DQO2_GS

April 23, 2023

1 DATA

2 CO CALIBRATION

[361]:
```
import pandas as pd
from pandas import MultiIndex, Int16Dtype
Ref=pd.read_csv('Ref.csv')
Ref["CO"] = 1000 * Ref["CO"]
Ref['Date'] = pd.to_datetime(Ref['Date_Time'])
Ref=Ref.set_index('Date')
Ref.drop('Date_Time',axis = 1, inplace = True)
Ref=Ref.resample('5min').mean()
Ref=Ref[76463:137376]
Ref_CO=Ref['CO'].to_list()
Ref_NO2=Ref['NO2'].to_list()
Ref_SO2=Ref['SO2'].to_list()
Ref_O3=Ref['O3'].to_list()
```

[362]:
```
import random
import pandas as pd
import scipy.io
import numpy as np
data = pd.read_csv('CO.txt', header = None,low_memory=False)
data.columns=['WE','AE','Temp','RH','Time']
Time=data['Time'].to_list()
time=[]
for i in range(len(Time)):
    time.append(float(abs(Time[i])))
Time=np.array(time)
Date=pd.to_datetime(Time-719529,unit='d').round('s')
data['Date'] = Date.tolist()
data=data.set_index('Date')
data.drop('Time',axis = 1, inplace = True)
data=data.resample('5min').mean()
Data_CO=data
Data_CO['Ref']=Ref_CO
index_names = Data_CO[ (Data_CO['WE'] >1000)].index
```

```
#Data_CO.drop(index_names, inplace = True)
WE=Data_CO['WE'].to_list()
AE=Data_CO['AE'].to_list()
signal=np.array(WE)-np.array(AE)
Data_CO['Net Signal']=signal
Data_CO['Month']=Data_CO.index.month
Data_CO['Day_of_week']=Data_CO.index.dayofweek
Data_CO['Day']=Data_CO.index.day
Data_CO['Hour']=Data_CO.index.hour
CO_Data=Data_CO
CO_Data=CO_Data[(CO_Data[CO_Data.columns] >= 0).all(axis=1)]
CO_Data=CO_Data.dropna()
data = pd.read_csv('Conc_CO.txt', header = None,low_memory=False)
data.columns=['Lab1','Temp','RH','Time','Ref']
Time=data['Time'].to_list()
time=[]
for i in range(len(Time)):
    time.append(float(abs(Time[i])))
Time=np.array(time)
Date=pd.to_datetime(Time-719529,unit='d').round('s')
data['Date'] = Date.tolist()
data=data.set_index('Date')
data.drop('Time',axis = 1, inplace = True)
data=data.resample('5min').mean()
Data_CO=data
#Data_CO.drop(index_names, inplace = True)
signal=np.array(WE)-np.array(AE)
Data_CO['Net Signal']=signal
Data_CO['Month']=Data_CO.index.month
Data_CO['Day_of_week']=Data_CO.index.dayofweek
Data_CO['Day']=Data_CO.index.day
Data_CO['Hour']=Data_CO.index.hour
CO_Data=Data_CO
CO_Data=CO_Data[(CO_Data[CO_Data.columns] >= 0).all(axis=1)]
CO_Data=CO_Data.dropna()
CO_Data=CO_Data.sample(frac=1)
```

[363]:
```
CO_Data=CO_Data.resample('5min').mean()
CO_Data=CO_Data.dropna()
CO_Data.head()
```

[363]:
```
                            Lab1       Temp         RH        Ref  Net Signal  \
Date
2019-10-02 11:55:00  3571.592599  26.378438  58.063437  312.70720  984.426875
2019-10-02 12:10:00  3541.294823  25.500000  48.612609  206.02900  984.224348
2019-10-02 12:15:00  2676.586421  25.765087  48.441408  170.30085  817.534721
2019-10-02 12:20:00  1694.726608  26.120078  47.716553  140.82115  509.284536
```

```
2019-10-02 12:25:00  3534.556213  25.502791  59.868837  397.72490  983.212857

                     Month  Day_of_week  Day  Hour
Date
2019-10-02 11:55:00   10.0          2.0  2.0  11.0
2019-10-02 12:10:00   10.0          2.0  2.0  12.0
2019-10-02 12:15:00   10.0          2.0  2.0  12.0
2019-10-02 12:20:00   10.0          2.0  2.0  12.0
2019-10-02 12:25:00   10.0          2.0  2.0  12.0
```

[364]:
```
#Ref=CO_Data['Ref'].to_list()
#CO_Data=CO_Data[CO_Data.Ref.between(np.mean(Ref)-0.7*np.std(Ref), np.
 ↪mean(Ref)+0.7*np.std(Ref))]
#CO_Data.shape
```

[365]:
```
subscript= str.maketrans("0123456789", "          ")
```

[366]:
```
print(r'$O_{2}$')
```

```
$O_{2}$
```

[367]:
```
import pandas as pd
import numpy as np
R1_data= pd.read_csv('R1_data.csv')
R1_data.columns=['Sen_2.5','Sen_10','Ref_2.5','Ref_10','Time','T','RH']
R1_data=R1_data.dropna()
Time=R1_data['Time'].to_list()
time=[]
for i in range(len(Time)):
    time.append(float(abs(Time[i])))
Time=np.array(time)
Date=pd.to_datetime(Time-719529,unit='d').round('s')
R1_data['Date'] = Date.tolist()
R1_data=R1_data.set_index('Date')
R1_data.drop('Time',axis = 1, inplace = True)
R1_data['Month']=R1_data.index.month
R1_data['Day_of_week']=R1_data.index.dayofweek
R1_data['Hour']=R1_data.index.hour
R1_data=R1_data.resample('5min').mean()
R1_data=R1_data.dropna()
R1_data.head()
```

[367]:
```
                        Sen_2.5      Sen_10   Ref_2.5    Ref_10          T  \
Date
2019-10-02 11:55:00  112.477418  112.477418  18.58330  32.75481  26.378438
2019-10-02 12:10:00   14.218595   58.035547  17.30462  31.54500  25.497143
2019-10-02 12:15:00    5.174785   22.242307  17.09769  31.13976  25.807733
2019-10-02 12:20:00    4.945599   29.365024  17.06241  31.07447  26.123333
```

```
2019-10-02 12:25:00  132.986920  133.789832  16.62954  30.29124  25.502791

                            RH  Month  Day_of_week  Hour
Date
2019-10-02 11:55:00  58.063437   10.0          2.0  11.0
2019-10-02 12:10:00  48.609524   10.0          2.0  12.0
2019-10-02 12:15:00  48.275000   10.0          2.0  12.0
2019-10-02 12:20:00  47.734643   10.0          2.0  12.0
2019-10-02 12:25:00  59.868837   10.0          2.0  12.0
```

[368]:

```
import pandas as pd
import numpy as np
N3_data= pd.read_csv('N3_data.csv')
N3_data.columns=['Sen_2.5','Sen_10','Ref_2.5','Ref_10','Time','T','RH']
N3_data=N3_data.dropna()
Time=N3_data['Time'].to_list()
time=[]
for i in range(len(Time)):
    time.append(float(abs(Time[i])))
Time=np.array(time)
Date=pd.to_datetime(Time-719529,unit='d').round('s')
N3_data['Date'] = Date.tolist()
N3_data=N3_data.set_index('Date')
N3_data.drop('Time',axis = 1, inplace = True)
N3_data['Month']=N3_data.index.month
N3_data['Day_of_week']=N3_data.index.dayofweek
N3_data['Hour']=N3_data.index.hour
N3_data=N3_data.resample('10min').mean()
N3_data=N3_data.dropna()
N3_data.head()
```

[368]:

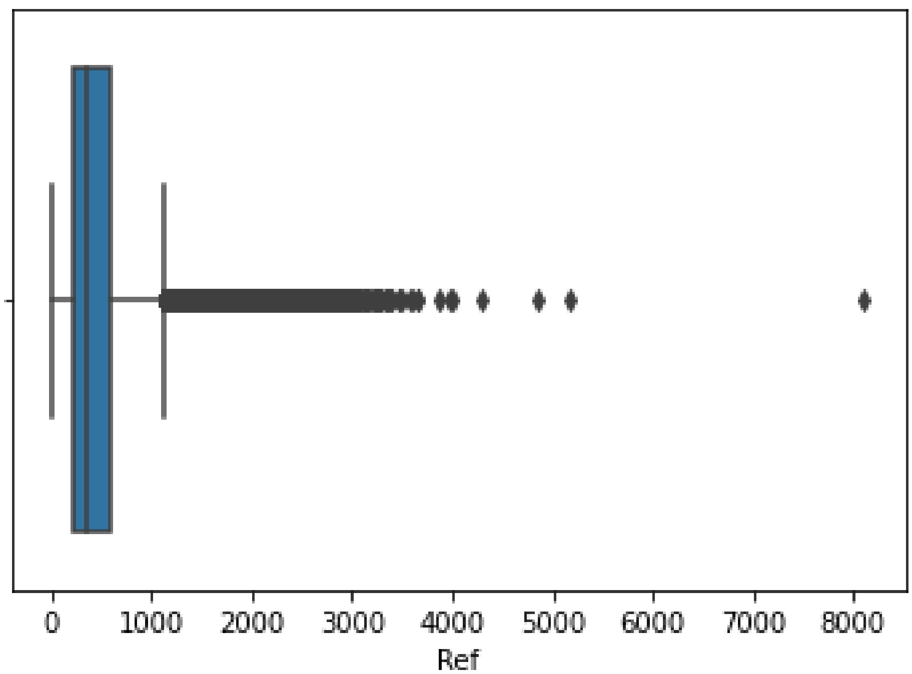
```
                      Sen_2.5     Sen_10    Ref_2.5     Ref_10          T  \
Date
2019-10-02 12:00:00  7.972913  17.284141  17.700490  31.956415  24.827483
2019-10-02 12:10:00  4.448633  10.763524  17.201155  31.342380  25.074930
2019-10-02 12:20:00  3.378485  17.141379  17.062410  31.074470  25.445921
2019-10-02 15:40:00  4.223667  13.522096  19.076640  35.864505  30.180843
2019-10-02 15:50:00  4.301400  16.168827  19.210635  34.961880  30.316215

                            RH  Month  Day_of_week  Hour
Date
2019-10-02 12:00:00  64.382667   10.0          2.0  12.0
2019-10-02 12:10:00  54.874831   10.0          2.0  12.0
2019-10-02 12:20:00  54.380000   10.0          2.0  12.0
2019-10-02 15:40:00  55.684552   10.0          2.0  15.0
2019-10-02 15:50:00  55.095438   10.0          2.0  15.0
```

3 Outlier detection and removal

[369]:
```
import numpy as np

import pandas as pd
import seaborn as sns
from scipy import stats
```

[370]:
```
sns.boxplot(x=CO_Data['Ref'])
z=np.abs(stats.zscore(CO_Data))
CO_data=CO_Data[(z < 3).all(axis=1)]
CO_data.shape,CO_Data.shape
```

[370]: ((43258, 9), (45117, 9))



[371]:
```
def MBE(true,pred):
    true=np.array(true)
    pred=np.array(pred)
    mbe=np.mean(true-pred)
    return mbe
def CRMSE(true,pred):
    true=np.array(true)
    pred=np.array(pred)
    crmse=np.sqrt(np.mean(((true-np.mean(true))-(pred-np.mean(pred)))**2))
    if np.std(pred)>np.std(true):
```

```
        crmse=crmse
    else:
        crmse=-crmse
    return crmse
import random
```

4 Relative Expanded Uncertainty(REU)

[372]:
```
def REF(pred,y_test,alpha):
    import random
    cal=np.array(pred)
    ref=np.array(y_test.to_list())
    ref_mean=np.mean(ref)
    cal_mean=np.mean(cal)
    prec=np.array([20 for i in range(len(ref))])
    u=0.05*ref
    #cal=np.log(cal)
    #ref=np.log(ref)
    sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
    sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
    sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
    beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
    beta_0=cal_mean-beta_1*ref_mean
    RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*u**2)
    du_s=RSS/(len(cal)-2)
    Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
    Beta_0=cal_mean-Beta_1*ref_mean
    P1=(RSS/(len(cal)-2))
    P2=(Beta_1**2+alpha)*u**2+(-2*Beta_1**2+2*Beta_1-1)*u**2
    P3=(Beta_0+(Beta_1-1)*ref)**2
    P=[]
    for i in range(len(P3)):
        P.append(P1+P2[i]+P3[i])
    for i in range(len(P)):
        if P[i]<0:
            P[i]=random.randint(1,100)
    u_cal=(2*np.sqrt(np.array(P))/cal)*100
    #u_cal=((2*np.sqrt((RSS/(len(cal)-2))+(1-(beta_1-1)**2)*(0.
 ↪08*ref)**2+(Beta_0+(Beta_1-1)*ref)**2))/cal)*100
    return u_cal
```

[373]:
```
def REF2(pred,y_test,alpha,LV):
    import random
    cal=np.array(pred)
    ref=np.array(y_test.to_list())
```

```
    for i in range(len(ref)):
        if ref[i]==0:
            ref[i]=np.mean(ref)
    ref_mean=np.mean(ref)
    cal_mean=np.mean(cal)
    for i in range(len(ref)):
        if ref[i]==0:
            ref[i]=ref_mean
    prec=np.array([20 for i in range(len(ref))])
    u=0.05*ref
    #cal=np.log(cal)
    #ref=np.log(ref)
    sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
    sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
    sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
    #beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
    beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
    beta_0=cal_mean-beta_1*ref_mean
    RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
    du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
    Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
    Beta_0=cal_mean-Beta_1*ref_mean
    P1=(RSS/(len(cal)-2))
    P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
    P3=(Beta_0+(Beta_1-1)*LV)**2
    P=P1+P2+P3
    if P<0:
        P=random.randint(1,100)
    u_cal=(2*np.sqrt(P)/(Beta_0+Beta_1*LV))*100
    #u_cal=((2*np.sqrt((RSS/(len(cal)-2))+(1-(beta_1-1)**2)*0.
 ↪1+(Beta_0+(Beta_1-1)*ref)**2))/cal)*100
    return u_cal
```

[374]:
```
def target(pred,y_test,alpha):
    import random
    cal=np.array(pred)
    ref=np.array(y_test.to_list())
    for i in range(len(ref)):
        if ref[i]==0:
            ref[i]=np.mean(ref)
    ref_mean=np.mean(ref)
    cal_mean=np.mean(cal)
    prec=np.array([20 for i in range(len(ref))])
    #u=np.maximum(prec, 0.001*ref)
    u=0.001*ref
```

```
    #cal=np.log(cal)
    #ref=np.log(ref)
    sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
    sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
    sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
    #beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
    beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
    beta_0=cal_mean-beta_1*ref_mean
    RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*u**2)
    du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
    Beta_1=((sy_s-alpha*sx_s-du_s)+np.
↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
    Beta_0=cal_mean-Beta_1*ref_mean
    P1=(RSS/(len(cal)-2))
    P2=(Beta_1**2+alpha)*u**2+(-2*Beta_1**2+2*Beta_1-1)*u**2
    P3=(Beta_0+(Beta_1-1)*ref)
    P=[]
    for i in range(len(P2)):
        P.append(P1+P2[i])
    for i in range(len(P)):
        if P[i]<0:
            P[i]=random.randint(1,50)
    A=(2*(np.array(P))**0.5/ref)*100
    #for i in range(len(P3)):
        #if P3[i]<0:
            #P3[i]=random.randint(0,50)
    B=(2*(np.array(P3))/ref)*100
    bias=[]
    random=[]
    Ref=[]
    part1=(Beta_0/ref)*100
    part=[beta_1-1 for i in range(len(ref))]
    part2=(np.array(part))*100
    PART1=[]
    PART2=[]
    for i in range(len(A)):
        if A[i]<500:
            random.append(A[i])
            bias.append(B[i])
            Ref.append(ref[i])
            PART1.append(part1[i])
            PART2.append(part2[i])
    return [random,bias,Ref, PART1,PART2]
```

```
[375]: def target(pred,y_test,alpha):
    import random
```

```
    cal=np.array(pred)
    ref=np.array(y_test.to_list())
    for i in range(len(ref)):
        if ref[i]==0:
            ref[i]=np.mean(ref)
    ref_mean=np.mean(ref)
    cal_mean=np.mean(cal)
    prec=np.array([20 for i in range(len(ref))])
    #u=np.maximum(prec, 0.001*ref)
    u=0.001*ref
    #cal=np.log(cal)
    #ref=np.log(ref)
    sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
    sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
    sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
    #beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
    beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
    beta_0=cal_mean-beta_1*ref_mean
    RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*u**2)
    du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
    Beta_1=((sy_s-alpha*sx_s-du_s)+np.
↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
    Beta_0=cal_mean-Beta_1*ref_mean
    P1=(RSS/(len(cal)-2))
    P2=(Beta_1**2+alpha)*u**2+(-2*Beta_1**2+2*Beta_1-1)*u**2
    P3=(Beta_0+(Beta_1-1)*ref)
    P=[]
    for i in range(len(P2)):
        P.append(P1+P2[i])
    for i in range(len(P)):
        if P[i]<0:
            P[i]=random.randint(1,50)
    A=(2*(np.array(P))**0.5/ref)*100
    #for i in range(len(P3)):
        #if P3[i]<0:
            #P3[i]=random.randint(0,50)
    B=(2*(np.array(P3))/ref)*100
    bias=[]
    random=[]
    Ref=[]
    part1=(Beta_0/ref)*100
    part=[beta_1-1 for i in range(len(ref))]
    part2=(np.array(part))*100
    PART1=[]
    PART2=[]
    for i in range(len(A)):
```

```
        if A[i]<500:
            random.append(A[i])
            bias.append(B[i])
            Ref.append(ref[i])
            PART1.append(part1[i])
            PART2.append(part2[i])
    return [random,bias,Ref, PART1,PART2]
```

[376]:
```
def REF10(pred,y_test,alpha):
    import random
    cal=np.array(pred)
    ref=np.array(y_test.to_list())
    for i in range(len(ref)):
        if ref[i]==0:
            ref[i]=np.mean(ref)
    ref_mean=np.mean(ref)
    cal_mean=np.mean(cal)
    prec=np.array([20 for i in range(len(ref))])
    u=np.maximum(prec,0.001*ref)
    u=0.001*ref
    #cal=np.log(cal)
    #ref=np.log(ref)
    sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
    sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
    sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
    beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
    beta_0=cal_mean-beta_1*ref_mean
    RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*u**2)
    du_s=RSS/(len(cal)-2)
    Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
    Beta_0=cal_mean-Beta_1*ref_mean
    P1=(RSS/(len(cal)-2))
    #P2=(Beta_1**2+alpha)*u**2+(-2*Beta_1**2+2*Beta_1-1)*u**2
    P2=-(u**2)
    P3=(Beta_0+(Beta_1-1)*ref)**2
    P=[]
    for i in range(len(P3)):
        P.append(P1+P2[i]+P3[i])
    U1=[]
    Ref=[]
    for i in range(len(P)):
        if P[i]>=0:
            U1.append(P[i])
            Ref.append(ref[i])
    #for i in range(len(P)):
        #if P[i]<0:
```

```
            # P[i]=np.mean(P1)
    u_cal_s=np.array(U1)
    return u_cal_s,Ref
```

[377]:
```
from sklearn import linear_model
import numpy as np
Y=[20,40,60,80,100]
X=np.array([10,30,50,70,90]).reshape(-1, 1)

regr = linear_model.LinearRegression()
regr.fit(X, Y)
print('Intercept: \n', regr.intercept_)
print('Coefficients: \n', regr.coef_)
```

```
Intercept:
 10.0
Coefficients:
 [1.]
```

[378]:
```
def target2(Y,X,u):
    from sklearn import linear_model
    import numpy as np
    x=np.array(Y).reshape(-1, 1)
    y=np.array(X).reshape(-1, 1)
    regr = linear_model.LinearRegression()
    regr.fit(x, y)
    b0=regr.intercept_
    b1=regr.coef_[0]
    RSS=sum((np.array(Y)-(b0[0]+b1[0]*np.array(X)))**2)
    RR=2*((RSS/((len(X)-2))-u**2)/np.array(X))**0.5
    RB=2*(b0/np.array(X)+(b1-1))
    return RR,RB
```

A=[200,360,288,290] B=[204,336,267,301] y=np.array(B).reshape(-1, 1) RSS=sum((np.array(A)-(b0[0]+b1[0]*np.array(B)))**2) RSS RR=2*((RSS/((len(X)-2))-5**2)/np.array(X))**0.5 RR**

x=np.array(A).reshape(-1, 1) y=np.array(B).reshape(-1, 1) regr = linear_model.LinearRegression() regr.fit(x, y) b0=regr.intercept_ b1=regr.coef_[0] b0[0] b1[0]

target2(A,B,5)

