EMISSÃO DE CO_2 DO SOLO EM ÁREAS AGRÍCOLAS: ABORDAGEM EM APRENDIZADO DE MÁQUINA ESTATÍSTICO

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Objetivo

O objetivo do repositório `tese-fco2-ml-2023` é promover a transparência, a reprodutibilidade e a colaboração em pesquisa. Você é incentivado a explorar o código-fonte, utilizar os dados e contribuir com melhorias, se desejar. Sinta-se à vontade para entrar em contato caso tenha alguma dúvida ou precise de mais informações sobre minha pesquisa.

Contribuições

Contribuições são bem-vindas! Se você deseja colaborar com melhorias nos códigos, correções de erros ou qualquer outro aprimoramento, sinta-se à vontade para abrir uma solicitação de `pull request`.

Licença

Base de dados

Apresentação do pacote `fco2r` construído para facilitar a divulgação e análise dos resultados obtidos ao longo de mais de 20 anos de ensaios em campo. Este pacote, permite a visualização dos dados, a execução de análises estatísticas avançadas e a geração de gráficos interativos para tornar os resultados mais acessíveis e compreensíveis para a comunidade científica.

Instalação

Você pode instalar uma versão de desenvolvimento do pacote `fco2r` a partir do GitHub (https://github.com/) com os seguintes comandos:

```
# install.packages("devtools")
# devtools::install_github("arpanosso/fco2r")
```

Problemas na instalação:

Possíveis problemas na instalação do pacote podem ser sanados com os seguintes comandos:

```
# Sys.getenv("GITHUB_PAT")
# Sys.unsetenv("GITHUB_PAT")
# Sys.getenv("GITHUB_PAT")
```

Carregando os pacotes

```
library(fco2r)
library(tidyverse)
library(patchwork)
library(ggspatial)
library(readxl)
library(skimr)
library(tidymodels)
library(ISLR)
library(modeldata)
library(vip)
library(ggpubr)
```

Conhecendo a base de dados de emissão de CO_2 do solo

Base proveniente de ensaios de campo.

```
help(data_fco2)
glimpse(data_fco2)
#> Rows: 15,397
#> Columns: 39
#> $ experimento       <chr> "Espacial", "Espacial", "Espacial", "Espacial", "Esp…
#> $ data              <date> 2001-07-10, 2001-07-10, 2001-07-10, 2001-07-10, 200…
#> $ manejo            <chr> "convencional", "convencional", "convencional", "con…
#> $ tratamento        <chr> "AD_GN", "AD_GN", "AD_GN", "AD_GN", "AD_GN", "AD_GN"…
#> $ revolvimento_solo <lgl> FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FALSE, FAL…
#> $ data_preparo      <date> 2001-07-01, 2001-07-01, 2001-07-01, 2001-07-01, 200…
#> $ conversao         <date> 1970-01-01, 1970-01-01, 1970-01-01, 1970-01-01, 197…
#> $ cobertura         <lgl> TRUE, TRUE, TRUE, TRUE, TRUE, TRUE, TRUE, TRUE, TRUE…
#> $ cultura           <chr> "milho_soja", "milho_soja", "milho_soja", "milho_soj…
#> $ x                 <dbl> 0, 40, 80, 10, 25, 40, 55, 70, 20, 40, 60, 10, 70, 3…
#> $ y                 <dbl> 0, 0, 0, 10, 10, 10, 10, 10, 20, 20, 20, 25, 25, 30,…
#> $ longitude_muni    <dbl> 782062.7, 782062.7, 782062.7, 782062.7, 782062.7, 78…
#> $ latitude_muni     <dbl> 7647674, 7647674, 7647674, 7647674, 7647674, 7647674…
#> $ estado            <chr> "SP", "SP", "SP", "SP", "SP", "SP", "SP", "SP", "SP"…
#> $ municipio         <chr> "Jaboticabal", "Jaboticabal", "Jaboticabal", "Jaboti…
#> $ ID                <int> 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 1…
#> $ prof              <chr> "0-0.1", "0-0.1", "0-0.1", "0-0.1", "0-0.1", "0-0.1"…
#> $ FCO2              <dbl> 1.080, 0.825, 1.950, 0.534, 0.893, 0.840, 1.110, 1.8…
#> $ Ts                <dbl> 18.73, 18.40, 19.20, 18.28, 18.35, 18.47, 19.10, 18.…
#> $ Us                <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, …
#> $ pH                <dbl> 5.1, 5.1, 5.8, 5.3, 5.5, 5.7, 5.6, 6.4, 5.3, 5.8, 5.…
#> $ MO                <dbl> 20, 24, 25, 23, 23, 21, 26, 23, 25, 24, 26, 20, 25, …
#> $ P                 <dbl> 46, 26, 46, 78, 60, 46, 55, 92, 55, 60, 48, 71, 125,…
#> $ K                 <dbl> 2.4, 2.2, 5.3, 3.6, 3.4, 2.9, 4.0, 2.3, 3.3, 3.6, 4.…
#> $ Ca                <dbl> 25, 30, 41, 27, 33, 38, 35, 94, 29, 36, 37, 29, 50, …
#> $ Mg                <dbl> 11, 11, 25, 11, 15, 20, 16, 65, 11, 17, 15, 11, 30, …
#> $ H_Al              <dbl> 31, 31, 22, 28, 27, 22, 22, 12, 31, 28, 28, 31, 18, …
#> $ SB                <dbl> 38.4, 43.2, 71.3, 41.6, 50.6, 60.9, 55.0, 161.3, 43.…
#> $ CTC               <dbl> 69.4, 74.2, 93.3, 69.6, 77.9, 82.9, 77.0, 173.3, 74.…
#> $ V                 <dbl> 55, 58, 76, 60, 65, 73, 71, 93, 58, 67, 67, 58, 82, …
#> $ Ds                <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, …
#> $ Macro             <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, …
#> $ Micro             <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, …
#> $ VTP               <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, …
#> $ PLA               <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, …
#> $ AT                <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, …
#> $ SILTE             <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, …
#> $ ARG               <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, …
#> $ HLIFS             <dbl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, …
```

Vamos conhecer, um pouco mais a nossa base de dados.

```
skimr::skim(data_fco2)
```

Name	data_fco2
Number of rows	15397
Number of columns	39
_______________________	
Column type frequency:	
character	7
Date	3
logical	2
numeric	27
________________________	
Group variables	None

Data summary

Variable type: character

skim_variable	n_missing	complete_rate	min	max	empty	n_unique	whitespace
experimento	0	1	8	8	0	2	0
manejo	0	1	6	15	0	10	0
tratamento	0	1	2	10	0	21	0

skim_variable	n_missing	complete_rate	min	max	empty	n_unique	whitespace
cultura	0	1	4	14	0	11	0
estado	0	1	2	2	0	2	0
municipio	0	1	7	20	0	6	0
prof	0	1	5	7	0	2	0

Variable type: Date

skim_variable	n_missing	complete_rate	min	max	median	n_unique
data	0	1	2001-07-10	2019-12-01	2014-07-12	205
data_preparo	0	1	1986-03-01	2019-04-01	2002-01-01	14
conversao	0	1	1970-01-01	2009-07-03	1986-03-01	11

Variable type: logical

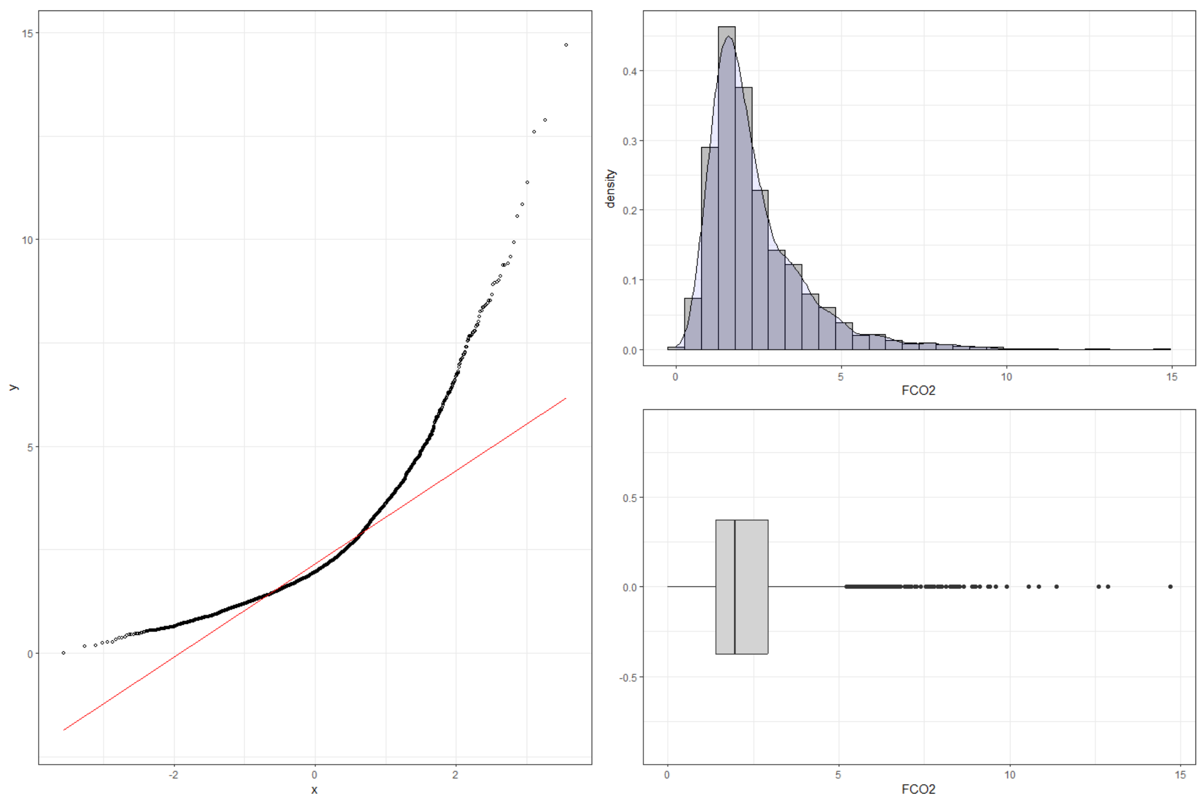
skim_variable	n_missing	complete_rate	mean	count
revolvimento_solo	0	1	0	FAL: 15397
cobertura	0	1	1	TRU: 15397

Variable type: numeric

skim_variable	n_missing	complete_rate	mean	sd	p0	p25	p50	p75	p100	hist
x	0	1.00	1392083.56	2923710.70	0.00	0.00	30.00	100.00	7749472.16	
y	0	1.00	495854.97	1722529.75	0.00	0.00	27.00	80.00	7630525.47	
longitude_muni	0	1.00	1067926.05	1796771.47	456798.63	458447.46	458447.46	792043.56	7638196.06	
latitude_muni	0	1.00	7231328.21	1754220.76	795907.06	7635356.70	7749398.84	7749821.85	7758831.37	
ID	0	1.00	40.52	31.52	1.00	13.00	35.00	60.00	141.00	
FCO2	110	0.99	2.78	2.08	-3.42	1.30	2.16	3.75	46.93	
Ts	317	0.98	21.84	6.76	1.00	19.33	22.50	26.15	195.63	
Us	1754	0.89	16.31	8.93	0.00	10.00	14.06	22.00	89.00	
pH	2802	0.82	4.64	1.13	3.50	4.00	4.50	5.15	52.00	
MO	1355	0.91	21.59	12.60	1.35	12.00	23.00	29.00	61.26	
P	1355	0.91	20.95	24.74	1.00	6.00	15.48	27.36	253.00	
K	1348	0.91	2.40	2.21	0.03	0.90	1.70	3.40	34.00	
Ca	1376	0.91	17.20	14.57	1.10	6.00	11.00	26.00	94.00	
Mg	1376	0.91	10.13	5.65	0.32	7.00	10.00	13.00	65.00	
H_Al	1362	0.91	46.89	29.38	0.00	26.00	42.29	72.00	121.00	
SB	1376	0.91	29.69	20.10	1.54	15.60	23.80	42.00	161.30	
CTC	1369	0.91	77.10	32.99	4.62	59.23	83.40	103.20	173.30	
V	1383	0.91	41.68	20.05	4.96	22.00	43.00	58.00	100.00	
Ds	3284	0.79	1.38	0.17	0.88	1.24	1.38	1.52	1.86	
Macro	3277	0.79	8.55	7.85	-45.30	0.15	8.13	13.64	49.77	
Micro	3298	0.79	25.30	17.13	0.07	0.37	33.86	38.30	52.42	
VTP	3298	0.79	42.34	15.65	-4.68	40.81	46.25	51.32	87.80	
PLA	3438	0.78	29.57	11.80	-47.30	21.27	32.41	38.15	79.80	
AT	8083	0.48	1013.33	1358.81	11.72	236.00	593.62	816.00	4542.73	
SILTE	8048	0.48	229.26	336.37	1.26	50.87	73.65	188.00	1395.00	
ARG	8055	0.48	995.41	1560.32	27.19	173.27	403.69	609.50	5244.76	
HLIFS	10872	0.29	14590.11	17253.55	158.39	1110.15	2409.80	29707.78	84692.90	

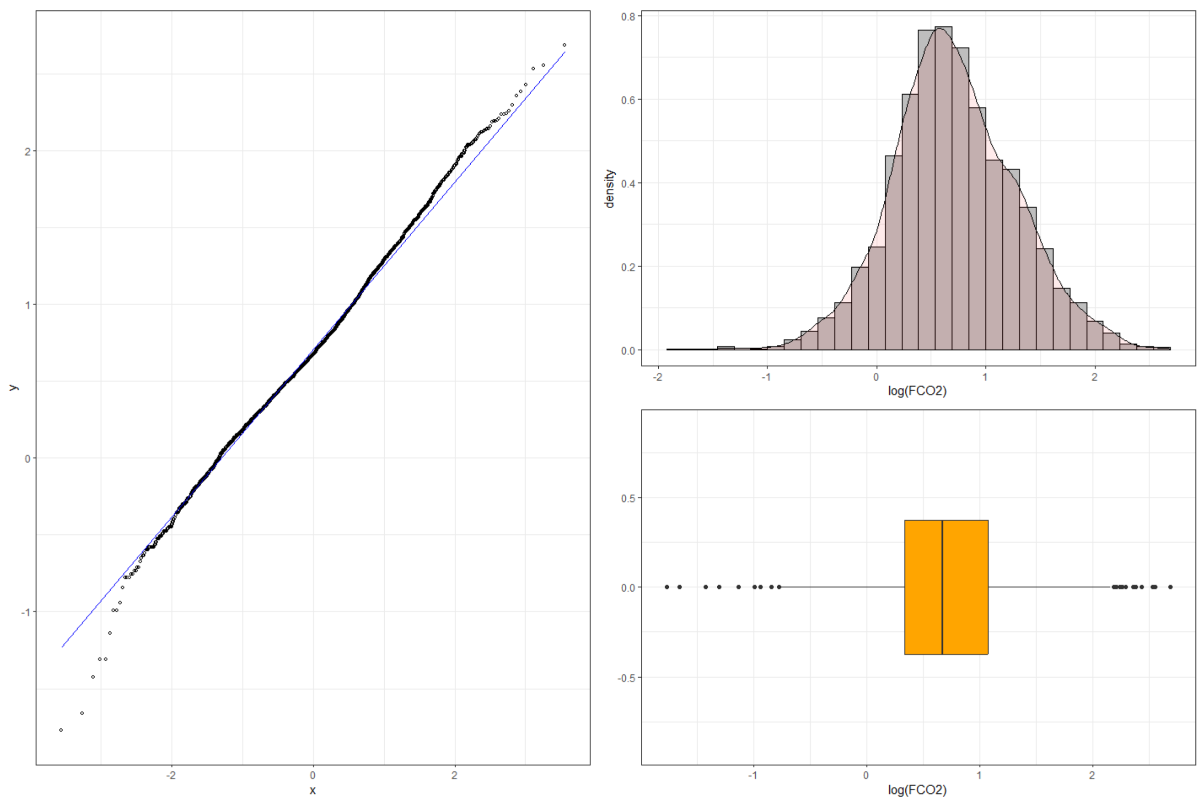
Alguns gráficos a respeito de nossa variável alvo, emissão de CO_2 do solo (FCO_2).

```
theme_set(theme_bw())
fco2_histograma <- data_fco2 %>%
  drop_na() %>%
  ggplot(aes(x=FCO2, y=..density..)) +
  geom_histogram(col="black",fill="gray") +
  geom_density(fill="blue",alpha=.08)

fco2_boxplot <- data_fco2 %>%
  drop_na() %>%
  ggplot(aes(x=FCO2)) +
  geom_boxplot(fill="lightgray") +
  coord_cartesian(ylim=c(-.9,.9))

fco2_qqplot <- data_fco2 %>%
  drop_na() %>%
  ggplot(aes(sample=FCO2)) +
  stat_qq(shape=1,size=1,color="black")+
  stat_qq_line(col="red")

fco2_qqplot | (fco2_histograma)/(fco2_boxplot)
```



