SummingUp ✓ 02.05.2018

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

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

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

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

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

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

minimize RSS: $RSS = \sum_{i=1}^n (y_i-\hat y_i)^2$ 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)

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

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

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

penalizing of training error

} can be used in model selection using "only" the training data
- best subset selection: all 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 (unpenalized) can be used.

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)

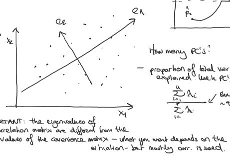
Have $\underset{n\times p}{X}$ with p large and/or many correlated covariates: want set of linear comb. of the X's that capture a large part of the variability – and where the sets are uncorrelated. → for interpretability, data reduction, visualization

Let Σ be covariance (or correlation) matrix of X, and (λ_i, e_i) eigenvalue/eigenvector pairs of Σ where $\lambda_1 \le \lambda_2 \le \dots \le \lambda_p$. Then

construct $Z_i = e_i^T X$ (principal component scores, loadings). 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



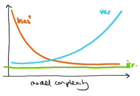
IMPORTANT: the eigenvalues of the correlation matrix are different from the eigenvalues of the covariance matrix – what you want depends on the situation – but mostly corr. is used.

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%?

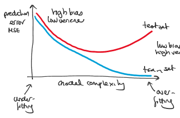
[M2+3] BIAS-VARIANCE trade-off in regression setting: $Y=f(x)+\varepsilon$

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 ($(f(x_0)-\hat f(x_0))^2$)

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

MODEL REGULARIZATION (M6)

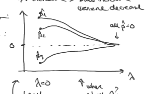
Motivation: LS regression gives unbiased $\hat\beta$, but variance might be large, e.g. when covariates are correlated (or p is large compared to n) → $(X^TX)^{-1}\sigma^2$. If we instead look at biased $\hat\beta$ (shrinkage) we might get smaller $Var(\hat\beta)+(\hat\beta-\beta)^2$? (brutto variance) 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; not scale invariant – useful to scale covariates before using ridge

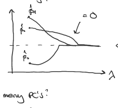
λ: tuning parameter ← decided by CV ← value giving min MSE

λ increase ⇒ bias increase, variance decrease

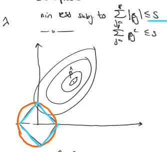
Interpretation of plots: ridge:



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



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



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

RESAMPLING METHODS (M5)

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

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

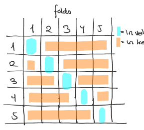
DATA not so rich = common situation:
- → Validation set approach (V+ B+)
- → Leave one out cross validation LOOCV (V+ due to corr., B÷)
- → k-fold cross validation (CV)

• biased estimate (as compared to using the whole 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.

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



$CV_k = \frac{1}{n}\sum_{j=1}^k MSE_j\cdot n_j$ (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

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 $1-(1-\frac{1}{n})^n \underset{n\to\infty}{\to} 0.632$

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

MOVING BEYOND LINEARITY (M7)

$Y=f(x)+\varepsilon$ and MLR $f(x) = X\beta$ → $\hat\beta = (X^TX)^{-1}X^TY$

X can be replaced by a set of basis functions $X^* = \begin{bmatrix}1 & b_1(x_1) & b_2(x_1) & \cdots & b_k(x_1)\\ \vdots & & & & \vdots\\ 1 & b_1(x_n) & \cdots & & b_k(x_n)\end{bmatrix}$ ← but we only look at one x at a time first; $x_1 = x$ for obs 1, $x_n = x$ 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: $b_k(x) = I(c_k \le x < c_{k+1})$ 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

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

$\lambda = 0$ g interpolates

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)

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)

5) Local regression: smoothed version of KNN regression

minimize$_\beta$ $\sum_{i=1}^n K_{i0}(y_i-\beta_0-\beta_1x_i-\beta_2x_i^2)^2$ ← close observation higher weight than far apart; different versions

6) Additive model: put 1-5 all together

$X = [1\ X_1\ X_2\ X_3]$ — 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 that class boundaries non-linear in X-space.

