Lecture Notes

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Prerequisites

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Chapter 1

A short path to GLM and GAM

1.1 Theory

This is a brief overview of popular regression models, based on Lyubchich et al. (2019).

Consider a general regression framework:

$$\mathbf{Y} = \mu + \epsilon, \tag{1.1}$$

where **Y** is an $n \times 1$ column vector comprising observations of the variable of interest (response variable); μ is an $n \times 1$ column vector of expected values $\mathrm{E}(Y_i) \equiv \mu_i$; ϵ is an $n \times 1$ column vector of zero-mean random deviations from the expected values, $i = 1, \ldots, n$; and n is the sample size.

1.1.1 Multiple linear regression

In case of a multiple linear regression, the mean response takes the form

$$\mu = \mathbf{X}\beta,\tag{1.2}$$

where **X** is an $n \times (d+1)$ matrix with one column of 1's for fitting an intercept in the model and the remaining d columns for d correlates (that is, explanatory variables) associated with the response variable; β is a $(d+1) \times 1$ column vector of regression coefficients.

The estimation of regression model (1.2) and further inference are based on a number of assumptions about the validity of the form of the model (i.e., linearity of relationships between Y and each X variable), linear independence of the variables in X, relatively equal importance of all the n observations, as well as

uncorrelatedness, homoscedasticity, and normality of errors ϵ (Chatterjee and Hadi, 2006). However, the assumption of normality is often violated, and model (1.2) in its classical formulation cannot be used in majority of applied problems.

1.1.2 Generalized linear model (GLM)

Generalized linear models (GLMs) help to overcome the violation of normality assumption by extending the applicability of model (1.2) to exponential-type distributions, such as Poisson, binomial, and gamma (Wood, 2006). In GLMs, distribution of Y_i belongs to a family of exponential distributions, and a smooth monotonic link function $g(\cdot)$ is applied to transform the response variable:

$$g(\mu) = \mathbf{X}\beta. \tag{1.3}$$

A distribution belongs to the exponential family of distributions if its probability density function can be written as:

$$f_{\theta}(y) = \exp[y\theta - b(\theta)/a(\phi) + c(y,\phi)],$$

where b, a, and c are arbitrary functions, ϕ and arbitrary 'scale' parameter, and θ is the 'canonical parameter' of the distribution. For normal distribution, $\theta = \mu$ and $a(\phi) = \phi = \sigma^2$ (Wood, 2006).

Canonical link functions are identity, ln, and inverse for normal, Poisson, and gamma distributions, respectively. After such transformation, however, model (1.3) still assumes linear relationships between each of the original variables in \mathbf{X} and the transformed response. Model (1.3) is applicable when the link function successfully linearizes the relationship between the risk variable and a predictor. In other cases, especially if there are multiple predictors, additional work on re-specifying the model may be required. For example, relationships between the response variable and different predictors may require different linearizing transformations, the relationships may be non-monotonic, and many of them may be thresholded (i.e., the effect of a covariate X is pronounced only when X takes on values from a certain range, such as the effect of daily precipitation on sediment concentrations in the streams is not noticeable below certain precipitation threshold).

1.1.3 Generalized additive model (GAM)

One way we can capture highly non-linear relationships is by inclusion of additional transformed X-variables, such as power transformed or thresholded variables (e.g., X_i^2 ; $\max(0, X_j - a)$). However, adding tightly linked variables into the design matrix \mathbf{X} may introduce multicollinearity and affect the inference. An alternative way of modeling non-linearities is replacing the original variables with those individually transformed using smooth (nonparametric) functions, such as in a generalized additive model (GAM):

$$g(\mu) = \mathbf{X}^* \beta^* + f_1(X_1) + f_2(X_2) + f_3(X_3, X_4) + \dots, \tag{1.4}$$

1.1. THEORY 9

where Y_i still follows one of the exponential-family distributions; \mathbf{X}^* and $\boldsymbol{\beta}^*$ are the remaining variables and associated coefficients in strictly parametric formulation; $f(\cdot)$ are smooth functions, often represented by regression splines (Wood, 2006). Model (1.4) can easily deal with deviations from normality and can accommodate non-linearity and non-monotonicity of individual relationships, however, the model still fails to address the issue of remaining dependencies in the errors, e.g., see Kohn et al. (2000).

