SummingUp2019 03.04.2019

TMA4268 STATISTICAL LEARNING

fit → TRAINING SET $\{(x_1,y_1),\dots,(x_n,y_n)\}$ (independent pairs)

assess → TEST SET: same format

model selection → VALIDATION

LINEAR REGRESSION (M3)

classical normal regression model: $\begin{cases} Y = X\beta + \varepsilon \\ \varepsilon \sim N_n(0,\sigma^2 I)\end{cases}$ (Y: $n\times 1$, X: $n\times(p+1)$, β: $(p+1)\times 1$, ε: $n\times 1$)

X has rank $(p+1)$ = full rank ($n >> p+1$)

$\hat\beta = (X^TX)^{-1}X^TY$ ← minimize RSS

$\hat\beta \sim N_{(p+1)}(\beta, \sigma^2(X^TX)^{-1})$

$\hat\sigma^2 = \frac{1}{n-p-1}\cdot RSS$

$TSS = \sum_{i=1}^n (y_i-\bar y)^2$, $\bar y = \frac{1}{n}\sum_{i=1}^n y_i$ — total sum of squares

$RSS = \sum_{i=1}^n (y_i-\hat y_i)^2$ — residual sum of squares

$\hat y_i = x_i^T\hat\beta$

$R^2 = \frac{TSS-RSS}{TSS} = 1-\frac{RSS}{TSS}$ — coeff. of determination, prop. of variance explained by regression

c_{jj} is jth diagonal element of $(X^TX)^{-1}$.

Inference for one β_j: based on $T_j = \frac{\hat\beta_j - \beta_j}{\hat\sigma\sqrt{c_{jj}}} \sim t_{n-p-1}$

$(1-\alpha)100\%$ Confidence interval for β_j: $[\hat\beta_j \pm t_{\frac{\alpha}{2},n-p-1}\sqrt{c_{jj}}\,\hat\sigma]$

Prediction interval for Y_0 at x_0: $[x_0^T\hat\beta \pm t_{\frac{\alpha}{2},n-p-1}\,\hat\sigma\sqrt{1+x_0^T(X^TX)^{-1}x_0}]$

Hypothesis test: $H_0: \beta_j = 0$ vs $H_1: \beta_j \neq 0$

Reject H_0 when $T_0 = \frac{\hat\beta_j - 0}{\hat\sigma\sqrt{c_{jj}}}$ ...

Is the regression significant?

$H_0: \beta_1=\beta_2=\dots=\beta_p=0$ vs H_1: at least one different

$F = \frac{(TSS-RSS)/p}{RSS/(n-p-1)} \sim F_{p,n-p-1}$ under H_0

P-value: $P(F > f_{obs})$, f_{obs} observed F. $F_{p,n-p-1}$

Residuals: $e_i = y_i - \hat y_i$ and scaled versions thereof → plot: $\hat y_i$ vs e_i → random, no trend; plot: qq plot e_i for normality → straight line

MODEL SELECTION (M6) VS. MODEL ASSESMENT

$R^2_{adj} = 1-\frac{RSS/(n-p-1)}{TSS/(n-1)}$

$AIC = -2\,\text{loglikelihood} + 2\,(\text{number of param.})$ ($p+1$)

$BIC = -2\,\text{loglikelihood} + \log(n)\cdot$ — " —

penalizing of training error

can be used in model selection using "only" the training data

- best subset selection: all "models" (2^p models)
- stepwise methods ← when p is large ($1+p(p+1)/2$ models)

When model selection is done on test set or with CV, then RSS, R^2, MSE can be used. (unpenalized)

RSS will always decrease (or stay unchanged) if new covariates are added to the regression (even if they are just noise — why?), and R^2 will always increase (or stay unchanged). Therefore R^2 can never be a criterion to choose between regr. models of different model complexity based on a training set alone.

DIMENSIONALITY REDUCTION: Principal component regression PCA (M6+10)

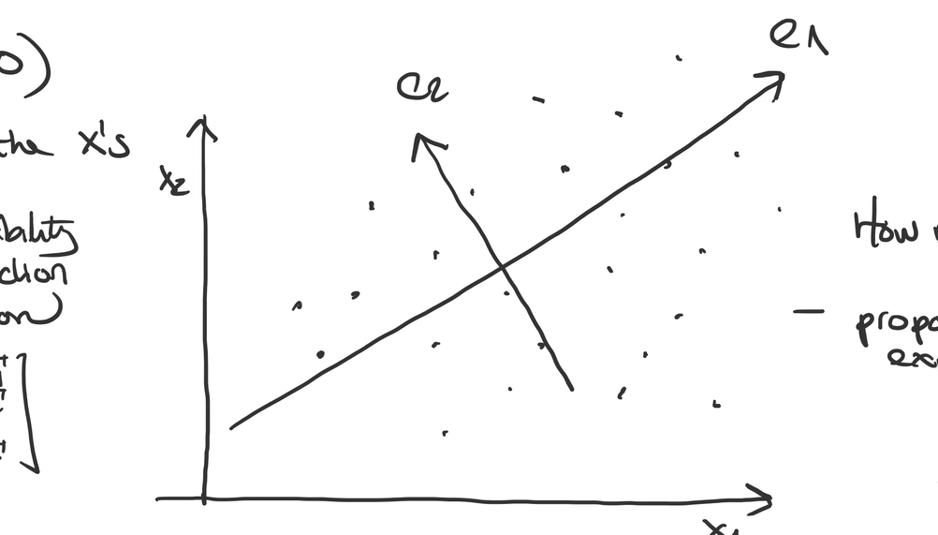
Have $X_{n\times p}$ with p large and/or many correlated covariates: want set of linear comb. of the X's that capture a large part of the variability — and where the sets are uncorrelated. → for interpretability, data reduction, visualization

