SummingUp v 23.05.2018

~~Saturday, 21 April 2018 13:45~~

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

VS. MODEL ASSESMENT

LINEAR REGRESSION (M3)

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

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

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)

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

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

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

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)

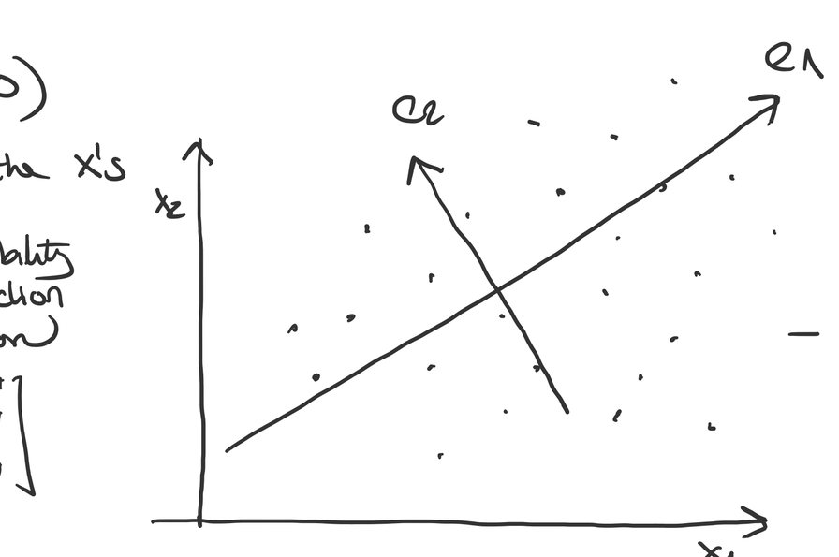
Have $X_{n\times p}$ with p large and/or many correlated covariates: want set of linear comb. of the X's that capture a large part of the variability – and where the sets are uncorrelated. → for interpretability, data reduction, visualization

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 $[e_1 e_2 \dots e_p]\begin{bmatrix}\lambda_1 & & 0\\ & \ddots & \\ 0 & & \lambda_p\end{bmatrix}\begin{bmatrix}e_1^T\\ \vdots \\ e_p^T\end{bmatrix}$

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%?

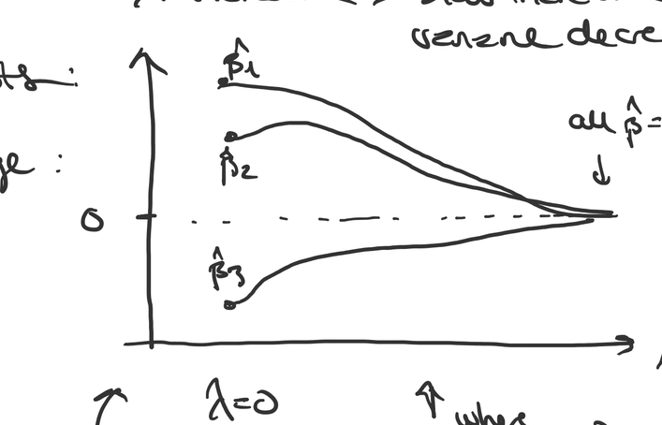
Partial least squares (PLS): Competitor to PCR, but now Z is found also taking Y into account. More details in MA8701.

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 $Var(\hat\beta) + (E(\hat\beta)-\beta)^2$ (bias-variance tradeoff). This also reduces the effective number of parameters.

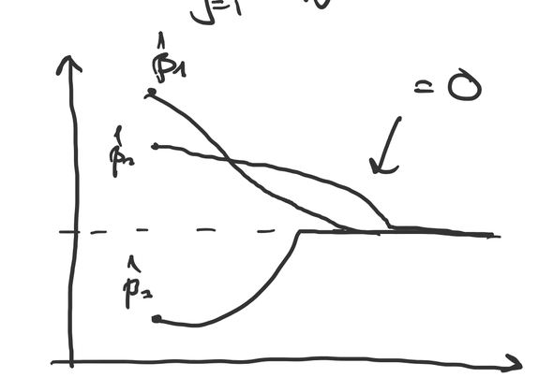
Ridge (L2) regression: minimize over β: $RSS + \lambda\sum_{j=1}^p \beta_j^2$
- not scale invariant – useful to scale covariates before using ridge
- β_0 not penalized
- λ: tuning parameter, decided by CV ← value giving min MSE
- λ increase ⇒ bias increase, variance decrease

