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2023-05-16

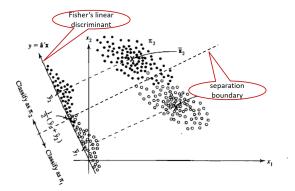
Section 1

Summary of LDA

Summary of LDA

knitr::include_graphics("img/FLDA.png")

Fisher's Linear Discriminant Analysis



LDA for two classes (Fisher's LDA)

- Fisher 1936 proposed a dichotomous discriminant analysis
- Fisher's linear discriminant function is a linear function
- The linear function has the maximum ability to discriminant between samples
- Once we find the linear function, we
 - project the data on to it
 - find the boundary of different classes
 - allocate new observations

FLDA: Assumptions

Summary of LDA

- Let's consider a two-class classification problem with n_1 and n_2 observations in classes 1 and 2, respectively.
- Suppose we have two independent random samples
 - Sample 1: $X_{1j} \stackrel{\textit{iid}}{\sim} (\mu_1, \Sigma)$, where $j = 1, \dots, n_1$
 - Sample 2: $X_{2j} \stackrel{iid}{\sim} (\mu_2, \mathbf{\Sigma})$, where $j = 1, \dots, n_2$
- Sample mean vectors:

$$ar{\mathbf{X}}_1 = rac{1}{n_1} \sum_{i=1}^{n_1} X_{1j}, ar{\mathbf{X}}_2 = rac{1}{n_2} \sum_{i=1}^{n_2} X_{2j}$$

FLDA: The Goal

Summary of LDA

- FLDA aims to find a linear combination of features that maximally separates two samples.
- How to define separability of a linear function?
- Consider a linear function with coefficients being denoted by a vector a.
 - $a^T \bar{\mathbf{X}}_1 \sim (a^T \mu_1, \frac{1}{n_1} a^T \mathbf{\Sigma} a)$
 - $a^T \bar{\mathbf{X}}_2 \sim (a^T \mu_2, \frac{1}{n_2} a^T \mathbf{\Sigma} a)$
- $a^T \bar{\mathbf{X}}_1 a^T \bar{\mathbf{X}}_2$ measures the difference but the variation of this difference depends on the scale of a and also the covariance structure
- We need to "standardize" it by its standard error

Subsection 1

FLDA: Maximum Separability

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FLDA: Maximum Separability

- Recall that we have two independent random samples. Therefore,
 - $\bar{\mathbf{X}}_1$ and $\bar{\mathbf{X}}_2$ are independent
 - As a result.

$$(a^T \mathbf{\bar{X}}_1 - a^T \mathbf{\bar{X}}_2) \sim \left(a^T \mu_1 - a^T \mu_2, \left(\frac{1}{n_1} + \frac{1}{n_2}\right) a^T \Sigma a\right)$$

The standardized version is

$$\frac{a^T \bar{\mathbf{X}}_1 - a^T \bar{\mathbf{X}}_2}{\sqrt{(\frac{1}{n_1} + \frac{1}{n_2})a^T \mathbf{\Sigma} a}}$$

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FLDA: Maximum Separability

The sign does not matter. So we consider the squared statistic

$$\frac{(a^T\bar{\mathbf{X}}_1 - a^T\bar{\mathbf{X}}_2)^2}{(\frac{1}{n_1} + \frac{1}{n_2})a^T\mathbf{\Sigma}a}$$

- Note that this is the squared t-statistic for testing $a^T \mu_1 = a^T \mu_2$
- The Fisher I DA aims to find a linear combination of features $Y = a^T X$ that maximally separates the classes while minimizing the within-class variance. This can be expressed as:

$$\frac{(a^T\bar{\mathbf{X}}_1 - a^T\bar{\mathbf{X}}_2)^2}{a^T\mathbf{\Sigma}a}$$

FLDA: Maximum Separability

• The maximization problem is

$$\underset{a}{\operatorname{argmin}} \ \frac{a^T (\bar{\mathbf{X}}_1 - \bar{\mathbf{X}}_2) (\bar{\mathbf{X}}_1 - \bar{\mathbf{X}}_2)^T a}{a^T \mathbf{\Sigma} a}$$

- Use an argument similar to PCA, such a is the first eigenvector of $\mathbf{\Sigma}^{-1}(\bar{\mathbf{X}}_1 \bar{\mathbf{X}}_2)(\bar{\mathbf{X}}_1 \bar{\mathbf{X}}_2)^T$.
- We can show that $a = \mathbf{S}_p^{-1}(\bar{\mathbf{X}}_1 \bar{\mathbf{X}}_2)$.
- The linear function

$$f(x) = a^T x$$
 where $a = \mathbf{S}_p^{-1} (\mathbf{\bar{X}}_1 - \mathbf{\bar{X}}_2)$

is called Fisher's linear discriminant function.

