analysis

January 12, 2023

0.0.1 Set variables

[ ]:
```
## Year of period split
anno = "2016"
## How much months casuality analysis looks back
TAU_MAX = 12
```

0.0.2 Load libraries

[ ]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import datetime as dt
import seaborn as sns
import statsmodels.api as sm
from scipy import stats
from scipy.stats import shapiro
from scipy.stats import spearmanr
from scipy import stats
from statsmodels.tsa.seasonal import seasonal_decompose
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import TimeSeriesSplit
from sklearn.decomposition import PCA
from sklearn.metrics import pairwise_distances
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error, r2_score
from matplotlib.ticker import FormatStrFormatter
```

0.0.3 Load and visualize data

[ ]:
```
data = pd.read_csv('data.csv', header=0, parse_dates=[0], sep=',')
data.columns = data.columns.str.strip()
data.rename(columns={'CO2_Con':'CO2'}, inplace=True)
data['Datetime'] = pd.to_datetime(data["date"])
data = data[["Datetime","O2", "CO2", "Temperature", "Salinity", "pH", "EC50"]]
data
```

```
[ ]:        Datetime         O2        CO2  Temperature   Salinity        pH   EC50
     0    2003-01-01  244.25089  33.043930    13.899383  37.763194  8.155155    NaN
     1    2003-02-01  252.53078  30.830639    12.228910  37.792016  8.181169  28.97
     2    2003-03-01  254.69466  31.928104    13.029431  37.878502  8.168952  39.77
     3    2003-04-01  254.88481  33.393970    14.144464  37.888187  8.152712  55.44
     4    2003-05-01  249.18790  39.920483    18.658495  37.799844  8.087382  24.15
     ..          …         …         …          …        …        …       …
     232  2022-05-01  247.31284  43.736410    18.932010  38.191498  8.055904    NaN
     233  2022-06-01  230.25885  53.264680    24.568462  38.182266  7.983217    NaN
     234  2022-07-01  222.63089  58.078090    27.196798  38.172510  7.951786    NaN
     235  2022-08-01  221.80557  56.470406    26.143705  38.213444  7.961412    NaN
     236  2022-09-01  212.18929  52.375122    24.981016  38.151127  7.988306    NaN

     [237 rows x 7 columns]
```

Fill missing values of EC50 by rolling mean.

```
[ ]: data["EC50"] =  data["EC50"].rolling(min_periods=1, center=True, window=12).
      ↪mean()
     df = data.dropna()
```

0.0.4 PCA anomaly detection

```
[ ]: X = df[[ "O2", "CO2", "Temperature", "Salinity", "pH","EC50"]]
     ### PCA ANOMALY DETECTION ###
     rec_errors_samples = {}
     rec_errors_features = {}
     for i, (past_id,future_id) in enumerate(
         TimeSeriesSplit(20, test_size=11).split(X)
     ):
         scaler = StandardScaler()
         pca = PCA(0.7)
         pca.fit(scaler.fit_transform(X.iloc[past_id]))
         Xt = pca.inverse_transform(
             pca.transform(
                 scaler.transform(X.iloc[future_id])
             )
         )
         rec_errors_samples[past_id[-1]] = \
             np.linalg.norm(scaler.transform(X.iloc[future_id]) - Xt, axis=1)
         rec_errors_features[past_id[-1]] = \
             np.linalg.norm(scaler.transform(X.iloc[future_id]) - Xt, axis=0)
```

0.0.5 Decompose and plot data

[ ]:
```
def decompose(df, data_colum_name):
    data_decompose = df.set_index("Datetime")
    decompose_result_mult = seasonal_decompose(data_decompose[data_colum_name],␣
↪model="multiplicative",extrapolate_trend='freq',period=12,two_sided=False)
    trend = decompose_result_mult.trend
    seasonal = decompose_result_mult.seasonal
    residual = decompose_result_mult.resid
    res=decompose_result_mult
    #res.plot()
    trend.to_csv("trend_" + data_colum_name + ".csv")
    return res, seasonal, trend, residual
```

[ ]:
```
ec50, seasonal_ec50, trend_ec50, residual_ec50 = decompose(df, "EC50")
temperature, seasonal_temperature, trend_temperature, residual_temperature =␣
↪decompose(df, "Temperature")
ph, seasonal_pH, trend_pH, residual_pH = decompose(df, "pH")
salinity, seasonal_salinity, trend_salinity, residual_salinity = decompose(df,␣
↪"Salinity")
o2, seasonal_o2, trend_o2, residual_o2 = decompose(df, "O2")
co2, seasonal_co2, trend_co2, residual_co2 = decompose(df, "CO2")

df_trend = df.copy()
df_trend["EC50"] = trend_ec50.values
df_trend["Temperature"] = trend_temperature.values
df_trend["pH"] = trend_pH.values
df_trend["Salinity"] = trend_salinity.values
df_trend["O2"] = trend_o2.values
df_trend["CO2"] = trend_co2.values
```

[ ]:
```
df_pre =  df[(df['Datetime'] < anno + "-01-01")]
df_post =  df[(df['Datetime'] >= anno + "-01-01")]

ec50_pre, seasonal_ec50_pre, trend_ec50_pre, residual_ec50_pre =␣
↪decompose(df_pre, "EC50")
temperature_pre, seasonal_temperature_pre, trend_temperature_pre,␣
↪residual_temperature_pre = decompose(df_pre, "Temperature")
ph_pre, seasonal_pH_pre, trend_pH_pre, residual_pH_pre = decompose(df_pre, "pH")
salinity_pre, seasonal_salinity_pre, trend_salinity_pre, residual_salinity_pre␣
↪= decompose(df_pre, "Salinity")
o2_pre, seasonal_o2_pre, trend_o2_pre, residual_o2_pre = decompose(df_pre, "O2")
co2_pre, seasonal_co2_pre, trend_co2_pre, residual_co2_pre = decompose(df_pre,␣
↪"CO2")

trend_df_pre = df_pre[["O2", "CO2", "Temperature", "Salinity", "pH", "EC50"]].
↪dropna()
```

```
trend_df_pre["EC50"] = trend_ec50_pre.to_frame().dropna().values
trend_df_pre["O2"] = trend_o2_pre.to_frame().dropna().values
trend_df_pre["CO2"] = trend_co2_pre.to_frame().dropna().values
trend_df_pre["Temperature"] = trend_temperature_pre.to_frame().dropna().values
trend_df_pre["Salinity"] = trend_salinity_pre.to_frame().dropna().values
trend_df_pre["pH"] = trend_pH_pre.to_frame().dropna().values

ec50_post, seasonal_ec50_post, trend_ec50_post, residual_ec50_post =␣
 ↪decompose(df_post, "EC50")
temperature_post, seasonal_temperature_post, trend_temperature_post,␣
 ↪residual_temperature_post = decompose(df_post, "Temperature")
ph_post, seasonal_pH_post, trend_pH_post, residual_pH_post = decompose(df_post,␣
 ↪"pH")
salinity_post, seasonal_salinity_post, trend_salinity_post,␣
 ↪residual_salinity_post = decompose(df_post, "Salinity")
o2_post, seasonal_o2_post, trend_o2_post, residual_o2_post = decompose(df_post,␣
 ↪"O2")
co2_post, seasonal_co2_post, trend_co2_post, residual_co2_post =␣
 ↪decompose(df_post, "CO2")


trend_df_post = df_post[["O2", "CO2", "Temperature", "Salinity", "pH", "EC50"]].
 ↪dropna()
trend_df_post["EC50"] = trend_ec50_post.to_frame().dropna().values
trend_df_post["O2"] = trend_o2_post.to_frame().dropna().values
trend_df_post["CO2"] = trend_co2_post.to_frame().dropna().values
trend_df_post["Temperature"] = trend_temperature_post.to_frame().dropna().values
trend_df_post["Salinity"] = trend_salinity_post.to_frame().dropna().values
trend_df_post["pH"] = trend_pH_post.to_frame().dropna().values
```

[ ]:

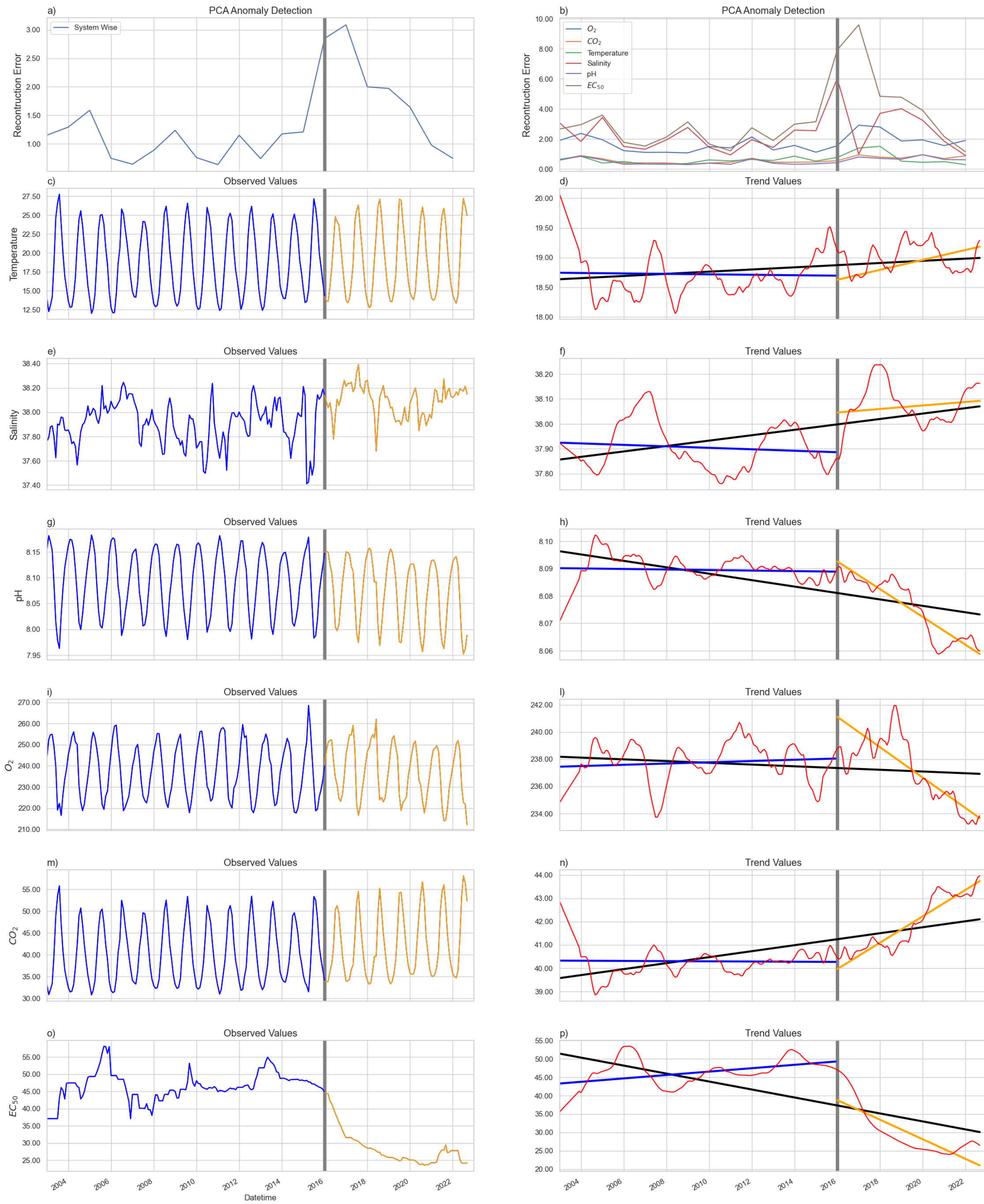
```
res2 = np.arange(np.datetime64("2003-01-01"), np.datetime64("2022-12-01"),  np.
 ↪timedelta64(1, 'Y'),  dtype='datetime64[M]')
res3 = np.arange(np.datetime64("2003-01-01"), np.datetime64("2022-12-01"),  np.
 ↪timedelta64(1, 'Y'),  dtype='datetime64[Y]')

