Linear Regression

$y_i = \beta_1 x_{i1} + ... + \beta_p x_{ip} + \epsilon_i$ ($x_{i1} \equiv 1$, so β_1 is intercept; Y: response var., x: predictor. n: sample size; p: number of predictors). Assumptions: $\epsilon_1, ..., \epsilon_n$ independent (uncorrelated), $E(\epsilon_1) = 0, \text{Var}(\epsilon_i) = \sigma^2$ (unknown; homoscedasticity)

Matrix Form: $\underset{n\times 1}{Y} = \underset{n\times p}{X} \cdot \underset{p\times 1}{\beta} + \underset{n\times 1}{\epsilon}$. $X = (x_{ij})_{i,j}$ is called design matrix.

LSE: $\hat\beta = \text{argmin}_\beta \|Y - Xb\|_2^2 = (X^\top X)^{-1} X^\top Y \sim \mathcal{N}_p(\beta, \sigma^2 (X^\top X)^{-1})$

$\hat\sigma^2 = \frac{1}{n-p}\sum_{i=1}^n (Y_i - (X\hat\beta)_i)^2 = \frac{1}{n-p} RSS$. Then $\mathbb{E}[\hat\sigma^2] = \sigma^2$ (unbiased). Moreover, $\mathbb{E}[\hat\beta] = \beta$, $\text{Var}[\hat\beta] = \sigma^2 (X^T X)^{-1}$. Thus if $\epsilon \sim N_p(0, \sigma^2 Id)$, then $\hat\beta \sim N_p(\beta, \sigma^2 (X^T X)^{-1})$. Also, if error Gaussian, then: $\hat Y \sim \mathcal{N}_n(X\beta, \sigma^2 P)$, error $e \sim \mathcal{N}_n(0, \sigma^2 (I - P))$, $\hat\sigma^2 \sim \sigma^2/(n-p) \cdot X_{n-p}$ where $P = X(X^\top X)^{-1} X^\top$

Categorical Variables: For two levels: $y_i = \beta_1 x_{i1} + ... + \beta_p x_{ip} + \lambda d_{is} + \epsilon_i$ so if i is in category, then $d_{is} = 1$ else $d_{is} = 0$. This acts as a different intercept ($E(y_i) - E(y_j) = \lambda$). If more categories, add more dummy variables ($n-1$ for n levels). **Interaction:** dummy can also influence slope: add term $\delta d_i x_i$, can influence interaction between predictors: add term $\delta x_{i2} x_{i3}$, can influence other categorical variable: add term $\delta d_{i1} d_{i2}$. Product of two predictors is also a predictor. In case of one categorical variable and one quantitative predictor, this leads to different slopes of the planes. But also other combinations possible.

Measuring Goodness of Fit

Proportion of variance that is explained by fitted linear model: $R^2 = 1 - {}^{RSS}/_{TSS} \in [0,1]$, where $TSS = \sum_{i=1}^n (y_i - \overline{y})^2$, $RSS = \sum_{i=1}^n (y_i - \hat y_i)^2$. In simple lin. reg.: $R^2 = r^2$, sample correlation. To account for more variables in model (R^2 decreases), $\text{adj}R^2 = 1 - {}^{RSS/(n-p)}/_{TSS/(n-1)}$.

$H_0 : y = X\beta + \epsilon$ with $\beta_j = 0$ $H_A : y = X\beta + \epsilon$ with $\beta_j \neq 0$

Under H_0 : ${}^{\hat\beta_j - (E[\hat\beta_j] = 0)}/_{\sqrt{\hat\sigma^2 (X^T X)^{-1}_{jj}}} \sim \mathcal{N}(0,1)$, t-statistic: ${}^{\hat\beta_j}/_{\sqrt{\widehat{\text{Var}}[\hat\beta_j]}} \sim t_{n-p}$

Test for significance of j-th predictor. H_0: $Y = X\beta + \epsilon$ with $\beta_j = 0$, H_1: $Y = X\beta + \epsilon$ with $\beta_j \neq 0$. Under H_0: $\hat\beta_j \sim N(0, \left[\sigma^2 (X^T X)^{-1}\right]_{jj})$. Thus ${}^{\hat\beta_j}/_{\sqrt{\widehat{\text{Var}}[\hat\beta_j]}} \sim N(0,1)$ and ${}^{\hat\beta_j}/_{\sqrt{\widehat{\text{Var}}[\hat\beta_j]}} \sim t_{n-p}$. Remark: $\widehat{\text{Var}}[\hat\beta_j] = \left[\hat\sigma^2 (X^T X)^{-1}\right]_{jj} = (se(\hat\beta))^2 = {}^{\hat\sigma^2}/_{(n-1)\text{Var}(X_j)} \cdot {}^{1}/_{1-R_j^2}$, where R_j^2 is the multiple R^2 from regression of X_j on all other predictors. One finds that an $1-\alpha$-C.I. for β_j is $\hat\beta_j \pm \widehat{\text{se}}(\hat\beta_j) t_{1-\alpha/2, n-p}$.

Let $X_0 = (x_{01}, ..., X0p$ be a new point. Then a $1-\alpha$-C.I. for $\mathbb{E}[Y_0]$ is $X_0^T \hat\beta \pm \hat\sigma \sqrt{X_0^T (X^T X)^{-1} X_0} t_{1-\alpha/2, n-p}$. A $1-\alpha$-C.I. (prediction Interval) for Y_0 is $X_0^T \hat\beta \pm \hat\sigma \sqrt{1 + X_0^T (X^T X)^{-1} X_0} t_{1-\alpha/2, n-p}$. Note: $\text{Var}(AY) = A \cdot \text{Var}(X) A^T$.