Interpretation of plots: ridge:

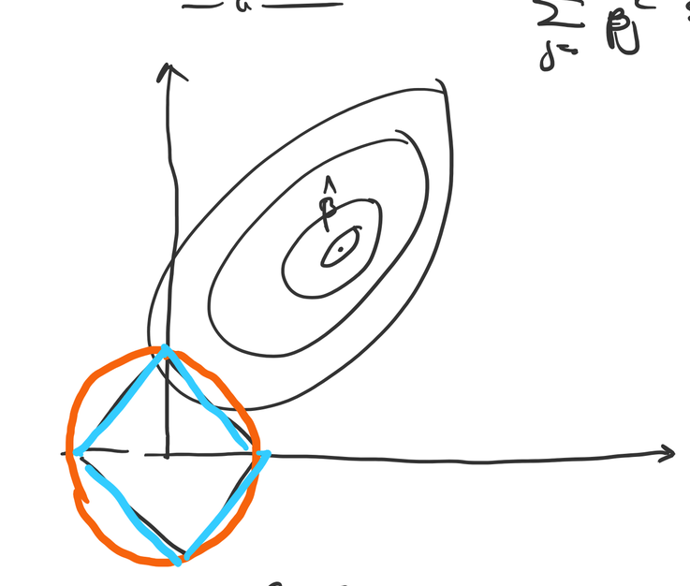


$\lambda = 0$ least squares; when is best λ?

Lasso (L1) regression: minimize over β: $RSS + \lambda\sum_{j=1}^p |\beta_j|$ — 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)
$$d_k(x) = \frac{(x-c_k)_+^3 - (x-c_{K+1})_+^3}{c_{K+1}-c_k}$$

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 how much g turns
$\lambda = 0$ 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)

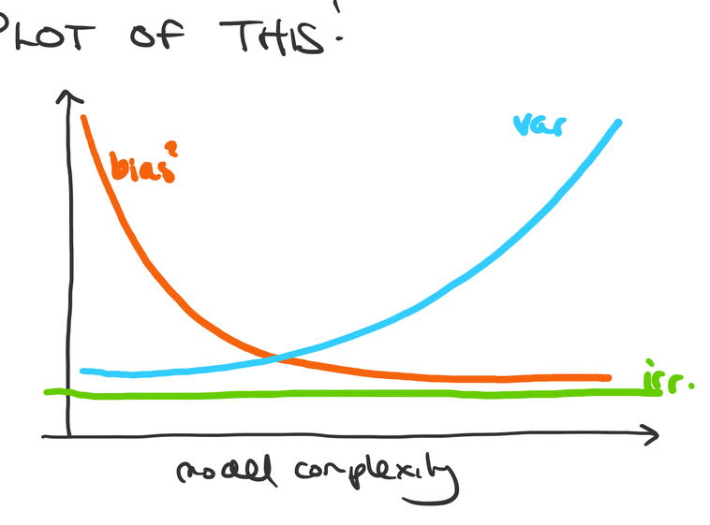
5) Local regression: smoothed version of KNN regression
minimize over β: $\sum_{i=1}^n K_{i0}(y_i - \beta_0 - \beta_1 x_i - \beta_2 x_i^2)^2$
close observation higher weight than far apart; different versions

6) Additive model: put it all together
$X = [1\ X_1\ X_2\ X_3]$ — choose for X_1 maybe poly?; choose for X_2, maybe natural cubic spline; choose 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 the class boundaries non-linear in x-space.