B=np.array([20,20]) A=np.array([1,30]) C=np.array([A,B]) np.maximum(A,B)

[379]:
```
Ref=CO_Data['Ref'].to_list()
#CO_Data=CO_Data[CO_Data.Ref.between(np.mean(Ref)-1*np.std(Ref), np.
 ↪mean(Ref)+1*np.std(Ref))]
#NO2_Data.shape
```

4.1 Model 1: Linear Regression

[380]:
```
df1=[x for _, x in CO_Data.groupby('Month')]
data_oct=df1[4]
#data_oct=data_oct.sample(frac=1)
data_nov=df1[5]
#data_nov=data_nov.sample(frac=1)
data_dec=df1[6]
#data_dec=data_dec.sample(frac=1)
data_jan=df1[0]
#data_jan=data_jan.sample(frac=1)
data_feb=df1[1]
#data_feb=data_feb.sample(frac=1)
data_mar=df1[2]

data_Oct=data_oct.resample('15min').mean()
data_Oct=data_Oct.dropna()
data_Oct1=data_Oct[:int(0.8*data_Oct.shape[0])]
data_Oct2=data_Oct[int(0.8*data_Oct.shape[0]):]
data_Nov=data_nov.resample('15min').mean()
data_Nov=data_Nov.dropna()
data_Nov1=data_Nov[:int(0.8*data_Nov.shape[0])]
data_Nov2=data_Nov[int(0.8*data_Nov.shape[0]):]
data_Dec=data_dec.resample('15min').mean()
data_Dec=data_Dec.dropna()
data_Dec1=data_Dec[:int(0.8*data_Dec.shape[0])]
data_Dec2=data_Dec[int(0.8*data_Dec.shape[0]):]
data_Jan=data_jan.resample('15min').mean()
data_Jan=data_Jan.dropna()
data_Jan1=data_Jan[:int(0.8*data_Jan.shape[0])]
data_Jan2=data_Jan[int(0.8*data_Jan.shape[0]):]
data_Feb=data_feb.resample('15min').mean()
data_Feb=data_Feb.dropna()
data_Feb1=data_Feb[:int(0.8*data_Feb.shape[0])]
data_Feb2=data_Feb[int(0.8*data_Feb.shape[0]):]
data_Mar=data_mar.resample('15min').mean()
data_Mar=data_Mar.dropna()
data_Mar1=data_Mar[:int(0.8*data_Mar.shape[0])]
data_Mar2=data_Mar[int(0.8*data_Mar.shape[0]):]
frame1=[data_Oct1,data_Nov1,data_Dec1,data_Jan1,data_Feb1,data_Mar1]
frame2=[data_Oct2,data_Nov2,data_Dec2,data_Jan2,data_Feb2,data_Mar2]
CO_data1=pd.concat(frame1)
CO_data2=pd.concat(frame2)
CO_data=pd.concat([CO_data1,CO_data2])
```

[381]:
```
from sktime.performance_metrics.forecasting import sMAPE, smape_loss
from sklearn.model_selection import train_test_split
```

```python
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_absolute_error as mae
import sklearn.metrics as sm
import matplotlib.pyplot as plt

X=CO_data[['Net Signal','Lab1','Temp','RH','Month','Day_of_week','Hour']]
y=CO_data['Ref']
#X=R1_data[['Sen_2.5','T','RH','Month','Day_of_week','Hour']]
#y=R1_data['Ref_2.5']
X_train, X_test, y_train, y_test =train_test_split(X, y, test_size = 0.
 ↪2,shuffle=True)
#train_test_split(X, y, test_size = 0.2)
```

[382]:
```python
X1=X[:int(0.4*(X.shape[0]))]
X2=X[int(0.6*(X.shape[0])):]
X_train=X[int(0.2*(X.shape[0])):]
X_test=X[:int(0.2*(X.shape[0]))]




y_train=y[int(0.2*(X.shape[0])):]
y_test=y[:int(0.2*(X.shape[0]))]
```

X1=X[:int(0.4*(X.shape[0]))] X2=X[int(0.6*(X.shape[0])):] X_train=pd.concat([X1,X2]) X_test=X[int(0.4*(X.shape[0])):int(0.6*(X.shape[0]))]*

y1=y[:int(0.4*(X.shape[0]))] y2=y[int(0.6*(X.shape[0])):] y_train=pd.concat([y1,y2]) y_test=y[int(0.4*(X.shape[0])):int(0.6*(X.shape[0]))]*

[383]:
```python
lr = LinearRegression()
from sklearn.ensemble import RandomForestRegressor

 # create regressor object
regressor = RandomForestRegressor(n_estimators = 500,min_samples_split=␣
 ↪2,min_samples_leaf= 1,max_features= 'sqrt',
                                  random_state =␣
 ↪0,max_depth=None,bootstrap=False)

# fit the regressor with x and y data
regressor=regressor.fit(X_train, y_train)
pred = regressor.predict(X_test)
u_c_s=REF10(pred,y_test,1)[0]
X=np.array(REF10(pred,y_test,1)[1])**2
X=X.reshape((-1, 1))
model = lr.fit(X,u_c_s )
m_CO=model.coef_
q_CO=model.intercept_
m_CO,q_CO
```

```
LV=10000
u_r=(np.sqrt(m_CO*y_test**2+q_CO)/y_test)*100
u_LV=(np.sqrt(m_CO*LV**2+q_CO)/LV)*100
T_LV=25
Beta=T_LV/u_LV
#Beta=T_LV-u_LV
LQ,median, UQ=np.percentile(y_test, [25,50,75])
u_25=(np.sqrt(m_CO*LQ**2+q_CO)/LQ)*100
T_25=u_25*Beta
u_50=(np.sqrt(m_CO*median**2+q_CO)/median)*100
T_50=u_50*Beta
u_75=(np.sqrt(m_CO*UQ**2+q_CO)/UQ)*100
T_75=u_75*Beta
T_25,T_50,T_75
```

[383]: (array([260.17584684]), array([185.2348942]), array([105.65607129]))

[384]:
```
lr = LinearRegression()
model = lr.fit(X_train.drop(['Lab1'], axis=1), y_train)
pred = model.predict(X_test.drop(['Lab1'], axis=1))
lab1=X_test['Lab1'].to_list()

index=[i for i in range(len(y_test))]
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =index)
Y_test
Pred=pd.Series(pred,index =index)
Lab1=pd.Series(lab1,index =index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_lr_CO=sMAPE_lr
RMSE_lr_CO=round(RMSE_lr/np.mean(np.array(y_test)),2)
Pearson_lr_CO=Pearson_lr
sMAPE_lab_CO=sMAPE_lab
RMSE_lab_CO=round(RMSE_lab/np.mean(np.array(lab1)),2)
Pearson_lab_CO=Pearson_lab
R2_lr_CO=round(sm.r2_score(y_test, pred), 2)
R2_lab_CO=round(sm.r2_score(y_test, lab1), 2)
RMSE_Lr_CO=RMSE_lr
RMSE_Lab_CO=RMSE_lab

A=len(y_test)-200
```

```
D=max(y_test[A:])-0.2*max(y_test[A:])
C=max(y_test[A:])-0.1*max(y_test[A:])
B=120
Pearson_lr,RMSE_Lr_CO
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

[384]: (0.92, 189.0)

[385]:
```
cal=np.array(pred)
ref=np.array(y_test.to_list())
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
    #cal=np.log(cal)
    #ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+1)*(0.08*ref)**2)
du_s=RSS/(len(cal)-2)
Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P1
```

[385]: 29157.53112696561

[386]:
```
import random
alpha=1.4
LV2=max(y_test)+400
Cal=0
for i in range(len(y_test)):
```

```
    if y_test[i]==LV2:
        Cal=lab1[i]
cal=np.array(lab1)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV2)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV2)**2
P3=(Beta_0+(Beta_1-1)*LV2)
P=P1+P2+P3
Bias=(2*(P3)/LV2)*100
Random=(2*(P1+P2)**0.5/LV2)*100


import random
alpha=1.4
LV=median
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(lab1)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
```

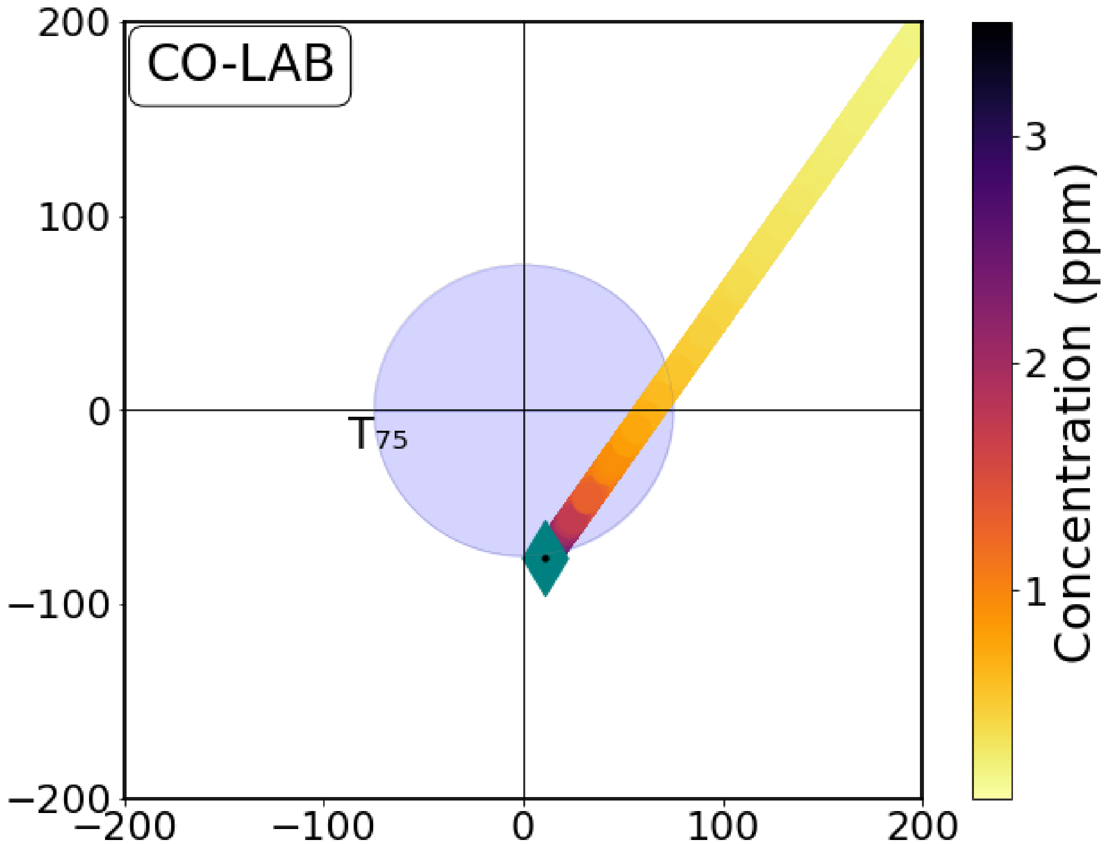
```
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=LQ
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(lab1)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
```

```
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[387]:
```
A4=target(lab1,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

#plt.fill_between(a1, b1, color='blue', alpha=0.17)
#plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)
```

```python
#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

#plt.plot(x1,y1, linewidth=0.2, color='grey')
#plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
#plt.plot(x2,y2, linewidth=0.2, color='grey')
#plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

#plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
#plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
#plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
#plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$_{0}$'+'/'+r'$ref_{i}$,␣
 ↪'+r'$(_{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-200)
plt.ylim(ymax=200)
plt.xlim(xmax=200)
plt.xlim(xmin=-200)
plt.xticks(np.arange(-75,75),fontsize=22)
plt.xticks([-200,-100,0,100,200],fontsize=22)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-200,-100,0,100,200],fontsize=22)
#plt.colorbar()
```

```
cbar = plt.colorbar(ticks=[0,1,2,3])
cbar.ax.tick_params(labelsize=22)
cbar.set_label('Concentration (ppm)', rotation=90,fontsize=27)
plt.scatter(Random,Bias+0.2,marker="d",s=900, color='teal')
textstr = 'CO-LAB'
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
 ↪rotation_mode='anchor')
#plt.text(-25,-7, 'T25'.translate(subscript),fontsize=18)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=18)
plt.text(-88,-20, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_CO_LAB.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[388]:
```
import random
alpha=1.4
LV=max(y_test)+400
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
```

```
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=median
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100
```

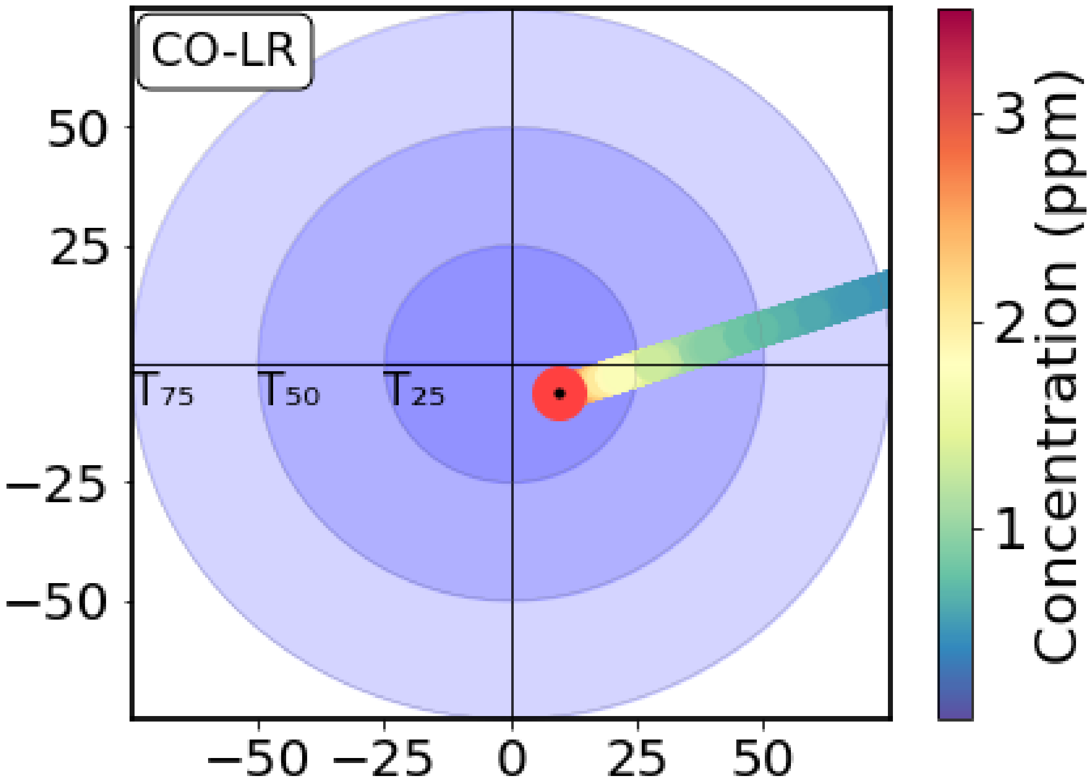
```
import random
alpha=1.4
LV=LQ
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[389]:
```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )
```

```
#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(6.5,5))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
```

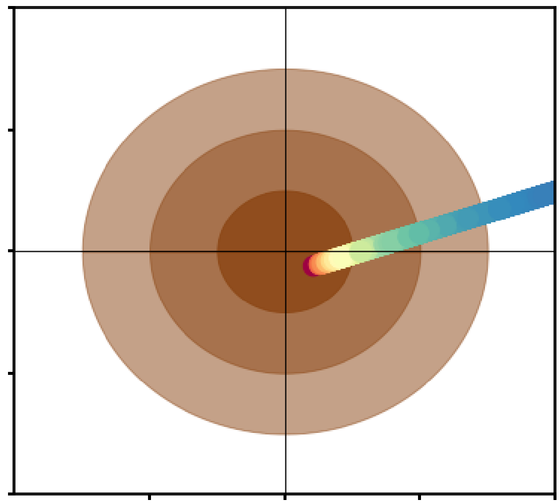
```
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$ _{0}$'+'/'+r'$ref_{i}$, '+r'$( _{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=600,c=np.array(A4[2])/1000,cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=20)
plt.xticks([-50,-25,0,25,50],fontsize=20)

plt.yticks(np.arange(-75,75),fontsize=20)
plt.yticks([-50,-25,25,50],fontsize=20)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,1,2,3])
cbar.ax.tick_params(labelsize=22)
cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)
plt.scatter(Random,Bias+0.2,marker="o",s=400, color='#FF4040')
textstr = 'CO-LR'
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.027, 0.972, textstr, transform=ax.transAxes, fontsize=18,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
```

```
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
↪rotation_mode='anchor')
plt.text(-25,-9, 'T25'.translate(subscript),fontsize=17)
plt.text(-50,-9, 'T50'.translate(subscript),fontsize=17)
plt.text(-75,-9, 'T75'.translate(subscript),fontsize=17)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_CO_LR.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



[390]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=25
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
```

```
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 25, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_CO_LR1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



fig= plt.figure(figsize=(8,6)) index=[i for i in range(1,201)] ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.2) plt.plot(index,y_test[A:], color='limegreen',linewidth=3) plt.plot(index,pred[A:], color='#513e00',linewidth=3) plt.plot(index,lab1[A:], color='#426eff',linewidth=3) plt.legend(['Ref', 'LR-Calibrated', 'Lab-Calibrated'], loc = 2, bbox_to_anchor = (0.74,1)) plt.ylabel('CO Concentration(ppb)',fontsize=18) #plt.text(B-20, C, r'$R^2(LR)$ ='+str(R2_lr_CO), fontsize = 14, color='#513e00') #plt.text(B-20, D, r'$R^2(Lab)$ =' +str(R2_lab_CO), fontsize = 14, color='#426eff') #plt.text(B-70, C, 'Pearson r(LR)='+str(Pearson_lr), fontsize = 14, color='#513e00') #plt.text(B-70, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') #plt.xlabel('Last 200 hours of testing period',fontsize=18) #plt.title('Visualization: Linear Regression Calibration vs Laboratory Calibration',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

[391]:
```
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),␣
↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),␣
↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))
pred_lr=pred
```

```
MBE_LR_CO=MBE(pred,y_test)/np.std(y_test)
CRMSE_LR_CO=CRMSE(y_test,pred)/np.std(y_test)
MBE_LAB_CO=MBE(lab1,y_test)/np.std(y_test)
CRMSE_LAB_CO=CRMSE(y_test,lab1)/np.std(y_test)
```

```
Regressor model performance:
Mean absolute error(MAE) = 103.97
Mean squared error(MSE) = 35721.44
Median absolute error = 68.85
Explain variance score = 0.83
R2 score = 0.82
```

4.2 Model 2 : Support Vector Regression (SVR)

[392]:
```
from sklearn.svm import SVR
from sklearn.preprocessing import StandardScaler
regressor = SVR(kernel = 'linear')
regressor.fit(X_train.drop(['Lab1'], axis=1), y_train)
pred = regressor.predict(X_test.drop(['Lab1'], axis=1))
for i in range(len(Pred)):
    if pred[i]<0:
        pred[i]=np.mean(np.array(pred))
pred_svr=pred
```

[393]:
```
Index=[i for i in range(len(y_test))]
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)

Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_svr_CO=sMAPE_lr
RMSE_svr_CO=round(RMSE_lr/np.mean(np.array(y_test)),2)
Pearson_svr_CO=Pearson_lr
R2_svr_CO=round(sm.r2_score(y_test, pred), 2)
RMSE_Svr_CO=RMSE_lr
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

fig= plt.figure(figsize=(8,6)) ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) plt.plot(index,y_test[A:], color='limegreen',linewidth=3) plt.plot(index,pred[A:], color='brown',linewidth=3) plt.plot(index,lab1[A:], color='#426eff',linewidth=3) plt.legend(['Ref', 'SVR-Calibrated', 'Lab-Calibrated'], loc = 2, bbox_to_anchor = (0.74,1)) plt.ylabel('CO Concentration(ppb)',fontsize=18) #plt.text(B-20, C,r'$R^2(SVR)$ ='+str(R2_svr_CO) , fontsize = 14, color='brown') #plt.text(B-20, D,r'$R^2(Lab)$ ='+str(R2_lab_CO) , fontsize = 14, color='#426eff') #plt.text(B-70, C, 'Pearson r(SVR)='+str(Pearson_lr), fontsize = 14, color='brown') #plt.text(B-70, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') #plt.xlabel('Last 200 hours of testing period',fontsize=18) #plt.title('Visualization: Support Vector Regression (SVR) Calibration vs Laboratory Calibration',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