def plotseasonal(res,res_pre, res_post, x1, x2, label , slopes, titoli,␣
 ↪etichetta=False):
    x1.set_ylabel(label , size='large')
    x1.set_title("Observed Values", size='large', loc='center')
    x2.set_title("Trend Values", size='large', loc='center')
    x1.set_title(titoli[0], size='large', loc='left')
    x2.set_title(titoli[1], size='large', loc='left')
    x1.yaxis.set_major_formatter(FormatStrFormatter('%.2f'))
    x2.yaxis.set_major_formatter(FormatStrFormatter('%.2f'))
    temp = res.trend.to_frame().dropna().reset_index()
    xx = temp['Datetime'].copy()
```

```
    temp['Datetime']=temp['Datetime'].map(dt.datetime.toordinal)
    X = temp["Datetime"].values.reshape(-1,1)
    X = sm.add_constant(X)
    Y = temp["trend"].values.reshape(-1,1)
    reg = sm.OLS(Y, X).fit()
    y_predicted = reg.predict(X)
    slope = str(reg.params[1])
    intercept = str(round(reg.params[0],5))
    x1.axvline(x=np.datetime64(anno + "-01-01"), color='gray', linewidth=5)
    x2.axvline(x=np.datetime64(anno + "-01-01"), color='gray', linewidth=5)
    res.observed.plot(ax=x1,  legend=False, color='blue')
    x2.plot(xx,y_predicted, color='black',linewidth=3)
    temp = res_pre.trend.to_frame().dropna().reset_index()
    xx = temp['Datetime'].copy()
    temp['Datetime']=temp['Datetime'].map(dt.datetime.toordinal)
    X = temp["Datetime"].values.reshape(-1,1)
    X = sm.add_constant(X)
    Y = temp["trend"].values.reshape(-1,1)
    reg = sm.OLS(Y, X).fit()
    y_predicted = reg.predict(X)
    slope_pre =  str(reg.params[1])
    intercept_pre = str(round(reg.params[0],5))
    res_pre.observed.plot(ax=x1, sharex=x1, legend=False, color='blue')
    x2.plot(xx,y_predicted, color='blue',linewidth=3)
    temp = res_post.trend.to_frame().dropna().reset_index()
    xx = temp['Datetime'].copy()
    temp['Datetime']=temp['Datetime'].map(dt.datetime.toordinal)
    X = temp["Datetime"].values.reshape(-1,1)
    X = sm.add_constant(X)
    Y = temp["trend"].values.reshape(-1,1)
    reg = sm.OLS(Y, X).fit()
    y_predicted = reg.predict(X)
    slope_post = str(reg.params[1])
    intercept_post = str(round(reg.params[0],5))
    res_post.observed.plot(ax=x1, legend=False, color='orange')
    x2.plot(xx,y_predicted, color='orange',linewidth=3)
    slopes = label + "2003-2022 S:" +  slope + " I:" + "    <" + anno +" S:" + slope_pre + "  - I:" + "   >=" + anno +" S:" +  slope_post
    print(slopes)
    res.trend.plot(ax=x2, legend=False, color='red')
    x2.axis(xmin=np.datetime64("2003-01-01"), xmax = np.datetime64("2023-01-01"))
    if etichetta:
        x2.set_xlabel("")
    else :
        x1.set_xlabel("")
        x2.set_xlabel("")
```

```python
fig, axes = plt.subplots(ncols=2, nrows=7, sharex=True, sharey=False, figsize=(25,35))
plt.subplots_adjust(hspace = 0.3)
slopes = ""
cols = ["$O_{2}$","$CO_{2}$", "Temperature","Salinity", "pH", "$EC_{50}$"]
rows = ["Measures","Trend","Seasonality"]
n_features = len(cols)
for ax, col in zip(axes[0], cols):
    ax.set_title(col)
rec =   [np.mean(r) for r in rec_errors_samples.values()]
ff = plt.subplot(6,2,1)
plt.plot(res2,rec,label="System Wise")
ff.set_title("PCA Anomaly Detection", size='large', loc='center')
ff.set_title("a)", size='large', loc='left')
plt.ylabel('Recontruction Error', size='large');
plt.legend(loc="upper left")
ff.set_xlabel("")
ff.yaxis.set_major_formatter(FormatStrFormatter('%.2f'))
ff.axvline(x=np.datetime64("2016-01-01"), color='gray', linewidth=5)
plt.xlim(np.datetime64("2003-01-01"), np.datetime64("2023-01-01"))
ff = plt.subplot(6,2,2)
for i in range(n_features):
    rec = []
    for r in rec_errors_features.values():
        rec.append(r[i])
    plt.plot(res2,rec,label=cols[i])
plt.ylabel('Recontruction Error', size='large');
ff.set_title("PCA Anomaly Detection", size='large', loc='center')
ff.set_title("b)", size='large', loc='left')
ff.set_xlabel("")
ff.yaxis.set_major_formatter(FormatStrFormatter('%.2f'))
ff.axvline(x=np.datetime64(anno + "-01-01"), color='gray', linewidth=5)
plt.legend(loc="upper left")
plt.xlim(np.datetime64("2003-01-01"), np.datetime64("2023-01-01"))

plotseasonal(temperature, temperature_pre, temperature_post, axes[1,0], axes[1,1], "Temperature",slopes, titoli=["c)","d)"], etichetta=False )
plotseasonal(salinity, salinity_pre, salinity_post, axes[2,0], axes[2,1],"Salinity",slopes, titoli=["e)","f)"], etichetta=False, )
plotseasonal(ph, ph_pre, ph_post, axes[3,0], axes[3,1],"pH",slopes, titoli=["g)","h)"], etichetta=False)
plotseasonal(o2, o2_pre, o2_post, axes[4,0], axes[4,1],"$O_{2}$",slopes, titoli=["i)","l)"], etichetta=False)
plotseasonal(co2, co2_pre, co2_post, axes[5,0], axes[5,1], "$CO_{2}$",slopes, titoli=["m)","n)"], etichetta=False)
```

```python
plotseasonal(ec50, ec50_pre, ec50_post, axes[6,0], axes[6,1], "$EC_{50}$",slopes, titoli=["o)","p)"], etichetta=True)

plt.show()
fig.savefig("plots-" + anno + ".pdf")
```

```
Temperature2003-2022 S:5.000209979992878e-05 I:    <2016
S:-1.0352591164280084e-05  - I:   >=2016 S:0.00022933807033885046
Salinity2003-2022 S:2.971129753407759e-05 I:    <2016 S:-8.063835246369512e-06
- I:   >=2016 S:1.9200192605092498e-05
pH2003-2022 S:-3.212400103011905e-06 I:    <2016 S:-2.678549282452385e-07  - I:
>=2016 S:-1.3880295630349163e-05
$O_{2}$2003-2022 S:-0.00017505420198396472 I:    <2016 S:0.00012713522130422105
- I:   >=2016 S:-0.0030613454499755733
$CO_{2}$2003-2022 S:0.0003516702559631684 I:    <2016 S:-1.1671179518476463e-05
- I:   >=2016 S:0.001549811868944639
$EC_{50}$2003-2022 S:-0.0029649707772495576 I:    <2016 S:0.0012651809968117578
- I:   >=2016 S:-0.0072796709446532985
```



0.0.6 Period split

We can perform Kruskal-Wallis and Mann-Whitneyu for EC50 values between and after 01-01-2016.

[ ]:
```
stats.kruskal(df_pre["EC50"],df_post["EC50"] )
```

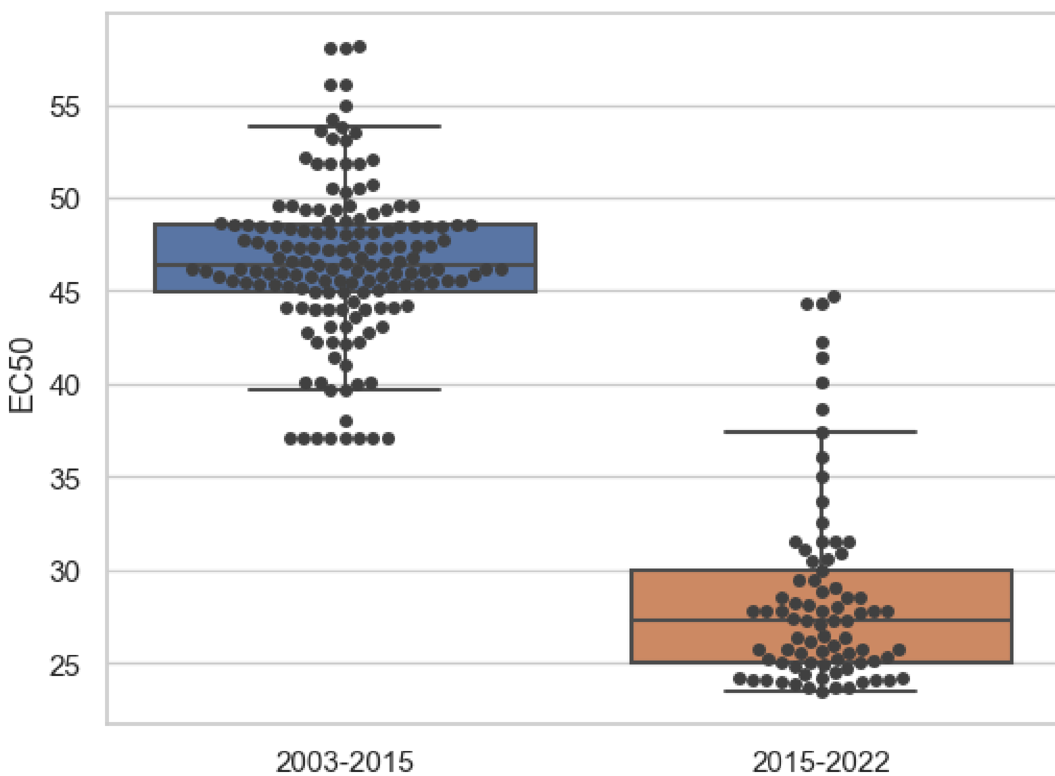
[ ]: KruskalResult(statistic=150.7374237488993, pvalue=1.1961316983628424e-34)

```
[ ]: stats.mannwhitneyu(df_pre["EC50"],df_post["EC50"])
```

[ ]: MannwhitneyuResult(statistic=12464.0, pvalue=1.2109868782577416e-34)

As pvalue is much greater than 0.05 we can refuse the null iphothesis that the medians of the two different periods are equal.