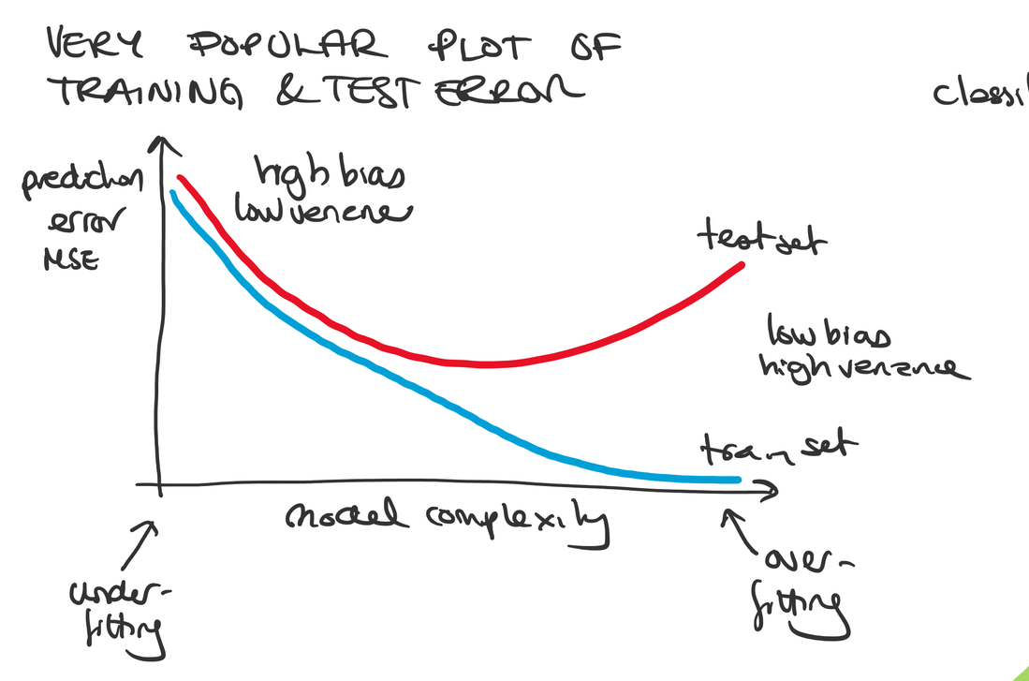
[M2+3] BIAS-VARIANCE trade-off in regression setting: $Y = f(x) + \varepsilon$

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 ($f(x_0) - \hat f(x_0)$)

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 $P(Y=k|X=x)$ – and in simulation experiments this is known.
Bayes–class boundary: boundary of Bayes classifier.
Bayes error = error rate of Bayes classifier

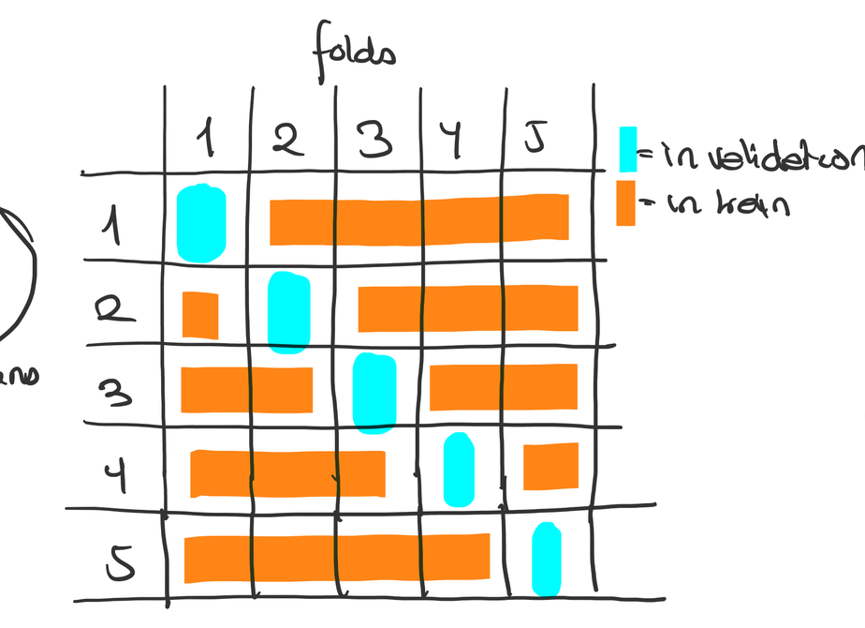
RESAMPLING METHODS (M5)

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 ($V+, B+$; due to corr. $V+, B\div$)
- → Leave one out cross validation LOOCV
- → k-fold cross validation (CV)
- • biased estimate (as compared to using the whole data 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.
$$\widehat{SD}(\hat\beta_j) = \sqrt{\frac{1}{B-1}\sum_{b=1}^B\left(\hat\beta_b - \frac{1}{B}\sum \hat\beta_b\right)^2}$$ 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)