Let Σ be covariance (or correlation) matrix of X, and (λ_i, e_i): $\Sigma = P\Lambda P^T$ eigenvalue/eigenvector pairs of Σ where $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p$. Then $[e_1 e_2 \dots e_p]\begin{bmatrix}\lambda_1 & & 0\\ & \ddots & \\ 0 & & \lambda_p\end{bmatrix}\begin{bmatrix}e_1^T\\ e_2^T\\ \vdots\\ e_p^T\end{bmatrix}$

construct $Z_i = e_i^T X$ (principal component scores; loadings; $p\times 1$ random vector). Property: $Cov(Z) = \begin{bmatrix}\lambda_1 & & 0\\ & \ddots & \\ 0 & & \lambda_p\end{bmatrix}$ uncorrelated with $Var(Z_i) = \lambda_i$.

MLR can then be performed with Z as covariates instead of X. ⇒ PCR

but remember the PC's are not selected based on Y only on X, so we assume variability in X is related to variability in Y



IMPORTANT: the eigenvalues of the correlation matrix are different from the eigenvalues of the covariance matrix — what you want depends on the situation — but mostly corr. is used.

How many PC's? — proportion of total variance explained by the k PC's $\frac{\sum_{i=1}^k \lambda_i}{\sum_{i=1}^p \lambda_i}$ ← should be ~95%?

Partial least squares (PLS): Competitor to PCR, but now Z is found also taking Y into account. More details in MA8701.

MODEL REGULARIZATION (M6)

Motivation: LS regression gives unbiased $\hat\beta$, but variance might be large, e.g. when covariates are correlated → $(X^TX)^{-1}\sigma^2$ (or p is large compared to n). If we instead look at biased $\hat\beta$ (shrunken) we might get smaller $Var(\hat\beta) + (E(\hat\beta)-\beta)^2$ (brutto variance). This also reduces the effective number of parameters.

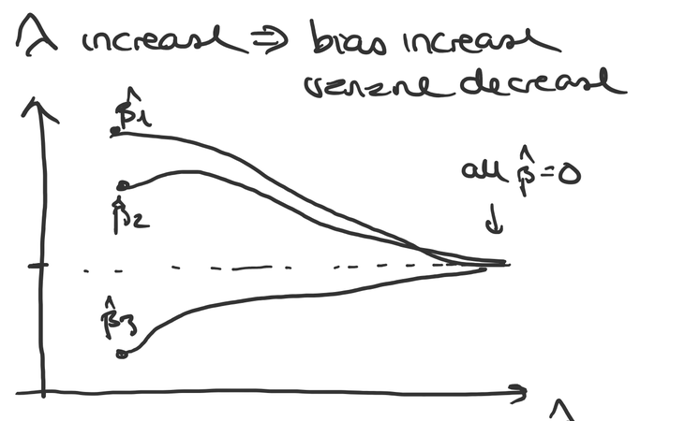
Ridge (L2) regression: minimize$_\beta$ $RSS + \lambda\sum_{j=1}^p \beta_j^2$ (β_0 not penalized)

λ: tuning parameter ← decided by CV ← value giving min $\widehat{MSE}$

not scale invariant — useful to scale covariates before using ridge

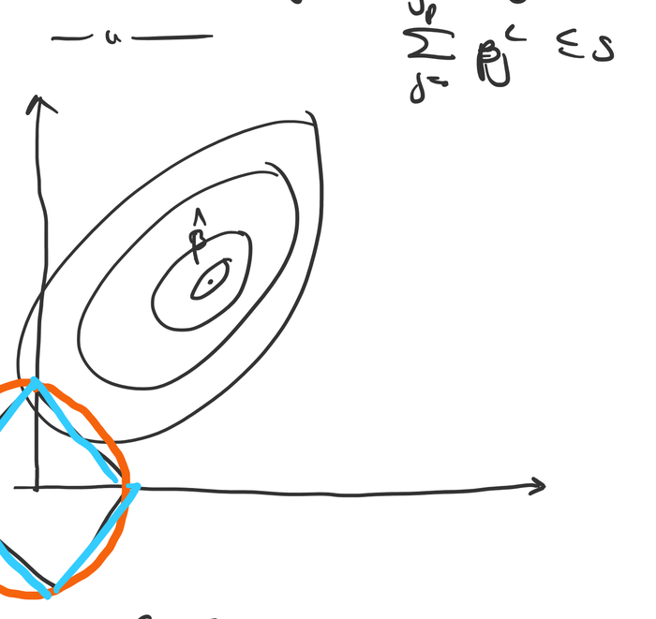
λ increase ⇒ bias increase, variance decrease

Interpretation of plots: ridge:



Lasso (L1) regression: minimize$_\beta$ $RSS + \lambda\sum_{j=1}^p |\beta_j|$ — automatically performs model selection

