Linear Regression

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Model Building: Overview

Model-Building Steps

- Data collection and processing
- Exploratory data analysis
- Preliminary model investigation
- Model selection
- Model diagnostics and validation

Case Study: Surgical Unit

A hospital surgical unit was interested in predicting survival times of patients (in days, ascertained in a follow-up study) undergoing a particular type of liver operation. 108 such patients were randomly selected for this study. The following variables were measured for each patient: blood clotting score, prognostic index, enzyme function test score, liver function test score, age (in years), gender (male or female) and history of alcohol use (none, moderate or severe). We use half of the data to build the model (**training data**) and use the other half to perform model validation (**validation data**) later.

Model Building:

Exploratory Data Analysis

Exploratory Data Analysis

- Type of each variable: quantitative or qualitative?
- Distribution of each variable: symmetric or skewed? outliers? *
  if error → fix
  - Quantitative: histogram, boxplot, summary statistics, etc.
  - Qualitative: pie chart, frequency table, etc.
- Relationships among variables:
  - scatter plot matrix, correlation matrix, side-by-side box plots
  - nonlinear pattern? clusters? outliers?

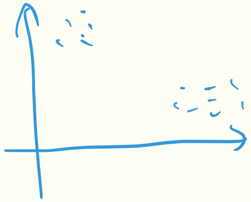


Figure: Histograms of quantitative variables

y

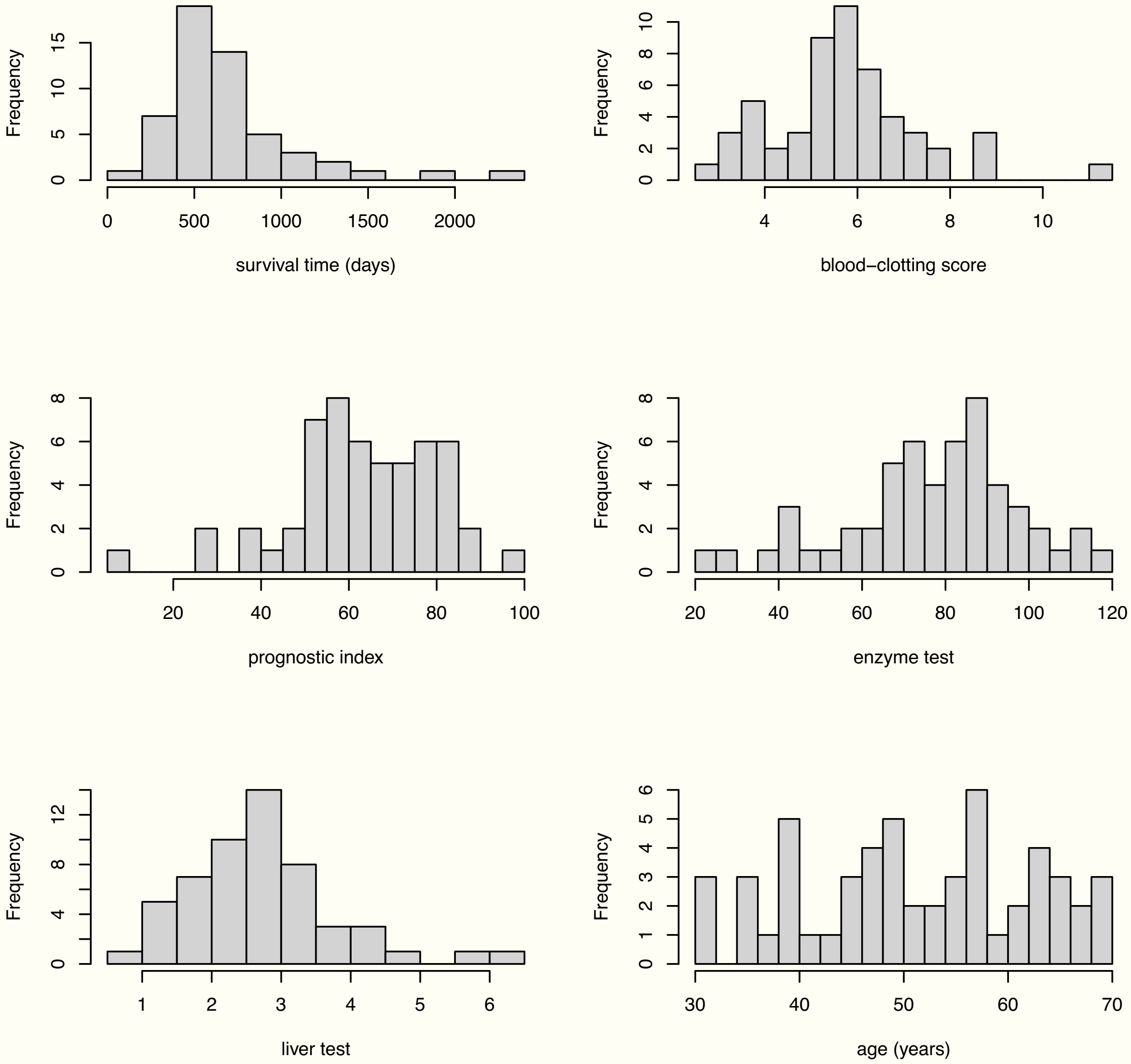


Figure: Scatter plot matrix of quantitative variables

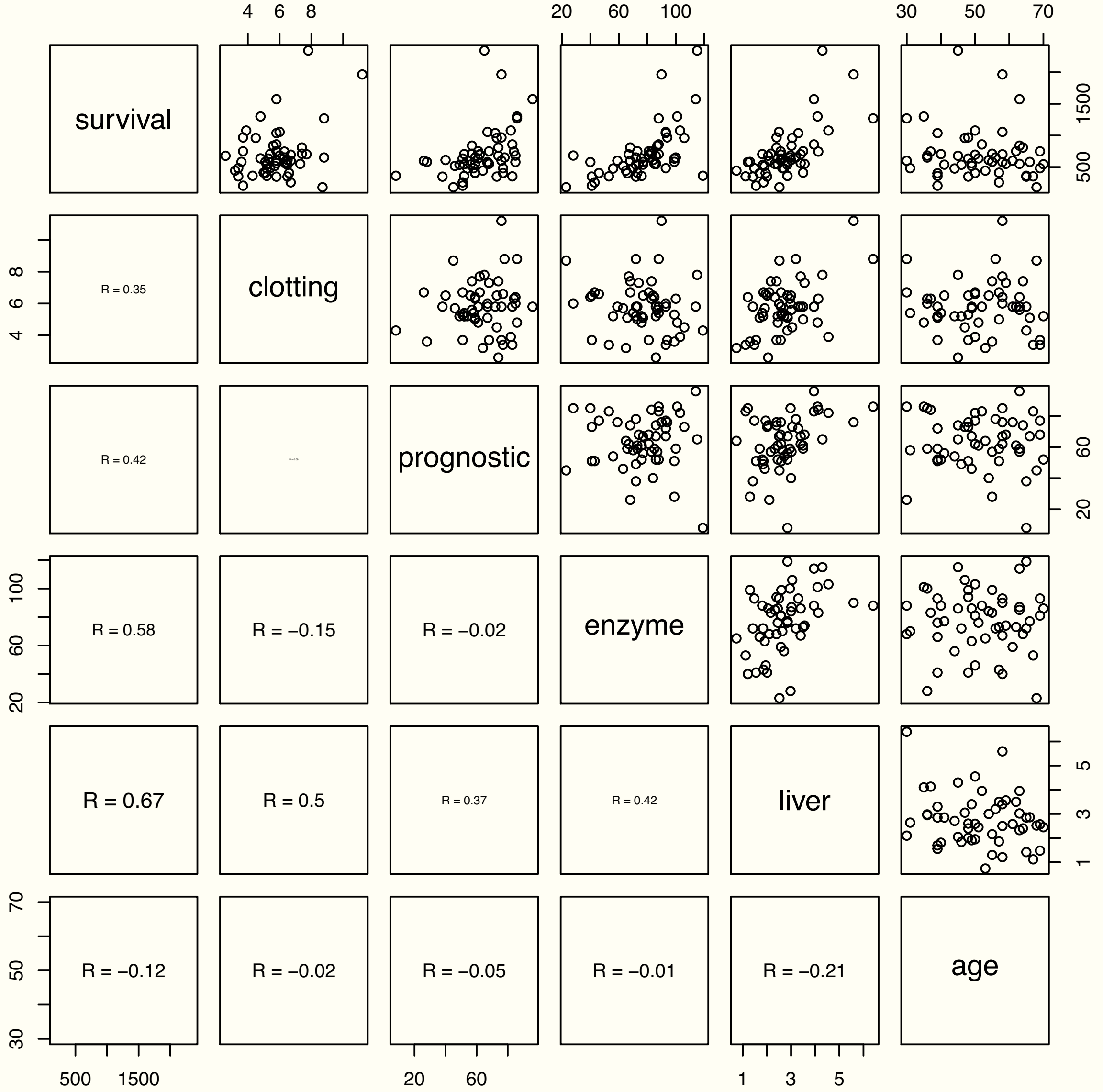


Figure: Pie charts of qualitative variables

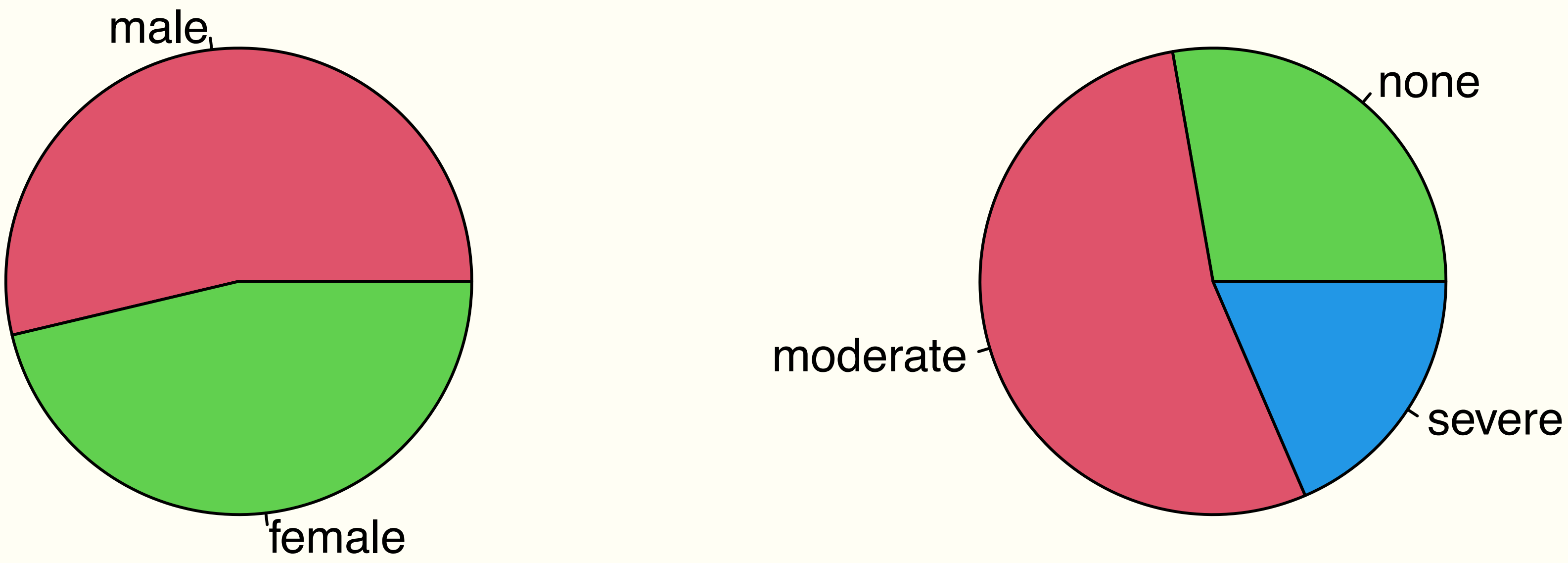
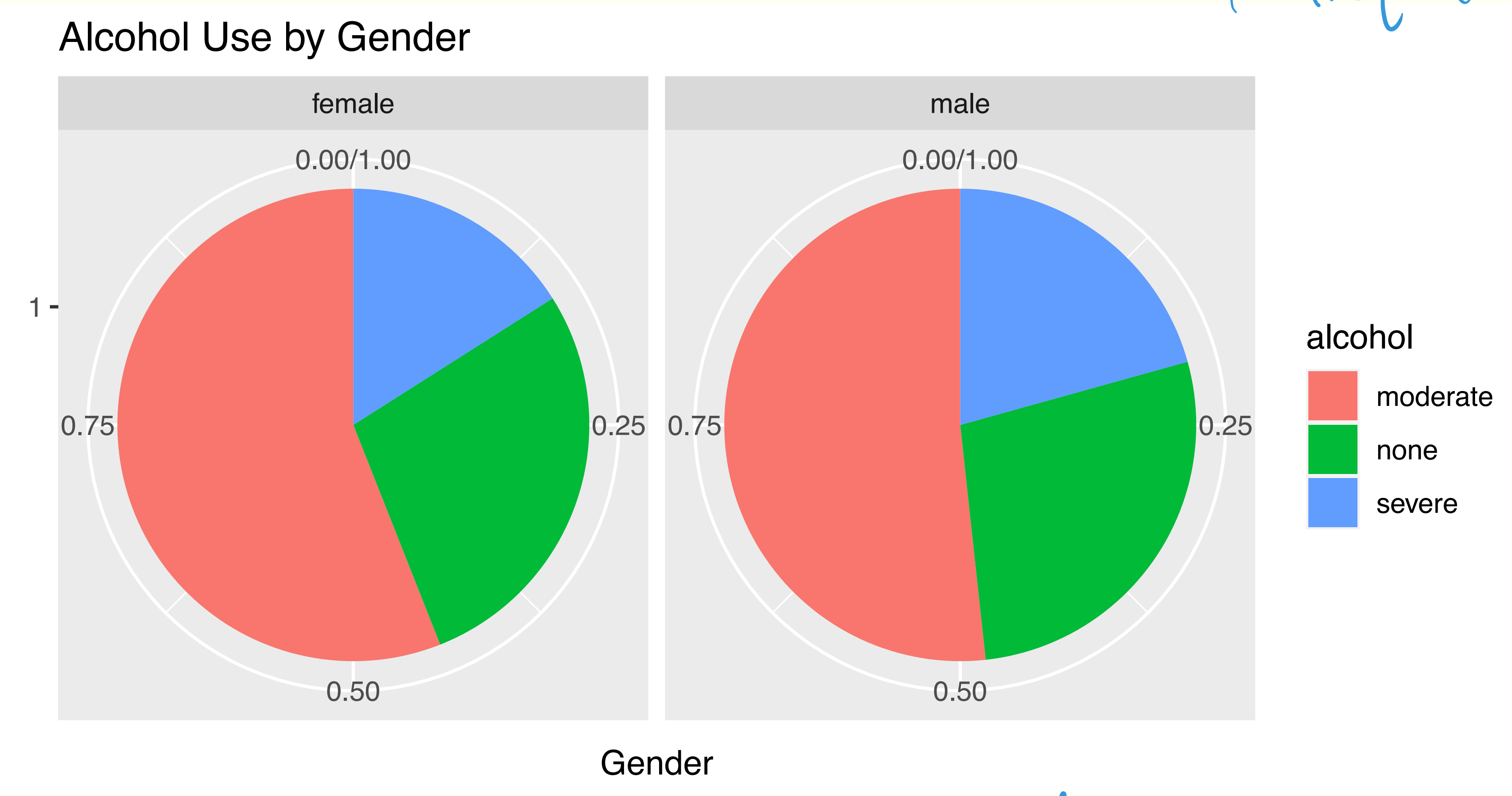


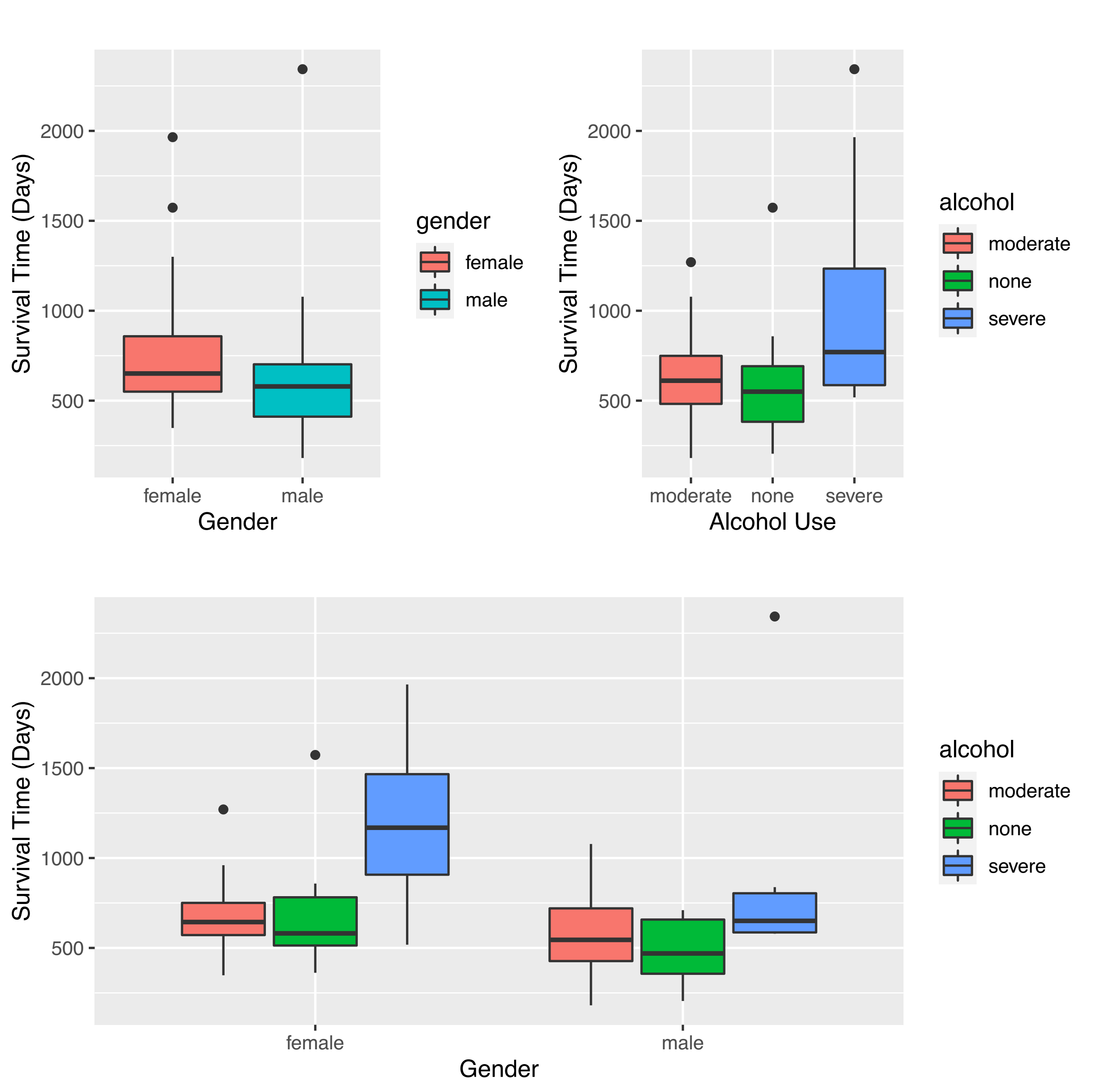
Figure: Side-by-side pie charts

P can use freq. table



no obvious diff. across gender

Figure: Side-by-side box plots



Model Building:

Preliminary Fit

Preliminary Model Fitting

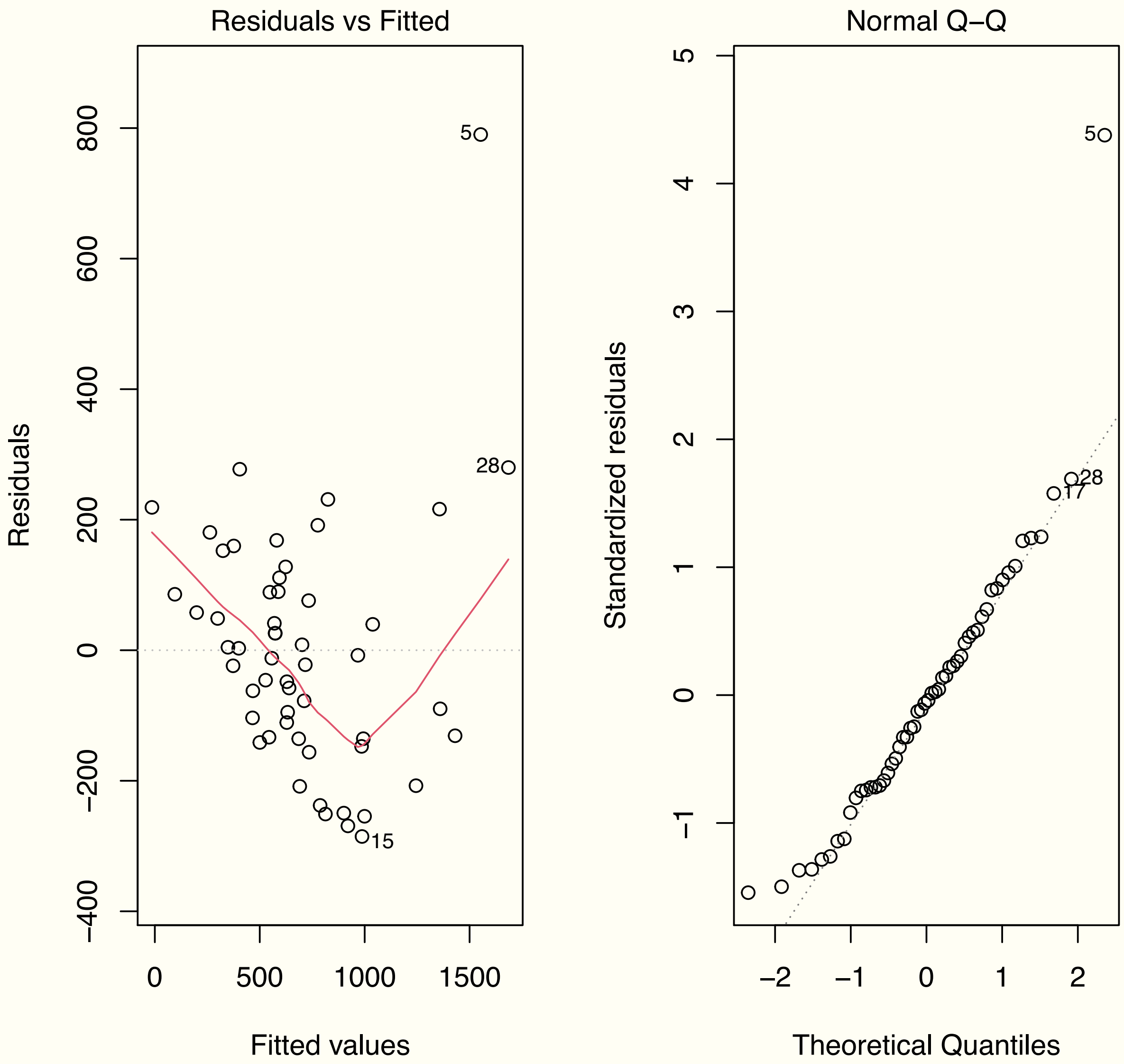
- Residual plots based on initial fits:
  - nonlinearity? departure from Normality? nonconstant error variance?
  - transformations needed? log make data closer (outlier ↓)
  - interaction terms and/or high-order power terms?
- The goal is to decide on:
  - Functional forms in which variables should enter the model;
  - Potential pool of *X* variables to be considered in subsequent analysis;
- This process should be aided by prior knowledge and domain expertise if available.

Surgical Unit: First-Order Model

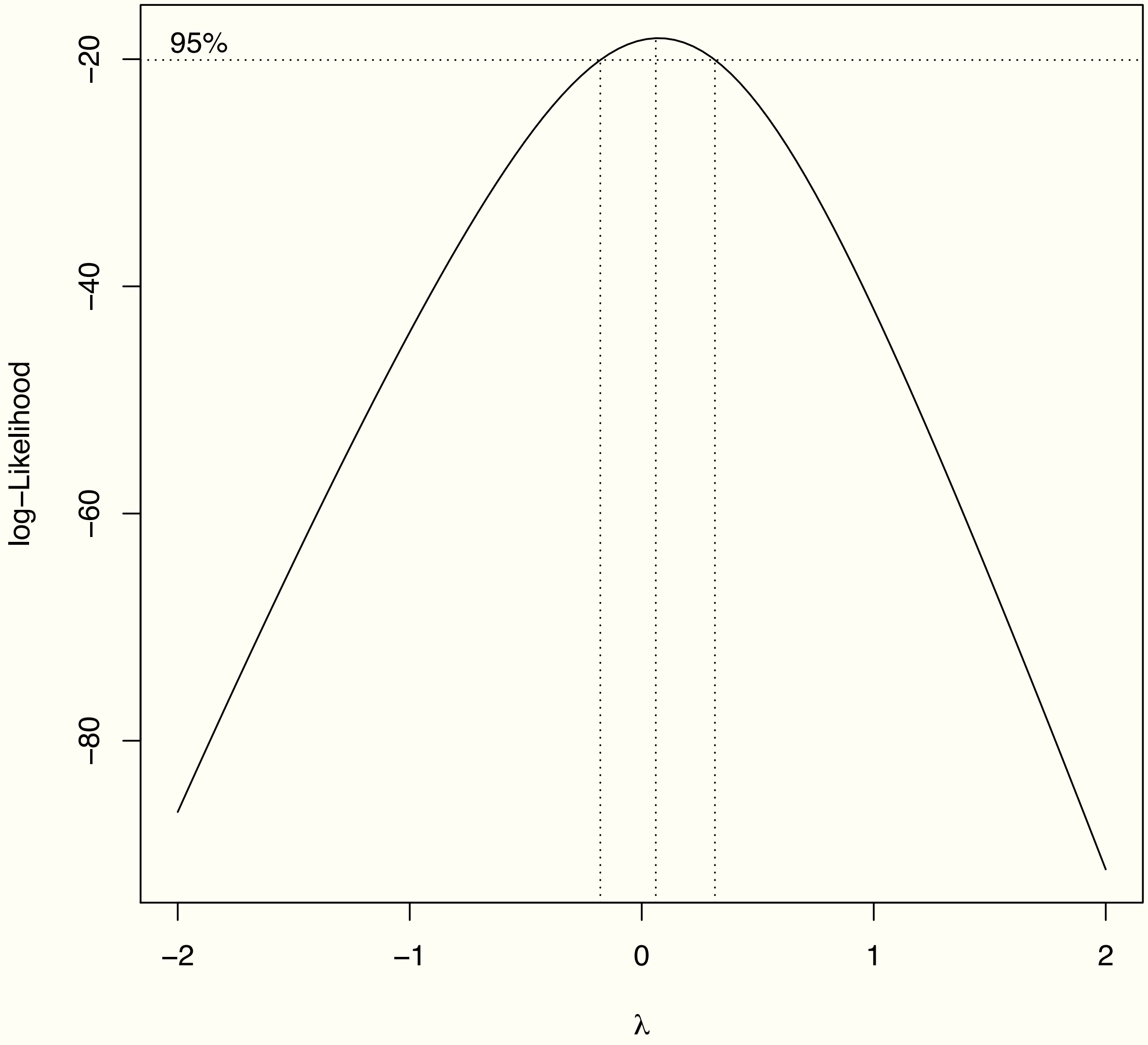
Fit a first-order model with survival time as response, and blood clotting score, prognostic index, enzyme function test score, liver function test score, age, gender (male or female) and history of alcohol use (none, moderate or severe) as X variables. Note that, gender and alcohol use should be treated as factors.

{ non - normal
model fix

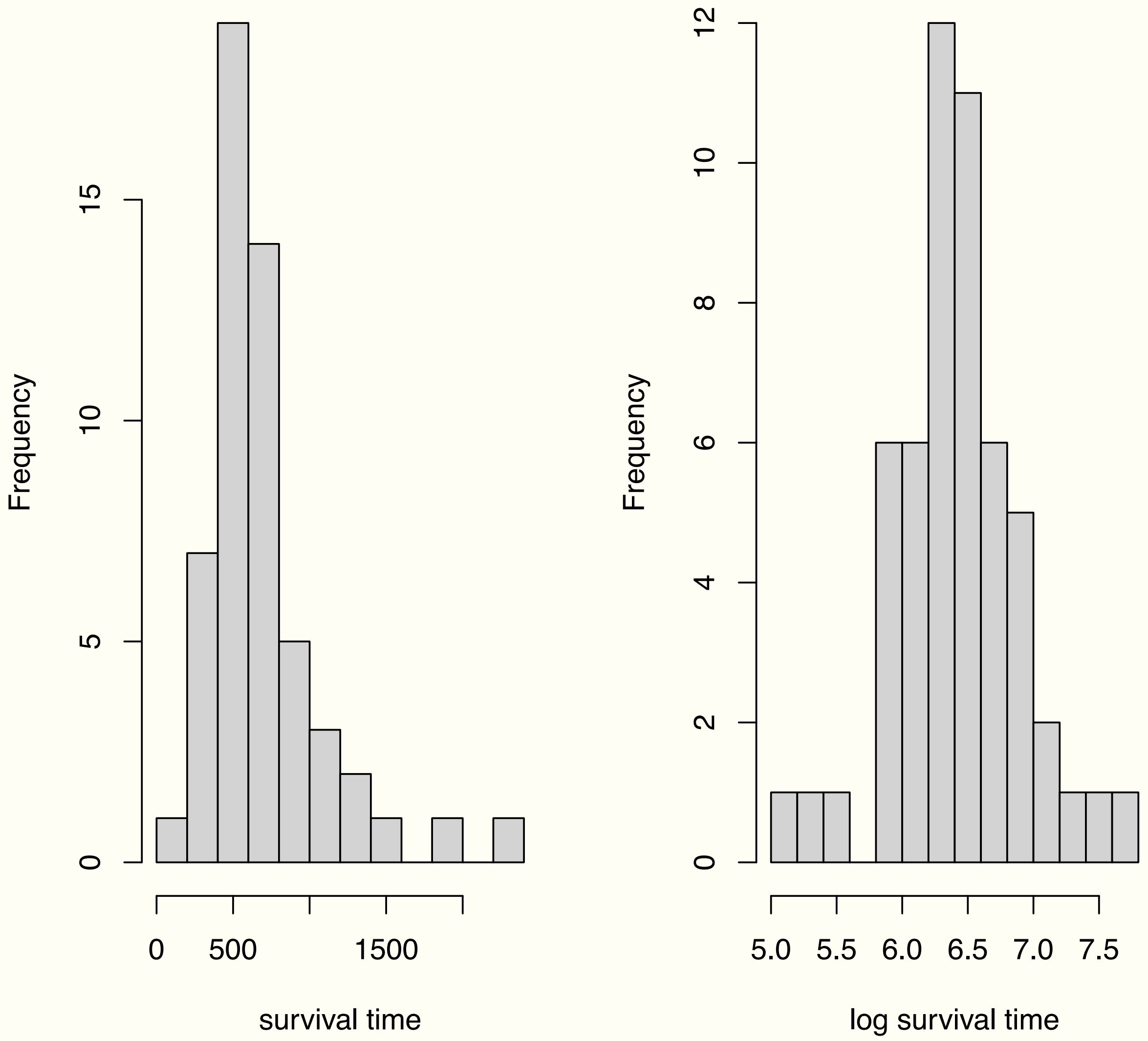
There appears to be non-linearity in regression relation. Residual Q-Q plot indicates outliers on the right tail.