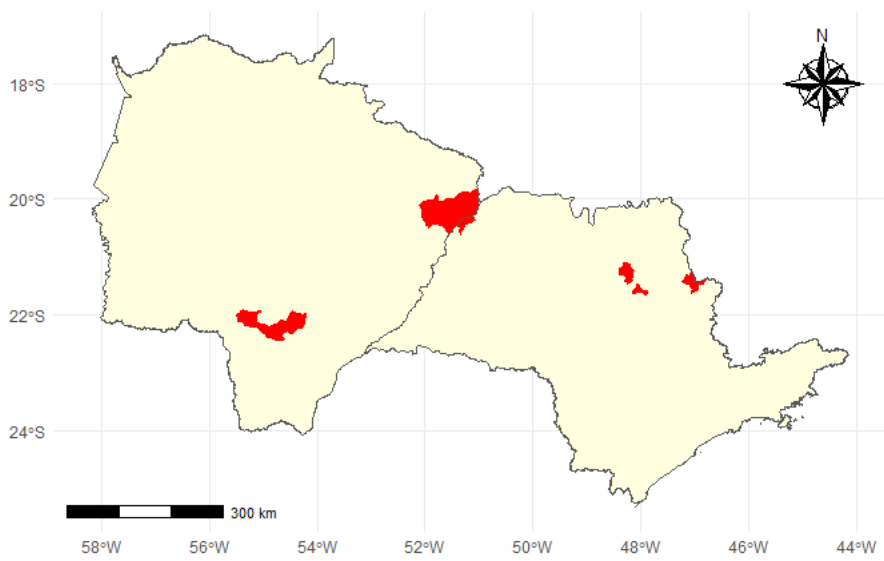
Aplicando a transformação logarítmica nos dados de FCO_2

```
ggplot2::theme_set(theme_bw())

fco2_histograma <- data_fco2 %>%
  drop_na() %>%
  ggplot(aes(x=log(FCO2), y=..density..)) +
  geom_histogram(col="black",fill="gray") +
  geom_density(fill="red",alpha=.08)

fco2_boxplot <- data_fco2 %>%
  drop_na() %>%
  ggplot(aes(x=log(FCO2))) +
  geom_boxplot(fill="orange") +
  coord_cartesian(ylim=c(-.9,.9))

fco2_qqplot <- data_fco2 %>%
  drop_na() %>%
  ggplot(aes(sample=log(FCO2))) +
  stat_qq(shape=1,size=1,color="black")+
  stat_qq_line(col="blue")

fco2_qqplot | (fco2_histograma)/(fco2_boxplot)
```




```
# brasil_geobr <- geobr::read_country()
# estados <- read_state(code_state = "all")
# write_rds(estados,"data/estados.rds")
# write_rds(brasil_geobr,"data/brasil_geobr.rds")
estados <- read_rds("data/estados.rds")
```

```r
# muni <- read_municipality()
# write_rds(muni,"data/municipios.rds")
muni <- read_rds("data/municipios.rds")

sp <- muni %>%
  filter(abbrev_state == "SP")

ms <- muni %>%
  filter(abbrev_state == "MS")

sp_ms <- muni %>%
  filter(abbrev_state == "SP" | abbrev_state == "MS")

fsp<-if_else(sp$name_muni == "Jaboticabal" |
             sp$name_muni == "Guariba" |
             sp$name_muni == "Padrópolis" |
             sp$name_muni == "Rincão"|
             sp$name_muni == "Mococa"|
             sp$name_muni == "Ilha Solteira"
             ,"red","lightyellow")

fms<-if_else(ms$name_muni == "Aparecida Do Taboado" |
             ms$name_muni == "Selvíria"|
             ms$name_muni == "Dourados"
             ,"red","lightyellow")

sp_ <- estados %>%
      filter(abbrev_state == "SP")

ms_ <- estados %>%
      filter(abbrev_state == "MS")

ggplot(sp_ms) +
  geom_sf(fill="lightyellow")+
  theme_minimal() +
  annotation_scale(location="bl")+
  annotation_north_arrow(location="tr",
                         style = north_arrow_nautical(),
                         width = unit(2,"cm"),
                         height = unit(2,"cm")) +
  geom_sf(data= sp, fill=fsp,col=fsp) +
  geom_sf(data=sp_,fill="transparent") +
  geom_sf(data= ms, fill=fms,col=fms) +
  geom_sf(data=ms_,fill="transparent")
```



Conhecendo a base de dados de concentração de CO_2 atmosférico, oriundo do sensor NASA-OCO2.

```
help(oco2_br)
glimpse(oco2_br)
#> Rows: 37,387
#> Columns: 18
#> $ longitude                                               <dbl> -70.5, -…
#> $ longitude_bnds                                          <chr> "-71.0:-…
#> $ latitude                                                <dbl> -5.5, -4…
#> $ latitude_bnds                                           <chr> "-6.0:-5…
#> $ time_yyyymmddhhmmss                                     <dbl> 2.014091…
#> $ time_bnds_yyyymmddhhmmss                                <chr> "2014090…
#> $ altitude_km                                             <dbl> 3307.8, …
#> $ alt_bnds_km                                             <chr> "0.0:661…
#> $ fluorescence_radiance_757nm_uncert_idp_ph_sec_1_m_2_sr_1_um_1 <dbl> 7.272876…
#> $ fluorescence_radiance_757nm_idp_ph_sec_1_m_2_sr_1_um_1       <dbl> 2.537127…
#> $ xco2_moles_mole_1                                       <dbl> 0.000394…
#> $ aerosol_total_aod                                       <dbl> 0.148579…
#> $ fluorescence_offset_relative_771nm_idp                  <dbl> 0.016753…
#> $ fluorescence_at_reference_ph_sec_1_m_2_sr_1_um_1        <dbl> 2.615319…
#> $ fluorescence_radiance_771nm_idp_ph_sec_1_m_2_sr_1_um_1       <dbl> 3.088582…
#> $ fluorescence_offset_relative_757nm_idp                  <dbl> 0.013969…
#> $ fluorescence_radiance_771nm_uncert_idp_ph_sec_1_m_2_sr_1_um_1 <dbl> 5.577878…
#> $ XCO2                                                    <dbl> 387.2781…
```

Breve resumo do banco de dados de X_{CO2}

```
skimr::skim(oco2_br)
```

Name	oco2_br
Number of rows	37387
Number of columns	18
_______________________	
Column type frequency:	
character	4
numeric	14
________________________	
Group variables	None

Data summary

Variable type: character

skim_variable	n_missing	complete_rate	min	max	empty	n_unique	whitespace
longitude_bnds	0	1	11	11	0	39	0
latitude_bnds	0	1	7	11	0	38	0
time_bnds_yyyymmddhhmmss	0	1	29	29	0	1765	0
alt_bnds_km	0	1	11	20	0	64	0

Variable type: numeric

skim_variable	n_missing	complete_rate	mean	sd	p0	
longitude	0	1	-5.120000e+01	8.280000e+00	-7.350000e+01	-5.65000
latitude	0	1	-1.179000e+01	7.850000e+00	-3.250000e+01	-1.75000
time_yyyymmddhhmmss	0	1	2.016952e+13	1.564571e+10	2.014091e+13	2.01602
altitude_km	0	1	3.123200e+03	1.108800e+02	2.555700e+03	3.05635
fluorescence_radiance_757nm_uncert_idp_ph_sec_1_m_2_sr_1_um_1	0	1	8.520719e+17	5.599367e+18	-9.999990e+05	6.32325
fluorescence_radiance_757nm_idp_ph_sec_1_m_2_sr_1_um_1	0	1	-1.358150e+18	1.946775e+20	-3.400736e+22	7.73515
xco2_moles_mole_1	0	1	0.000000e+00	0.000000e+00	0.000000e+00	0.00000
aerosol_total_aod	0	1	4.828100e+02	7.848572e+04	2.000000e-02	1.10000
fluorescence_offset_relative_771nm_idp	0	1	-4.814400e+02	2.193698e+04	-9.999990e+05	1.00000

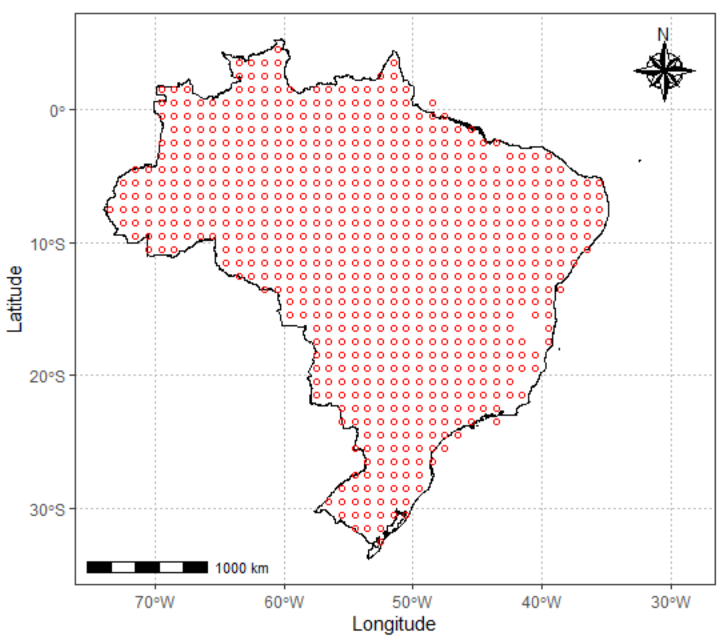
skim_variable	n_missing	complete_rate	mean	sd	p0	
fluorescence_at_reference_ph_sec_1_m_2_sr_1_um_1	0	1	1.296932e+18	2.245185e+18	-8.394901e+19	2.01456
fluorescence_radiance_771nm_idp_ph_sec_1_m_2_sr_1_um_1	0	1	1.904438e+18	2.236381e+18	-8.453983e+19	9.6947
fluorescence_offset_relative_757nm_idp	0	1	-3.744400e+02	1.934763e+04	-9.999990e+05	1.0000
fluorescence_radiance_771nm_uncert_idp_ph_sec_1_m_2_sr_1_um_1	0	1	5.235574e+17	7.580471e+16	-9.999990e+05	4.6954
XCO2	0	1	3.858900e+02	3.120000e+00	3.383400e+02	3.8441

Manipulando a base `oco2_br` para criação das variáveis temporais e ajuste de unidade de xco2.

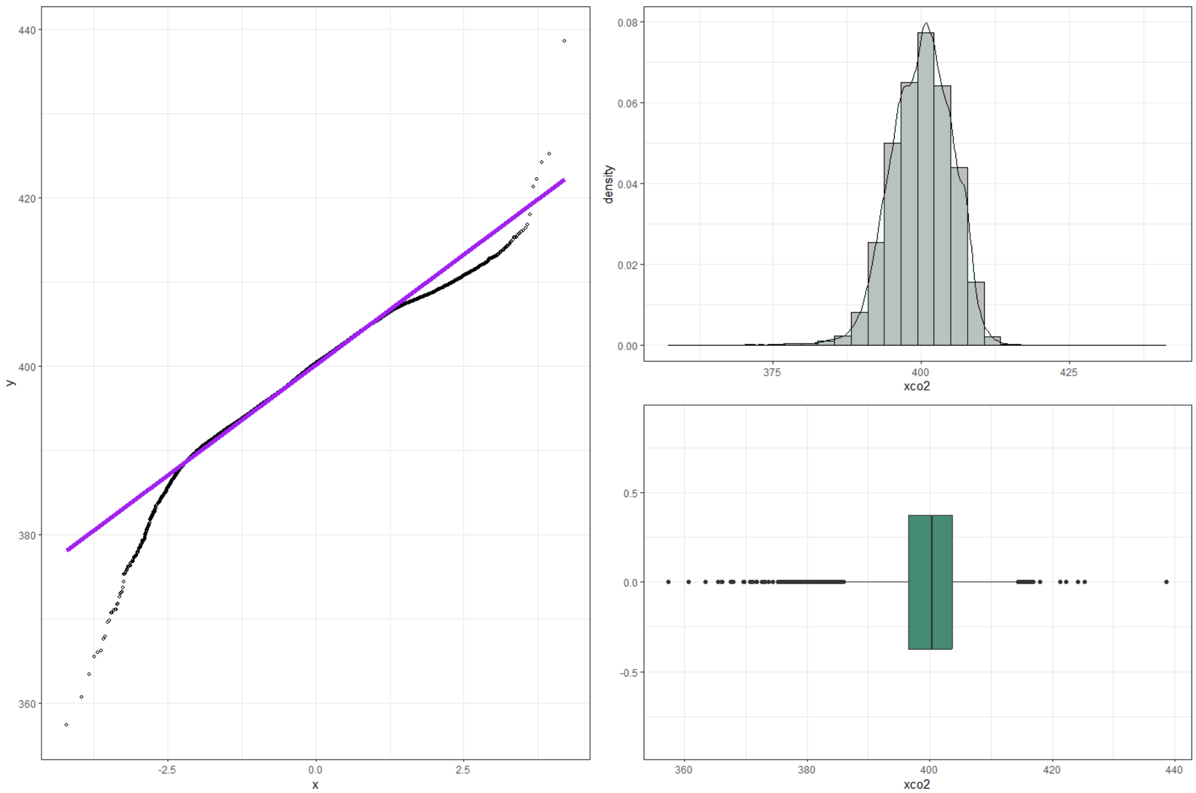
```
oco2_br <- oco2_br  %>%
        mutate(
           xco2 = xco2_moles_mole_1*1e06,
           data = ymd_hms(time_yyyymmddhhmmss),
           ano = year(data),
           mes = month(data),
           dia = day(data),
           dia_semana = wday(data))
```