[394]:
```python
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),␣
 ↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),␣
 ↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
 ↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
 ↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))
pred_svr=pred
MBE_SVR_CO=MBE(pred,y_test)/np.std(y_test)
CRMSE_SVR_CO=CRMSE(y_test,pred)/np.std(y_test)
```

```
Regressor model performance:
Mean absolute error(MAE) = 100.9
Mean squared error(MSE) = 34408.42
Median absolute error = 66.0
Explain variance score = 0.84
R2 score = 0.83
```

[395]:
```python
import random
alpha=1.4
LV=max(y_test)+400
Cal=0
```

```
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=median
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
```

```
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=LQ
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
```

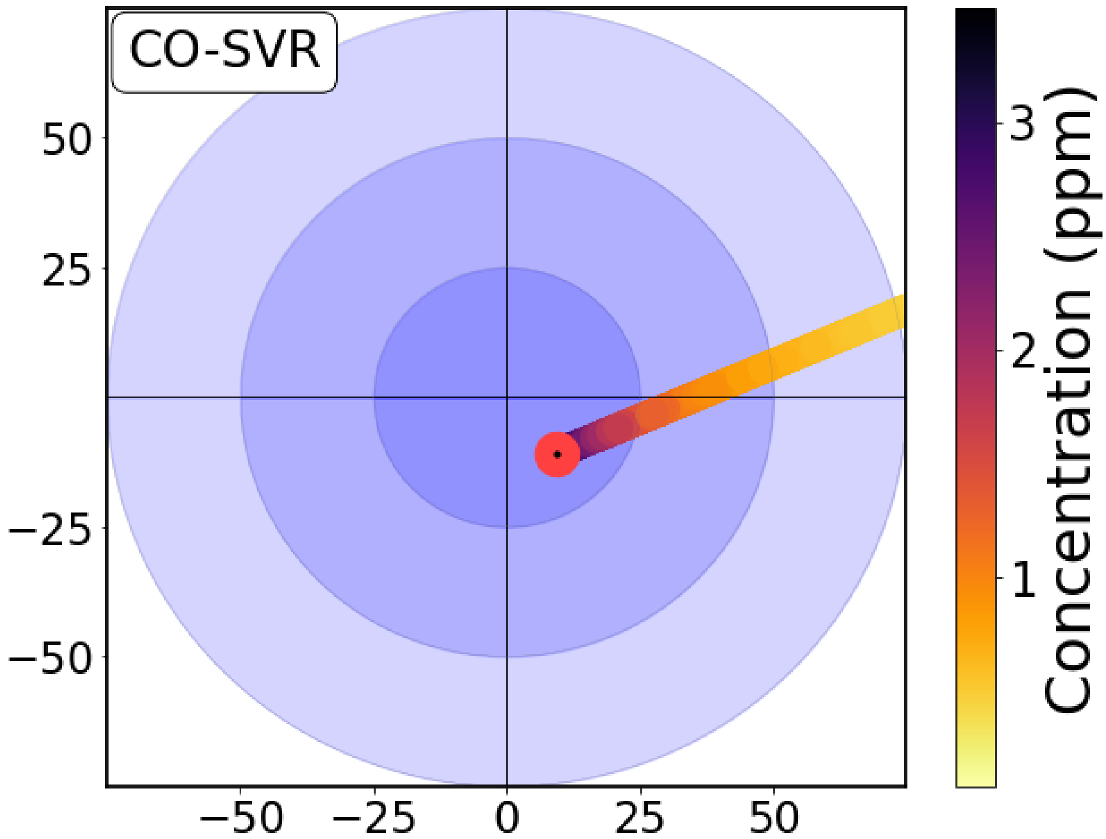
```
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[396]:

```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)
```

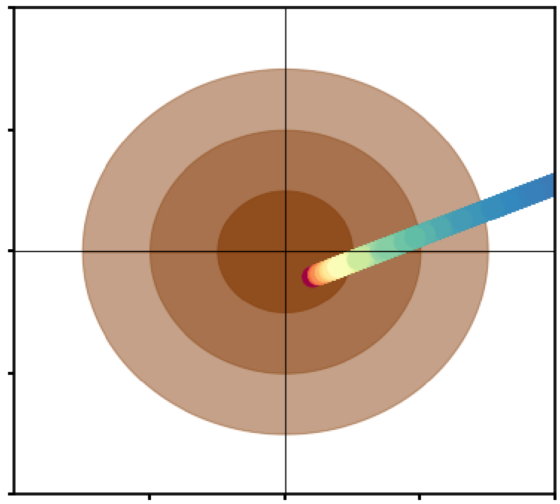
```
#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$_{0}$'+'/'+r'$ref_{i}$, 
 ↪'+r'$(_{1}-1)$'+'
#in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=24)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=24)
```

```
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,1,2,3])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppm)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = 'CO-SVR'
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
 ↪rotation_mode='anchor')
#plt.text(-25,-7, 'T25'.translate(subscript),fontsize=24)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
#plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_CO_SVR.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[397]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=25
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 25, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
```

```
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_CO_SVR1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



4.3 Model 3 : Random Forest

[398]:
```
from sklearn.ensemble import RandomForestRegressor

 # create regressor object
regressor =RandomForestRegressor(max_features=0.5687641759232935,␣
 ↪max_leaf_nodes=1450,
                              n_estimators=313, n_jobs=-1)


# fit the regressor with x and y data
regressor=regressor.fit(X_train.drop(['Lab1'], axis=1), y_train)
pred = regressor.predict(X_test.drop(['Lab1'], axis=1))
```

[399]:
```
features_CO=regressor.feature_importances_
pred = regressor.predict(X_test.drop(['Lab1'], axis=1))
pred_rf_co=pred
Index=[i for i in range(len(y_test))]
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
```

```
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_rf_CO=sMAPE_lr
RMSE_rf_CO=round(RMSE_lr/np.mean(np.array(y_test)),2)
Pearson_rf_CO=Pearson_lr
R2_rf_CO=round(sm.r2_score(y_test, pred), 2)
RMSE_Rf_CO=RMSE_lr
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

[400]:
```
import random
alpha=1.4
LV=max(y_test)+400
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
```

```
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100


import random
alpha=1.4
LV=median
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
```

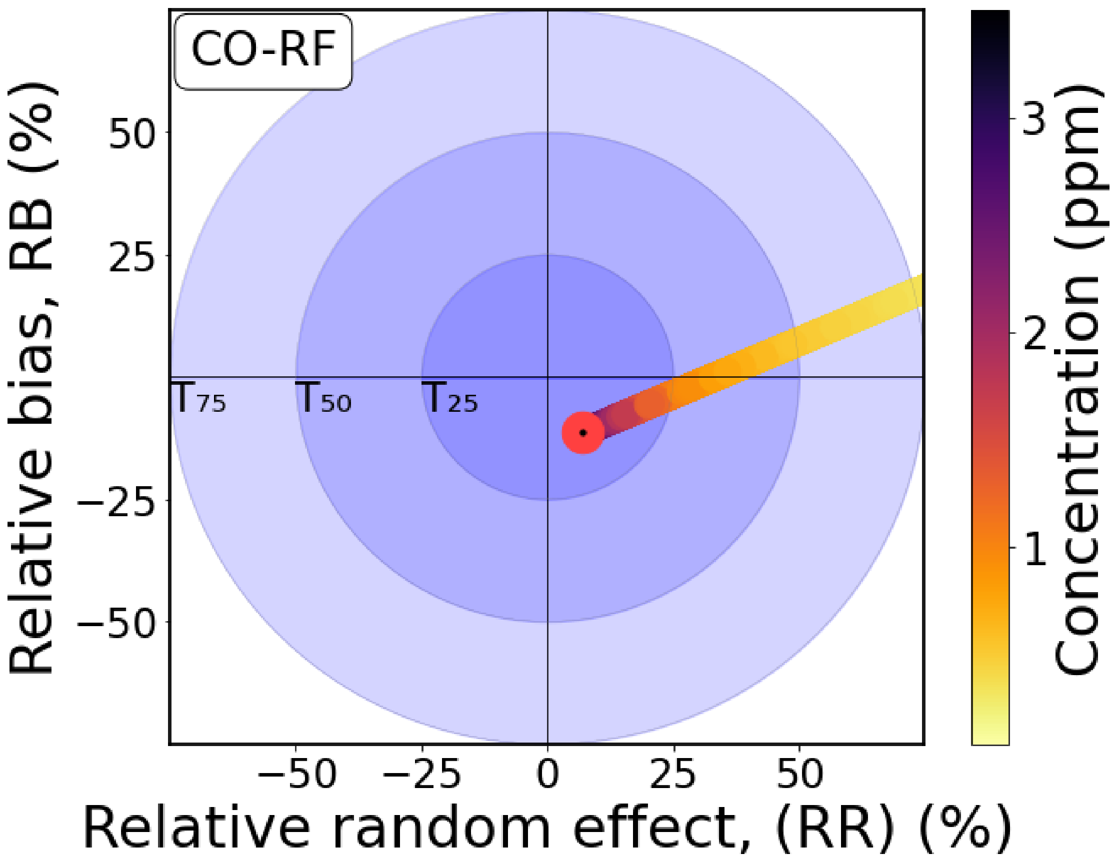
```
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=LQ
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[401]:
```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )
```

```
#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
```

```
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

plt.xlabel('Relative random effect, (RR) (%)' ,fontsize=34)
plt.ylabel('Relative bias, RB (%)',fontsize=34)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=24)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=24)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,1,2,3])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppm)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = 'CO-RF'
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
```

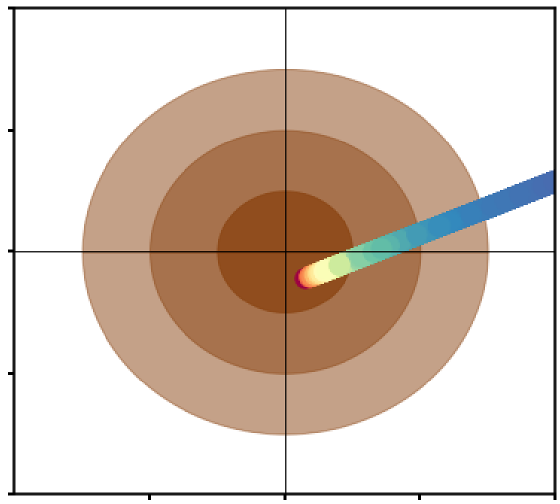
```
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
↪rotation_mode='anchor')
plt.text(-25,-7, 'T25'.translate(subscript),fontsize=24)
plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_CO_RF.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[402]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=25
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
```

```
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 25, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')
#plt.title('Case3')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
```

```
plt.savefig("dqo_CO_RF1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



X_Train, X_Test, y_Train, y_Test =train_test_split(X, y, test_size = 0.001) REU_CO=[] for i in range(1,30): regressor=regressor.fit(X_train[:120*i].drop([‘Lab1’], axis=1), y_train[:120*i]) pred = regressor.predict(X_test.drop([‘Lab1’], axis=1)) reu=REF2(pred,y_test,1.35,30000) REU_CO.append(reu)

4.4 Model 5: ANN

[403]:

```
from keras.models import Sequential
from keras.layers import Dense
from keras import optimizers
from sklearn.preprocessing import StandardScaler
model = Sequential()
model.add(Dense(3, input_shape = (6,),kernel_initializer='normal', activation=␣
↪'linear'))
model.add(Dense(128,kernel_initializer='normal', activation= 'relu'))
model.add(Dense(128, kernel_initializer='normal',activation= 'relu'))
model.add(Dense(100, kernel_initializer='normal',activation= 'relu'))
model.add(Dense(1,kernel_initializer='normal',activation='linear',))
sgd = optimizers.Adam(learning_rate=0.01)
```

```
model.compile(optimizer = sgd, loss = 'mean_squared_error', metrics= ['mse',␣
↪'mae'])
model.summary()
```

```
Model: "sequential_8"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense_38 (Dense)             (None, 3)                 21
_________________________________________________________________
dense_39 (Dense)             (None, 128)               512
_________________________________________________________________
dense_40 (Dense)             (None, 128)               16512
_________________________________________________________________
dense_41 (Dense)             (None, 100)               12900
_________________________________________________________________
dense_42 (Dense)             (None, 1)                 101
=================================================================
Total params: 30,046
Trainable params: 30,046
Non-trainable params: 0
_________________________________________________________________
```

[404]:
```
scaler = StandardScaler()
scaler.fit(X_train.drop(['Lab1'], axis=1))
X_train_scaled=scaler.transform(X_train.drop(['Lab1'], axis=1))
X_test_scaled=scaler.transform(X_test.drop(['Lab1'], axis=1))
hist=model.fit(X_train_scaled, y_train, batch_size= 10, epochs=40, verbose=␣
↪0)#,validation_split=0.2
```

[405]:
```
train_pred = model.predict(X_train_scaled)
test_pred = model.predict(X_test_scaled)
pred=[]
for i in range(len(test_pred)):
    pred.append(sum(list(test_pred[i])))
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_ann_CO=sMAPE_lr
```

```
RMSE_ann_CO=round(RMSE_lr/np.mean(np.array(y_test)),2)
Pearson_ann_CO=Pearson_lr
R2_ann_CO=round(sm.r2_score(y_test, pred), 2)
RMSE_Ann_CO=RMSE_lr
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

fig= plt.figure(figsize=(8,6)) ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) plt.plot(index,y_test[A:], color='limegreen',linewidth=3) plt.plot(index,pred[A:], color='tomato',linewidth=3) plt.plot(index,lab1[A:], color='#426eff',linewidth=3) plt.legend(['Ref', 'ANN-Calibrated', 'LAB-Calibrated'], loc = 2, bbox_to_anchor = (0.74,1)) plt.ylabel('CO Concentration(ppb)',fontsize=18) #plt.text(B-200, C, r'$R^2(ANN)$ ='+str(R2_ann_CO), fontsize = 14, color='tomato') #plt.text(B-200, D, r'$R^2(Lab)$ ='+str(R2_lab_CO), fontsize = 14, color='#426eff') #plt.text(B-800, C, 'Pearson r(ANN)='+str(Pearson_lr), fontsize = 14, color='tomato') #plt.text(B-800, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') #plt.xlabel('Last 200 hours of testing period',fontsize=18) #plt.title('ANN Calibration vs Laboratory Calibration',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

[406]:
```
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),
 ↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),
 ↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),
 ↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,
 ↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))
pred_ann=pred
MBE_ANN_CO=MBE(pred,y_test)/np.std(y_test)
CRMSE_ANN_CO=CRMSE(y_test,pred)/np.std(y_test)
```

```
Regressor model performance:
```

```
Mean absolute error(MAE) = 101.03
Mean squared error(MSE) = 32623.1
Median absolute error = 71.28
Explain variance score = 0.84
R2 score = 0.84
```

fig= plt.figure(figsize=(50,6)) ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) plt.plot(index[A:],y_test[A:], color='limegreen',linewidth=3) plt.plot(index[A:],lab1[A:], color='#426eff',linewidth=3) plt.plot(index[A:],pred_lr[A:], color='goldenrod',linewidth=3) plt.plot(index[A:],pred_svr[A:], color='brown',linewidth=3) plt.plot(index[A:],pred_rf[A:], color='indigo',linewidth=3) plt.plot(index[A:],pred_ann[A:], color='tomato',linewidth=3)

plt.xlabel('Last 200 hours of testing period',fontsize=18) plt.ylabel('CO Concentration(ppb)',fontsize=18) plt.legend(['Ref', 'LAB', 'LR','SVR','RF','ANN'], loc = 2, bbox_to_anchor = (0.95,1)) #plt.title('CO Sensor',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3)

[407]:
```
REF2(pred,y_test,1,30000)
```

[407]:
```
43.28375711695745
```

[408]:
```
import random
alpha=1.4
LV=max(y_test)+400
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
```

```
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=median
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=LQ
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
```

```
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

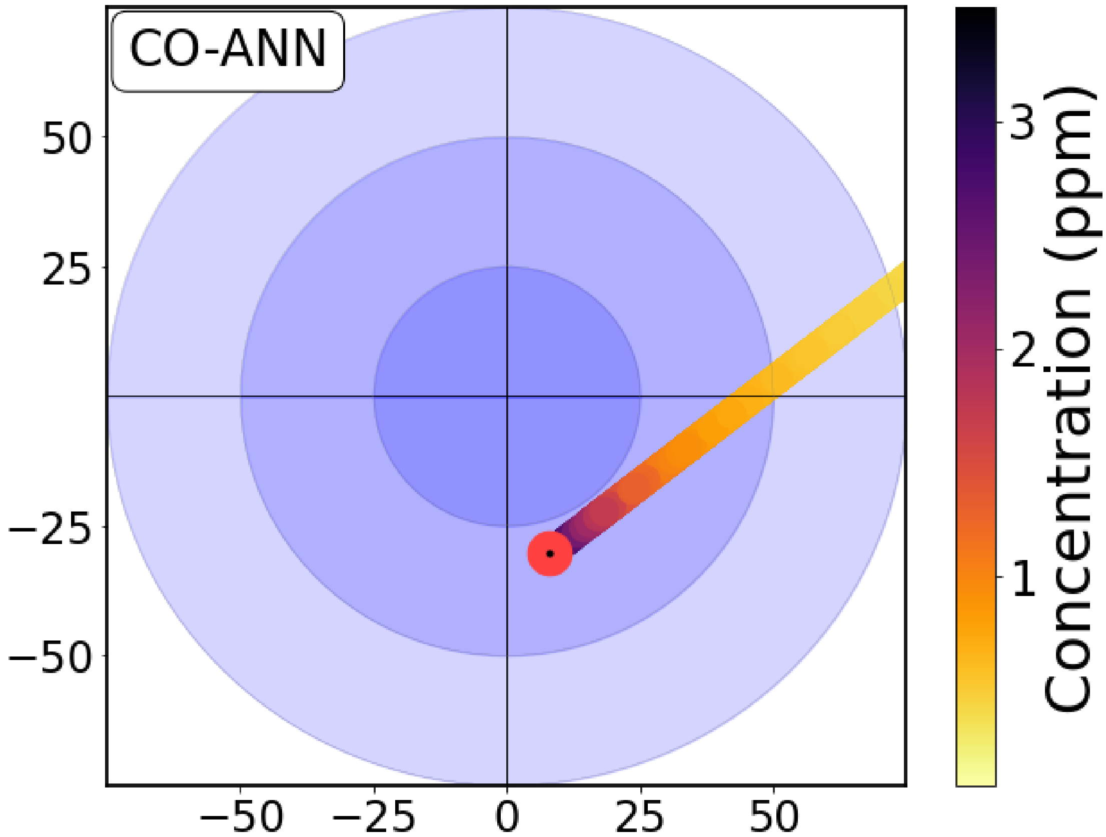
[409]:

```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
```

```
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')
```

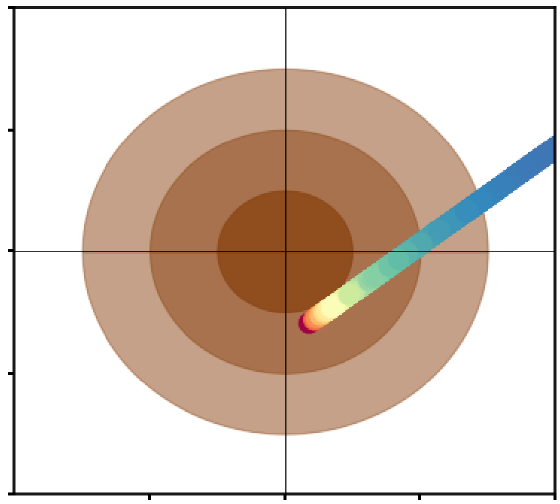
```
#plt.xlabel('Relative random effect (RR), ' + r'$ _{0}$'+'/'+r'$ref_{i}$, '+r'$( _{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.array(A4[2])/1000,cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=24)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=24)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,1,2,3])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppm)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = 'CO-ANN'
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90, rotation_mode='anchor')
#plt.text(-25,-7, 'T25'.translate(subscript),fontsize=24)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
#plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
```

```
plt.savefig("dqo_CO_ANN.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[410]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=25
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 25, color='wheat')
```

```
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_CO_ANN1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