Allocate New Observations

Subsection 2

Allocate New Observations

Allocate New Observations

Allocate New Observations

• Consider an observation X_0 . We compute

$$f(X_0) = a^T X_0$$

where
$$a = \mathbf{S}_p^{-1}(\mathbf{\bar{X}}_1 - \mathbf{\bar{X}}_2)$$

Let

$$m = a^{T} \frac{\bar{\mathbf{X}}_{1} + \bar{\mathbf{X}}_{2}}{2} = (\bar{\mathbf{X}}_{1} - \bar{\mathbf{X}}_{2})^{T} \mathbf{S}_{p}^{-1} \frac{\bar{\mathbf{X}}_{1} + \bar{\mathbf{X}}_{2}}{2}$$

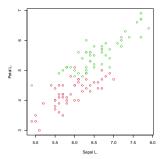
- Allocate X_0 to
 - class 1 if $f(X_0) > m$
 - class 2 if $f(x_0) < m$

Section 2

PCA vs LDA: An Example

PCA vs LDA: An Example

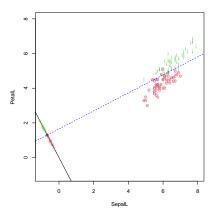
```
sample1=iris3[,c(1,3),2] #Versicolor
sample2=iris3[,c(1,3),3] #Virginica
sample12=rbind(sample1, sample2)
pch=c("e","i"); col=c(2,3); xlab="SepalL"; ylab="PetalL"
par(pty="s")
points(sample12,type="n")
points(sample12, col=col[1]); points(sample2, col=col[2])
```



```
n1=dim(sample1)[1]
n2=dim(sample2)[1]
#T.DA
mean.diff=c( colMeans(sample1)-colMeans(sample2) )
data.center=c( (colMeans(sample1)+colMeans(sample2))/2 )
S.pooled=((n1-1)*cov(sample1)+(n2-1)*cov(sample2))/(n1+n2-2)
lda.coeff=solve(S.pooled)%*% mean.diff
#rescale it so that is has norm 1
lda.coeff=lda.coeff/sqrt(sum(lda.coeff^2))
m=c(t(lda.coeff)%*%data.center)
#PCA
pca.coeff=eigen(cov(sample12))$vector[,1]
#project data to LDA and PCA
proj.lda=(sample12%*%lda.coeff)%*%matrix(lda.coeff, 1,2)
proj.pca=(sample12%*%pca.coeff)%*%matrix(pca.coeff, 1,2)
lda_coeff
                  Γ.17
## Sepal L. 0.4610660
## Petal I. -0.8873658
pca.coeff
```

Visualize the LDA

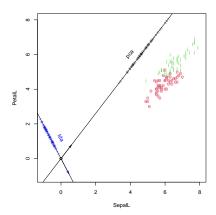
Visualize the LDA Allocations



Project Data to LDA and PCA

```
par(pty="s")
plot(sample12, xlim=c(-1,8), ylim=c(-1,8), xlab=xlab, ylab=ylab, type="n")
points(sample1, pch=pch[1], col=col[1])
points(sample2, pch=pch[2], col=col[2])
points(0, 0)
arrows(0, 0, lda.coeff[1], lda.coeff[2], length = 0.1, angle=15, col="blue")
abline(a=0, b=lda.coeff[2]/lda.coeff[1])
arrows(0, 0, pca.coeff[1], pca.coeff[2], length = 0.1, angle=15, col="black")
abline(a=0, b=pca.coeff[2]/pca.coeff[1])
for(i in 1: (n1+n2)){
 text(x=proj.lda[i,1],y=proj.lda[i,2], labels="|", col="blue",
       srt=atan(lda.coeff[2]/lda.coeff[1])*180/pi, cex=0.5)
 text(x=proj.pca[i,1],y=proj.pca[i,2], labels="|", col="black",
       srt=atan(pca.coeff[2]/pca.coeff[1])*180/pi, cex=0.5)}
text(x=0, y=1.2, "lda", srt=-60, col="blue")
text(x=4, v=6, "pca", srt=45, col="black")
```