Mapa das leituras do satélite OCO2-NASA

```
source("R/graficos.R")
brasil_geobr <- read_rds("data/brasil_geobr.rds")
brasil_geobr %>%
  ggplot() +
  geom_sf(fill="white", color="black",
          size=.15, show.legend = FALSE) +
  tema_mapa() +
  geom_point(data=oco2_br %>%
                        sample_n(20000) ,
             aes(x=longitude,y=latitude),
             shape=1,
             col="red",
             alpha=01)+
  labs(x="Longitude",y="Latitude")
```

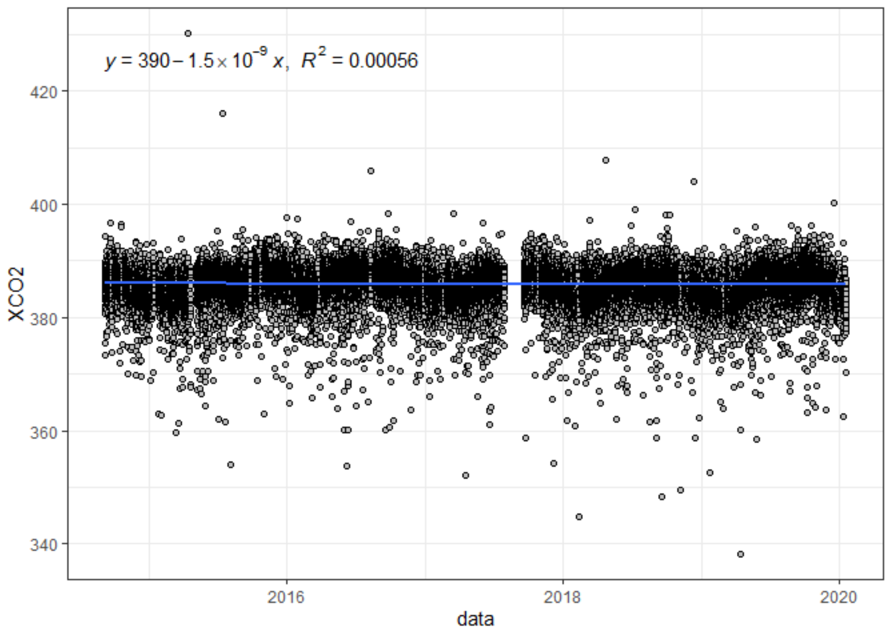


```
xco2_histograma <- oco2_br %>%
  drop_na() %>%
  ggplot(aes(x=xco2, y=..density..)) +
  geom_histogram(col="black",fill="gray") +
  geom_density(fill="aquamarine2",alpha=.08)

xco2_boxplot <- oco2_br %>%
  drop_na() %>%
  ggplot(aes(x=xco2)) +
  geom_boxplot(fill="aquamarine4") +
  coord_cartesian(ylim=c(-.9,.9))

xco2_qqplot <- oco2_br %>%
  drop_na() %>%
  ggplot(aes(sample=xco2)) +
  stat_qq(shape=1,size=1,color="black")+
  stat_qq_line(col="purple",lwd=2)

xco2_qqplot | (xco2_histograma)/(xco2_boxplot)
```

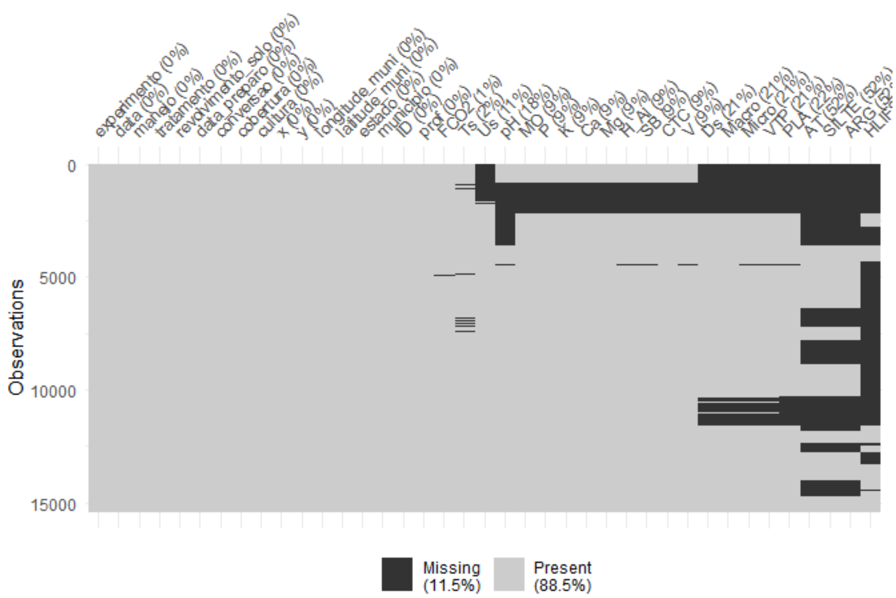



```
# Definindo o plano de multisession
future::plan("multisession")
```

```
oco2_br  %>%
  ggplot(aes(x=data,y=XCO2)) +
  geom_point(shape=21,color="black",fill="gray") +
  geom_smooth(method = "lm") +
  stat_regline_equation(ggplot2::aes(
  label =  paste(..eq.label.., ..rr.label.., sep = "*plain(\",\")~~")))
```




```
visdat::vis_miss(data_fco2)
```



Listando as datas dos arquivos

```
lista_data_fco2 <- unique(data_fco2$data)
lista_data_oco2 <- unique(oco2_br$data)
datas_fco2 <- paste0(lubridate::year(lista_data_fco2),"-",lubridate::month(lista_data_fco2)) %>% unique()

datas_oco2 <- paste0(lubridate::year(lista_data_oco2),"-",lubridate::month(lista_data_oco2)) %>% unique()
datas <- datas_fco2[datas_fco2 %in% datas_oco2]
```

Chaves para mesclagem

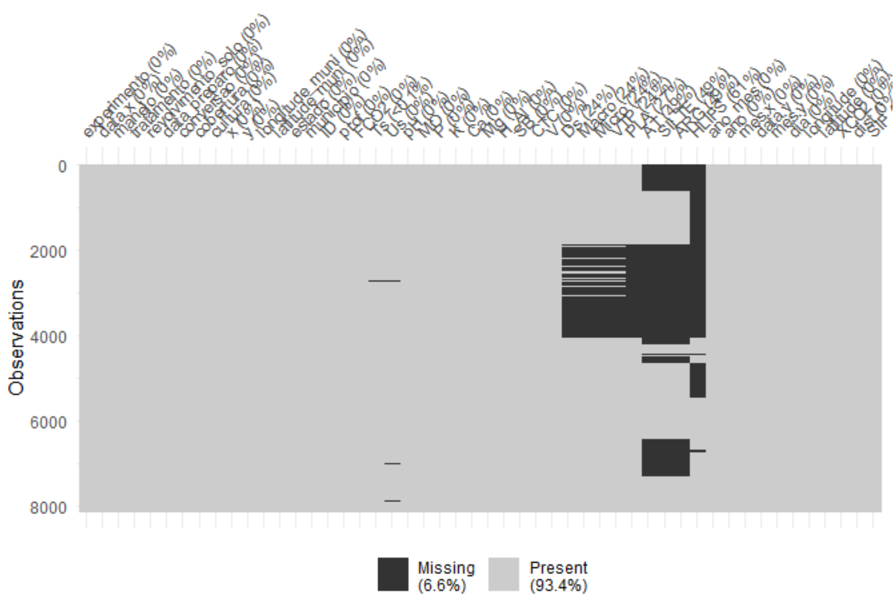
```
fco2 <- data_fco2 %>%
  mutate(ano_mes = paste0(lubridate::year(data),"-",lubridate::month(data))) %>%
  dplyr::filter(ano_mes %in% datas)

xco2 <- oco2_br %>%
  mutate(ano_mes=paste0(ano,"-",mes)) %>%
  dplyr::filter(ano_mes %in% datas)
```

Coordenadas das cidades

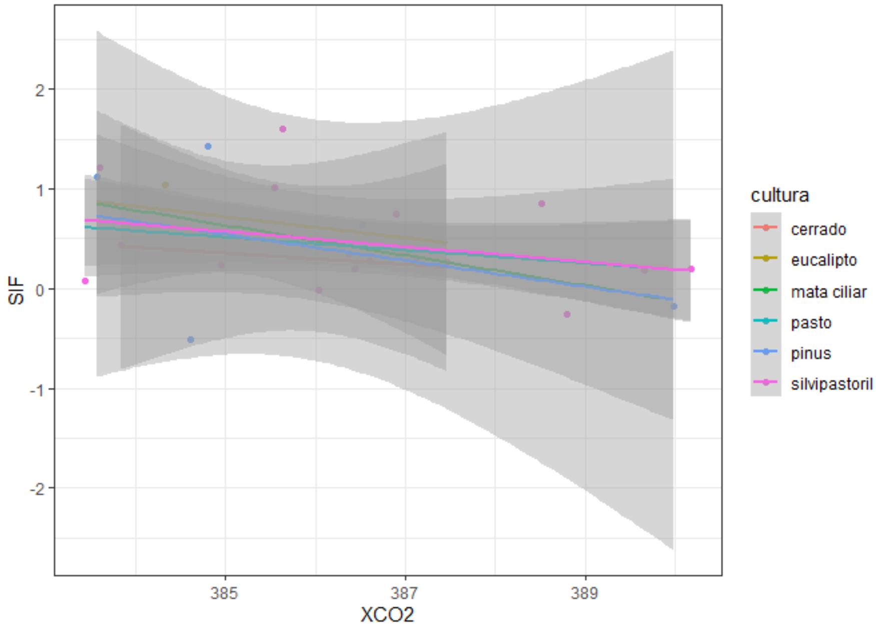
```r
unique(xco2$ano_mes)[unique(xco2$ano_mes) %>% order()] ==
unique(fco2$ano_mes)[unique(fco2$ano_mes) %>% order()]
#>  [1] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
#> [16] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
```

```r
data_set <- left_join(fco2 %>%
            mutate(ano = lubridate::year(data),
                   mes = lubridate::month(data)
                   ),
          xco2 %>%
            select(data,mes,dia,longitude,latitude,XCO2,fluorescence_radiance_757nm_idp_ph_sec_1_m_2_sr_1_um_1,fl
uorescence_radiance_771nm_idp_ph_sec_1_m_2_sr_1_um_1, ano_mes), by = "ano_mes") %>%
  mutate(dist = sqrt((longitude-(-51.423519))^2+(latitude-(-20.362911))^2),
         SIF = (fluorescence_radiance_757nm_idp_ph_sec_1_m_2_sr_1_um_1*2.6250912*10^(-19)  + 1.5*fluorescence_rad
iance_771nm_idp_ph_sec_1_m_2_sr_1_um_1* 2.57743*10^(-19))/2)


data_set<-data_set %>%
  select(-fluorescence_radiance_757nm_idp_ph_sec_1_m_2_sr_1_um_1, -fluorescence_radiance_771nm_idp_ph_sec_1_m_2_s
r_1_um_1 )  %>%
  filter(dist <= .16, FCO2 <= 30 )
```

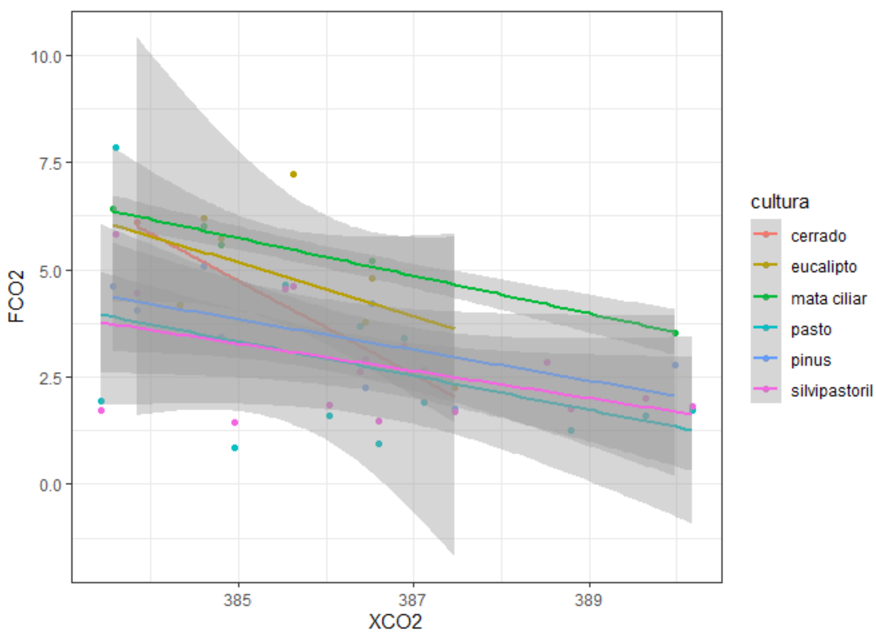
```r
visdat::vis_miss(data_set)
```



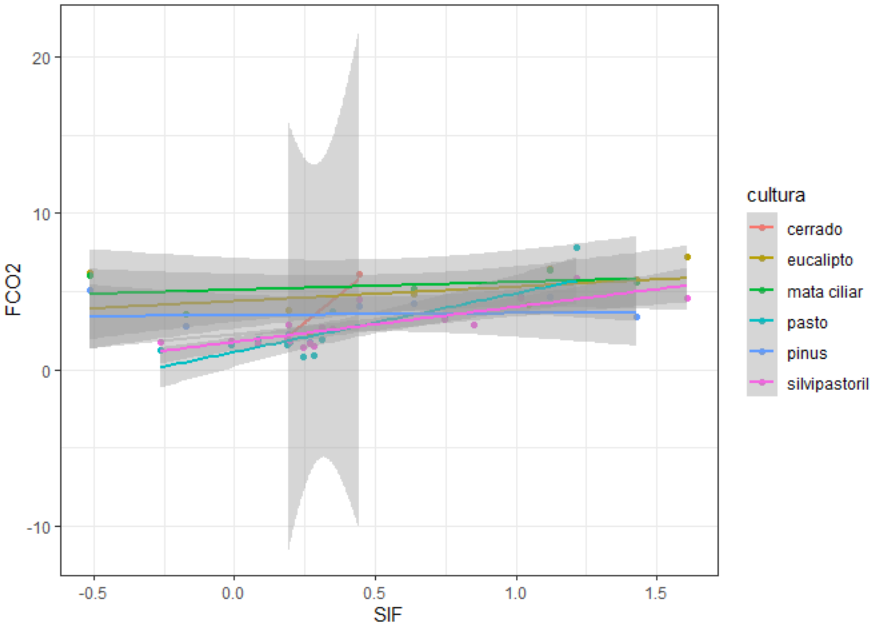

```r
tab_medias <- data_set %>%
  # mutate(SIF = ifelse(SIF <=0, mean(data_set$SIF, na.rm=TRUE),SIF)) %>%
  group_by(ano_mes, cultura) %>%
  summarise(FCO2 = mean(FCO2, na.rm=TRUE),
            XCO2 = mean(XCO2, na.rm=TRUE),
            SIF = mean(SIF, na.rm=TRUE))

tab_medias %>%
  ggplot(aes(x=XCO2, y=SIF,color=cultura)) +
  geom_point()+
  geom_smooth(method = "lm")+
  theme_bw()
```




```
tab_medias %>%
  ggplot(aes(x=XCO2, y=FCO2,col=cultura)) +
  geom_point()+
  geom_smooth(method = "lm")+
  theme_bw()
```