```
[ ]: sns.set(style="whitegrid")
df["2016-2022"] = (df['Datetime'] >= anno + "-01-01")
fig = plt.figure()
ax = sns.boxplot(x="2016-2022", y="EC50", data=df, showfliers = False)
ax = sns.swarmplot(x="2016-2022", y="EC50", data=df, color=".25")
plt.xticks([0, 1], ['2003-2015', '2015-2022'])
ax.set_xlabel('')

plt.show()
```



0.0.7 Correlation analysis

Test for if trends are normal distributed.

```
[ ]: print("EC50 - " + str(shapiro(trend_ec50)))
print("O2 - " + str(shapiro(trend_o2)))
print("CO2 - " + str(shapiro(trend_co2)))
print("Temperature - " + str(shapiro(trend_temperature)))
print("Salinity - " + str(shapiro(trend_salinity)))
print("pH - " + str(shapiro(trend_pH)))
```

```
EC50 - ShapiroResult(statistic=0.8668988943099976,
pvalue=1.6791276214508238e-13)
O2 - ShapiroResult(statistic=0.9687227010726929, pvalue=4.4526823330670595e-05)
CO2 - ShapiroResult(statistic=0.875939667224884, pvalue=5.556552397020798e-13)
Temperature - ShapiroResult(statistic=0.9771444201469421,
pvalue=0.0007096421322785318)
Salinity - ShapiroResult(statistic=0.9620153307914734,
pvalue=6.227187896001851e-06)
pH - ShapiroResult(statistic=0.8612942695617676, pvalue=8.223283843146814e-14)
```

They are not normal distributed. We have to use Spearman's algorithm to estimate the correlations between them.

```
[ ]: trend_df = data[["O2", "CO2", "Temperature", "Salinity", "pH", "EC50"]].dropna()
trend_df["EC50"] = trend_ec50.to_frame().dropna().values
trend_df["O2"] = trend_o2.to_frame().dropna().values
trend_df["CO2"] = trend_co2.to_frame().dropna().values
trend_df["Temperature"] = trend_temperature.to_frame().dropna().values
trend_df["Salinity"] = trend_salinity.to_frame().dropna().values
trend_df["pH"] = trend_pH.to_frame().dropna().values
```

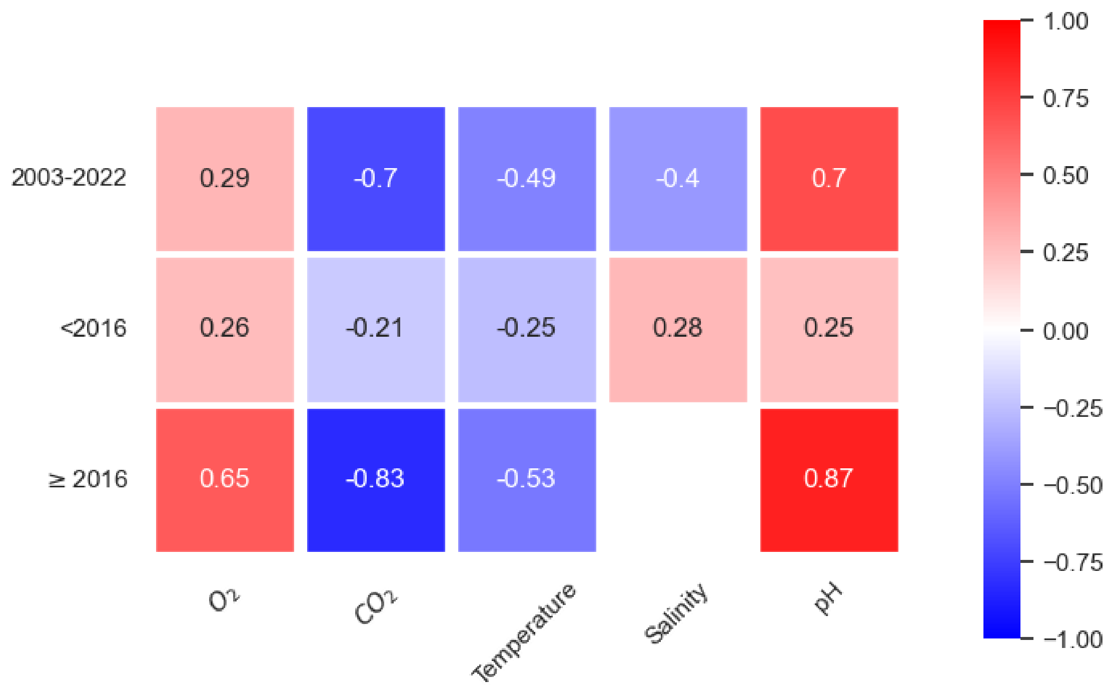
```
[ ]: def my_heat(corr, ax1) :
    axes = sns.heatmap(  corr, vmin=-1,
                            #mask=mask,
                            vmax=1,
                            #annot=annot,
                            linewidths=2, linecolor='black',
                            square=True, #linewidths=.5,
                            cbar_kws={"shrink": .5},
                            annot=True,
                            annot_kws={ "size": 12,
                                        #"color":"black",
                                        "weight":"bold"},
                            #shapesize=pval,
                            cmap='bwr',
                            rasterized=True,
                            ax=ax1)

def display_correlation(df, label):
    corr = df.corr(method="spearman")
    pval = df.corr(method=lambda x, y: spearmanr(x, y)[1]) - np.eye(*corr.shape)
```

```
    mask = np.triu(np.ones_like(corr, dtype=bool),  k=0)
    mask |= pval >= 0.05
    corr = corr[~mask]  # fill in NaN in the non-desired cells
    remove_empty_rows_and_cols = False
    if remove_empty_rows_and_cols:
        wanted_cols = np.flatnonzero(np.count_nonzero(~mask, axis=1))
        wanted_rows = np.flatnonzero(np.count_nonzero(~mask, axis=0))
        corr = corr.iloc[wanted_cols, wanted_rows]
    fig, ax = plt.subplots()
    heatmap = my_heat(corr,ax)
    plt.close()
    return(corr,pval)

def display_corr_pairs(df,label,color="cyan"):
    from decimal import Decimal
    s = set_title = np.vectorize(lambda ax,r,rho: ax.title.set_text("r = " +
                                        "{:.2f}".format(r) +
                                        '\n $\\rho$ = ' +
                                        #"{:.2f}".format(rho)
                                        '%.2E' % Decimal(rho)

                                        )
                                        if ax!=None else None
                              )

    r,pval= display_correlation(df,label)
    return(r)

heat_map_all = display_corr_pairs(trend_df, "ALL DATA")
heat_map_post = display_corr_pairs(trend_df_post, "POST " + anno)
heat_map_pre = display_corr_pairs(trend_df_pre, "PRE " + anno)
```

[ ]:

```
cols = ["$O_{2}$","$CO_{2}$", "Temperature","Salinity", "pH",  "$EC_{50}$"]
ycol= ["$EC_{50}$ Correlation"]
f,(ax1, axcb) = plt.subplots(1,2,
            gridspec_kw={'width_ratios':[1,0.05]},
             figsize=(7,5))
temp =heat_map_all.loc['EC50',:]
#display(temp)
temp_pre =heat_map_pre.loc['EC50',:]
temp_post =heat_map_post.loc['EC50',:]
ycol_all= ["2003-2022","<" + anno,"$\geq$" + anno ]
temp2 = np.vstack((temp,temp_pre,temp_post))
g3 = sns.heatmap( temp2, vmin=-1,
                            #mask=mask,
                            vmax=1,
                            #annot=annot,
```

```
                              xticklabels=cols, yticklabels=ycol_all,
                              linewidths=2, linecolor='black',
                              square=True,
                              annot=True,
                              cmap='bwr',
                              rasterized=True,
                              ax=ax1,
                              cbar_ax=axcb)
for i in range(temp2.shape[0] + 1):
    g3.axhline(i, color='white', lw=3)
for i in range(temp2.shape[1] + 1):
    g3.axvline(i, color='white', lw=6)
for ax in [g3]:
    tl = ax.get_xticklabels()
    ax.set_xticklabels(tl, rotation=45)
    tly = ax.get_yticklabels()
    ax.set_yticklabels(tly, rotation=0)
    ax.set_xlim(0,5)
plt.show()
f.savefig("heatmaps-" + anno + ".pdf")



heat_map_all = display_corr_pairs(trend_df, "ALL DATA")
```



```
[ ]:
```

0.0.8 Causality analysis

Stationarity To indagate causality we should work with stationary time series, so we test data.

```
[ ]: from statsmodels.tsa.stattools import adfuller, kpss
import pmdarima as pmd
# Stationarity
ALPHA = 0.05
# We apply the ADF and KPSS tests of statsmodels.stattools:
# statsmodels - ADF test
# null hypothesis: There is a unit root and the series is NOT stationary
# Low p-values are preferable
# get results as a dictionary
def ADF_statt(x):
     adf_test = adfuller(x, autolag="aic")
     t_stat, p_value, _, _, _, _  = adf_test
     conclusion = "non-stationary (unit root)" if p_value > ALPHA else␣
 ↪"stationary"
     res_dict = {"ADF statistic":t_stat, "p-value":p_value, "should we␣
 ↪difference?": (p_value > ALPHA), "conclusion": conclusion}
     return res_dict

# statsmodels - KPSS test
# more detailed output than pmdarima
# null hypothesis: There series is (at least trend-)stationary
# High p-values are preferable
# get results as a dictionary
def KPSS_statt(x):
     kpss_test = kpss(x)
     t_stat, p_value, _, critical_values  = kpss_test
     conclusion = "stationary" if p_value > ALPHA else "not stationary"
     res_dict = {"KPSS statistic":t_stat, "p-value":p_value, "should we␣
 ↪difference?": (p_value < ALPHA), "conclusion": conclusion}
     return res_dict

def test_stationary(data, variable) :
    # call the KPSS test:
    resKPSS = KPSS_statt(data[variable])
    print("---------" + variable + "----------------")
    # print dictionary of test results:
    print("KPSS test result for " + variable + " original data:")
    for key,value in (resKPSS.items()) :
        if key == "conclusion": print(key, ":", value)

import warnings
```

```
warnings.simplefilter("ignore")

# pmdarima also offers methods that suggest the order of first differencing,␣
 ↪based on either ADF or the KPSS test
test_stationary(df, "EC50")
test_stationary(df, "Temperature")
test_stationary(df, "pH")
test_stationary(df, "Salinity")
test_stationary(df, "CO2")
test_stationary(df, "O2")
```