Linear Regression

```
fit <- lm(y~x1+x2) # Fit only x1 and x2 (so p=3)
predict(fit, pred.data.frame)
X <- cbind(1, x1, x2) # p = 3
XtX.inv <- solve(t(X) %*% X) # Manual fit
beta.hat <- XtX.inv %*% t(X.int) %*% y
res <- y - X.int %*% beta.hat # Residuals
RSE <- sqrt(sum(res^2)/(n-p)) # Residual std. error: Est. of the
↪  sd of the noise in the linear model
se.x1 <- RSE * sqrt(XtX.inv[2, 2]) # Std. error of x1
t.val.x1 <- beta.hat[2] / se.x1 # T value of x1
p.val.x1 <- 2*pt(abs(t.val.x1), df=n-p, lower=F)
RSE <- sqrt(sum(residuals(fit)^2)/(n-p))
RSS <- sum(res^2) # Residual sum of squares
TSS <- sum((y - mean(y))^2) # Total sum of squares
R.sq <- 1 - RSS / TSS # R^2
AdjR2 <- 1 - (RSS/(n-p))/(TSS/(n-1))
# Alternative t-value
coef <- summary(fit1)$coefficients
  t1 <- coef["x1","Estimate"]/coef["x1","Std. Error"]
  # Finding p-values
  fit.smaller <- lm(y ~ x1)
  anova(fit.smaller, fit, fit.all)
  # Overall F-Test
  fit.empty <- lm(y ~ 1, data=...) # Empty model
  anova(fit.empty, fit) # Compare models
  # Alternative F-test
  Ftest <- summary(fit)$fstatistic
pval <- 1 - pf(Ftest[1], df1=Ftest[2], df2=Ftest[3])
# Categ. var. by hand & LOOCV
a1 <- (levels(shelveloc)[2]==shelveloc)*1
lcv<-mean((residuals(fit)/(1-lm.influence(fit)$h))^2)
```

R Diagnostic plots: #1 Tukey-Anscombe Plot `plot(fit, which=1)` the points follow the line, else $E(\epsilon) = 0$ violated. #2 Q-Q Plot should follow line, else error not Gaussian (still all fine). #3 Scale-Location: should be flat, else $\text{Var}(\epsilon_i) = \sigma^2$ violated (p-values wrong). #4/#5 Cook distance: shows if some data points have a larger impact on the fit than others (outliers). Note: cannot detect if the residuals are correlated with these plots!

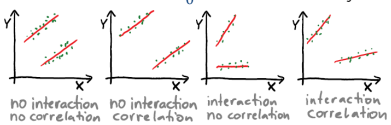
Tests & Confidence Intervals

Want to calculate: $P\left(t_{\alpha/2, n-p} < {}^{\hat\beta_j - \beta_j}/_{\hat{se}(\hat\beta_j)} < t_{1-\alpha/2, n-p}\right) = 1 - \alpha$. $CI = \hat\beta_j \pm \hat{se}(\hat\beta_j) \cdot t_{1-\alpha/2, n-p} = \hat\beta_j \pm \hat\sigma \sqrt{x_0^\top (X^\top X)^{-1} x_0} \cdot t_{1-\alpha/2, n-p}$

Prediction Interval

For new point x_0: $\hat y_0 = x_0^\top \beta \pm \hat\sigma^2 \sqrt{1 + x_0^\top (X^\top X)^{-1} x_0} \cdot t_{1-\alpha/2, n-p}$

P-Value: P(obs. a value of the test stat. that is as extreme or more extreme than the one we saw if H_0 is true). If $< \alpha$ then reject H_0.



Bias Variance Trade-Off

Expected Test MSE at x_0: $\mathbb{E}[(y_0 - \hat f(x_0))^2] = \text{Bias}^2(\hat f(x_0)) + \text{Var}(\hat f(x_0)) + \sigma^2$, where $\text{Bias}^2(\hat f(x_0)) = (f(x_0) - \mathbb{E}[\hat f(x_0)])^2$, $Bias = \mathbb{E}[\hat f(x_0)] - f(x_0)$ (see code).

Notation $Y_i = f(X_i) + \epsilon_i$, where ϵ_i iid, $\mathbb{E}[\epsilon_i] = 0$, $\text{Var}(\epsilon_i) = \sigma^2$. f is arbitrary fixed unknown function. Consider estimator $\hat f$ trained/fitted on $(x_1, y_1), ..., (x_n, y_n)$. Then Training MSE: $\frac{1}{n}\sum_{i=1}^n (y_i - \hat f(x_i))^2$. Test MSE on new sample $(\tilde x_1, \tilde y_1), ..., (\tilde x_m, \tilde y_m)$: $\frac{1}{m}\sum_{i=1}^m (\tilde y_i - \hat f(\tilde x_i))^2$.

Trade off Consider new pair (x_0, y_0): Then $\mathbb{E}[(y_0 - \hat f(x_0))^2] = (f(x_0) - \mathbb{E}[\hat f(x_0)])^2 + \text{Var}(\hat f(x_0)) + \text{Var}(\epsilon) = (\text{Bias}(\hat f(x_0)))^2 + \text{Var}(\hat f(x_0)) + \sigma^2$, σ^2irr. err., where Exp. is over different training sets.

Confidence Intervals & p-value

```
# P-value: variant 1, 1 sided, H0: <= 6
res <-  replicate(nsimul, simulateSomething())
pval.1 <- (1+sum(res.1 <= 6))/(nsimul+1)
# P-value: variant 2
pval.2 <- 2*pt(qt(1-alpha/2,n-p), df=n-p, lower=FALSE)
confint(fit) # Automatic CI.
# Manual CI (for intercept):
se.intercept <- summary(fit)$coef[1,2]
  coef(fit)[1] - qt(.975, n-2)*se.intercept
  coef(fit)[1] + qt(.975, n-2)*se.intercept
  # Predict value and C.I. (c for $\Ex[Y_0]$, p for $Y_0$):
  # Automatic Prediction CI
  predict(fit,newdata=data.frame(name=5), level=.95,
  ↪  interval="p")
  # Automatic CI
  predict(fit,newdata=data.frame(name=5), level=.95,
  ↪  interval="c")
  # Manual Prediction CI
  fitted <- fit$coef[1] + fit$coef[2]*x0
  quant <- qt(.975,n-2) # Quantile of t distribution
  sigma.hat <- sqrt(sum((fit$resid)^2/(n-2)))
X <- as.matrix(cbind(1,thuesen[,1]))
XtXi <- solve(t(X) %*% X) # (X^T X)^{-1}
X00 <- as.matrix(c(1,x0), nrow=2)
se <- sigma.hat * sqrt(t(X00) %*% XtXi %*% x00)
lower <- fitted - quant * se
upper <- fitted + quant * se
# Bias Variance Trade-Off of a Method
Bias <- mean(EstimateUsingCV) - TrueValueSimulated
MSE <- Bias^2 + var(EstimateUsingCV)
```

K Nearest Neighbors

Non-parametric method: $\hat f(x_0) = \frac{1}{k}\sum_{x_i \in N_0} y_i$, where N_0 is the set of k training observations with x-values closest to x_0. If k is larger has less variance, more bias. If k is smaller has more variance, less bias. Fails if there are lots of useless predictors.