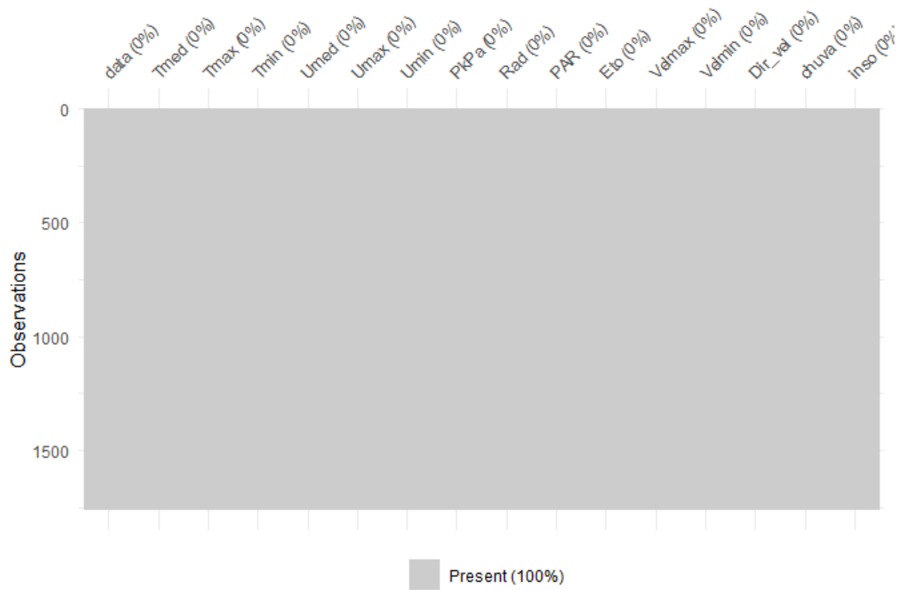

```
tab_medias %>%
  ggplot(aes(y=FCO2, x=SIF, color=cultura)) +
  geom_point()+
  geom_smooth(method = "lm") +
  theme_bw()
```




```
data_set_temporal <- data_set %>%
  filter(experimento == "Temporal")

data_set_espacial <- data_set %>%
  filter(experimento == "Espacial")
```

Carregando dados Meteorológicos de Ilha Solteira

```
dados_estacao <- read_excel("data-raw/xlsx/estacao_meteorologia_ilha_solteira.xlsx", na = "NA")
glimpse(dados_estacao)
#> Rows: 1,826
#> Columns: 16
#> $ data    <dttm> 2015-01-01, 2015-01-02, 2015-01-03, 2015-01-04, 2015-01-05, 2…
#> $ Tmed    <dbl> 30.5, 30.0, 26.8, 27.1, 27.0, 27.6, 30.2, 28.2, 28.5, 29.9, 30…
#> $ Tmax    <dbl> 36.5, 36.7, 35.7, 34.3, 33.2, 36.4, 37.2, 32.4, 37.1, 38.1, 38…
#> $ Tmin    <dbl> 24.6, 24.5, 22.9, 22.7, 22.3, 22.8, 22.7, 24.0, 23.0, 23.3, 24…
#> $ Umed    <dbl> 66.6, 70.4, 82.7, 76.8, 81.6, 75.5, 65.8, 70.0, 72.9, 67.6, 66…
#> $ Umax    <dbl> 89.6, 93.6, 99.7, 95.0, 98.3, 96.1, 99.2, 83.4, 90.7, 97.4, 90…
#> $ Umin    <dbl> 42.0, 44.2, 52.9, 43.8, 57.1, 47.5, 34.1, 57.4, 42.7, 38.3, 37…
#> $ PkPa    <dbl> 97.2, 97.3, 97.4, 97.5, 97.4, 97.5, 97.4, 97.4, 97.4, 97.4, 97…
#> $ Rad     <dbl> 23.6, 24.6, 20.2, 21.4, 17.8, 19.2, 27.0, 15.2, 21.6, 24.3, 24…
#> $ PAR     <dbl> 496.6, 513.3, 430.5, 454.0, 378.2, 405.4, 565.7, 317.2, 467.5,…
#> $ Eto     <dbl> 5.7, 5.8, 4.9, 5.1, 4.1, 4.8, 6.2, 4.1, 5.5, 5.7, 5.9, 6.1, 6.…
#> $ Velmax  <dbl> 6.1, 4.8, 12.1, 6.2, 5.1, 4.5, 4.6, 5.7, 5.8, 5.2, 5.2, 4.7, 6…
#> $ Velmin  <dbl> 1.0, 1.0, 1.2, 1.0, 0.8, 0.9, 0.9, 1.5, 1.2, 0.8, 0.8, 1.2, 1.…
#> $ Dir_vel <dbl> 17.4, 261.9, 222.0, 25.0, 56.9, 74.9, 53.4, 89.0, 144.8, 303.9…
#> $ chuva   <dbl> 0.0, 0.0, 3.3, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.…
#> $ inso    <dbl> 7.9, 8.7, 5.2, 6.2, 3.4, 4.5, 10.5, 1.3, 6.3, 8.4, 8.6, 7.9, 1…
dados_estacao <- dados_estacao %>%
                   drop_na()
visdat::vis_miss(dados_estacao)
```




```
data_set_est_isa <- left_join(data_set %>%
                         rename(data=data.x), dados_estacao, by = "data") %>%                          mutate(ra
nge_T = Tmax-Tmin)
```

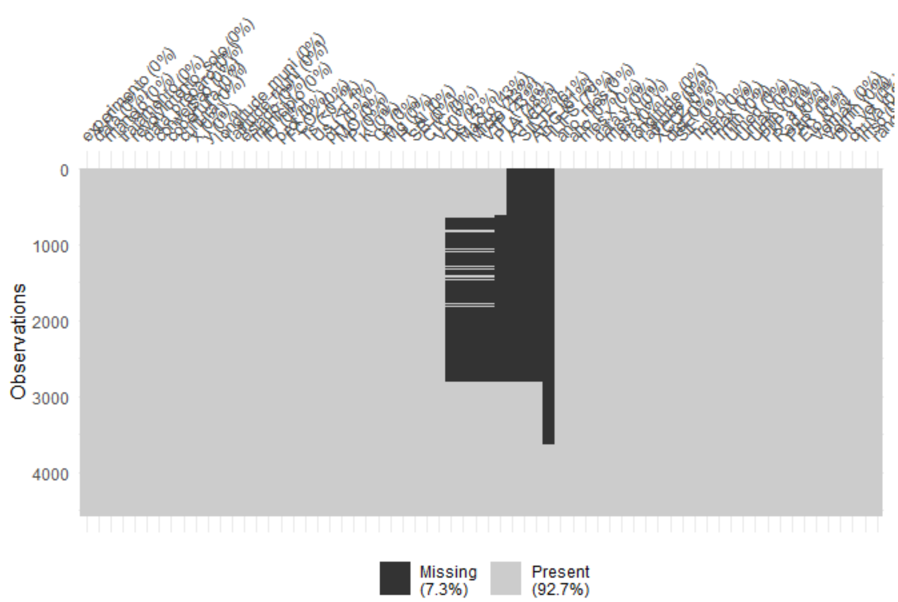
```
data_set_temporal <- data_set_est_isa %>%
  filter(experimento == "Temporal")

data_set_espacial <- data_set_est_isa %>%
  filter(experimento == "Espacial")
```

Quinta Aproximação

- Alvo: FCO2 - espacial
- restrição dados após 2014
- Features: Atributos do Solo + Xco2 e SIF + Dados da Estação de ISA
- Modelo mais simples e geral
- Testar 3 métodos baseados em árvores de decisão

visualização do banco de dados

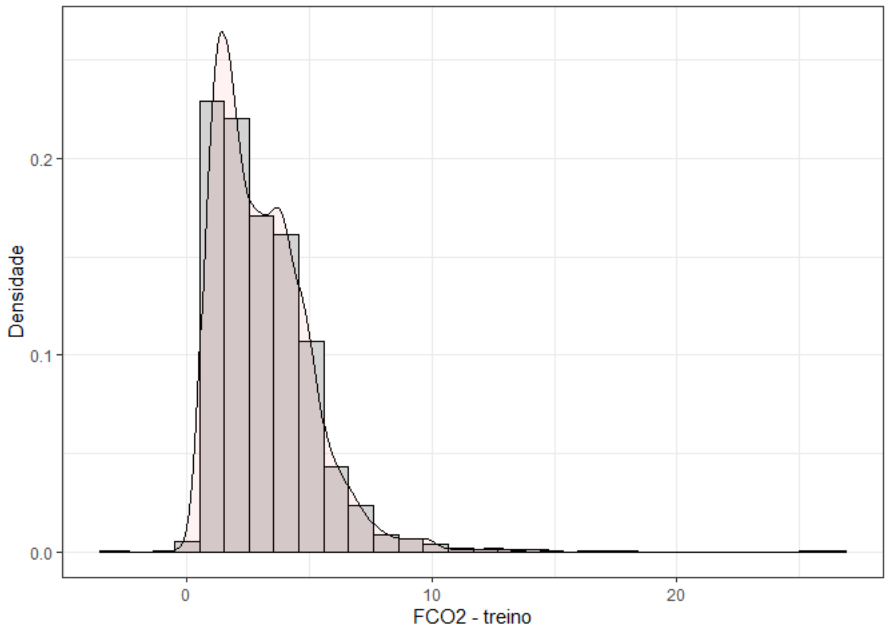
```
visdat::vis_miss(data_set_espacial)
```



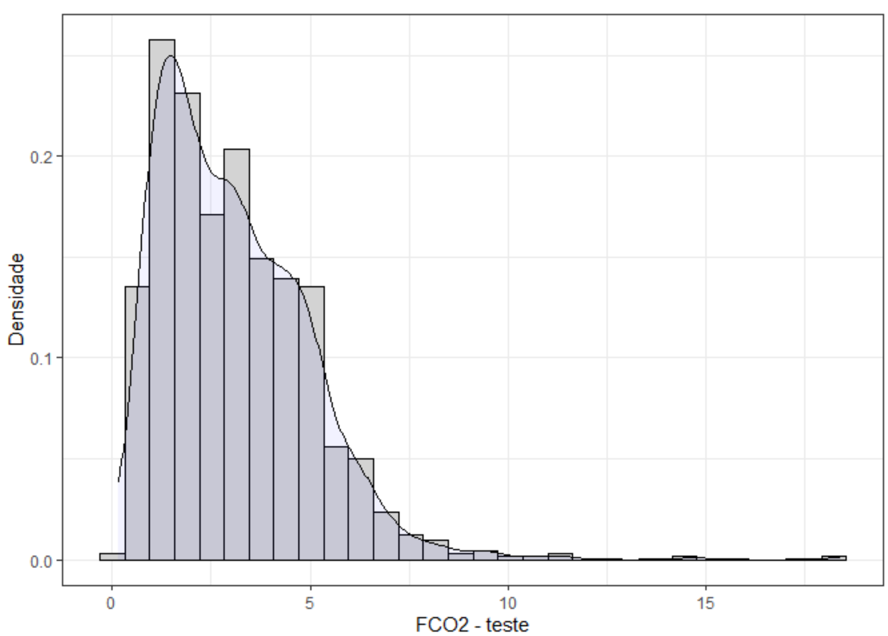
Definindo a Base de treino e teste

```
data_set_ml <- data_set_espacial  # <-------
fco2_initial_split <- initial_split(data_set_ml, prop = 0.75)
```

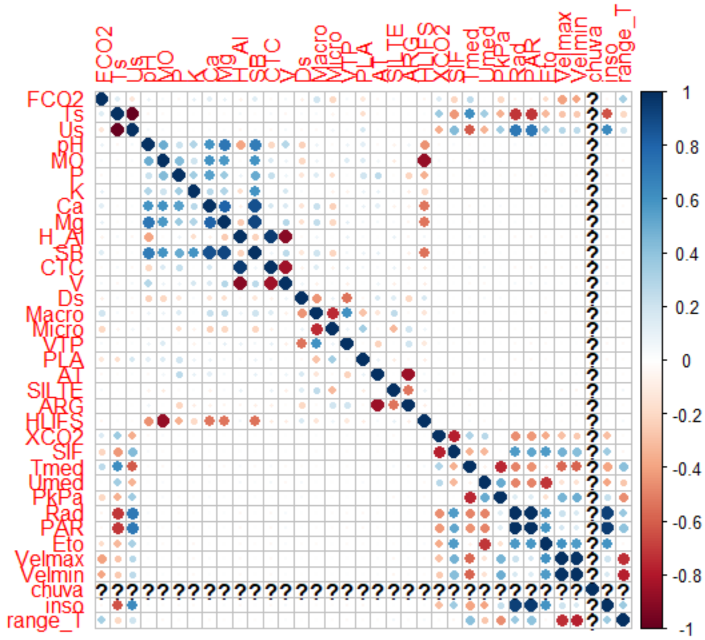
```
fco2_train <- training(fco2_initial_split)
# fco2_test <- testing(fco2_initial_split)
# visdat::vis_miss(fco2_test)
fco2_train  %>%
  ggplot(aes(x=FCO2, y=..density..))+
  geom_histogram(bins = 30, color="black",  fill="lightgray")+
  geom_density(alpha=.05,fill="red")+
  theme_bw() +
  labs(x="FCO2 - treino", y = "Densidade")
```




```
fco2_testing <- testing(fco2_initial_split)
fco2_testing  %>%
  ggplot(aes(x=FCO2, y=..density..))+
  geom_histogram(bins = 30, color="black",  fill="lightgray")+
  geom_density(alpha=.05,fill="blue")+
  theme_bw() +
  labs(x="FCO2 - teste", y = "Densidade")
```



