Supervised Learning: Classification

Logistic Regression and Discriminant Analysis

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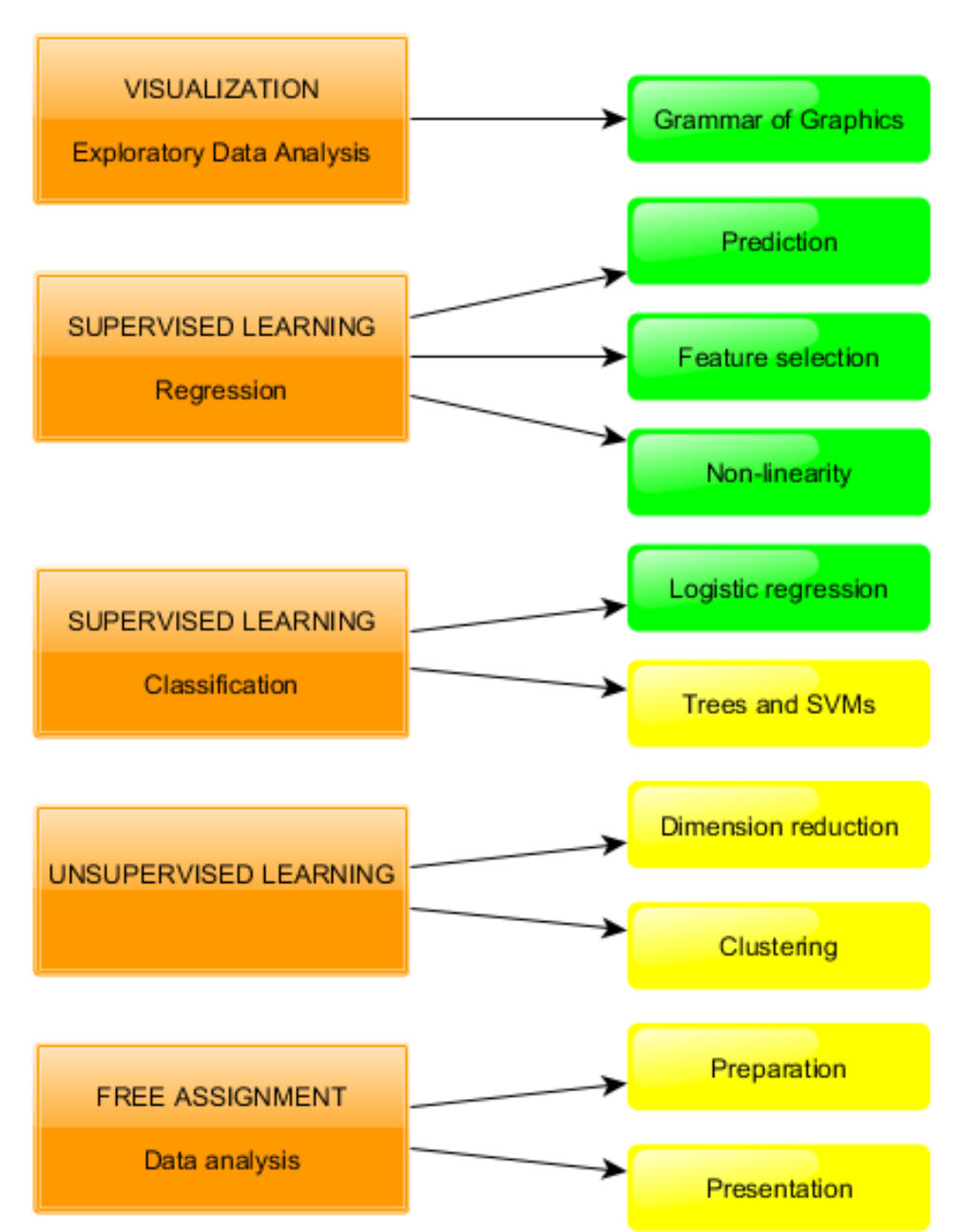
Program


VISUALIZATION
Exploratory Data Analysis
Grammar of Graphics
SUPERVISED LEARNING
Regression
Prediction
Feature selection
Non-linearity
SUPERVISED LEARNING
Classification
Logistic regression
Trees and SVMs
UNSUPERVISED LEARNING
Dimension reduction
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Preparation
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Content

1. Logistic regression
2. Linear discriminant analysis
3. Quadratic dicriminant analysis
4. Classification criteria
5. Model comparisons

What's classification?