Project Data to LDA and PCA





Three-Class LDA 0000

Three-Class LDA

Three-Class Classification

- Using the same strategy, we can construct linear discriminants for a three-class problem
- Suppose there are 3 independent random samples

- sample sizes n_1, n_2, n_3
- mean vectors μ_1, μ_2, μ_3
- a common covariance matrix **\Sigma**

Subsection 1

The Linear Discriminants

The Linear Discriminants

• Sample mean vectors

$$\boldsymbol{\bar{X}}_1,\boldsymbol{\bar{X}}_2,\boldsymbol{\bar{X}}_3$$

Pooled sample covariance

$$\mathbf{S}_{p} = \frac{(n_{1}-1)S_{1} + (n_{2}-1)S_{2} + (n_{3}-1)S_{3}}{n_{1} + n_{2} + n_{3} - 3}$$

- Let a₁₂, a₁₃, and a₂₃ denote the linear discriminants for the three pairs, respectively
- Let m_{12} , m_{13} , and m_{23} denote the projected centers

The Linear Disriminants

• Following from FLDA, we have

$$a_{ij} = \mathbf{S}_p^{-1}(\bar{\mathbf{X}}_i - \bar{\mathbf{X}}_j), m_{ij} = a_{ij}^T \frac{\bar{\mathbf{X}}_i + \bar{\mathbf{X}}_j}{2}$$

• The three linear boundaries are given by the three equations

$$f_{ij}(x) = a_{ij}^T x = m_{ij}$$

Allocate New Observations

- Let X_0 be a new observation
- We allocate X_0 to
 - class 1 if $f_{12}(X_0) > m_{12}$ and $f_{13}(X_0) > m_{13}$
 - ullet class 2 if $f_{23}(X_0) > m_{23}$ and $f_{12}(X_0) < m_{12}$
 - class 3 if $f_{13}(X_0) < m_{13}$ and $f_{23}(X_0) < m_{23}$

Minimum Distance Approach

Subsection 2

Minimum Distance Approach

Minimum Distance Approach

Minimum Distance Approach

- Following the argument we used for minimum distance in the two-class problem, the allocation rule in the previous slide is equivalent to allocate X_0 to
 - class 1 if $D_{S_p}(X_0, \overline{\mathbf{X}}_1) < D_{S_p}(X_0, \overline{\mathbf{X}}_2)$ and $D_{S_p}(X_0, \overline{\mathbf{X}}_1) < D_{S_p}(X_0, \overline{\mathbf{X}}_3)$
 - class 2 if $D_{S_p}(X_0, \bar{\mathbf{X}}_2) < D_{S_p}(X_0, \bar{\mathbf{X}}_1)$ and $D_{S_p}(X_0, \bar{\mathbf{X}}_2) < D_{S_p}(X_0, \bar{\mathbf{X}}_3)$
 - class 3 if $D_{S_p}(X_0, \bar{\mathbf{X}}_3) < D_{S_p}(X_0, \bar{\mathbf{X}}_1)$ and $D_{S_p}(X_0, \bar{\mathbf{X}}_3) < D_{S_p}(X_0, \bar{\mathbf{X}}_2)$
- In summary, we allocate X_0 to the group with the minimum Mahalanobis distance.

Maximum Likelihood Approach

Subsection 3

Maximum Likelihood Approach

Maximum Likelihood Approach

Maximum Likelihood Approach

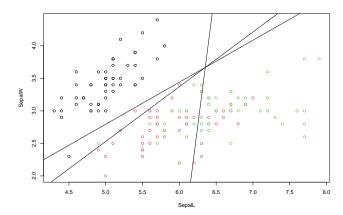
- ullet Again, following the argument used in the two-class problem, we allocate X_0 to
 - class 1 if $\frac{L_1}{L_2} > 1$ and $\frac{L_1}{L_2} > 1$
 - class 2 if $\frac{L_2}{L_3} > 1$ and $\frac{L_2}{L_3} > 1$
 - ullet class 3 if $rac{L_3}{L_1}>1$ and $rac{L_3}{L_2}>1$
- Therefore, the LDA is equivalent to the maximum likelihood approach.

