R Minicourse Workshop
White River Case Study

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White River Case Study

Preliminaries

- The R scripts for this lecture are called `whiteriver01.r` and `whiteriver02.r`.
- The first script does one reach, distance, and parameter, interactively.
- The second does all combinations of reach, distance, and several parameters and saves the results into files. `whiterivertext.txt` and `whiteriverplot.pdf`
- Greg Pelletier provided a spreadsheet `Q2KW_White_River_observed_and_predicted_data.xlsx`
- I saved the two pages of the spreadsheet into two csv files:
  - `Q2KW_White_River_observed_data.csv`
  - `Q2KW_White_River_predicted_data.csv`

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Loading the Data

```
predicted <- read.table("Q2KW_White_River_predicted_data.csv",
                        header=T,
                        sep=",",
                        stringsAsFactors=F)
observed <- read.table("Q2KW_White_River_observed_data.csv",
                       header=T,
                       sep=",",
                       stringsAsFactors=F)
# We want to load "5/5/12" as a string, rather than a factor,
# to make subsequent conversion to dates a bit easier.
# Now replace date strings with actual dates:
predicted$Date.time <- strptime(predicted$Date.time,
                                format="%m/%d/%y %H:%M")
observed$Date.time <- strptime(observed$Date.time,
                               format="%m/%d/%y %H:%M")
```

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Large size of the dataset makes it hard to view interactively.

```
dim(observed)
[1] 47265    54
dim(predicted)
[1] 48450    79
names(observed)
[1] "Reach.number"
[2] "Distance..Km."
[3] "Date.time"
[4] "Temperature..degC."
[5] "Conductivity..uS.cm.25C." ...
names(predicted)
[1] "Reach"
[2] "Distance..Km."
[3] "Date.time"
[4] "Temperature..degC."
[5] "Conductivity..uS.cm.25C." ...
```

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Observed *vs.* predicted reaches

- We want to use reach and distance as a site.
- Examining reaches in both observed and predicted shows that the observed reaches are a subset of the predicted reaches.
- So we can use the same reach, *e.g.* 23, for both files.

```
observed.reaches <- unique(sort(observed$Reach.number))
observed.reaches
[1]  3  8 13 20 21 22 23 25 27 28 31 33
predicted.reaches <- unique(sort(predicted$Reach))
predicted.reaches
[1]  0  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28
my.reach <- 23
```

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Observed *vs.* predicted distances

- Distances are not the same in the two files.
- We will have to find a closest distance in the predicted file to match any distance in the observed file.

```
observed.distances
[1]  0.03574664  2.15476664  5.81305664  7.90000000  9.37570664 12.01200000 13.31981664 16
[9] 24.72141000 31.85200000 39.69900000
predicted.distances
[1]  0.04  1.12  2.15  3.35  4.51  5.81  7.09  8.28  9.38 10.72 11.83 13.32 15.25 16.20 17
[18] 20.75 22.08 23.44 24.72 26.12 27.46 28.73 30.23 31.85 33.58 34.85 36.57 38.21 39.70 4
my.observed.distance <- observed.distances[6]
min.difference.index <- which.min(abs(predicted.distances - my.observed.distance))
my.predicted.distance <- predicted.distances[min.difference.index]
```

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Parameter names and columns

```
observed.parameter.name <- "pH"
observed.parameter.column <- which(names(observed) == observed.parameter.name)
predicted.parameter.name <- "pH"
predicted.parameter.column <- which(names(predicted) == predicted.parameter.name)
```

- Now we can use any of the following:
  - `observed[[observed.parameter.column]]`
  - `observed[,observed.parameter.column]`
  - `observed$pH`
  - `observed[[observed.parameter.name]]`
- And similarly for `predicted`

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Creating an ID for selected parameter, reach, distance

- We have now selected a parameter, a reach, and a distance.
- It will be helpful to print these out here and there, so we make a string with all this information in it.

```
my.id <- paste( observed.parameter.name,
                " reach:", my.reach,
                " distance:", my.observed.distance)
cat(paste("Sample ID: ", my.id, "\n"))
```