Outcome variable is categorical

- Predict **class membership** from feature set

Estimation

1. Estimate $P(class = j|X)$
2. Assign observation to class with largest probability

Models

- Logistic regression, Discriminant analysis, Trees, Random Forests, Bagging, Boosting, SVM's, etc.

Logistic Regression

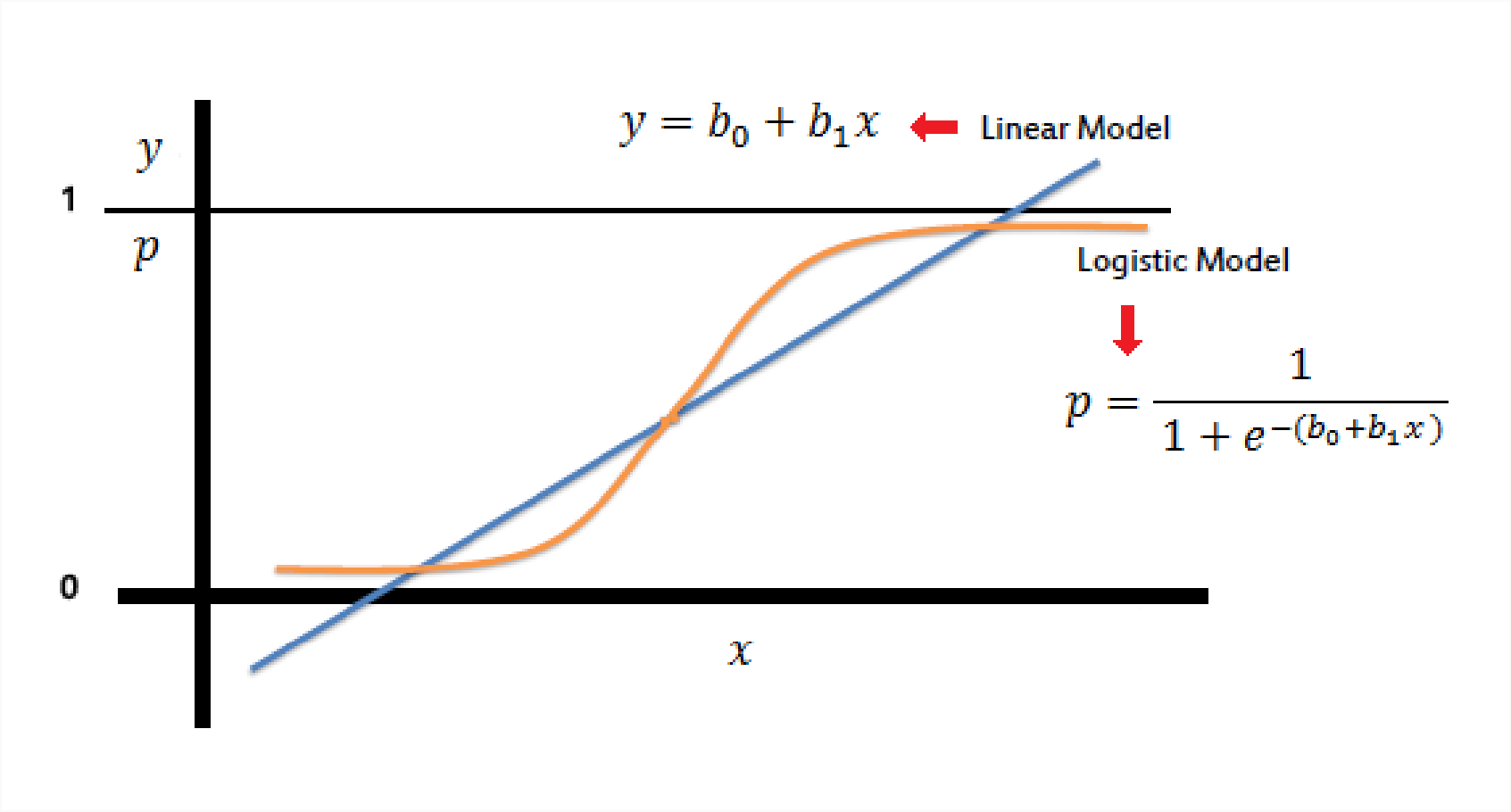
Binary logistic regression (BLR)