```
---------EC50----------------
KPSS test result for EC50 original data:
conclusion : not stationary
---------Temperature----------------
KPSS test result for Temperature original data:
conclusion : stationary
---------pH----------------
KPSS test result for pH original data:
conclusion : stationary
---------Salinity----------------
KPSS test result for Salinity original data:
conclusion : not stationary
---------CO2----------------
KPSS test result for CO2 original data:
conclusion : stationary
---------O2----------------
KPSS test result for O2 original data:
conclusion : stationary
```

We need to differenciate EC50 and Salinity.

[ ]:
```
df["EC50_diff"] = df["EC50"].diff().dropna()
df["Salinity_diff"] = df["Salinity"].diff().dropna()

df_pre["EC50_diff"] = df_pre["EC50"].diff().dropna()
df_pre["Salinity_diff"] = df_pre["Salinity"].diff().dropna()
df_post["EC50_diff"] = df_post["EC50"].diff().dropna()
df_post["Salinity_diff"] = df_post["Salinity"].diff().dropna()
```

0.0.9 Forecast

Senarios

[ ]:
```
import statsforecast
from statsforecast import StatsForecast
```

```python
from statsforecast.models import AutoARIMA, ETS
```

[ ]:
```python
data_mean = data.mean()
data_mean
```

[ ]:
```
O2             237.615534
CO2             40.895385
Temperature     18.805030
Salinity        37.968813
pH               8.084307
EC50            40.416074
dtype: float64
```

[ ]:
```python
import numpy as np
import pandas as pd
dataset = pd.DataFrame()
forecast_dates = np.arange(np.datetime64("2023-01-01"), np.
 ↪datetime64("2042-01-01"),  np.timedelta64(1, 'M'),  dtype='datetime64[M]')
dataset["Datetime"] = pd.to_datetime(forecast_dates)
dataset["O2"] =  data_mean["O2"]
dataset["CO2"] =  data_mean["CO2"]
dataset["EC50"] =  data_mean["EC50"]
n = dataset.shape[0]
dataset_bad, dataset_mean, dataset_good = dataset.copy(), dataset.copy(),␣
 ↪dataset.copy()
```

[ ]:
```python
dataset_bad_temperature = np.linspace(data_mean["Temperature"], 22.48, n)
dataset_bad_salinity = np.linspace(data_mean["Salinity"], 38.84, n)
dataset_bad_ph = np.linspace(data_mean["pH"],  7.626, n)

display(dataset_bad_temperature )

dataset_bad["Temperature"] = dataset_bad_temperature
dataset_bad["Salinity"] = dataset_bad_salinity
dataset_bad["pH"] = dataset_bad_ph



dataset_good_temperature = np.linspace(data_mean["Temperature"], 19.48, n)
dataset_good_salinity = np.linspace(data_mean["Salinity"], 38.43, n)
dataset_good_ph = np.linspace(data_mean["pH"], 7.98916, n)

dataset_good["Temperature"] = dataset_good_temperature
dataset_good["Salinity"] = dataset_good_salinity
dataset_good["pH"] = dataset_good_ph
```

```python
dataset_mean_temperature = np.linspace(data_mean["Temperature"], 20.98, n)
dataset_mean_salinity = np.linspace(data_mean["Salinity"], 38.608, n)
dataset_mean_ph = np.linspace(data_mean["pH"], 7.80758, n)

dataset_mean["Temperature"] = dataset_mean_temperature
dataset_mean["Salinity"] = dataset_mean_salinity
dataset_mean["pH"] = dataset_mean_ph

dataset_bad.to_csv('data_LSTMS_bad2.csv')
dataset_mean.to_csv('data_LSTMS_mean2.csv')
dataset_good.to_csv('data_LSTMS_good2.csv')
len(seasonal_o2)
```

```
array([18.80502953, 18.82121882, 18.83740812, 18.85359742, 18.86978672,
       18.88597601, 18.90216531, 18.91835461, 18.93454391, 18.9507332 ,
       18.9669225 , 18.9831118 , 18.99930109, 19.01549039, 19.03167969,
       19.04786899, 19.06405828, 19.08024758, 19.09643688, 19.11262617,
       19.12881547, 19.14500477, 19.16119407, 19.17738336, 19.19357266,
       19.20976196, 19.22595126, 19.24214055, 19.25832985, 19.27451915,
       19.29070844, 19.30689774, 19.32308704, 19.33927634, 19.35546563,
       19.37165493, 19.38784423, 19.40403353, 19.42022282, 19.43641212,
       19.45260142, 19.46879071, 19.48498001, 19.50116931, 19.51735861,
       19.5335479 , 19.5497372 , 19.5659265 , 19.58211579, 19.59830509,
       19.61449439, 19.63068369, 19.64687298, 19.66306228, 19.67925158,
       19.69544088, 19.71163017, 19.72781947, 19.74400877, 19.76019806,
       19.77638736, 19.79257666, 19.80876596, 19.82495525, 19.84114455,
       19.85733385, 19.87352315, 19.88971244, 19.90590174, 19.92209104,
       19.93828033, 19.95446963, 19.97065893, 19.98684823, 20.00303752,
       20.01922682, 20.03541612, 20.05160541, 20.06779471, 20.08398401,
       20.10017331, 20.1163626 , 20.1325519 , 20.1487412 , 20.1649305 ,
       20.18111979, 20.19730909, 20.21349839, 20.22968768, 20.24587698,
       20.26206628, 20.27825558, 20.29444487, 20.31063417, 20.32682347,
       20.34301276, 20.35920206, 20.37539136, 20.39158066, 20.40776995,
       20.42395925, 20.44014855, 20.45633785, 20.47252714, 20.48871644,
       20.50490574, 20.52109503, 20.53728433, 20.55347363, 20.56966293,
       20.58585222, 20.60204152, 20.61823082, 20.63442012, 20.65060941,
       20.66679871, 20.68298801, 20.6991773 , 20.7153666 , 20.7315559 ,
       20.7477452 , 20.76393449, 20.78012379, 20.79631309, 20.81250238,
       20.82869168, 20.84488098, 20.86107028, 20.87725957, 20.89344887,
       20.90963817, 20.92582747, 20.94201676, 20.95820606, 20.97439536,
       20.99058465, 21.00677395, 21.02296325, 21.03915255, 21.05534184,
       21.07153114, 21.08772044, 21.10390973, 21.12009903, 21.13628833,
       21.15247763, 21.16866692, 21.18485622, 21.20104552, 21.21723482,
       21.23342411, 21.24961341, 21.26580271, 21.281992  , 21.2981813 ,
       21.3143706 , 21.3305599 , 21.34674919, 21.36293849, 21.37912779,
       21.39531709, 21.41150638, 21.42769568, 21.44388498, 21.46007427,
       21.47626357, 21.49245287, 21.50864217, 21.52483146, 21.54102076,
```

```
       21.55721006, 21.57339935, 21.58958865, 21.60577795, 21.62196725,
       21.63815654, 21.65434584, 21.67053514, 21.68672444, 21.70291373,
       21.71910303, 21.73529233, 21.75148162, 21.76767092, 21.78386022,
       21.80004952, 21.81623881, 21.83242811, 21.84861741, 21.86480671,
       21.880996  , 21.8971853 , 21.9133746 , 21.92956389, 21.94575319,
       21.96194249, 21.97813179, 21.99432108, 22.01051038, 22.02669968,
       22.04288897, 22.05907827, 22.07526757, 22.09145687, 22.10764616,
       22.12383546, 22.14002476, 22.15621406, 22.17240335, 22.18859265,
       22.20478195, 22.22097124, 22.23716054, 22.25334984, 22.26953914,
       22.28572843, 22.30191773, 22.31810703, 22.33429632, 22.35048562,
       22.36667492, 22.38286422, 22.39905351, 22.41524281, 22.43143211,
       22.44762141, 22.4638107 , 22.48      ])
```

[ ]: 237

```
[ ]: df = data
###apply seasonal to scenarios
ss_temperature = seasonal_temperature.to_numpy()[len(seasonal_temperature)-n:]
tt_temperature = 1.0#trend.to_numpy()[len(trend)-n:]
#tt = sklearn.preprocessing.minmax_scale(tt, feature_range=(1,1.001))

ss_pH = seasonal_pH.to_numpy()[len(seasonal_pH)-n:]
tt_pH = 1.0#trend.to_numpy()[len(trend)-n:]
#tt = sklearn.preprocessing.minmax_scale(tt, feature_range=(1,1.001))

ss_salinity= seasonal_salinity.to_numpy()[len(seasonal_salinity)-n:]
tt_salinity = 1.0#trend.to_numpy()[len(trend)-n:]
#tt = sklearn.preprocessing.minmax_scale(tt, feature_range=(1,1.001))

ss_o2 = seasonal_o2.to_numpy()[len(seasonal_o2)-n:]
tt_o2 = 1.0#trend.to_numpy()[len(trend)-n:]
#tt = sklearn.preprocessing.minmax_scale(tt, feature_range=(1,1.001))

ss_co2 = seasonal_co2.to_numpy()[len(seasonal_co2)-n:]
tt_co2 = 1.0#trend.to_numpy()[len(trend)-n:]
#tt = sklearn.preprocessing.minmax_scale(tt, feature_range=(1,1.001))


dataset_bad["Temperature"] = dataset_bad["Temperature"].mul(ss_temperature,
 ↪axis=0).mul(tt_temperature, axis=0)
dataset_bad["Salinity"] = dataset_bad["Salinity"].mul(ss_salinity, axis=0).
 ↪mul(tt_salinity, axis=0)
dataset_bad["pH"] = dataset_bad["pH"].mul(ss_pH, axis=0).mul(tt_pH, axis=0)
dataset_bad["O2"] = dataset_bad["O2"].mul(ss_o2, axis=0).mul(tt_o2, axis=0)
dataset_bad["CO2"] = dataset_bad["CO2"].mul(ss_co2, axis=0).mul(tt_co2, axis=0)
```