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Selecting the rows

- We want only the data from the selected reach and distance, which also has a valid date and a valid datum.
- So we select just those rows.
- If the number of rows is too small, we can try a different reach and distance.
- Note that reach has different names in the two datasets.

```
observed.rows <- (observed$Reach.number == my.reach) &
  (observed$Distance == my.observed.distance) &
  (!is.na(observed$Date.time)) &
  (!is.na(observed[,observed.parameter.column]))

predicted.rows <- (predicted$Reach == my.reach) &
  (predicted$Distance == my.predicted.distance) &
  (!is.na(predicted$Date.time))&
  (!is.na(predicted[,predicted.parameter.column]))
```

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Subsetting the rows and columns of the data

- We can now select just the rows and columns we want.
- This will be the data we analyze, it has been "cleaned" so that we don't have to worry about missing numbers, *etc.*

```
date.name <- "Date.time"
observed.date.column <- which(names(observed) == date.name)
predicted.date.column <- which(names(predicted) == date.name)

observed.columns <- c(observed.date.column, observed.parameter.column)
predicted.columns <- c(predicted.date.column, predicted.parameter.column)

observed.subset <- observed[observed.rows, observed.columns]
predicted.subset <- predicted[predicted.rows, predicted.columns]
```

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Plotting observed and predicted data

- We want plots of observed and predicted to have the same x and y range, so we find the biggest range needed for each.

```
x.range <- as.numeric(range(c(observed.subset$Date.time,
                              predicted.subset$Date.time)))
y.range <- range(c(observed.subset[[observed.parameter.name]],
                   predicted.subset[[predicted.parameter.name]]))
```

- Now we can plot the data.

```
plot(observed.subset,
     type="l",
     xlim=x.range,
     ylim=y.range,
     main=paste("Observed", my.id,
                "N=",length(which(observed.rows))))
```

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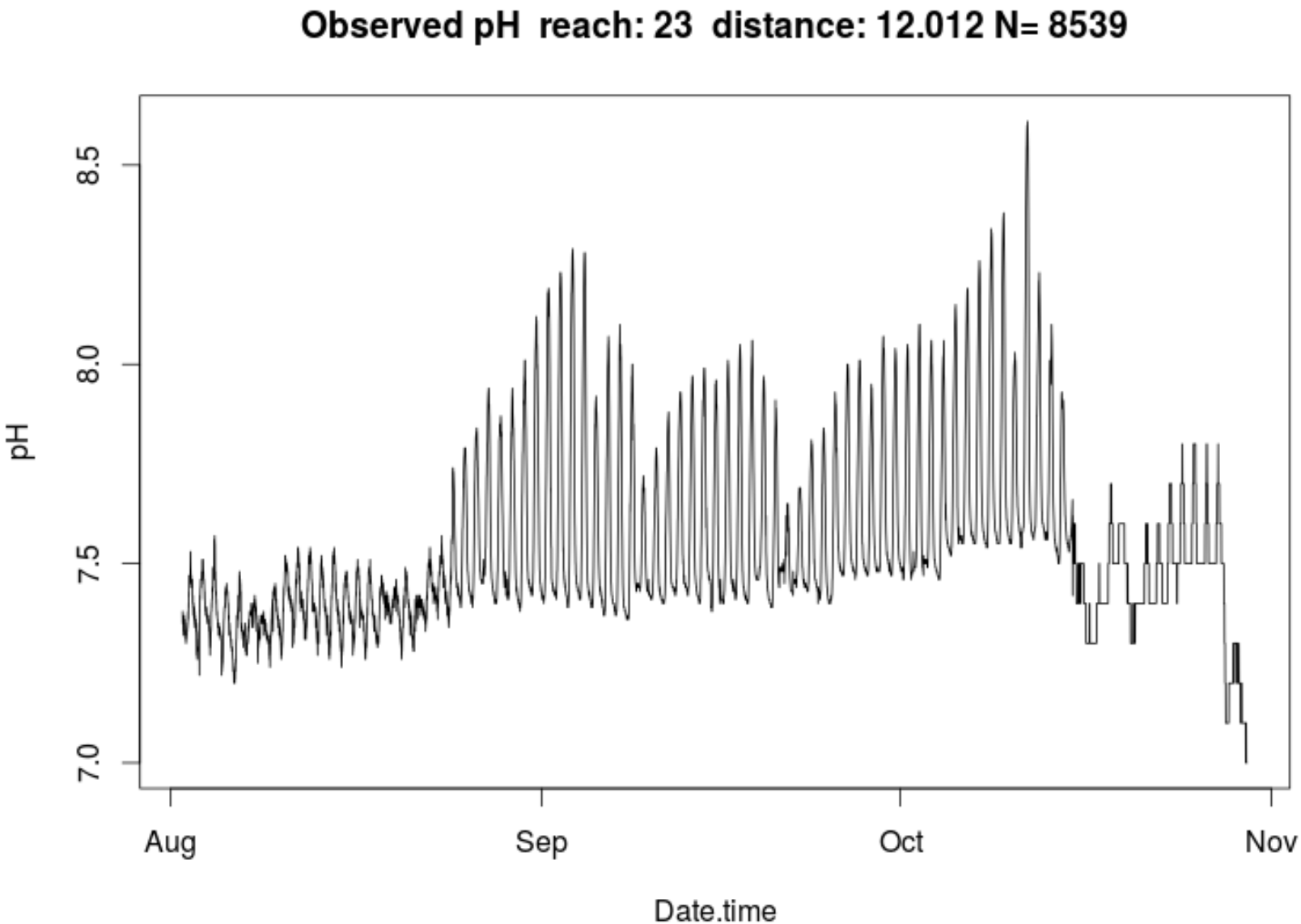
Observed plot