BLR predicts probability of a "success" with the logistic function

$$P(Y = \text{success}) = \frac{e^{\beta_0+\beta_1 x_1+\dots}}{1 + e^{\beta_0+\beta_1 x_1+\dots}} = \frac{1}{1 + e^{-(\beta_0+\beta_1 x_1+\dots)}}$$

- Y is coded as "1 = success" and "0 = failure"
- logistic (sigmoid) function ensures $\hat{P}(Y) \in (0, 1)$

Logistic vs linear regression



Reparametrizations

Logistic model is *generalized linear model* with link function

$$\text{logit}(Y) = \beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k$$

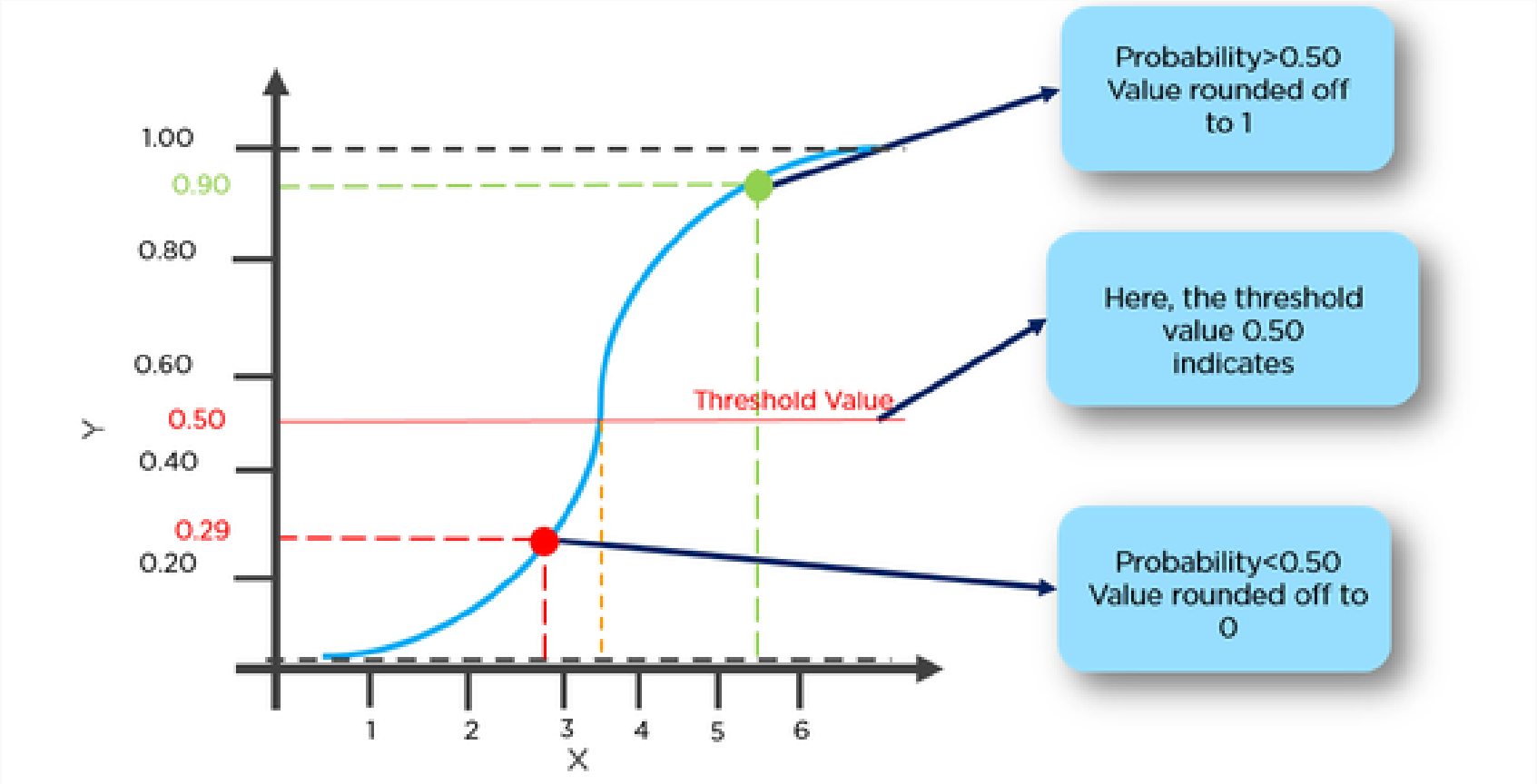
The "logit" is the log of the odds, so that