LOESS smoother Similar, but smooth weight function, α controls smoothing. α small means less smoothing. See also: GAM

KNN & LOESS

```
library(kknn)
dfTrain=data.frame(y=Ytrain,x=Xtrain)
dfTest=data.frame(x=Xtest)
fit.kknn <- kknn(y ~ ., dfTrain,dfTest,k=8)
predTest=predict(fit.kknn) # predictions on dfTest
library(class) # Alternative library for knn
knn(train, test, k=5)
lo <- loess(y ~ x, span=alpha) # for loess (smoother)
prediction <- predict(object=lo, x)
```

Cross Validation

Can be used for *model assessment* (estimate test MSE) and *model selection* (choose tuning parameters, variable selection). But not both at the same time (use double CV instead).

Validation set: split data into two halves, train on one, test on the other (most bias). Pros: "fair"estimate of test MSE. Cons: Too pessimistic (because only trained on half of the data), thus biased estimate. Varies a lot depending on split, large variance. **k-Fold:** same, but with many folds. Try all folds for test and average metrics over the folds (in between). $\widehat{\text{Var}}(\hat\theta_k) = 1/K \cdot \widehat{\text{Var}}(MSEs)$ K-fold CV estimator: $\frac{1}{K}\sum_{k=1}^K MSE_k$ with $MSE_k = \frac{1}{|F_k|}\sum_{i \in F_k} (y_i - \hat f^{(-k)}(x_i))^2$.

Leave one out cross validation (LOOCV): extreme version where each data point is a fold (least bias). For $i = 1, ..., n$: train $\hat f$ on (x_j, y_j), $j \in \{1, ..., n\} \setminus \{i\}$; evaluate $\hat f$ at $x_i \to \hat f^{(-i)}(x_i)$; $MSE_i = (y_i - \hat f^{(-i)}(x_i))^2$. LOOCV estimator of expected test MSE is $\sum_{i=1}^n MSE_i$.

$\theta_k = \frac{1}{k}\sum_{i=1}^k \frac{1}{|I_k|}\sum_{i \in I_k} (y_i - \hat f^{-I_k}(x_i))^2$, $\theta_L = \frac{1}{n}\sum_{i=1}^n (y_i - \hat f^{-i}(x_i))^2$

Pros: Less biased, no randomness due to split. Cons: computationally intensive (but sometimes shortcut).

Bootstrap

Sample uniform from data points with replacement, compute bootstrapped estimator. For a large dataset $x_1, ..., x_n$ the probability that x_1 is contained in a random bootstrap dataset is:

$1 - (1 - 1/n)^n \approx 2/3$ (for large n, limit goes to $1 - 1/e$).

Bootstrap Consistency

For an increasing sequence a_n (often $\sqrt{n}$) where a_n^{-1} is the convergence rate of $\hat\theta_n$: $P(a_n(\hat\theta_n - \theta) \le x) - P^*(a_n(\hat\theta_n - \hat\theta_n) \le x) \to^P 0$ as $n \to \infty$. This holds when $\sqrt{n}(\hat\theta_n - \theta)$ is asympt. normal. Allows to estimate $\text{Bias}(\hat\theta_n) = E[\hat\theta_n] - \theta$ by $E^*[\hat\theta_n^*] - \hat\theta_n$. Can also estimate $\text{Var}^*(\hat\theta_n)$ by $\text{Var}^*(\hat\theta_n^*)$. With bootstrap consistency, we have ${}^{\text{Var}^*(\hat\theta_n^*)}/_{\text{Var}(\hat\theta_n)} \to^P 1$ and ${}^{\mathbb{E}^*[\hat\theta_n^*] - \hat\theta_n}/_{\mathbb{E}[\hat\theta_n] - \theta} \to^P 1$.

Resersed Quantile Bootstrap CI: $[\hat\theta_n - Q_{\hat\theta^* - \hat\theta}(1-\alpha/2), \hat\theta_n - Q_{\hat\theta^* - \hat\theta}(\alpha/2)]$ (type="basic"), **Normal Bootstrap CI:** Assums $\hat\theta_n$ to be asympt. normal: $\hat\theta_n \pm Q_z(1-\alpha/2)\hat{sd}(\hat\theta_n)$ where $z \sim \mathcal{N}(0,1)$ and $\hat{sd}(\hat\theta_n) = \sqrt{(\text{Var}(\hat\theta_n^*))}$ (type="norm"), **Quantile Bootstrap CI:** not theoret. justified unless $\hat\theta_n$ is symm.: $[Q_{\theta_n^*}(\alpha/2), Q_{\theta_n^*}(1-\alpha/2)]$ (type="perc"). Same as *reversed quantile bootstrap CI* if $\hat\theta_n^* - \hat\theta_n$ is symm. around 0, **Bootstrap T:** Rely on $t = {}^{\hat\theta_n - \theta}/_{\hat{sd}(\hat\theta_n)}$ and $t* = {}^{\hat\theta_n^* - \theta_n}/_{\hat{sd}(\hat\theta_n^*)}$ to be asympt. equal: $[\hat\theta_n - \hat{sd}(\hat\theta_n) \cdot Q_{t*}(1-\alpha/2), \hat\theta_n - \hat{sd}(\hat\theta_n) \cdot Q_{t*}(\alpha/2)]$. Note: $\hat{sd}(\hat\theta_n)$ is computed as above and $\hat{sd}(\hat\theta_n^*)$ is computed using a 2nd layer bootstrap.

Parametric Bootstrap: Assume data is generated by some parametric distr. (e.g. $\mathcal{N}(\mu, \sigma^2)$), est. the param., then create new data sets from this distr. (with or whithout replacement). Works only well if distr. is approx. correct. Pros: good if parametric model is approximately true. Cons: Bad if not. (then non.param. bootstrap is better).

