Machine Learning for informing climate change

The CalCOFI dataset represents the longest (1949 - present) and most complete (more than 50,000 sampling stations) time series of oceanographic and larval fish data captured in the world. This database contains oceanographic data measured using CTD casts from seawater samples collected at CalCOFI stations.

CTD stands for conductivity, temperature, and depth, and refers to a package of electronic instruments that measure oceanographic properties (i.e., the physical features of seawater such as salinity, dissolved oxygen, chlorophyll-a, nutrients, and many more). A CTD cast gives scientists a precise and comprehensive charting of the distribution and variation of water oceanographic properties that helps to understand how the oceans affect life.

Salinity plays a key role in analyzing the water cycle, ocean circulation, and climate change, as it drives ocean currents and circulation patterns. Variations in salinity affect the density of seawater, which in turn influences its movement and mixing. Many marine organisms have adapted to specific salinity levels, so variations in salinity can directly impact their distribution, reproduction, and survival.

Obtaining the data

The dataset used for this project can be downloaded from :
https://drive.google.com/file/d/1EspgcE5t9VHvk338_uNesCfhNZWDPVnB/view?usp=drive_link

The dataset contains 325,281 rows and 16 oceanographic features and one outcome variable - salinity of the water (Salnty). Description of all the variables:

1. Salnty: Salinity (Practical Salinity Scale 1978) (outcome)
2. Depthm: cast depth in meters
3. O2mlL: Milliliters oxygen per liter of seawater
4. STheta: Potential Density (Sigma Theta), Kg/M3
5. O2Sat: Oxygen percent saturation
6. Oxyµmol/Kg: Oxygen micromoles per kilogram seawater
7. ChlorA: Migrograms Chlorophyll-a per liter seawater, measured fluorometrically
8. Phaeop: Micrograms Phaeopigment per liter seawater, measured fluormetrically
9. PO4uM: Micromoles Phosphate per liter of seawater
10. SiO3uM: Micromoles Silicate per liter of seawater
11. NO2uM: Micromoles Nitrite per liter of seawater
12. NH3uM: Micromoles Ammonia per liter of seawater

13. C14As1: 14C Assimilation of Replicate 1 (milligrams carbon per cubic meter of seawater per half light day)
14. C14As2: 14C Assimilation of Replicate 2 (milligrams carbon per cubic meter of seawater per half light day)
15. DarkAs: 14C Assimilation of Dark/Control Bottle (milligrams carbon per cubic meter of seawater per half light day)
16. LightP : Light intensities of the incubation tubes in the primary productivity experiment, expressed as percentages
17. Year: The year the sample was collected

In this project, I will attempt to use a linear regression model to predict the salinity of the ocean water based on the 16 features, analyze its efficacy and explore alternatives. For this purpose, I will be using the data from 1980-2013 as the training data and test the model on the data from 2014-2016.

In [1]:
```
df <- read.csv("final.csv")
head(df)
```

A data.frame: 6 x 17

	Depthm	Salnty	O2ml_L	STheta	O2Sat	Oxymol	ChlorA	Phaeop	PO4uM	SiO3uM
	<int>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
1	0	33.418	NA	24.287	NA	NA	NA	NA	NA	NA
2	10	33.419	NA	24.302	NA	NA	NA	NA	NA	NA
3	20	33.420	NA	24.318	NA	NA	NA	NA	NA	NA
4	30	33.400	NA	24.410	NA	NA	NA	NA	NA	NA
5	40	33.380	NA	24.470	NA	NA	NA	NA	NA	NA
6	50	33.360	NA	24.503	NA	NA	NA	NA	NA	NA

Exploratory Data Analysis and Pre-processing

In [2]:
```
summary(df)
```

```
     Depthm           Salnty          O2ml_L           STheta     
 Min.   :   0.0   Min.   :28.43   Min.   :-0.010   Min.   : 20.93  
 1st Qu.:  32.0   1st Qu.:33.39   1st Qu.: 2.040   1st Qu.: 24.86  
 Median : 100.0   Median :33.67   Median : 3.970   Median : 25.81  
 Mean   : 165.1   Mean   :33.70   Mean   : 3.759   Mean   : 25.69  
 3rd Qu.: 250.0   3rd Qu.:34.07   3rd Qu.: 5.690   3rd Qu.: 26.55  
 Max.   :4442.0   Max.   :37.03   Max.   :11.130   Max.   :250.78  
                  NA's   :3270    NA's   :26357    NA's   :5510    
     O2Sat            Oxymol            ChlorA           Phaeop      
 Min.   : -0.10   Min.   : -0.435   Min.   : 0.00    Min.   :-3.89   
 1st Qu.: 30.80   1st Qu.: 88.742   1st Qu.: 0.05    1st Qu.: 0.05   
 Median : 62.60   Median :172.421   Median : 0.16    Median : 0.11   
 Mean   : 62.63   Mean   :163.631   Mean   : 0.44    Mean   : 0.19   
 3rd Qu.:101.00   3rd Qu.:247.942   3rd Qu.: 0.39    3rd Qu.: 0.23   
 Max.   :214.10   Max.   :485.702   Max.   :66.11    Max.   :10.66   
 NA's   :26964    NA's   :26970     NA's   :116829   NA's   :116832  
     PO4uM          SiO3uM           NO2uM           NH3uM       
 Min.   :0.00   Min.   :  0.00   Min.   :0.00    Min.   : 0.00   
 1st Qu.:0.41   1st Qu.:  3.10   1st Qu.:0.00    1st Qu.: 0.00   
 Median :1.46   Median : 17.42   Median :0.01    Median : 0.00   
 Mean   :1.47   Mean   : 25.52   Mean   :0.04    Mean   : 0.08   
 3rd Qu.:2.30   3rd Qu.: 40.80   3rd Qu.:0.03    3rd Qu.: 0.06   
 Max.   :5.21   Max.   :181.60   Max.   :8.19    Max.   :15.63   
 NA's   :35625  NA's   :34752    NA's   :37090   NA's   :260319  
     C14As1           C14As2            DarkAs           LightP      
 Min.   : -0.24   Min.   : -0.20   Min.   :-0.01    Min.   : 0.00   
 1st Qu.:  0.93   1st Qu.:  0.93   1st Qu.: 0.06    1st Qu.: 0.28   
 Median :  2.60   Median :  2.60   Median : 0.10    Median : 1.80   
 Mean   :  9.76   Mean   :  9.76   Mean   : 0.16    Mean   :18.36   
 3rd Qu.:  8.00   3rd Qu.:  8.06   3rd Qu.: 0.17    3rd Qu.:24.00   
 Max.   :584.50   Max.   :948.30   Max.   : 6.90    Max.   :99.90   
 NA's   :310849   NA's   :310867   NA's   :302632   NA's   :306630  
      Year     
 Min.   :1980  
 1st Qu.:1988  
 Median :1997  
 Mean   :1997  
 3rd Qu.:2006  
 Max.   :2016  
```

From the above summary, it is clear that each column has a lot of NA values. So first, I am attempting to clean the data. Salnty has 3270 NA values, and since this is the outcome variable, these rows have to be deleted since they cannot be used to create or evaluate the model.