5 Model 6: XGBoost

[411]:
```
from xgboost import  XGBRegressor
from numpy import absolute
from pandas import read_csv
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import RepeatedKFold
# create an xgboost regression model
#n_estimators=10000, max_depth=5, eta=0.01, subsample=0.9,colsample_bytree=0.
↪4,alpha=10
model =XGBRegressor(base_score=0.5, booster='gbtree',
             colsample_bylevel=0.5325799047395141, colsample_bynode=1,
             colsample_bytree=1.0, gamma=0, gpu_id=-1, grow_policy='lossguide',
             importance_type='gain', interaction_constraints='',
             learning_rate=0.09162995757195729, max_delta_step=0, max_depth=0,
             max_leaves=10, min_child_weight=1.4762838570024215,
                    monotone_constraints='()', n_estimators=970, n_jobs=-1,
             num_parallel_tree=1, random_state=0, reg_alpha=0.09065596443403534,
             reg_lambda=0.0009765625, scale_pos_weight=1,
             subsample=0.7601526809022708, tree_method='hist',
             use_label_encoder=False, validate_parameters=1, verbosity=0)
model.fit(X_train.drop(['Lab1'], axis=1), y_train)
```

[411]: XGBRegressor(base_score=0.5, booster='gbtree',
             colsample_bylevel=0.5325799047395141, colsample_bynode=1,
             colsample_bytree=1.0, gamma=0, gpu_id=-1, grow_policy='lossguide',
             importance_type='gain', interaction_constraints='',
             learning_rate=0.09162995757195729, max_delta_step=0, max_depth=0,
             max_leaves=10, min_child_weight=1.4762838570024215, missing=nan,
             monotone_constraints='()', n_estimators=970, n_jobs=-1,
             num_parallel_tree=1, random_state=0, reg_alpha=0.09065596443403534,
             reg_lambda=0.0009765625, scale_pos_weight=1,
             subsample=0.7601526809022708, tree_method='hist',
             use_label_encoder=False, validate_parameters=1, verbosity=0)

[412]:
```
pred = model.predict(X_test.drop(['Lab1'], axis=1))
pred_xgb_co=pred
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_xgb_CO=sMAPE_lr
RMSE_xgb_CO=RMSE_lr/np.mean(np.array(y_test))
Pearson_xgb_CO=Pearson_lr
R2_xgb_CO=round(sm.r2_score(y_test, pred), 2)
RMSE_Xgb_CO=RMSE_lr
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

[413]:
```
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),␣
↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),␣
↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))
pred_xgb=pred
MBE_XGB_CO=MBE(pred,y_test)/np.std(y_test)
CRMSE_XGB_CO=CRMSE(y_test,pred)/np.std(y_test)
```

```
Regressor model performance:
Mean absolute error(MAE) = 87.93
Mean squared error(MSE) = 24902.85
Median absolute error = 54.51
Explain variance score = 0.88
R2 score = 0.88
```

[414]:
```
import random
alpha=1.4
LV=max(y_test)+400
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
```

```
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=median
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=LQ
Cal=0
for i in range(len(y_test)):
```

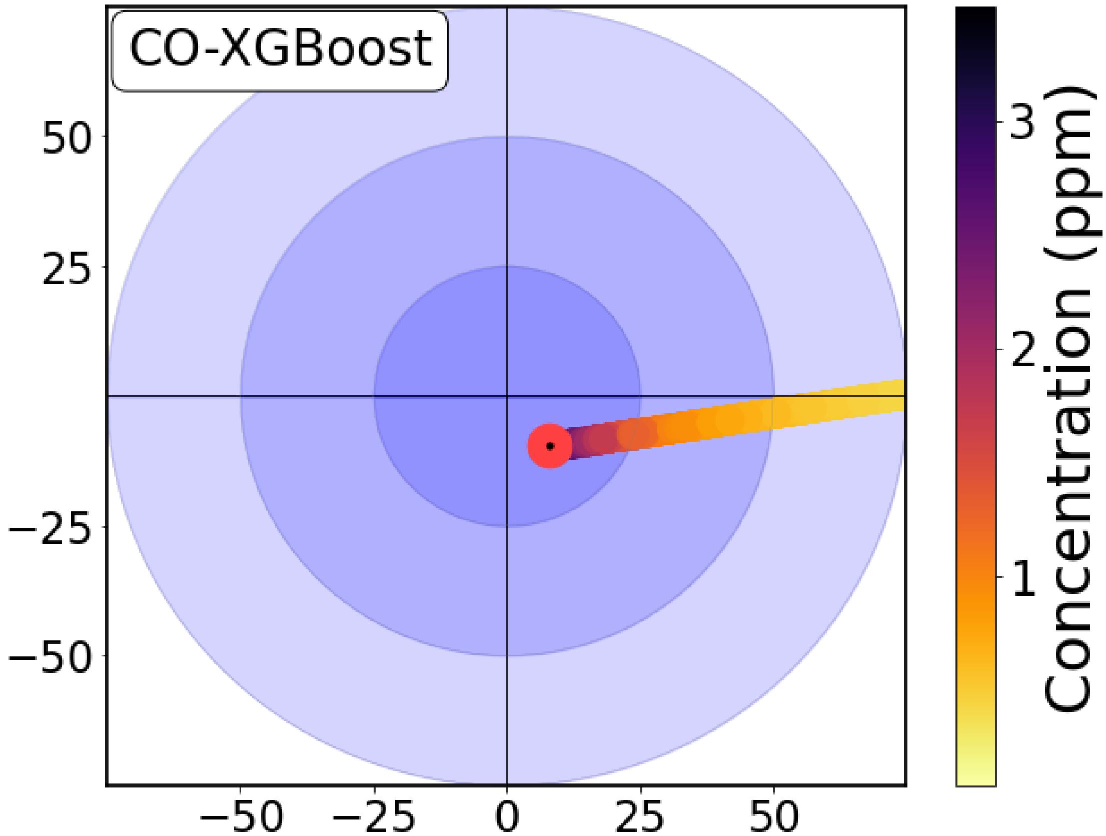
```
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[415]:
```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
```

```
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')
```

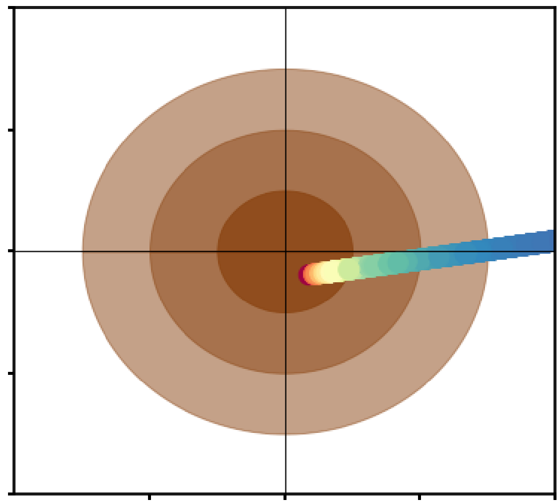
```
#plt.xlabel('Relative random effect (RR), ' + r'$ _{0}$'+'/'+r'$ref_{i}$,␣
↪'+r'$( _{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=24)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=24)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,1,2,3])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppm)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = 'CO-XGBoost'
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
↪rotation_mode='anchor')
#plt.text(-25,-7, 'T25'.translate(subscript),fontsize=24)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
#plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
```

```
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_CO_XGB.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[416]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=25
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
```

```python
plt.Circle((0, 0), 25, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_CO_XGB1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



6 NO2 Calibration

[417]:
```python
import pandas as pd
import scipy.io
import numpy as np
data = pd.read_csv('O3.txt', header = None,low_memory=False)
data.columns=['AE','WE','Temp','RH','Time']
Time=data['Time'].to_list()
time=[]
for i in range(len(Time)):
    time.append(float(abs(Time[i])))
Time=np.array(time)
Date=pd.to_datetime(Time-719529,unit='d').round('s')
data['Date'] = Date.tolist()
data=data.set_index('Date')
data.drop('Time',axis = 1, inplace = True)
data=data.resample('5min').mean()
Data_O3=data
Data_O3['Ref']=Ref_O3
WE=Data_O3['WE'].to_list()
AE=Data_O3['AE'].to_list()
signal=np.array(WE)-np.array(AE)
Data_O3['Net Signal']=signal
```

```
Data_03['Month']=Data_03.index.month
Data_03['Day_of_week']=Data_03.index.dayofweek
Data_03['Day']=Data_03.index.day
Data_03['Hour']=Data_03.index.hour
O3_Data=Data_03
O3_Data=O3_Data[(O3_Data[O3_Data.columns] >= 0).all(axis=1)]
O3_Data=O3_Data.dropna()
data = pd.read_csv('Conc_03.txt', header = None,low_memory=False)
data.columns=['Lab1','Temp','RH','Time','Ref']
Time=data['Time'].to_list()
time=[]
for i in range(len(Time)):
    time.append(float(abs(Time[i])))
Time=np.array(time)
Date=pd.to_datetime(Time-719529,unit='d').round('s')
data['Date'] = Date.tolist()
data=data.set_index('Date')
data.drop('Time',axis = 1, inplace = True)
data=data.resample('5min').mean()
Data_03=data
signal=np.array(WE)-np.array(AE)
Data_03['Net Signal']=signal
Data_03['Month']=Data_03.index.month
Data_03['Day_of_week']=Data_03.index.dayofweek
Data_03['Day']=Data_03.index.day
Data_03['Hour']=Data_03.index.hour
O3_Data=Data_03
O3_Data=O3_Data[(O3_Data[O3_Data.columns] >= 0).all(axis=1)]
O3_Data=O3_Data.dropna()
O3_Data=O3_Data.resample('5min').mean()
O3_Data=O3_Data.dropna()
O3_Data.head()

ref_03=Data_03['Ref'].to_list()
len(ref_03)
```

[417]: 60913

[418]:
```
import pandas as pd
import scipy.io
import numpy as np
data = pd.read_csv('NO2.txt', header = None,low_memory=False)
data.columns=['WE','AE','Temp','RH','Time']
Time=data['Time'].to_list()
time=[]
for i in range(len(Time)):
    time.append(float(abs(Time[i])))
```

```
Time=np.array(time)
Date=pd.to_datetime(Time-719529,unit='d').round('s')
data['Date'] = Date.tolist()
data=data.set_index('Date')
data.drop('Time',axis = 1, inplace = True)
data=data.resample('5min').mean()
Data_NO2=data
Data_NO2['Ref']=Ref_NO2
WE=Data_NO2['WE'].to_list()
AE=Data_NO2['AE'].to_list()
signal=np.array(WE)-np.array(AE)
Data_NO2['Net Signal']=signal
Data_NO2['Month']=Data_NO2.index.month
Data_NO2['Day_of_week']=Data_NO2.index.dayofweek
Data_NO2['Day']=Data_NO2.index.day
Data_NO2['Hour']=Data_NO2.index.hour
NO2_Data=Data_NO2
NO2_Data=NO2_Data[(NO2_Data[NO2_Data.columns] >= 0).all(axis=1)]
NO2_Data=NO2_Data.dropna()
data = pd.read_csv('Conc_NO2.txt', header = None,low_memory=False)
data.columns=['Lab1','Temp','RH','Time','Ref']
Time=data['Time'].to_list()
time=[]
subscript = str.maketrans("0123456789", "      ")
for i in range(len(Time)):
    time.append(float(abs(Time[i])))
Time=np.array(time)
Date=pd.to_datetime(Time-719529,unit='d').round('s')
data['Date'] = Date.tolist()
data=data.set_index('Date')
data.drop('Time',axis = 1, inplace = True)
data=data.resample('5min').mean()
Data_NO2=data
signal=np.array(WE)-np.array(AE)
Data_NO2['Net Signal']=signal
Data_NO2['Month']=Data_NO2.index.month
Data_NO2['Day_of_week']=Data_NO2.index.dayofweek
Data_NO2['Day']=Data_NO2.index.day
Data_NO2['Hour']=Data_NO2.index.hour
Data_NO2['Ref_O3']=ref_O3
NO2_Data=Data_NO2
NO2_Data=NO2_Data[(NO2_Data[NO2_Data.columns] >= 0).all(axis=1)]
NO2_Data=NO2_Data.dropna()
NO2_Data=NO2_Data.resample('5min').mean()
NO2_Data=NO2_Data.dropna()
NO2_Data.head()
```

[418]:

```
                           Lab1       Temp         RH        Ref  Net Signal  \
Date
2019-10-02 11:55:00   460.448301  26.378438  58.063437  15.230400    7.850000
2019-10-02 12:10:00  1364.583446  25.500000  48.612609   6.665136   37.815652
2019-10-02 12:15:00   224.159154  25.765087  48.441408   6.642805   12.275893
2019-10-02 12:20:00    82.998996  26.120078  47.716553   2.844210   13.152720
2019-10-02 15:45:00   566.301152  30.418466  50.153181  10.084125    9.323533

                     Month  Day_of_week  Day  Hour     Ref_O3
Date
2019-10-02 11:55:00   10.0          2.0  2.0  11.0  46.094860
2019-10-02 12:10:00   10.0          2.0  2.0  12.0  55.810810
2019-10-02 12:15:00   10.0          2.0  2.0  12.0  57.907075
2019-10-02 12:20:00   10.0          2.0  2.0  12.0  58.880540
2019-10-02 15:45:00   10.0          2.0  2.0  15.0  40.068225
```

[419]:

```
#Ref=NO2_Data['Ref'].to_list()
#NO2_Data=NO2_Data[NO2_Data.Ref.between(np.mean(Ref)-1*np.std(Ref), np.
 ↪mean(Ref)+1*np.std(Ref))]
#NO2_Data.shape
```

6.1 Model 1: Linear Regression (LR)

[420]:

```
df1=[x for _, x in NO2_Data.groupby('Month')]
data_oct=df1[4]
#data_oct=data_oct.sample(frac=1)
data_nov=df1[5]
#data_nov=data_nov.sample(frac=1)
data_dec=df1[6]
#data_dec=data_dec.sample(frac=1)
data_jan=df1[0]
#data_jan=data_jan.sample(frac=1)
data_feb=df1[1]
#data_feb=data_feb.sample(frac=1)
data_mar=df1[2]

data_Oct=data_oct.resample('15min').mean()
data_Oct=data_Oct.dropna()
data_Oct1=data_Oct[:int(0.8*data_Oct.shape[0])]
data_Oct2=data_Oct[int(0.8*data_Oct.shape[0]):]
data_Nov=data_nov.resample('15min').mean()
data_Nov=data_Nov.dropna()
data_Nov1=data_Nov[:int(0.8*data_Nov.shape[0])]
data_Nov2=data_Nov[int(0.8*data_Nov.shape[0]):]
data_Dec=data_dec.resample('15min').mean()
data_Dec=data_Dec.dropna()
data_Dec1=data_Dec[:int(0.8*data_Dec.shape[0])]
```

```
data_Dec2=data_Dec[int(0.8*data_Dec.shape[0]):]
data_Jan=data_jan.resample('15min').mean()
data_Jan=data_Jan.dropna()
data_Jan1=data_Jan[:int(0.8*data_Jan.shape[0])]
data_Jan2=data_Jan[int(0.8*data_Jan.shape[0]):]
data_Feb=data_feb.resample('15min').mean()
data_Feb=data_Feb.dropna()
data_Feb1=data_Feb[:int(0.8*data_Feb.shape[0])]
data_Feb2=data_Feb[int(0.8*data_Feb.shape[0]):]
data_Mar=data_mar.resample('15min').mean()
data_Mar=data_Mar.dropna()
data_Mar1=data_Mar[:int(0.8*data_Mar.shape[0])]
data_Mar2=data_Mar[int(0.8*data_Mar.shape[0]):]
frame1=[data_Oct1,data_Nov1,data_Dec1,data_Jan1,data_Feb1,data_Mar1]
frame2=[data_Oct2,data_Nov2,data_Dec2,data_Jan2,data_Feb2,data_Mar2]
NO2_data1=pd.concat(frame1)
NO2_data2=pd.concat(frame2)
NO2_data=pd.concat([NO2_data1,NO2_data2])
```

[421]:
```
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_absolute_error as mae
import sklearn.metrics as sm
import matplotlib.pyplot as plt
#X=R1_data[['Sen_10','T','RH','Month','Day_of_week','Hour']]
#y=R1_data['Ref_10']
X=NO2_data[['Net␣
↪Signal','Lab1','Temp','RH','Month','Day_of_week','Hour','Ref_O3']]#'Ref_O3'
y=NO2_data['Ref']
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.
↪2,shuffle=False)
len(X_test)
```

[421]: 2608

[422]:
```
lr = LinearRegression()
from sklearn.ensemble import RandomForestRegressor

 # create regressor object
regressor = RandomForestRegressor(n_estimators = 500,min_samples_split=␣
↪2,min_samples_leaf= 1,max_features= 'sqrt',
                                  random_state =␣
↪0,max_depth=None,bootstrap=False)

# fit the regressor with x and y data
regressor=regressor.fit(X_train, y_train)
pred = regressor.predict(X_test)
```

```
u_c_s=REF10(pred,y_test,1)[0]
X=np.array(REF10(pred,y_test,1)[1])**2
X=X.reshape((-1, 1))
model = lr.fit(X,u_c_s )
m_CO=model.coef_
q_CO=model.intercept_
m_CO,q_CO

LV=200
u_r=(np.sqrt(m_CO*y_test**2+q_CO)/y_test)*100
u_LV=(np.sqrt(m_CO*LV**2+q_CO)/LV)*100
T_LV=25
Beta=T_LV/u_LV
#Beta=T_LV-u_LV
LQ,median, UQ=np.percentile(y_test, [25,50,75])
u_25=(np.sqrt(m_CO*LQ**2+q_CO)/LQ)*100
T_25=u_25*Beta
u_50=(np.sqrt(m_CO*median**2+q_CO)/median)*100
T_50=u_50*Beta
u_75=(np.sqrt(m_CO*UQ**2+q_CO)/UQ)*100
T_75=u_75*Beta
T_25,T_50,T_75
```

```
<ipython-input-422-18bf9c5d0518>:21: RuntimeWarning: invalid value encountered
in sqrt
  u_LV=(np.sqrt(m_CO*LV**2+q_CO)/LV)*100
```

[422]:
```
(array([nan]), array([nan]), array([nan]))
```

[423]:
```
lr = LinearRegression()
model = lr.fit(X_train.drop(['Lab1'], axis=1), y_train)
pred = model.predict(X_test.drop(['Lab1'], axis=1))
lab1=X_test['Lab1'].to_list()
for i in range(len(lab1)):
    if lab1[i]>100:
        lab1[i]=np.mean(lab1)
index=[i for i in range(len(y_test))]
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =index)
Y_test
Pred=pd.Series(pred,index =index)
Lab1=pd.Series(lab1,index =index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
```

```
sMAPE_lr_NO2=sMAPE_lr
RMSE_lr_NO2=round(RMSE_lr/np.mean(np.array(y_test)),2)
Pearson_lr_NO2=Pearson_lr
sMAPE_lab_NO2=sMAPE_lab
RMSE_lab_NO2=round(RMSE_lab/np.mean(np.array(lab1)),2)
Pearson_lab_NO2=Pearson_lab
R2_lr_NO2=round(sm.r2_score(y_test, pred), 2)
R2_lab_NO2=round(sm.r2_score(y_test, lab1), 2)
RMSE_Lr_NO2=RMSE_lr
RMSE_Lab_NO2=RMSE_lab

A=len(y_test)-200
B=120
D=max(y_test[A:])-0.15*max(y_test[A:])
C=max(y_test[A:])-0.05*max(y_test[A:])
Pearson_lr_NO2,R2_lr_NO2,RMSE_Lr_NO2
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

[423]: (0.9, 0.81, 5.0)

subscript = str.maketrans("0123456789", " ") fig= plt.figure(figsize=(8,6)) index=[i for i in range(1,201)] ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) plt.plot(index,y_test[A:], color='limegreen',linewidth=3) plt.plot(index,pred[A:], color='#513e00',linewidth=3) plt.plot(index,lab1[A:], color='#426eff',linewidth=3) plt.legend(['Ref', 'LR-Calibrated', 'LAB-Calibrated'], loc = 2, bbox_to_anchor = (0.75,1)) plt.ylabel('NO2 Concentration(ppb)'.translate(subscript),fontsize=18) #plt.text(B-150, C,r'$R^2(LR)$ ='+str(R2_lr_NO2) , fontsize = 14, color='#513e00') #plt.text(B-150, D,r'$R^2(Lab)$ ='+str(R2_lab_NO2) , fontsize = 14, color='#426eff') #plt.text(B-700, C, 'Pearson r(LR)='+str(Pearson_lr), fontsize = 14, color='#513e00') #plt.text(B-700, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') #plt.xlabel('Last 200 hours of testing period',fontsize=18) #plt.title('Linear Regression Calibration vs Laboratory Calibration',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

```
[424]: print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),␣
 ↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),␣
 ↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
 ↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
 ↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))

MBE_LR_NO2=MBE(pred,y_test)/np.std(y_test)
CRMSE_LR_NO2=CRMSE(y_test,pred)/np.std(y_test)
MBE_LAB_NO2=MBE(lab1,y_test)/(2.6*np.std(y_test))
CRMSE_LAB_NO2=CRMSE(y_test,lab1)/(2.6*np.std(y_test))
pred_lr=pred
```

```
Regressor model performance:
Mean absolute error(MAE) = 3.88
Mean squared error(MSE) = 24.9
Median absolute error = 3.25
Explain variance score = 0.82
R2 score = 0.81
```

```
[425]: import random
alpha=1.4
LV=max(y_test)+2
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(lab1)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([0.4 for i in range(len(ref))])
u=0.005*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
```

```
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=median
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(lab1)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
```