Section 4

Example Iris

Iris Data: three species, two features: SepalL SepalW

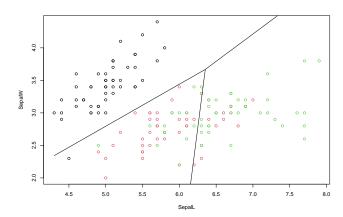
```
plot(iris3[,i,1], iris3[,j,1], xlim=c(min(iris3[,i,]),max(iris3[,i,])), xlab="SepalL", ylab="SepalL", ylab
```



```
# slopes
k12=a12[2]/a12[1]
k13=a13[2]/a13[1]
k23=a23[2]/a23[1]

# the joint point
joint.point=solve(rbind(a12,a13))%*%c(m12,m13) # point at which the three lines cross
```

```
### remove extra lines
plot(iris3[.i.1], iris3[.i.1], xlim=c(min(iris3[.i.]),max(iris3[.i.])), xlab="SepalL", ylab="SepalL",
vlim=c(min(iris3[,j,]),max(iris3[,j,])))
points(iris3[,i,2], iris3[,j,2], col=2)
points(iris3\lceil .i.3 \rceil, iris3\lceil .i.3 \rceil, col=3)
#classes 1 us 2
lines(
c(min(iris3[,i,]), joint.point[1]).
c(1/k12*(x1.bar[1]+x2.bar[1])/2 + (x1.bar[2]+x2.bar[2])/2 -min(iris3[.i.])/k12.
1/k12*(x1.bar[1]+x2.bar[1])/2 + (x1.bar[2]+x2.bar[2])/2 - joint.point[1]/k12))
#classes 1 us 3
lines(
c(joint.point[1],max(iris3[,i,])),
c(1/k13*(x1.bar[1]+x3.bar[1])/2 + (x1.bar[2]+x3.bar[2])/2 - ioint.point[1]/k13.
1/k13*(x1.bar[1]+x3.bar[1])/2 + (x1.bar[2]+x3.bar[2])/2 -max(iris3[.i.])/k13))
#classes 2 us 3
lines(
c(min(iris3[,i,]), joint.point[1]),
c(1/k23*(x2.bar[1]+x3.bar[1])/2 + (x2.bar[2]+x3.bar[2])/2 -min(iris3[.i.])/k23.
1/k23*(x2.bar[1]+x3.bar[1])/2 + (x2.bar[2]+x3.bar[2])/2 - ioint.point[1]/k23))
```



Subsection 1

The Three Boundaries Meet at Same Point

• The linear discriminants for groups (1,2) and (1,3) are:

$$(\bar{\mathbf{X}}_{1} - \bar{\mathbf{X}}_{2})^{T} \mathbf{\Sigma}^{-1} x = \frac{1}{2} (\bar{\mathbf{X}}_{1} - \bar{\mathbf{X}}_{2})^{T} \mathbf{\Sigma}^{-1} (\bar{\mathbf{X}}_{1} + \bar{\mathbf{X}}_{2})$$
$$(\bar{\mathbf{X}}_{1} - \bar{\mathbf{X}}_{3})^{T} \mathbf{\Sigma}^{-1} x = \frac{1}{2} (\bar{\mathbf{X}}_{1} - \bar{\mathbf{X}}_{3})^{T} \mathbf{\Sigma}^{-1} (\bar{\mathbf{X}}_{1} + \bar{\mathbf{X}}_{3})$$

Subtracting the first equation from the second equation

$$(\bar{\mathbf{X}}_2 - \bar{\mathbf{X}}_3)^T \mathbf{\Sigma}^{-1} \mathbf{X} = \frac{1}{2} (\bar{\mathbf{X}}_2^T \mathbf{\Sigma}^{-1} \bar{\mathbf{X}}_2 - \bar{\mathbf{X}}_3^T \mathbf{\Sigma}^{-1} \bar{\mathbf{X}}_3)$$
$$= \frac{1}{2} (\bar{\mathbf{X}}_2 - \bar{\mathbf{X}}_3)^T \mathbf{\Sigma}^{-1} (\bar{\mathbf{X}}_2 - \bar{\mathbf{X}}_3)$$