In [3]:
```
df <- subset(df, !is.na(df$Salnty))
summary(df)
nrow(df)
```

```
     Depthm          Salnty          O2ml_L           STheta
 Min.   :   0.0   Min.   :28.43   Min.   :-0.010   Min.   : 20.93
 1st Qu.:  35.0   1st Qu.:33.39   1st Qu.: 2.040   1st Qu.: 24.86
 Median : 101.0   Median :33.67   Median : 3.970   Median : 25.81
 Mean   : 166.4   Mean   :33.70   Mean   : 3.758   Mean   : 25.69
 3rd Qu.: 250.0   3rd Qu.:34.07   3rd Qu.: 5.690   3rd Qu.: 26.55
 Max.   :4442.0   Max.   :37.03   Max.   :11.130   Max.   :250.78
                                  NA's   :23312    NA's   :2240
     O2Sat            Oxymol            ChlorA           Phaeop
 Min.   : -0.10   Min.   : -0.435   Min.   : 0.00    Min.   :-3.89
 1st Qu.: 30.80   1st Qu.: 88.742   1st Qu.: 0.05    1st Qu.: 0.05
 Median : 62.60   Median :172.421   Median : 0.16    Median : 0.11
 Mean   : 62.63   Mean   :163.631   Mean   : 0.44    Mean   : 0.19
 3rd Qu.:101.00   3rd Qu.:247.942   3rd Qu.: 0.39    3rd Qu.: 0.23
 Max.   :214.10   Max.   :485.702   Max.   :66.11    Max.   :10.66
 NA's   :23694    NA's   :23700     NA's   :116245   NA's   :116248
     PO4uM          SiO3uM           NO2uM            NH3uM
 Min.   :0.00    Min.   :  0.00   Min.   :0.00    Min.   : 0.00
 1st Qu.:0.41    1st Qu.:  3.20   1st Qu.:0.00    1st Qu.: 0.00
 Median :1.47    Median : 17.60   Median :0.01    Median : 0.00
 Mean   :1.47    Mean   : 25.58   Mean   :0.04    Mean   : 0.08
 3rd Qu.:2.31    3rd Qu.: 40.90   3rd Qu.:0.03    3rd Qu.: 0.06
 Max.   :5.21    Max.   :181.60   Max.   :8.19    Max.   :15.63
 NA's   :33167   NA's   :32297    NA's   :34634   NA's   :257052
     C14As1           C14As2            DarkAs           LightP
 Min.   : -0.24   Min.   : -0.20   Min.   :-0.01    Min.   : 0.00
 1st Qu.:  0.88   1st Qu.:  0.88   1st Qu.: 0.05    1st Qu.: 0.20
 Median :  2.60   Median :  2.50   Median : 0.09    Median : 0.96
 Mean   :  9.52   Mean   :  9.55   Mean   : 0.15    Mean   :16.72
 3rd Qu.:  7.80   3rd Qu.:  7.87   3rd Qu.: 0.17    3rd Qu.:18.00
 Max.   :584.50   Max.   :948.30   Max.   : 6.90    Max.   :99.30
 NA's   :309085   NA's   :309085   NA's   :301921   NA's   :305931
      Year
 Min.   :1980
 1st Qu.:1988
 Median :1997
 Mean   :1997
 3rd Qu.:2007
 Max.   :2016
```

322011

Total number of rows = 322011 We see that for the following features:

- NH3uM missing: 257052 = 79.82%
- C14As1 missing: 309085 = 95.99 %
- C14As2 missing: 309085 = 95.99 %
- DarkAs missing: 301921 = 93.76%
- LightP missing: 305931 = 95.01 %

a large proportion of the samples have NA values. Thus, these features cannot be used to build an effective model, and have to be dropped from the dataset.

In [4]:
```
df <- subset(df, select = -c(12, 13, 14, 15, 16))
summary(df)
```

```
     Depthm           Salnty          O2ml_L           STheta      
 Min.   :   0.0   Min.   :28.43   Min.   :-0.010   Min.   : 20.93  
 1st Qu.:  35.0   1st Qu.:33.39   1st Qu.: 2.040   1st Qu.: 24.86  
 Median : 101.0   Median :33.67   Median : 3.970   Median : 25.81  
 Mean   : 166.4   Mean   :33.70   Mean   : 3.758   Mean   : 25.69  
 3rd Qu.: 250.0   3rd Qu.:34.07   3rd Qu.: 5.690   3rd Qu.: 26.55  
 Max.   :4442.0   Max.   :37.03   Max.   :11.130   Max.   :250.78  
                                  NA's   :23312    NA's   :2240    
     O2Sat            Oxymol            ChlorA           Phaeop      
 Min.   : -0.10   Min.   : -0.435   Min.   : 0.00    Min.   :-3.89   
 1st Qu.: 30.80   1st Qu.: 88.742   1st Qu.: 0.05    1st Qu.: 0.05   
 Median : 62.60   Median :172.421   Median : 0.16    Median : 0.11   
 Mean   : 62.63   Mean   :163.631   Mean   : 0.44    Mean   : 0.19   
 3rd Qu.:101.00   3rd Qu.:247.942   3rd Qu.: 0.39    3rd Qu.: 0.23   
 Max.   :214.10   Max.   :485.702   Max.   :66.11    Max.   :10.66   
 NA's   :23694    NA's   :23700     NA's   :116245   NA's   :116248  
     PO4uM          SiO3uM           NO2uM            Year     
 Min.   :0.00    Min.   :  0.00   Min.   :0.00    Min.   :1980  
 1st Qu.:0.41    1st Qu.:  3.20   1st Qu.:0.00    1st Qu.:1988  
 Median :1.47    Median : 17.60   Median :0.01    Median :1997  
 Mean   :1.47    Mean   : 25.58   Mean   :0.04    Mean   :1997  
 3rd Qu.:2.31    3rd Qu.: 40.90   3rd Qu.:0.03    3rd Qu.:2007  
 Max.   :5.21    Max.   :181.60   Max.   :8.19    Max.   :2016  
 NA's   :33167   NA's   :32297    NA's   :34634                 
```

For the remaining missing values, I'm filling them with the mean values of the respective columns.

In [5]:
```
for (i in 1 : 12){
  df[which(is.na(df[i])), i] <- colMeans(df, na.rm = TRUE)[i]
}
summary(df)
```

```
     Depthm           Salnty          O2ml_L           STheta     
 Min.   :   0.0   Min.   :28.43   Min.   :-0.010   Min.   : 20.93  
 1st Qu.:  35.0   1st Qu.:33.39   1st Qu.: 2.193   1st Qu.: 24.86  
 Median : 101.0   Median :33.67   Median : 3.758   Median : 25.79  
 Mean   : 166.4   Mean   :33.70   Mean   : 3.758   Mean   : 25.69  
 3rd Qu.: 250.0   3rd Qu.:34.07   3rd Qu.: 5.650   3rd Qu.: 26.54  
 Max.   :4442.0   Max.   :37.03   Max.   :11.130   Max.   :250.78  
     O2Sat            Oxymol             ChlorA             Phaeop       
 Min.   : -0.10   Min.   : -0.4349   Min.   :-0.0010   Min.   :-3.8900  
 1st Qu.: 33.30   1st Qu.: 95.6516   1st Qu.: 0.1100   1st Qu.: 0.0800  
 Median : 62.64   Median :163.6312   Median : 0.4395   Median : 0.1908  
 Mean   : 62.64   Mean   :163.6312   Mean   : 0.4395   Mean   : 0.1908  
 3rd Qu.:100.50   3rd Qu.:246.1283   3rd Qu.: 0.4395   3rd Qu.: 0.1908  
 Max.   :214.10   Max.   :485.7018   Max.   :66.1100   Max.   :10.6600  
     PO4uM           SiO3uM           NO2uM              Year     
 Min.   :0.000   Min.   :  0.00   Min.   :0.00000   Min.   :1980  
 1st Qu.:0.460   1st Qu.:  3.60   1st Qu.:0.00000   1st Qu.:1988  
 Median :1.473   Median : 22.72   Median :0.01000   Median :1997  
 Mean   :1.473   Mean   : 25.58   Mean   :0.04113   Mean   :1997  
 3rd Qu.:2.210   3rd Qu.: 37.80   3rd Qu.:0.04113   3rd Qu.:2007  
 Max.   :5.210   Max.   :181.60   Max.   :8.19000   Max.   :2016  
```

Splitting the data

I am spliiting the data such that the data from 1980 - 2013 is the training set, and the data from 2014 - 2016 is the test set.

