13. Model selection and model validation

- *•* model selection aspects
- *•* bias and variance
- *•* model selection: criterions, cross-validation
- *•* model validation: whiteness test, cross-correlation test

Factors in model selection

objective: obtain a good model at a low cost

- 1. **quality of the model:** defined by a measure of the goodness, e.g., the mean-squared error, log-likelihood
	- *•* MSE consists of a *bias* and a *variance* contribution
	- a complex model has small bias but higher variance (than a simple model)
	- *•* the best model structure is therefore a trade-off between *flexibility* and *parsimony*
- 2. **price of the model:** an estimation method (which typically results in an optimization problem) highly depends on the model structures, which influences:
	- algorithm complexity
	- *•* properties of the loss function
- 3. **intended use of the model:** prediction, controller design, inference

Bias-variance decomposition

assume that the observation *Y* obeys

$$
Y = f(X) + \nu
$$
, $\mathbf{E}\nu = 0$, $\mathbf{cov}(\nu) = \sigma^2$

the mean-squared error of a regression fit $\hat{f}(X)$ at $X = x_0$ is

$$
MSE = \mathbf{E}[(Y - \hat{f}(x_0))^2 | X = x_0]
$$

= $\sigma^2 + [\mathbf{E}\hat{f}(x_0) - f(x_0)]^2 + \mathbf{E}[\hat{f}(x_0) - \mathbf{E}\hat{f}(x_0)]^2$
= $\sigma^2 + \text{Bias}^2(\hat{f}(x_0)) + \text{Var}(\hat{f}(x_0))$

- *•* this relation is known as **bias-variance decomposition**
- \bullet no matter how well we estimate $f(x_0)$, σ^2 represents *irreducible error*
- typically, the more complex we make model \hat{f} , the lower the bias, but the higher the variance

proof of bias-variance decomposition: note that

- *•* the true *f* is deterministic
- $\mathbf{var}(Y|X=x) = \sigma^2$ and $\mathbf{E}[Y|X=x] = f(x)$
- \bullet $\hat{f}(x)$ is random

we will omit the notation of conditioning on $X = x$

$$
\mathbf{E}[(Y - \hat{f}(X))^2] = \mathbf{E}[Y^2] + \mathbf{E}[\hat{f}(x)^2] - \mathbf{E}[2Y\hat{f}(x)]
$$

\n
$$
= \mathbf{var}(Y) + \mathbf{E}[Y]^2 + \mathbf{var}\,\hat{f}(x) + \mathbf{E}[\hat{f}(x)]^2 - 2f(x)\mathbf{E}[\hat{f}(x)]
$$

\n
$$
= \mathbf{var}(Y) + f(x)^2 + \mathbf{var}\,\hat{f}(x) + \mathbf{E}[\hat{f}(x)]^2 - 2f(x)\mathbf{E}[\hat{f}(x)]
$$

\n
$$
= \sigma^2 + \mathbf{var}\,\hat{f}(x) + (f(x) - \mathbf{E}[\hat{f}(x)])^2
$$

\n
$$
= \sigma^2 + \mathbf{var}\,\hat{f}(x) + (\mathbf{E}[f(x) - \hat{f}(x)])^2
$$

\n
$$
= \sigma^2 + \mathbf{var}\,\hat{f}(x) + [\text{Bias}(\hat{f}(x))]^2
$$

Bias and variance in linear models

two nested linear regression models: predictor X in \mathcal{M}_1 is also contained in \mathcal{M}_2

$$
\mathcal{M}_1: y = X\beta \quad \text{VS} \quad \mathcal{M}_2: y = \begin{bmatrix} X & \tilde{x} \end{bmatrix} \begin{bmatrix} \beta \\ \alpha \end{bmatrix} \triangleq Z\gamma
$$

setting: two models are estimated by LS method, denoted by *β*ˆ and *γ*ˆ

- 1. *M*² has lower MSE in predicting *y* than the MSE of *M*¹
- 2. **cov** $(\hat{\beta})$ of \mathcal{M}_2 is larger than $\mathbf{cov}(\hat{\beta})$ of \mathcal{M}_1
- 3. variance of \hat{y} from \mathcal{M}_2 is higher than that of \mathcal{M}_1