Smoothed Bootstrap: Given data $Z_1, ..., Z_n \sim_{i.i.d} P$, we estimate P by some smooth (non-parametric) estimate $\tilde P_n$, then generate bootstrap samples from $\tilde P_n$. In between non-param. and param. bootstrap. Works well if P is indeed smooth.

Confidence intervals: Quantile: $[q_{\hat\theta_n^*}(\alpha/2), q_{\hat\theta_n^*}(1-\alpha/2)]$ Same as Rev. quant. if distr. of $\hat\theta_n^* - \hat\theta_n$ is symm. In R: `perc`.

Normal: $\hat\theta_n \pm q_Z(1-\alpha/2)\widehat{\text{sd}}(\hat\theta_n)$, where $Z \sim N(0,1)$, $\text{sd}(\hat\theta_n) = \sqrt{\widehat{\text{Var}}^*(\hat\theta_n^*)}$. In R: `norm`

Reversed quantile: $[\hat\theta_n - q_{\hat\theta_n^* - \hat\theta_n}(1-\alpha/2), \hat\theta_n - q_{\hat\theta_n^* - \hat\theta_n}(\alpha/2)] = [2\hat\theta_n - q_{\hat\theta_n^*}(1-\alpha/2), 2\hat\theta_n - q_{\hat\theta_n^*}(\alpha/2)]$. In R: `basic`

Bootstrap T: $[\hat\theta_n - q_{\hat\theta_n^* - \hat\theta_n/\widehat{\text{sd}}(\hat\theta_n^*)}(1-\alpha/2)\widehat{\text{sd}}(\hat\theta_n), \hat\theta_n - q_{\hat\theta_n^* - \hat\theta_n/\widehat{\text{sd}}(\hat\theta_n^*)}(\alpha/2)\widehat{\text{sd}}(\hat\theta_n)]$, where $\widehat{\text{sd}}(\hat\theta_n^*)$ is obtained via second layer of bootstrap. In R: `stud`. **Bootstrap for regression:** Model: $\mathbb{E}[Y|X = x] = \mu(x)$. Let $\hat\mu(x)$ be an estimate of $\mu(x)$. Let $r_i = y_i - \hat\mu(x_i)$ denote the residuals. Different options:

-Simulate new X-values from the model's estimated distribution for X. Then draw Y-values from the model's estimated distribution of $Y|X$.

-Hold the x's fixed, and draw $Y|X$ from the model's estimated distribution of $Y|X$.

-Hold the x's fixed and set $Y = \hat\mu(x)$ plus a randomly resampled residual r_j.

-Resample (x_i, y_i) pairs.

Options range from fully parametric to fully non parametric.

Bootstrap

```
library(boot)
sample(c(1:n), n, replace=T) # bootstrap sample
res.boot <- boot(Portfolio, f, R=1000)# f's args: (data, idx)
res.boot$t0 # Estimates on original data
res.boot$t # Estimates on bootstrapped data
# Confidence intervals for variable i
boot.ci(res.boot, type="basic", index=i)
# Example to find all confidence intervals
tm <- function(x, ind) {mean(x[ind], trim = 0.1)}
tmv <- function(x, ind) {
   # bootstrap Var, required for the bootstrap T CI
   t2 <- var(boot(data=x[ind], statistic=tm, R=50)$t)
   return(c(tm(x, ind), t2)) }
res<-boot(data=..,statistic=tmv,R=10,sim="ordinary")
boot.ci(res, conf=0.95, type=c("basic","norm", "perc","stud"),
↪  var.t0=var(res.boot$t[,1]))
# Intervals by hand (t0: estimate, t: bootstrapped)
quantile.CI <- quantile(t,probs=c(0.025,0.975))
norm<-c(t0-qnorm(0.975)*sd(t),t0+qnorm(0.975)*sd(t))
reversed.CI <- t0-quantile(t-t0,probs=c(0.975,0.025))
# Parametric Bootstrap
# f1 is the bootstrap function: args (data)
# f2 returns a random dataset: args (data, mle)
res.boot <- boot(data, f1, R=1000, ran.gen=f2, sim="parametric",
↪  mle=1/mean(x1))
```

Permutation Test

Pros/Cons - Advantages: Idea is simple and elegant, flexible, no parametric/distribution assumption, use any test statistic, p-values and type I error control are exact, not asymptotic (if all permut. are considered).

- Limitations: Need computational power; not everything can be formulated as perm. test. (example: indiv. coefficients in regression).

Paired/unpaired two sample Paired: two measurements on same object/-person, etc. **Parametric vs. non parametric tests** Parametric: assumes form of distribution, e.g. T-test. Non parametric: No assumption about distribution, e.g. Wilcoxon rank sum test, Randomization/permutation tests. Non-parametric, simple model that works with any test statistic. P-values and type I error control exact/approximate (not asymptotic), but needs computational power and not everything can be modeled in this way (e.g. individual coefficients in LR)

1. Pick a test stat. that measures some difference between groups
2. Consider all possible permutations (or randomly permute) to obtain a permutation distribution.
3. Compare observed value to permutation distribution

Wilcoxon Test

Non-parametric, unpaired, robust test. $H_0 : F_1 = F_2$, $H_A : F_1$ shifted compared to F_2. Compute ranks of randomly switched sign (different group assignment), reject H_0 if observed rank over critical value of rank distribution. Determine the ranks of all data points $(1, ..., n_1 + n_2)$. Compute U: sum of ranks in one group. Distr. of U under H_0 in R or simulate: Permute Y values among two groups in all possible ways (or simulate large number). For each such group assignement compute the sum of ranks in one group. Idea: under H_0 treatment has no effect, thus assignment has no effect.

Wilcoxon signed rank test: $V = \sum_i \text{rank}(|D_i|) \cdot 1_{D_i > 0}$. D_i difference on ith object.