In [6]:
```
traindf <- df[df["Year"] <= 2013, ]
testdf <- df[df["Year"] > 2013, ]
cat("Number of rows in training set :", nrow(traindf), "\n")
cat("Number of rows in test set :", nrow(testdf))
```

```
Number of rows in training set : 298558
Number of rows in test set : 23453
```

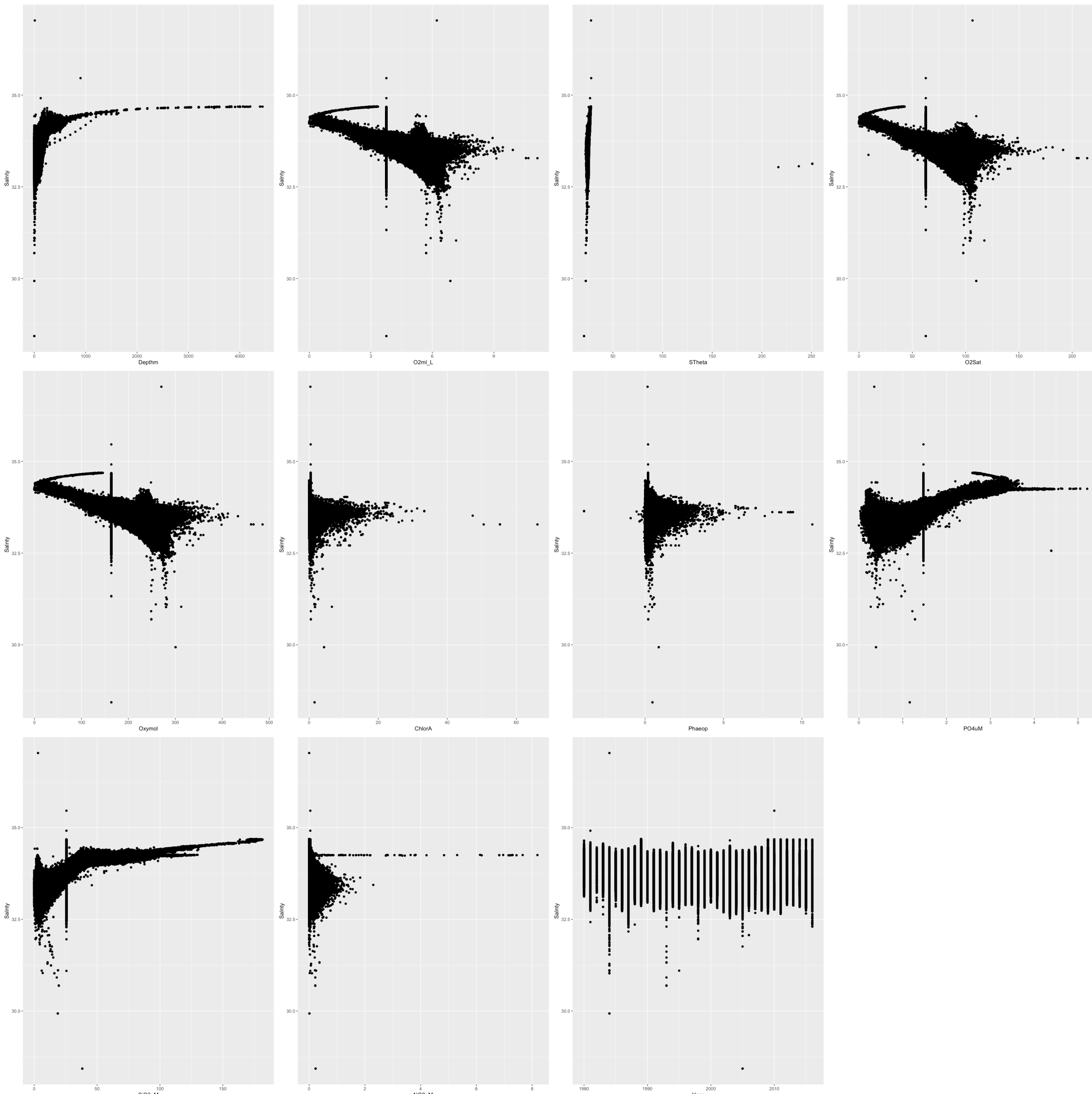
Plots and correlations

In [7]:
```
library(ggplot2)
```

In [8]:
```
p1 <- ggplot(data = df) + geom_point(aes(x = Depthm, y = Salnty))
p2 <- ggplot(data = df) + geom_point(aes(x = O2ml_L, y = Salnty))
p3 <- ggplot(data = df) + geom_point(aes(x = STheta, y = Salnty))
p4 <- ggplot(data = df) + geom_point(aes(x = O2Sat, y = Salnty))

p5 <- ggplot(data = df) + geom_point(aes(x = Oxymol, y = Salnty))
p6 <- ggplot(data = df) + geom_point(aes(x = ChlorA, y = Salnty))
p7 <- ggplot(data = df) + geom_point(aes(x = Phaeop, y = Salnty))
p8 <- ggplot(data = df) + geom_point(aes(x = PO4uM, y = Salnty))

p9 <- ggplot(data = df) + geom_point(aes(x = SiO3uM, y = Salnty))
p10 <- ggplot(data = df) + geom_point(aes(x = NO2uM, y = Salnty))
p11 <- ggplot(data = df) + geom_point(aes(x = Year, y = Salnty))
```

In [9]:
```
library(patchwork)
```

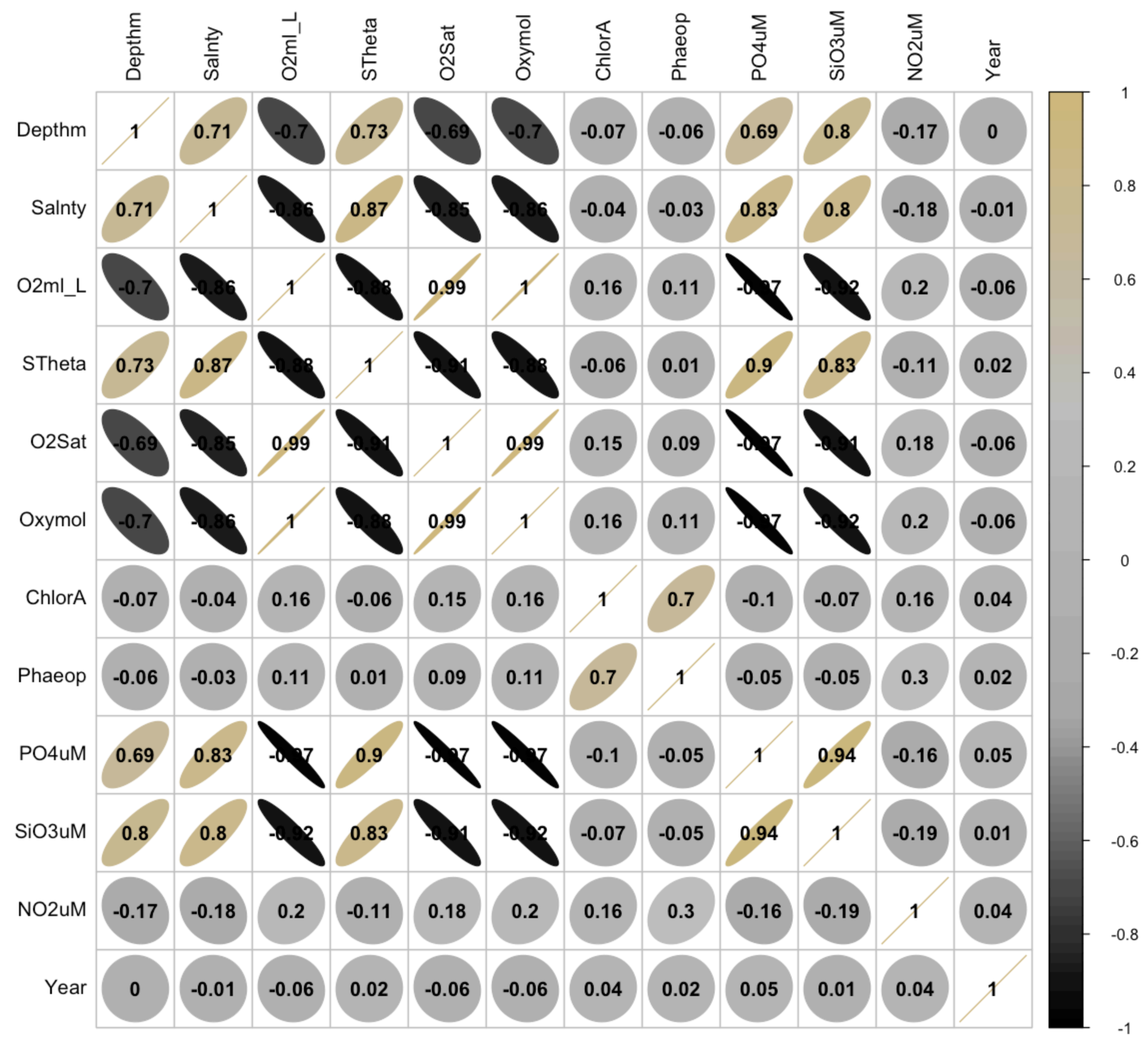
In [13]:
```
plots <- p1 + p2 + p3 + p4 + p5 + p6 + p7 + p8 + p9 + p10 + p11
options(repr.plot.width = 30, repr.plot.height = 30)
wrap_plots(plots)
```