1.1.4 Generalized additive model for location scale and shape (GAMLSS)

An extension of model (1.4) by Stasinopoulos and Rigby (2007) to k = 1, 2, 3, 4 parameters θ_k of a distribution (not just the location parameter μ_i , but also scale σ_i , and shape – skewness and kurtosis; can be generalized for k > 4) allows fitting k individual models

$$g_k(\theta_k) = h_k\left(\mathbf{X}_k, \boldsymbol{\beta}_k\right) + \sum_{i=1}^{J_k} h_{jk}(\mathbf{x}_{jk}), \tag{1.5}$$

where k=1 produces model for the mean; $h_k(\cdot)$ and $h_{jk}(\cdot)$ are non-linear functions; β_k is a parameter vector of length J_k ; \mathbf{X}_k is an $n \times J_k$ design matrix; \mathbf{x}_{jk} are vectors of length n. The additive terms in this generalized additive model for location scale and shape (GAMLSS) provide a flexible framework to specify random effects and correlation structure as in mixed effects models (Zuur et al., 2009); see Table 3 by Stasinopoulos and Rigby (2007) for other possible specifications of the additive terms. Hence, models of the form (1.5) may be a good choice for insurance problems, because such models accommodate non-normal distributions, possibly highly non-linear relationships, and spatiotemporal dependencies in the data.

1.1.5 Generalized autoregressive moving average (GARMA)

Another group of models, called generalized autoregressive moving average (GARMA), was developed by Benjamin et al. (2003) as a combination of GLM (1.3) with Box–Jenkins approach of modeling temporal dependence:

$$g(\boldsymbol{\mu}_t) = \eta_t = \mathbf{X}_t \boldsymbol{\beta} + \sum_{i=1}^p \phi_j \{g(y_{t-j}) - \mathbf{X}_{t-j} \boldsymbol{\beta}\} + \sum_{i=1}^q \theta_j \left\{g(y_{t-j}) - \eta_{t-j}\right\}, \quad (1.6)$$

where $t=1,\ldots,n$ is the time index; $\phi_j,\ j=1,\ldots,p$, are autoregressive coefficients; $\theta_j,\ j=1,\ldots,q$, are moving average coefficients, and p and q are the autoregressive and moving average orders, respectively. Model (1.6) is efficient for dealing with individual time series.

1.1.6 Summary

Notice that the issue of different reliability of individual measurements can be solved in models (1.2)–(1.6) by introducing pre-defined weights in the estimation process. An automatic tuning of weights for improved model performance is possible with a number of boosting algorithms, such as AdaBoost.M1 (Hastie et al., 2009).

Overall, model (1.5) is a powerful and flexible choice for a variety of applied problems, when data exhibit complex spatiotemporal dependence and do not adhere to commonly used distributions, such as normal or Poisson.

The challenges of using the above statistical models include the choice of predictors, their transformations, distribution of the response variable, and model specification, which can be attempted with a variety of criteria (for example, Akaike and Bayesian information criteria – AIC and BIC) ubiquitous in statistical literature. Machine learning approaches offer more flexibility by relaxing the assumptions about distributions and forms of relationships, and providing automated solutions for learning meta-features from large amounts of data. At the same time, the large number of tuning parameters that inhere in a machine learning (especially in deep learning) method and their ability of changing the output or extending the computing time dramatically put out a warning for cautious implementation and interpretation of those methods.

1.2 Data example

```
library(dplyr)
library(GGally)
library(plotly)
set.seed(123)
```

Select average water quality measurements in Chesapeake Bay for December 2010:

- Station: station at which the measurements were taken. There are 133 stations in the data file; at this time, we disregard the spatial patterns;
- DO: concentration of dissolved oxygen;
- CHLA: concentration of chlorophyll-a;
- SALINITY: water salinity;
- WTEMP: water temperature;
- TSS: concentration of total suspended solids;
- TN: concentration of total nitrogen;
- TP: concentration of total phosphorus.