Permutation Test & Wilcoxon Signed Rank Sum Test

```
# Permutation test
fit <- lm(y~X)
obsF <- summary(fit)$fstatistic[1]
  res.f <- rep(NA, 10000)
  for (i in 1:10000){
      y <- y[sample(1:nrow(X), nrow(X))]
      fit.tmp <- lm(y~X)
      res.f[i] <- summary(fit.tmp)$fstatistic[1]
    }
  pval<-(sum(obsF<=res.f,na.rm=T)+1)/(length(res.f)+1)
  # Permutation Wilcoxon Signed Rank Sum Test
  diff <- immer$Y1 - immer$Y2
V.obs <- sum(rank(abs(diff)) * (diff > 0))
V <- numeric(100000)
for(i in 1:100000){
    perm<-diff * sample(c(1,-1),nrow(immer),replace=T)
    V[i] <- sum(rank(abs(perm)) * (perm > 0))
  }
p.value <- table(V >= V.obs)["TRUE"]/length(V)
# Automatic
wilcox.test(diff, alternative = "greater")
wilcox.test(control, treatment , alternative = c("two.sided",
↪  "less", "greater") # for unpaired two sample Wilc. test.
```

Multiple Testing

	H_0 true	H_A true	
H_0 not reject.	U true neg.	T false neg. Type II error	$m - R$
H_0 reject.	V false pos. Type I error	S true pos.	$R = V + S$
	m_0	$m - m_0$	m

Capital letters represent RV. Only R is observable. m is fixed and known, m_0 is fixed and unknown. If $m_0 = m$ then *global null*.

$P(\text{type I error}) = P(\text{rejecting } H_0 \text{ when } H_0 \text{ is true}) = \alpha$

$P(\text{type II error}) = P(\text{not rejecting } H_0 \text{ when } H_A \text{ is true}) = \beta$

Power of a test $1-\beta$ **False discovery proportion (FDP):** $Q = V/R$ (note: $V/R = 0$ if $V = R = 0$) **False discovery rate (FDR):** $E(Q)$ Expected proportion of false discoveries among all disc. **Family wise error rate (FWER):** $P(V \ge 1)$ Prob. of making one or more false discoveries. Note: controlling the FWER is more strict than controlling the FDR: if $V \ge 1$, then $Q = V/R \le 1$ and if $V = 0$, then $Q = V/R = 0$. So $\mathbb{1}_{\{V \ge 1\}} \ge Q$: FWER $= P(V \ge 1) = E[\mathbb{1}_{\{V \ge 1\}}] \ge E[Q] =$ FDR. If $m = m_0$/under global null, then FWER = FDR. Generaly, $\alpha m \ge$ FWER $\ge$ FDR.

Bonferroni Correction

Idea: FWER $= P(V \ge 1) = P(\text{at least one false rejection among tests } T_1, ..., T_m) = P(\cup_{i=1}^m \{\text{false rejection in test } T_i\}) \le \sum_{i=1}^m P(\{\text{false rej. in test}\}) \le \sum_{i=1}^m \alpha = m \cdot \alpha$ so we set the signif. level of individual tests to $\alpha' = \alpha/m$ (or, equiv.: $p_{bonf} = min(1, n \cdot p)$), then FWER $\le m\alpha' = \alpha$. **Power:** if the tests are indep. and $m = m_0$ then FWER $= 1 - (1-\alpha)^m$ which is $\approx \alpha \cdot m$ for small α and moderate m. If the tests are dependent/correlated: too conservative.

Benjamini-Hochberg

Let $p(1) \le p(2) \le ... \le p(m)$ be ordered p-values. Let i_0 be the largest i, s.t. $p(i) \le q \cdot i/m$. Reject all $H_{(i)}$ with $i \le i_0$. For independent test statistics (or p-values) this controls the FDR at level q, i.e. FDR $= q \cdot m_0/m \le q$.

Westfall Young Permutation Procedure

Provides *weak control of the FWER* (i.e. under the global null).

Given a data $X \in \mathbb{R}^{n\times(m+1)}$ size and $y \in \{0,1\}^n$. If $m = m_0$ then one can permute the y-values:

1. Repeat many times: premute y-cols, do a two sample test (e.g. Wilcoxon) for each x_j col. (comparing $x_j[y==1]$ and $x_j[y==0]$). Let p_j for $j = 0,...,m$ be the corresp. p-value. Store $\min(p_1,...,p_m)$.
2. Set δ to the empirical α-quantile of the permutation distribution of $min(p_1,...,p_m)$.
3. Reject any null hypothesis where the two-sample test on the original data has p-value $\leq \delta$.

Westfall Young Permutation Procedure

```
nr.sim <- 1000
min.p.values <- numeric(nr.sim)
for(sim in 1:nr.sim) {
  y_perm = sample(y, length(y), replace = FALSE)
  min.p.values[sim] <- min(apply(x, 2, function(j) chisq.test(x
  ↪  = j, y = y_perm)$p.value))
}
delta <- quantile(min.p.values, probs = 0.05)
table(p.values < delta)
```

Model Selection

Criteria for model selection (for linear models): Mallow's $C_p = \frac{1}{n}(RSS + 2d\cdot\hat{\sigma}^2)$, $AIC = \frac{1}{n\hat{\sigma}^2}(RSS + 2d\cdot\hat{\sigma}^2)$, $BIC = \frac{1}{n\hat{\sigma}^2}(RSS + \log(n)d\cdot\hat{\sigma}^2) = -2\cdot\log(\hat{L}) + d\cdot\log(n)$ where $\hat{L}$ is the maximized value of the likelihood of the model, $AdjR^2 = 1 - \frac{RSS/(n-d-1)}{TSS/(n-1)}$.

Shrinkage Methods

Assume centered variable (no intercept). Remark: Ridge does not really do model selection, Lasso does, because L^1-spheres have "corners". Note: first standartize variables to have variance 1: $\tilde{x}_{ij} = x_{ij}/\sqrt{\frac{1}{n}\sum_i (x_{ij}-\overline{x}_j)^2}$ **Ridge regression:** $\hat{\beta}_s^{ridge} = \text{argmin}_\beta RSS(\beta) + \lambda\|\beta\|_2^2 = (X^\top X + \lambda I)^{-1} X^\top y$ (if X- matrix has no intercept (i.e. center variables before)) **Lasso:** $\hat{\beta}_s^{lasso} \text{argmin}_\beta RSS(\beta) + \lambda\|\beta\|_1$.