 \mathcal{M}_2 (complex model) has less bias but more variance both in estimator and prediction our proof will use subscript 1 for \mathcal{M}_1 and and 2 for \mathcal{M}_2

Inverse of block matrices

the inverse of a block matrix

$$
X = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \succ 0
$$

 can be obtained in block using Schur complement: $S = (D - CA^{-1}B)^{-1} \succ 0$

$$
X^{-1} = \begin{bmatrix} A^{-1} + A^{-1}B(D - CA^{-1}B)^{-1}CA^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -(D - CA^{-1}B)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{bmatrix} (1)
$$

we often encounter the difference of two quadratic forms

$$
\begin{bmatrix} u \\ v \end{bmatrix}^T \begin{bmatrix} A & B \\ B^T & D \end{bmatrix}^{-1} \begin{bmatrix} u \\ v \end{bmatrix} - u^T A^{-1} u = (v - B^T A^{-1} u)^T S^{-1} (v - B^T A^{-1} u) \ge 0 \tag{2}
$$

which is always non-negative

Model selection and model validation 13-6

proof of MSE² *≤* **MSE**¹

- let P_1 and P_2 be orthogonal projection of *y* onto $\mathcal{R}(X)$ and $\mathcal{R}(Z)$, resp
- \bullet it can be shown that $\mathsf{MSE}_1 = \|y\|_2^2 y^T P_1 y$ and $\mathsf{MSE}_2 = \|y\|_2^2 y^T P_2 y$
- \bullet it is left to show that $y^TP_2y \geq y^TP_1y$

$$
P_2 = Z(Z^T Z)^{-1} Z^T = \begin{bmatrix} X & \tilde{x} \end{bmatrix} \begin{bmatrix} X^T X & X^T \tilde{x} \\ \tilde{x}^T X & \tilde{x}^T \tilde{x} \end{bmatrix}^{-1} \begin{bmatrix} X^T \\ \tilde{x}^T \end{bmatrix}, \quad P_1 = X(X^T X)^{-1} X^T
$$

• apply the inverse of block matrix

$$
P_2 - P_1 = (\tilde{x} - X(X^T X)^{-1} X^T \tilde{x}) S^{-1} (\tilde{x} - X(X^T X)^{-1} X^T \tilde{x})^T \succeq 0
$$

where
$$
S = \tilde{x}^T \tilde{x} - \tilde{x}^T X (X^T X)^{-1} X^T \tilde{x}
$$

 $\mathbf{proof of } \mathbf{cov}(\hat{\beta}_2) \succeq \mathbf{cov}(\hat{\beta}_1)$

- \bullet $\mathbf{cov}(\hat{\beta}_2)$ is the leading $(1,1)$ block of $\mathbf{cov}(\hat{\gamma})$, while $\mathbf{cov}(\hat{\beta}_1) = (X^TX)^{-1}$
- \bullet use $\mathbf{cov}(\hat{\gamma}) = (Z^TZ)^{-1}$ and the inverse of block matrix

$$
(Z^T Z)^{-1} = \begin{bmatrix} X^T X & X^T \tilde{x} \\ \tilde{x}^T X & \tilde{x}^T \tilde{x} \end{bmatrix}^{-1} \triangleq \begin{bmatrix} A & B \\ B^T & D \end{bmatrix}^{-1} = \begin{bmatrix} A^{-1} + A^{-1} B S^{-1} B^T A^{-1} & \times \\ \times & \times & \end{bmatrix}
$$

where $S = D - B^T A^{-1} B \succeq 0$

 \bullet ${\bf cov}(\hat\beta_2)$ is bigger than ${\bf cov}(\hat\beta_1)$ because

$$
\mathbf{cov}(\hat{\beta}_2) - \mathbf{cov}(\hat{\beta}_1) = A^{-1} + A^{-1}BS^{-1}B^T A^{-1} - A^{-1} = A^{-1}BS^{-1}B^T A^{-1} \succeq 0
$$