```
dataset_good["Temperature"] = dataset_good["Temperature"].mul(ss_temperature,␣
↪axis=0).mul(tt_temperature, axis=0)
dataset_good["Salinity"] = dataset_good["Salinity"].mul(ss_salinity, axis=0).
↪mul(tt_salinity, axis=0)
dataset_good["pH"] = dataset_good["pH"].mul(ss_pH, axis=0).mul(tt_pH, axis=0)
dataset_good["O2"] = dataset_good["O2"].mul(ss_o2, axis=0).mul(tt_o2, axis=0)
dataset_good["CO2"] = dataset_good["CO2"].mul(ss_co2, axis=0).mul(tt_co2,␣
↪axis=0)

dataset_mean["Temperature"] = dataset_mean["Temperature"].mul(ss_temperature,␣
↪axis=0).mul(tt_temperature, axis=0)
dataset_mean["Salinity"] = dataset_mean["Salinity"].mul(ss_salinity, axis=0).
↪mul(tt_salinity, axis=0)
dataset_mean["pH"] = dataset_mean["pH"].mul(ss_pH, axis=0).mul(tt_pH, axis=0)
dataset_mean["O2"] = dataset_mean["O2"].mul(ss_o2, axis=0).mul(tt_o2, axis=0)
dataset_mean["CO2"] = dataset_mean["CO2"].mul(ss_co2, axis=0).mul(tt_co2,␣
↪axis=0)
```

Forecast with ARIMA: CO2

[ ]:
```
def plot_with_int_all(a,label_a, b, label_b, c, label_c, real, label_real,␣
↪rename) :
    fig, ax = plt.subplots(1, 1, figsize = (20, 7))

    df_plot = pd.concat([Y_train_df, a]).set_index('ds')
    df_plot.rename(columns = {'AutoARIMA':label_a}, inplace = True)
    df_plot.rename(columns = {real:rename}, inplace = True)
    df_plot[[rename]].plot(ax=ax, linewidth=2, color='blue')
    df_plot[[label_a]].plot(ax=ax, linewidth=2, label=label_a, color='green')
    ax.fill_between(df_plot.index,
                    df_plot['AutoARIMA-lo-95'],
                    df_plot['AutoARIMA-hi-95'],
                    alpha=.1,
                    color='green'#,
                    #label='auto_arima_level_95' + label_a
                    )

    df_plot = pd.concat([Y_train_df, b]).set_index('ds')
    df_plot.rename(columns = {'AutoARIMA':label_b}, inplace = True)
    df_plot[[label_b]].plot(ax=ax, linewidth=2, label=label_b,color='orange')
    ax.fill_between(df_plot.index,
                    df_plot['AutoARIMA-lo-95'],
                    df_plot['AutoARIMA-hi-95'],
                    alpha=.1,
                    color='orange'#,
                    #label='auto_arima_level_95' + label_b
                    )
```

```
    df_plot = pd.concat([Y_train_df, c]).set_index('ds')
    df_plot.rename(columns = {'AutoARIMA':label_c}, inplace = True)
    df_plot[[label_c]].plot(ax=ax, linewidth=2, label=label_c,color='red')
    ax.fill_between(df_plot.index,
                    df_plot['AutoARIMA-lo-95'],
                    df_plot['AutoARIMA-hi-95'],
                    alpha=.1,
                    color='red'#,
                    #label='auto_arima_level_95' + label_c
                    )


    #ax.set_title('EC50 Forecast', fontsize=22)
    ax.set_ylabel(label_real, fontsize=20)
    ax.set_xlabel('Date', fontsize=20)
    ax.legend(prop={'size': 15})
    plt.xlim(np.datetime64("2003-01-01"), np.datetime64("2040-01-01"))
    ax.set_ylim([0, 80])

    ax = plt.gca()
    ax.grid(True)
    for label in (ax.get_xticklabels() + ax.get_yticklabels()):
        label.set_fontsize(20)
    fig.savefig("forecast.pdf")
```

[ ]:

```
Y_df = pd.DataFrame({'unique_id': np.ones(len(df)),
                     'ds': df["Datetime"],
                     #'EC50': df["EC50"],
                     'CO2': df["CO2"],
                     #'O2': df["EC50"],
                     #'Salinity': df["Salinity"],
                     #'pH': df["pH"],
                     #'Temperature': df["Temperature"]
                     })
Y_df_full = pd.DataFrame({'unique_id': np.ones(len(df)),
                     'ds': df["Datetime"],
                     #'EC50': df["EC50"],
                     'CO2': df["CO2"],
                     #'O2': df["O2"],
                     'Salinity': df["Salinity"],
                     'pH': df["pH"],
                     'Temperature': df["Temperature"]
                     })

Y_df_woEC50 = pd.DataFrame({'unique_id': np.ones(len(df)),
                     'ds': df["Datetime"],
```

```
                      #'EC50': df["EC50"],
                      #'CO2': df["CO2"],
                      #'O2': df["O2"],
                      'Salinity': df["Salinity"],
                      'pH': df["pH"],
                      'Temperature': df["Temperature"]
                      })

Y_train_df = Y_df_full[Y_df_full.ds<='2022-01-01']
Y_train_df_woEC50 = Y_df[Y_df_full.ds<='2022-01-01']
Y_test_df_woEC50 = Y_df[Y_df_full.ds>'2022-01-01']

scenario_bad = pd.DataFrame({'unique_id': np.ones(len(dataset_bad)),
                      'ds': dataset_bad["Datetime"],
                      #'EC50': df["EC50"],
                      #'CO2': dataset_bad["CO2"],
                      #'O2': dataset_bad["O2"],
                      'Salinity': dataset_bad["Salinity"],
                      'pH': dataset_bad["pH"],
                      'Temperature': dataset_bad["Temperature"]
                      })

scenario_good = pd.DataFrame({'unique_id': np.ones(len(dataset_good)),
                      'ds': dataset_good["Datetime"],
                      #'EC50': df["EC50"],
                      #'CO2': dataset_good["CO2"],
                      #'O2': dataset_good["O2"],
                      'Salinity': dataset_good["Salinity"],
                      'pH': dataset_good["pH"],
                      'Temperature': dataset_good["Temperature"]
                      })

scenario_mean = pd.DataFrame({'unique_id': np.ones(len(dataset_mean)),
                      'ds': dataset_mean["Datetime"],
                      #'EC50': df["EC50"],
                      #'CO2': dataset_mean["CO2"],
                      #'O2': dataset_mean["O2"],
                      'Salinity': dataset_mean["Salinity"],
                      'pH': dataset_mean["pH"],
                      'Temperature': dataset_mean["Temperature"]
                      })

xreg_test = Y_df_woEC50[Y_df_full.ds>'2022-01-01']

xreg_test =  pd.concat([xreg_test], ignore_index=True)
xreg_test["ds"] = pd.date_range(start='2022-01-01', periods=len(xreg_test),
  ↪freq='M')
```

```
[ ]: #Define the parameters that you want to use in your models.
season_length = 12
# Note: For all models the following parameters are passed automaticly and␣
 ↪don't need to be declared: (X, h, future_xreg)

models = [
    AutoARIMA(season_length=season_length)#,
    #ETS(season_length=season_length, model='ZMZ')
]
model = StatsForecast(
    df=Y_train_df,
    models=models,
    freq='M',
    n_jobs=-1,
)
```

```
[ ]: horizon = len(xreg_test)
Y_hat_df_xreg = model.forecast(horizon, X_df=xreg_test.set_index('unique_id'))
#Y_hat_df_xreg = model.forecast(horizon)
Y_hat_df_xreg = Y_hat_df_xreg.reset_index()
df_plot = pd.concat([Y_train_df, Y_hat_df_xreg]).set_index('ds')
df_plot.columns = df_plot.columns.str.replace('AutoARIMA', 'TEST')
```

```
[ ]: horizon = len(scenario_bad)
Y_hat_df_xreg_bad = model.forecast(horizon, X_df=scenario_bad.
 ↪set_index('unique_id'))
#Y_hat_df_xreg = model.forecast(horizon)
Y_hat_df_xreg_bad = Y_hat_df_xreg_bad.reset_index()
df_plot_bad = pd.concat([Y_train_df, Y_hat_df_xreg_bad]).set_index('ds')
df_plot_bad.columns = df_plot_bad.columns.str.replace('AutoARIMA', 'BAD')
```

```
[ ]: horizon = len(scenario_good)
Y_hat_df_xreg_good = model.forecast(horizon, X_df=scenario_good.
 ↪set_index('unique_id'))
#Y_hat_df_xreg = model.forecast(horizon)
Y_hat_df_xreg_good = Y_hat_df_xreg_good.reset_index()
df_plot_good = pd.concat([Y_train_df, Y_hat_df_xreg_good]).set_index('ds')
df_plot_good.columns = df_plot_good.columns.str.replace('AutoARIMA', 'GOOD')
```

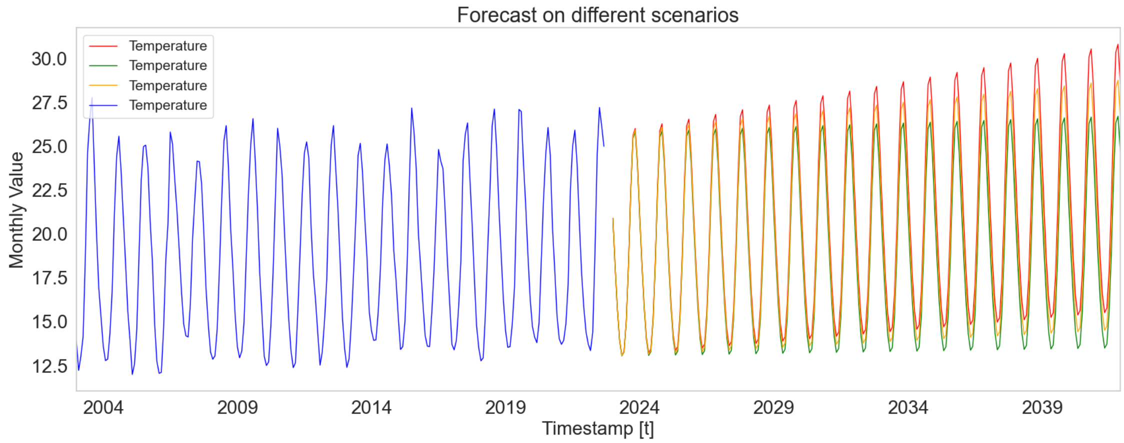
```
[ ]: horizon = len(scenario_mean)
Y_hat_df_xreg_mean = model.forecast(horizon, X_df=scenario_mean.
 ↪set_index('unique_id'))
#Y_hat_df_xreg = model.forecast(horizon)
Y_hat_df_xreg_mean = Y_hat_df_xreg_mean.reset_index()
df_plot_mean = pd.concat([Y_train_df, Y_hat_df_xreg_mean]).set_index('ds')
df_plot_mean.columns = df_plot_mean.columns.str.replace('AutoARIMA', 'MEAN')
```

```
[ ]: Y_hat_df_intervals_good = model.forecast(horizon, level=(80, 95),␣
     ↪X_df=scenario_good.set_index('unique_id'))
     df_plot = pd.concat([Y_train_df, Y_hat_df_intervals_good]).set_index('ds')
```

```
[ ]: #We are going to plot the models againts the real values of test.

     fig, ax = plt.subplots(1, 1, figsize = (20, 7))

     #df_plot[['EC50', 'TEST']].plot(ax=ax, linewidth=10)
     #df_plot_good[['GOOD']].plot(ax=ax, linewidth=1, color='green')
     #df_plot_mean[['MEAN']].plot(ax=ax, linewidth=1, color='orange')
     #df_plot_bad[['BAD']].plot(ax=ax, linewidth=1, color='red')

     bad_temp = scenario_bad[["ds", "Temperature"]]

     display(bad_temp)

     bad_temp = bad_temp.set_index('ds')
     bad_temp["Temperature"].plot(ax=ax, linewidth=1, color='red')

     good_temp = scenario_good[["ds", "Temperature"]]
     good_temp = good_temp.set_index("ds")
     good_temp["Temperature"].plot(ax=ax, linewidth=1, color='green')

     mean_temp = scenario_mean[["ds", "Temperature"]]
     mean_temp = mean_temp.set_index("ds")
     mean_temp["Temperature"].plot(ax=ax, linewidth=1, color='orange')