Elastic Net: $\hat{\beta}_s^{glastic} = \text{argmin}_\beta RSS(\beta) + (1-\alpha)\lambda\|\beta\|_1 + \alpha\lambda\|\beta\|_2^2 (\alpha = 1$: ridge, $\alpha = 0$: lasso),

Adaptive Lasso: Lasso with penalty weights: $\hat{\beta}_s^{adapt.lasso} \text{argmin}_\beta RSS(\beta) + \lambda\sum_{j=1}^p w_j|\beta_j|$. Take a $\sqrt{n}$ consistent estimate $\hat{\beta}$ of β (e.g. least squares Choose $\gamma > 0$, then set $\hat{w}_j = 1/|\hat{\beta}|^\gamma$. This asymptotically selects the right covariates and has optimal estimation rate.

Group Lasso: Predictors are divided into L groups of size $p_1,...,p_L$ s.t. $\sum p_i = p$. $\hat{\beta}_\lambda^{gr.lasso} = \text{argmin}_\beta RSS(\beta) + \lambda\sum_{l=1}^L \sqrt{p_l}\|\beta\|_2$. (if L=p, we get Lasso). Acts like Lasso on a group level. Useful if there are categorical variables with > 2 categories (put all corresponding dummy variables in a group).

Best subset selection:

$\hat{\beta}_s^{subset} = \text{argmin}_{\beta,\|\beta\|_0\leq s} RSS(\beta)$. 1) Fit M_0 (null model = sample mean. 2) For $k = 1,...,p$ fit $\binom{p}{k}$models that contain exactly k predictors and select best (smallest RSS): M_k. 3) Select best among $M_0,...,M_p$ using CV or criteria.

1. Let $\mathcal{M}_0$ denote the *null model*, which contains no predictors (i.e. simply predicts the sample mean).
2. For $k = 1,2,...,p$: (a) Fit all $\binom{p}{k}$ models that contain exactly k predictors. (b) Pick the best among these $\binom{p}{k}$ models, call it $\mathcal{M}_k$, i.e. having the smallest RSS (equiv. largest R^2)
3. Select a single best model from among $\mathcal{M}_0,...,\mathcal{M}_p$, using CV, C_p (AIC), BIC, or adj. R^2.

To reduce computational cost, do in step 2. forward/backward stepwise selection.

Forward stepwise: 1) Fit M_0 2) For $k = 0,...,p-1$ fit all $p-k$ models with 1 additional predictor and select best (smallest RSS): M_k. 3) Select best among $M_0,...,M_p$ using CV or criteria.

Backward stepwise: 1) Fit M_p (full model). 2) For $k = p,p-1,...,1$: fit all k models that drop one perdictor in M_k. Choose best (smallest RSS): M_{k-1}. 3) Select best among $M_0,...,M_p$ using CV or criteria.

Model Selection

```
# Lasso/Ridge
library(glmnet)
grid <- 10^seq(from=10,to=-2,length=100)
# x must be matrix, e.g. model.matrix(Salary . , Hitters)[, -1]
ridge <- glmnet(x[train,], y[train], alpha=0, lambda=grid)
lasso <- glmnet(x[train,], y[train], alpha=1, lambda=grid)
# Predict for new $\lambda = 35$ and for new data use
predict(ridge.mod, s=35, type="coefficients", newx=x[test,])
# for CV to choose $\lambda$
c <- cv.glmnet(x[train,], y[train], alpha=0, nfolds=10)
c$lambda.min # gives best lambda. Plot coefficient paths:
↪  plot(fit.lasso)
```

```
# Best subset. method="forward" or "backward" for stepwise
regfit.full=regsubsets(Salary~., data=..., nvmax=19)
# Mallow Cp
library(leaps)
m <- leaps::regsubsets(y~., data=train, nvmax=10)
mo <- which.min(summary(m)$cp)
form <- as.formula(paste("y~",
paste(names(coef(m,mo))[-1],collapse="+"), sep = ""))
fit <- lm(form, data=test)
# Workaround for categorical variables
predict.regsubsets <- function(reg, new.data, id) {
  form <- as.formula(reg$call[[2]])
  mat <- model.matrix(form, new.data)
  coefi <- coef(reg, id=id)
  return(mat[,names(coefi)]%*%coefi)
}
n <- nrow(data)
folds <- sample(cut(1:n, 10, labels=F), n, replace=F)
for (fold in 1:10) {
test.fold <- which(folds == fold)
data.train <- data[-test.fold,]
data.test <- data[test.fold,]
m <- nrow(data.train)
cv.f <- sample(cut(1:m, 10, labels=F), m, replace=F)
cv.errors <- matrix(nrow=10, ncol=19)
for (k in 1:10) {
  cv.tf <- (cv.f == k)
  cv.m <- regsubsets(Salary~., data.train[-cv.tf,], nvmax=19)
  for (i in 1:19) {
  pred <- predict(cv.m, data.train[cv.tf,], id=i)
  cv.errors[k, i] <- mean((pred-data.train[cv.tf,]$Salary)^2)
  }
}
m <- regsubsets(Salary~., data=data.train, nvmax=19)
best.cp <- which.min(summary(m)$cp)
best.cv <- which.min(apply(cv.errors, 2, mean))
pred.cp <- predict.regsubsets(m, data.test, best.cp)
pred.cv <- predict.regsubsets(m, data.test, best.cv)
}
# For double CV with glmnet, can use cv.glmnet
inner.folds <- factors(folds[folds!=i])
levels(inner.folds) <- 1:(k-1)
inner.folds <- as.numeric(inner.folds)
```

Beyond Linearity

Basis Functions: $y_i = \beta_0 + \beta_1 b_1(x_i) + ... + \beta_k b_k(x_i) + \epsilon_i$

Polynomial Regression: $y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + ... + \beta_d x_i^d + \epsilon_i$. Easy to fit, but unstable near boundaries. As basis function: $b_j(x_i) = (x_i)^j$. Can also use better (orthogonal) basis functions (R automatically uses these). Using orth. polynomials implies that coefficients do not change when adding higher degree → can check until which coefficient it is significant. Gives same result and accuracy as monomial basis.

Step Functions: Create k cut points $c_1,...,c_k$ in the range of x. Then basis functions: $b_j(x_i) = 1_{\{c_j < x_i \leq c_{j+1}\}}$.