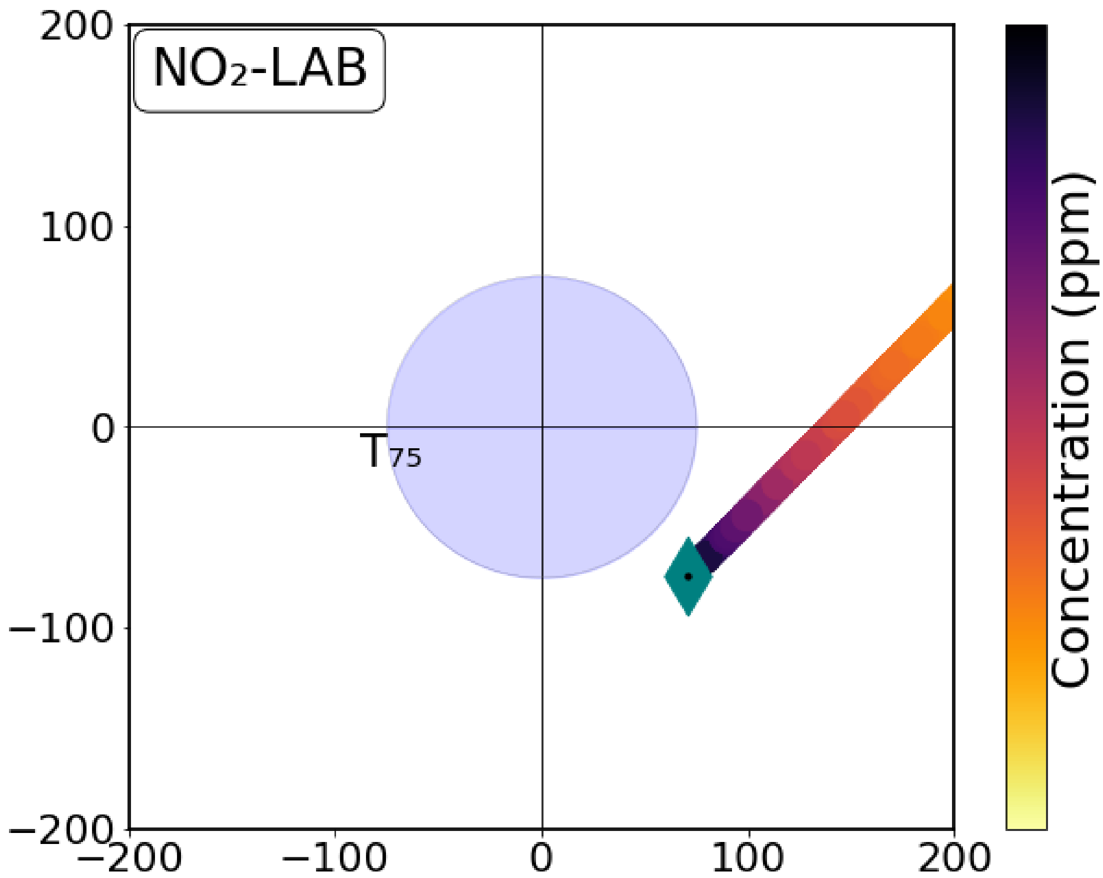
```
LV=LQ
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(lab1)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[426]:
```
A4=target(lab1,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
```

```python
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

#plt.fill_between(a1, b1, color='blue', alpha=0.17)
#plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

#plt.plot(x1,y1, linewidth=0.2, color='grey')
#plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
#plt.plot(x2,y2, linewidth=0.2, color='grey')
#plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

#plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
#plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
#plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
#plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
```

```
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$ _{0}$'+'/'+r'$ref_{i}$, '+r'$( _{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.array(A4[2])/1000,cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-200)
plt.ylim(ymax=200)
plt.xlim(xmax=200)
plt.xlim(xmin=-200)
plt.xticks(np.arange(-75,75),fontsize=22)
plt.xticks([-200,-100,0,100,200],fontsize=22)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-200,-100,0,100,200],fontsize=22)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,1,2,3])
cbar.ax.tick_params(labelsize=22)
cbar.set_label('Concentration (ppm)', rotation=90,fontsize=27)
plt.scatter(Random,Bias+0.2,marker="d",s=900, color='teal')
textstr = 'NO2-LAB'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90, rotation_mode='anchor')
#plt.text(-25,-7, 'T25'.translate(subscript),fontsize=18)
```

```python
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=18)
plt.text(-88,-20, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_NO2_LAB.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[427]:

```python
import random
alpha=1.4
LV=max(y_test)+5
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([0.4 for i in range(len(ref))])
```

```
u=0.005*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=median
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
```

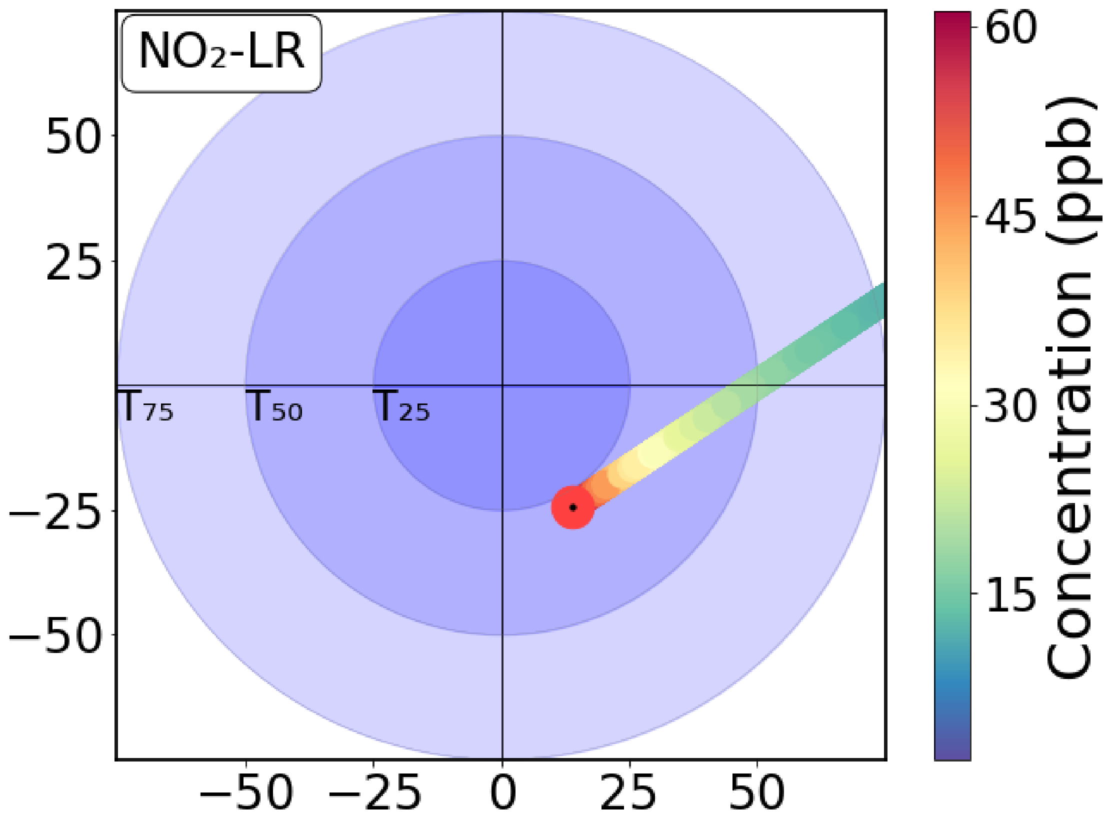
```
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=LQ
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[428]:
```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
```

```
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
```

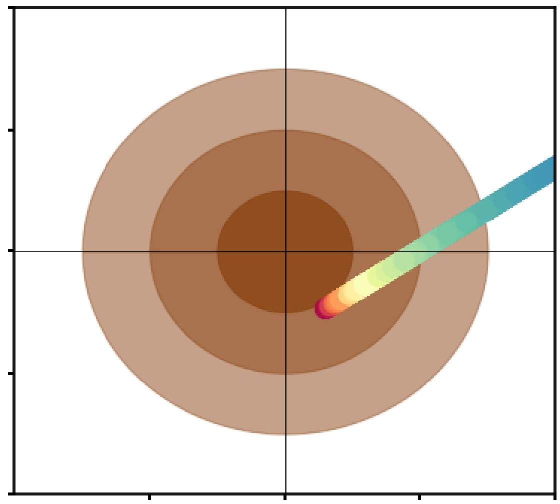
```
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$_{0}$'+'/'+r'$ref_{i}$,␣
↪'+r'$(_{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.
↪array(A4[2]),cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=28)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=28)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,15,30,45,60,75])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = textstr = 'NO2-LR'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
```

```
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
 ↪rotation_mode='anchor')
plt.text(-25,-7, 'T25'.translate(subscript),fontsize=24)
plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_NO2_LR.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



```
[429]: theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=25
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 25, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
```

```
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_NO2_LR1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



6.2 Model 2: Support Vector Regression (SVR)

[430]:
```
from sklearn.svm import SVR
from sklearn.preprocessing import StandardScaler
regressor = SVR(kernel = 'poly')
regressor.fit(X_train.drop(['Lab1'], axis=1), y_train)
pred = regressor.predict(X_test.drop(['Lab1'], axis=1))
for i in range(len(Pred)):
    if pred[i]<0:
        pred[i]=np.mean(np.array(pred))
```

[431]:
```python
Index=[i for i in range(len(y_test))]
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_svr_NO2=sMAPE_lr
RMSE_svr_NO2=round(RMSE_lr/np.mean(np.array(y_test)),2)
Pearson_svr_NO2=Pearson_lr
R2_svr_NO2=round(sm.r2_score(y_test, pred), 2)
RMSE_Svr_NO2=RMSE_lr
Pearson_svr_NO2,R2_svr_NO2,RMSE_Svr_NO2
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

[431]:
```
(0.92, 0.85, 4.5)
```

fig= plt.figure(figsize=(8,6)) ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) plt.plot(index,y_test[A:], color='limegreen',linewidth=3) plt.plot(index,pred[A:], color='brown',linewidth=3) plt.plot(index,lab1[A:], color='#426eff',linewidth=3) plt.legend(['Ref', 'SVR-Calibrated', 'LAB-Calibrated'], loc = 2, bbox_to_anchor = (0.74,1)) plt.ylabel('NO2 Concentration(ppb)'.translate(subscript),fontsize=18) #plt.text(B-150, C, r'$R^2(SVR)$ ='+str(R2_svr_NO2), fontsize = 14, color='brown') #plt.text(B-150, D, r'$R^2(Lab)$ ='+str(R2_lab_NO2), fontsize = 14, color='#426eff') #plt.text(B-700, C, 'Pearson r(SVR)='+str(Pearson_lr), fontsize = 14, color='brown') #plt.text(B-700, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') #plt.xlabel('Last 200 hours of testing period',fontsize=18) #plt.title('Support Vector Regression (SVR) Calibration vs Laboratory

Calibration',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

[432]:
```
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),␣
 ↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),␣
 ↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
 ↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
 ↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))

MBE_SVR_NO2=MBE(pred,y_test)/np.std(y_test)
CRMSE_SVR_NO2=CRMSE(y_test,pred)/np.std(y_test)
pred_svr=pred
```

```
Regressor model performance:
Mean absolute error(MAE) = 3.39
Mean squared error(MSE) = 20.2
Median absolute error = 2.69
Explain variance score = 0.85
R2 score = 0.85
```

[433]:
```
import random
alpha=1.4
LV=max(y_test)+5
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([0.4 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
```

```
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=median
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=LQ
```

```
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

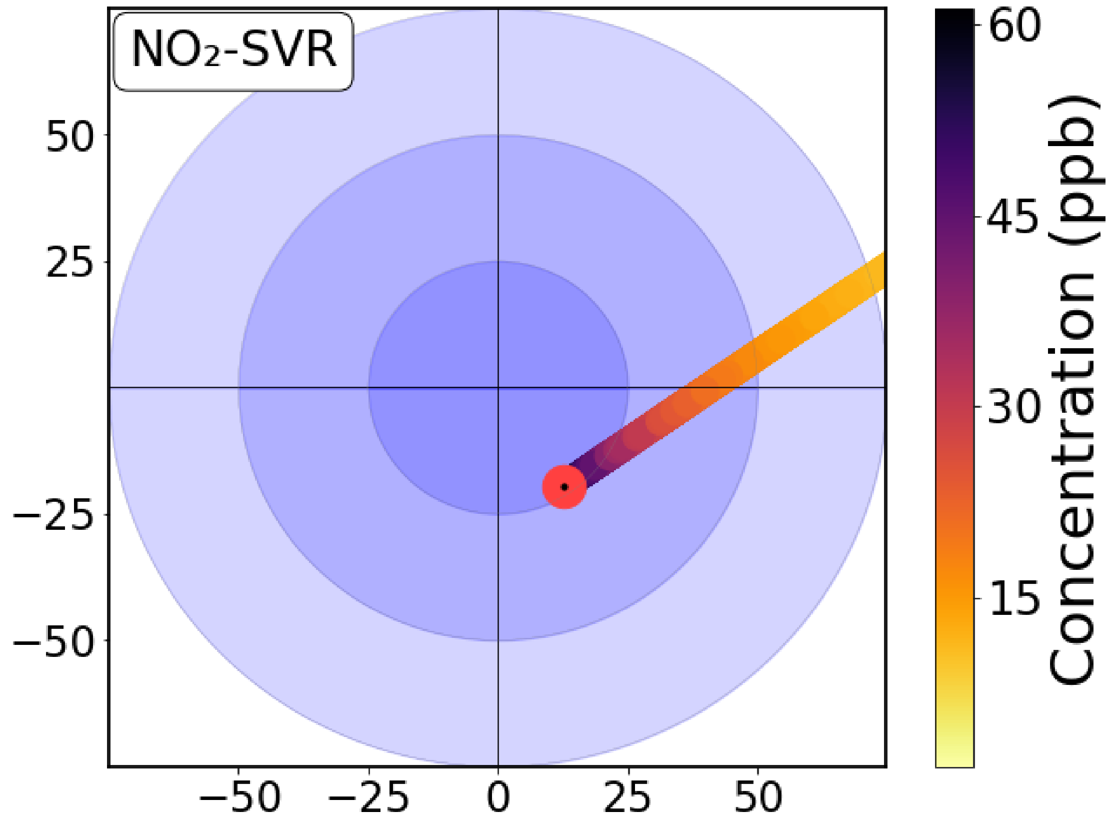
[434]:

```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
```

```python
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
```

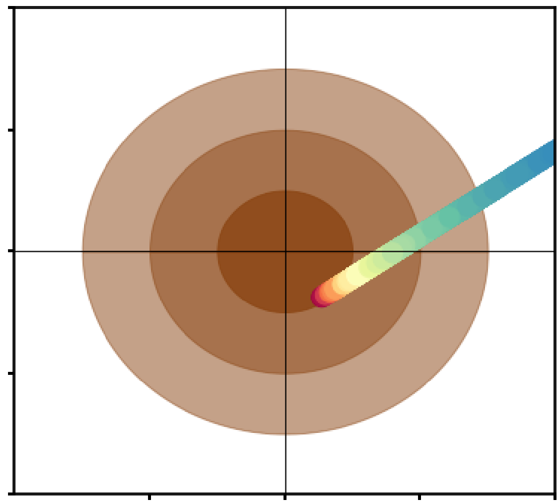
```
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$_{0}$'+'/'+r'$ref_{i}$,␣
↪'+r'$(_{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.
↪array(A4[2]),cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=24)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=24)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,15,30,45,60,75])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = textstr = 'NO2-SVR'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
↪rotation_mode='anchor')
#plt.text(-25,-7, 'T25'.translate(subscript),fontsize=24)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
```

```
#plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_NO2_SVR.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[435]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=25
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )
```

```python
fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 25, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_NO2_SVR1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



6.3 Model 3: Random Forest

[436]:
```
from sklearn.ensemble import RandomForestRegressor

 # create regressor object
regressor = RandomForestRegressor(max_features=0.30888259687906783,␣
↪max_leaf_nodes=1564,
                      n_estimators=194, n_jobs=-1,min_samples_split=␣
↪2,min_samples_leaf= 1,
                                  random_state =␣
↪0,max_depth=None,bootstrap=False)

# fit the regressor with x and y data
regressor.fit(X_train.drop(['Lab1'], axis=1), y_train)
```

[436]:
```
RandomForestRegressor(bootstrap=False, max_features=0.30888259687906783,
                      max_leaf_nodes=1564, n_estimators=194, n_jobs=-1,
                      random_state=0)
```

[437]:
```
Index=[i for i in range(len(y_test))]
features_NO2=regressor.feature_importances_
pred = regressor.predict(X_test.drop(['Lab1'], axis=1))
pred_rf_no2=pred
Y_test=y_test.to_list()
```

```
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_rf_NO2=sMAPE_lr
RMSE_rf_NO2=round(RMSE_lr/np.mean(np.array(y_test)),2)
Pearson_rf_NO2=Pearson_lr
R2_rf_NO2=round(sm.r2_score(y_test, pred), 2)
RMSE_Rf_NO2=RMSE_lr
Pearson_rf_NO2,R2_rf_NO2,RMSE_Rf_NO2
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

[437]:
```
(0.96, 0.9, 3.6)
```

fig= plt.figure(figsize=(10,5))

ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) plt.plot(index,y_test[A:], color='limegreen',linewidth=3) plt.plot(index,pred[A:], color='indigo',linewidth=3) plt.plot(index,lab1[A:], color='#426eff',linewidth=3) plt.legend(['Ref', 'RF-Calibrated', 'LAB-Calibrated'], loc = 2, bbox_to_anchor = (0.79,1)) plt.ylabel('NO2 Concentration(ppb)'.translate(subscript),fontsize=18) plt.text(B-15, C,r'$R^2(RF)$ ='+str(R2_rf_NO2) , fontsize = 14, color='indigo') plt.text(B-15, D,r'$R^2(Lab)$ ='+str(R2_lab_NO2) , fontsize = 14, color='#426eff') plt.text(B-73, C, 'Pearson r(RF)='+str(Pearson_lr), fontsize = 14, color='indigo') plt.text(B-73, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') #plt.xlabel('Last 200 hours of testing period',fontsize=18) #plt.title('Random Forest(RF) Calibration vs Laboratory Calibration',fontsize=18) plt.xlabel('Last 100 hours of testing period',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

[438]:
```
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),␣
 ↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),␣
 ↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
 ↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
 ↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))

MBE_RF_NO2=MBE(pred,y_test)/np.std(y_test)
CRMSE_RF_NO2=CRMSE(y_test,pred)/np.std(y_test)
pred_rf=pred
```

```
Regressor model performance:
Mean absolute error(MAE) = 2.92
Mean squared error(MSE) = 13.18
Median absolute error = 2.6
Explain variance score = 0.91
R2 score = 0.9
```

[439]:
```
import random
alpha=1.4
LV=max(y_test)+5
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([0.4 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
```