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

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

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

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

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

Sampling paradigm: LDA & QDA

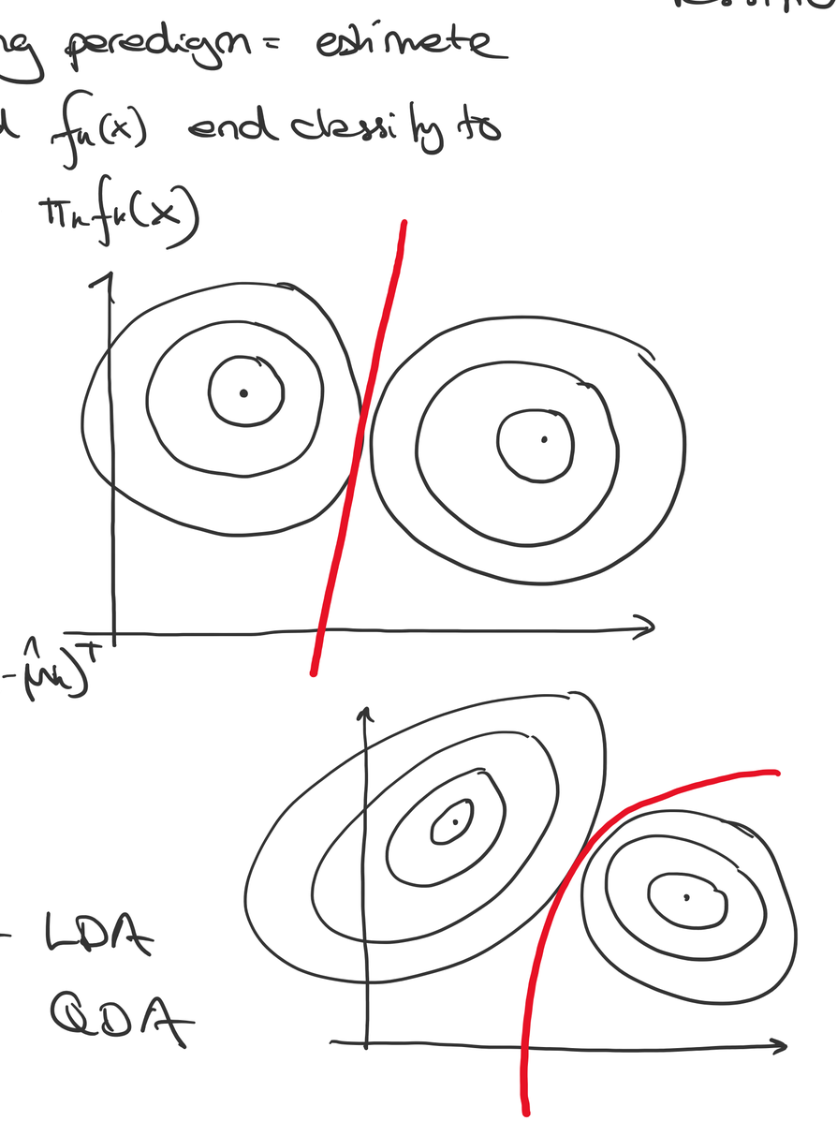
LDA: $f_k(x)$ is $N(\mu_k, \Sigma)$. $\hat\mu_k = \frac{1}{n_k}\sum_{i:\{y_i=k\}} x_i$
QDA: $f_k(x)$ is $N(\mu_k, \Sigma_k)$

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

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

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

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



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

KNN: $\hat P(Y=j|X=x_0) = \frac{1}{K}\sum_{i\in N_0} I(y_i=j)$, 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 $p_i = \frac12$ gives odds 1, and is relevant because:
$$\frac{P(Y_i=1|x_{i1}+1)}{P(Y_i=0|x_{i1}+1)} = \frac{P(Y_i=1|x_{i1})}{P(Y_i=0|x_{i1})}\cdot\exp(\beta_1)$$

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.

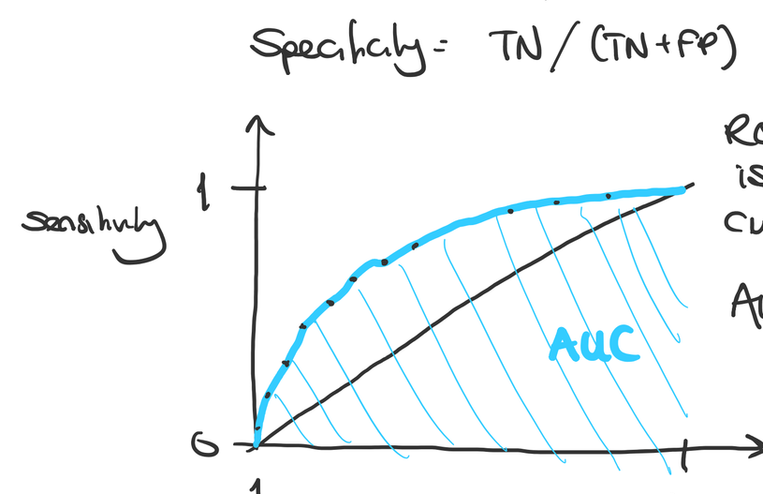
Assessment of classification → given a cut-off on p (maybe 0.5); n observations; on test data