proof of $var(\hat{y}_2) \geq var(\hat{y}_1)$

- suppose $\hat{y}_1 = u^T \hat{\beta}$ and $\hat{y}_2 = w^T \hat{\gamma}$ where $w = (u, v)$
- *•* we test prediction of *y* from new regressors *u* and (*u, v*)
- since the model is simply linear, the variance can be obtained by

$$
\mathbf{var}(\hat{y}_2) - \mathbf{var}(\hat{y}_1) = w^T \mathbf{cov}(\gamma)w - u^T \mathbf{cov}(\beta)u
$$

$$
= \begin{bmatrix} u \\ v \end{bmatrix}^T \begin{bmatrix} X^T X & X^T \tilde{x} \\ \tilde{x}^T X & \tilde{x}^T \tilde{x} \end{bmatrix}^{-1} \begin{bmatrix} u \\ v \end{bmatrix} - u^T (X^T X)^{-1} u
$$

• the difference is non-negative (using result on page 13-6)

Model properties

consider bias and variance of model with different structures

(T. Hastie *et.al. The Elements of Statistical Learning*, Springer, 2010 page 225)

a simple model has less flexibility (more bias) but easy to interpret and has less variance

U-shape of generalization error

models are estimated on training data set and evaluated on test set (unseen data)

- *•* training errors always decrease as model complexity increase
- *•* generalization error initially decreases as model picks up relevant features of data
- however, if the model complexity exceeds a certain degree, the generalization error can rise up again $-$ this is when we observe overfitting

Model fitting versus model complexity

- true AR model has order $p=5$
- *•* estimate AR model using LS method
- *•* plot loss function (MSE) at different model orders

- *•* the minimized loss is a decreasing function of the model order
- loss function begins to decrease as the model picks up the relevant features
- *•* as *p* increases, the model tends to *over fit* the data
- in practice, we look for the "knee" in the curve (around $p=5$)

Estimation data Test data 2 1.6 $-f(x)$ \bullet data 0_o $-Linear$ 1.4 1.5 -Quadratic -Smoothing spline 1.2 \hat{p} \mathcal{L} $\overline{1}$ 1 f \circ 0.5 0.8 $0.6\frac{1}{0}$ $0 - 2$ 0 0.5 1 1.5 2 -0.2 0 0.2 0.4 0.6 0.8 1 $\hat{\mathcal{L}}$ \boldsymbol{x} **Polynomial models Smoothing splines** 0.08 0.1 **B**-Estimation \leftarrow Test 0.08 0.06 ് ^{0.06}
S MSE 0.04 \mid 0.04 0.02 $0.02\frac{1}{0}$ $0\frac{L}{0}$ 0 2 4 6 8 10 0 5 10 15 20 Model complexity Model complexity

Observe overfitting on test error

- *•* too complex models cannot generalize well on test (unseen) data
- overfitting occurs when MSE on test set decreases but starts to rise again

Does overfitting always occur?

- when the true description is highly nonlinear, test MSE does not significantly increase
- overfitting is apparent when the estimated model is more complex (than it should be) in order to explain a simpler ground-truth model

Model selection

- *•* model selection criterions
- *•* cross-validation

Model selection criterion

parsimony principle: among competing models which all explain the data well, the model with the smallest number of parameters should be chosen

a model selction criterion consists of two parts:

 $loss function + model complexity$

- the first term is to assess the quality of the model, e.g., likelihood function, RSS, MSE, Fit Percent (1 *− ∥y−y*ˆ*∥ ∣*^{*y*}−*y*^{*∥*}</sup>/ *×* 100%
- *•* the second term is to penalize the model order and grows as the number of parameters increases
- *•* we choose the best model as the one with the lowest model selection score

What exactly do we choose in a model?

consider an additive error model

$$
y_i = g(x_i; \theta) + e_i, \quad e_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, 2, \dots, N
$$

model selection can be choosing

- *•* a list of predictors *x*
- *•* a degree of polynomial function *g*
- *•* a number of basis functions used to decompose *g*

consider a dynamical model with additive noise (*e.g.*, ARX, FIR)

$$
y(t) = g(t, Z^{t-1}; \theta) + e(t), \quad e(t) \sim \mathcal{N}(0, \Sigma), \quad t = 1, 2, ..., N
$$

model selection can be choosing order (*p, q, r*) in ARMA model, or order of FIR

let α be a parameter that indicates model complexity

- *•* ARX or FIR orders
- *•* penalty parameter in regularized regression
- the number of predictors in regression models

what can be a function of *α* ?