In [11]:
```
library(corrplot)
```

```
corrplot 0.92 loaded
```

In [15]:
```
col4 <- colorRampPalette(c("black", "darkgrey", "grey", "#CFB87C"))
par(bg = "white")
options(repr.plot.width = 10, repr.plot.height = 10)
corrplot(cor(traindf), method = "ellipse", col = col4(100),
         addCoef.col = "black", tl.col = "black")
```



From the second row of the above correlation plot (which corresponds to correlation with Salnty), we see that almost all except 4 features seem highly linearly correlated with the outcome. From the rest of the plot, we see that some of the features seem to be intra-correlated as well, so I suspect some of the features might be redundant in fitting a linear regression model.

Multiple Linear Regression modelling

Starting off with fitting a full linear model with all the features.

In [17]:
```
fullmodel <- lm(Salnty ~ ., data = traindf)
summary(fullmodel)
```

```
Call:
lm(formula = Salnty ~ ., data = traindf)

Residuals:
    Min      1Q  Median      3Q     Max 
-2.8546 -0.0649  0.0088  0.0682  5.1596 

Coefficients:
              Estimate Std. Error  t value Pr(>|t|)    
(Intercept)  2.513e+01  5.867e-02  428.342  < 2e-16 ***
Depthm       1.175e-04  2.562e-06   45.878  < 2e-16 ***
O2ml_L      -1.805e-01  3.295e-03  -54.787  < 2e-16 ***
STheta       4.808e-01  9.203e-04  522.423  < 2e-16 ***
O2Sat        5.473e-02  1.174e-04  466.293  < 2e-16 ***
Oxymol      -1.811e-02  8.638e-05 -209.656  < 2e-16 ***
ChlorA       1.598e-02  3.696e-04   43.249  < 2e-16 ***
Phaeop       5.132e-03  1.541e-03    3.330 0.000868 ***
PO4uM        1.107e-01  1.641e-03   67.469  < 2e-16 ***
SiO3uM      -6.464e-03  4.399e-05 -146.931  < 2e-16 ***
NO2uM       -8.784e-03  2.672e-03   -3.287 0.001013 ** 
Year        -1.796e-03  2.550e-05  -70.443  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.1302 on 298546 degrees of freedom
Multiple R-squared:  0.8955,	Adjusted R-squared:  0.8955 
F-statistic: 2.325e+05 on 11 and 298546 DF,  p-value: < 2.2e-16
```

F and t-tests

The full F-test has the following as the null and alternative hypotheses:

$$H_0 : \beta_1 = \beta_2 = .. = \beta_{11} = 0$$
$$H_1 : \beta_k \neq 0 \text{ for some k in } 1, 2, .. 11$$

From the summary of the above full model, we see that the F-statistic for the full model is 2.325e+05 which is very large. The p-value for this is very small (< 2.2e-16). Thus, the null hypothesis that none of the features are necessary, can be rejected. This shows that atleast some of the feature variables are necessary to model the salinity of the ocean water.

We also see that the p-values of the t-tests of all the features are very small (<0.05), suggesting that all of them might be useful in predicting the outcome, but a more rigorous analysis needs to be done to see if some of them can be removed. Further down, I will be performing model diagnostics and model selection to identify a reduced model.

Now, partial F-tests for each feature need to be done individually. The partial (individual) F-test for a feature k is as follows:

$$H_0 : \beta_i = 0 \text{ for i} \neq \text{k}$$
$$H_1 : \beta_i \neq 0 \text{ for some i} \neq \text{k}$$

In [18]:
```
partial1 <- lm(Salnty ~ Depthm, data = traindf)
partial2 <- lm(Salnty ~ O2ml_L, data = traindf)
partial3 <- lm(Salnty ~ STheta, data = traindf)
partial4 <- lm(Salnty ~ O2Sat, data = traindf)

partial5 <- lm(Salnty ~ Oxymol, data = traindf)
partial6 <- lm(Salnty ~ ChlorA, data = traindf)
partial7 <- lm(Salnty ~ Phaeop, data = traindf)
partial8 <- lm(Salnty ~ PO4uM, data = traindf)

partial9 <- lm(Salnty ~ SiO3uM, data = traindf)
partial10 <- lm(Salnty ~ NO2uM, data = traindf)
partial11 <- lm(Salnty ~ Year, data = traindf)

anova(partial1, fullmodel)
anova(partial2, fullmodel)
anova(partial3, fullmodel)
anova(partial4, fullmodel)

anova(partial5, fullmodel)
anova(partial6, fullmodel)
anova(partial7, fullmodel)
anova(partial8, fullmodel)

anova(partial9, fullmodel)
anova(partial10, fullmodel)
anova(partial11, fullmodel)
```

A anova: 2 x 6

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
1	298556	23736.301	NA	NA	NA	NA
2	298546	5064.784	10	18671.52	110060.1	0

A anova: 2 x 6

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
1	298556	12529.173	NA	NA	NA	NA
2	298546	5064.784	10	7464.389	43999.18	0

A anova: 2 x 6

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
1	298556	12109.072	NA	NA	NA	NA
2	298546	5064.784	10	7044.287	41522.87	0

A anova: 2 x 6

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
1	298556	13370.711	NA	NA	NA	NA
2	298546	5064.784	10	8305.927	48959.66	0

A anova: 2 x 6

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
1	298556	12563.277	NA	NA	NA	NA
2	298546	5064.784	10	7498.492	44200.2	0

A anova: 2 x 6

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
1	298556	48363.200	NA	NA	NA	NA
2	298546	5064.784	10	43298.42	255224.5	0

A anova: 2 x 6

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
1	298556	48407.427	NA	NA	NA	NA
2	298546	5064.784	10	43342.64	255485.2	0

A anova: 2 x 6

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
1	298556	14895.915	NA	NA	NA	NA
2	298546	5064.784	10	9831.13	57950.04	0

A anova: 2 x 6

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
1	298556	17275.336	NA	NA	NA	NA
2	298546	5064.784	10	12210.55	71975.65	0

A anova: 2 x 6

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
1	298556	46836.317	NA	NA	NA	NA
2	298546	5064.784	10	41771.53	246224.2	0

A anova: 2 x 6

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
1	298556	48439.891	NA	NA	NA	NA
2	298546	5064.784	10	43375.11	255676.5	0

From the partial F-tests of each feature, we see that the p-values for each of the reduced models with only one feature is very small (last column of secomd row of each anova table = almost 0), which shows that the null hypothesis for each of the partial F-tests, which states that the model can be explained using just that one variable, needs to be rejected. Thus, the alternate hypothesis that a combination of features is necessary is accepted.