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Predicted plot

```
plot(predicted.subset,
     type="l",
     xlim=x.range,
     ylim=y.range,
     main=paste("Predicted", my.id,
                "N=",length(which(predicted.rows))))
```

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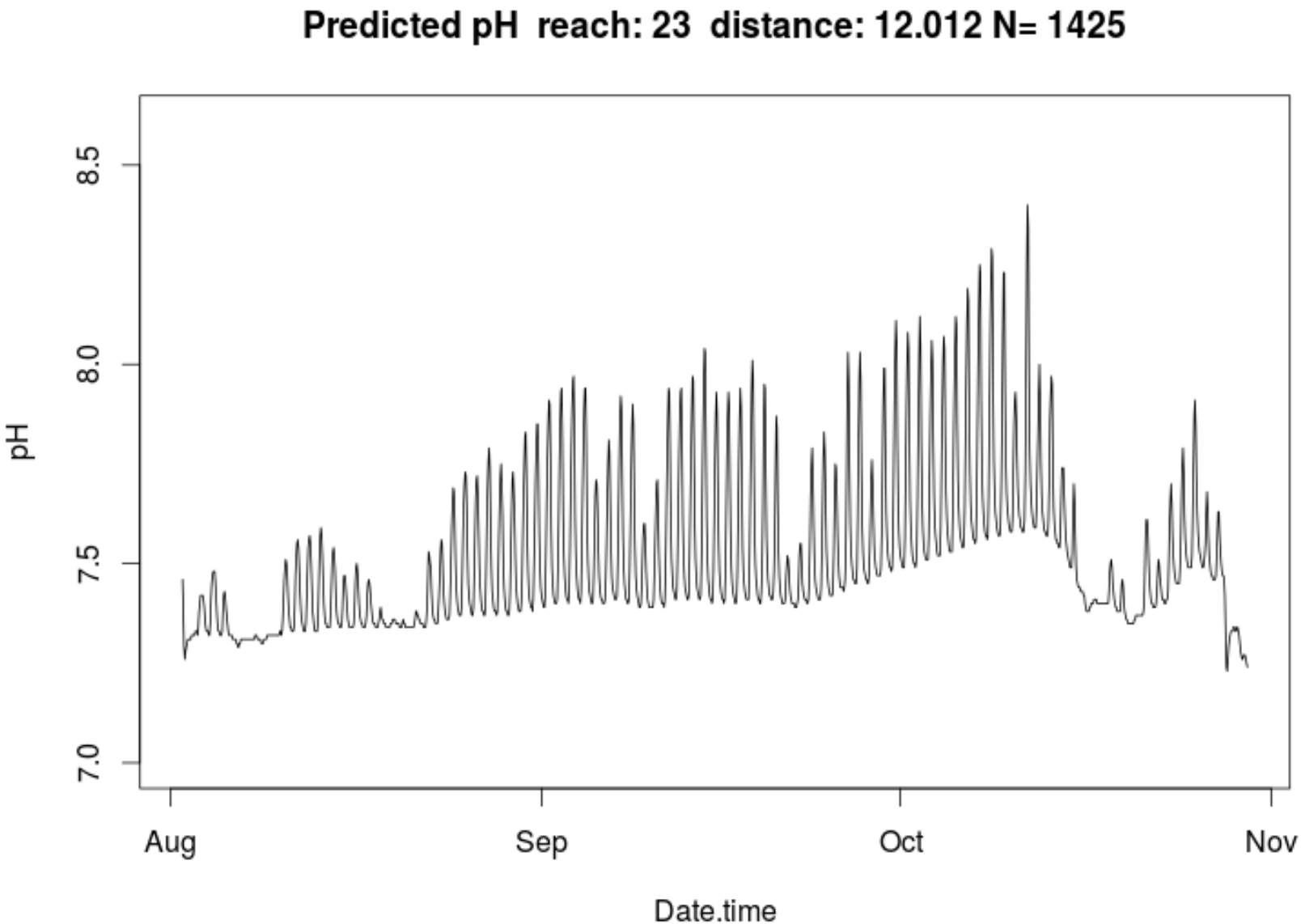
Predicted plot