```
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=median
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=LQ
```

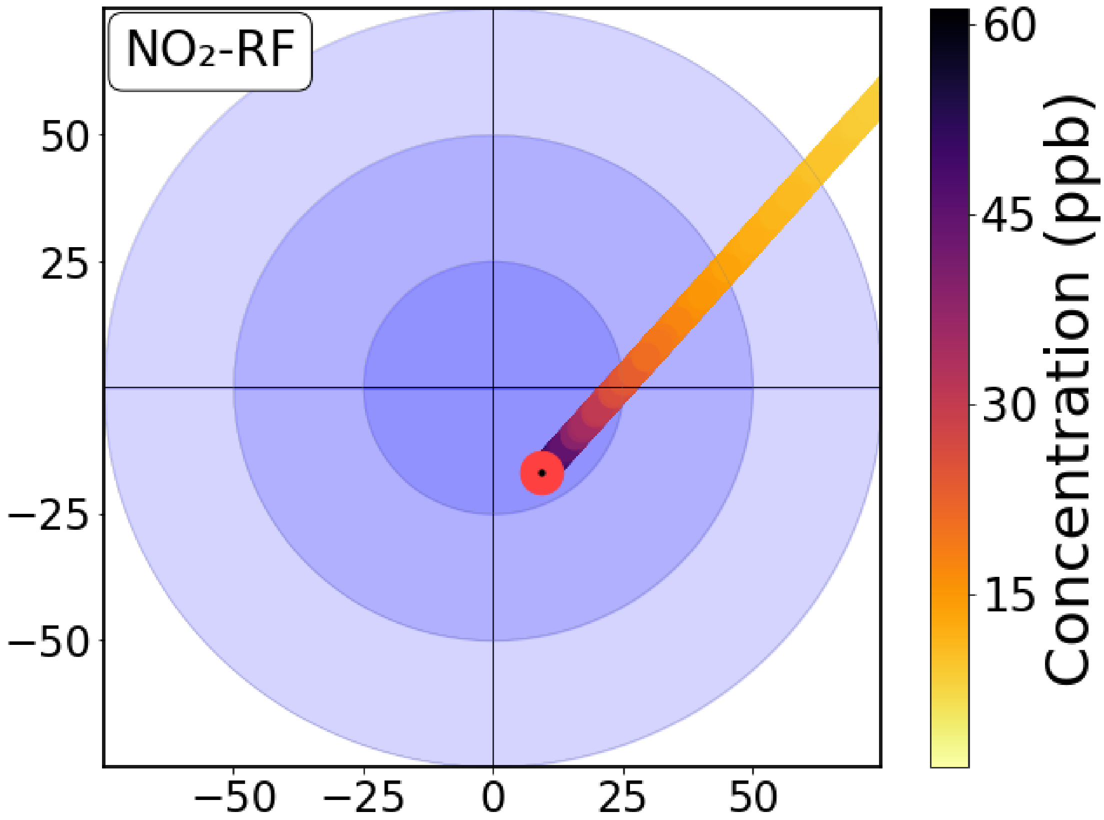
```
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[440]:
```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
```

```
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
```

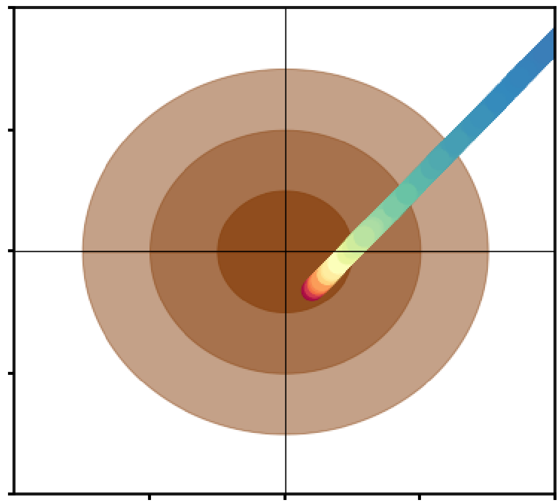
```
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$ _{0}$'+'/'+r'$ref_{i}$, '+r'$( _{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.array(A4[2]),cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=24)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=24)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,15,30,45,60,75])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = textstr = 'NO2-RF'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,rotation_mode='anchor')
#plt.text(-25,-7, 'T25'.translate(subscript),fontsize=24)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
```

```
#plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_NO2_RF.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[441]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=25
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )
```

```
fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 25, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_NO2_RF1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



6.4 Model 4 : ANN

[442]:
```
from keras.models import Sequential
from keras.layers import Dense
from keras import optimizers
from sklearn.preprocessing import StandardScaler
model = Sequential()
model.add(Dense(6, input_shape = (7,),kernel_initializer='normal', activation=␣
 ↪'linear'))
model.add(Dense(128,kernel_initializer='normal', activation= 'relu'))
model.add(Dense(128, kernel_initializer='normal',activation= 'relu'))
model.add(Dense(100, kernel_initializer='normal',activation= 'relu'))
model.add(Dense(1,kernel_initializer='normal',activation='linear',))
sgd = optimizers.Adam(learning_rate=0.01)

model.compile(optimizer = sgd, loss = 'mean_squared_error', metrics= ['mse',␣
 ↪'mae'])
model.summary()
```

```
Model: "sequential_9"

_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense_43 (Dense)             (None, 6)                 48
```

```
_________________________________________________________________
dense_44 (Dense)             (None, 128)               896
_________________________________________________________________
dense_45 (Dense)             (None, 128)               16512
_________________________________________________________________
dense_46 (Dense)             (None, 100)               12900
_________________________________________________________________
dense_47 (Dense)             (None, 1)                 101
=================================================================
Total params: 30,457
Trainable params: 30,457
Non-trainable params: 0
_________________________________________________________________
```

[443]:
```
scaler = StandardScaler()
scaler.fit(X_train.drop(['Lab1'], axis=1))
X_train_scaled=scaler.transform(X_train.drop(['Lab1'], axis=1))
X_test_scaled=scaler.transform(X_test.drop(['Lab1'], axis=1))
model.fit(X_train_scaled, y_train, batch_size= 100, epochs=100, verbose= 0)
```

[443]: <tensorflow.python.keras.callbacks.History at 0x137859b20>

[444]:
```
train_pred = model.predict(X_train_scaled)
test_pred = model.predict(X_test_scaled)
pred=[]
for i in range(len(test_pred)):
    pred.append(sum(list(test_pred[i])))
len(y_test)
```

[444]: 2608

[445]:
```
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_ann_NO2=sMAPE_lr
RMSE_ann_NO2=round(RMSE_lr/np.mean(np.array(y_test)),2)
Pearson_ann_NO2=Pearson_lr
R2_ann_NO2=round(sm.r2_score(y_test, pred), 2)
RMSE_Ann_NO2=RMSE_lr
Pearson_ann_NO2,R2_ann_NO2,RMSE_Ann_NO2
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

[445]:
```
(0.94, 0.86, 4.3)
```

fig= plt.figure(figsize=(8,6)) ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) plt.plot(index,y_test[A:], color='limegreen',linewidth=3) plt.plot(index,pred[A:], color='tomato',linewidth=3) plt.plot(index,lab1[A:], color='#426eff',linewidth=3) plt.legend(['Ref', 'ANN-Calibrated', 'LAB-Calibrated'], loc = 2, bbox_to_anchor = (0.74,1)) plt.ylabel('NO2 Concentration(ppb)',fontsize=18) #plt.text(B-150, C, r'$R^2(ANN)$ ='+str(R2_ann_NO2), fontsize = 14, color='tomato') #plt.text(B-150, D, r'$R^2(Lab)$ ='+str(R2_lab_NO2), fontsize = 14, color='#426eff') #plt.text(B-700, C, 'Pearson r(ANN)='+str(Pearson_lr), fontsize = 14, color='tomato') #plt.text(B-700, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') #plt.xlabel('Last 200 hours of testing period',fontsize=18) #plt.title(' Artificial Neural Network(ANN) Calibration vs Laboratory Calibration',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

[446]:
```python
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),
 ↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),
 ↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),
 ↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,
 ↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))

MBE_ANN_NO2=MBE(pred,y_test)/np.std(y_test)
CRMSE_ANN_NO2=CRMSE(y_test,pred)/(np.std(y_test))
pred_ann=pred
```

```
Regressor model performance:
Mean absolute error(MAE) = 3.28
Mean squared error(MSE) = 18.19
```

```
Median absolute error = 2.67
Explain variance score = 0.88
R2 score = 0.86
```

[447]:
```python
import random
alpha=1.4
LV=max(y_test)+5
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([0.4 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=median
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
```

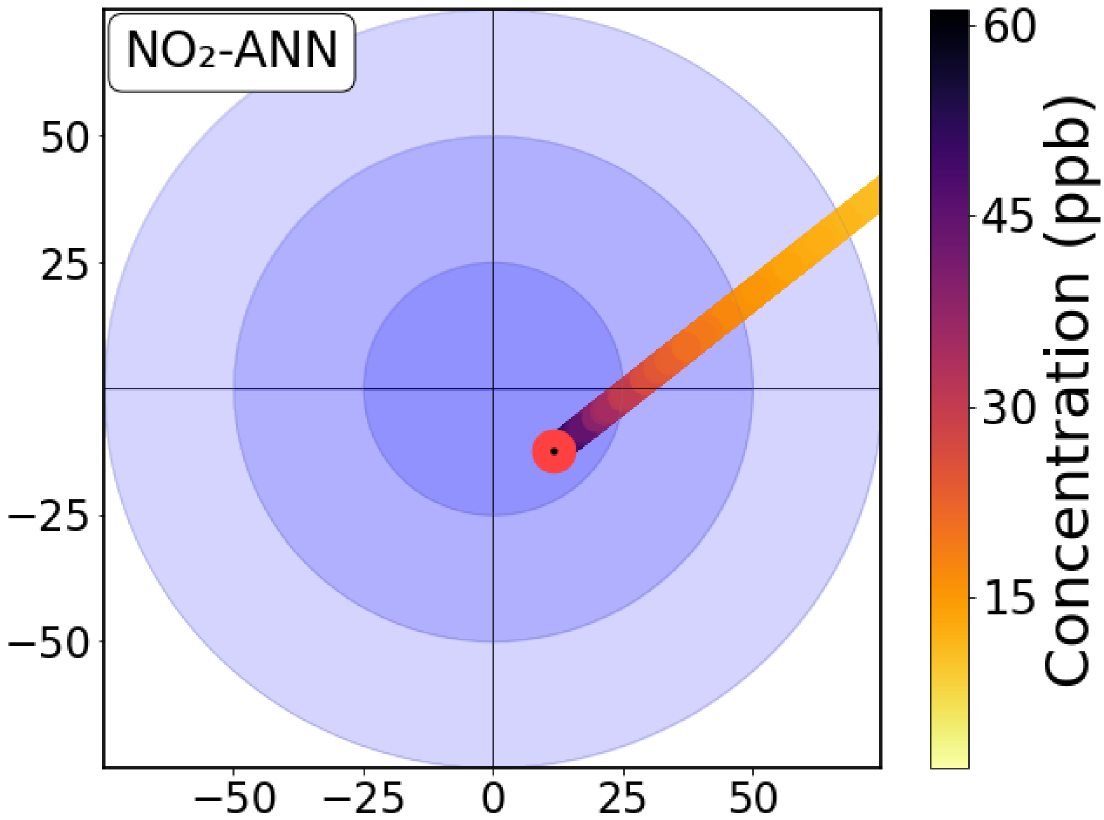
```
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=LQ
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
```

```
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[448]:
```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
```

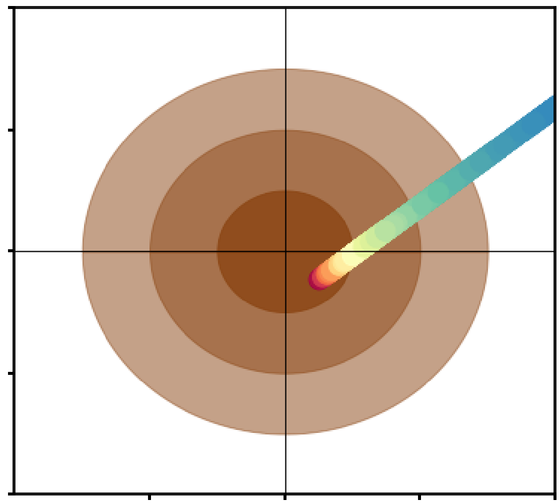
```
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$_{0}$'+'/'+r'$ref_{i}$,␣
↪'+r'$(_{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('C0',fontsize=18)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.
↪array(A4[2]),cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
```

```python
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=24)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=24)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,15,30,45,60,75])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = textstr = 'NO2-ANN'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
 ↪rotation_mode='anchor')
#plt.text(-25,-7, 'T25'.translate(subscript),fontsize=24)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
#plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_NO2_ANN.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[449]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=25
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 25, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
```

```
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_NO2_ANN1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



7 Model 5: XGBoost

[450]:
```
from xgboost import  XGBRegressor
from numpy import absolute
from pandas import read_csv
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import RepeatedKFold
# create an xgboost regression model
#n_estimators=10000, max_depth=5, eta=0.01, subsample=0.9,colsample_bytree=0.
 ↪4,alpha=10
model =XGBRegressor(base_score=0.5, booster='gbtree',
             colsample_bylevel=0.6707587713163239, colsample_bynode=1,
             colsample_bytree=0.8537810552612592, gamma=0, gpu_id=-1,
             grow_policy='lossguide', importance_type='gain',
             interaction_constraints='', learning_rate=0.03751721359159872,
             max_delta_step=0, max_depth=0, max_leaves=65,
             min_child_weight=2.7540944694192047,
             monotone_constraints='()', n_estimators=499, n_jobs=-1,
             num_parallel_tree=1, random_state=0,
             reg_alpha=0.0017451960573349064, reg_lambda=0.0014745070199918,
             scale_pos_weight=1, subsample=0.5146065456700301,
             tree_method='hist', use_label_encoder=False, validate_parameters=1,
             verbosity=0)
```

```
model.fit(X_train.drop(['Lab1'], axis=1),y_train)
```

[450]:
```
XGBRegressor(base_score=0.5, booster='gbtree',
             colsample_bylevel=0.6707587713163239, colsample_bynode=1,
             colsample_bytree=0.8537810552612592, gamma=0, gpu_id=-1,
             grow_policy='lossguide', importance_type='gain',
             interaction_constraints='', learning_rate=0.03751721359159872,
             max_delta_step=0, max_depth=0, max_leaves=65,
             min_child_weight=2.7540944694192047, missing=nan,
             monotone_constraints='()', n_estimators=499, n_jobs=-1,
             num_parallel_tree=1, random_state=0,
             reg_alpha=0.0017451960573349064, reg_lambda=0.0014745070199918,
             scale_pos_weight=1, subsample=0.5146065456700301,
             tree_method='hist', use_label_encoder=False, validate_parameters=1,
             verbosity=0)
```

[451]:
```
pred = model.predict(X_test.drop(['Lab1'], axis=1))
pred_xgb_no2=pred
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_xgb_NO2=sMAPE_lr
RMSE_xgb_NO2=RMSE_lr/np.mean(np.array(y_test))
Pearson_xgb_NO2=Pearson_lr
R2_xgb_NO2=round(sm.r2_score(y_test, pred), 2)
RMSE_Xgb_NO2=RMSE_lr
Pearson_xgb_NO2,R2_xgb_NO2,RMSE_Xgb_NO2
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
```

```
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

[451]:
```
(0.96, 0.91, 3.5)
```

fig= plt.figure(figsize=(8,6)) ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) plt.plot(index,y_test[A:], color='limegreen',linewidth=3) plt.plot(index,pred[A:], color='darkgoldenrod',linewidth=3) plt.plot(index,lab1[A:], color='#426eff',linewidth=3) plt.legend(['Ref', 'XGBoost-Calibrated', 'LAB-Calibrated'], loc = 2, bbox_to_anchor = (0.69,1)) plt.ylabel('NO2 Concentration(ppb)'.translate(subscript),fontsize=18) #plt.text(B-150, C, r'$R^2(XGB)$ ='+str(R2_xgb_NO2), fontsize = 14, color='darkgoldenrod') #plt.text(B-150, D, r'$R^2(Lab)$ ='+str(R2_lab_NO2), fontsize = 14, color='#426eff') #plt.text(B-700, C, 'Pearson r(XGB)='+str(Pearson_lr), fontsize = 14, color='darkgoldenrod') #plt.text(B-700, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') #plt.xlabel('Last 200 hours of testing period',fontsize=18) #plt.title('XGBoost Calibration vs Laboratory Calibration',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

[452]:
```python
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),␣
 ↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),␣
 ↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
 ↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
 ↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))

MBE_XGB_NO2=MBE(pred,y_test)/np.std(y_test)
CRMSE_XGB_NO2=CRMSE(y_test,pred)/np.std(y_test)
pred_xgb=pred
```

```
Regressor model performance:
Mean absolute error(MAE) = 2.78
Mean squared error(MSE) = 12.54
Median absolute error = 2.32
Explain variance score = 0.91
R2 score = 0.91
```

[453]:
```python
import random
alpha=1.4
LV=max(y_test)+5
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
```

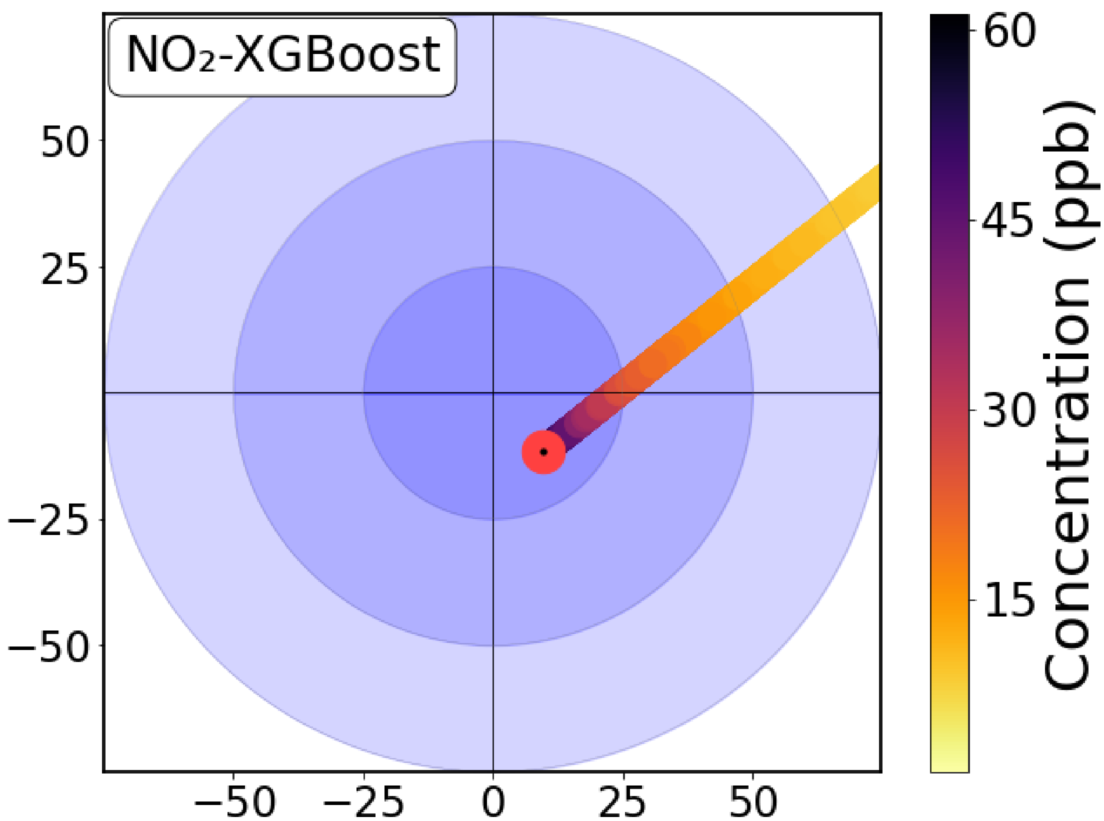
```
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([0.4 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=median
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
```

```
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=LQ
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[454]:
```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)
```

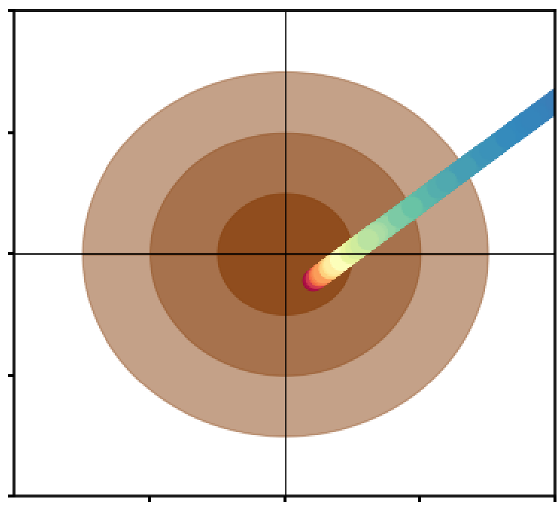
```
plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$ _{0}$'+'/'+r'$ref_{i}$, '+r'$( _{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.array(A4[2]),cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=24)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=24)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,15,30,45,60,75])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
```

```
textstr = textstr = 'NO2-XGBoost'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
 ↪rotation_mode='anchor')
#plt.text(-25,-7, 'T25'.translate(subscript),fontsize=24)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
#plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_NO2_XGB.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[455]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=25
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 25, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')
```

```
#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_NO2_XGB1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



SO2 Calibration

[456]:
```
import pandas as pd
Ref=pd.read_csv('Ref.csv')
Ref["CO"] = 1000 * Ref["CO"]
Ref['Date'] = pd.to_datetime(Ref['Date_Time'])
Ref=Ref.set_index('Date')
Ref.drop('Date_Time',axis = 1, inplace = True)
Ref=Ref.resample('5min').mean()
Ref=Ref[76463:137376]
Ref_CO=Ref['CO'].to_list()
```