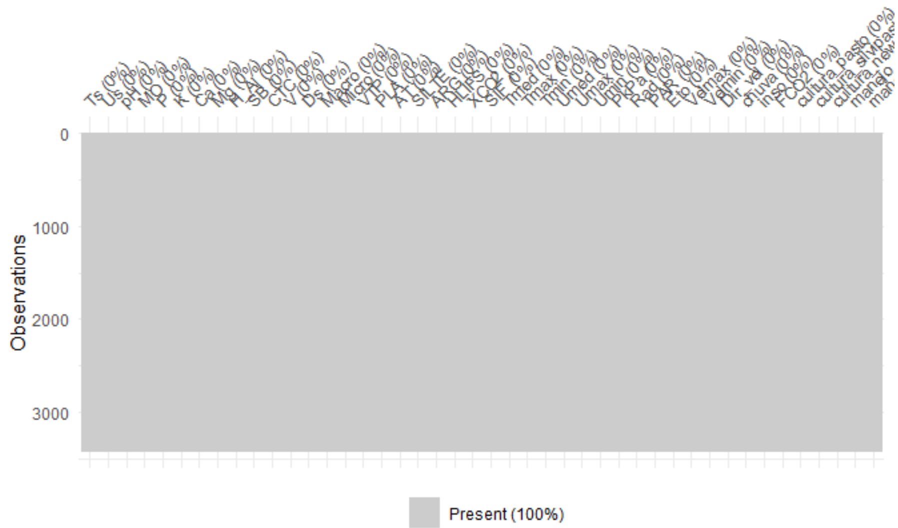
```r
fco2_train   %>%    select(FCO2:HLIFS,XCO2,SIF,Tmed:inso) %>%
  mutate(range_T = Tmax-Tmin) %>% select(-c(Tmax,Tmin,Umax,Umin,Dir_vel)) %>%   select(where(is.numeric)) %>%
  drop_na() %>%
  cor()  %>%
  corrplot::corrplot()
```



data prep

```r
fco2_recipe <- recipe(FCO2 ~ .,
                      data = fco2_train %>%
                        select(cultura, manejo, cobertura, FCO2:HLIFS,XCO2,SIF,Tmed:inso)
) %>%
  step_normalize(all_numeric_predictors())  %>%
  step_novel(all_nominal_predictors()) %>%
  step_zv(all_predictors()) %>%
  #step_naomit(c(Ts, Us)) %>%
  step_impute_median(where(is.numeric)) %>% # inputação da mediana nos numéricos
  #step_poly(c(Us,Ts), degree = 2)  %>%
  step_dummy(all_nominal_predictors())
bake(prep(fco2_recipe), new_data = NULL)
#> # A tibble: 3,428 × 44
#>         Ts      Us       pH       MO       P       K      Ca      Mg     H_Al      SB
#>      <dbl>   <dbl>    <dbl>    <dbl>   <dbl>   <dbl>   <dbl>   <dbl>    <dbl>   <dbl>
#>  1  0.746  -0.992 -0.207    1.24     0.944 -0.115 -0.181 -0.537  0.505   -0.317
#>  2 -1.59    0.872 -0.207   -0.393   -0.910 -0.311 -0.371 -1.22    1.13    -0.696
#>  3 -1.08    0.587 -0.207   -0.542   -0.601  0.539 -0.560 -0.764  1.13    -0.603
#>  4 -0.771   0.161 -0.161    0.348   -0.910  1.72   -0.560 -0.991  0.505   -0.546
#>  5 -0.0256 -1.10   0.0206  1.24     1.25   -0.442  1.05    1.74  -0.261    1.29
#>  6  0.283  -0.524 -0.0703  0.496   -0.292  0.932 -0.465  0.373  0.226   -0.132
#>  7 -0.334  -0.196 -0.116   0.496    0.326 -0.377  0.765  0.827 -0.0523  0.795
#>  8 -1.13    0.395 -0.207   0.348   -0.601  0.278 -0.465 -0.537  0.783   -0.489
#>  9  1.31    1.57  -0.207   0.200   -0.601  0.408 -0.655 -0.991  1.13    -0.760
#> 10  1.26   -0.565 -0.161   0.0513 -0.601  1.26   -0.465 -0.537  0.505   -0.382
#> # ℹ 3,418 more rows
#> # ℹ 34 more variables: CTC <dbl>, V <dbl>, Ds <dbl>, Macro <dbl>, Micro <dbl>,
#> #   VTP <dbl>, PLA <dbl>, AT <dbl>, SILTE <dbl>, ARG <dbl>, HLIFS <dbl>,
#> #   XCO2 <dbl>, SIF <dbl>, Tmed <dbl>, Tmax <dbl>, Tmin <dbl>, Umed <dbl>,
#> #   Umax <dbl>, Umin <dbl>, PkPa <dbl>, Rad <dbl>, PAR <dbl>, Eto <dbl>,
#> #   Velmax <dbl>, Velmin <dbl>, Dir_vel <dbl>, chuva <dbl>, inso <dbl>,
#> #   FCO2 <dbl>, cultura_pasto <dbl>, cultura_silvipastoril <dbl>, …
```

```r
visdat::vis_miss(bake(prep(fco2_recipe), new_data = NULL))
```



Reamostragem definida e será padrão para todos os modelos

```
fco2_resamples <- vfold_cv(fco2_train, v = 5) # 10 fold
grid <- grid_regular(
  penalty(range = c(-8, 0)),
  levels = 20
)
```

Árvore de Decisão

Definição do modelo

```
fco2_dt_model <- decision_tree(
  cost_complexity = tune(),
  tree_depth = tune(),
  min_n = tune()
)  %>%
  set_mode("regression")  %>%
  set_engine("rpart")
```

Workflow

```
fco2_dt_wf <- workflow()   %>%
  add_model(fco2_dt_model) %>%
  add_recipe(fco2_recipe)
```

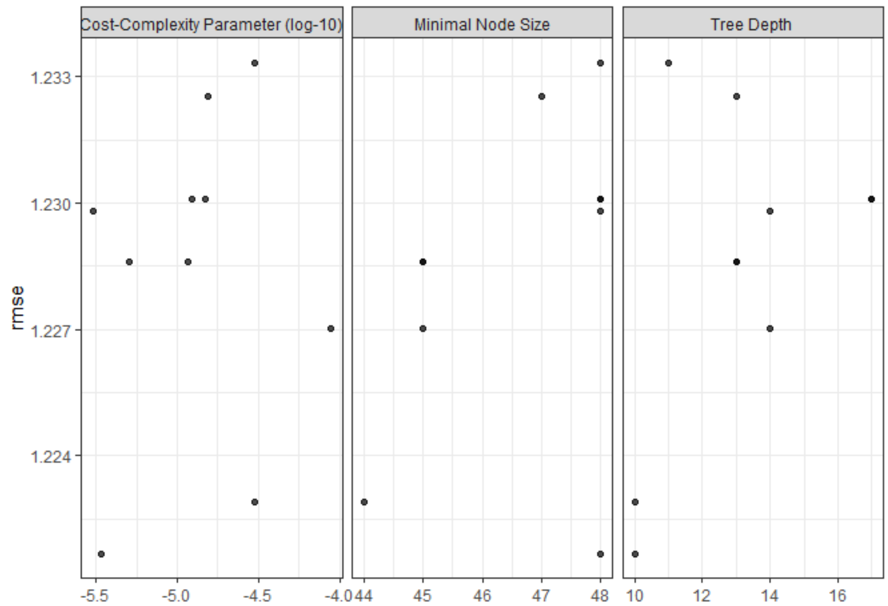
Criando a matriz (grid) com os valores de hiperparâmetros a serem testados

```
grid_dt <- grid_random(
  cost_complexity(c(-6, -4)),
  tree_depth(range = c(8, 18)),
  min_n(range = c(42, 52)),
  size = 10 # <------------------------------
)
glimpse(grid_dt)
#> Rows: 10
#> Columns: 3
#> $ cost_complexity <dbl> 1.497271e-05, 3.016738e-05, 1.233316e-05, 1.557756e-05…
#> $ tree_depth      <int> 17, 10, 17, 13, 13, 14, 13, 11, 10, 14
#> $ min_n           <int> 48, 44, 48, 47, 45, 45, 45, 48, 48, 48
```

Tuning de hiperparâmetros

```
fco2_dt_tune_grid <- tune_grid(
  fco2_dt_wf,
  resamples = fco2_resamples,
  grid = grid_dt,
  metrics = metric_set(rmse)
)
```

```
autoplot(fco2_dt_tune_grid)
```



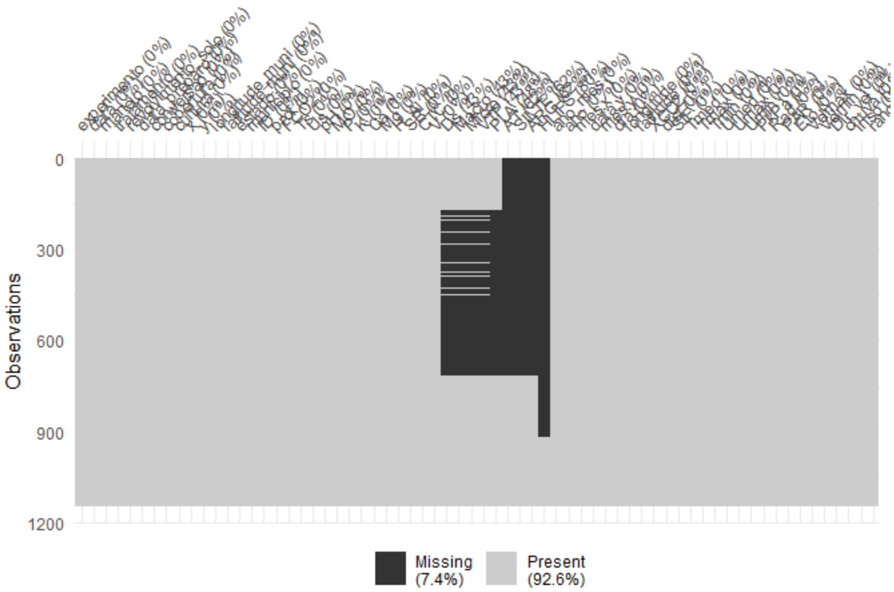

```
collect_metrics(fco2_dt_tune_grid)
#> # A tibble: 10 × 9
#>    cost_complexity tree_depth min_n .metric .estimator  mean     n std_err
#>              <dbl>      <int> <int> <chr>   <chr>      <dbl> <int>   <dbl>
#>  1       0.0000150         17    48 rmse    standard    1.23     5  0.0603
#>  2       0.0000302         10    44 rmse    standard    1.22     5  0.0579
#>  3       0.0000123         17    48 rmse    standard    1.23     5  0.0603
#>  4       0.0000156         13    47 rmse    standard    1.23     5  0.0599
#>  5       0.00000510        13    45 rmse    standard    1.23     5  0.0599
#>  6       0.0000875         14    45 rmse    standard    1.23     5  0.0587
#>  7       0.0000116         13    45 rmse    standard    1.23     5  0.0599
#>  8       0.0000300         11    48 rmse    standard    1.23     5  0.0585
#>  9       0.00000340        10    48 rmse    standard    1.22     5  0.0596
#> 10       0.00000304        14    48 rmse    standard    1.23     5  0.0587
#> # ℹ 1 more variable: .config <chr>
```

Desempenho dos modelos finais

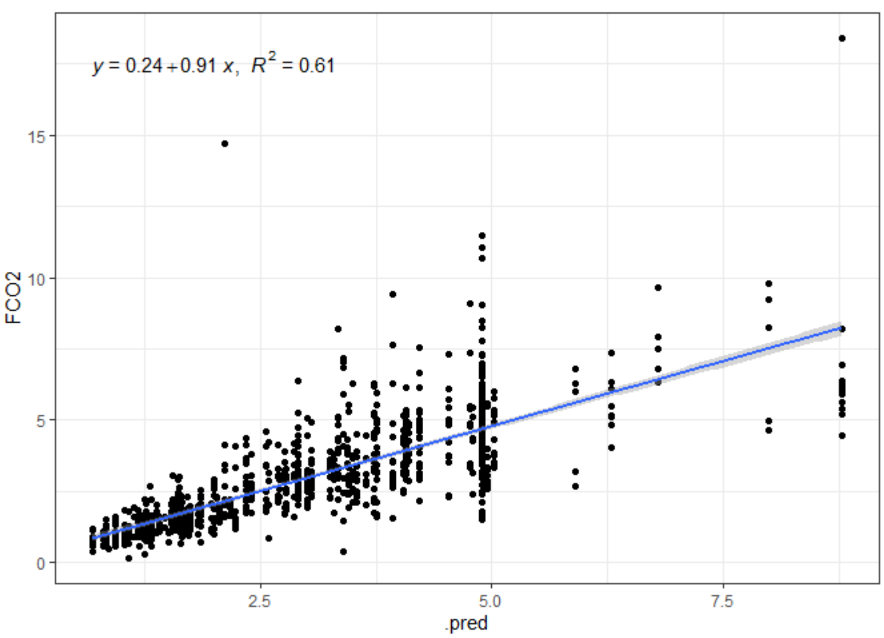
```
fco2_dt_best_params <- select_best(fco2_dt_tune_grid, "rmse")
fco2_dt_wf <- fco2_dt_wf %>% finalize_workflow(fco2_dt_best_params)
fco2_dt_last_fit <- last_fit(fco2_dt_wf, fco2_initial_split)
```

Criando os preditos

```
fco2_test_preds <- bind_rows(
  collect_predictions(fco2_dt_last_fit)  %>%   mutate(modelo = "dt")
)

fco2_test <- testing(fco2_initial_split)
visdat::vis_miss(fco2_test)
```

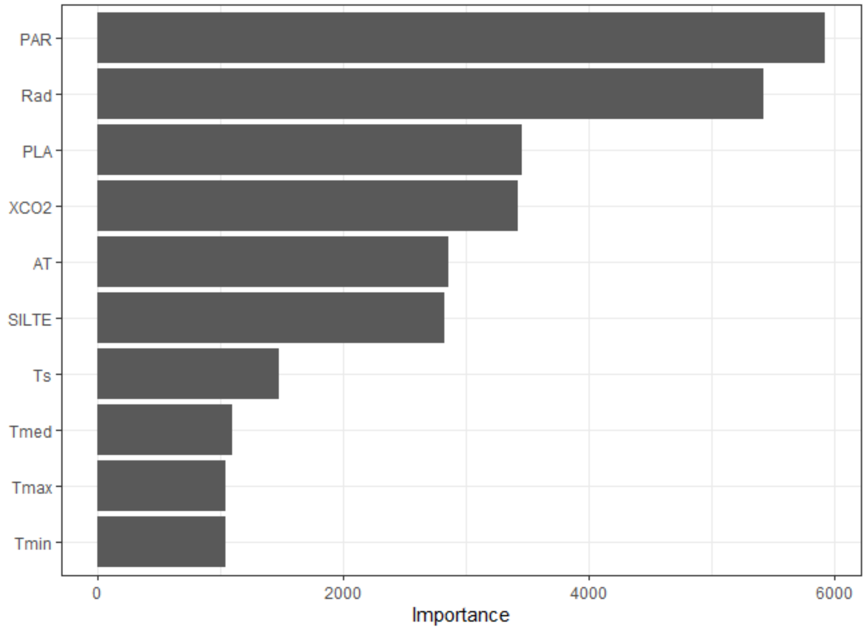



```
fco2_test_preds %>%
  ggplot(aes(x=.pred, y=FCO2)) +
  geom_point()+
  theme_bw() +
  geom_smooth(method = "lm") +
  stat_regline_equation(ggplot2::aes(
  label =  paste(..eq.label.., ..rr.label.., sep = "*plain(\",\")~~")))
```