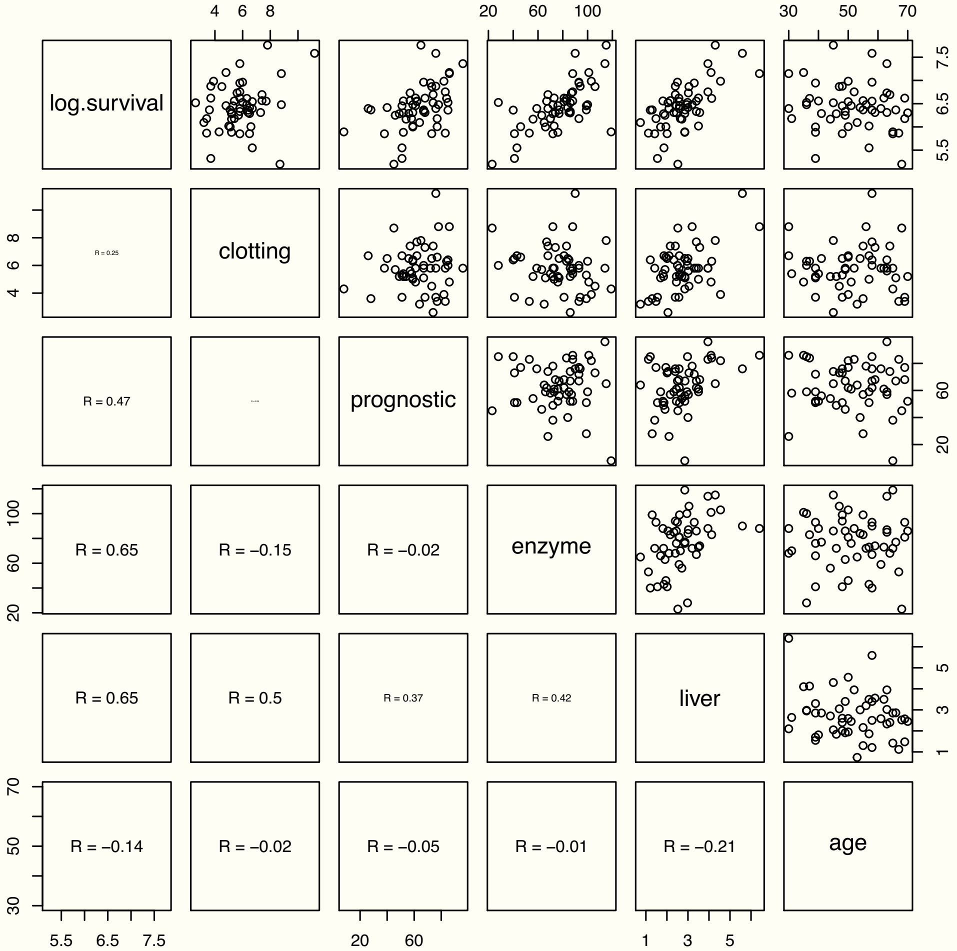
Box-cox procedure suggests logarithm transformation of the response variable.



Surgical Unit: Log-Transformation

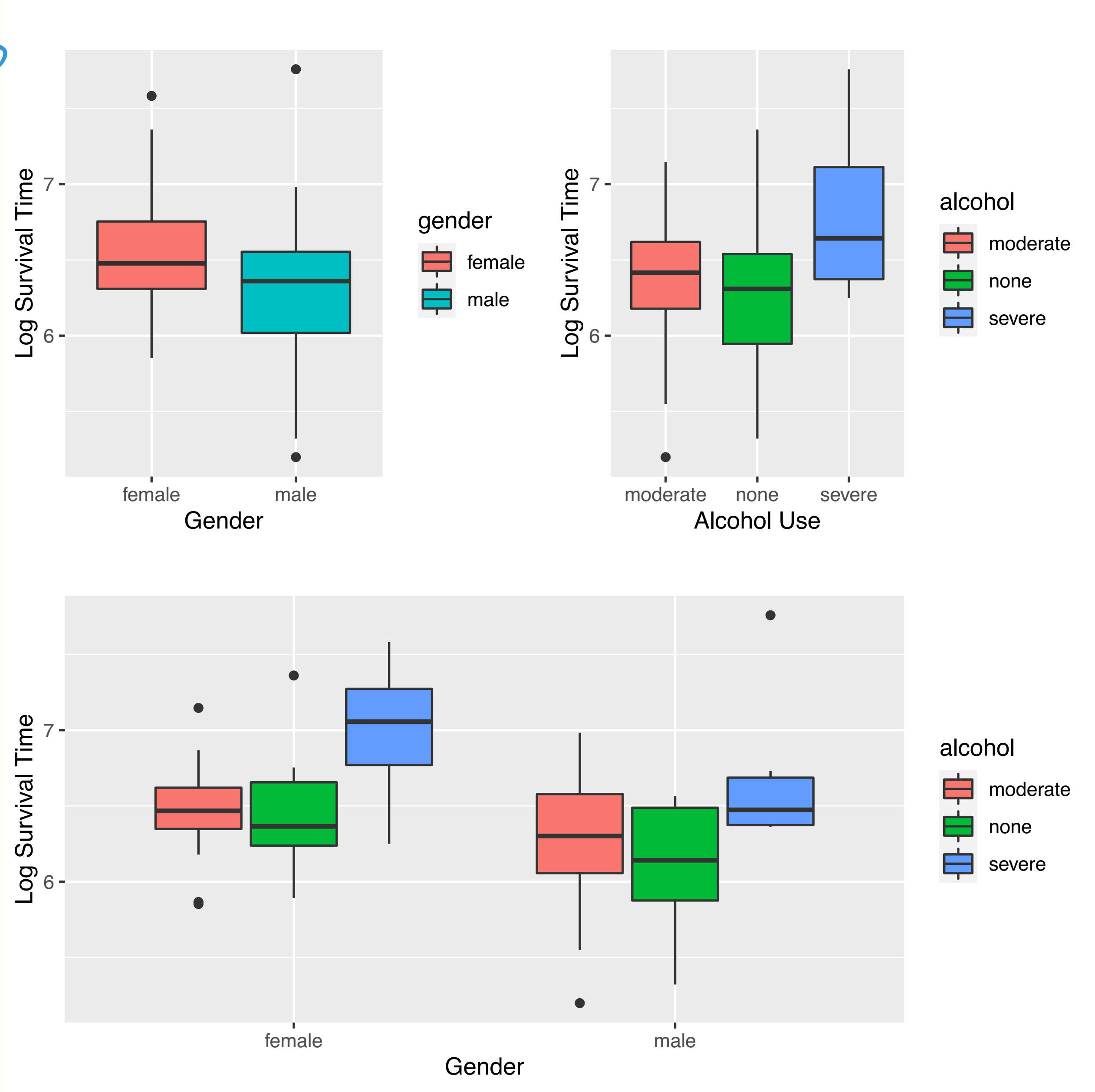


No obvious nonlinearity between log-survival-time and the quantitative X variables:



outlier less extreme ,

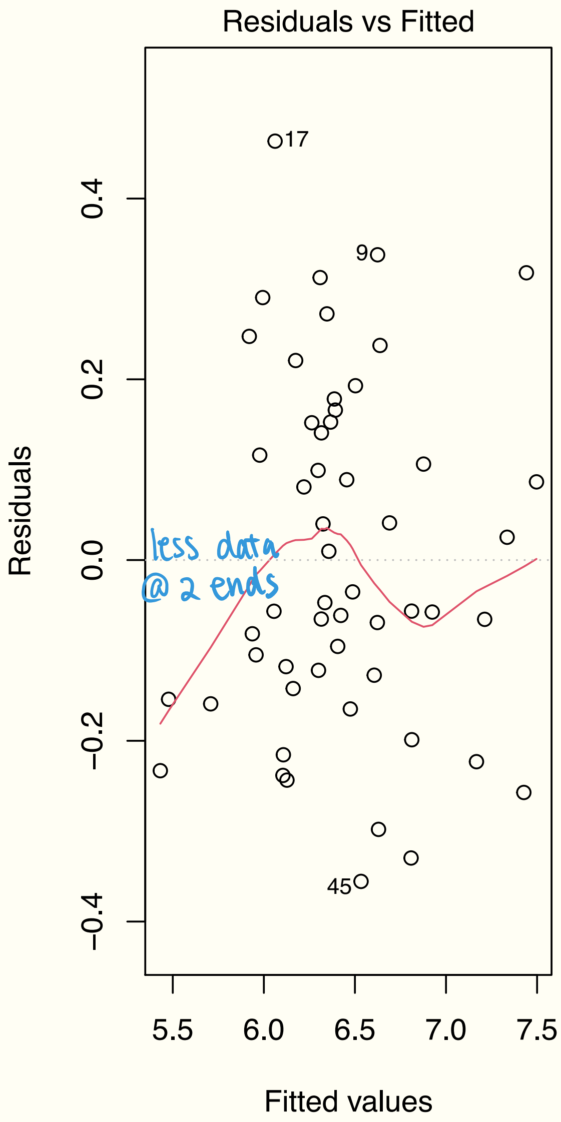
overall distrib. similar

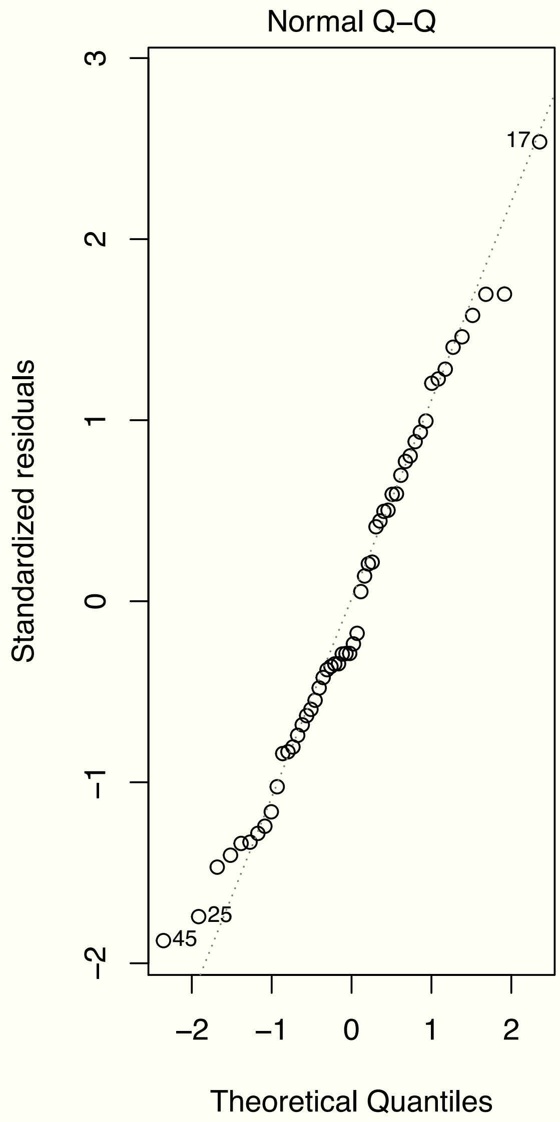


Fit the first-order model with log-survival-time as response: model assumptions appear to hold better.

no clear pattern

good





Based on these preliminary fits, we decided to:

- use log-survival-time as the response variable;
- not include any interaction terms: this could be further examined by plotting residuals versus various interaction terms (e.g., those involving significant predictors).

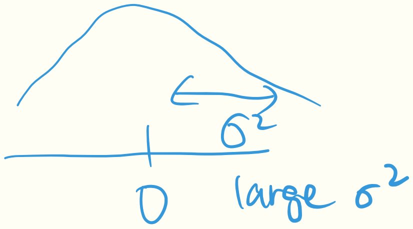
Next, we should examine whether all predictors are needed or a subset of them is adequate in explaining log-survival-time $\Longrightarrow$ **model selection**

Bias-Variance Trade-off

Correct Models vs. Good Models

- Correct models are those that contain all important X variables $\Longrightarrow$ little model bias.
- However, a correct model is not necessarily a good model because it may include too many nuisance variables $\Longrightarrow$ large sampling variability and overfitting.
- A good model should contain all important X variables (correct: little bias), and at the same time it should have few nuisance variables (simple: small variability) $\Longrightarrow$ achieves *bias-variance trade-off.*

Example



$$Y = 1 + 2X_1 + 3X_2 + \epsilon$$

- Any model contains (X_1, X_2) is a correct model, e.g., eg.

  $\{X_1, x_2\}, \{X_1, X_2, X_1X_2\}$,v$\{X_1, X_2, X_1^2, X_2^2\}$, $\{X_1, X_2, \underline{X_3, X_4, X_5}\}$.

  - These models have unbiased estimates.
  - However, some of them may have very large model variance such that the estimates behave erratically with even very small perturbation of the data.

- The models $\{X_1\}$ or $\{X_2\}$ both have an important X variable omitted and thus have substantial model bias. (omitted variable bias)

$Y = \mu + \varepsilon$, $var(\varepsilon) = \sigma^2 \cdot I_n$

i.e. $var(y_i) = \sigma^2$

$cov(y_i, y_j) = 0$

In the following:

$\begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$

- Assume the response vector **Y** has $Var(\mathbf{Y}) = \sigma^2\mathbf{I}_n$.

Notations

- Let $\boldsymbol{\mu} = E(\mathbf{Y})$ denote the mean of the response vector. $\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_n \end{pmatrix} = \begin{pmatrix} E(y_1) \\ \vdots \\ E(y_n) \end{pmatrix}$
- Let $\mathbb{M} = \mathbb{M}(X_1, \cdots, X_{p-1})$ denote an arbitrary model (**not necessarily** a correct model) and **X** denote its corresponding design matrix. $(\vec{1}, \vec{x}_1, \vec{x}_2 \cdots \vec{x}_{p-1})_{n \times p}$
- Let $H(\mathbf{X}) = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ be the hat matrix and $\hat{\mathbf{Y}} = \hat{\mathbf{Y}}(\mathbf{X}) = H(\mathbf{X})\mathbf{Y}$ be the fitted values vector.

$= M(X)$

not true for arbitrary

Def: Note that, $\mathbb{M}$ being a correct model means that there exists a vector $\boldsymbol{\beta}$ such that $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$. $\Leftrightarrow$ (iff) $\mu \in col(X)$

mean response

Model Variance

$\hat{y} = H(x) \cdot y$

$H(X) = X(X^TX)^{-1}X^T$

assump: $var(y) = \sigma^2 \cdot I_n$

assump: $rank(X) = p$

$var(\hat{y}) = H(x) \cdot var(y) \cdot H(x)^T$

$H(x) \cdot (\sigma^2 \cdot I_n) \cdot H(x)^T = \sigma^2 \cdot H(x)$

$$\begin{pmatrix} var(\hat{y}_1) & cov(\hat{y}_1, \hat{y}_2) & \\ & \ddots & \\ & & var(\hat{y}_n) \end{pmatrix}$$ var. of fitted values

- The (in-sample) variance of $\mathbb{M}$ is the overall variances of the fitted values:

  arbitrary

  summation

$$Var_{in}(\mathbb{M}) \overset{\text{def.}}{:=} \sum_{i=1}^{n} Var(\hat{Y}_i) = Tr(Var(\hat{\mathbf{Y}})) = \sigma^2 \underline{\overset{=p}{Tr(H(\mathbf{X}))}} = p\sigma^2$$

↳ # of regr. coefficients in M

- Therefore, larger models always have larger variances, whether they are correct or not.

∵ larger (complex) model
↳ larger var.

Model Bias

bias vector $= \overset{H(x)\cdot\vec{u}}{E(\hat{y})} - \overset{\vec{u}}{E(y)} = \begin{pmatrix} E(\hat{y}_1)-E(y_1) \\ \vdots \\ E(\hat{y}_n)-E(y_n) \end{pmatrix} =$

$(H(x)-I_n)\cdot\vec{u}$

recall $E(y)=\vec{u}$
$\hat{y}=H(x)\cdot y$
$E(\hat{y})=H(x)\cdot E(y)$
$=H(x)\cdot u$

- The (in-sample) bias of $\mathbb{M}$ is the overall biases of the fitted values:

(ℓ_2- norm / length of vector
$\|y\|_2 = \sqrt{\sum_{i=1}^{n} v_i^2}$
$= \sqrt{v^T v}$)

$$bias_{in}(\mathbb{M}) \overset{\text{def}}{:=} \|E(\hat{\mathbf{Y}}) - E(\mathbf{Y})\|_2 = \|(\underset{X(X^TX)^{-1}X^T}{H(\mathbf{X})} - \mathbf{I})\boldsymbol{\mu}\|_2$$

- Model bias depends on how well the column space $\langle \mathbf{X} \rangle$ approximates the mean response vector $\boldsymbol{\mu}$:

$$\boldsymbol{\mu} = E(\mathbf{Y}) = \underset{}{\overset{H(x)\cdot\vec{u}}{\boldsymbol{\mu}_X}} + \overset{(I_n-H(x))\cdot\vec{u}}{\boldsymbol{\mu}_{X^\perp}}, \quad \boldsymbol{\mu}_X \in \langle \mathbf{X} \rangle, \ \boldsymbol{\mu}_{X^\perp} \in \langle \mathbf{X} \rangle^\perp$$

$=((H(x)-I_n)\cdot u)^T\cdot(Hx-I)u) = u^T\cdot(I-H(x))\cdot u$

$$(H(\mathbf{X}) - \mathbf{I})\boldsymbol{\mu} = -\boldsymbol{\mu}_{X^\perp}, \quad bias^2_{in}(\mathbb{M}) = \boldsymbol{\mu}^T(\mathbf{I} - H(\mathbf{X}))\boldsymbol{\mu} = \underset{\text{squared length}}{\|\boldsymbol{\mu}_{X^\perp}\|_2^2}$$

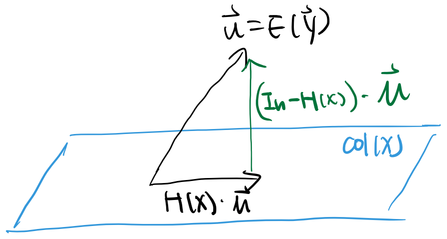
- If $\mathbb{M}$ is a correct model, then $bias_{in}(\mathbb{M}) = 0$ because:

$$\boldsymbol{\mu} = E(\mathbf{Y}) = \mathbf{X}\boldsymbol{\beta} \in \langle \mathbf{X} \rangle, \quad so, \quad \boldsymbol{\mu}_{X^\perp} = \mathbf{0}$$

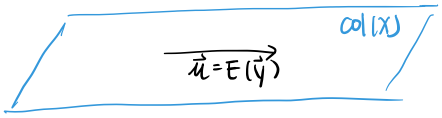
if μ is a correct model, ie $\mu \in col(X)$

so $H\mu = \vec{\mu}$, so $(H - I_n)\cdot\vec{\mu} = \vec{0}$.

so $bias_{In}(\mu) = ||\vec{0}||_2 = 0$



correct model



$M = M(X)$

↓ length of $(I_n - H)\vec{u}$

→ $bias_{In}(\mu)$

Msee

parameter / target: θ, estimator $\hat{\theta}$

↑ goal ↑ Statistic

$$\boxed{(a+b)^2 = a^2 + 2ab + b^2}$$

msee of $\hat{\theta}$ in estimator, θ is defined as:

$$\underbrace{E}_{\text{mean}}\Big(\underbrace{(\theta - \hat{\theta})}_{\text{estimation error}}{}^{2}\Big) \text{ squared } = E\Big[\big(\underbrace{\theta - E(\hat{\theta})} + \underbrace{E(\hat{\theta}) - \hat{\theta}}\big)^2\Big]$$

bias$(\hat{\theta}) = E(\hat{\theta}) - \theta$

$$= E\Big[(\theta - E(\hat{\theta}))^2 + 2(\theta - E(\hat{\theta}))\cdot(E(\hat{\theta}) - \hat{\theta}) + (E(\hat{\theta}) - \hat{\theta})^2\Big)$$

$$= \underbrace{(\theta - E(\hat{\theta}))^2} + \underbrace{2\cdot(\theta - E(\hat{\theta}))\cdot E(E(\hat{\theta}) - \hat{\theta})}_{0} + \underbrace{E(E(\hat{\theta}) - \hat{\theta})^2)}$$

msee $= bias^2(\hat{\theta})$ + 0 + var$(\hat{\theta})$

$$\boxed{E(E(\hat{\theta}) - \hat{\theta}) = E(\hat{\theta}) - E(\hat{\theta}) = 0}$$