Regression Splines: Combines polynomial regression with continuity constraint. A piecewise degree d polynomial with continuity in dimensions $0,...,d-1$. Generally has $(k+1)(d+1)$ parameters and $k\cdot d$ constraints, so $k+d+1$ degrees of freedom. (e.g. **piecewise cubic** has $4(k+1)$ parameters and $3k$ constraint, so $k+4$ degrees of freedom. Basis functions: $h(x,\xi) = (x-\xi)_+^3$ (0 for all values $\leq \xi$). $y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \gamma_1 h(x_i,\xi_1) + ... + \gamma_k h(x_i,\xi_k) + \epsilon_i$.

Natural splines: Regression splines with additional boundary constraints: linear outside of outer knots (so k degrees of freedom).

Smoothing Splines: $G = \{g : [a,b] \to \mathbb{R} : g''$ exists and $\int_a^b g''(x)^2 dx < \infty\}$ is the class of functions to consider: $\hat{g} = \text{argmin}_{g\in G}\sum_{i=1}^n (y_i - g(x_i))^2 + \lambda\int_a^b g''(x)^2 dx$. Note: if $\lambda = 0$, $\hat{g}$ is any function in G that passes through all data points. If $\lambda = \infty$, we get the least squares estimate. Shrunken version of natural spline with knots at $x_1,...,x_n$.

Generalized Additive Models: $y_i = \beta_0 + \sum_{j=1}^p f_j(x_{ij}) + \epsilon_i$. More general than linear model, does not allow for interactions automatically → no curse of dimensionality.

Local Regression: Algorithm for local regression at $X = x_0$: 1) Gather the fraction $s = k/n$ of trianing points there x_i are closest to x_0. 2) Assign weight $K_{i0} = K(x_i, x_0)$ to each point in this neighborhood, so that the point furthest from x_0 has weight zero and the closest has the highest weight. All but these k nearest neighbors get weight zero. 3) Fit a weighted least squares regression of the y_i on the x_i using the weights, by finding $\hat{\beta}_0$ and $\hat{\beta}_1$ that minimize $\sum_{i=1}^n K_{i0}(y_i - \beta_0 - \beta_1 x_i)^2$. 4) The fitted value of x_0 is given by $\hat{f}(x_0) = \hat{\beta}_0 + \hat{\beta}_1 x_0$.

Backfitting: Let $s_j : (u_1,...,u_n)^T \to (\hat{u}_1,...,\hat{u}_n)^T$ be a smoother (e.g. multiple linear regression). Order influences #iterations. Initialize $\hat{\mu} = \frac{1}{n}\sum_{i=1}^n y_i$, $\hat{g}_j = 0 \quad \forall j$

Do until convergence (measure of conv. e.g.: $\max_j \frac{\|\hat{g}_{j,new} - \hat{g}_{j,old}\|}{\|\hat{g}_{j,old}\|}$):

for each $j = 1,...,p$: $\hat{g}_j \leftarrow s_j(y - \hat{\mu}\mathbb{1} - \sum_{k\neq j}\hat{g}_k)$, $\hat{g}_j \leftarrow \hat{g}_j - \frac{1}{n}\sum_{i=1}^n \hat{g}_j(x_{ij})\vec{1}$

Using GAMs and KNN

```
# Specify k+3 dof for cubic splines and k+1 dof for nat.
↪  splines.
lm(wage~poly(age,4)) # Orthogonal polynomials
lm(wage~poly(age, 4, raw=T)) # Monomial basis
lm(wage~age+I(age^2)+I(age^3)+I(age^4)) # Alternative
# Polynomial regression
fit <- lm(wage ~ poly(age, 4), data=Wage)
fit2 <- lm(wage ~ poly(age, 3), data=Wage)
anova(fit, fit2) # Check if significantly better
# Automatically check significance (if orthognal)
round(coef(summary(fit2), 2), 4)
library(splines) # Regular spline
fit <- lm(wage ~ bs(age, knots=c(25,40,60)), data=Wage)
# Natural spline
fit <- lm(wage ~ ns(age, df=4), data=Wage)
# Smoothing spline
fit <- smooth.spline(age, wage, df=16)
fit <- smooth.spline(age, wage, cv=T) # to do CV
# DOF/lambda: fit$df, fit$lambda
library(gam)
# s() for smoothing spline, lo() for loess
model.gam <- gam(y~s(X1, 4), data = dtrain)
mse.gam <- mean((ytest - predict(model.gam, dtest))^2) #
↪  predict.gam
```

Backfitting Algorithm for MLR

```
backfit <- function(x, y, n, p, o, eps) {
  mu.hat <- mean(y) # Compute overall mean
  g <- matrix(0, nrow=n, ncol=p) # Initialize g
  converged <- FALSE
  while(!converged) {
    old.g <- g
    beta0.hat <- mu.hat
    beta.hat <- numeric(p+1)
    for(i in o) { # o: order e.g. 1:p
      r <- y - mu.hat - rowSums(g[,-i])
      fit <- lm(r~x[,i])
      g[,i] <- fit$fitted
      beta0.hat <- beta0.hat + fit$coeff[1]
      beta.hat[1+i] <- fit$coeff[2]
    }
    if(max(colSums((old.g - g)^2)/colSums(old.g^2)) < eps)
      { converged <- TRUE }
    beta.hat[1] <- beta0.hat
  }
  return(beta.hat)
}
```

Classification and regression trees (CART)

$y_i = \sum_{r=1}^M \beta_r 1_{x_i\in R_r} + \epsilon_i$. where $\mathcal{P} = \{R_1,...,R_M\}$ is a partition of $\mathbb{R}^p$. If the partition is given, estimation is easy: $\hat{\beta}_j = \frac{\sum_{i=1}^n Y_i 1_{x_i\in R_j}}{\sum_{i=1}^n 1_{x_i\in R_j}}$ = average y value among obs. in R_j.

Recursive Binary Splitting: Greedy method to find the regions: For all predictors find the best cutting point, then take the cutting point that minimizes the error $\sum_{i:x\in R_1}(y_i - \overline{y}_{R_1})^2 + \sum_{i:x\in R_2}(y_i - \overline{y}_{R_2})^2$. Stop when region contains less than 5 elements.