 The result indicates that the three lines meet at the same point

Example Iris: SepalL SepalW: Performance

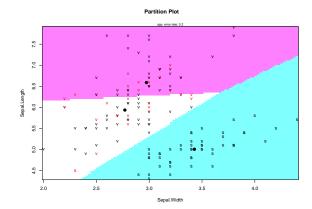
```
lda.iris = lda(Species ~., data = iris[, c(1,2,5)])
con.mat=table(Pred = predict(lda.iris, iris[, c(1,2,5)])$class,
              True = iris$Species)
#Confusion Matrix
con.mat
##
               True
## Pred
                setosa versicolor virginica
##
                    49
                                0
     setosa
##
    versicolor
                               36
                                          15
                                         35
##
    virginica
                               14
#Training Error
sum(diag(con.mat))/sum(con.mat)
## [1] 0.8
```

Example Iris: Visualization

library(klaR)

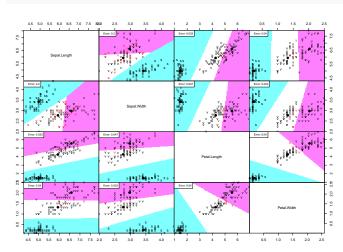
Warning: package 'klaR' was built under R version 4.2.3

partimat(Species ~ Sepal.Length + Sepal.Width, data = iris, method = "lda")



Example Iris: All Features

partimat(Species ~ ., data = iris, method = "lda", plot.matrix=TRUE)



Iris All Features: Performance

```
lda.iris = lda(Species ~ ., data = iris)
con.mat=table(Pred = predict(lda.iris, iris)$class,
              True = iris$Species)
#Confusion Matrix
con.mat
               True
##
## Pred
                setosa versicolor virginica
     setosa
                    50
                                0
##
    versicolor
                               48
   virginica
                                          49
##
#Training Error
sum(diag(con.mat))/sum(con.mat)
## [1] 0.98
```

Iris Data: PCA vs LDA

Subsection 2

Iris Data: PCA vs LDA

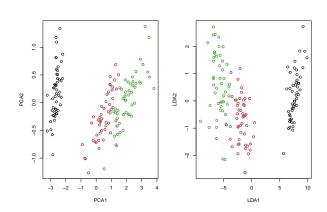
Iris Data: PCA vs LDA

Iris Data: PCA vs LDA

```
pca.iris = princomp(iris[,1:4], cor = FALSE, scores = TRUE)
par(mfrow=c(1,2))
plot(pca.iris$scores[,1:2], xlab="PCA1", ylab="PCA2")
points(pca.iris$scores[5i:100,1:2], col=2)
points(pca.iris$scores[101:150,1:2], col=3)
plot(predict(lda.iris, iris)$x, xlab="LDA1", ylab="LDA2")
points(predict(lda.iris, iris)$x, xlab="LDA1", ylab="LDA2")
points(predict(lda.iris, iris)$x[5i:100,], col=2)
points(predict(lda.iris, iris)$x[101:150,], col=3)
```

Iris Data: PCA vs LDA

Iris Data: PCA vs LDA



Section 5

Multi-Class LDA

Extend FLDA to g Classes

• Consider g classes. We have g independent random samples:

$$X_{1j} \stackrel{iid}{\sim} (\mu_1, \Sigma), j = 1, \cdots, n_1$$

 $X_{2j} \stackrel{iid}{\sim} (\mu_2, \Sigma), j = 1, \cdots, n_2$
 $\cdots \cdots$
 $X_{\sigma i} \stackrel{iid}{\sim} (\mu_{\sigma}, \Sigma), j = 1, \cdots, n_{\sigma}$

• Want to find a linear function
$$Y_{ij}^{(1)} = a^T X_{ij}$$
 that leads to maximum separation