Mean-Squared-Estiamtion-Error

- Mean squared estimation error (msee) of $\hat{Y}_i$:

$$msee_i(\mathbb{M}) := E((\hat{Y}_i - \mu_i)^2)$$

$$= Var(\hat{Y}_i) + (E(\hat{Y}_i) - \mu_i)^2$$

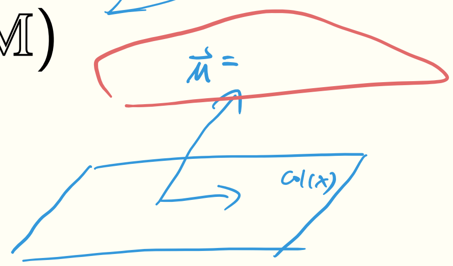
$$\text{var} + \text{bias}^2$$

- The (in-sample) msee of $\mathbb{M}$ equals model variance plus squared model bias:

$$= \|E(\hat{y}) - E(y)\|_2^2$$

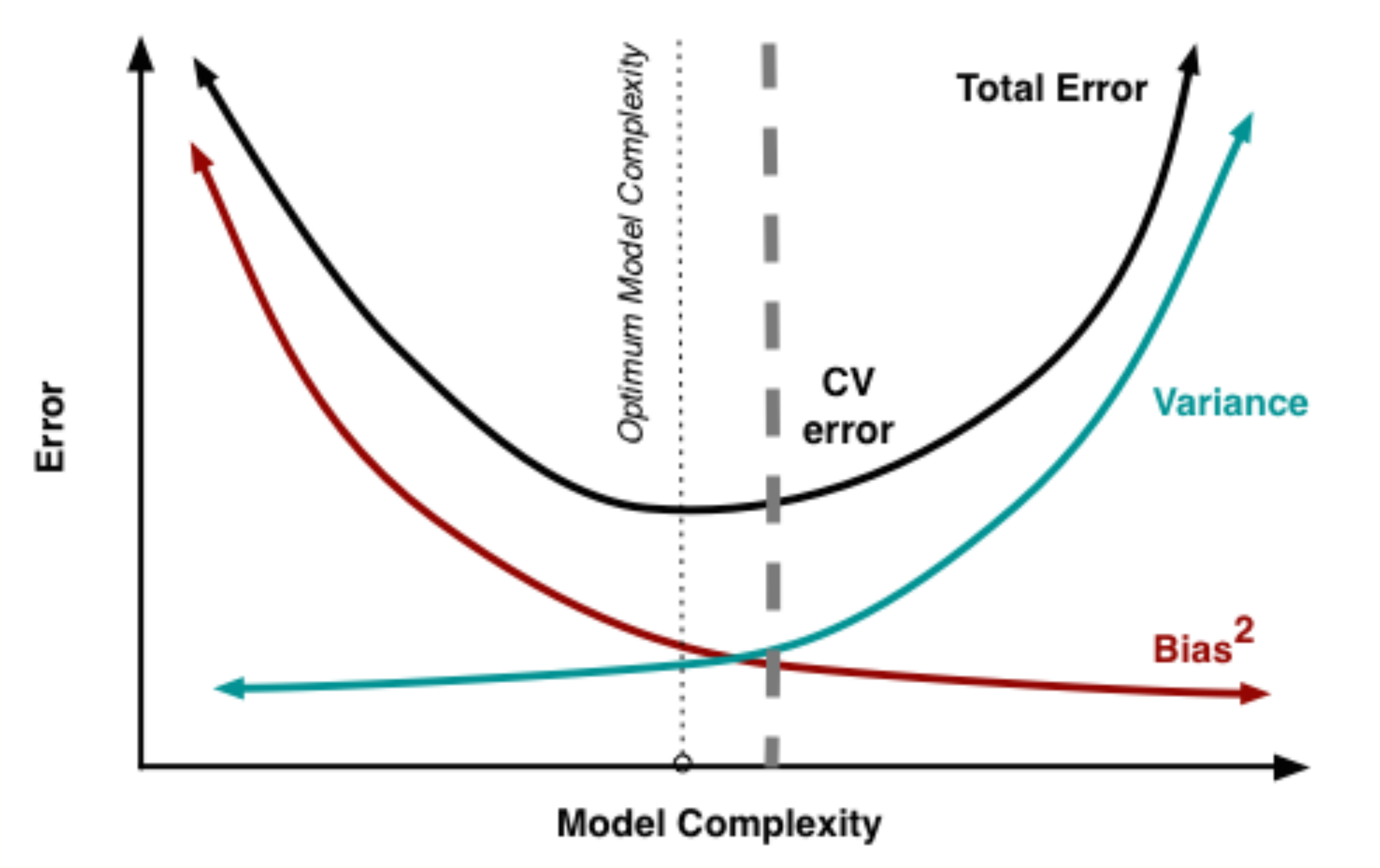
$$msee_{in}(\mathbb{M}) \overset{\text{def}}{:=} \sum_{i=1}^{n} msee_i(\mathbb{M}) = \sum_{i=1}^{n} var(\hat{y}_i) + \sum_{i=1}^{n} (E(\hat{y}_i) - \mu_i)^2$$

$$= Var_{in}(\mathbb{M}) + bias^2_{in}(\mathbb{M})$$



$$= \underset{\uparrow \text{ w/ p}}{p\sigma^2} + \underset{\downarrow \text{ w/ expanding col(x)}}{\|\boldsymbol{\mu}_{X^\perp}\|_2^2}$$

Bias-Variance Trade-off



$E(SSE)$ of a Model

- $SSE = \mathbf{e}^T\mathbf{e} = \mathbf{Y}^T(\mathbf{I} - H(\mathbf{X}))\mathbf{Y}$, is a measure of *goodness-of-fit* of the model to the **observed data Y**.
- $E(SSE)$ is affected by three factors: (i) model complexity p; (ii) error variance σ^2; (iii) and model bias $bias_{in}$.

$$
\begin{aligned}
E(SSE) &= E(Tr((\mathbf{I} - H(\mathbf{X}))\mathbf{Y}\mathbf{Y}^T)) = Tr((\mathbf{I} - H(\mathbf{X}))E(\mathbf{Y}\mathbf{Y}^T)) \\
&= Tr((\mathbf{I} - H(\mathbf{X}))(\sigma^2\mathbf{I} + \boldsymbol{\mu}\boldsymbol{\mu}^T)) \\
&= (n-p)\sigma^2 + \boldsymbol{\mu}^T(\mathbf{I} - H(\mathbf{X}))\boldsymbol{\mu} \\
&= (n-p)\sigma^2 + bias_{in}^2 \geq (n-p)\sigma^2
\end{aligned}
$$

↓ as p ↑, fit better [Msee also larger] [eg. overfitting]

(goal: small msee)

- If $\mathbb{M}$ is a correct model, then $bias_{in}(\mathbb{M}) = 0$ and thus $E(SSE) = (n - p)\sigma^2$ and $E(MSE) = \sigma^2$.
- If $\mathbb{M}$ is an incorrect model, i.e., $\boldsymbol{\mu} = E(\mathbf{Y}) \notin \langle \mathbf{X} \rangle$, then $E(SSE) > (n - p)\sigma^2$ and $E(MSE) > \sigma^2$.

Summary

- Larger models have larger variances.
- Model bias depends on how well the column space of its design matrix approximates the mean response vector.
- For two correct models, the larger model has a smaller $E(SSE)$, but a larger variance and thus a larger overall msee mean-squared-estimation-error. So it tends to *overfit* the observed data.
- Incorrect models have larger $E(SSE)$ than correct models of the same size, so they tend to *underfit* the observed data.

Model Selection: Overview

Full Model vs. Candidate Model

(either in / not)

2^{p-1} potential

↗ Sub-models

Setup

- *Full model*: The model that contains all $P - 1$ potential X variables in the pool.
    - ☆ **Assume the full model is a correct model.**
- *Candidate model*: A model that contains a subset of $p - 1$ X variables with $1 \leq p \leq P$.
- The goal is to choose good model(s) (subset(s) of X variables) that balances bias and variance.

Key Components for Model Selection

Subset

- **Criterion to compare models**:
  - $R_a^2, C_p, AIC_p, BIC_p, Press_p$, etc.
- **Procedure to search for good model(s):**
  - *Best subset selection*: Exhaustive search; Applicable when the number of potential X variables is not too big ;
  - *Stepwise regression*: Greedy search; The number of potential X variables can be large;

$2^{p-1} = 2^4 = 16$

$p=5$

Surgical Unit

If `clotting` (X_1), `prognostic` (X_2), `enzyme` (X_3), `liver` (X_4) form the potential pool of X variables, then there are 16 sub-models.

```
p   intercept X1 X2 X3 X4     sse   R^2 R^2_a      Cp      aic      bic    press
1           1  0  0  0  0 12.805 0.000 0.000 151.569  -75.716  -73.727 13.292
2           1  0  0  1  0  7.334 0.427 0.416  66.518 -103.811  -99.833  8.329
2           1  0  0  0  1  7.408 0.421 0.410  67.696 -103.268  -99.290  8.024
2           1  0  1  0  0  9.974 0.221 0.206 108.469  -87.205  -83.227 10.738
2           1  1  0  0  0 12.028 0.061 0.043 141.093  -77.096  -73.118 13.508
3           1  0  1  1  0  4.313 0.663 0.650  20.523 -130.479 -124.512  5.066
3           1  0  0  1  1  5.132 0.599 0.583  33.536 -121.089 -115.122  6.123
3           1  1  0  1  0  5.783 0.548 0.531  43.873 -114.644 -108.677  6.989
3           1  0  1  0  1  6.620 0.483 0.463  57.175 -107.342 -101.375  7.474
3           1  1  0  0  1  7.299 0.430 0.408  67.961 -102.070  -96.103  8.472
3           1  1  1  0  0  9.437 0.263 0.234 101.937  -88.194  -82.227 11.055
4           1  1  1  1  0  3.109 0.757 0.743*  3.388* -146.161* -138.205* 3.914*
4           1  0  1  1  1  3.615 0.718 0.701  11.434 -138.011 -130.055  4.598
4           1  1  0  1  1  4.970 0.612 0.589  32.960 -120.823 -112.867  6.209
4           1  1  1  0  1  6.568 0.487 0.456  58.358 -105.763  -97.807  7.902
5           1  1  1  1  1  3.084 0.759* 0.739  5.000 -144.587  -134.642 4.069
```

best for all criteria:

Cp, AIC, BIC

close to p

full: Cp = p (def)

Model Selection: Criteria

Mallows' C_p Criterion

$$C_p := \underbrace{\frac{SSE_p}{\hat{\sigma}^2}}_{\substack{\text{goodness of fit:} \\ \text{monotone} \uparrow \text{ in SSE}}} \overbrace{-\,(n - 2p)}^{\substack{\text{penalty on complexity:} \\ \uparrow \text{ with } p}}$$

- n : sample size
- p: number of regression coefficients in the candidate model
- SSE_p: error sum of squares of the candidate model
- $\hat{\sigma}^2$: an unbiased estimator of the error variance σ^2:

$$\hat{\sigma}^2 = MSE_{\text{full model}}$$

→ need assumpt: full model is correct

Mallows' C_p: Interpretation

Let $\mathbb{M} = \mathbb{M}(X_1, \cdots, X_{p-1})$ denote the candidate model, then

don't do this

$$E(C_p(\mathbb{M})) \overset{\text{very rough}}{\approx} \frac{E(SSE(\mathbb{M}))}{\sigma^2} - (n - 2p)$$

$$\| $$

$$E\left(\frac{SSE}{\hat{\sigma}^2}\right) - (n-2p)$$

$$E(\hat{\sigma}^2) = \sigma^2$$

$$= \frac{(n-p)\sigma^2 + bias^2_{in}(\mathbb{M})}{\sigma^2} - (n - 2p)$$

$$= \frac{p\sigma^2 + bias^2_{in}(\mathbb{M})}{\sigma^2}$$

$$= \frac{Var_{in}(\mathbb{M}) + bias^2_{in}(\mathbb{M})}{\sigma^2} = \frac{msee_{in}(\mathbb{M})}{\sigma^2}$$

if: $bias(\mathbb{M}) = 0$

then: $E(C_p) \approx p$

So C_p can be viewed as an rough estimator of the overall mean-squared-estimation-error divided by the error variance.

How to Use C_p?

- If a model has no bias, i.e., a correct model, then $E(C_p) \approx p$; Otherwise $E(C_p)$ tends to be larger than p.
- When C_p is plotted against p, then models with little bias will tend to fall near the diagonal line $C_p = p$.
- On the other hand, models with substantial bias will tend to fall considerably above this line.
- Look for models with (i) the C_p value not far above p and (ii) less X variables $\Longrightarrow$ small bias and small variance

?

AIC_p and BIC_p Criteria

- *Akaike's information criterion (AIC)*:

$$AIC_p = n \log \frac{SSE_p}{n} + 2p$$

- *Bayesian information criterion (BIC)*:

more penalty on complexity

$$BIC_p = n \log \frac{SSE_p}{n} + (\log n)p$$

- How to use: Look for models with small AIC (BIC)

AIC_p and BIC_p: Interpretation

- The first term: $n \log \frac{SSE_p}{n}$ reflects the *goodness-of-fit* of the model to the **observed data**:
  - decreases by adding more X variables into the model
- The second term, $2p$ for AIC and $(\log n)p$ for BIC, reflects model complexity:
  - increases by adding more X variables into the model
  - If $n \geq 8$, then $\log n > 2$ and BIC puts more penalty on model complexity and tends to choose smaller models than AIC.

- Overly simplified models have small model complexity (p), but they tend to have large SSE (underfitting, high bias).
- Overly complicated models may have a small SSE, but they have large model complexity (overfitting, high variance).
- By minimizing AIC (or BIC), we are trying to find a model that balances between model complexity and the goodness-of-fit.

$Press_p$ Criterion

Predicted residual sum of squares ($Press_p$):

$$Press_p = \sum_{i=1}^{n} (Y_i - \widehat{Y}_{i(i)})^2.$$

- Y_i is the observed response of the *ith* case.
- $\widehat{Y}_{i(i)}$ is the predicted value for the ith case obtained by fitting the model only using $n - 1$ cases excluding case i.
- $Press_p$ is also known as *leave-one-out-cross-validation (LOOCV)*.
- Models with small $Press_p$ are considered good in terms of predictive ability.

Press$_p$: Calculation

Press$_p$ can be calculated without actually performing n regressions because the *deleted residual* for the *ith* case:

$$d_i := Y_i - \widehat{Y}_{i(i)} = \frac{e_i}{1 - h_{ii}}, \quad i = 1, \cdots, n.$$

where $e_i = Y_i - \widehat{Y}_i$ is the residual of the *ith* case and h_{ii} is the *ith* diagonal element of the hat matrix **H**, both from the regression fit using **all** n cases. So

$$Press_p = \sum_{i=1}^{n} \frac{(Y_i - \widehat{Y}_i)^2}{(1 - h_{ii})^2}.$$

Surgical Unit: Full Model

```
lm(formula = log(Y) ~ X1 + X2 + X3 + X4, data = data.o)

Coefficients:

Estimate Std. Error t value Pr(>|t|)

(Intercept) 3.851933   0.266263  14.467  < 2e-16 ***

X1          0.083739   0.028834   2.904  0.00551 **

X2          0.012671   0.002315   5.474 1.50e-06 ***

X3          0.015627   0.002100   7.440 1.38e-09 ***

X4          0.032056   0.051466   0.623  0.53627
```

$\sqrt{MSE}$

```
Residual standard error: 0.2509 on 49 degrees of freedom

Multiple R-squared: 0.7591,     Adjusted R-squared: 0.7395

F-statistic: 38.61 on 4 and 49 DF,  p-value: 1.398e-14


Analysis of Variance Table

Df Sum Sq Mean Sq  F value    Pr(>F)

X1         1 0.7770  0.7770  12.3443 0.0009618 ***

X2         1 2.5904  2.5904  41.1565 5.341e-08 ***

X3         1 6.3286  6.3286 100.5490 1.838e-13 ***

X4         1 0.0244  0.0244   0.3879 0.5362698

Residuals 49 3.0841  0.0629
```

- Full model has $P = 5$ and or $\frac{SSE}{df}$

  $\sqrt{MSE} = 0.2509$

  $$SSE = 3.0841, \quad MSE = 0.0629, \quad R^2 = 0.7591, \quad R_a^2 = 0.7395$$

- By definition, for the full model, $C_P = P = 5$
- Sample size $n = 54$, so for the full model:

  $$AIC_P = 54\log(3.0841/54) + 2 \times 5 = -144.5871 \text{ and}$$

  $$BIC_P = 54\log(3.0841/54) + \log(54) \times 5 = -134.6422$$
- $Press_p = 4.069$

```
> e.f=fit.f$residuals  ## residuals

> h.f=influence(fit.f)$hat  ## diagonals of hat matrix

> press.f= sum(e.f^2/(1-h.f)^2)  ## calculate press
```

Model Selection: Stepwise Regression

Model Search Procedures

- The number of possible models, 2^{P-1}, grows very fast with the number potential X variables $P - 1$.
- Evaluating every possible model can be computationally infeasible even for moderate P.
- A variety of search procedures have been developed to efficiently search for the "best" model(s) in the model space.
  - *Stepwise regression procedures*
  - *Best subsets algorithms*: Not applicable when the pool of potential X variables is large.

Stepwise Regression Procedures

- Use “greedy” search strategies to examine a sequence of models by adding or deleting only one X variable according to a pre-specified criterion (e.g., AIC) at each search step.
- Could end up with a *local optimal model* rather than the global “best” model.
- Commonly used stepwise procedures: *forward stepwise*, *forward selection*, *backward stepwise* and *backward elimination*.

Forward Stepwise Procedure

Inputs:

- A model selection criterion, e.g., *AIC*.
- An initial model $\mathbb{M}_0$, usually a small model, e.g., the null-model with no X variable.
- The pool of potential X variables $\mathcal{X}$.
- The set of terms that will always be in the model $\mathcal{X}_0$, e.g., the intercept term.

Starting from the initial model $\mathbb{M}_0$, at each step:

(a) Consider the X variables in the pool $\mathcal{X}$ that are not currently in the model. Examine the change of the criterion by adding each such variable into the current model.

(b) Consider the X variables that are already in the model but not in the set $\mathcal{X}_0$. Examine the change of the criterion by dropping each such variable out of the current model.

(c) Choose the operation that improves the criterion the most and update the current model accordingly.

Repeat steps (a) – (c) until there is no operation that can improve the criterion anymore.

Forward Selection and Backward Elimination

- *Forward selection* is a simplified version of forward stepwise procedure by omitting the considerations of dropping a variable currently in the model at each step.
- *Backward elimination* is the opposite of the forward selection:
  - Start with a “big” initial model, e.g., the full model.
  - At each step, examine the change of the criterion by dropping a variable currently in the model.
- *Backward stepwise procedure*: opposite of forward stepwise.

Stepwise Procedures: Comparisons

- Forward stepwise procedure often works better than forward selection when there is high multicollinearity among the potential X variables.
- Backward procedures are not good when the number of potential X variables is large. Particularly, they are not feasible when $P > n$, since then the full model can not be fitted.
- A commonly used alternative to forward stepwise procedure is to perform one pass of forward selection, followed by one pass of backward elimination.

`stepAIC()` Function in R library *MASS*

- `direction=‘‘both"` corresponds to forward stepwise procedure or backward stepwise procedure (depending on the initial model); `direction=‘‘forward"` corresponds to froward selection; `direction=‘‘backward"` corresponds to backward elimination.
- The option `scope` specifies the potential pool of *X* variables (`upper`) and the *X* variables that should always be included in the model (`lower`).
- `k=2` corresponds to *AIC* criterion; `k=log(n)` corresponds to *BIC* criterion.

