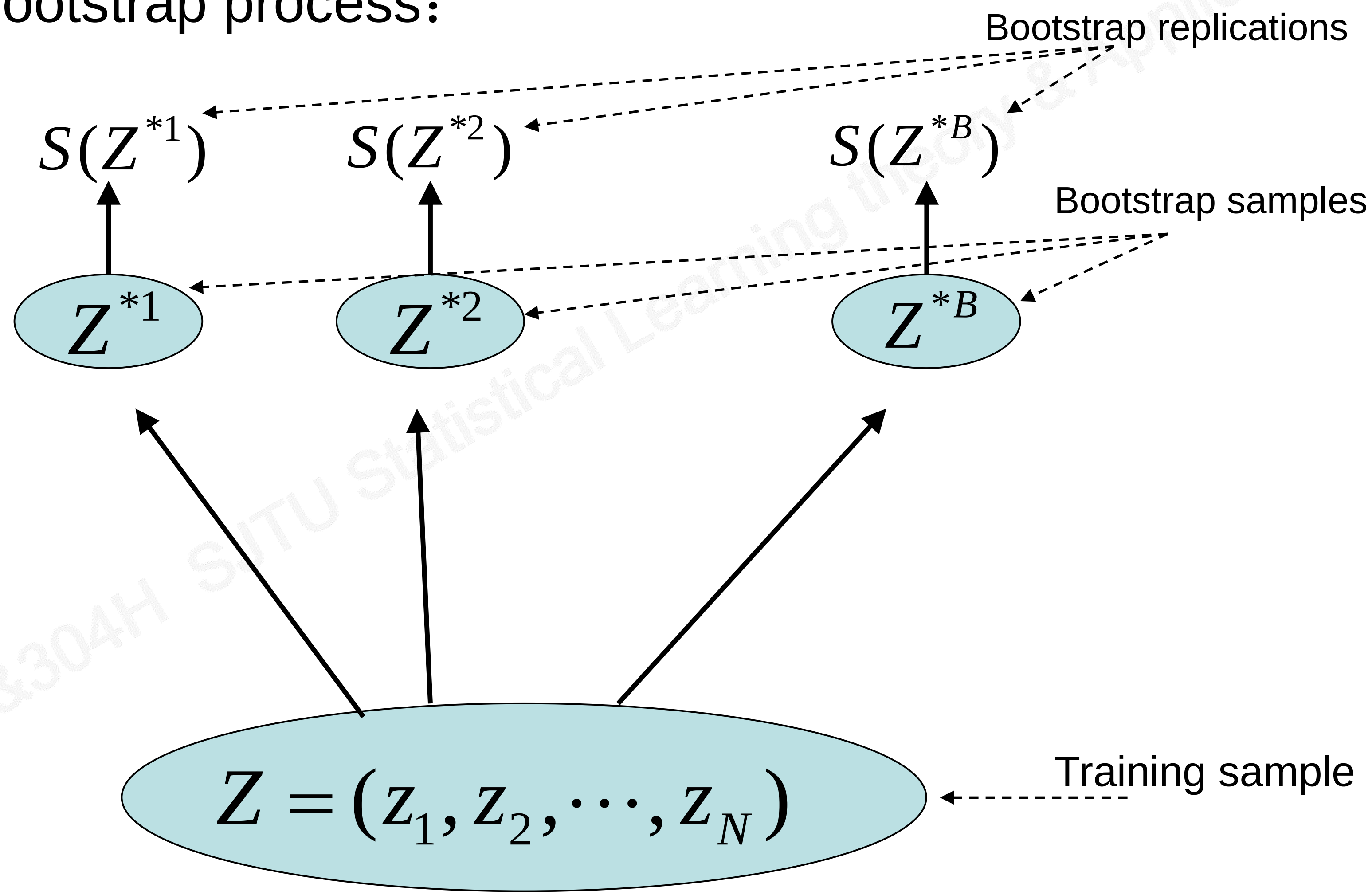
Bootstrap Methods

- Schematic of the bootstrap process：



Bootstrap Methods

- Basic Idea：The basic idea is to randomly draw datasets with replacement from the training data, each sample the same size as the original training set。
- B times (B = 100 say), producing B bootstrap datasets

$$\hat{f}^{*b}(x_i) \text{ is the prediction function at } x_i$$

- The bootstrap error

$$Err_{boot} = \frac{1}{B}\frac{1}{N}\sum_{b=1}^{B}\sum_{i=1}^{N} L(y_i, \hat{f}^{*b}(x_i))$$

Review of the Talk

- Model selection and assessment
- How to derive model selection criterion
  - In-sample error
- What are the most popular model selection criteria
  - AIC; BIC; MDL; VC
- CV for model selection
- Bootstrap method

The End