Then try modeling TP with different methods.

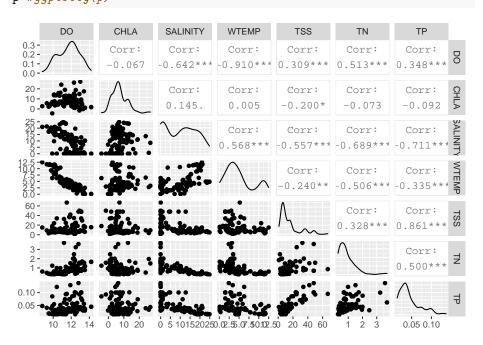
```
D <- read.csv("./data/CBmonthly.csv") %>%
    dplyr::filter(., Year == 2010 & Month == 12) %>%
```

```
dplyr::select(Station, DO, CHLA, SALINITY, WTEMP, TSS, TN, TP)
str(D)
```

```
##
   'data.frame':
                     133 obs. of 8 variables:
##
                     "CB1.1" "CB2.1" "CB2.2" "CB3.1" ...
    $ Station : chr
                     14.2 14.2 13.4 12.7 12.2 ...
              : num
    $ CHLA
                     1.78 1.78 1.07 1.87 2.56 ...
              : num
    $ SALINITY: num
                     0 0 0.9 3.12 5.63 ...
##
    $ WTEMP
                     0.1 0.1 0.6 0.9 1.6 ...
              : num
    $ TSS
              : num
                     15.6 15.6 16.2 18.4 12 ...
                     1.66 1.66 1.55 1.25 1.12 ...
##
     TN
              : num
    $
                     0.045 0.045 0.0403 0.0436 0.036 ...
              : num
```

Plot data

```
p <- ggpairs(D[,-1])
p #ggplotly(p)</pre>
```



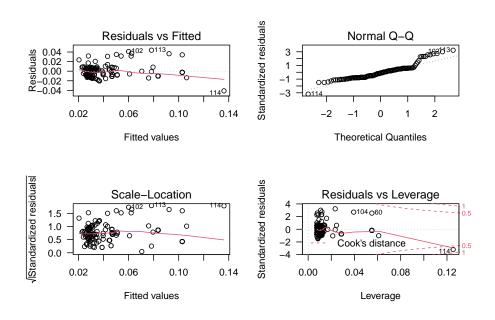
1.2.1 Simple linear regression

For the simplest model, select a variable with the strongest correlation with TP: it is TSS. Our simple linear regression model is

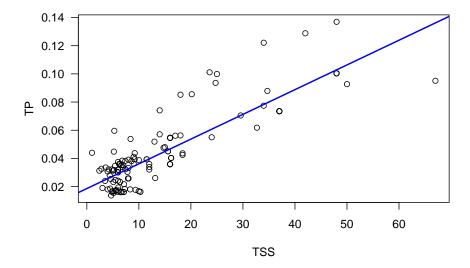
$$TP_i = \beta_0 + \beta_1 TSS_i + \epsilon_i,$$

where i = 1, ..., n (n = 133 is the sample size).

```
m1 \leftarrow lm(TP \sim TSS, data = D)
summary(m1)
##
## Call:
## lm(formula = TP ~ TSS, data = D)
## Residuals:
##
         Min
                    1Q
                           Median
                                         3Q
                                                  Max
## -0.041079 -0.010033 -0.001276 0.006457
                                            0.043831
##
## Coefficients:
                Estimate Std. Error t value Pr(>|t|)
##
## (Intercept) 1.860e-02 1.801e-03
                                       10.33
                                               <2e-16 ***
## TSS
               1.755e-03 9.059e-05
                                       19.37
                                               <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.01375 on 131 degrees of freedom
## Multiple R-squared: 0.7412, Adjusted R-squared: 0.7393
## F-statistic: 375.3 on 1 and 131 DF, p-value: < 2.2e-16
par(mfrow = c(2, 2))
plot(m1, las = 1)
```



```
plot(TP ~ TSS, data = D, las = 1)
abline(m1, lwd = 2, col = "blue")
```



The model clearly has problems.