Surgical Unit

```
> fit.0=lm(log(survival)˜1, data=data.o) ##initial model, only intercept
> step.aic=stepAIC(fit.0, scope=list(upper=˜clotting+prognostic+enzyme+liver+age+gender
+alcohol.mod+alcohol.sev, lower=˜1), direction="both", k=2, trace=FALSE)
> step.aic$anova
Stepwise Model Path
Analysis of Deviance Table
Initial Model:
log(survival) ˜ 1
Final Model:
log(survival) ˜ enzyme + prognostic + alcohol.sev + clotting + gender + age
Step            Df   Deviance Resid. Df Resid. Dev        AIC
1                                    53  12.804509  -75.71608
2      + enzyme  1 5.47078352        52   7.333726 -103.81102
3  + prognostic  1 3.02085553        51   4.312870 -130.47855
4 + alcohol.sev  1 1.47089284        50   2.841977 -151.00214
5    + clotting  1 0.66416961        49   2.177808 -163.37593
6      + gender  1 0.09659084        48   2.081217 -163.82569
7         + age  1 0.07688125        47   2.004335 -163.85826
```

Model Validation

Model Validation

- *Internal validation*: Check validity using **the same data** used to fit the model.
- *External validation*: Check validity using **new data** – either newly collected or a holdout sample.

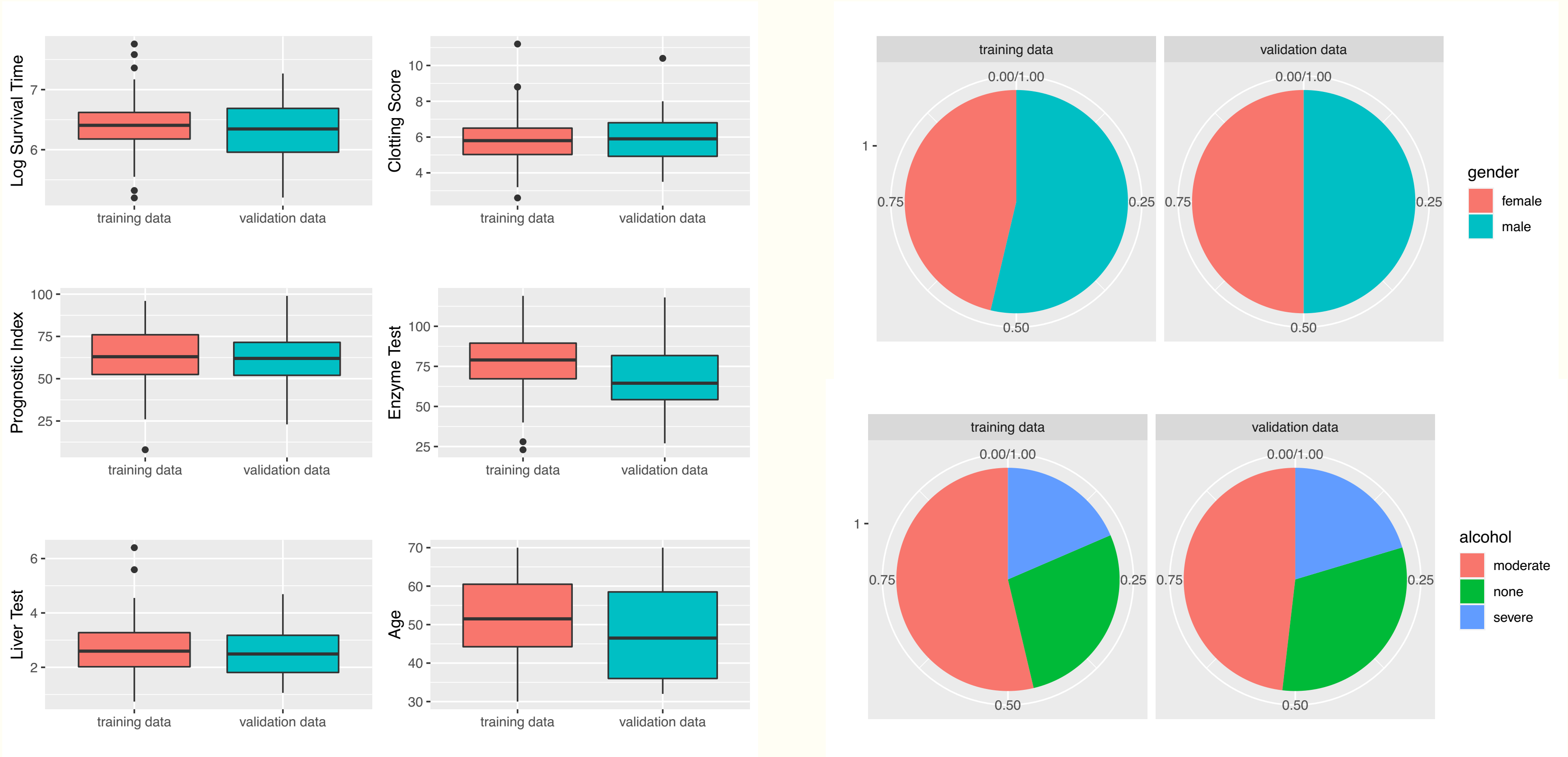
Training Data vs. Validation Data

When sample size is sufficiently large, an option is to split the data into two sets, a *training data* used to build the model and a *validation data* used to check model validity.

- Training data should be sufficiently large so that a reliable model can be built from it. Sometimes, the validation data will have to be smaller.
- Once a final model has been validated and chosen, it is a common practice to use the entire data set to re-fit the final model.

Surgical Unit: Training Data vs. Validation Data

Figure: Distributions of variables in training data ($n = 54$) and validation data ($n = 54$)



Internal Validation by $Press_p$ and C_p

- $Press_p$ is a measure of the predictive ability of the model: $Press_p$ not much larger than SSE_p means there is no severe over-fitting by the model.
- $C_p \approx p$ indicates little bias in the model, whereas $C_p >> p$ indicates substantial model bias.

External Validation by Mean Squared Prediction Error

$$MSPE_v := \frac{\sum_{j=1}^{m}(Y_j - \widehat{Y_j})^2}{m},$$

where m is the sample size of the validation data, Y_j is the *jth* observation in the validation data, and $\widehat{Y_j}$ is the predicted value of the *jth* case in the validation data based on the model fitted on the training data.

- $MSPE_v$ is a measure of the predictive ability of the model.
- $MSPE_v$ is usually larger than SSE/n: $MSPE_v$ not much larger than SSE/n indicates no severe over-fitting by the model.

Surgical Unit: Internal Validation

Three “best” models according to various criteria:

- By BIC_p and $Press_p$: Model 1, $\log Y \sim X_1, X_2, X_3, X_8$.
  - $p = 5, SSE_p = 2.178, C_p = 5.734, Press_p = 2.736$.
- By C_p: Model 2, $\log Y \sim X_1, X_2, X_3, X_6, X_8$.
  - $p = 6, SSE_p = 2.081, C_p = 5.528, Press_p = 2.782$.
- By $R^2_{a,p}$ and AIC_p: Model 3, $\log Y \sim X_1, X_2, X_3, X_5, X_6, X_8$.
  - $p = 7, SSE_p = 2.004, C_p = 5.772, Press_p = 2.771$.
- For all three models, $Press_p$ and SSE_p are reasonably close and $C_p \approx p$, supporting their validity.

Surgical Unit: Model 1 External Validation

```
Training             Validation
Estimate Std. Error Estimate Std. Error
(Intercept)    3.853      0.193    3.635      0.289
X1             0.073      0.019    0.096      0.032
X2             0.014      0.002    0.016      0.002
X3             0.015      0.001    0.016      0.002
X8             0.353      0.077    0.186      0.096

sse   mse  R2_a press press/n  mspe
Training   2.178 0.044 0.816 2.736  0.051   --
Validation 3.794 0.077 0.682  --     --     0.077
```

Surgical Unit: Model 2 External Validation

```
Training              Validation
Estimate    Std. Error Estimate Std. Error
(Intercept)    3.867      0.191    3.614      0.291
X1             0.071      0.019    0.100      0.032
X2             0.014      0.002    0.016      0.002
X3             0.015      0.001    0.015      0.002
X6             0.087      0.058    0.073      0.079
X8             0.363      0.077    0.189      0.097

sse   mse  R2_a press press/n  mspe
Training   2.081 0.043 0.821 2.782   0.052   --
Validation 3.728 0.078 0.682  --      --   0.076
```

Surgical Unit: Model 3 External Validation

```
Training              Validation
Estimate    Std. Error Estimate Std. Error
(Intercept)    4.054      0.235    3.470      0.347
X1             0.072      0.019    0.099      0.032
X2             0.014      0.002    0.016      0.002
X3             0.015      0.001    0.016      0.002
X5        →   -0.003      0.003    0.003      0.003
X6             0.087      0.058    0.073      0.079
X8             0.351      0.076    0.193      0.097
```

```
sse   mse  R2_a press press/n  mspe
Training   2.004 0.043 0.823 2.771   0.051  --
Validation 3.681 0.078 0.679  --      --   0.079
```

Surgical Unit: Choice of Final Model

- $MSPE_v$ of the three models have similar values, indicating that they have similar predictive ability.
- Model 3 has one estimated regression coefficient changing sign due to relatively large SE of this coefficient.
- Models 1 and 2 perform similarly in validation.
- Based on the **principle of parsimony (“Occam’s Razor”)**, choose Model 1 as the final model and re-fit Model 1 on all data.

Surgical Unit: Model 1 Fitted on All Data

```
lm(formula = log(Y) ˜ X1 + X2 + X3 + X8, data = rbind(data.o,data.v))
Estimate Std. Error t value Pr(>|t|)
(Intercept) 3.756276   0.162825  23.069  < 2e-16 ***
X1          0.083744   0.016781   4.990 2.46e-06 ***
X2          0.014988   0.001409  10.641  < 2e-16 ***
X3          0.015690   0.001134  13.839  < 2e-16 ***
X8          0.265096   0.060045   4.415 2.50e-05 ***
Residual standard error: 0.2446 on 103 degrees of freedom
Multiple R-squared: 0.7642,     Adjusted R-squared: 0.755
F-statistic: 83.45 on 4 and 103 DF,  p-value: < 2.2e-16


Analysis of Variance Table
Df  Sum Sq Mean Sq F value    Pr(>F)
X1          1  1.0809  1.0809  18.064 4.703e-05 ***
X2          1  6.5415  6.5415 109.322 < 2.2e-16 ***
X3          1 11.1859 11.1859 186.940 < 2.2e-16 ***
X8          1  1.1663  1.1663  19.492 2.498e-05 ***
Residuals 103  6.1632  0.0598
```