Pruning: A deep tree T_0 can overfit. Pruning is a possible solution: For $\alpha > 0$: find $\text{argmin}_{T\subset T_0} err(T) + \alpha|T|$. α is tuning parameter, find via CV: Apply cost complexity pruning to the large tree to obtain a seq. of best subtrees as a function of α. Use K-fold CV to choose α, i.e. for $k = 1,...,K$: on all but k-th fold make a tree and prune it back for same α's as above, evaluate MSE on k-th fold. Average for each value of α and pick minimizing α. Return the subtree of the full tree corresponding to minimal α.

Classification Trees: At each split, try to improve node purity measured by gini index: $I(D) = [\frac{n_L}{n}I(D_L) + \frac{n_R}{n}I(D_R)] > 0$ where the subtrees are $I(D_R) = \hat{p}(1-\hat{p})$ where $\hat{p} = \frac{\#yes}{\#yes+\#no}$. Can predict class probability $\hat{p}_k(x) =$ *proportion of observations with class k in leaf node that contains x.*

Using Trees

```
# Create and plot tree
library(tree)
cs.tree <- tree(Sales ~ . , \textit{train_data})
plot(cs.tree); text(cs.tree, pretty=1)
# Predict using tree, type="class" for classification
test.pred <- predict(cs.tree, \textit{test_data})
(MSE <- mean((test.data$Sales - test.pred)^2))
  # Prune tree. FUN=prune.misclass, $dev for nr. of
  ↪  misclassifications
cv.carseats = cv.tree(cs.tree, FUN=prune.tree)
best.size <- cv.carseats$size [which.min(cv.carseats$dev)]
pruned.tree <- prune.tree(cs.tree, best = best.size)
```

Bootstrap Aggregating (Bagging)

Bagging for Regression: For data $(X_1,Y_1),...,(X_n,Y_n)$ and base procedure $\hat{g}(\cdot) : \mathbb{R}^p \to \mathbb{R}$, take B bootstrap samples $\hat{g}_{bag}(x) = \frac{1}{B}\sum_{b=1}^B \hat{g}^{*b}(x)$ where $\hat{g}^{*b}$ is the estimate based on the b-th bootstrap sample. No pruning, since variance of single tree not a problem as we average. Linear predictions are the same under bagging, so only interesting for non-linear estimates. For regression can only improve or stay the same.

Bagging for Classification: $\hat{g}(\cdot) : \mathbb{R}^p \to \{1,...,k\}$. $\hat{g}(x) = \text{argmax}_{k=1,...,K}\sum_{b=1}^B 1_{\hat{g}^{*b}(x)=k}$ (majority vote). Can also get class probability: $\hat{p}_k^{bag}(x) = \frac{1}{B}\sum_{b=1}^B \hat{p}_k^{*b}(x)$. Can also be formulated as $\hat{g}^{bag}(x) = \text{argmax}_{k=1,...,K}\hat{p}_k^{bag}(x)$ (better if interested in class probabilities, sometimes even helps accuracy). Has the advantages that we get the estimated class probabilities; bagging a good classifier can improve performance (bad classifier can decrease).

Random Forests: Essentially bagged trees. Have B bootstrap samples → create trees. They reduce dependence between tree estimates by only allowing a random subset of predictors at each split. Default: regression $p/3$, classification $\sqrt{p}$. (in R option mtry).

Out-of-Bag Error: Some bags have not trained on a particular sample. Can predict this only by the bags that have not been trained on it (should be $\sim 1/3$) for all samples and average to get a valid estimate for the test error.

	Tree	Bagging	Random Forest
Performance	-	+	++
Computation	+	-	+/-
Interpretation	+	-	-
Out-of-bag error	-	+	+

Random Forests

```
library(randomForest)
cs.bag <- randomForest(Sales ~ . , train.data, mtry=p-1) #
↪  Bagging
cs.forest <- randomForest(Sales ~ . , train.data, mtry=p/3) #
↪  Random Forest
importance(cs.forest) # Importance of predictors. Plot:
↪  varImpPlot(...
```

General R commands

Packages used: boot, leaps, gam, glmnet, ISLR, rpart, tree, randomForest, kknn, class, splines, MASS, Datasets

R-Help

```
is.na(x) # returns Boolean vector of size length(x)
na.omit(x) # removes rows with missing values from dataset.
qt(), rt(), qf(), rf() # etc. for student/r distr.
cut(seq(1,n),breaks=K,labels=FALSE) # to get K (roughly) equally
↪  sized folds.
which(x, arr.ind = TRUE) # gives vector of indices for which
↪  x==TRUE
par(mfrow=c(1,1)) # for division of plot window.
unique(x) # vector with elements of x # without duplicates.
names(object) # gives the stuff that can be returned by
↪  object$...
abline(v=...) # for vertical line in plot (h for horizontal)
cbind(), rbind() # combine
hist(..., freq=F) # for probab. scale
levels() # access to the levels attribute of a variable
complete.cases(data) # removes NA's
stripchart(..., method="stack") # for small data sets
fitdistr(data, densfun,...) # fits MLE do data (e.g.
↪  densfun="'gamma"')
which.max(...) # returns indices of maxima
# Test if an element is in a list
if ("X1" %in% names(coef(m,mo)))
# Creating categorical variables
High=ifelse(Carseats$Sales<=8,"No","Yes")
# Standardize data
scaled.dat <- scale(dat)
# Anova test to determine if there is a significant
# difference between models. Anova uses RSS and DoF
# of largest (last) model, so use ascending order!
anova(fit.0, fit.1, fit.2, fit.3)
# Given fixed x, error distribution and true param.:
# Power of test simulation. Know that y ~ poly(x, 3) + err (for
↪  typeI error: do same with y = err)
results.power <- numeric(n.sim)
for (i in 1:n.sim) {
    err <- rgamma(n, ...) - 2
    y <- beta.0 + beta.1 * I(x) + beta.2 * I(x^2) + beta.3 +
    ↪  I(x^3) + err
    fit.power <- lm(y ~ I(x) + I(x^2) + I(x^3))
    f1 <- summary(fit.power)$fstatistic
    p.val.power <- 1 - pf(f1[1], f1[2], f1[3])
    results.power[i] <- p.val.power < 0.05
  }
power <- mean(results.power)
# draw density and CDF
grid <- seq(from=0,to=5,length=200)
plot(grid, dlnorm(grid), type="l", main="density")
plot(grid, plnorm(grid), type="l", main="CDF")
```