1.2.2 Polynomial regression

Without modifying the response variable, apply a polynomial transformation to the explanatory variable, for example quadratic (informed by the plot). Our polynomial regression model is

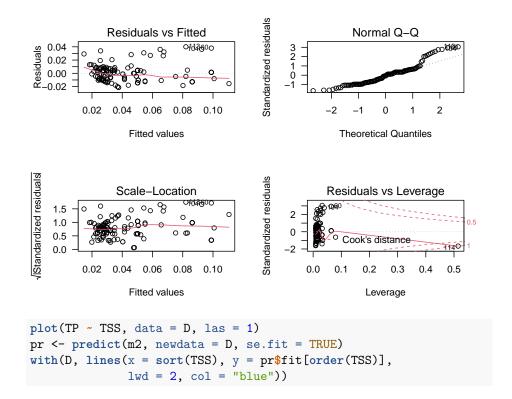
$$TP_i = \beta_0 + \beta_1 TSS_i + \beta_2 TSS_i^2 + \epsilon_i,$$

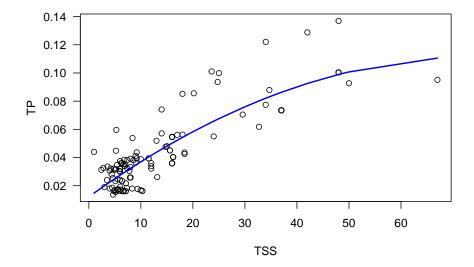
Use function poly to create orthogonal polynomials:

```
m2 <- lm(TP ~ poly(TSS, 2), data = D)
summary(m2)</pre>
```

```
##
## Call:
## lm(formula = TP ~ poly(TSS, 2), data = D)
##
## Residuals:
## Min 1Q Median 3Q Max
## -0.021327 -0.010286 -0.000931 0.005123 0.040019
##
```

```
## Coefficients:
##
                  Estimate Std. Error t value Pr(>|t|)
                  0.044747
                                        38.72 < 2e-16 ***
## (Intercept)
                             0.001156
## poly(TSS, 2)1 0.266399
                             0.013327
                                        19.99
                                              < 2e-16 ***
## poly(TSS, 2)2 -0.041043
                                        -3.08 0.00253 **
                             0.013327
## ---
## Signif. codes:
                  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.01333 on 130 degrees of freedom
## Multiple R-squared: 0.7588, Adjusted R-squared: 0.7551
## F-statistic: 204.5 on 2 and 130 DF, p-value: < 2.2e-16
par(mfrow = c(2, 2))
plot(m2, las = 1)
```

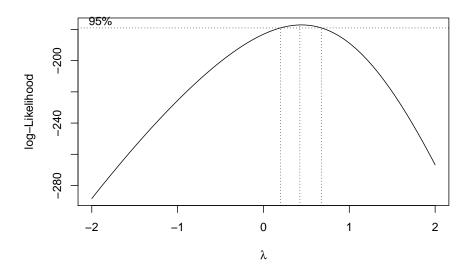




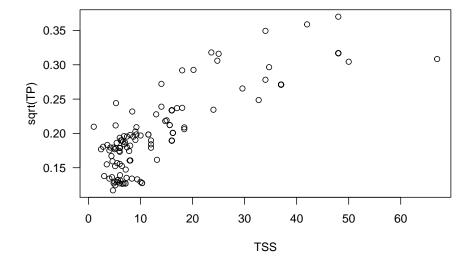
1.2.3 Power transformation

Apply Box–Cox method to select a power transformation for the response variable:

```
library(MASS)
boxcox(m1)
```