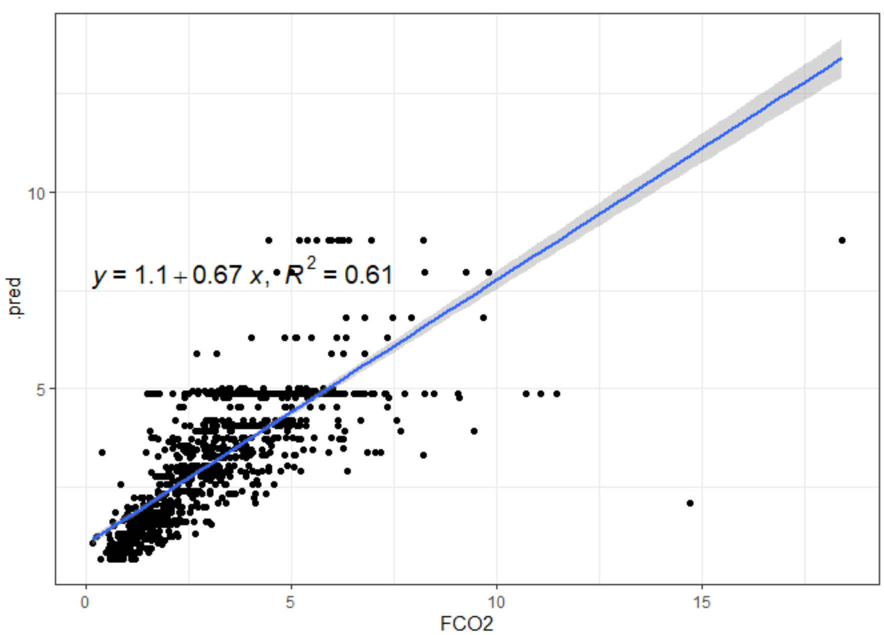
Importância

```
fco2_dt_last_fit_model <-fco2_dt_last_fit$.workflow[[1]]$fit$fit
vip(fco2_dt_last_fit_model)
```



Métricas

```
da <- fco2_test_preds %>%
  filter(FCO2 > 0, .pred>0 )

my_r <- cor(da$FCO2,da$.pred)
my_r2 <- my_r*my_r
my_mse <- Metrics::mse(da$FCO2,da$.pred)
my_rmse <- Metrics::rmse(da$FCO2,
                         da$.pred)
my_mae <- Metrics::mae(da$FCO2,da$.pred)
my_mape <- Metrics::mape(da$FCO2,da$.pred)*100


fco2_test_preds %>%
  ggplot(aes(x=FCO2,y=.pred))+
  geom_point()+
  geom_smooth(method = "lm")+
  stat_regline_equation(ggplot2::aes(
    label =  paste(..eq.label.., ..rr.label.., sep = "*plain(\",\")~~")),size=5)
```



```
  # ggplot2::annotate('text',x=10.4,y=16.7,label=paste0('RMSE = ',round(my_rmse,2),', MAPE = '
  #                                                       ,round(my_mape,2),'%'),size=5)+
  # theme_bw()
vector_of_metrics <- c(r=my_r, R2=my_r2, MSE=my_mse, RMSE=my_rmse, MAE=my_mae, MAPE=my_mape)
print(data.frame(vector_of_metrics))
#>      vector_of_metrics
#> r            0.7817922
#> R2           0.6111991
#> MSE          1.3956239
#> RMSE         1.1813653
#> MAE          0.7420816
#> MAPE        27.6461279
```

Random Forest

Definição do modelo

```
fco2_rf_model <- rand_forest(
  min_n = tune(),
  mtry = tune(),
  trees = tune()
)   %>%
  set_mode("regression")  %>%
  set_engine("randomForest")
```

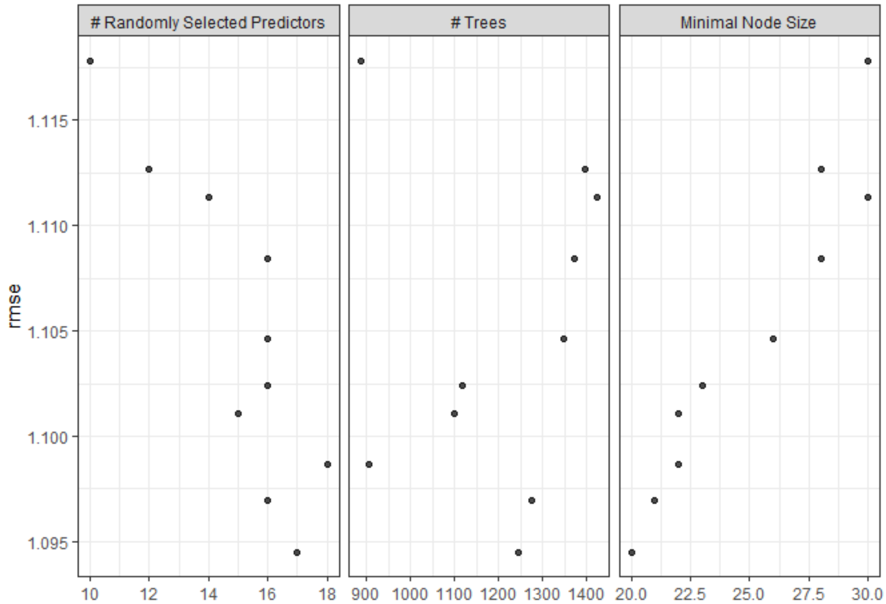
Workflow

```
fco2_rf_wf <- workflow()   %>%
  add_model(fco2_rf_model) %>%
  add_recipe(fco2_recipe)
```

Tune

```
grid_rf <- grid_random(
  min_n(range = c(20, 30)),
  mtry(range = c(10,20)),
  trees(range = c(769,1500) ),
  size = 10 #<-----------------------
)
```

```
fco2_rf_tune_grid <- tune_grid(
 fco2_rf_wf,
  resamples = fco2_resamples,
  grid = grid_rf,
  metrics = metric_set(rmse)
)
autoplot(fco2_rf_tune_grid)
```



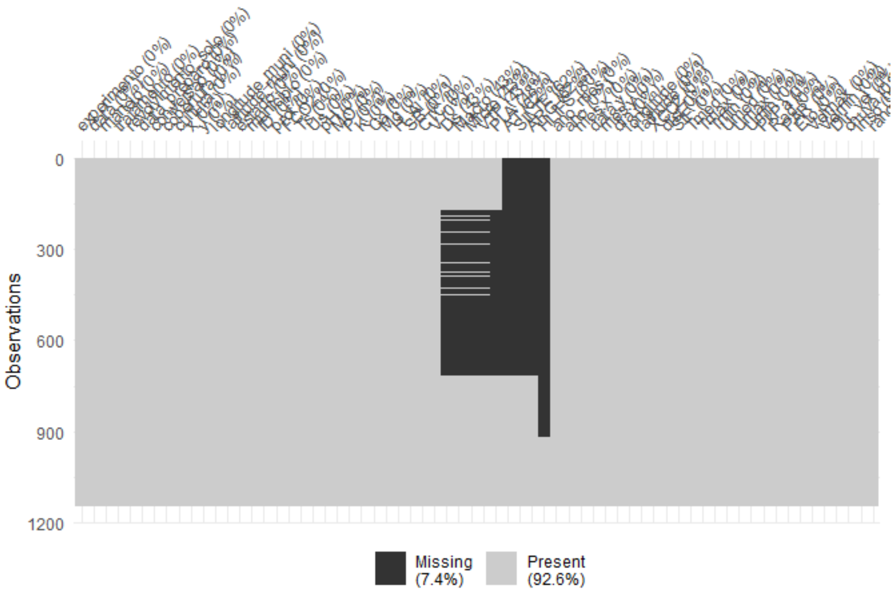

```
collect_metrics(fco2_rf_tune_grid)
#> # A tibble: 10 × 9
#>     mtry trees min_n .metric .estimator  mean     n std_err .config
#>    <int> <int> <int> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
#>  1    18   906    22 rmse    standard    1.10     5  0.0663 Preprocessor1_Model…
#>  2    16  1276    21 rmse    standard    1.10     5  0.0660 Preprocessor1_Model…
#>  3    15  1099    22 rmse    standard    1.10     5  0.0659 Preprocessor1_Model…
#>  4    12  1395    28 rmse    standard    1.11     5  0.0670 Preprocessor1_Model…
#>  5    16  1371    28 rmse    standard    1.11     5  0.0658 Preprocessor1_Model…
#>  6    16  1348    26 rmse    standard    1.10     5  0.0665 Preprocessor1_Model…
#>  7    14  1425    30 rmse    standard    1.11     5  0.0664 Preprocessor1_Model…
#>  8    16  1118    23 rmse    standard    1.10     5  0.0661 Preprocessor1_Model…
#>  9    10   887    30 rmse    standard    1.12     5  0.0662 Preprocessor1_Model…
#> 10    17  1245    20 rmse    standard    1.09     5  0.0665 Preprocessor1_Model…
```

Desempenho modelo final

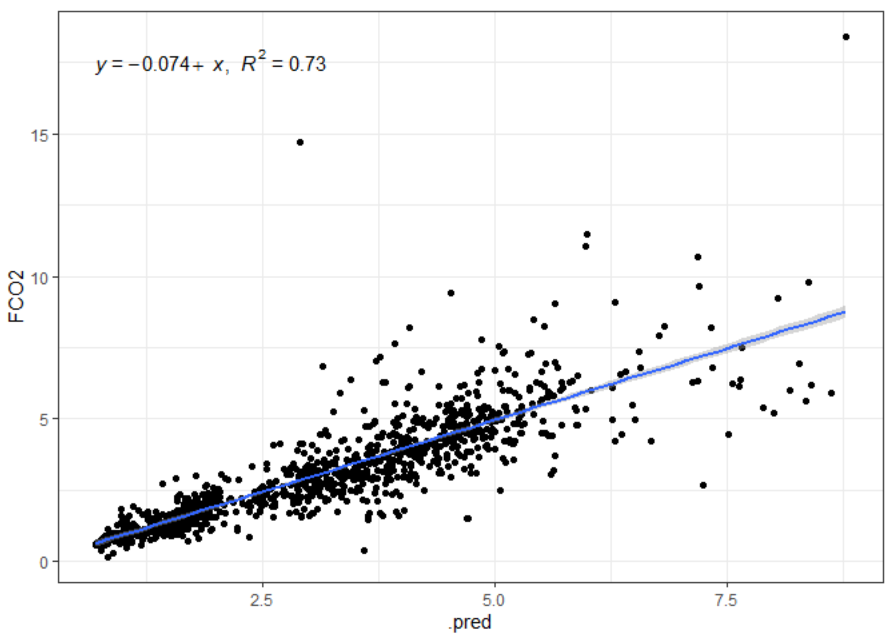
```
fco2_rf_best_params <- select_best(fco2_rf_tune_grid, "rmse")
fco2_rf_wf <- fco2_rf_wf %>% finalize_workflow(fco2_rf_best_params)
fco2_rf_last_fit <- last_fit(fco2_rf_wf, fco2_initial_split)
```

Criando os preditos

```
fco2_test_preds <- bind_rows(
  collect_predictions(fco2_rf_last_fit)  %>%   mutate(modelo = "rf")
)

fco2_test <- testing(fco2_initial_split)
visdat::vis_miss(fco2_test)
```

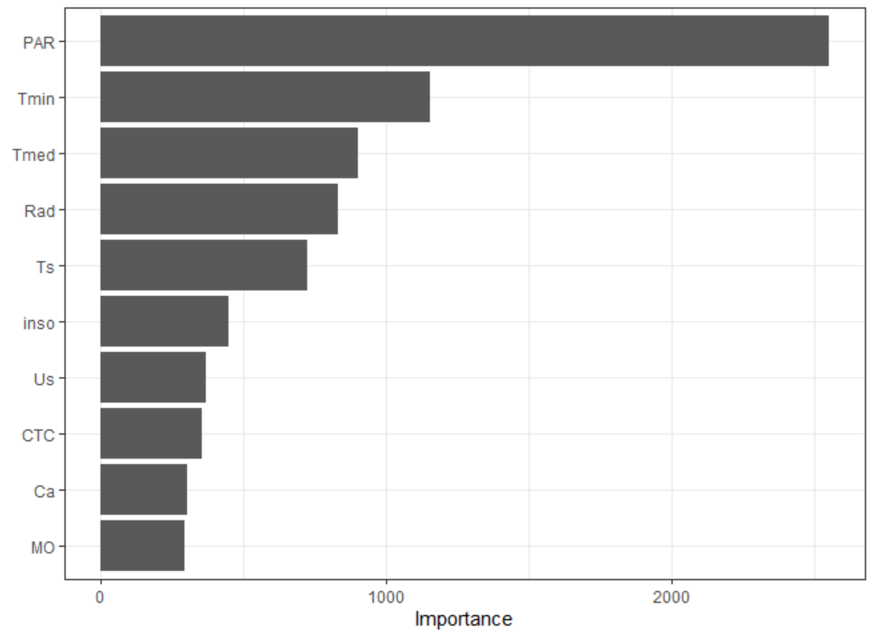



```
fco2_test_preds %>%
  ggplot(aes(x=.pred, y=FCO2)) +
  geom_point()+
  theme_bw() +
  geom_smooth(method = "lm") +
  stat_regline_equation(ggplot2::aes(
  label =  paste(..eq.label.., ..rr.label.., sep = "*plain(\",\")~~")))
```



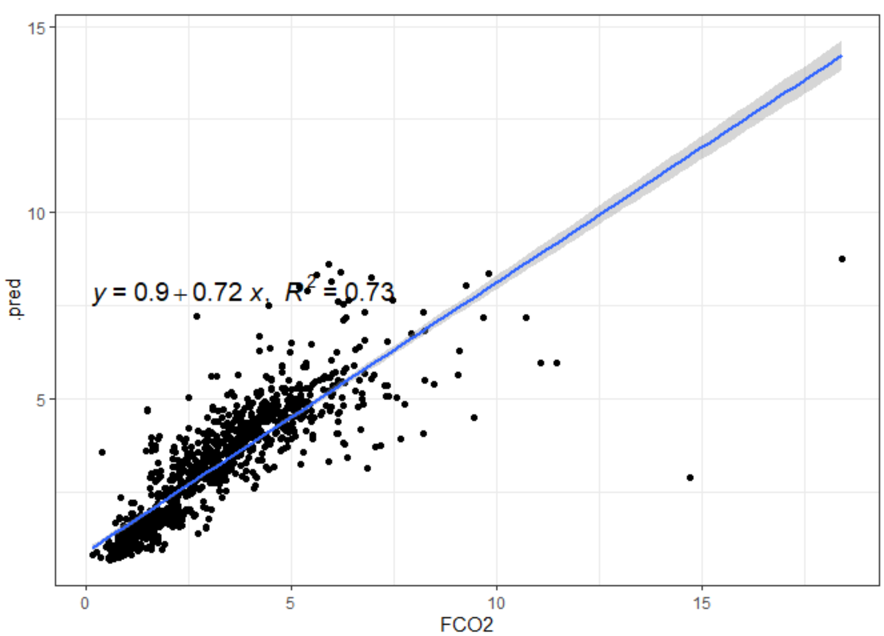
Importância

```
fco2_rf_last_fit_model <-fco2_rf_last_fit$.workflow[[1]]$fit$fit
vip(fco2_rf_last_fit_model)
```