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Predicted and observed plot

```
plot(observed.subset,
     type="l",
     xlim=x.range,
     ylim=y.range,
     col="blue",
     main=paste(my.id))
lines(predicted.subset,
     type="l",
     col="red")
legend(x=min(x.range), y=ypos, yjust=yjus,
       lty=1,
       col=c("blue","red"),
       legend=c("Observed","Predicted"))
```

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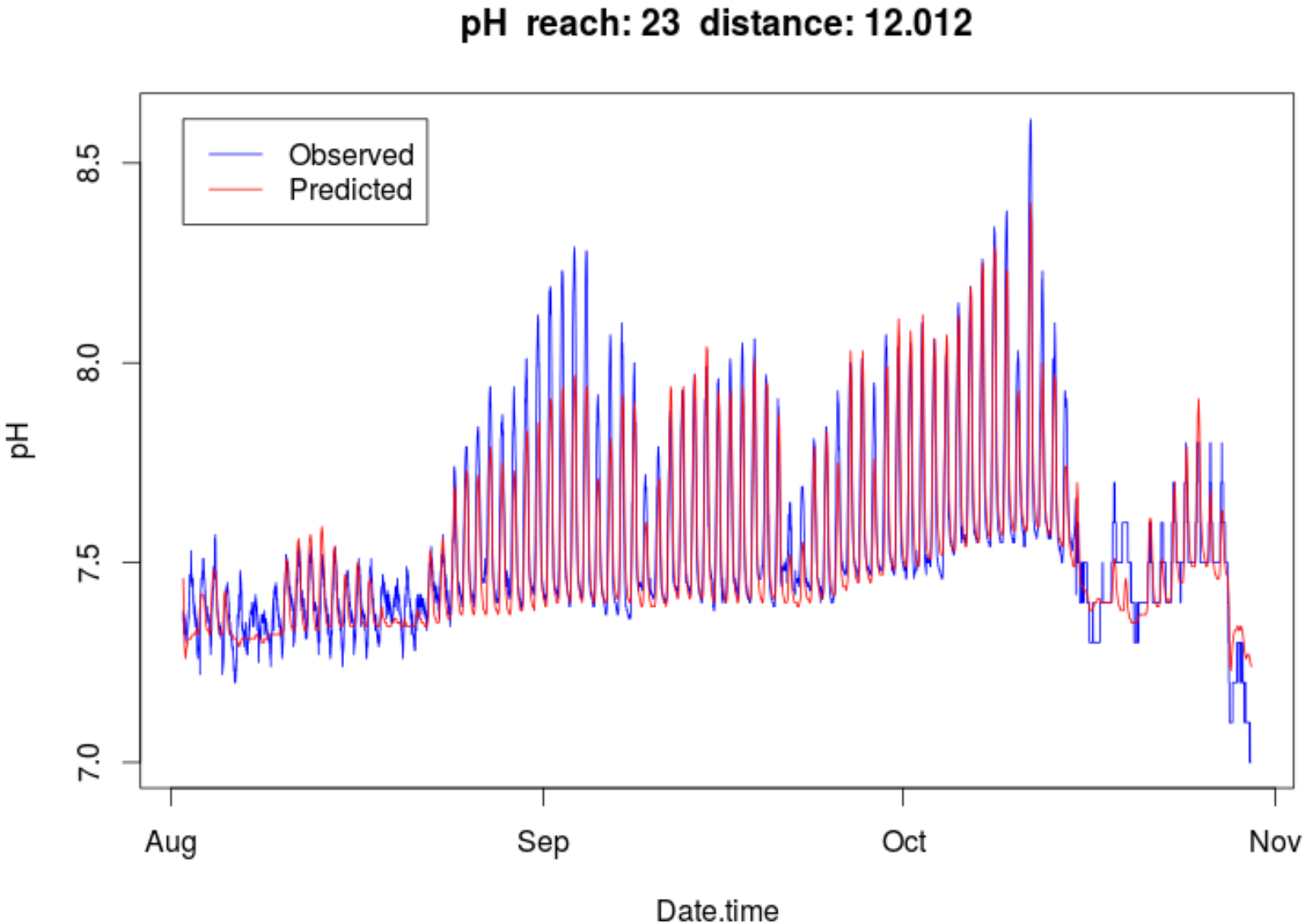
Predicted and observed plot