$$\text{odds}(Y) = \frac{P(Y)}{1 - P(Y)} = e^{\beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k}$$

Classification procedure in R

```
fit.glm  <- glm(y ~ x1 + x2 . . .,
                family = "binomial",
                data   = <data>)

pred.glm  <- predict(fit.glm,
                     data = <data>,
                     type = "response")  # alternative is "link"

class.glm <- factor(pred.glm > 0.5,
                    labels = c("success", "failure"))
```

Schematically

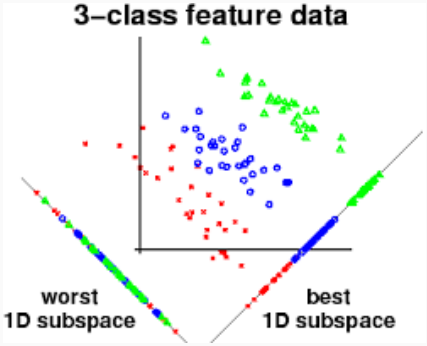


Discriminant Analysis

What's discriminant analysis

Estimation of discriminant functions

- directions in feature space that best separate between classes
- number of functions is $\min(J-1, p-1)$
  - J is number of classes
  - p is number of features



Linear Discriminant Analysis (LDA)

1. Estimate *posterior* probability $P(X = x|Y = j)$ of class $j = 1, \ldots, J$

$$P(Y = j|X = x) = \frac{\pi_j P(X = x|Y = j)}{\sum_{k=1}^{J} \pi_k P(X = x|Y = k)}$$

2. Use Bayes Theorem to find $P(Y = j|X = x)$

3. Assign x to class j with highest posterior probability

- π_j is *posterior probability* class j (estimated by sample proportion)
- $P(X = x|Y = j)$ estimated by conditional sample means

Linear discriminant functions

Linear discriminant functions

$$LD_j = c_{1j}X_1 + \cdots + c_{pj}X_p$$

- LD_1 separates the classes best, LD_2 second best, and so on
- LD's are orthogonal

Assumption $X|Y \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

- X is multivariate normal within each class
- X has covariance matrix $\boldsymbol{\Sigma}$ within each class

Quadratic Discriminant Analysis (QDA)

Estimates covariance matrix $\mathbf{\Sigma}_j$ for each class, with

- quadratic dicriminant functions
- more parameters, so less bias but higher variance