Confusion matrix:

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

may report misclassification rate $1-\frac{(TN+TP)}{n}$ og 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

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

SUPPORT VECTOR MACHINES (M9)

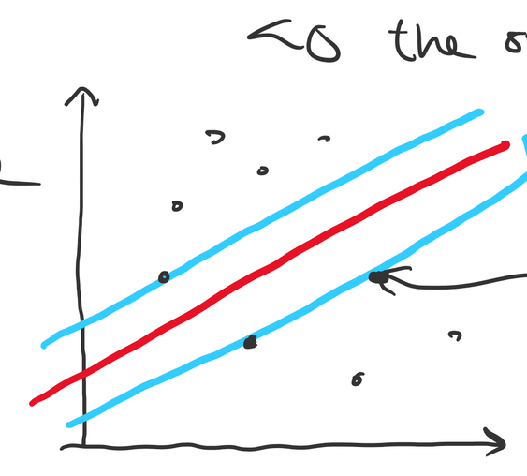
A method both for regression and classification, but we only consider classification, and two classes (coded as $\{-1,1\}$). Standardized x's are preferred!

Aim: find (high dimensional) hyperplane that separate (perfectly) the two classes

$\beta_0 + x^T\beta = 0$ 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 $\sum_1^p\beta_j^2 = 1$, $y_i(\beta_0 + x_i^T\beta) \geq M$ $\forall i = 1,\dots,n$

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

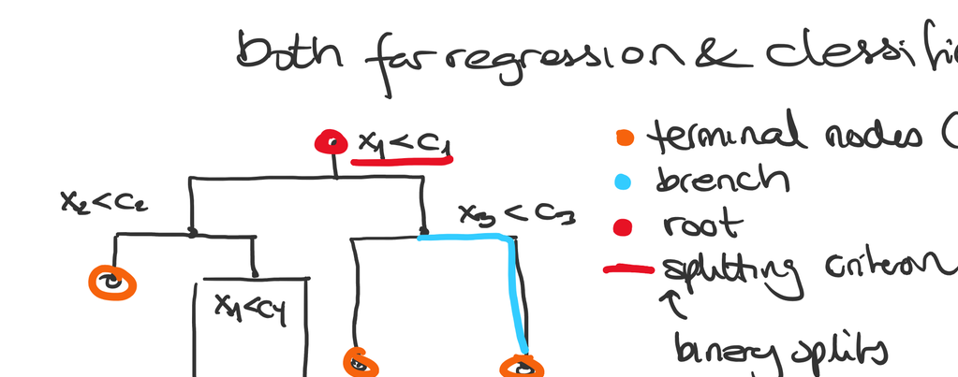
Support vector classifier: non-separable case – $\varepsilon_1,\dots,\varepsilon_n$: slack variables
$\max_{\beta_0,\beta_1,\dots,\beta_p,\varepsilon_1,\dots,\varepsilon_n,M} M$ subject to $\sum_1^p\beta_j^2 = 1$, $y_i(\beta_0 + x_i^T\beta) \geq M(1-\varepsilon_i)$ $\forall i$, $\varepsilon_i \geq 0$, $\sum_{i=1}^n \varepsilon_i \leq C$ — 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: $K(x_i, x_i') = \exp\left(-\gamma\sum_{j=1}^p (x_{ij}-x_{i'j})^2\right)$

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.
$R_1(j,s) = \{x|x_j < s\}$, $R_2(j,s) = \{x|x_j \geq s\}$: 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 regions 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: R_j region (leaf) $\hat y = \frac{1}{N_j}\sum_{i:x_i\in R_j} y_i$ ← y_i's in the training set
b) classification $\hat y$ = majority vote among all y_i's in R_j, or $\hat p_{kj} = \frac{1}{N_j}\sum_{i:x_i\in R_j} I(y_i = k)$ 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 $C_\alpha(T) = Q(T) + \alpha\cdot|T|$ (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.