Métricas

```
da <- fco2_test_preds %>%
  filter(FCO2 > 0, .pred>0 )

my_r <- cor(da$FCO2,da$.pred)
my_r2 <- my_r*my_r
my_mse <- Metrics::mse(da$FCO2,da$.pred)
my_rmse <- Metrics::rmse(da$FCO2,
                         da$.pred)
my_mae <- Metrics::mae(da$FCO2,da$.pred)
my_mape <- Metrics::mape(da$FCO2,da$.pred)*100


fco2_test_preds %>%
  ggplot(aes(x=FCO2,y=.pred))+
  geom_point()+
  geom_smooth(method = "lm")+
  stat_regline_equation(ggplot2::aes(
    label =  paste(..eq.label.., ..rr.label.., sep = "*plain(\",\")~~")),size=5)
```



```
  # ggplot2::annotate('text',x=10.4,y=16.7,label=paste0('RMSE = ',round(my_rmse,2),', MAPE = '
  #                                                      ,round(my_mape,2),'%'),size=5)+
  # theme_bw()
vector_of_metrics <- c(r=my_r, R2=my_r2, MSE=my_mse, RMSE=my_rmse, MAE=my_mae, MAPE=my_mape)
print(data.frame(vector_of_metrics))
#>      vector_of_metrics
#> r            0.8540438
#> R2           0.7293909
#> MSE          0.9579750
#> RMSE         0.9787620
#> MAE          0.5753262
#> MAPE        21.6829855
```

Boosting gradient tree (xgb)

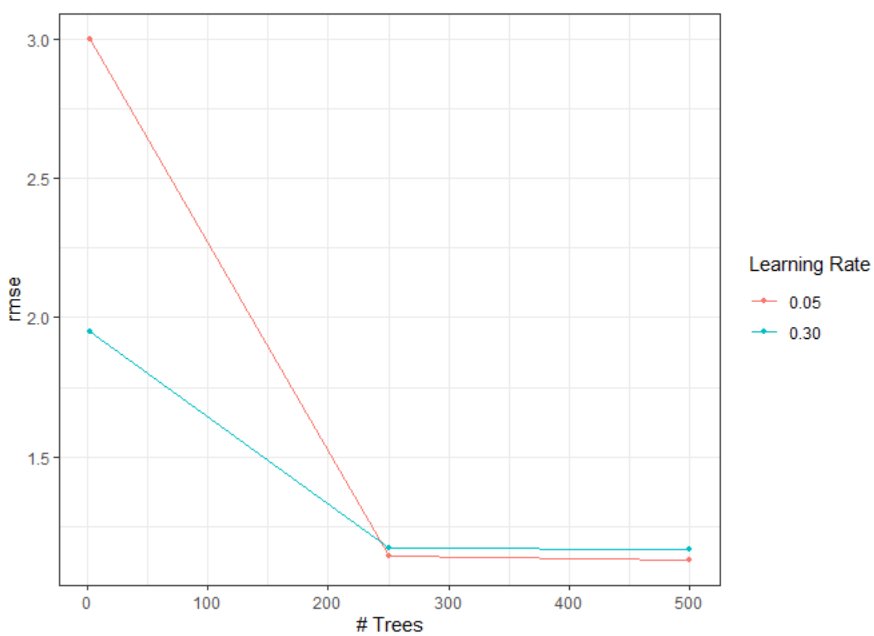
```
cores = 4
fco2_xgb_model <- boost_tree(
  mtry = 0.8,
  trees = tune(), # <---------------
  min_n = 5,
  tree_depth = 4,
  loss_reduction = 0, # lambda
  learn_rate = tune(), # epsilon
  sample_size = 0.8
)  %>%
  set_mode("regression")  %>%
  set_engine("xgboost", nthread = cores, counts = FALSE)
```

```
fco2_xgb_wf <- workflow()  %>%
  add_model(fco2_xgb_model) %>%
  add_recipe(fco2_recipe)
```

```
grid_xgb <- expand.grid(
  learn_rate =  c(0.05, 0.3),
  trees = c(2, 250, 500)
)
```

Passo 1

```
fco2_xgb_tune_grid <- tune_grid(
 fco2_xgb_wf,
  resamples = fco2_resamples,
  grid = grid_xgb,
  metrics = metric_set(rmse)
)
autoplot(fco2_xgb_tune_grid)
```

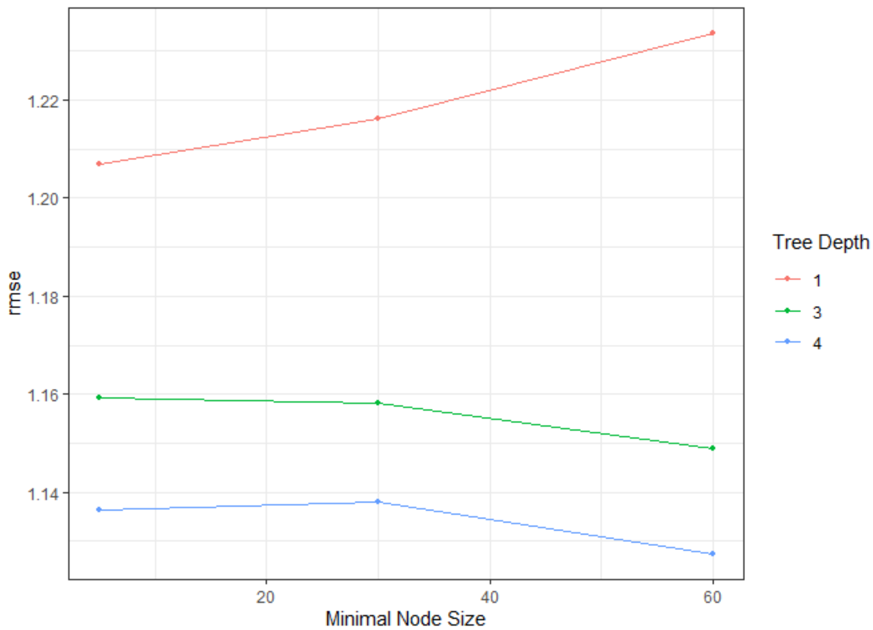


```r
fco2_xgb_tune_grid   %>%   show_best(metric = "rmse", n = 6)
#> # A tibble: 6 × 8
#>   trees learn_rate .metric .estimator  mean     n std_err .config
#>   <dbl>      <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
#> 1   500       0.05 rmse    standard    1.13     5  0.0583 Preprocessor1_Model3
#> 2   250       0.05 rmse    standard    1.15     5  0.0548 Preprocessor1_Model2
#> 3   500       0.3  rmse    standard    1.17     5  0.0564 Preprocessor1_Model6
#> 4   250       0.3  rmse    standard    1.17     5  0.0559 Preprocessor1_Model5
#> 5     2       0.3  rmse    standard    1.95     5  0.0724 Preprocessor1_Model4
#> 6     2       0.05 rmse    standard    3.00     5  0.0766 Preprocessor1_Model1
```

```r
fco2_xgb_select_best_passo1 <- fco2_xgb_tune_grid %>%
  select_best(metric = "rmse")
fco2_xgb_select_best_passo1
#> # A tibble: 1 × 3
#>   trees learn_rate .config
#>   <dbl>      <dbl> <chr>
#> 1   500       0.05 Preprocessor1_Model3
```

Passo 2

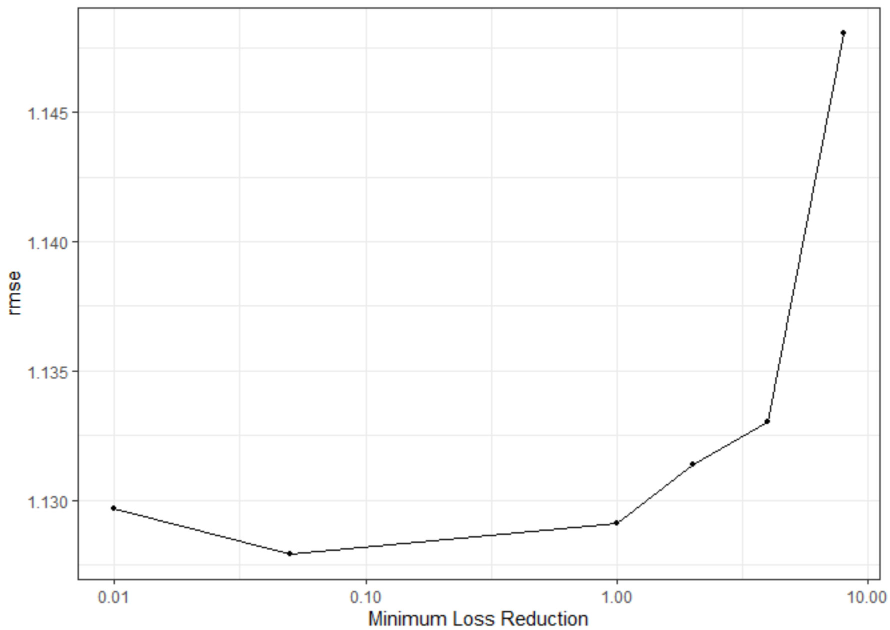
```r
fco2_xgb_model <- boost_tree(
  mtry = 0.8,
  trees = fco2_xgb_select_best_passo1$trees,
  min_n = tune(),
  tree_depth = tune(),
  loss_reduction = 0,
  learn_rate = fco2_xgb_select_best_passo1$learn_rate,
  sample_size = 0.8
) %>%
  set_mode("regression")  %>%
  set_engine("xgboost", nthread = cores, counts = FALSE)

#### Workflow
fco2_xgb_wf <- workflow() %>%
    add_model(fco2_xgb_model)   %>%
    add_recipe(fco2_recipe)

#### Grid
fco2_xgb_grid <- expand.grid(
  tree_depth = c(1, 3, 4),
  min_n = c(5, 30, 60)
)

fco2_xgb_tune_grid <- fco2_xgb_wf   %>%
  tune_grid(
    resamples =fco2_resamples,
    grid = fco2_xgb_grid,
    control = control_grid(save_pred = TRUE, verbose = FALSE, allow_par = TRUE),
    metrics = metric_set(rmse)
  )

#### Melhores hiperparâmetros
autoplot(fco2_xgb_tune_grid)
```




```
fco2_xgb_tune_grid  %>%   show_best(metric = "rmse", n = 5)
#> # A tibble: 5 × 8
#>   min_n tree_depth .metric .estimator  mean     n std_err .config
#>   <dbl>      <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
#> 1    60          4 rmse    standard    1.13     5  0.0556 Preprocessor1_Model9
#> 2     5          4 rmse    standard    1.14     5  0.0557 Preprocessor1_Model3
#> 3    30          4 rmse    standard    1.14     5  0.0540 Preprocessor1_Model6
#> 4    60          3 rmse    standard    1.15     5  0.0554 Preprocessor1_Model8
#> 5    30          3 rmse    standard    1.16     5  0.0544 Preprocessor1_Model5
fco2_xgb_select_best_passo2 <- fco2_xgb_tune_grid  %>%   select_best(metric = "rmse")
fco2_xgb_select_best_passo2
#> # A tibble: 1 × 3
#>   min_n tree_depth .config
#>   <dbl>      <dbl> <chr>
#> 1    60          4 Preprocessor1_Model9
```

Passo 3

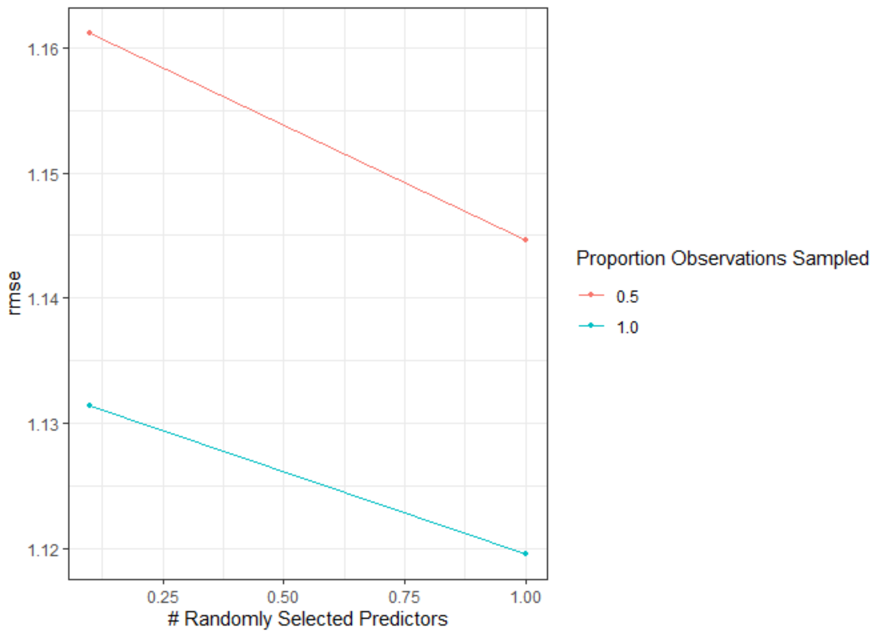
```
fco2_xgb_model <- boost_tree(
  mtry = 0.8,
  trees = fco2_xgb_select_best_passo1$trees,
  min_n = fco2_xgb_select_best_passo2$min_n,
  tree_depth = fco2_xgb_select_best_passo2$tree_depth,
  loss_reduction =tune(),
  learn_rate = fco2_xgb_select_best_passo1$learn_rate,
  sample_size = 0.8
)  %>%
  set_mode("regression")  %>%
  set_engine("xgboost", nthread = cores, counts = FALSE)

#### Workflow
fco2_xgb_wf <- workflow()  %>%
    add_model(fco2_xgb_model)  %>%
    add_recipe(fco2_recipe)

#### Grid
fco2_xgb_grid <- expand.grid(
  loss_reduction = c(0.01, 0.05, 1, 2, 4, 8)
)

fco2_xgb_tune_grid <- fco2_xgb_wf   %>%
  tune_grid(
    resamples = fco2_resamples,
    grid = fco2_xgb_grid,
    control = control_grid(save_pred = TRUE, verbose = FALSE, allow_par = TRUE),
    metrics = metric_set(rmse)
  )

#### Melhores hiperparâmetros
autoplot(fco2_xgb_tune_grid)
```




```
fco2_xgb_tune_grid   %>%   show_best(metric = "rmse", n = 5)
#> # A tibble: 5 × 7
#>   loss_reduction .metric .estimator  mean     n std_err .config
#>            <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
#> 1           0.05 rmse    standard    1.13     5  0.0573 Preprocessor1_Model2
#> 2           1    rmse    standard    1.13     5  0.0566 Preprocessor1_Model3
#> 3           0.01 rmse    standard    1.13     5  0.0558 Preprocessor1_Model1
#> 4           2    rmse    standard    1.13     5  0.0564 Preprocessor1_Model4
#> 5           4    rmse    standard    1.13     5  0.0593 Preprocessor1_Model5
fco2_xgb_select_best_passo3 <- fco2_xgb_tune_grid %>% select_best(metric = "rmse")
fco2_xgb_select_best_passo3
#> # A tibble: 1 × 2
#>   loss_reduction .config
#>            <dbl> <chr>
#> 1           0.05 Preprocessor1_Model2
```