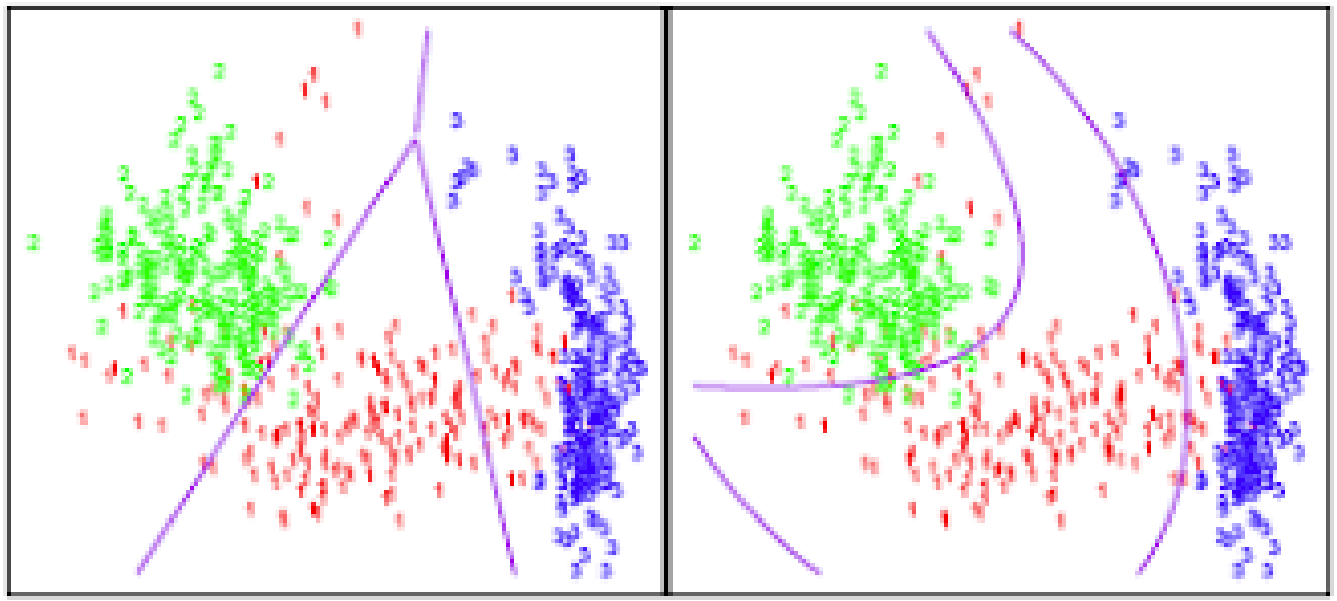


Figure 1: Linear vs quadratic discriminant functions

DA in R

`lda()`and `qda()`

- for LDA:

```
fit.lda   <- lda(formula, data = <data>)

pred.lda  <- predict(fit.lda, newdata = <data>)

prob.lda  <- pred.lda$posterior

class.lda  <- pred.lda$class
```

Functions in basic R package `MASS`

Classification criteria

Goodness-of-fit criteria

a. Deviance statistic $dev = 2 \sum y \log(y/\hat{P}(y))$
   - distance measure observed and estimated

b. AIC
   - deviance plus penalty model complexity (2 times # parameters)

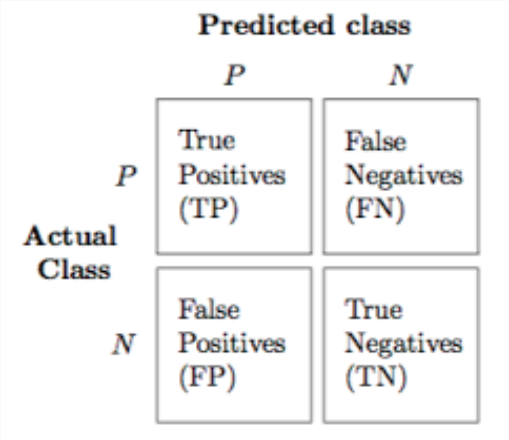
c. Confusion matrix
   - proportions correctly/incorrectly classified

d. ROC curve/AUC
   - Receiving Operation Characteristic (ROC) curve
   - Area Under Curve (AUC)