Check linearity after applying the transformation

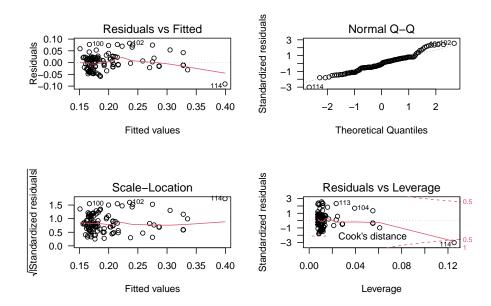


Hence, the model looks like

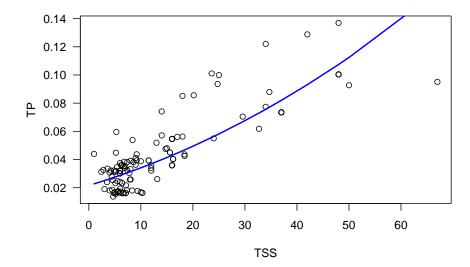
$$\sqrt{TP_i} = \beta_0 + \beta_1 TSS_i + \epsilon_i$$

```
m3 <- lm(sqrt(TP) ~ TSS, data = D)
summary(m3)
```

```
##
## Call:
## lm(formula = sqrt(TP) ~ TSS, data = D)
##
## Residuals:
##
        Min
                   1Q
                         Median
                                      3Q
                                               Max
## -0.090920 -0.017810 -0.002486 0.018862 0.082065
##
## Coefficients:
               Estimate Std. Error t value Pr(>|t|)
## (Intercept) 0.1470414 0.0042308 34.76 <2e-16 ***
              0.0037651 0.0002128 17.69 <2e-16 ***
## TSS
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 0.03231 on 131 degrees of freedom
## Multiple R-squared: 0.7049, Adjusted R-squared: 0.7027
## F-statistic: 313 on 1 and 131 DF, p-value: < 2.2e-16
par(mfrow = c(2, 2))
plot(m3, las = 1)
```



When plotting the fitted values, remember to back-transform

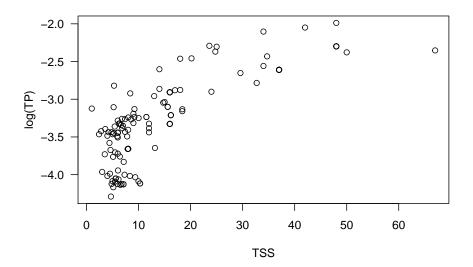


1.2.4 Generalized linear model (GLM)

Review the distribution of the response variable and select an appropriate one <code>?family</code>

Check linearity after applying the transformation (link function for the selected distribution)

```
plot(log(TP) ~ TSS, data = D, las = 1)
```



```
m4 <- glm(TP ~ TSS, data = D, family = Gamma(link = "log"))
summary(m4)
##</pre>
```

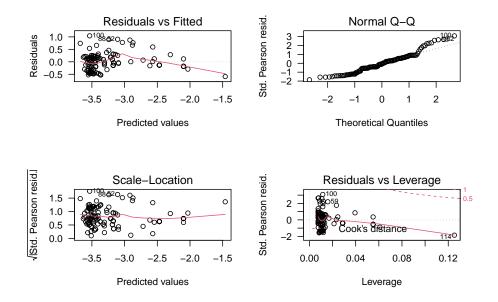
```
## Call:
## glm(formula = TP ~ TSS, family = Gamma(link = "log"), data = D)
## Deviance Residuals:
       Min
                  1Q
                        Median
## -0.77706 -0.20733 -0.01593
                                 0.17525
                                           0.80973
##
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -3.71136
                           0.04453
                                   -83.34
                                            <2e-16 ***
## TSS
               0.03359
                          0.00224
                                    15.00
                                            <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for Gamma family taken to be 0.1156311)
##
##
      Null deviance: 42.986 on 132 degrees of freedom
## Residual deviance: 15.270 on 131 degrees of freedom
## AIC: -771.27
##
## Number of Fisher Scoring iterations: 5
```