Model Selection

Backward selection

First, I'm going to try backward selection with $\alpha_{crit} = 0.15$. In backward selection, we start with the full model, and update the model step-by-step; at each step, the feature with the highest p-value ($> \alpha_{crit}$) is removed.

In [19]:
```
summary(fullmodel)
```

```
Call:
lm(formula = Salnty ~ ., data = traindf)

Residuals:
    Min      1Q  Median      3Q     Max 
-2.8546 -0.0649  0.0088  0.0682  5.1596 

Coefficients:
              Estimate Std. Error  t value Pr(>|t|)    
(Intercept)  2.513e+01  5.867e-02  428.342  < 2e-16 ***
Depthm       1.175e-04  2.562e-06   45.878  < 2e-16 ***
O2ml_L      -1.805e-01  3.295e-03  -54.787  < 2e-16 ***
STheta       4.808e-01  9.203e-04  522.423  < 2e-16 ***
O2Sat        5.473e-02  1.174e-04  466.293  < 2e-16 ***
Oxymol      -1.811e-02  8.638e-05 -209.656  < 2e-16 ***
ChlorA       1.598e-02  3.696e-04   43.249  < 2e-16 ***
Phaeop       5.132e-03  1.541e-03    3.330 0.000868 ***
PO4uM        1.107e-01  1.641e-03   67.469  < 2e-16 ***
SiO3uM      -6.464e-03  4.399e-05 -146.931  < 2e-16 ***
NO2uM       -8.784e-03  2.672e-03   -3.287 0.001013 ** 
Year        -1.796e-03  2.550e-05  -70.443  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.1302 on 298546 degrees of freedom
Multiple R-squared:  0.8955,	Adjusted R-squared:  0.8955 
F-statistic: 2.325e+05 on 11 and 298546 DF,  p-value: < 2.2e-16
```

The p-values of every feature is less than α_{crit}. Thus, according to backward selection, the best model is the full model itself.

Model selection using "regsubsets"

I am going to compute the best model of size 1, best model of size 2, etc. up through the best model of size 11 (full model). I will then compare these 11 best models on the basis of their MSPE, BIC and R2a values to decide the best model.

In [20]:
```
library(leaps)
```

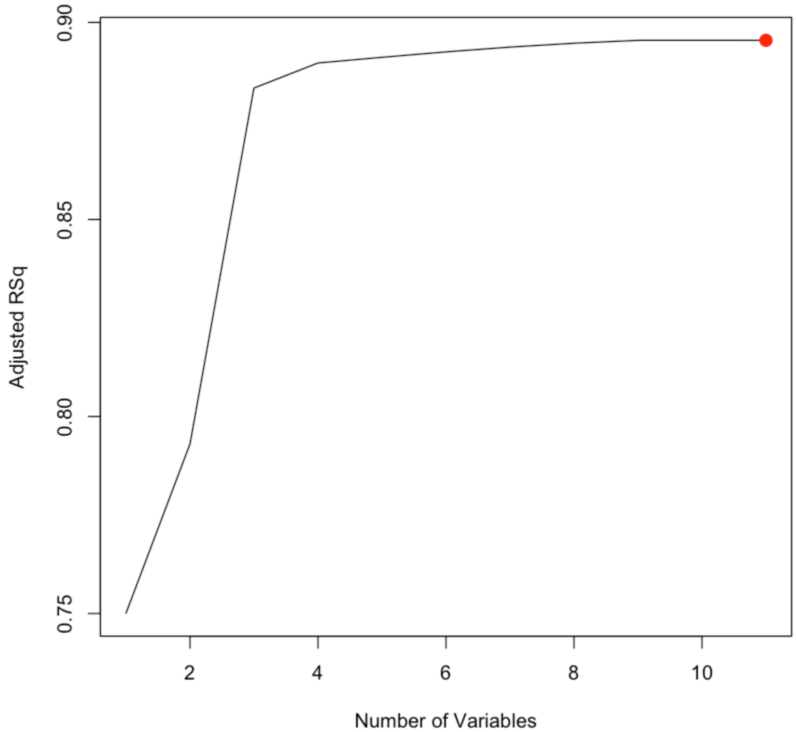
In [21]:
```
reg <- regsubsets(Salnty ~ ., data = traindf, nvmax = 11)
rs <- summary(reg)
rs$which
```

A matrix: 11 x 12 of type lgl

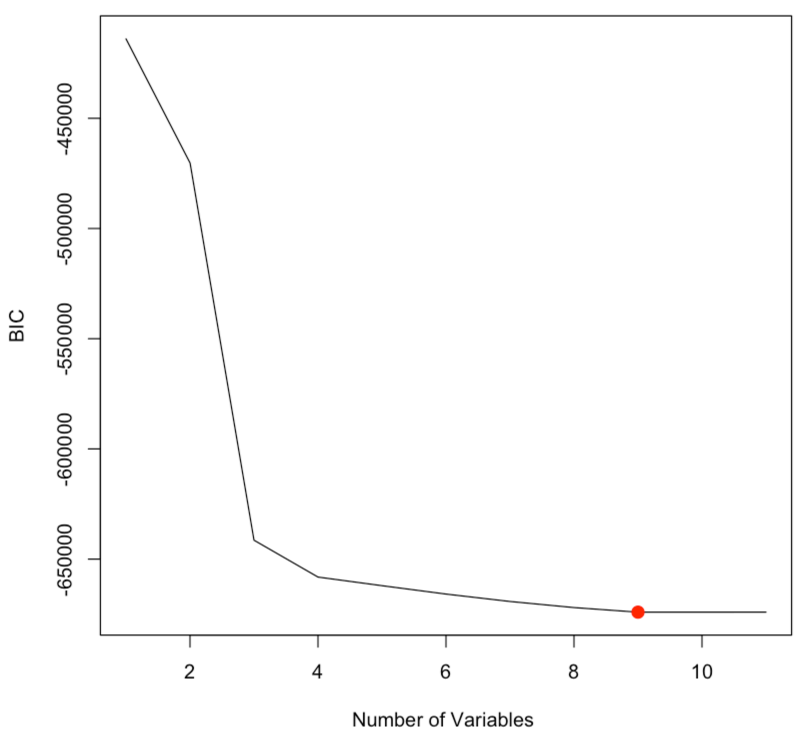
	(Intercept)	Depthm	O2ml_L	STheta	O2Sat	Oxymol	ChlorA	Phaeop	PO4uM	Si
1	TRUE	FALSE	FALSE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	
2	TRUE	FALSE	TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	
3	TRUE	FALSE	FALSE	TRUE	TRUE	TRUE	FALSE	FALSE	FALSE	
4	TRUE	FALSE	FALSE	TRUE	TRUE	TRUE	FALSE	FALSE	FALSE	
5	TRUE	FALSE	FALSE	TRUE	TRUE	TRUE	FALSE	FALSE	TRUE	
6	TRUE	FALSE	FALSE	TRUE	TRUE	TRUE	FALSE	FALSE	TRUE	
7	TRUE	FALSE	TRUE	TRUE	TRUE	TRUE	TRUE	FALSE	FALSE	
8	TRUE	FALSE	TRUE	TRUE	TRUE	TRUE	TRUE	FALSE	TRUE	
9	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	FALSE	TRUE	
10	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	
11	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	

In [22]:
```
options(repr.plot.width = 7, repr.plot.height = 7)
par(bg = "white")


plot(rs$adjr2, xlab = "Number of Variables", ylab = "Adjusted RSq", type = "
which.max(rs$adjr2)
points(which.max(rs$adjr2), rs$adjr2[which.max(rs$adjr2)],
       col = "red", cex = 2, pch = 20)

plot(rs$bic, xlab = "Number of Variables ", ylab = "BIC", type = "l")
which.min(rs$bic)
points(which.min(rs$bic), rs$bic[which.min(rs$bic)],
       col = "red", cex = 2, pch = 20)
```