     Y_df = pd.DataFrame({
                         'ds': df["Datetime"],
                         'Temperature': df["Temperature"]})
     Y_df = Y_df.set_index("ds")
     display(Y_df)


     Y_df["Temperature"].plot(ax=ax, linewidth=1, color='blue')

     dataset_good["CO2"]= df_plot_good[['GOOD']]['GOOD'].array[-horizon:]
     dataset_mean["CO2"] = df_plot_mean[['MEAN']]['MEAN'].array[-horizon:]
     dataset_bad["CO2"] = df_plot_bad[['BAD']]['BAD'].array[-horizon:]

     #ax.fill_between(df_plot.index,
     #                 df_plot['AutoARIMA-lo-95'],
     #                 df_plot['AutoARIMA-hi-95'],
     #                 alpha=.2,
```

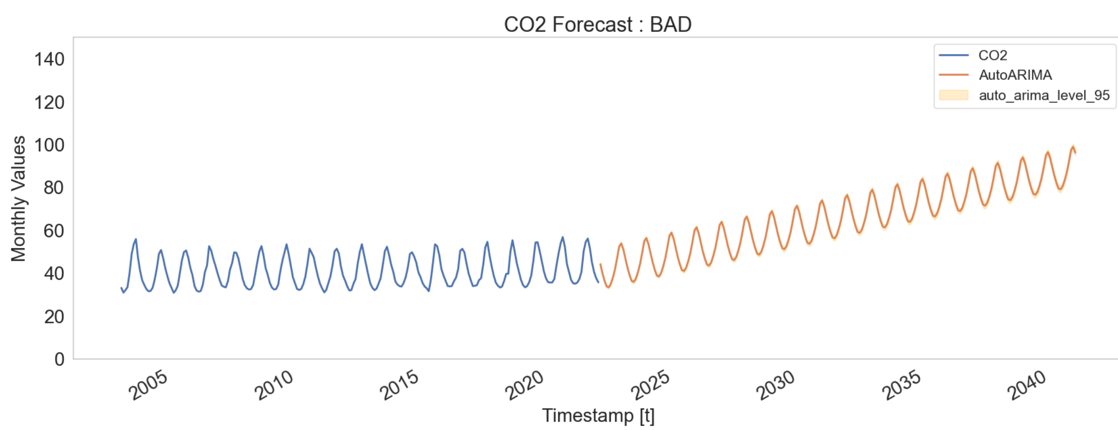
```
#                 color='orange',
#                 label='GOOD_level_95')

#df_plot.plot(ax=ax, linewidth=10)
fd_plot_real = Y_df_full.set_index('ds')
#fd_plot_real[['EC50']].plot(ax=ax, linewidth=5)
ax.set_title('Forecast on different scenarios', fontsize=22)
ax.set_ylabel('Monthly Value', fontsize=20)
ax.set_xlabel('Timestamp [t]', fontsize=20)
ax.legend(prop={'size': 15})
ax.grid()
for label in (ax.get_xticklabels() + ax.get_yticklabels()):
    label.set_fontsize(20)
```

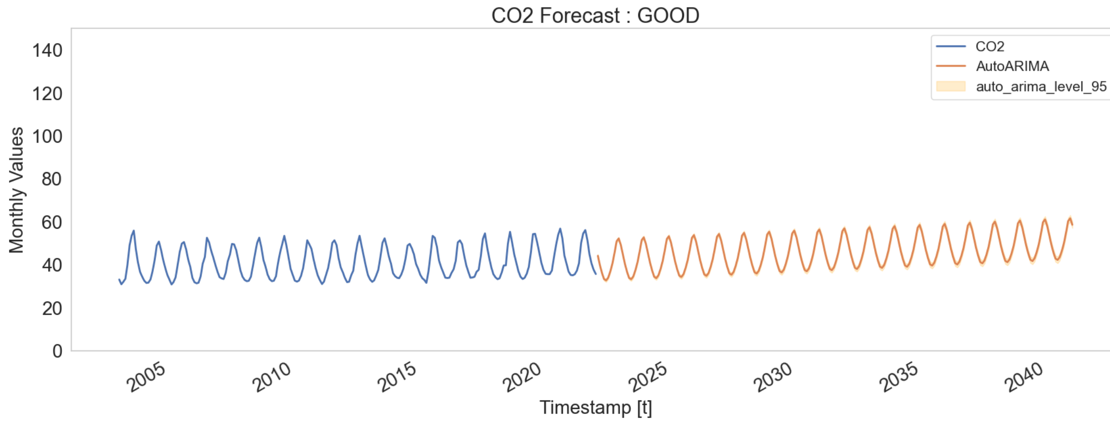
```
            ds  Temperature
0   2023-01-01    20.892152
1   2023-02-01    18.186433
2   2023-03-01    15.767156
3   2023-04-01    13.970393
4   2023-05-01    13.086998
..         …          …
223 2041-08-01    21.714358
224 2041-09-01    26.668356
225 2041-10-01    30.335540
226 2041-11-01    30.798026
227 2041-12-01    28.533934

[228 rows x 2 columns]

            Temperature
ds
2003-01-01    13.899383
2003-02-01    12.228910
2003-03-01    13.029431
2003-04-01    14.144464
2003-05-01    18.658495
…                 …
2022-05-01    18.932010
2022-06-01    24.568462
2022-07-01    27.196798
2022-08-01    26.143705
2022-09-01    24.981016

[237 rows x 1 columns]
```

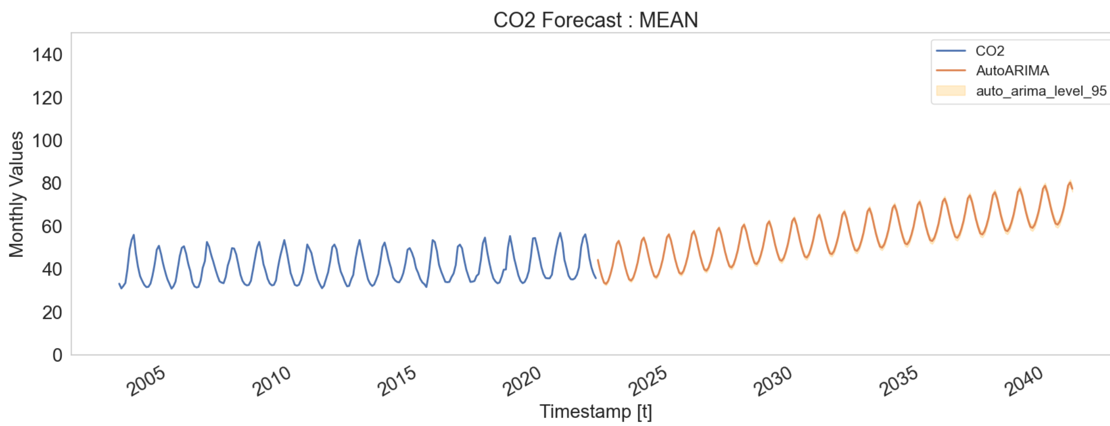


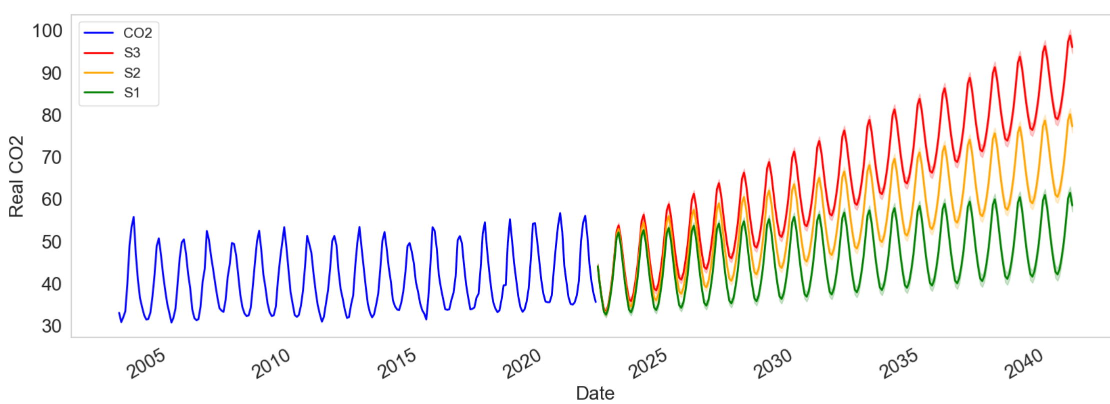

```
[ ]: # Then we plot the intervals
def plot_with_int(Y_hat_df_intervals,label) :
    fig, ax = plt.subplots(1, 1, figsize = (20, 7))
    df_plot = pd.concat([Y_train_df, Y_hat_df_intervals]).set_index('ds')
    df_plot[['CO2', 'AutoARIMA']].plot(ax=ax, linewidth=2)
    #ax.fill_between(df_plot.index,
    #                df_plot['AutoARIMA-lo-80'],
    #                df_plot['AutoARIMA-hi-80'],
    #                alpha=.35,
    #                color='orange',
    #                label='auto_arima_level_80')
    ax.fill_between(df_plot.index,
                    df_plot['AutoARIMA-lo-95'],
                    df_plot['AutoARIMA-hi-95'],
                    alpha=.2,
                    color='orange',
                    label='auto_arima_level_95')
    ax.set_title('CO2 Forecast : ' + label, fontsize=22)
    ax.set_ylabel('Monthly Values', fontsize=20)
    ax.set_xlabel('Timestamp [t]', fontsize=20)
    ax.legend(prop={'size': 15})
    ax.set_ylim([0, 150])
    ax.grid()
    for label in (ax.get_xticklabels() + ax.get_yticklabels()):
        label.set_fontsize(20)

###BAD
# You just need to add the `level` argument to the `forecast` method
# as folloows
Y_hat_df_intervals = model.forecast(horizon, level=(80, 95), X_df=scenario_bad.
 ↪set_index('unique_id'))
plot_with_int(Y_hat_df_intervals, "BAD")
```

```
#####GOOD
# You just need to add the `level` argument to the `forecast` method
# as folloows
Y_hat_df_intervals = model.forecast(horizon, level=(80, 95), X_df=scenario_good.
 ↪set_index('unique_id'))
plot_with_int(Y_hat_df_intervals, "GOOD")
# Then we plot the intervals