- model quality: it indicate the model fitting at such degree of complexity such as $\mathcal{L}(\alpha)$ *,* RSS(α)
- prediction error: $\varepsilon(t, \theta) = y(t) \hat{y}(t, \theta)$
- *•* the effective number of parameters (*d*)

other parameters that involve in model selection scores: *N* (samples) and output dimension

Model selection scores

model quality: *L*: log-likelihood, *V* : loss function **model complexity:** *d*: effective number of parameters

- *•* Akaike information criterion (AIC): AIC(*α*) = *−*2*L*(*α*) + 2*d*
- corrected Akaike information (AICc): $\text{AICc}(\alpha) = -2\mathcal{L}(\alpha) + 2d + \frac{2d(d+1)}{N-d-1}$ *N−d−*1
- *•* Bayesian information criterion (BIC): BIC(*α*) = *−*2*L*(*α*) + *d* log *N*
- \bullet Akaike's final prediction-error criterion (FPE): $\mathsf{FPE}(\alpha) = V(\hat{\theta}) \left(\frac{1+d/N}{1-d/N} \right)$ 1*−d*/*N* $\overline{}$
- Mallow's C_p : $C_p(\alpha) = \frac{1}{N}$ $[RSS(\alpha) + 2d\hat{\sigma}^2]$
- *•* adjusted *^R*² : 1 *−* RSS(*α*)/(*N−d−*1) TSS/(*N−*1)

Variable selection in linear regression

model: $\hat{y} = \sum_{k=1}^{n} a_k \cos(kx) + b_k \sin(kx)$ for $n = 1, 2, \ldots, 20$ and $N = 50$

- *•* aim to choose the number of basis function (*n*)
- set the effective number of parameters $d = 2n$ (the number of $sin(kx)$, $cos(kx)$)
- *•* compute [∆]AIC, [∆]AICc, [∆]BIC (subtracted by its minimum), *^Cp*, adjusted *^R*²

- AIC and adjusted R^2 chose a complex model, while AICc and BIC picked 4 basis functions (simpler), and *C^p* chose 7 basis functions
- $\bullet\,$ train MSE always decreases, as well as, R^2 always increases but the curves have a knee around $n = 4$

Choosing AR lag order

fitting AR model of order $p = 1, 2, \ldots, 20$ to unemployment rate time series

- the effective number of parameters is chosen as $d = p$
- *•* compute ∆AIC, ∆AICc, ∆BIC, FPE, train MSE, and Fit Percent
- *•* data samples: *N* = 245, examine two cases: (i) use all data (ii) use only half

left: use all data right: use half of data

- left: AIC, AICc and FPE tend to choose a higher order model ($p = 13$) but BIC prefers a simpler model (*p* = 2)
- *•* right: AICc chose a lower order model when *N* is halved (sample size was corrected)
- *•* both *train* MSE and Fit Percent are not good indicators for model selection

Log-likelihood based scores (AIC, AICc)

AIC, AICc, BIC use negative log-likelihood to indicate model quality

$$
AIC(\alpha) = -2\mathcal{L}(\alpha) + 2d
$$

\n
$$
AICc(\alpha) = -2\mathcal{L}(\alpha) + 2d + \frac{2d(d+1)}{N - d - 1}
$$

\n
$$
BIC(\alpha) = -2\mathcal{L}(\alpha) + d \log N
$$

• AIC is an approximation of Kullback-Leibler (KL) divergence between the true $\textsf{density}\,\left(f(x)\textsf{ and the model}\left(g(x|\hat{\theta})\right)\right)$

$$
\begin{array}{lcl} I(f,g) & = & \displaystyle \int f(x) \log(f(x)/g(x|\theta)) dx \\ \\ -\mathcal{L}(\hat{\theta}) + d & \approx & \mathbf{E}_{\hat{\theta}}[I(f(x),g(x|\hat{\theta}))] + \text{constant} \end{array}
$$