11



9



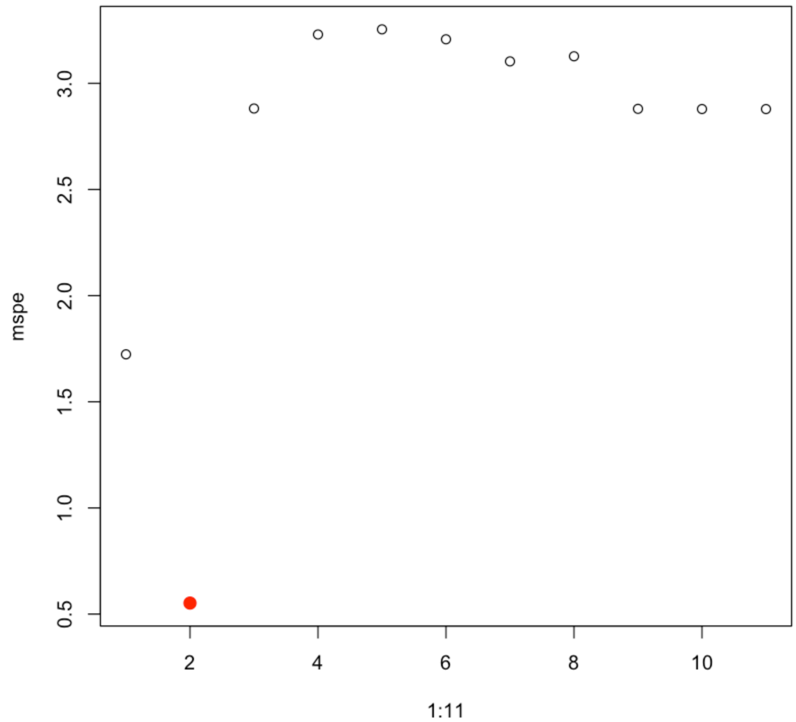
In [23]:
```
## Calculating MSPE of each of the 11 models

# Assigning the best models best on the truth values of the features
m1 <- lm(Salnty ~ STheta, data = traindf)
```

```
m2 <- lm(Salnty ~ STheta + O2ml_L, data = traindf)
m3 <- lm(Salnty ~ STheta + O2Sat + Oxymol, data = traindf)
m4 <- lm(Salnty ~ STheta + O2Sat + Oxymol + SiO3uM, data = traindf)

m5 <- lm(Salnty ~ STheta + O2Sat + Oxymol + SiO3uM + PO4uM, data = traindf)
m6 <- lm(Salnty ~ STheta + O2Sat + Oxymol +
           SiO3uM + PO4uM + Year, data = traindf)
m7 <- lm(Salnty ~ STheta + O2Sat + Oxymol +
           SiO3uM + O2ml_L + ChlorA + Year, data = traindf)
m8 <- lm(Salnty ~ STheta + O2Sat + Oxymol + PO4uM +
           SiO3uM + O2ml_L + ChlorA + Year, data = traindf)

m9 <- lm(Salnty ~ STheta + O2Sat + Oxymol + PO4uM +
           SiO3uM + O2ml_L + ChlorA + Year + Depthm, data = traindf)

m10 <- lm(Salnty ~ STheta + O2Sat + Oxymol + PO4uM +
            SiO3uM + O2ml_L + ChlorA + Year + Depthm + Phaeop, data = trainc

m11 <- lm(Salnty ~ ., data = traindf)


pred1 <- predict(m1, newdata = testdf)
pred2 <- predict(m2, newdata = testdf)
pred3 <- predict(m3, newdata = testdf)
pred4 <- predict(m4, newdata = testdf)

pred5 <- predict(m5, newdata = testdf)
pred6 <- predict(m6, newdata = testdf)
pred7 <- predict(m7, newdata = testdf)
pred8 <- predict(m8, newdata = testdf)

pred9 <- predict(m9, newdata = testdf)
pred10 <- predict(m10, newdata = testdf)
pred11 <- predict(m11, newdata = testdf)



mspe <- rep(NA, 11)
mspe[1] <- mean((testdf$Salnty - pred1)^2)
mspe[2] <- mean((testdf$Salnty - pred2)^2)
mspe[3] <- mean((testdf$Salnty - pred3)^2)
mspe[4] <- mean((testdf$Salnty - pred4)^2)

mspe[5] <- mean((testdf$Salnty - pred5)^2)
mspe[6] <- mean((testdf$Salnty - pred6)^2)
mspe[7] <- mean((testdf$Salnty - pred7)^2)
mspe[8] <- mean((testdf$Salnty - pred8)^2)

mspe[9] <- mean((testdf$Salnty - pred9)^2)
mspe[10] <- mean((testdf$Salnty - pred10)^2)
mspe[11] <- mean((testdf$Salnty - pred11)^2)
```

In [24]:

```
par(bg = "white")
plot(x = 1:11, y = mspe)
```

```
points(which.min(mspe), mspe[which.min(mspe)],
       col = "red", cex = 2, pch = 20)
```



From the above plots, the best performing models are the ones with 11, 9 and 2 features respectively for R2a, BIC and MSPE.

Checking for collinearity

In [25]:
```
library(car)
```

```
Loading required package: carData
```

In [26]:
```
vif(m11)
vif(m9)
vif(m2)
```

Depthm: 4.36950253896657 **O2ml_L:** 690.265045637104 **STheta:** 13.286548515554 **O2Sat:** 284.325620807596 **Oxymol:** 900.411157271409 **ChlorA:** 2.09321230611346 **Phaeop:** 2.13726850149583 **PO4uM:** 41.2943716810368 **SiO3uM:** 20.0382135780015 **NO2uM:** 1.18710363246507 **Year:** 1.03651556355834

STheta: 13.2737553779942 **O2Sat:** 280.839461890357 **Oxymol:** 896.282480353494 **PO4uM:** 41.2177108808897 **SiO3uM:** 20.0263710177101 **O2ml_L:** 690.225362148234 **ChlorA:** 1.13772578343519 **Year:** 1.03376892309575 **Depthm:** 4.36001062439453

STheta: 4.46696896001851 **O2ml_L:** 4.46696896001851

We see that the models with 9 and 11 features have high collinearity, since the VIF values are greater than 5 for many of the variables in those models. Whereas for the model with 2 features, both the VIF values are less than 5 which suggests no collinearity between the features.

Also considering parsimony, I believe model 2 is the best model, since it has the best performance based on MSPE, performs relatively well in terms of BIC and R2a and does not have any redundant features. Thus, the chosen best model is:

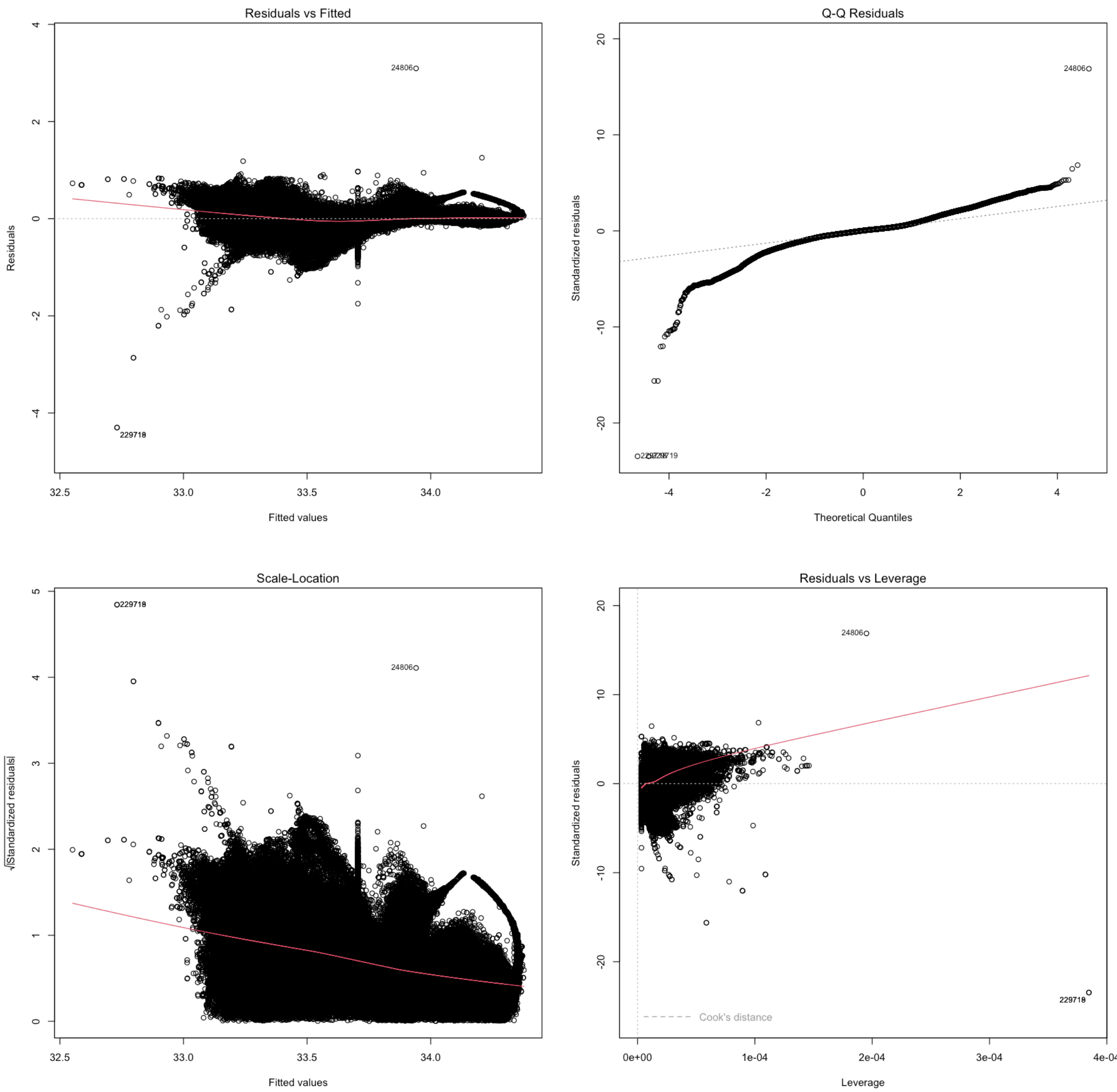
$$\text{Salnty} = 28.7911722 + 0.2048749 \times \text{STheta} - 0.0928460 \times \text{O2ml\\\_L}$$

In [27]:
```
summary(m2)
```

```
Call:
lm(formula = Salnty ~ STheta + O2ml_L, data = traindf)

Residuals:
    Min      1Q  Median      3Q     Max 
-4.3001 -0.0792  0.0064  0.0781  3.0933 

Coefficients:
              Estimate Std. Error t value Pr(>|t|)    
(Intercept) 28.7911722  0.0205452  1401.4   <2e-16 ***
STheta       0.2048749  0.0007508   272.9   <2e-16 ***
O2ml_L      -0.0928460  0.0003730  -248.9   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.1833 on 298555 degrees of freedom
Multiple R-squared:  0.793,	Adjusted R-squared:  0.793 
F-statistic: 5.719e+05 on 2 and 298555 DF,  p-value: < 2.2e-16
```

Model diagnostics

In [30]:
```
par(mfrow = c(2, 2))
par(bg = "white")
options(repr.plot.width = 15, repr.plot.height = 15)
plot(m2)
```



From the Residuals vs Fitted plot, we see that the residuals are pretty random, but there is a slight pattern where the variance of the residual values decrease when the fitted values are high, suggesting that they may not be fully independent.

The pattern in the residual plot also suggests that the constant variance assumption might be erroneous since we should have expected a band of uniform width in that case.

The Q-Q plot suggests the normality assumption may also be violated, since at the edges, the model deviates quite a bit.

From the leverage plot, there are no points with Cook's distance > 0.5, indicating the absense of influential points which is a good thing.

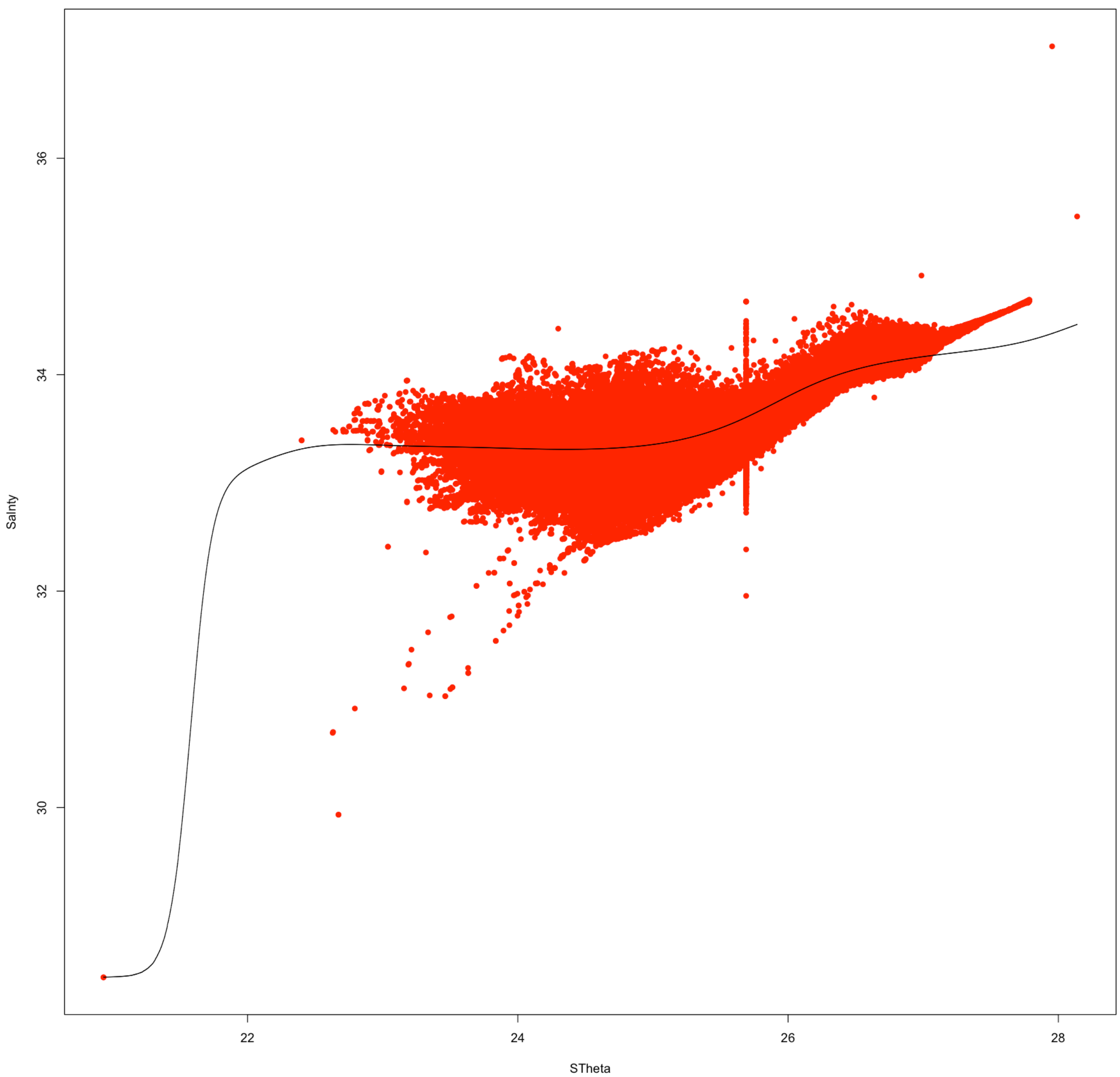
Kernel Regression

With some of the violations of the assumptions of the linear regression model, I would like to consider a kernel regression model with STheta as the variable. I'm choosing this, since the coefficient of STheta is higher than that of O2ml_L, despite the fact that the scale of the STheta variable is higher (20.93 to 28.14 for Stheta compared to -0.01 to 11.13 for O2ml_L). This suggests that STheta is a stronger influencer on Salnty (higher increase in Salnty for unit change in STheta compared to unit change in O2ml_L).