#####MEAN
# You just need to add the `level` argument to the `forecast` method
# as folloows
Y_hat_df_intervals = model.forecast(horizon, level=(80, 95), X_df=scenario_mean.
 ↪set_index('unique_id'))
plot_with_int(Y_hat_df_intervals, "MEAN")



bad = model.forecast(horizon, level=(80, 95), X_df=scenario_bad.
 ↪set_index('unique_id'))
good= model.forecast(horizon, level=(80, 95), X_df=scenario_good.
 ↪set_index('unique_id'))
mean = model.forecast(horizon, level=(80, 95), X_df=scenario_mean.
 ↪set_index('unique_id'))

plot_with_int_all(bad, "S3",mean, "S2",good, "S1", "CO2", "Real CO2")
```









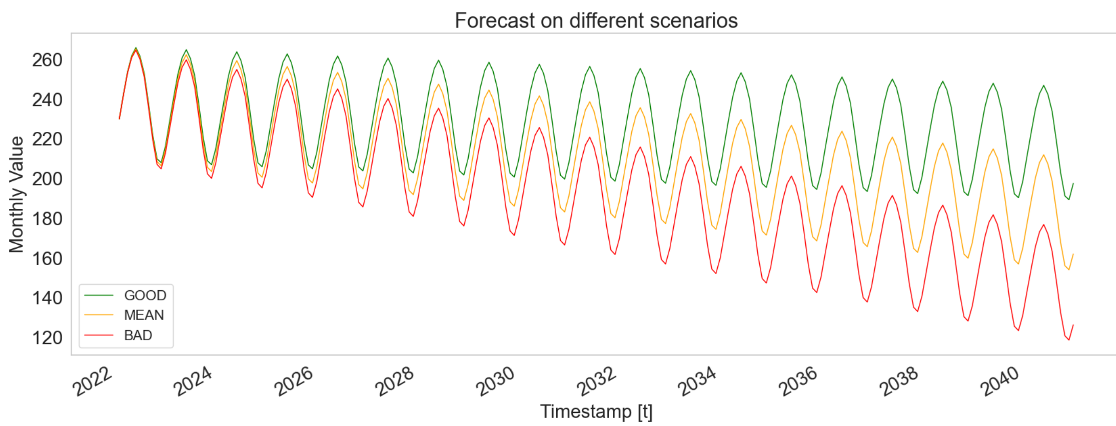
Forecast with ARIMA: O2

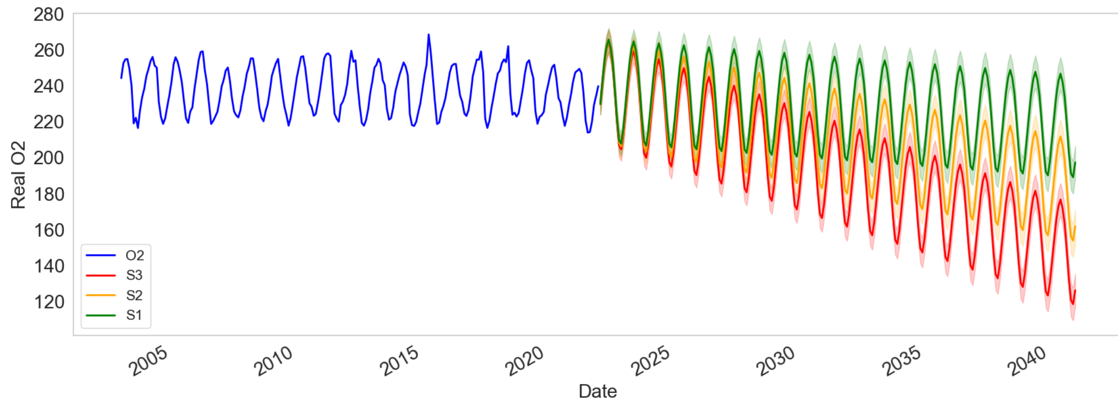
```
[ ]: Y_df = pd.DataFrame({'unique_id': np.ones(len(df)),
                         'ds': df["Datetime"],
                         #'EC50': df["EC50"],
                         #'CO2': df["CO2"],
                         'O2': df["EC50"],
                         #'Salinity': df["Salinity"],
                         #'pH': df["pH"],
                         #'Temperature': df["Temperature"]
                         })
     Y_df_full = pd.DataFrame({'unique_id': np.ones(len(df)),
                         'ds': df["Datetime"],
                         #'EC50': df["EC50"],
                         #'CO2': df["CO2"],
                         'O2': df["O2"],
                         'Salinity': df["Salinity"],
                         'pH': df["pH"],
                         'Temperature': df["Temperature"]
                         })

     Y_df_woEC50 = pd.DataFrame({'unique_id': np.ones(len(df)),
                         'ds': df["Datetime"],
                         #'EC50': df["EC50"],
                         #'CO2': df["CO2"],
                         #'O2': df["O2"],
                         'Salinity': df["Salinity"],
                         'pH': df["pH"],
                         'Temperature': df["Temperature"]
                         })

     Y_train_df = Y_df_full[Y_df_full.ds<='2022-01-01']
     Y_train_df_woEC50 = Y_df[Y_df_full.ds<='2022-01-01']
     Y_test_df_woEC50 = Y_df[Y_df_full.ds>'2022-01-01']

     scenario_bad = pd.DataFrame({'unique_id': np.ones(len(dataset_bad)),
                         'ds': dataset_bad["Datetime"],
                         #'EC50': df["EC50"],
                         #'CO2': dataset_bad["CO2"],
                         #'O2': dataset_bad["O2"],
                         'Salinity': dataset_bad["Salinity"],
                         'pH': dataset_bad["pH"],
                         'Temperature': dataset_bad["Temperature"]
                         })

     scenario_good = pd.DataFrame({'unique_id': np.ones(len(dataset_good)),
                         'ds': dataset_good["Datetime"],
                         #'EC50': df["EC50"],
                         #'CO2': dataset_good["CO2"],
```

```
                     #'O2': dataset_good["O2"],
                     'Salinity': dataset_good["Salinity"],
                     'pH': dataset_good["pH"],
                     'Temperature': dataset_good["Temperature"]
                     })

scenario_mean = pd.DataFrame({'unique_id': np.ones(len(dataset_mean)),
                     'ds': dataset_mean["Datetime"],
                     #'EC50': df["EC50"],
                     #'CO2': dataset_mean["CO2"],
                     #'O2': dataset_mean["O2"],
                     'Salinity': dataset_mean["Salinity"],
                     'pH': dataset_mean["pH"],
                     'Temperature': dataset_mean["Temperature"]
                     })

xreg_test = Y_df_woEC50[Y_df_full.ds>'2022-01-01']

xreg_test =  pd.concat([xreg_test], ignore_index=True)
xreg_test["ds"] = pd.date_range(start='2022-01-01', periods=len(xreg_test),␣
↪freq='M')

#Define the parameters that you want to use in your models.
season_length = 12
# Note: For all models the following parameters are passed automaticly and␣
↪don't need to be declared: (X, h, future_xreg)

models = [
    AutoARIMA(season_length=season_length)#,
    #ETS(season_length=season_length, model='ZMZ')
]
model = StatsForecast(
    df=Y_train_df,
    models=models,
    freq='M',
    n_jobs=-1,
)

horizon = len(xreg_test)
Y_hat_df_xreg = model.forecast(horizon, X_df=xreg_test.set_index('unique_id'))
#Y_hat_df_xreg = model.forecast(horizon)
Y_hat_df_xreg = Y_hat_df_xreg.reset_index()
df_plot = pd.concat([Y_train_df, Y_hat_df_xreg]).set_index('ds')
df_plot.columns = df_plot.columns.str.replace('AutoARIMA', 'TEST')

horizon = len(scenario_bad)
```

```python
Y_hat_df_xreg_bad = model.forecast(horizon, X_df=scenario_bad.
 ↪set_index('unique_id'))
#Y_hat_df_xreg = model.forecast(horizon)
Y_hat_df_xreg_bad = Y_hat_df_xreg_bad.reset_index()
df_plot_bad = pd.concat([Y_train_df, Y_hat_df_xreg_bad]).set_index('ds')
df_plot_bad.columns = df_plot_bad.columns.str.replace('AutoARIMA', 'BAD')

horizon = len(scenario_good)
Y_hat_df_xreg_good = model.forecast(horizon, X_df=scenario_good.
 ↪set_index('unique_id'))
#Y_hat_df_xreg = model.forecast(horizon)
Y_hat_df_xreg_good = Y_hat_df_xreg_good.reset_index()
df_plot_good = pd.concat([Y_train_df, Y_hat_df_xreg_good]).set_index('ds')
df_plot_good.columns = df_plot_good.columns.str.replace('AutoARIMA', 'GOOD')

horizon = len(scenario_mean)
Y_hat_df_xreg_mean = model.forecast(horizon, X_df=scenario_mean.
 ↪set_index('unique_id'))
#Y_hat_df_xreg = model.forecast(horizon)
Y_hat_df_xreg_mean = Y_hat_df_xreg_mean.reset_index()
df_plot_mean = pd.concat([Y_train_df, Y_hat_df_xreg_mean]).set_index('ds')
df_plot_mean.columns = df_plot_mean.columns.str.replace('AutoARIMA', 'MEAN')


Y_hat_df_intervals_good = model.forecast(horizon, level=(80, 95),␣
 ↪X_df=scenario_good.set_index('unique_id'))
df_plot = pd.concat([Y_train_df, Y_hat_df_intervals_good]).set_index('ds')


#We are going to plot the models againts the real values of test.

fig, ax = plt.subplots(1, 1, figsize = (20, 7))

#df_plot[['EC50', 'TEST']].plot(ax=ax, linewidth=10)
df_plot_good[['GOOD']].plot(ax=ax, linewidth=1, color='green')
df_plot_mean[['MEAN']].plot(ax=ax, linewidth=1, color='orange')
df_plot_bad[['BAD']].plot(ax=ax, linewidth=1, color='red')

dataset_good["O2"]= df_plot_good[['GOOD']]['GOOD'].array[-horizon:]
dataset_mean["O2"] = df_plot_mean[['MEAN']]['MEAN'].array[-horizon:]
dataset_bad["O2"] = df_plot_bad[['BAD']]['BAD'].array[-horizon:]

#ax.fill_between(df_plot.index,
#                 df_plot['AutoARIMA-lo-95'],
#                 df_plot['AutoARIMA-hi-95'],
#                 alpha=.2,
#                 color='orange',
```

```
#                 label='GOOD_level_95')

#df_plot.plot(ax=ax, linewidth=10)
fd_plot_real = Y_df_full.set_index('ds')
#fd_plot_real[['EC50']].plot(ax=ax, linewidth=5)
ax.set_title('Forecast on different scenarios', fontsize=22)
ax.set_ylabel('Monthly Value', fontsize=20)
ax.set_xlabel('Timestamp [t]', fontsize=20)
ax.legend(prop={'size': 15})
ax.grid()
for label in (ax.get_xticklabels() + ax.get_yticklabels()):
    label.set_fontsize(20)

bad = model.forecast(horizon, level=(80, 95), X_df=scenario_bad.
 ↪set_index('unique_id'))
good= model.forecast(horizon, level=(80, 95), X_df=scenario_good.
 ↪set_index('unique_id'))
mean = model.forecast(horizon, level=(80, 95), X_df=scenario_mean.
 ↪set_index('unique_id'))

plot_with_int_all(bad, "S3",mean, "S2",good, "S1", "02", "Real 02")
```





Forecast with ARIMA: EC50