```
Ref_NO2=Ref['NO2'].to_list()
Ref_SO2=Ref['SO2'].to_list()
Ref_O3=Ref['O3'].to_list()
```

import pandas as pd import scipy.io import numpy as np data = pd.read_csv(‘SO2.txt’, header = None,low_memory=False) data.columns=[‘WE’,‘AE’,‘Temp’,‘RH’,‘Time’] Time=data[‘Time’].to_list() time=[] for i in range(len(Time)): time.append(float(abs(Time[i]))) Time=np.array(time) Date=pd.to_datetime(Time-719529,unit=‘d’).round(‘s’) data[‘Date’] = Date.tolist() data=data.set_index(‘Date’) data.drop(‘Time’,axis = 1, inplace = True) data=data.resample(‘5min’).mean() Data_SO2=data Data_SO2[‘Ref’]=Ref_SO2 WE=Data_SO2[‘WE’].to_list() AE=Data_SO2[‘AE’].to_list() signal=np.array(WE)-np.array(AE) Data_SO2[‘Net Signal’]=signal Data_SO2[‘Month’]=Data_SO2.index.month Data_SO2[‘Day_of_week’]=Data_SO2.index.dayofweek Data_SO2[‘Day’]=Data_SO2.index.day Data_SO2[‘Hour’]=Data_SO2.index.hour SO2_Data=Data_SO2 SO2_Data=SO2_Data[(SO2_Data[SO2_Data >= 0).all(axis=1)] SO2_Data=SO2_Data.dropna() data = pd.read_csv(‘Conc_SO2.txt’, header = None,low_memory=False) data.columns=[‘Lab2’,‘Temp’,‘RH’,‘Time’,‘Ref’] Time=data[‘Time’].to_list() time=[] for i in range(len(Time)): time.append(float(abs(Time[i]))) Time=np.array(time) Date=pd.to_datetime(Time-719529,unit=‘d’).round(‘s’) data[‘Date’] = Date.tolist() data=data.set_index(‘Date’) data.drop(‘Time’,axis = 1, inplace = True) data=data.resample(‘5min’).mean() Data_SO2=data signal=np.array(WE)-np.array(AE) Data_SO2[‘Net Signal’]=signal Data_SO2[‘Month’]=Data_SO2.index.month Data_SO2[‘Day_of_week’]=Data_SO2.index.dayofweek Data_SO2[‘Day’]=Data_SO2.index.day Data_SO2[‘Hour’]=Data_SO2.index.hour SO2_Data=Data_SO2 SO2_Data=SO2_Data[(SO2_Data[SO2_Data >= 0).all(axis=1)] SO2_Data=SO2_Data.dropna() SO2_Data=SO2_Data.resample(‘h’).mean() SO2_Data=SO2_Data.dropna() SO2_Data.head()

[457]:
```
import pandas as pd
import scipy.io
import numpy as np
data = pd.read_csv('Conc_SO2.txt', header = None,low_memory=False)
data.columns=['Lab2','Temp','RH','Time','Ref']
Time=data['Time'].to_list()
time=[]
for i in range(len(Time)):
    time.append(float(abs(Time[i])))
Time=np.array(time)
Date=pd.to_datetime(Time-719529,unit='d').round('s')
data['Date'] = Date.tolist()
data=data.set_index('Date')
data.drop('Time',axis = 1, inplace = True)
data=data.resample('5min').mean()
Data_SO2=data
Data_so2=data
signal=np.array(WE)-np.array(AE)
Data_SO2['Net Signal']=signal
Data_SO2['Month']=Data_SO2.index.month
Data_SO2['Day_of_week']=Data_SO2.index.dayofweek
```

```
Data_SO2['Day']=Data_SO2.index.day
Data_SO2['Hour']=Data_SO2.index.hour
SO2_Data=Data_SO2
SO2_Data=SO2_Data.resample('5min').mean()
SO2_Data=SO2_Data[(SO2_Data[SO2_Data.columns] >= 0).all(axis=1)]
SO2_Data=SO2_Data.dropna()
data = pd.read_csv('SO2.txt', header = None,low_memory=False)
data.columns=['WE','AE','Temp','RH','Time']
Time=data['Time'].to_list()
time=[]
for i in range(len(Time)):
    time.append(float(abs(Time[i])))
Time=np.array(time)
Date=pd.to_datetime(Time-719529,unit='d').round('s')
data['Date'] = Date.tolist()
data=data.set_index('Date')
data.drop('Time',axis = 1, inplace = True)
data=data.resample('5min').mean()
Data_SO2=data
Data_SO2['Ref']=Ref_SO2
WE=Data_SO2['WE'].to_list()
AE=Data_SO2['AE'].to_list()
signal=np.array(WE)-np.array(AE)
Data_SO2['Lab2']=Data_so2['Lab2'].to_list()
Data_SO2['Net Signal']=signal
Data_SO2['Month']=Data_SO2.index.month
Data_SO2['Day_of_week']=Data_SO2.index.dayofweek
Data_SO2['Day']=Data_SO2.index.day
Data_SO2['Hour']=Data_SO2.index.hour
SO2_Data=Data_SO2
SO2_Data=SO2_Data[(SO2_Data[SO2_Data.columns] >= 0).all(axis=1)]
SO2_Data=SO2_Data.dropna()
CO_Data=CO_Data.resample('5min').mean()
CO_Data=CO_Data.dropna()
SO2_Data.head()
```

[457]:

```
                             WE          AE       Temp         RH       Ref  \
Date
2019-10-10 04:15:00  342.991196  342.255475  18.268917  81.793083  1.085790
2019-10-10 04:45:00  345.767413  342.543745  18.359000  82.451958  1.163473
2019-10-10 04:50:00  343.919310  342.689191  18.348826  82.572044  1.200187
2019-10-10 04:55:00  343.377326  342.448811  18.353612  82.675760  1.312772
2019-10-10 05:00:00  343.358621  342.322426  18.351611  82.723472  1.237584

                         Lab2  Net Signal  Month  Day_of_week  Day  Hour
Date
2019-10-10 04:15:00  7.660248    0.735722     10            3   10     4
```

2019-10-10 04:45:00	15.077802	3.223668	10	3	10	4
2019-10-10 04:50:00	9.035877	1.230119	10	3	10	4
2019-10-10 04:55:00	8.189301	0.928515	10	3	10	4
2019-10-10 05:00:00	8.546278	1.036195	10	3	10	5

8 Model 1: Linear Regression (LR)

[458]:
```
df1=[x for _, x in SO2_Data.groupby('Month')]
data_oct=df1[4]
#data_oct=data_oct.sample(frac=1)
data_nov=df1[5]
#data_nov=data_nov.sample(frac=1)
data_dec=df1[6]
#data_dec=data_dec.sample(frac=1)
data_jan=df1[0]
#data_jan=data_jan.sample(frac=1)
data_feb=df1[1]
#data_feb=data_feb.sample(frac=1)
data_mar=df1[2]

data_Oct=data_oct.resample('5min').mean()
data_Oct=data_Oct.dropna()
data_Oct1=data_Oct[:int(0.8*data_Oct.shape[0])]
data_Oct2=data_Oct[int(0.8*data_Oct.shape[0]):]
data_Nov=data_nov.resample('5min').mean()
data_Nov=data_Nov.dropna()
data_Nov1=data_Nov[:int(0.8*data_Nov.shape[0])]
data_Nov2=data_Nov[int(0.8*data_Nov.shape[0]):]
data_Dec=data_dec.resample('5min').mean()
data_Dec=data_Dec.dropna()
data_Dec1=data_Dec[:int(0.8*data_Dec.shape[0])]
data_Dec2=data_Dec[int(0.8*data_Dec.shape[0]):]
data_Jan=data_jan.resample('5min').mean()
data_Jan=data_Jan.dropna()
data_Jan1=data_Jan[:int(0.8*data_Jan.shape[0])]
data_Jan2=data_Jan[int(0.8*data_Jan.shape[0]):]
data_Feb=data_feb.resample('5min').mean()
data_Feb=data_Feb.dropna()
data_Feb1=data_Feb[:int(0.8*data_Feb.shape[0])]
data_Feb2=data_Feb[int(0.8*data_Feb.shape[0]):]
data_Mar=data_mar.resample('5min').mean()
data_Mar=data_Mar.dropna()
data_Mar1=data_Mar[:int(0.8*data_Mar.shape[0])]
data_Mar2=data_Mar[int(0.8*data_Mar.shape[0]):]
frame1=[data_Oct1,data_Nov1,data_Dec1,data_Jan1,data_Feb1,data_Mar1]
frame2=[data_Oct2,data_Nov2,data_Dec2,data_Jan2,data_Feb2,data_Mar2]
```

```
SO2_data1=pd.concat(frame1)
SO2_data2=pd.concat(frame2)
SO2_data=pd.concat([SO2_data1,SO2_data2])
```

[459]:
```
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_absolute_error as mae
import sklearn.metrics as sm
import matplotlib.pyplot as plt
#'Ref_CO','Ref_NO2','Ref_O3',
#X=N3_data[['Sen_2.5','T','RH','Month','Day_of_week','Hour']]
#y=N3_data['Ref_2.5']
X=SO2_data[['Net Signal','Lab2','Temp','RH','Month','Day_of_week','Hour']]
y=SO2_data['Ref']
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.
 ↪2,shuffle=False)
len(X_test)
```

[459]: 3471

[460]:
```
lr = LinearRegression()
model = lr.fit(X_train, y_train)
pred = model.predict(X_test)
lab1=X_test['Lab2'].to_list()
Index=[i for i in range(len(y_test))]
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_lr_SO2=sMAPE_lr
RMSE_lr_SO2=RMSE_lr/np.mean(np.array(y_test))
Pearson_lr_SO2=Pearson_lr
sMAPE_lab_SO2=sMAPE_lab
RMSE_lab_SO2=RMSE_lab/np.mean(np.array(lab1))
Pearson_lab_SO2=Pearson_lab
R2_lr_SO2=round(sm.r2_score(y_test, pred), 2)
R2_lab_SO2=round(sm.r2_score(y_test, lab1), 2)
RMSE_Lr_SO2=RMSE_lr
RMSE_Lab_SO2=RMSE_lab
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
```

```
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

[461]:
```
import random
alpha=1.4
LV=25
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=lab1[i]
cal=np.array(lab1)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/(LV))*100
```

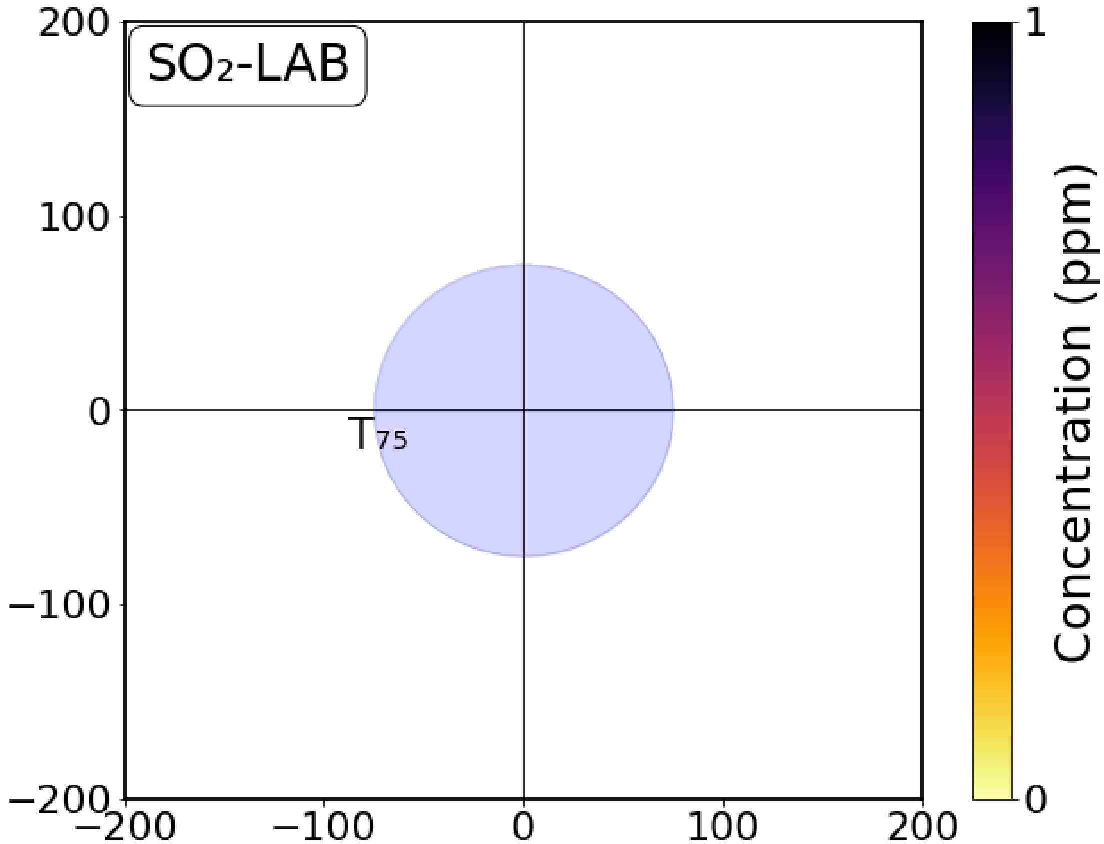
```
Random=(2*(P1+P2)**0.5/(LV))*100


import random
alpha=1.4
LV=max(y_test)
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(lab1)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=17.5
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(lab1)
ref=np.array(y_test)
ref_mean=np.mean(ref)
```

```
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[462]:
```
A4=target(lab1,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)
```

```
plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

#plt.fill_between(a1, b1, color='blue', alpha=0.17)
#plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

#plt.plot(x1,y1, linewidth=0.2, color='grey')
#plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
#plt.plot(x2,y2, linewidth=0.2, color='grey')
#plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

#plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
#plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
#plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
#plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$_{0}$'+'/'+r'$ref_{i}$, 
 ↪'+r'$(_{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
```

```
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-200)
plt.ylim(ymax=200)
plt.xlim(xmax=200)
plt.xlim(xmin=-200)
plt.xticks(np.arange(-75,75),fontsize=22)
plt.xticks([-200,-100,0,100,200],fontsize=22)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-200,-100,0,100,200],fontsize=22)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,1,2,3])
cbar.ax.tick_params(labelsize=22)
cbar.set_label('Concentration (ppm)', rotation=90,fontsize=27)
plt.scatter(Random,Bias+0.2,marker="d",s=900, color='teal')
textstr = 'SO2-LAB'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
 ↪rotation_mode='anchor')
#plt.text(-25,-7, 'T25'.translate(subscript),fontsize=18)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=18)
plt.text(-88,-20, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_SO2_LAB.pdf", format="pdf", bbox_inches="tight")
plt.show()
```

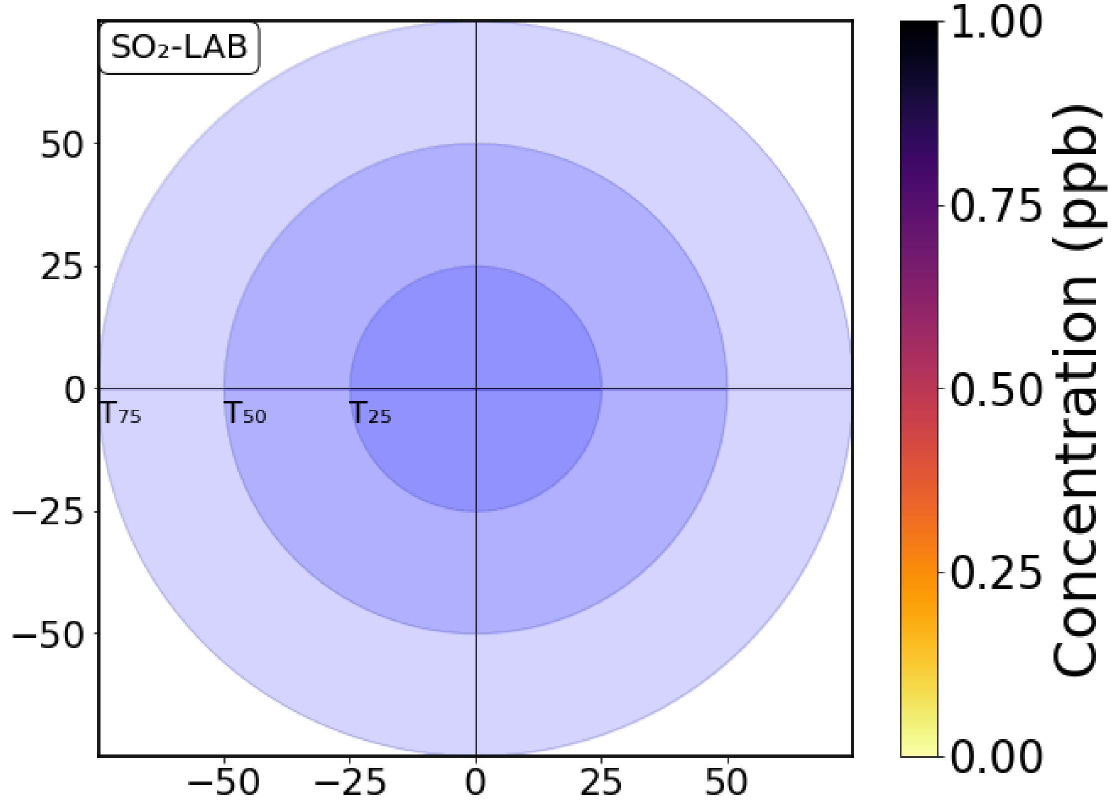


[463]:
```
A4=target(lab1,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
```

```
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$ _{0}$'+'/'+r'$ref_{i}$,␣
↪'+r'$( _{1}-1)$'+' in (%)' ,fontsize=22)
```

```
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.
 ↪array(A4[2]),cmap=reversed_color_map )
plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.
 ↪array(A4[2]),cmap=reversed_color_map)
plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.
 ↪array(A4[2]),cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,75),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=22)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,0,25,50],fontsize=22)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75,1])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="*",s=600, color='teal')
textstr = 'SO2-LAB'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.015, 0.985, textstr, transform=ax.transAxes, fontsize=20,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
 ↪rotation_mode='anchor')
plt.text(-25,-7, 'T25'.translate(subscript),fontsize=18)
plt.text(-50,-7, 'T50'.translate(subscript),fontsize=18)
plt.text(-75,-7, 'T75'.translate(subscript),fontsize=18)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_SO2_LAB.pdf", format="pdf", bbox_inches="tight")
```

```
plt.show()
```




```
[464]: import random
alpha=1.4
LV=max(y_test)
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=y_test[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
```