• AICc penalizes more on complexity for small *N* (as quadratic term in *d*); it approaches AIC for large samples (large *N*)

Log-likelihood based score (BIC)

- *•* BIC penalizes more on complexity than AIC (as indicated by log *N >* 2)
- *•* when model candidates contain a true model, BIC is consistent (probability of choosing the correct model \rightarrow 1 as $N \rightarrow \infty$)
- *•* model with minimum BIC *⇔* model with *highest* posterior density

$$
\text{posterior odds} = \frac{P(\mathcal{M}_m|\text{data})}{P(\mathcal{M}_l|\text{data})} = \underbrace{\frac{P(\mathcal{M}_m)}{P(\mathcal{M}_l)}}_{\text{prior}} \cdot \underbrace{\frac{P(\text{data}|\mathcal{M}_m)}{P(\text{data}|\mathcal{M}_l)}}_{\text{Bayes factor}}
$$

model prior tells which model is more likely to be preferred (by users)

- *•* when prior is not available (all models have equal probabilities), Bayes factor directly affects the posterior odds
- *•* BIC (with *−*2 factor) is an approximate of Bayes factor (see Hastie et al. book)
- for nested models \mathcal{M}_1 (complex), \mathcal{M}_2 (simple) with $d(\mathcal{M}_1) = d(\mathcal{M}_2) + m$
	- **–** AIC picks complex model if *L*(*M*1) *− L*(*M*2) *>* 2*m* (it's worth to use complex model since model quality improved much more)
	- **–** BIC picks complex model if *L*(*M*1) *− L*(*M*2) *> m* log *N*
- *•* improved gap of log-likelihood required by AIC is less than that of BIC; hence, AIC is prone to choosing a complex model more easily than BIC
- *•* for LR (log-likelihood ratio) test, with test statistic

$$
2(\mathcal{L}(\mathcal{M}_1)-\mathcal{L}(\mathcal{M}_2))\sim\mathcal{X}^2(m)
$$

- $-$ LR test picks \mathcal{M}_1 (complex) if $2\mathcal{L}(\mathcal{M}_1) > 2\mathcal{L}(\mathcal{M}_2)$ by $\mathcal{X}_{0.05}^2(m)$
- $-$ for $m < 7$, we have $2m < \mathcal{X}_{0.05}^2(m)$; hence, AIC tends to pick a complex model more easily than LR test in this case

Akaike's final prediction (FPE)

denote $V(\hat{\theta})$ a loss function used in prediction error method (*e.g.*, det or trace of error covariance)

$$
\text{FPE}(\alpha) = V(\hat{\theta}) \left(\frac{1+d/N}{1-d/N} \right)
$$

- *•* model complexity is cooperated in *multiplicative form* (as compared to additive form in AIC, BIC)
- $\bullet\,$ when model output is scalar, $V(\hat\theta)$ is simply MSE and FPE reduces to

$$
\text{FPE} = \frac{1}{N} \sum_{t=1} \varepsilon^2(t, \hat{\theta}) \cdot \frac{1 + d/N}{1 - d/N}
$$

• it was shown in Ljung book that FPE is a way to approximate of lim*^N→∞* **E**[*V* (*θ*)] (population), which can be estimated using $V(\hat{\theta})$ evaluated on *estimation data*

Mallow's *C^p*

C^p is mostly used in linear regression with *d* predictors and homoskedastic noise

$$
C_p(\alpha) = \frac{1}{N} \left[\text{RSS}(\alpha) + 2d\hat{\sigma}^2 \right]
$$