Dual problem: min RSS subj. to $\sum_{j=1}^p |\beta_j| \leq s$ lasso; $\sum_{j=1}^p \beta_j^2 \leq s$ ridge



MOVING BEYOND LINEARITY (M7)

$Y = f(x)+\varepsilon$ and MLR $f(x) = X\beta$. → $\hat\beta = (X^TX)^{-1}X^TY$ (but we only look at one x at a time first)

X can be replaced by a set of basis functions $X^* = \begin{bmatrix}1 & b_1(x_1) & b_2(x_1) & \cdots & b_k(x_1)\\ \vdots & & & & \vdots\\ 1 & b_1(x_n) & & \cdots & b_k(x_n)\end{bmatrix}$ ($x_1 = x$ for obs 1, $x_n = x$ for obs n)

So we still have linearity in β's — but now $f(x) = X^*\beta$, So $\hat\beta = (X^{*T}X^*)^{-1}X^{*T}Y$

1) POLYNOMIAL regression: $b_k(x) = x^k$

2) STEP FUNCTIONS: $b_k(x) = I(c_k \leq x < c_{k+1})$ — similar to dummy variable coding, but now x might be continuous

3) REGRESSION SPLINES: combine polynomials & steps at knots

order-M spline: $b_j(x) = x^j$, $j = 1,\dots,M-1$; $b_{M-1+k}(x) = (x-c_k)_+^{M-1}$, $k = 1,\dots,K$

where knots $c_1,\dots,c_K$ are chosen (not estimated). The resulting curve is smooth and deriv. up to order M−2 continuous (also in knots). Cubic spline popular.

NATURAL cubic spline = cubic spline that is linear at ends. Now bases as $b_1(x) = x$, $b_{k+2}(x) = d_k(x) - d_K(x)$ (small k, small k, capital K)

$d_k(x) = \frac{(x-c_k)_+^3 - (x-c_K)_+^3}{c_K - c_k}$

4) SMOOTHING SPLINE ← penalization problem (similar to ridge & lasso). $g(x)$ smoothing spline

min $\sum_{i=1}^n (y_i - g(x_i))^2 + \lambda\int g''(t)^2 dt$ (tuning; penalize variation in g; how much g varies)

$\lambda = 0$ g interpolates

It turns out (MA8701) that a smoothing spline is a natural cubic spline with knots at the unique values of x. → lovely maths with smoother matrix! (beyond our scope in this course)

λ can be chosen by CV, or some version of AIC. Then effective number of parameters is calculated from the trace of the smoother matrix. (beyond our scope)

5) Local regression: smoothed version of KNN regression

minimize$_\beta$ $\sum_{i=1}^n K_{i0}(y_i - \beta_0 - \beta_1 x_i - \beta_2 x_i^2)^2$ ← close observation higher weight than far apart; different versions

6) Additive model: put 1-5 all together

$X = [1\ X_1\ X_2\ X_3]$ ← choice for X_1, maybe poly? choice for X_2, maybe natural cubic spline; choice for X_3, maybe smoothing spline?

EXTENSION: this additive model can be used on $p_i = \frac{\exp(x_i^T\beta)}{1+\exp(x_i^T\beta)}$ (new X) to generalize to logistic regression and make that class boundaries non-linear in X-space.

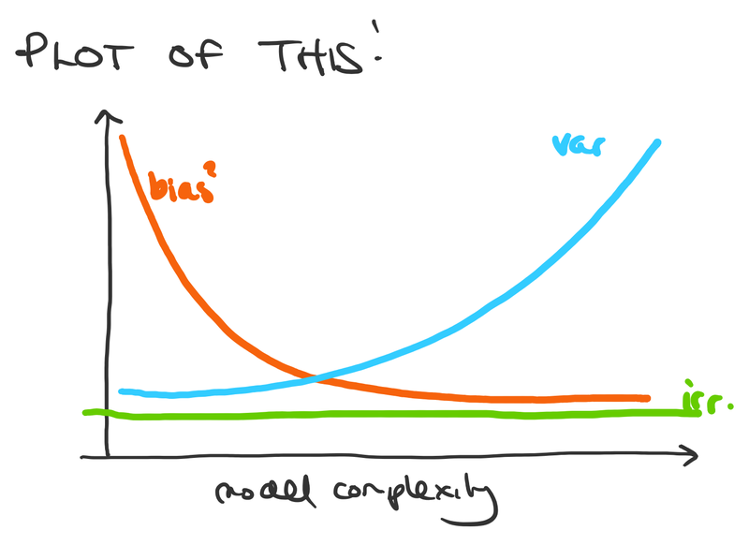
[M2+3] BIAS-VARIANCE trade-off in regression setting: $Y = f(x)+\varepsilon$

Expected test mean squared error at x_0:

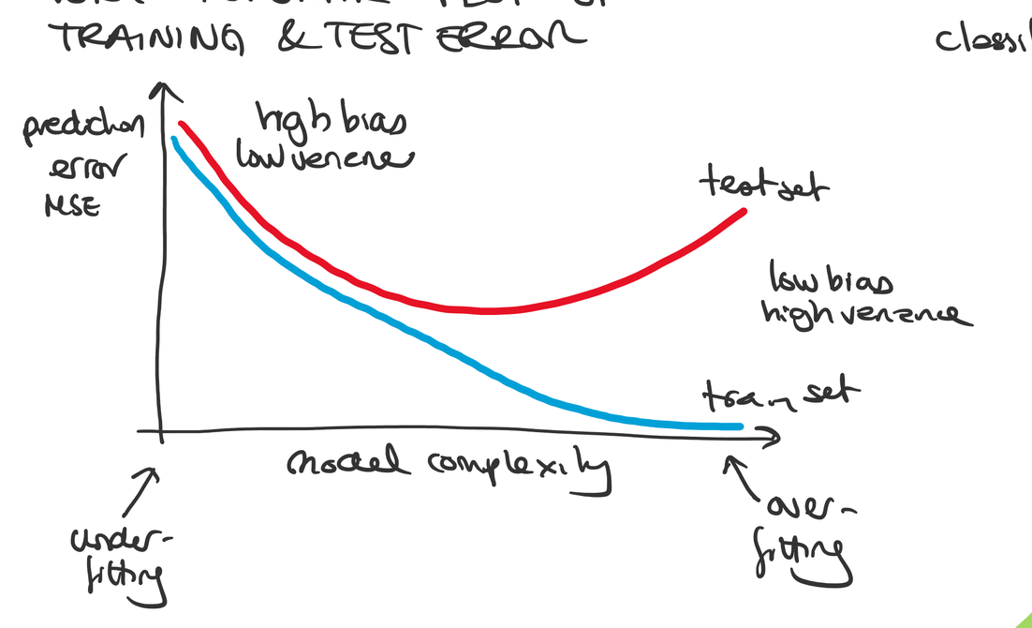
$E[(Y-\hat f(x_0))^2] = \dots = Var(\varepsilon) + Var[\hat f(x_0)] + Bias(\hat f(x_0))^2$

irreducible error; variance of prediction at x_0; bias of prediction at x_0 ($(f(x_0)-\hat f(x_0))^2$, $\hat f(x)$ from ...)

PLOT OF THIS:



VERY POPULAR PLOT OF TRAINING & TEST ERROR



Loss function:

regression: Quadratic: $\sum_{i=1}^n (y_i - f(x_i))^2$

classification: 0/1: $y_i = f(x_i) \to 0$ loss; $y_i \neq f(x_i) \to 1$ loss

minimize 0/1 loss → Bayes classifier: classify to the class with the highest probability $P(Y=k \mid X=x)$ — and in simulation experiments this is known.

Bayes class boundary: boundary of Bayes classifier.

Bayes error = error rate of Bayes classifier

RESAMPLING METHODS (M5)

DATA rich situation (sometimes, e.g. when we generate data ourselves)

TRAIN	VALIDATE	TEST
↑ fit model	↑ model selection (complexity)	↑ model assessment

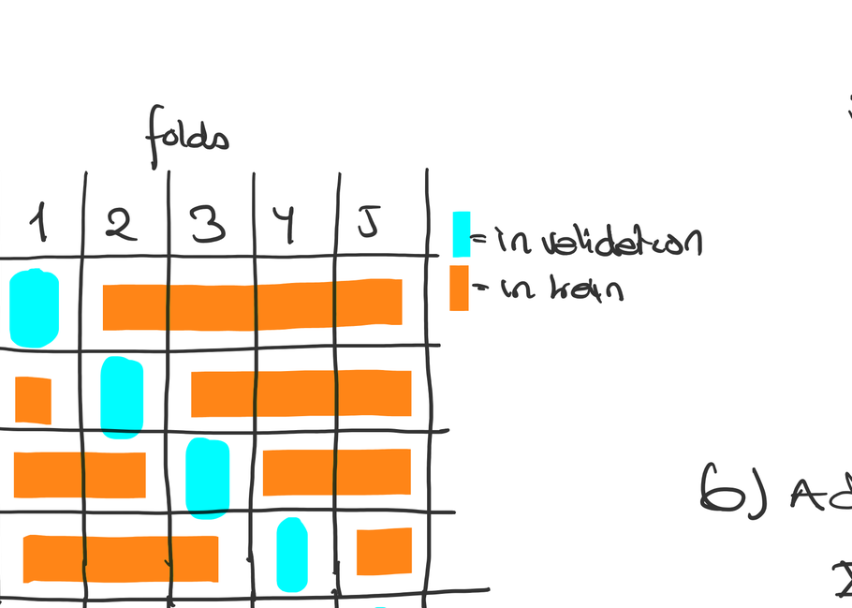
DATA not so rich = common situation:

- → Validation set approach (V↑ B↑)
- → Leave one out cross validation LOOCV (V↑ due to corr., B↓)
- → k-fold cross validation (CV)

• biased estimate (as compared to using the whole d.s. to train) • high/low variance • randomness • comp. issues — expensive

pros and cons of the three methods ⇓ compromise 5 or 10-fold CV

Assess with $MSE_i = (y_i - \hat y_i)^2$ for each obs ← regression; or 0/1: $I(y_i \neq \hat y_i)$ ← classification. Sum over folds and average.



$CV = \frac{1}{n}\sum_{j=1}^k MSE_j \cdot n_j$ (regr.)