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Subsample the data

- There are tens of thousands of rows for some of these plots.
- We make analysis more tractable by subsampling.

```
n <- min(200, nrow(observed.subset))
sample.rows <- sort(sample(1:nrow(observed.subset), n))
observed.sample <- observed.subset[sample.rows,]
predictions <- rep(0,n)
for (row in 1:n) {
  obs.time <- observed.sample$Date.time[row]
  pred.row <- which.min(abs(predicted.subset$Date.time-obs.time))
  predictions[row] <- predicted.subset[[predicted.parameter.name]][pred.row]
}
```

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Plot the observed and predicted subsample

```
plot(observed.sample,
     type="l",
     xlim=x.range,
     ylim=y.range,
     col="blue",
     main=paste("Subsampled",my.id))
lines(observed.sample$Date.time,predictions,
      type="l",
      col="red")
legend(x=min(x.range), y=ypos, yjust=yjus,
       lty=1,
       col=c("blue","red"),
       legend=c("Observed","Predicted")
       )
```

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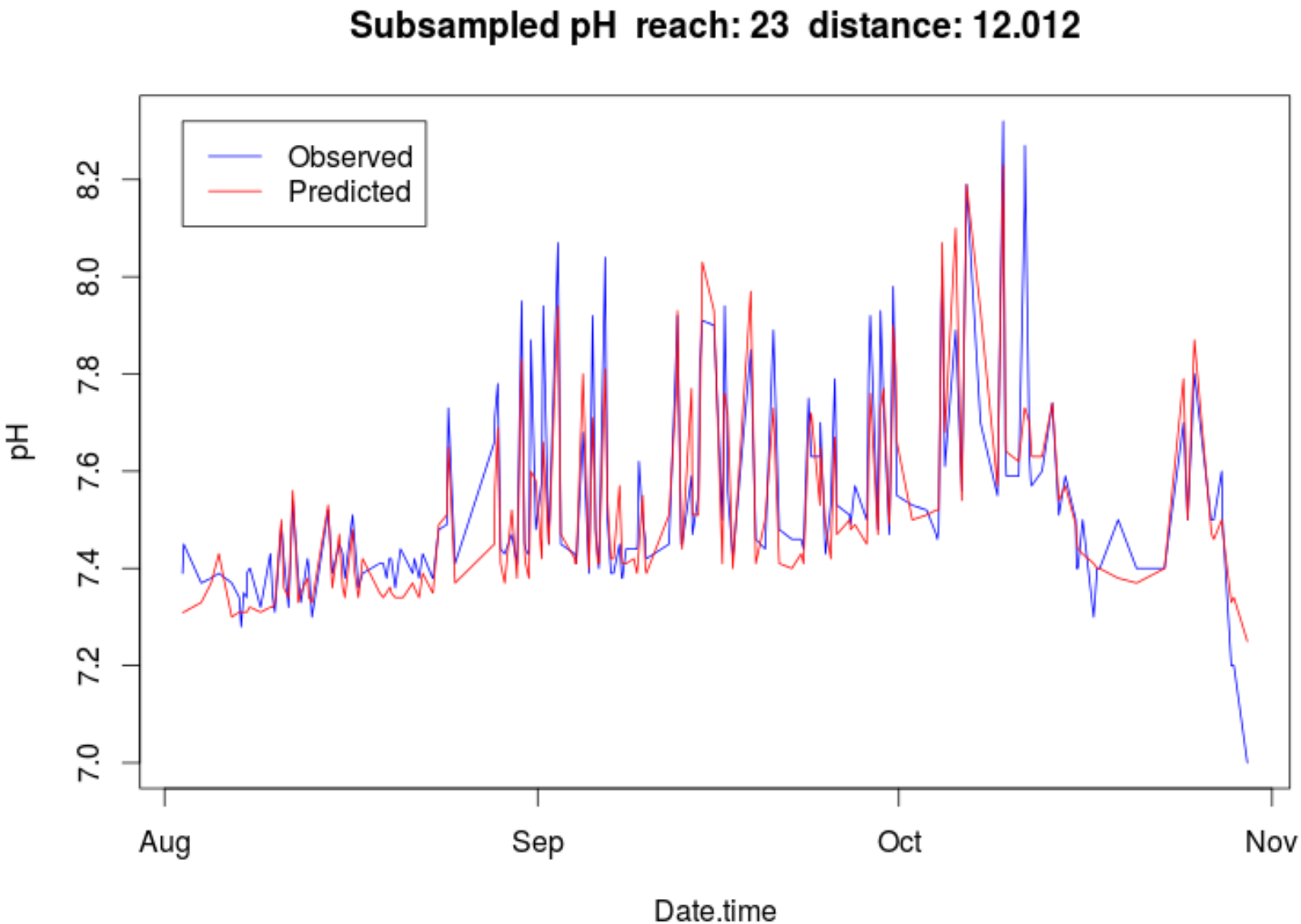
Plot the observed and predicted subsample



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Fit a linear model

```