Quantify Separation in a g-Class Problem

• Measure separation using F statistic

$$F(a) = \frac{MSB}{MSW} = \frac{SSB/(g-1)}{SSW/(n-g)}$$

$$= \frac{\sum_{i=1}^{g} n_i (\bar{Y}_{i.}^{(1)} - \bar{Y}_{..}^{(1)})^2/(g-1)}{\sum_{i=1}^{g} (n_i - 1)S_{Y_i^{(1)}}^2/(n-g)}$$

$$= \frac{a^T \sum_{i=1}^{g} n_i (\bar{X}_{i.} - \bar{X}_{..})(\bar{X}_{i.} - \bar{X}_{..})^T a}{a^T \sum_{i=1}^{g} \sum_{j=1}^{n_i} (X_{ij} - \bar{X}_{i.})(X_{ij} - \bar{X}_{i.})^T a} \frac{n-g}{g-1}$$

$$= \frac{a^T \mathbf{B} a}{a^T \mathbf{W} a} \frac{n-g}{g-1}$$

where $n = \sum_{i=1}^{g} n_i$, **B** is the between-group sample covariance matrix, and **W** is the within-group sample covariance matrix.

Linear Discriminants

 The first linear discriminant is the linear function that maximizes F(a). It can also be shown that the first linear discriminant is given by the first eigenvector of $\mathbf{W}^{-1}\mathbf{B}$, i.e.,

$$Y_{ij}^{(1)} = \gamma_1^T X_{ij}$$

where γ_1 is the first eigenvector of $\mathbf{W}^{-1}\mathbf{B}$.

• Similarly, for $k = 1, \dots, rank(\mathbf{B})$, the kth linear discriminant is given by the kth eigenvector of $\mathbf{W}^{-1}\mathbf{B}$

$$Y_{ij}^{(k)} = \gamma_k^T X_{ij}$$

- Allocate an observation to the group with the minimum distance defined by the Euclidean distance in space spanned by the linear discriminants.
- Let X_0 be a new observation.
- Calculate $Y_0^{(k)} = \gamma_k^T X_0$, the projection of X_0 to the kth linear discriminant for $k = 1, \dots, rank(B)$.
- Calculate the distances

$$D^2(X_0,g) = \sum_{k=1}^{rank(B)} [Y_0^{(k)} - \bar{Y}_{g.}^{(k)}]^2$$

Allocate X₀ to

$$\underset{g}{\operatorname{argmin}} D^2(X_0,g)$$

The Number of Linear Discriminants

- Recall that rank(B) = min(p, g 1) (Lecture 8). The number of total linear discriminants is min(p, g 1).
- In the two-class, rank(B) = 1. Thus, there is only one linear discrminant.
- When rank(B) is large, it is often helpful to use all linear discriminants.
- A scree plot of the eigenvalues of $\mathbf{W}^{-1}\mathbf{B}$ can be used to find an elbow point, if there is one

Section 6

Example Crude Oil

Example Crude Oil

```
urlfile='https://raw.githubusercontent.com/yu-zhaoxia/teaching-multivariate/d87ce8b30ecb15fc09aa543047b3b
co=read.table(urlfile, header=F)
names(co)=c("V1","V2","V3","V4","V5","type")
```

Exploratory analysis shows that transformation might be helpful

```
co[,2]=sqrt(co[,2])
co[,3]=sqrt(co[,3])
co[,4]=1/co[,4]
```

Example Crude Oil

```
par(mfrow=c(2,2))
par(vaxt="n")
plot(ld1, rep(0,56), xlab="LD1", ylab="", type="n")
points(ld1[1:7], rep(0, 7), pch="w", col=1)
points(ld1[8:18], rep(0, 11), pch="s", col=2)
points(ld1[19:56], rep(0, 38), pch="u", col=3)
plot(ld2, rep(0,56), xlab="LD2", ylab="", type="n")
points(ld2[1:7], rep(0, 7), pch="w", col=1)
points(ld2[8:18], rep(0, 11), pch="s", col=2)
points(ld2[19:56], rep(0, 38), pch="u", col=3)
par(vaxt="t")
plot(ld1, ld2, xlab="LD1", ylab="LD2", type="n")
points(ld1[1:7], ld2[1:7], pch="w", col=1)
points(ld1[8:18], ld2[8:18], pch="s", col=2)
points(ld1[19:56], ld2[19:56], pch="u", col=3)
#### scree plot
plot(lambda, type="b", ylab="", main="eigenvalues of BW^{-1}")
```

Example Crude Oil