$MSE_j = \frac{1}{n_j}\sum_{i\in j\text{th fold}} (y_i - \hat y_i)^2$ ← prediction when trained without jth fold

How to PERFORM CV: ALL PARTS of model fitting must be (inside) CV loop unless → selection bias. Eg: cancer predicted perfectly from 5 genes example

MORE RESAMPLING (M5)

BOOTSTRAPPING: data set of n observations. Estimate $\hat f$ by $\frac{1}{n}$. Draw random sample from $\hat f$ → draw with replacement from data → one bootstrap sample

The probability that x_i is in bootstrap sample is $1-(1-\frac{1}{n})^n \xrightarrow{n\to\infty} 0.632$

We may estimate $SD(\hat\beta_j)$ from regression — using bootstrapping. CI's in TMA4300 Comp. stat.

$\widehat{SD}(\hat\beta_j) = \sqrt{\frac{1}{B-1}\sum_{b=1}^B(\hat\beta_{jb} - \frac{1}{B}\sum\hat\beta_{jb})^2}$ B = total no. of bootstrap samples

CLASSIFICATION (M4)

(Y_i, x_i) with $Y_i \in \{1,\dots,K\}$ or $Y_i = \{0,1\}$ or $\{-1,1\}$ (as in M9)

$p_k(x_0) = P(Y=k \mid X = x_0)$ posterior class probability

$\pi_k = P(Y=k)$ prior class probability

$f_k(x) = "P(X=x \mid Y=k)"$ is pdf of x in class k, class conditional distribution

diagnostic paradigm = directly estimate $P(Y=k \mid X=x)$

Sampling paradigm = estimate π_k and $f_k(x)$ and classify to largest $\pi_k f_k(x)$

● Sampling paradigm: LDA & QDA

LDA: $f_k(x)$ is $N(\mu_k, \Sigma)$. $\hat\mu_k = \frac{1}{n_k}\sum_{i:y_i=k} x_i$

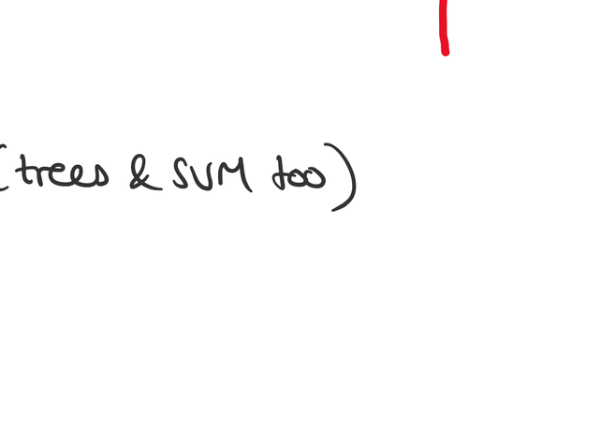
QDA: $f_k(x)$ is $N(\mu_k, \Sigma_k)$

$\hat\Sigma_k = \frac{1}{n_k-1}\sum_{i:y_i=k}(x_i-\hat\mu_k)(x_i-\hat\mu_k)^T$

$\hat\pi_k = \frac{n_k}{n}$

$\hat\Sigma = \sum_{k=1}^K \frac{n_k-1}{n-K}\cdot\hat\Sigma_k$

$\pi_k\cdot f_k(x) = \pi_j f_j(x)$ → linear class boundaries for LDA, quadratic QDA



● Diagnostic paradigm: KNN & logistic regression (trees & SVM too)

KNN: $\hat P(Y=j \mid X=x_0) = \frac{1}{K}\sum_{i\in N_0} I(y_i = j)$ — N_0 = neighborhood of x_0

Logistic regression ($K=2$): $Y_i = \begin{cases}0 & \text{with prob. } (1-p_i)\\ 1 & p_i\end{cases}$

where $p_i = \frac{\exp\{x_i^T\beta\}}{1+\exp\{x_i^T\beta\}}$ ← logistic function aka sigmoid; $x_i = \begin{bmatrix}1\\x_{i1}\\ \vdots\\ x_{ip}\end{bmatrix}$, $X = \begin{bmatrix}x_1^T\\ \vdots\\ x_n^T\end{bmatrix}$

Prediction at x_0: $\hat p(x_0) = \frac{\exp(x_0^T\hat\beta)}{1+\exp(x_0^T\hat\beta)}$

Parameter estimates found by maximum likelihood (TMA4315 GLM) not on closed form.

$odds = \frac{p_i}{1-p_i}$ so $p_i = \frac{1}{2}$ gives odds 1, and is relevant because:

$\frac{P(Y_i=1 \mid x_{i1}+1)}{P(Y_i=0 \mid x_{i1}+1)} = \frac{P(Y_i=1 \mid x_{i1})}{P(Y_i=0 \mid x_{i1})}\cdot\exp(\beta_1)$

If x_1 increase to x_1+1, but all other x's are kept fixed then the odds is multiplied by $\exp(\beta_1)$.

Class boundary is linear in x-space, because $\log\left(\frac{p(x)}{1-p(x)}\right) = x^T\beta$ and set a cut-off on $p(x)$ (e.g. 0.5) and solve: $0 = x^T\beta = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p$ is the eq. for a hyperplane.