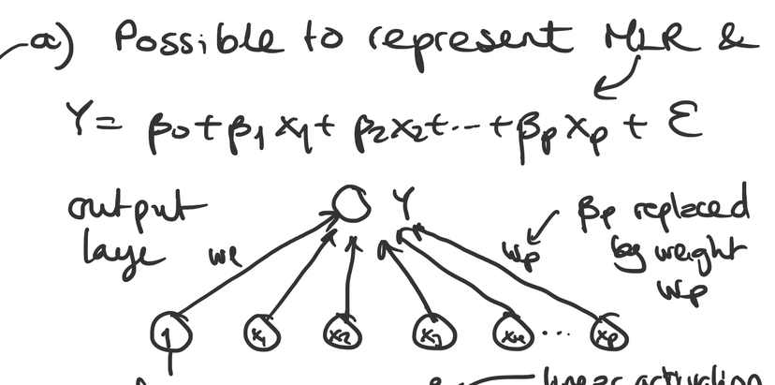
OOB = out-of-bag: for each bootstrap sample there are on average $\frac23$ of the observations in the sample (bag). The last $\frac13$ are used for prediction. We will then have $\approx\frac{B}{3}$ predictions for observation i – which we average.

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

C) BOOSTING: many variants, but we only considered boosting for trees.
Fit one tree – make residuals – fit a tree to the residuals → update
with d splits $\hat f^b(x)$; $\hat f(0) = 0$
$\hat f(x) \leftarrow \hat f(x) + \lambda\cdot\hat f^b(x)$
$r \leftarrow r - \lambda\hat f^b(x)$
$\hat f(x) = \sum_{b=1}^B \lambda\hat f^b(x)$
Tuning parameters: B = number of trees; λ = shrinkage parameter; d = number of tree splits

NEURAL NETWORKS (M11)

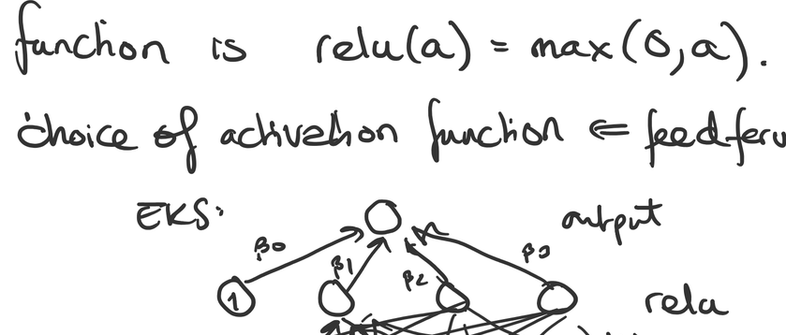
a) Possible to represent MLR & logistic regression as graph (one input and one output layer)
$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_p x_p + \varepsilon$
$\log\left(\frac{p}{1-p}\right) = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p$ ⟺ $p = \frac{\exp(\beta_0+\dots)}{1+\exp(\beta_0+\dots)} = \frac{\exp(a)}{1+\exp(a)}$



$Y = \sum_{j=0}^p w_j x_j$ linear activation function; β_p replaced by weight w_p; bias = intercept term
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:



$Y = \beta_0 + \sum_{j=1}^3\max\left(\alpha_{0j} + \sum_{i=1}^4 w_{ij}x_i, 0\right)\cdot\beta_j$ — these are often also called w's (but I wanted to avoid many indices)
number of unknown parameters? 4 in hidden to output, 15 in input to hidden, 19; $p=4$ inputs + bias

technical issue: data represented as tensors (generalization of vector, matrix). Does calc. in the network easy to perform, also for images & text.

model level library keras in R: use to setup and call backend (Tensorflow,...)
use "pipe" type notation to set up model architecture and send to estimation and then to evaluation

c) How to find/estimate the unknown weight (= parameters)?
– minimize loss (as before): quadratic loss for regression = "mse"
K=2 classes: "binary crossentropy" = as in tree and logistic regression: $-y_i\log(p_{i1}) - (1-y_i)\log(1-p_{i1})$
K classes: "categorical crossentropy": $-\sum_{j=1}^K y_{ij}\log(p_{ij})$
– optimization: rmsprop (adjust gradient), adam,...
gradient based: lower method, with stoch. version with "batches" of observations (can use chain rule for differentiation)
popular: mini-batch stochastic gradient descent
epoch: one run through all observations

d) Evaluation of performance: "metrics"
mae = mean abs. error, accuracy = avg correct class.

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?

f) many cool extensions – we have briefly looked at recurrent nets & convolution nets

g) data types popular: images, text that M1-10 not have solved.

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 weighted Mahlanobis)
Generalizations to medoids 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.