```
[ ]: dataset_good["O2"]= df_plot_good[['GOOD']]['GOOD'].array[-horizon:]
     dataset_mean["O2"] = df_plot_mean[['MEAN']]['MEAN'].array[-horizon:]
     dataset_bad["O2"] = df_plot_bad[['BAD']]['BAD'].array[-horizon:]
```

```
[ ]: Y_df = pd.DataFrame({'unique_id': np.ones(len(df)),
                          'ds': df["Datetime"],
                          'EC50': df["EC50"],
                          #'CO2': df["CO2"],
                          #'O2': df["EC50"],
                          #'Salinity': df["Salinity"],
                          #'pH': df["pH"],
                          #'Temperature': df["Temperature"]
                          })
     Y_df_full = pd.DataFrame({'unique_id': np.ones(len(df)),
                          'ds': df["Datetime"],
                          'EC50': df["EC50"],
                          'CO2': df["CO2"],
                          'O2': df["O2"],
                          'Salinity': df["Salinity"],
                          'pH': df["pH"],
                          'Temperature': df["Temperature"]
                          })

     Y_df_woEC50 = pd.DataFrame({'unique_id': np.ones(len(df)),
                          'ds': df["Datetime"],
                          #'EC50': df["EC50"],
                          'CO2': df["CO2"],
                          'O2': df["O2"],
                          'Salinity': df["Salinity"],
                          'pH': df["pH"],
                          'Temperature': df["Temperature"]
```

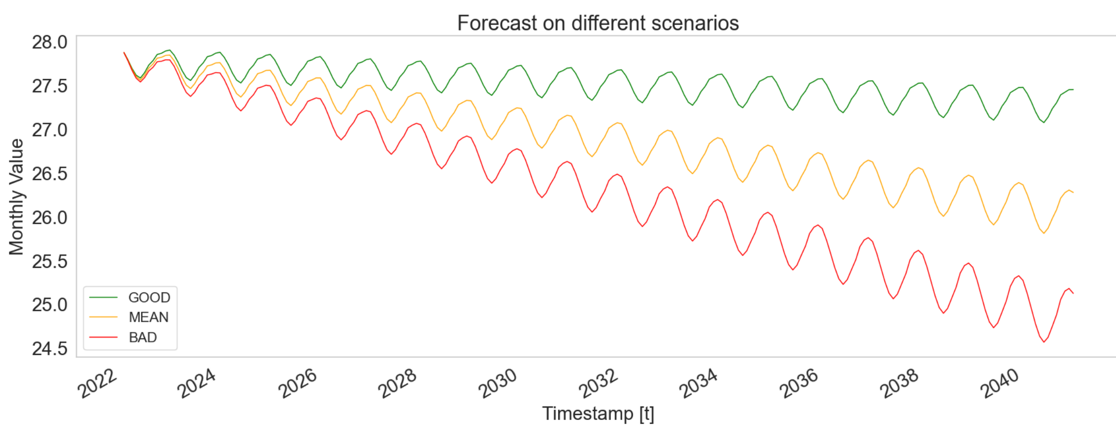
```
                     })

Y_train_df = Y_df_full[Y_df_full.ds<='2022-01-01']
Y_train_df_woEC50 = Y_df[Y_df_full.ds<='2022-01-01']
Y_test_df_woEC50 = Y_df[Y_df_full.ds>'2022-01-01']

scenario_bad = pd.DataFrame({'unique_id': np.ones(len(dataset_bad)),
                     'ds': dataset_bad["Datetime"],
                     #'EC50': df["EC50"],
                     'CO2': dataset_bad["CO2"],
                     'O2': dataset_bad["O2"],
                     'Salinity': dataset_bad["Salinity"],
                     'pH': dataset_bad["pH"],
                     'Temperature': dataset_bad["Temperature"]
                     })

scenario_good = pd.DataFrame({'unique_id': np.ones(len(dataset_good)),
                     'ds': dataset_good["Datetime"],
                     #'EC50': df["EC50"],
                     'CO2': dataset_good["CO2"],
                     'O2': dataset_good["O2"],
                     'Salinity': dataset_good["Salinity"],
                     'pH': dataset_good["pH"],
                     'Temperature': dataset_good["Temperature"]
                     })

scenario_mean = pd.DataFrame({'unique_id': np.ones(len(dataset_mean)),
                     'ds': dataset_mean["Datetime"],
                     #'EC50': df["EC50"],
                     'CO2': dataset_mean["CO2"],
                     'O2': dataset_mean["O2"],
                     'Salinity': dataset_mean["Salinity"],
                     'pH': dataset_mean["pH"],
                     'Temperature': dataset_mean["Temperature"]
                     })

xreg_test = Y_df_woEC50[Y_df_full.ds>'2022-01-01']

xreg_test =  pd.concat([xreg_test], ignore_index=True)
xreg_test["ds"] = pd.date_range(start='2022-01-01', periods=len(xreg_test),
 ↪freq='M')

#Define the parameters that you want to use in your models.
season_length = 12
# Note: For all models the following parameters are passed automaticly and
 ↪don't need to be declared: (X, h, future_xreg)
```

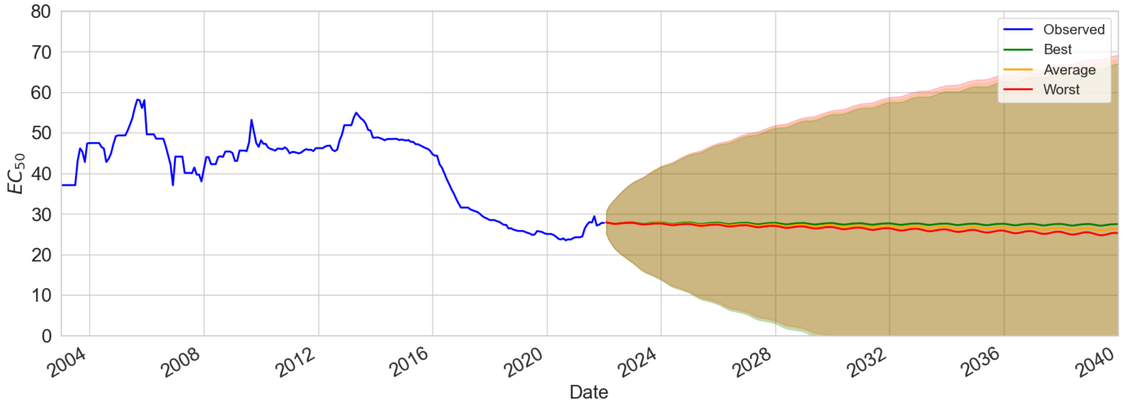
```
models = [
    AutoARIMA(season_length=season_length)#,
    #ETS(season_length=season_length, model='ZMZ')
]
model = StatsForecast(
    df=Y_train_df,
    models=models,
    freq='M',
    n_jobs=-1,
)
```

[ ]:
```
horizon = len(xreg_test)
Y_hat_df_xreg = model.forecast(horizon, X_df=xreg_test.set_index('unique_id'))
#Y_hat_df_xreg = model.forecast(horizon)
Y_hat_df_xreg = Y_hat_df_xreg.reset_index()
df_plot = pd.concat([Y_train_df, Y_hat_df_xreg]).set_index('ds')
df_plot.columns = df_plot.columns.str.replace('AutoARIMA', 'TEST')

horizon = len(scenario_bad)
Y_hat_df_xreg_bad = model.forecast(horizon, X_df=scenario_bad.
 ↪set_index('unique_id'))
#Y_hat_df_xreg = model.forecast(horizon)
Y_hat_df_xreg_bad = Y_hat_df_xreg_bad.reset_index()
df_plot_bad = pd.concat([Y_train_df, Y_hat_df_xreg_bad]).set_index('ds')
df_plot_bad.columns = df_plot_bad.columns.str.replace('AutoARIMA', 'BAD')

horizon = len(scenario_good)
Y_hat_df_xreg_good = model.forecast(horizon, X_df=scenario_good.
 ↪set_index('unique_id'))
#Y_hat_df_xreg = model.forecast(horizon)
Y_hat_df_xreg_good = Y_hat_df_xreg_good.reset_index()
df_plot_good = pd.concat([Y_train_df, Y_hat_df_xreg_good]).set_index('ds')
df_plot_good.columns = df_plot_good.columns.str.replace('AutoARIMA', 'GOOD')

horizon = len(scenario_mean)
Y_hat_df_xreg_mean = model.forecast(horizon, X_df=scenario_mean.
 ↪set_index('unique_id'))
#Y_hat_df_xreg = model.forecast(horizon)
Y_hat_df_xreg_mean = Y_hat_df_xreg_mean.reset_index()
df_plot_mean = pd.concat([Y_train_df, Y_hat_df_xreg_mean]).set_index('ds')
df_plot_mean.columns = df_plot_mean.columns.str.replace('AutoARIMA', 'MEAN')
```

[ ]:
```
Y_hat_df_intervals_good = model.forecast(horizon, level=(80, 95),␣
 ↪X_df=scenario_good.set_index('unique_id'))
df_plot = pd.concat([Y_train_df, Y_hat_df_intervals_good]).set_index('ds')
```

```python
#We are going to plot the models againts the real values of test.

fig, ax = plt.subplots(1, 1, figsize = (20, 7))

#df_plot[['EC50', 'TEST']].plot(ax=ax, linewidth=10)
df_plot_good[['GOOD']].plot(ax=ax, linewidth=1, color='green')
df_plot_mean[['MEAN']].plot(ax=ax, linewidth=1, color='orange')
df_plot_bad[['BAD']].plot(ax=ax, linewidth=1, color='red')


#ax.fill_between(df_plot.index,
#                 df_plot['AutoARIMA-lo-95'],
#                 df_plot['AutoARIMA-hi-95'],
#                 alpha=.2,
#                 color='orange',
#                 label='GOOD_level_95')

#df_plot.plot(ax=ax, linewidth=10)
fd_plot_real = Y_df_full.set_index('ds')
#fd_plot_real[['EC50']].plot(ax=ax, linewidth=5)
ax.set_title('Forecast on different scenarios', fontsize=22)
ax.set_ylabel('Monthly Value', fontsize=20)
ax.set_xlabel('Timestamp [t]', fontsize=20)
ax.legend(prop={'size': 15})
ax.grid()
for label in (ax.get_xticklabels() + ax.get_yticklabels()):
    label.set_fontsize(20)
```






```
[ ]: ###BAD
bad = model.forecast(horizon, level=(80, 95), X_df=scenario_bad.
  ↪set_index('unique_id'))
good= model.forecast(horizon, level=(80, 95), X_df=scenario_good.
  ↪set_index('unique_id'))
mean = model.forecast(horizon, level=(80, 95), X_df=scenario_mean.
  ↪set_index('unique_id'))

plot_with_int_all(good, "Best",mean, "Average",bad, "Worst", "EC50",␣
  ↪"$EC_{50}$","Observed")
```