Assessment of classification → given a cut-off on p (maybe 0.5) — n observations — on test data

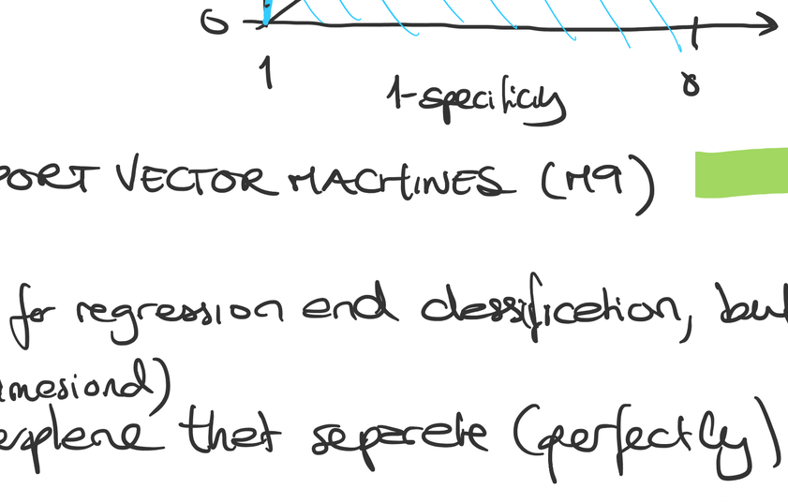
Confusion matrix:

		predicted class 0	predicted class 1	
true class	0	TN	FP	N
	1	FN	TP	P

may report misclassification rate $1-\frac{(TN+TP)}{n}$ or accuracy = rate of correct classifications: $\frac{TN+TP}{n}$

Sensitivity = $TP/(FN+TP)$

Specificity = $TN/(TN+FP)$



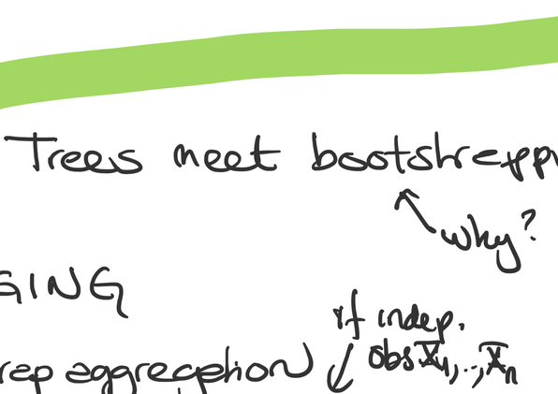
ROC-curve, each • is based on one cut-off on p.

AUC: area under ROC-curve

AUC = ½ = random guessing

TREE-BASED METHODS (M8)

both for regression & classification — and we have nonlinearities & interactions between covariates!



1) Want to minimize an error criterion on the whole tree construction — but since computationally infeasible a greedy approach "recursive binary splitting" is used.

$R_1(j,s) = \{x \mid x_j < s\}$, $R_2(j,s) = \{x \mid x_j \geq s\}$: find predictor (j) and splitting point (s) that minimize "RSS"

Regression: $\sum_{i:x_i\in R_1}(y_i - \hat y_{R_1})^2 + \sum_{i:x_i\in R_2}(y_i - \hat y_{R_2})^2$ ($RSS(R_1)$, $RSS(R_2)$) — $\hat y_{R_1}$ = mean of training resp. in R_1

Classification: similar, but using impurity measure ← $\hat p_{jk} = \frac{1}{N_j}\sum_{i:x_i\in R_j} I(y_i = k)$ (n_{jk})

• Gini index: In region R_j (leaf node) with N_j obs. $G = \sum_{k=1}^K \hat p_{jk}(1-\hat p_{jk})$

• Cross entropy: $D = -\sum_{k=1}^K \hat p_{jk}\cdot\log\hat p_{jk} = -\sum_{k=1}^K\left(\frac{n_{jk}}{N_j}\cdot\log\left(\frac{n_{jk}}{N_j}\right)\right)$

• Deviance: $-2\sum_{k=1}^K n_{jk}\cdot\log(\hat p_{jk}) = -2\sum_{k=1}^K n_{jk}\cdot\log\left(\frac{n_{jk}}{N_j}\right)$ } gives the same tree

2) Continue splitting until we reach decided stopping criterion. Eg: reduction in RSS not big, less than 5 obs in a terminal node.

3) This full tree is used for prediction by dropping a new obs down the tree and predict as

a) regression: $\hat y = \frac{1}{N_j}\sum_{i:x_i\in R_j} y_i$ (R_j region (leaf)) ← y_i's in the training set

b) classification: $\hat y$ = majority vote among all y_i's in R_j

or $\hat p_{kj} = \frac{1}{N_j}\sum_{i:x_i\in R_j} I(y_i = k)$ (n_{jk}) and classify to the class with the highest probability.

4) From a full tree to a pruned tree. Reduce the size of the tree by cutting branches. Cost complexity pruning: for a complexity param α

minimize$_T$ $C_\alpha(T) = Q(T) + \alpha\cdot|T|$ (tree; cost function from the fitting (Gini, deviance, ...); number of terminal nodes) α found by CV.

5) Evaluate model fit on a test set! Same criteria as regression (RSS) or classification (ROC, AUC, misclassification rate).