- *• C^p* uses *quadratic loss* to measure model quality
- \bullet $\hat{\sigma}^2$ is an estimate of noise variance using **full** model
- \bullet RSS/ N always decreases when d increases; penalty on complexity is put on $2d\hat{\sigma}^2$
- *•* in Hastie et al. book, it showed that *C^p* is an estimate of test MSE
- \bullet other form of C_p exists: $C_p = \mathrm{RSS}/\hat{\sigma}^2 + 2d N$ but result in choosing the same d

Adjusted *R*²

 \mathbb{R}^2 (coefficient of determination) is based on the decomposition:

$$
\underbrace{\sum_{i} (y_i - \bar{y})^2}_{\text{TSS}} = \underbrace{\sum_{i} (y_i - \hat{y}_i)^2}_{\text{RSS}} + \underbrace{\sum_{i} (\hat{y}_i - \bar{y})^2}_{\text{ESS}} + 2 \underbrace{\sum_{i} (y_i - \hat{y}_i)(\hat{y}_i - \bar{y})}_{\text{zero if model has a constant}}
$$

 R^2 is the proportion of the total variation in Y that can be linearly predicted by X

$$
R^2 = 1 - \frac{\text{RSS}}{\text{TSS}}, \quad \text{adjusted } R^2 = 1 - \frac{\text{RSS}(\alpha)/(N - d - 1)}{\text{TSS}/(N - 1)}
$$

• for linear model, ⁰ *[≤] ^R*² *[≤]* ¹ and always increases for larger models

- *•* the presence of *d* penalizes the criterion for the number of predictor variables
- $\bullet\,$ adjusted R^2 increases if the added predictor variables decrease RSS enough to compensate for the increase in *d*

Score relations

for Gaussian noise additive model, we can show that log-likelihood (up to constant) is

$$
-2\mathcal{L}(\theta) = \begin{cases} N \log \det \left(\frac{1}{N} \sum_{t=1} \varepsilon(t,\theta) \varepsilon(t,\theta)^T\right), & \text{if noise covariance is a parameter} \\ \frac{\text{RSS}(\theta)}{\sigma^2}, & \text{if noise variance is given} \end{cases}
$$

• for scalar output and noise variance is a parameter

$$
\mathsf{AIC}_{\mathsf{scaled}} = \mathsf{AIC}/N = \log(\mathsf{MSE}) + 2d/N \approx \log(\mathsf{FPE}), \text{ for } d \ll N
$$

 $\bullet\,$ for scalar output and noise variance is given as $\hat{\sigma}^2$ (as computed from full model)

$$
\text{AIC}_{\text{scaled}} = \text{AIC}/N = \frac{1}{N} \left(\frac{\text{RSS}(\theta)}{\hat{\sigma}^2} + 2d \right) = \hat{\sigma}^2 \cdot C_p
$$

AIC and *C^p* choose the same model in this case

Cross validation

- training error rate: the average error that results from using a trained model (or method) back on the training data set
- test error rate: the average error that results from using a statistical learning method to predict the response on a **new observation**
- *•* training error can be quite different from the test error rate
- *•* **cross validation** can be used to estimate *test error rate* using available data: split into training and validation sets
	- **–** validation set approach
	- **–** leave-one-out cross validation
	- **–** *k*-fold cross validation

Splitting data

- training set: used for fitting a model
- validation set: used for predicting the response from the fitted model

- validation set approach or hold out (left): randomly split data
- leave-one-out or LOOCV (middle): leave 1 sample for validation set
- k -fold (right): randomly split data into k folds; leave 1 fold for validation
	- repeat k times where each time a different fold is regarded as validation set and compute MSE_1 , MSE_2 , ..., MSE_k
	- the test error rate is estimated by **averaging** the k MSE's

Cross validation on polynomial order

 $N = 500$, show 7 runs of holdout, and 5-fold

- *•* result of holdout has high variation since it depends on random splitting
- *•* 5-fold results has less variation because MSE is averaged over *k* folds
- \bullet <code>LOOCV</code> requires N loops (high computation cost); <code>MSE</code> $_i$'s are highly correlated