Hence, the model is

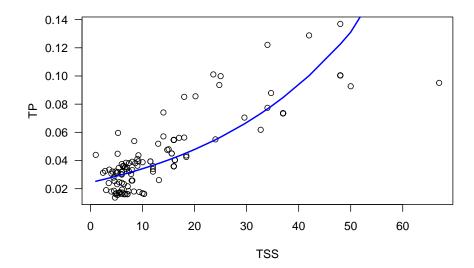
$$TP_i \sim Gamma$$

$$\ln(\mathbf{E}(TP_i)) = \beta_0 + \beta_1 TSS_i$$

```
par(mfrow = c(2, 2))
plot(m4, las = 1)
```



When plotting the fitted values, remember to back-transform



1.2.5 Generalized additive model (GAM)

```
library(mgcv)
m5 <- gam(TP ~ s(TSS), data = D, family = Gamma(link = log))
summary(m5)
##
## Family: Gamma
## Link function: log
## Formula:
## TP ~ s(TSS)
##
## Parametric coefficients:
##
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -3.22297
                          0.02675 -120.5
                                           <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Approximate significance of smooth terms:
           edf Ref.df
                          F p-value
## s(TSS) 5.597 6.614 43.63 <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

```
##
## R-sq.(adj) = 0.789 Deviance explained = 71.9%
## GCV = 0.10045 Scale est. = 0.095193 n = 133
```

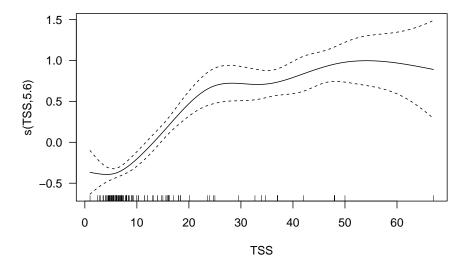
The model is

$$TP_i \sim Gamma$$

$$\ln(\mathrm{E}(TP_i)) = \beta_0 + f(TSS_i)$$

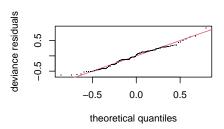
Visualize the smooth term. For identifiability, sum of the values of each curve, at the observed covariate values, must be zero.

$$plot(m5, las = 1)$$

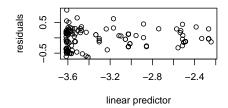


Diagnostics

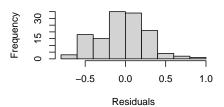
```
gam.check(m5)
```



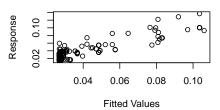
Resids vs. linear pred.



Histogram of residuals

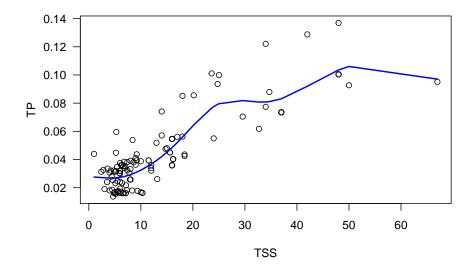


Response vs. Fitted Values



```
##
## Method: GCV
                 Optimizer: outer newton
## full convergence after 3 iterations.
## Gradient range [1.729043e-10,1.729043e-10]
## (score 0.1004541 & scale 0.09519291).
## Hessian positive definite, eigenvalue range [0.0008269258,0.0008269258].
## Model rank = 10 / 10
##
## Basis dimension (k) checking results. Low p-value (k-index<1) may
## indicate that k is too low, especially if edf is close to k'.
##
##
           k' edf k-index p-value
                     0.91
## s(TSS) 9.0 5.6
```

If family is not Gaussian (more specifically, if the link function is not identity), remember to back-transform



1.2.6 Generalized additive model for location scale and shape (GAMLSS)

Note that variance of residuals slightly increases with TSS. We can

- use generalized least squares (GLS) to transform the variables and stabilize the variance, or
- fit a separate model for variance, similar to the model for the mean.

Use the second approach in GAMLSS:

```
library(gamlss)
m6 <- gamlss(
   TP ~ pb(TSS)
   ,sigma.formula = ~TSS
   ,family = GA
   ,data = D
   #,control = gamlss.control(n.cyc = 100, c.crit = 0.9)
)

## GAMLSS-RS iteration 1: Global Deviance = -821.986
## GAMLSS-RS iteration 2: Global Deviance = -825.3166
## GAMLSS-RS iteration 3: Global Deviance = -825.8326
## GAMLSS-RS iteration 4: Global Deviance = -825.8686
## GAMLSS-RS iteration 5: Global Deviance = -825.8733
## GAMLSS-RS iteration 6: Global Deviance = -825.874</pre>
```

```
summary (m6)
## Family: c("GA", "Gamma")
##
## Call: gamlss(formula = TP ~ pb(TSS), sigma.formula = ~TSS,
##
    family = GA, data = D)
##
## Fitting method: RS()
## -----
## Mu link function: log
## Mu Coefficients:
          Estimate Std. Error t value Pr(>|t|)
## pb(TSS)
         0.03220
                   0.00112 28.75 <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## -----
## Sigma link function: log
## Sigma Coefficients:
           Estimate Std. Error t value Pr(>|t|)
                  0.092819 -9.926 < 2e-16 ***
## (Intercept) -0.921346
## TSS
          -0.023435
                  0.004775 -4.908 2.82e-06 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## -----
## NOTE: Additive smoothing terms exist in the formulas:
## i) Std. Error for smoothers are for the linear effect only.
## ii) Std. Error for the linear terms maybe are not accurate.
## -----
## No. of observations in the fit: 133
## Degrees of Freedom for the fit: 8.420713
      Residual Deg. of Freedom: 124.5793
##
##
                 at cycle: 6
##
## Global Deviance:
                 -825.874
          AIC:
                 -809.0326
                 -784.6938
##
          SBC:
```

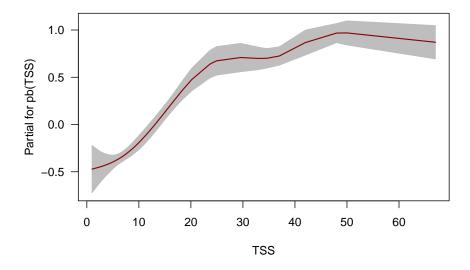
In this case, we model both parameters of the distribution:

```
TP_i \sim Gamma(\mu_i, \sigma_i)
```

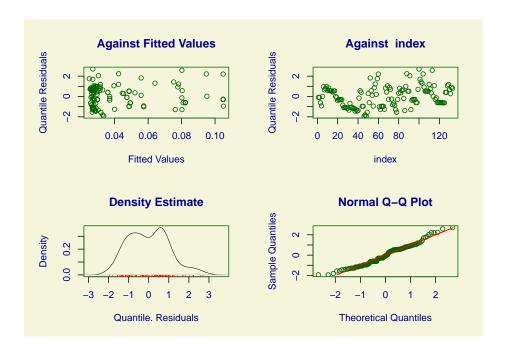
$$\ln(\mathrm{E}(TP_i)) = \ln(\mu_i) = \beta_0 + f(TSS_i)$$

$$\ln(\sigma_i) = c_0 + c_1 T S S_i$$

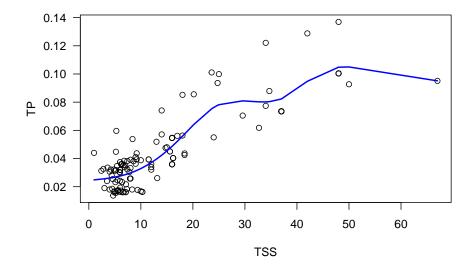
term.plot(m6, las = 1, se = TRUE, ylim = "common")



plot(m6)