my.model <- lm(predictions ~ observed.sample[[observed.parameter.name]])
summary(my.model)
Call:
lm(formula = predictions ~ observed.sample[[observed.parameter.name]])

Residuals:
     Min       1Q   Median       3Q      Max
-0.25823 -0.03804 -0.00541  0.04324  0.24426

Coefficients:
                                          Estimate Std. Error t value Pr(>|t|)
(Intercept)                                1.26902    0.19073   6.653 2.74e-10 ***
observed.sample[[observed.parameter.name]]  0.82893    0.02526  32.815  < 2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.07581 on 198 degrees of freedom
Multiple R-squared:  0.8447, Adjusted R-squared:  0.8439
F-statistic:  1077 on 1 and 198 DF,  p-value: < 2.2e-16
```

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Plot the observed *vs.* predicted and the linear fit

```
plot(observed.sample[[observed.parameter.name]], predictions,
     xlab="Observed",
     ylab="Predicted",
     main=paste("Linear model for", my.id))
# Add the best fit line and legend
abline(my.model,col="red")
legend(x=min(observed.sample[[observed.parameter.name]]),
       y=max(predictions),
       legend=c(paste("Slope:", round(my.model$coefficients[2],2)),
                paste("Intercept:", round(my.model$coefficients[1],2))))
```