Deviance/AIC

```
Call:
glm(formula = type ~ glu, family = binomial, data = Pima.te)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.2343  -0.7270  -0.4985   0.6663   2.3268

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) -5.946808   0.659839  -9.013   <2e-16 ***
glu          0.042421   0.005165   8.213   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 420.30  on 331  degrees of freedom
Residual deviance: 325.99  on 330  degrees of freedom
AIC: 329.99
```

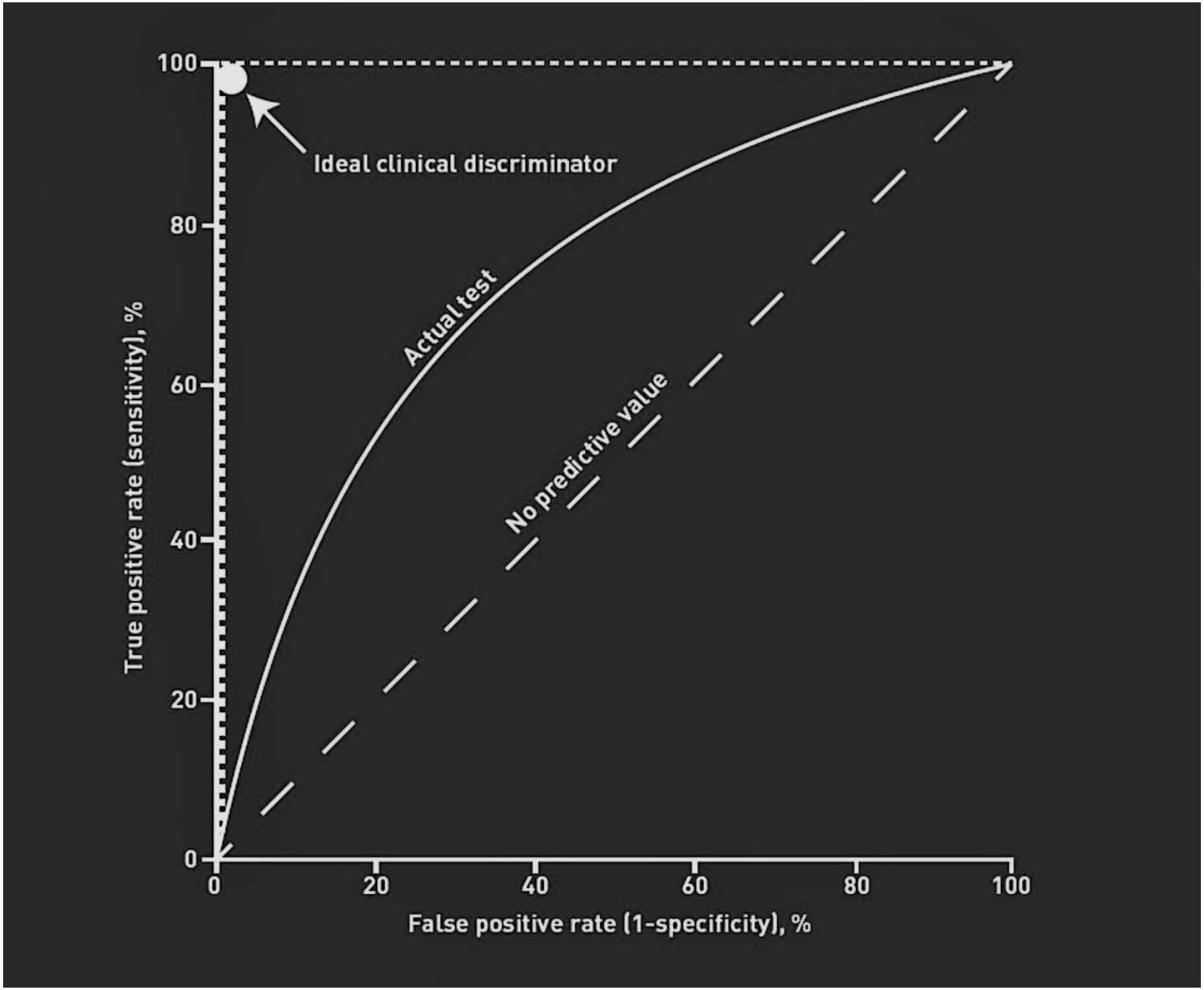
Confusion matrix



- Accuracy: $(TP + TN)/(TP + TN + FP + FN)$
- Sensitivity: $TP/(TP + FN)$
- Specificity: $TN/(TN + FP)$

Misclassification error rate: 1 - Accuracy

ROC and AUC


100
80
60
40
20
0
0
20
40
60
80
100
True positive rate (sensitivity), %
False positive rate (1-specificity), %
Ideal clinical discriminator
Actual test
No predictive value

Cross validation with `train()`

```
fit_cv <- train(formula   = y ~ .,
                data      = <data>,
                method    = c("glm", "lda", "qda"),
                metric    = "Accuracy",
                trControl = trainControl(method = "cv",
                                         number = 5))
```

Cross-validated accuracy:

- `fit_cv$results$Accuracy`

Estimates of model fitted to <data>:

- `fit_cv$finalModel`

Model comparisons

Example data `Pima.te`

Data set on Indian tribe where women often have diabetes

- 332 observations
- 7 predictors

Small data set and no tuning parameters, so

- no train/test partition
- just cross validation with 'caret::train()‘

Estimates BLR

```
Call:  NULL

Coefficients:
(Intercept)        npreg          glu           bp         skin