Trees meet bootstrapping ⇒ FORESTS ← why? More powerful prediction models — but loose in interpretation

A) BAGGING

Bootstrap aggregation (if indep. obs $X_1,\dots,X_n$)

Motivation: $Var(\bar X) = \frac{\sigma^2}{n}$ → we construct many trees and average them to define $\hat y$. The B trees we grow (full) from B bootstrap samples. $\hat f_{bag}(x) = \frac{1}{B}\sum_{b=1}^B \hat f^{*b}(x)$ ← one tree!

B) RANDOM FOREST — but not maximal effect of bagging because trees are not independent ⇒ we make them more uncorrelated by not allowing all p covariates to be chosen in each binary split.

Rule of thumb: $m = \sqrt{p}$ classification and $m = \frac{p}{3}$ for regression

OOB = out-of-bag: for each bootstrap sample there are on average $\frac{2}{3}$ of the observations in the sample (bag). The last $\frac{1}{3}$ are used for prediction. We will then have $\approx\frac{B}{3}$ predictions for observation i — which we average.

Variable importance plots: — give the total amount of RSS (or Gini) decrease over splits of a predictor — averaged over all B trees

C) BOOSTING: many variants, but we only considered boosting regression trees

Fit one tree — make residuals — fit a tree to the residuals → update

$\hat f(0) = 0$, $\hat f^b(x)$ with d splits

$\hat f(x) \leftarrow \hat f(x) + \lambda\cdot\hat f^b(x)$

$r_i \leftarrow r_i - \lambda\hat f^b(x_i)$

$\hat f(x) = \sum_{b=1}^B \lambda\hat f^b(x)$

Tuning parameters: B = number of trees; λ = shrinkage parameter; d = number of tree splits

SUPPORT VECTOR MACHINES (M9)

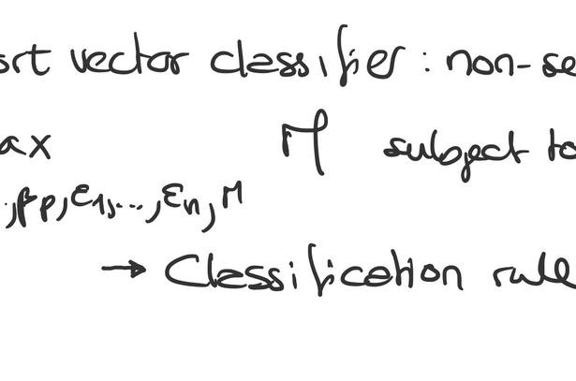
A method both for regression and classification, but we only consider classification, and two classes } standardized x's are preferred!

Aim: find (high dimensional) hyperplane that separate (perfectly) the two classes (coded as $\{-1,1\}$)

$\beta_0 + x^T\beta = 0$ with normalized βs $\sum_{j=1}^p \beta_j^2 = 1$

$\beta_0 + x^T\beta > 0$ one side of hyperplane; < 0 the other side } $y_i\cdot(\beta_0 + x_i^T\beta) > 0$ if correct classified x_i

separable problem



Maximal margin classifier: $\max_{\beta_0,\beta_1,\dots,M} M$ subject to $\sum_1^p \beta_j^2 = 1$; $y_i(\beta_0 + x_i^T\beta) \geq M$ $\forall i = 1,\dots,n$

CONNECTION SVM & logistic regression (ridge version)

SVM: $\min_\beta\left\{\sum_{i=1}^n \max(0, 1-y_i f(x_i)) + \lambda\sum_{j=1}^p \beta_j^2\right\}$ (hinge loss; ridge penalty)

logistic regr has $\log(1+\exp(-y_i f(x_i)))$ which looks similar; $f(x_i)$ might contain nonlinear terms

result: the hyperplane only depends on the observations that lie on the margin or on the wrong side of the margin = "support vectors"

Support vector classifier: non-separable case — $\varepsilon_1,\dots,\varepsilon_n$: slack variables

$\max_{\beta_0,\beta_1,\dots,\beta_p,\varepsilon_1,\dots,\varepsilon_n,M} M$ subject to $\sum_1^p \beta_j^2 = 1$, $y_i(\beta_0 + x_i^T\beta) \geq M(1-\varepsilon_i)$ $\forall i$, $\varepsilon_i \geq 0$, $\sum_1^n \varepsilon_i \leq C$ { C is tuning parameter chosen by CV

→ Classification rule: $f(x^*) = \beta_0 + x^{*T}\beta$ and: if $f(x^*) < 0$ set $y^* = -1$; > 0 set $y^* = 1$

to understand skills in optimization is needed (Lagrange primal & dual problem)

Support vector machine: $f(x) = \beta_0 + \sum_{i\in S}\alpha_i K(x, x_i)$ — $x_i^T\beta$ replaced by more general nonlinear functions that are written as sums of kernels (generalization of inner products)

$\max_{\beta_0,\alpha_1,\dots,\alpha_n,\varepsilon_1,\dots,\varepsilon_n,M} M$, $y_i(f(x_i)) \geq M(1-\varepsilon_i)$, $\varepsilon_i \geq 0$, $\sum\varepsilon_i \leq C$, $\sum_1^p \beta_j^2 = 1$ where $f(x) = \beta_0 + \sum_{i\in S}\alpha_i K(x, x_i)$

tuning: (C,γ) by CV

popular kernel: radial kernel: $K(x_i, x_i') = \exp\left(-\gamma\sum_{j=1}^p (x_{ij} - x_{i'j})^2\right)$

UNSUPERVISED LEARNING (M10)

Look for underlying structure or groupings in data — no Y only $X_{n\times p}$.