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

$f_k(x) = \text{"}P(X=x\mid Y=k)\text{"}$ 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 $N(\mu_k, \Sigma)$. $\hat\mu_k = \frac{1}{n_k}\sum_{i:y_i=k}x_i$

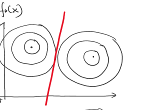
QDA: $f_k(x)$ is $N(\mu_k, \Sigma_k)$

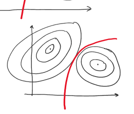
$\hat\Sigma_k = \frac{1}{n_k-1}\sum_{i:y_i=k}(x_i-\hat\mu_k)(x_i-\hat\mu_k)^T$

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

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

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





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

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

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

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

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: $0 = x^T\beta = \beta_0+\beta_1x_1+\dots+\beta_px_p$ is the eq. for a hyperplane.

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

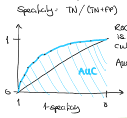
Confusion matrix:

		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

SUPPORT VECTOR MACHINES (M9)

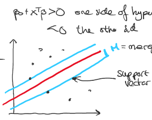
A method both for regression and classification, but we only consider classification, and two classes

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

CONNECTION SVM & logistic regression (ridge version)

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

logistic regr. has $\log(1+\exp(-y_if(x_i)))$ 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 $\sum_1^p\beta_j^2=1$, $y_i(\beta_0+x_i^T\beta)\ge M(1-\varepsilon_i)$ $\forall i$, $\varepsilon_i\ge0$, $\sum_1^n\varepsilon_i\le C$ — C is tuning parameter chosen by CV

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

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

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

$\max_{\beta_0,\alpha_1,\dots,\alpha_n,\varepsilon_1,\dots,\varepsilon_n,M} M$, $y_i(f(x_i))\ge M(1-\varepsilon_i)$, $\varepsilon_i\ge0$, $\sum\varepsilon_i\le C$ where $f(x) = \beta_0+\sum_{i\in S}\alpha_iK(x,x_i)$ 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 $\underset{n\times p}{X}$.

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

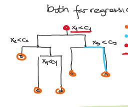
Euclidean distance popular (but also Mahalanobis (weighted))

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.

TREE-BASED METHODS (M8)

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



• terminal nodes (leaves) • branch • root — splitting criterion, binary splits

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

$R_1(j,s) = \{x\mid x_j<s\}$, $R_2(j,s) = \{x\mid x_j\ge s\}$: 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 responses 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: $D = -\sum_{k=1}^K\hat p_{jk}\log\hat p_{jk} = -\sum_{k=1}^K\left(\frac{n_{jk}}{N_j}\cdot\log\left(\frac{n_{jk}}{N_j}\right)\right)$

• Deviance: $-2\sum_{k=1}^K n_{jk}\log(\hat p_{jk}) = -2\sum_{k=1}^K n_{jk}\cdot\log\left(\frac{n_{jk}}{N_j}\right)$ } 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$_T$ $C_\alpha(T) = Q(T)+\alpha\cdot|T|$ — 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. Motivation: $Var(\bar X) = \frac{\sigma^2}{n}$ (if indep. obs $X_1,\dots,X_n$) → 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 (or Gini) decrease 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

$\hat f(0)=0$, $\hat f^b(x)$ with d splits → $\hat f(x) \leftarrow \hat f(x)+\lambda\cdot\hat f^b(x)$, $r\leftarrow r-\lambda\hat f^b(x)$

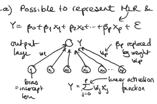
$\hat f(x) = \sum_{b=1}^B\lambda\hat f^b(x)$

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)

$Y = \beta_0+\beta_1x_1+\beta_2x_2+\dots+\beta_px_p+\varepsilon$



$Y = \sum_{j=0}^p w_jx_j$

$\log\left(\frac{p}{1-p}\right) = \beta_0+\beta_1x_1+\dots+\beta_px_p \iff p = \frac{\exp(\beta_0+\dots)}{1+\exp(\beta_0+\dots)} = \frac{\exp(a)}{1+\exp(a)}$

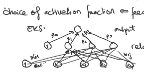
same graph, but now output layer has logistic activation function (sigmoid) used for two-class classification problems

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

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

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:



$Y = \beta_0+\sum_{j=1}^3\max\left(\alpha_{0j}+\sum_{i=1}^4 w_{ji}x_i, 0\right)\beta_j$ — 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, 21. p=4 inputs + bias

keras in R: use to setup and call backend (Tensorflow, ...) ← model level library. 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: $-y_i\log(p_i)-(1-y_i)\log(1-p_i)$
  - K classes: "categorical crossentropy": $-\sum_{j=1}^K y_j\log(p_j)$
- 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 = avg 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?

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.