```
***********************
##
##
        Summary of the Quantile Residuals
##
                                  -0.0008679401
                          mean
                                  1.007634
##
                      variance
##
               coef. of skewness
                                  0.3308549
               coef. of kurtosis
                                  2.612453
## Filliben correlation coefficient
                                  0.988048
## *************
plot(TP ~ TSS, data = D, las = 1)
pr <- predict(m6, type = "response")</pre>
with(D, lines(x = sort(TSS), y = pr[order(TSS)],
            lwd = 2, col = "blue"))
```



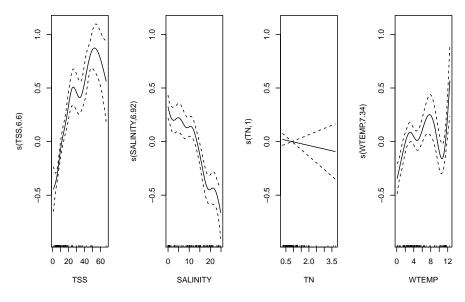
1.2.7 Next steps

We have considered several models for the pair TP \sim TSS, without considering other variables yet. Need to carefully select an appropriate distribution family for modeling.

When modeling with smoothers we should consider the issue of concurvity (an analogue of collinearity in linear models), when smooth transformations of predictors 'look alike.' There are functions to check concurvity in R.

```
m7 <- gam(TP ~ s(TSS) + s(SALINITY) + s(TN) + s(WTEMP),
data = D, family = Gamma(link = log))
summary(m7)
```

```
##
## Approximate significance of smooth terms:
                edf Ref.df
                                F p-value
              6.595 7.617 29.353 < 2e-16 ***
## s(TSS)
## s(SALINITY) 6.923 7.966 10.892 4.79e-12 ***
## s(TN)
              1.000
                    1.000 0.519
                                     0.473
## s(WTEMP)
              7.342 8.298 7.683 6.73e-08 ***
## ---
                 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Signif. codes:
##
## R-sq.(adj) = 0.886
                        Deviance explained = 92.4%
## GCV = 0.035873 Scale est. = 0.032206 n = 133
par(mfrow = c(1, 4))
plot(m7)
```



concurvity(m7)

```
## para s(TSS) s(SALINITY) s(TN) s(WTEMP)
## worst 2.255338e-24 0.8492033 0.9328362 0.9342809 0.8218917
## observed 2.255338e-24 0.6554349 0.9203188 0.7103660 0.3510102
## estimate 2.255338e-24 0.5150905 0.8471733 0.5209155 0.7415149
concurvity(m7, full = FALSE)$estimate
```

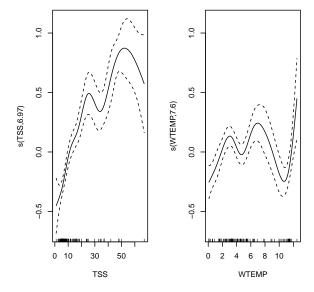
```
## para s(TSS) s(SALINITY) s(TN) s(WTEMP)
## para 1.000000e+00 1.696166e-27 1.054164e-28 2.357477e-28 6.180660e-28
```

```
## s(TSS) 7.907947e-25 1.000000e+00 4.507004e-01 2.590425e-01 1.895382e-01 ## s(SALINITY) 6.370609e-26 2.829094e-01 1.000000e+00 3.382813e-01 6.017203e-01 ## s(TN) 1.318787e-25 2.477700e-01 7.128446e-01 1.000000e+00 5.096872e-01 ## s(WTEMP) 4.200428e-25 2.441318e-01 4.495728e-01 2.178949e-01 1.000000e+00
```

Variable selection in GAM is more tedious than in linear models. A general recommendation for GAM is to do forward-selection: include only relevant meaningful variables, do not just throw everything into the model. Note that the model can hold a mix of smoothed and non-smoothed terms. For example, remove TN, do not smooth SALINITY:

```
## para s(TSS) s(WTEMP)
## para 1.000000e+00 1.696166e-27 6.180660e-28
## s(TSS) 7.944119e-25 1.0000000e+00 1.895382e-01
## s(WTEMP) 4.226487e-25 2.441318e-01 1.000000e+00
```

```
#gam.check(m8)
```



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