In [34]:
```
summary(traindf)
```

```
     Depthm           Salnty          O2ml_L           STheta     
 Min.   :   0.0   Min.   :28.43   Min.   :-0.010   Min.   :20.93  
 1st Qu.:  37.0   1st Qu.:33.40   1st Qu.: 2.210   1st Qu.:24.88  
 Median : 101.0   Median :33.68   Median : 3.758   Median :25.80  
 Mean   : 166.8   Mean   :33.71   Mean   : 3.765   Mean   :25.70  
 3rd Qu.: 250.0   3rd Qu.:34.07   3rd Qu.: 5.660   3rd Qu.:26.54  
 Max.   :4442.0   Max.   :37.03   Max.   :11.130   Max.   :28.14  
     O2Sat            Oxymol             ChlorA            Phaeop       
 Min.   : -0.10   Min.   : -0.4349   Min.   :-0.0010   Min.   :-3.8900  
 1st Qu.: 33.60   1st Qu.: 96.1958   1st Qu.: 0.1100   1st Qu.: 0.0800  
 Median : 62.64   Median :163.6312   Median : 0.4395   Median : 0.1908  
 Mean   : 62.70   Mean   :163.9198   Mean   : 0.4422   Mean   : 0.1916  
 3rd Qu.:100.50   3rd Qu.:246.4232   3rd Qu.: 0.4395   3rd Qu.: 0.1908  
 Max.   :214.10   Max.   :485.7018   Max.   :66.1100   Max.   :10.6600  
     PO4uM           SiO3uM           NO2uM              Year     
 Min.   :0.030   Min.   :  0.00   Min.   :0.00000   Min.   :1980  
 1st Qu.:0.470   1st Qu.:  3.70   1st Qu.:0.00000   1st Qu.:1987  
 Median :1.473   Median : 22.90   Median :0.01000   Median :1996  
 Mean   :1.474   Mean   : 25.65   Mean   :0.04090   Mean   :1996  
 3rd Qu.:2.200   3rd Qu.: 37.80   3rd Qu.:0.04113   3rd Qu.:2004  
 Max.   :5.210   Max.   :181.60   Max.   :8.19000   Max.   :2013  
```

In [35]:
```
par(bg = 'white')
with(traindf, plot(Salnty ~ STheta, pch = 16, col = "red"))
with(traindf, lines(ksmooth(STheta, Salnty, "normal", 1)))
```



In [43]:
```
library(mgcv)
```

```
Loading required package: nlme

This is mgcv 1.9-1. For overview type 'help("mgcv-package")'.
```

In [44]:
```
kern <- gam(Salnty ~ s(STheta, bs = "cr", k = 1),
            data = traindf, method = "REML")

pred_kern <- predict(kern, newdata = testdf, type = "response")
mspe_lin <- mean((testdf$Salnty - pred2)^2)
mspe_kern <- mean((testdf$Salnty - pred_kern)^2)
mspe_lin    # Linear model
mspe_kern   # Kernel model
```

```
Warning message in smooth.construct.cr.smooth.spec(object, dk$data, dk$knot
s):
"basis dimension, k, increased to minimum possible
"
```

0.551914139113923

7.81093318075351

Synopsis

Background :

I was interested in this problem because of my childhood interest in Marine Biology. I found a dataset that was tangential to this field, where I could study how oceanographic quantities affect species diversity in the ocean. The CalCOFI dataset represents the longest (1949 - present) and most complete (more than 50,000 sampling stations) time series of oceanographic and larval fish data captured in the world. This database contains oceanographic data measured using CTD casts from seawater samples collected at CalCOFI stations.

CTD stands for conductivity, temperature, and depth, and refers to a package of electronic instruments that measure oceanographic properties (i.e., the physical features of seawater such as salinity, dissolved oxygen, chlorophyll-a, nutrients, and many more). A CTD cast gives scientists a precise and comprehensive charting of the distribution and variation of water oceanographic properties that helps to understand how the oceans affect life.

Salinity plays a key role in analyzing the water cycle, ocean circulation, and climate change, as it drives ocean currents and circulation patterns. Variations in salinity affect the density of seawater, which in turn influences its movement and mixing. Many marine organisms have adapted to specific salinity levels, so variations in salinity can directly impact their distribution, reproduction, and survival.

The dataset used for this project can be downloaded from :
https://drive.google.com/file/d/1EspgcE5t9VHvk338_uNesCfhNZWDPVnB/view?usp=drive_link

The dataset contains 325,281 rows and 16 oceanographic features and one outcome variable - salinity of the water (Salnty). Description of all the variables:

1. Salnty: Salinity (Practical Salinity Scale 1978) (outcome)
2. Depthm: cast depth in meters
3. O2mlL: Milliliters oxygen per liter of seawater
4. STheta: Potential Density (Sigma Theta), Kg/M3
5. O2Sat: Oxygen percent saturation

6. Oxyµmol/Kg: Oxygen micromoles per kilogram seawater
7. ChlorA: Migrograms Chlorophyll-a per liter seawater, measured fluorometrically
8. Phaeop: Micrograms Phaeopigment per liter seawater, measured fluormetrically
9. PO4uM: Micromoles Phosphate per liter of seawater
10. SiO3uM: Micromoles Silicate per liter of seawater
11. NO2uM: Micromoles Nitrite per liter of seawater
12. NH3uM: Micromoles Ammonia per liter of seawater
13. C14As1: 14C Assimilation of Replicate 1 (milligrams carbon per cubic meter of seawater per half light day)
14. C14As2: 14C Assimilation of Replicate 2 (milligrams carbon per cubic meter of seawater per half light day)
15. DarkAs: 14C Assimilation of Dark/Control Bottle (milligrams carbon per cubic meter of seawater per half light day)
16. LightP : Light intensities of the incubation tubes in the primary productivity experiment, expressed as percentages
17. Year: The year the sample was collected

In this project, I have attempted to obtain a reliable model to predict the salinity of ocean water using a subset of these oceanographic features. Accurate prediction of salinity at any location in the ocean can be used to identify more efficient mechanisms to optimally conserve the habitat of marine species and thereby enhance stability and preservation of the environment in the face of global climate change.

Methods and Conclusion

For exploaratory data analysis, I looked at the individual plots of each feature against the outcome, and the correlation between all the features. The scatter plots conveyed the presence of patterns (seemingly linear) and the correlation heatmap concurred. Thus, I decided to create a linear regression model to predict the salinity.

Initially, I had to perform pre-processing on the data to clean it and fill in any missing values. Some of the features had few rows of data available, so I decided to remove those features and work with a smaller subset of features. I then filled any missing values in the other features with their respective column means to prepare for linear regression modelling. I also split the dataset into training and test datasets based on the year (before 2013 as training and after that as test), since I wanted to mimic reality to predict the salinity in the future years based on the past.

On performing Multiple Linear Regression, I fit a full model with all the features. I then performed F-tests on the model to identify that a trivial model with no features will indeed not predict the outcome as well as a linear model would.

I performed model selection to obtain the best model for different numbers of features. Out of these models, I used different evaluation criteria like BIC, MSPE and R2a to identify the best performing model. The final model I landed on was:

$$\text{Salnty} = 28.7911722 + 0.2048749 \times \text{STheta} - 0.0928460 \times \text{O2ml\textbackslash\_L}$$

I then performed model diagnostics, and found that some of the assumptions for MLR were violated. I then fit a kernel regression model using just the STheta feature and saw that it explained the behaviour a little better. However, its MSPE performance was not as good as that of the linear model.

In conclusion, I believe the above linear model is a good predictor for the salinity of ocean water.