Passo 4

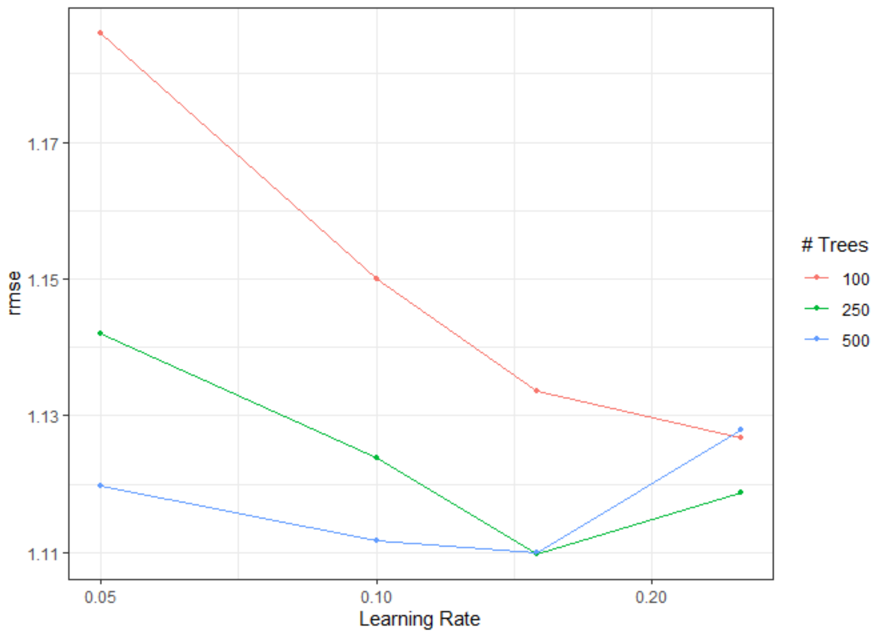
```
fco2_xgb_model <- boost_tree(
  mtry = tune(),
  trees = fco2_xgb_select_best_passo1$trees,
  min_n = fco2_xgb_select_best_passo2$min_n,
  tree_depth = fco2_xgb_select_best_passo2$tree_depth,
  loss_reduction = fco2_xgb_select_best_passo3$loss_reduction,
  learn_rate = fco2_xgb_select_best_passo1$learn_rate,
  sample_size = tune()
)%>%
  set_mode("regression")  |>
  set_engine("xgboost", nthread = cores, counts = FALSE)

#### Workflow
fco2_xgb_wf <- workflow()  %>%
    add_model(fco2_xgb_model)  %>%
    add_recipe(fco2_recipe)

#### Grid
fco2_xgb_grid <- expand.grid(
    sample_size = seq(0.5, 1.0, length.out = 2), ## <---
    mtry = seq(0.1, 1.0, length.out = 2) ## <---
)

fco2_xgb_tune_grid <- fco2_xgb_wf   %>%
  tune_grid(
    resamples = fco2_resamples,
    grid = fco2_xgb_grid,
    control = control_grid(save_pred = TRUE, verbose = FALSE, allow_par = TRUE),
    metrics = metric_set(rmse)
  )

autoplot(fco2_xgb_tune_grid)
```




```
fco2_xgb_tune_grid  |>  show_best(metric = "rmse", n = 5)
#> # A tibble: 4 × 8
#>    mtry sample_size .metric .estimator  mean     n std_err .config
#>   <dbl>       <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
#> 1   1           1   rmse    standard    1.12     5  0.0562 Preprocessor1_Model4
#> 2   0.1         1   rmse    standard    1.13     5  0.0555 Preprocessor1_Model2
#> 3   1           0.5 rmse    standard    1.14     5  0.0578 Preprocessor1_Model3
#> 4   0.1         0.5 rmse    standard    1.16     5  0.0624 Preprocessor1_Model1
fco2_xgb_select_best_passo4 <- fco2_xgb_tune_grid   %>%   select_best(metric = "rmse")
fco2_xgb_select_best_passo4
#> # A tibble: 1 × 3
#>    mtry sample_size .config
#>   <dbl>       <dbl> <chr>
#> 1     1           1 Preprocessor1_Model4
```

Passo 5

```
fco2_xgb_model <- boost_tree(
  mtry = fco2_xgb_select_best_passo4$mtry,
  trees = tune(),
  min_n = fco2_xgb_select_best_passo2$min_n,
  tree_depth = fco2_xgb_select_best_passo2$tree_depth,
  loss_reduction = fco2_xgb_select_best_passo3$loss_reduction,
  learn_rate = tune(),
  sample_size = fco2_xgb_select_best_passo4$sample_size
) |>
  set_mode("regression")  %>%
  set_engine("xgboost", nthread = cores, counts = FALSE)

#### Workflow
fco2_xgb_wf <- workflow() %>%
    add_model(fco2_xgb_model)  %>%
    add_recipe(fco2_recipe)

#### Grid
fco2_xgb_grid <- expand.grid(
    learn_rate = c(0.05, 0.10, 0.15, 0.25),
    trees = c(100, 250, 500)
)

fco2_xgb_tune_grid <- fco2_xgb_wf   %>%
  tune_grid(
    resamples = fco2_resamples,
    grid = fco2_xgb_grid,
    control = control_grid(save_pred = TRUE, verbose = FALSE, allow_par = TRUE),
    metrics = metric_set(rmse)
  )

#### Melhores hiperparâmetros
autoplot(fco2_xgb_tune_grid)
```




```
fco2_xgb_tune_grid  %>%   show_best(metric = "rmse", n = 5)
#> # A tibble: 5 × 8
#>   trees learn_rate .metric .estimator  mean     n std_err .config
#>   <dbl>      <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
#> 1   250       0.15 rmse    standard    1.11     5  0.0545 Preprocessor1_Model08
#> 2   500       0.15 rmse    standard    1.11     5  0.0576 Preprocessor1_Model09
#> 3   500       0.1  rmse    standard    1.11     5  0.0566 Preprocessor1_Model06
#> 4   250       0.25 rmse    standard    1.12     5  0.0573 Preprocessor1_Model11
#> 5   500       0.05 rmse    standard    1.12     5  0.0562 Preprocessor1_Model03
fco2_xgb_select_best_passo5 <- fco2_xgb_tune_grid   %>%   select_best(metric = "rmse")
fco2_xgb_select_best_passo5
#> # A tibble: 1 × 3
#>   trees learn_rate .config
#>   <dbl>      <dbl> <chr>
#> 1   250       0.15 Preprocessor1_Model08
```

Desempenho dos modelos finais

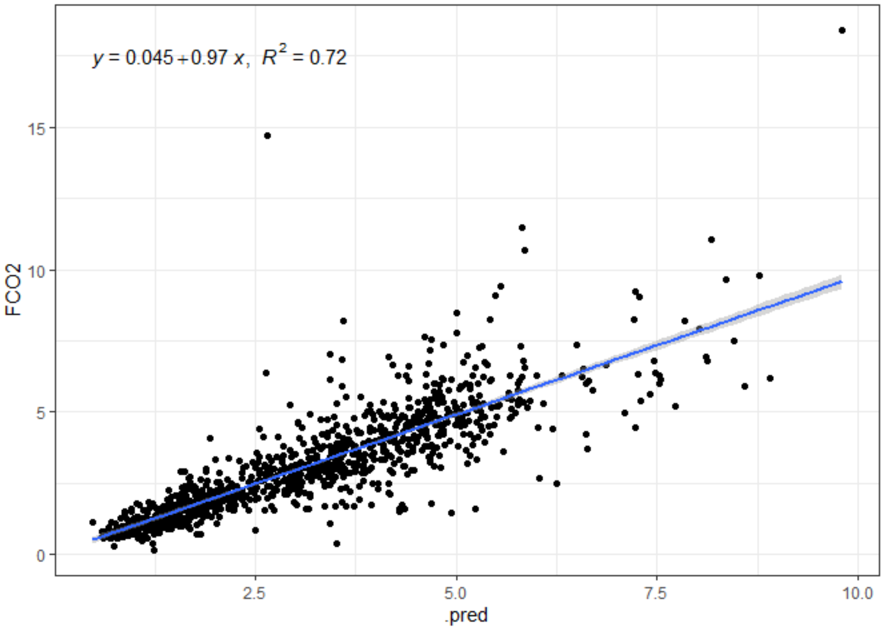
```
fco2_xgb_model <- boost_tree(
  mtry = fco2_xgb_select_best_passo4$mtry,
  trees = fco2_xgb_select_best_passo5$trees,
  min_n = fco2_xgb_select_best_passo2$min_n,
  tree_depth = fco2_xgb_select_best_passo2$tree_depth,
  loss_reduction = fco2_xgb_select_best_passo3$loss_reduction,
  learn_rate = fco2_xgb_select_best_passo5$learn_rate,
  sample_size = fco2_xgb_select_best_passo4$sample_size
) %>%
  set_mode("regression")  %>%
  set_engine("xgboost", nthread = cores, counts = FALSE)
```

```
df <- data.frame(
  mtry = fco2_xgb_select_best_passo4$mtry,
  trees = fco2_xgb_select_best_passo5$trees,
  min_n = fco2_xgb_select_best_passo2$min_n,
  tree_depth = fco2_xgb_select_best_passo2$tree_depth,
  loss_reduction = fco2_xgb_select_best_passo3$loss_reduction,
  learn_rate = fco2_xgb_select_best_passo5$learn_rate,
  sample_size = fco2_xgb_select_best_passo4$sample_size
)
fco2_xgb_wf <- fco2_xgb_wf %>% finalize_workflow(df) # <------
fco2_xgb_last_fit <- last_fit(fco2_xgb_wf, fco2_initial_split) # <--------
```

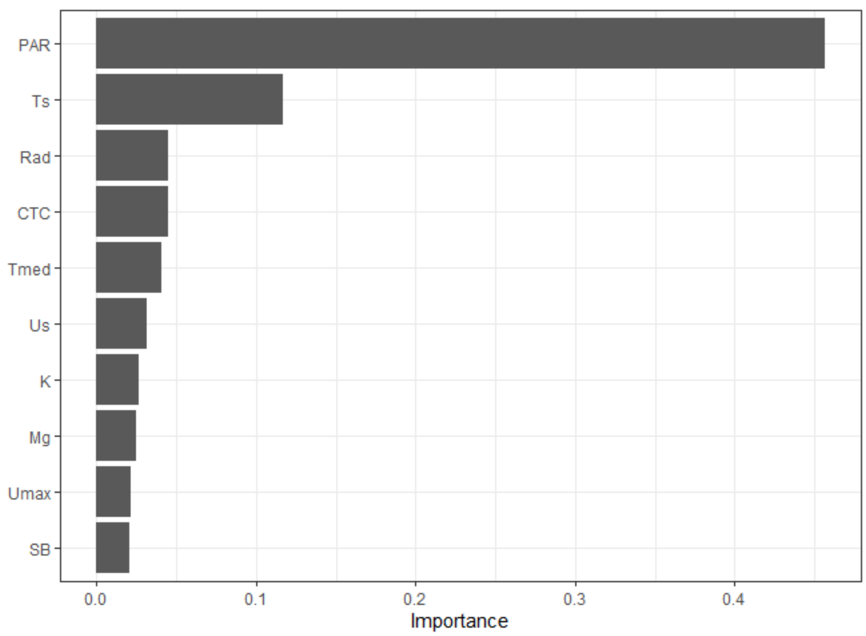
Criar Preditos

```
fco2_test_preds <- bind_rows(
  collect_predictions(fco2_xgb_last_fit)  %>%   mutate(modelo = "xgb")
)
```

```
fco2_test_preds %>%
  ggplot(aes(x=.pred, y=FCO2)) +
  geom_point()+
  theme_bw() +
  geom_smooth(method = "lm") +
  stat_regline_equation(ggplot2::aes(
  label =  paste(..eq.label.., ..rr.label.., sep = "*plain(\",\")~~")))
```

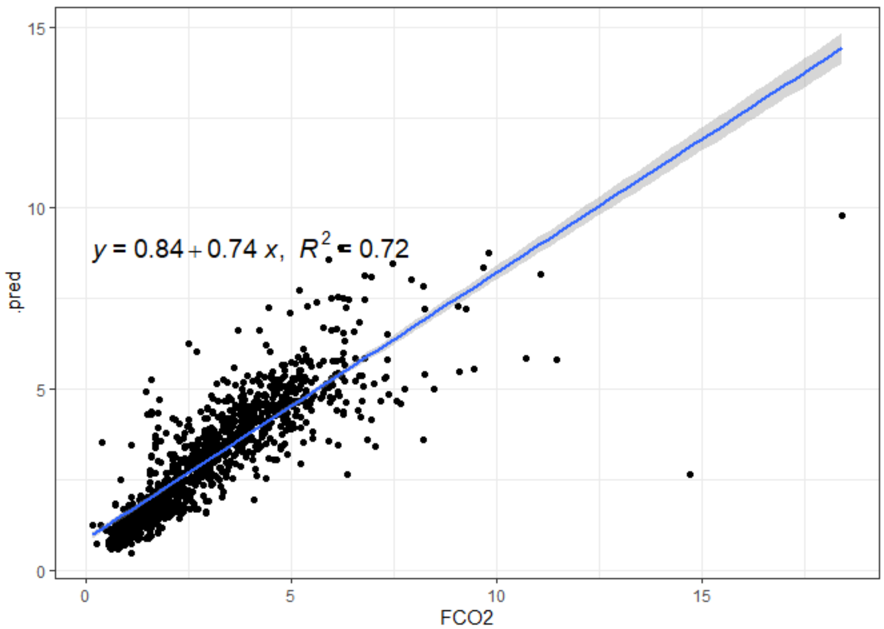



```
fco2_xgb_last_fit_model <-fco2_xgb_last_fit$.workflow[[1]]$fit$fit
vip(fco2_xgb_last_fit_model)
```



Métricas

```
da <- fco2_test_preds %>%
  filter(FCO2 > 0, .pred>0 )

my_r <- cor(da$FCO2,da$.pred)
my_r2 <- my_r*my_r
my_mse <- Metrics::mse(da$FCO2,da$.pred)
my_rmse <- Metrics::rmse(da$FCO2,
                         da$.pred)
my_mae <- Metrics::mae(da$FCO2,da$.pred)
my_mape <- Metrics::mape(da$FCO2,da$.pred)*100


fco2_test_preds %>%
  ggplot(aes(x=FCO2,y=.pred))+
  geom_point()+
  geom_smooth(method = "lm")+
  stat_regline_equation(ggplot2::aes(
    label =  paste(..eq.label.., ..rr.label.., sep = "*plain(\",\")~~")),size=5)
```




```
  # ggplot2::annotate('text',x=10.4,y=16.7,label=paste0('RMSE = ',round(my_rmse,2),', MAPE = '
  #                                                     ,round(my_mape,2),'%'),size=5)+
  # theme_bw()
vector_of_metrics <- c(r=my_r, R2=my_r2, MSE=my_mse, RMSE=my_rmse, MAE=my_mae, MAPE=my_mape)
print(data.frame(vector_of_metrics))
#>      vector_of_metrics
#> r            0.8479290
#> R2           0.7189837
#> MSE          0.9951377
#> RMSE         0.9975659
#> MAE          0.6028209
#> MAPE        23.0930305
```