Principal component analysis (see M6)

PC loadings: interpret effect of each covariate on each component — average effect, diff between A and B etc

PC score: (plot) observations in PC1 & PC2, ... can be used for quality control

PC scores → MLR = PCR (M6)

K-means clustering (non-overlapping clusters)

- * Number of clusters given (or selected separately)
- * Define cluster centroids → classify observations to clusters (closest)
- * Recalculate centroids

Euclidean distance popular (but also (weighed) Mahlanobis)

Generalizations to medioids etc.

Hierarchical clustering — work in a sequential way by connecting observations that are similar

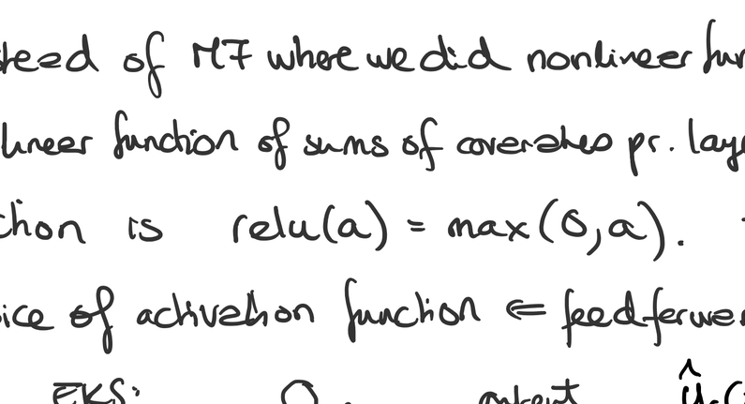
- * Similarity measures (dissimilarity): Euclidean, Correlation
- * Linkage: how to calculate dissimilarity between groups of observations?
  - single: minimum
  - average: average
  - complete: maximum
- * Presented in a dendrogram — choose where to cut the dendrogram to get a number of clusters.

NEURAL NETWORKS (M11)

nnet or keras are R packages to be used

a) Possible to represent MLR & logistic regression as graph (one input and one output layer)

$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_p x_p + \varepsilon$



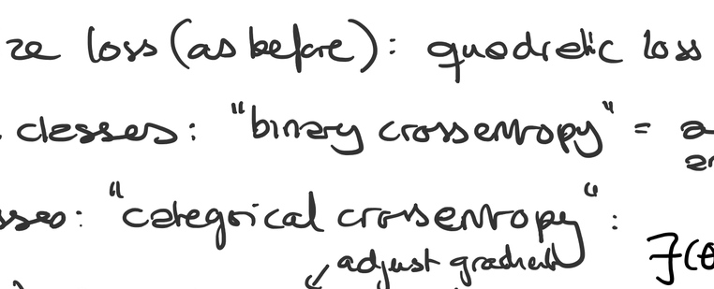
$\log\left(\frac{p}{1-p}\right) = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p$ ⟺ $p = \frac{\exp(\beta_0 + \dots)}{1+\exp(\beta_0+\dots)} = \frac{\exp(a)}{1+\exp(a)}$

same graph, but now output layer has logistic activation function (sigmoid) used for two-class classification problems

for K classes: K outputs (dummy) and softmax activation $\frac{\exp(a_k)}{\sum_{k=1}^K \exp(a_k)}$ ensure sum to 1

b) Instead of M7 where we did nonlinear function of each covariate, we instead look at nonlinear function of sums of covariates pr. layer — and add many layers. Popular non-linear activation function is $relu(a) = \max(0,a)$. For each layer we specify number of nodes and choice of activation function ⇐ feedforward network.

EKS:



$\hat y_c(x) = \phi_o\left(\beta_{0c} + \sum_{m=1}^M \beta_{mc}\phi_h\left(\alpha_{0m} + \sum_{j=1}^p \alpha_{jm}x_j\right)\right)$

number of unknown parameters? 4 in hidden to output, 15 in input to hidden, 19 ($p=4$ inputs + bias)

c) How to find/estimate the unknown weight (= parameters)?

— minimize loss (as before): quadratic loss for regression = "mse" $J(\theta) = \frac{1}{n}\sum_{i=1}^n (y_i - \hat y(x_i))^2$

K=2 classes: "binary crossentropy" = as in tree and logistic regression $J(\theta) = -\frac{1}{n}\sum_{i=1}^n (y_i\ln(\hat y(x_i)) + (1-y_i)\ln(1-\hat y(x_i)))$

K classes: "categorical crossentropy": $J(\theta) = -\frac{1}{n}\sum_{i=1}^n \frac{1}{C}\sum_{c=1}^C (y_{ic}\ln(\hat y_c(x_i)))$

— optimization: (rmsprop; adjust gradient), adam, ...

gradient based: (order method), can use chain rule for differentiation, with stoch. version with "batches" of observations

popular: mini-batch stochastic gradient descent

epoch: one run through all observations

d) Evaluation of performance: "metrics"

mae = mean abs. error, accuracy = average correct classif.

e) avoiding overfitting:

- smaller network or more data
- regularization (L1, L2, combine)
- drop-out
- early stopping

⊗ "unsolved": how do we assess the uncertainty in the network fitted?