Estimate a true test MSE by CV

accuracy of test error rate (on simulation data set): using model of smoothing splines

compute the *true test MSE* (assume to know true *f*) as a function of complexity

- *•* (left): cv estimates have the correct general U shape but underestimate test MSE
- *•* (center): cv gives overestimate of test MSE at high flexibility
- *•* (right): the true test MSE and the cv estimates are almost identical

Choosing penalty parameter in lasso

lasso can be used for feature selection by choosing a right amount of penalty

- *•* each penalty parameter *γ* corresponds to a sparsity pattern of *β*
- *•* vary *γ* and evaluate model selection scores and CV
- *• k*-fold, LOOCV, AIC and AICc chose smaller *γ* than the one selected by BIC
- \bullet solution path show the significant β_i 's selected from all methods

Model validation

the parameter estimation procedure picks out the *best* model

a problem of model validation is to verify whether *this best* model is "good enough" general aspects of model validation

- validation with respect to the purpose of the modeling
- *•* feasibility of physical parameters
- *•* consistency of model input-output behavior
- model order reduction
- *•* parameter confidence intervals
- *•* simulation and prediction

Validation of dynamical models

dgp: $y = Gu + He$ **model**: $\hat{y} = \tilde{G}u + \tilde{H}e$ *residual error:* $\varepsilon(t) = y(t) - \hat{y}(t)$

common validation approaches based on residual analysis

- whiteness test of residuals
- *•* cross-correlation test (between residual and input)
- *•* examination of model order

Whiteness test of residuals

residual error contain mismatch in *G* (system dynamic) and *H* (noise dynamic)

$$
\varepsilon(t)=(G-\hat{G})u+(H-\hat{H})e,\qquad R_{\varepsilon}(\tau)=\frac{1}{N}\sum_{t=\tau}^{N}\varepsilon(t)\varepsilon(t-\tau)
$$

- \bullet $\varepsilon(t)$ can be regarded as filtered noise if there is a model mismatch in *H* and $R_{\varepsilon}(\tau)$ is not significantly small at $\tau \neq 0$ ($y(t)$ could have been better predicted)
- apply hypothesis test $(H_0: \varepsilon$ is white) with test statistic

$$
W=\frac{N}{R_{\varepsilon}^2(0)}\sum_{\tau=1}^mR_{\varepsilon}^2(\tau)\overset{d}{\to}\chi^2(m)
$$

 $\bullet\,$ if $W>\mathcal{X}^{2}_{\alpha}(m)$, we reject H_{0} (reject the model and improve $\hat{H})$

Cross-correlation test

if *G*ˆ perfectly matches *G*, residual *ε* contains no dynamic of *u*, so the cross-correlation

$$
R_{\varepsilon u}(\tau) = \frac{1}{N} \sum_{t=\tau}^N \varepsilon(t) u(t-\tau)
$$

must be zero for all *τ*

- form a hypothesis test with $H_0: R_{\varepsilon u}(\tau)$ is zero
- *•* we can compute the test statistic

$$
W = Nr^{T}[R_{\varepsilon}(0)R_{u}]^{-1}r \stackrel{d}{\to} \chi^{2}(m)
$$

r is a sample cross-correlation, *R^ε* and *R^u* are auto-correlation

 $\bullet\,$ if $W>\mathcal{X}^2_\alpha(m)$, we reject H_0 (reject the model and improve $\hat{G})$

Residual analysis of ARMAX model

true system: ARMAX(2,2,3) and consider models ARX(3,3) and ARMAX(3,3,3)

- *•* ARX has a significant *Rε*(3) (more apparent than ARMAX) because ARX does not incorporate noise dynamic in the model
- **•** $R_{\varepsilon u}$ of both model stay inside the acceptable region (G [∂] was suitably estimated)

Model order examination

if a model is *overparametrized*, it is more likely to see zero-pole cancellation

compare ARMAX models of order (3,3,3) and (6,6,6)

Example of MATLAB commands

- *•* resid: residual analysis
- *•* compare: compare the prediction with the measurement
- *•* iopzplot: plots of zeros and poles

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