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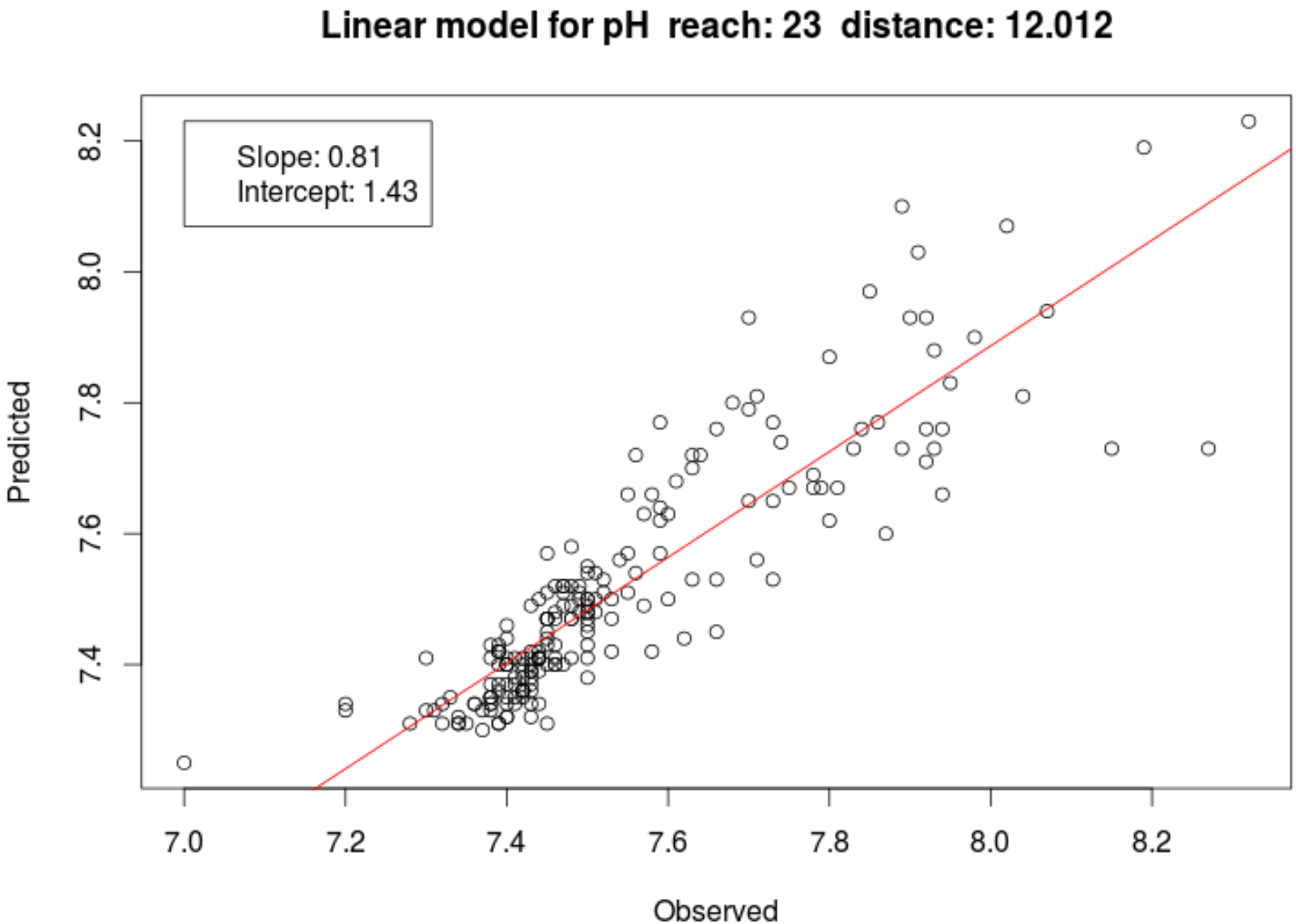
Plot the observed *vs.* predicted and the linear fit



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ANOVA on the model

```
anova(my.model)
Analysis of Variance Table

Response: predictions
                                          Df Sum Sq Mean Sq F value    Pr(>F)
observed.sample[[observed.parameter.name]]  1 6.1881  6.1881  1076.8 < 2.2e-16 ***
Residuals                                 198 1.1378  0.0057
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
```

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Plot the residuals for the linear model

```
par(mfrow=c(2,2))
plot(my.model, main=my.id)
par(mfrow=c(1,1))
```

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Plot the residuals for the linear model