  -9.514019     0.140944     0.037481    -0.008675     0.013167
        bmi          ped          age
   0.078951     1.110131     0.018055

Degrees of Freedom: 331 Total (i.e. Null);  324 Residual
Null Deviance:      420.3
Residual Deviance: 285.8    AIC: 301.8
```

Estimates LDA

```
Call:
lda(x, grouping = y)

Prior probabilities of groups:
       No       Yes
0.6716867 0.3283133

Group means:
       npreg      glu       bp     skin      bmi       ped      age
No  2.932735 108.1883 70.13004 27.34081 31.63991 0.4645650 29.21525
Yes 4.614679 141.9083 74.77064 32.88991 36.51284 0.6589633 35.61468

Coefficients of linear discriminants:
               LD1
npreg  0.099984437
glu    0.028389957
bp    -0.004602843
skin   0.004726554
bmi    0.052002256
ped    0.615724201
age    0.012235784
```

Estimates QDA

```
Call:
qda(x, grouping = y)

Prior probabilities of groups:
       No       Yes
0.6716867 0.3283133

Group means:
       npreg      glu       bp     skin      bmi       ped      age
No  2.932735 108.1883 70.13004 27.34081 31.63991 0.4645650 29.21525
Yes 4.614679 141.9083 74.77064 32.88991 36.51284 0.6589633 35.61468
```

Confusion matrices of final models

BLR

```
        estimated
observed  No Yes
     No  201  22
     Yes  46  63
```

LDA

```
        estimated
observed  No Yes
     No  199  24
     Yes  47  62
```

QDA

```
        estimated
observed  No Yes
     No  199  24
     Yes  40  69
```

Accuracy

Accuracy crossvalidation versus final model

	CV	Final model
BLR	0.783	0.795
LDA	0.786	0.786
QDA	0.765	0.807

- BLR best CV accuracy
- QDA best final model accuracy

ROC's and AUC's