```
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/(LV))*100
Random=(2*(P1+P2)**0.5/(LV))*100

import random
alpha=1.4
LV=12.5
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
```

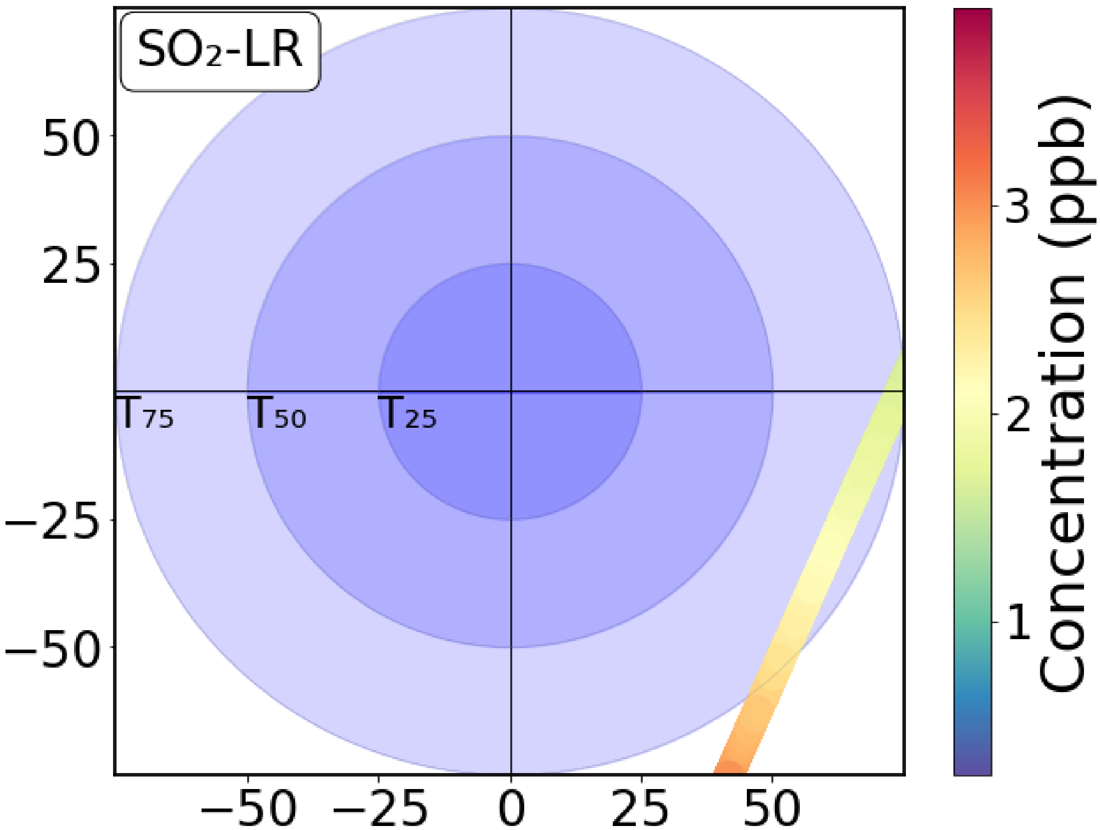
```
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=17.5
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[465]:
```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )
```

```
#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
```

```
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$_{O}$'+'/'+r'$ref_{i}$,␣
↪'+r'$(_{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.
↪array(A4[2]),cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=28)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=28)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,1,2,3,4,5])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = textstr = 'SO2-LR'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
```

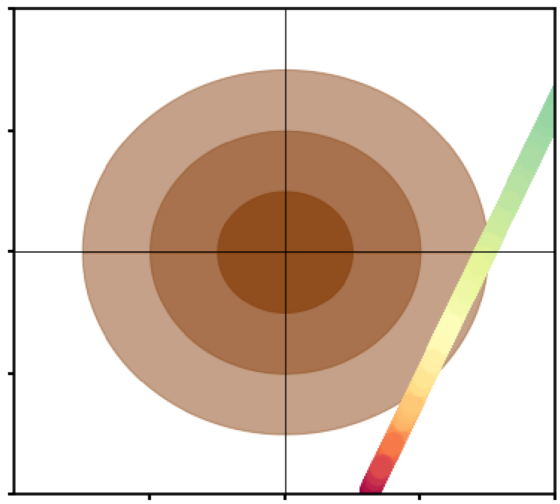
```
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
 ↪rotation_mode='anchor')
plt.text(-25,-7, 'T25'.translate(subscript),fontsize=24)
plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_SO2_LR.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[466]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=25
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
```

```
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 25, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_SO2_LR1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
```

```
plt.show()
```



8.1 Scaling Laboratory Calibration

For the purpose of visual comparison with the ref and calibrated measurements, the lab measurement was scaled by a factor of 0.05

[467]:
```
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),␣
↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),␣
↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))
MBE_LR_SO2=MBE(pred,y_test)/np.std(y_test)
CRMSE_LR_SO2=CRMSE(y_test,pred)/np.std(y_test)
MBE_LAB_SO2=MBE(lab1,y_test)/(25*np.std(y_test))
CRMSE_LAB_SO2=CRMSE(y_test,lab1)/25*(np.std(y_test))
pred_lr=pred
```

```
Regressor model performance:
Mean absolute error(MAE) = 0.5
Mean squared error(MSE) = 0.38
Median absolute error = 0.43
Explain variance score = 0.23
R2 score = 0.19
```

9 Model 2: SVR

[468]:
```python
from sklearn.svm import SVR
from sklearn.preprocessing import StandardScaler
regressor = SVR(kernel = 'poly',degree=3)
regressor.fit(X_train, y_train)
pred = regressor.predict(X_test)
```

[469]:
```python
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_svr_SO2=sMAPE_lr
RMSE_svr_SO2=RMSE_lr/np.mean(np.array(y_test))
Pearson_svr_SO2=Pearson_lr
R2_svr_SO2=round(sm.r2_score(y_test, pred), 2)
RMSE_Svr_SO2=RMSE_lr
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

fig= plt.figure(figsize=(8,6)) ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) plt.plot(index,y_test[A:], color='limegreen',linewidth=3) plt.plot(index,pred[A:], color='brown',linewidth=3) plt.plot(index,LAB1[A:], color='#426eff',linewidth=3) plt.legend(['Ref', 'SVR-Calibrated', 'LAB-Calibrated(Scaled)'], loc = 2, bbox_to_anchor = (0.65,1)) plt.ylabel('SO2 Concentration(ppb)'.translate(subscript),fontsize=18) #plt.text(B-200, C,r'$R^2(SVR)$ ='+str(R2_svr_SO2) , fontsize = 14, color='brown') #plt.text(B-200, D, r'$R^2(Lab)$ ='+str(R2_lab_SO2), fontsize = 14, color='#426eff') #plt.text(B-420, C, 'Pearson r(SVR)='+str(Pearson_lr), fontsize = 14, color='brown') #plt.text(B-420, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') #plt.xlabel('Last 200 hours of testing period',fontsize=18) #plt.title('Support Vector Regression (SVR) Calibration vs Laboratory Calibration',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

[470]:
```
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),␣
↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),␣
↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))

MBE_SVR_SO2=MBE(pred,y_test)/np.std(y_test)
CRMSE_SVR_SO2=CRMSE(y_test,pred)/np.std(y_test)
pred_svr=pred
```

```
Regressor model performance:
Mean absolute error(MAE) = 0.45
Mean squared error(MSE) = 0.33
Median absolute error = 0.39
Explain variance score = 0.32
R2 score = 0.29
```

[471]:
```
import random
alpha=1.4
LV=max(y_test)
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=y_test[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
```

```python
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/(LV))*100
Random=(2*(P1+P2)**0.5/(LV))*100

import random
alpha=1.4
LV=12.5
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
```

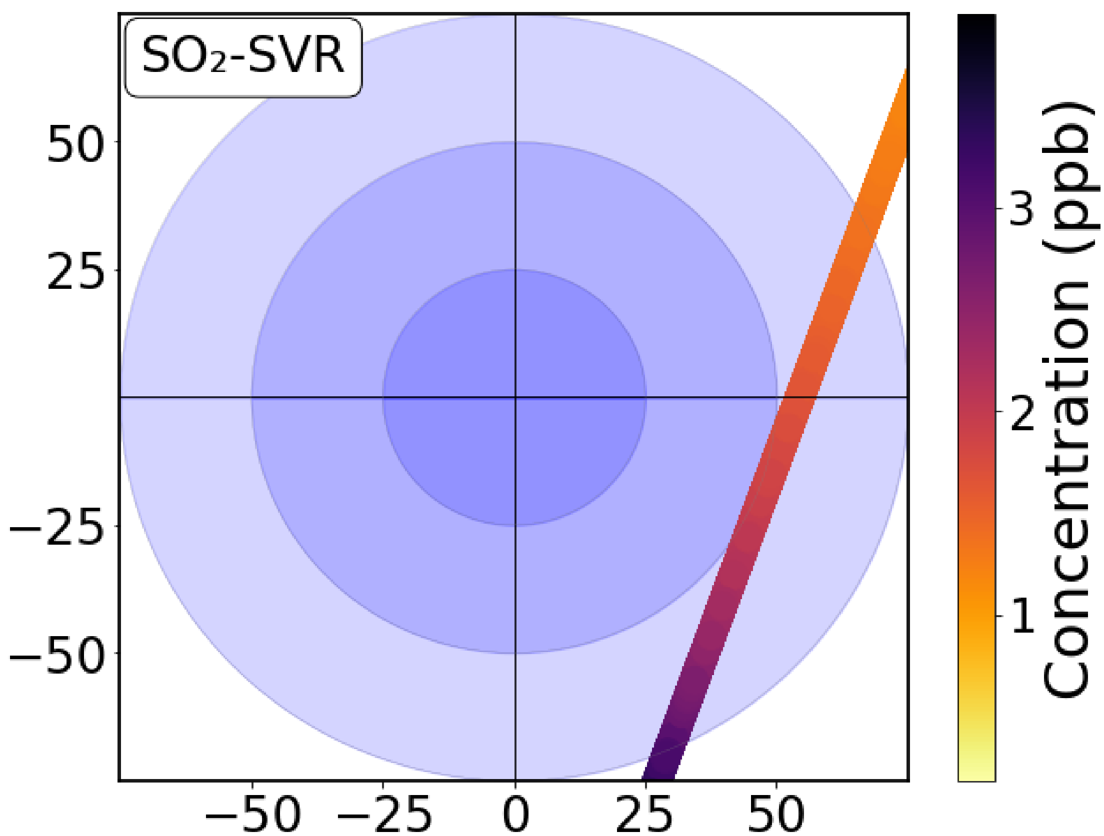
```
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=17.5
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[472]:
```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
```

```
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
```

```
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$_{0}$'+'/'+r'$ref_{i}$, '+r'$(_{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.array(A4[2]),cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=28)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=28)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,1,2,3,4,5])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = textstr = 'SO2-SVR'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
```

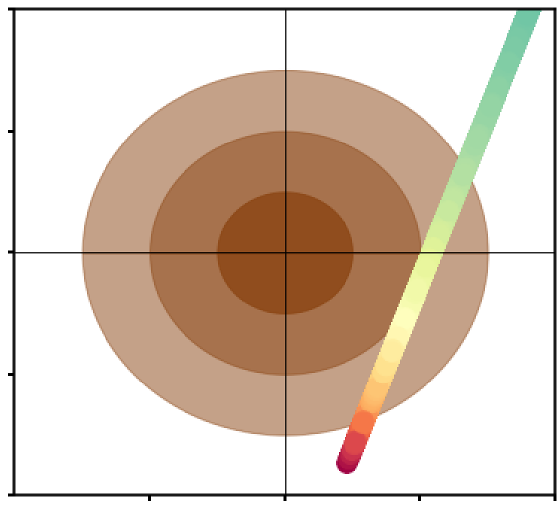
```
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
↪rotation_mode='anchor')
#plt.text(-25,-7, 'T25'.translate(subscript),fontsize=24)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
#plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_SO2_SVR.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[473]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=25
```

```
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 25, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)
```

```
#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_SO2_SVR1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



Model 3: Random Forest

[474]:
```
from sklearn.ensemble import RandomForestRegressor

 # create regressor object
regressor = RandomForestRegressor(max_features=0.28087865827498987,␣
 ↪max_leaf_nodes=776,
                      n_estimators=1291, n_jobs=-1)

# fit the regressor with x and y data
regressor=regressor.fit(X_train, y_train)
```

[475]:
```
Index=[i for i in range(len(y_test))]
features_SO2=regressor.feature_importances_
pred = regressor.predict(X_test)
pred_rf_so2=pred
```

```
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_rf_SO2=sMAPE_lr
RMSE_rf_SO2=RMSE_lr/np.mean(np.array(y_test))
Pearson_rf_SO2=Pearson_lr
R2_rf_SO2=round(sm.r2_score(y_test, pred), 2)
RMSE_Rf_SO2=RMSE_lr
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

fig= plt.figure(figsize=(10,5)) ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) plt.plot(index,y_test[A:], color='limegreen',linewidth=3) plt.plot(index,pred[A:], color='indigo',linewidth=3) plt.plot(index,LAB1[A:], color='#426eff',linewidth=3) plt.legend(['Ref', 'RF-Calibrated', 'LAB-Calibrated(Scaled)'], loc = 2, bbox_to_anchor = (0.72,1)) plt.ylabel('SO2 Concentration(ppb)'.translate(subscript),fontsize=18) plt.text(B-20, C,r'$R^2(RF)$ ='+str(R2_rf_SO2) , fontsize = 14, color='indigo') plt.text(B-20, D,r'$R^2(Lab)$ ='+str(R2_lab_SO2) , fontsize = 14, color='#426eff') plt.text(B-70, C, 'Pearson r(RF)='+str(Pearson_lr), fontsize = 14, color='indigo') plt.text(B-70, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') #plt.xlabel('Last 200 hours of testing period',fontsize=18) #plt.title('Visualization: Random Forest(RF) Calibration vs Laboratory Calibration',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

[476]:
```
print("Regressor model performance:")
```

```
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),␣
 ↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),␣
 ↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
 ↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
 ↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))

MBE_RF_SO2=MBE(pred,y_test)/np.std(y_test)
CRMSE_RF_SO2=CRMSE(y_test,pred)/np.std(y_test)
pred_rf=pred
```

```
Regressor model performance:
Mean absolute error(MAE) = 0.48
Mean squared error(MSE) = 0.38
Median absolute error = 0.4
Explain variance score = 0.21
R2 score = 0.18
```

[477]:
```
import random
alpha=1.4
LV=max(y_test)
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=y_test[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
```

```
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/(LV))*100
Random=(2*(P1+P2)**0.5/(LV))*100

import random
alpha=1.4
LV=12.5
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=17.5
Cal=0
for i in range(len(y_test)):
```

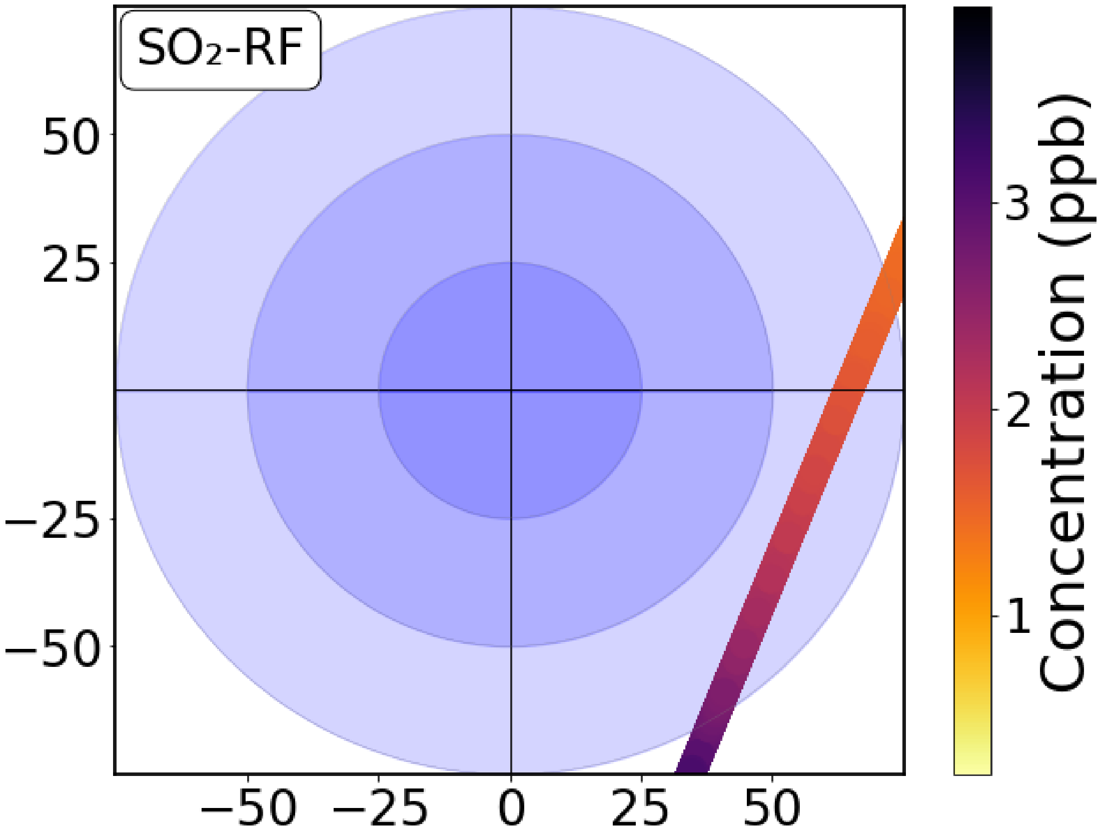
```
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[478]:
```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
```

```
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')
```

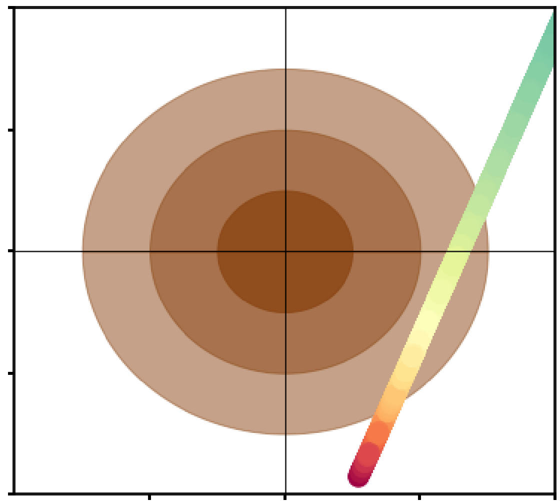
```python
#plt.xlabel('Relative random effect (RR), ' + r'$ _{0}$'+'/'+r'$ref_{i}$, '+r'$( _{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.array(A4[2]),cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=28)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=28)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,1,2,3,4,5])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = textstr = 'SO2-RF'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90, rotation_mode='anchor')
#plt.text(-25,-7, 'T25'.translate(subscript),fontsize=24)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
#plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
```

```
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_SO2_RF.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[479]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=25
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
```

```
plt.Circle((0, 0), 25, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_SO2_RF1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



10 Model 4 : ANN

[480]:
```
from keras.models import Sequential
from keras.layers import Dense
from keras import optimizers
from sklearn.preprocessing import StandardScaler
model = Sequential()
model.add(Dense(6, input_shape = (7,),kernel_initializer='normal', activation=␣
↪'linear'))
model.add(Dense(128,kernel_initializer='normal', activation= 'relu'))
model.add(Dense(50, kernel_initializer='normal',activation= 'relu'))
#model.add(Dense(100, kernel_initializer='normal',activation= 'relu'))
model.add(Dense(1,kernel_initializer='normal',activation='linear',))
sgd = optimizers.Adam(learning_rate=0.01)

model.compile(optimizer = sgd, loss = 'mean_squared_error', metrics= ['mse',␣
↪'mae'])
model.summary()
```

```
Model: "sequential_10"

_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense_48 (Dense)             (None, 6)                 48
```

```
_________________________________________________________________
dense_49 (Dense)             (None, 128)               896
_________________________________________________________________
dense_50 (Dense)             (None, 50)                6450
_________________________________________________________________
dense_51 (Dense)             (None, 1)                 51
=================================================================
Total params: 7,445
Trainable params: 7,445
Non-trainable params: 0
_________________________________________________________________
```

[481]:
```
scaler = StandardScaler()
scaler.fit(X_train)
X_train_scaled=scaler.transform(X_train)
X_test_scaled=scaler.transform(X_test)
model.fit(X_train_scaled, y_train, batch_size= 200, epochs=100, verbose= 0)
```

[481]:
```
<tensorflow.python.keras.callbacks.History at 0x160383580>
```

[482]:
```
train_pred = model.predict(X_train_scaled)
test_pred = model.predict(X_test_scaled)
pred=[]
for i in range(len(test_pred)):
    pred.append(sum(list(test_pred[i])))
len(y_test)
```

[482]:
```
3471
```

[483]:
```
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_ann_SO2=sMAPE_lr
RMSE_ann_SO2=RMSE_lr/np.mean(np.array(y_test))
Pearson_ann_SO2=Pearson_lr
R2_ann_SO2=round(sm.r2_score(y_test, pred), 2)
RMSE_Ann_SO2=RMSE_lr
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
```

```
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

fig= plt.figure(figsize=(8,6)) ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) plt.plot(index,y_test[A:], color='limegreen',linewidth=3) plt.plot(index,pred[A:], color='tomato',linewidth=3) plt.plot(index,LAB1[A:], color='#426eff',linewidth=3) plt.legend(['Ref', 'ANN-Calibrated', 'LAB-Calibrated(Scaled)'], loc = 2, bbox_to_anchor = (0.65,1)) plt.ylabel('SO2 Concentration(ppb)'.translate(subscript),fontsize=18) #plt.text(B-200, C,r'$R^2(ANN)$ ='+str(R2_ann_SO2) , fontsize = 14, color='tomato') #plt.text(B-200, D,r'$R^2(Lab)$ ='+str(R2_lab_SO2) , fontsize = 14, color='#426eff') #plt.text(B-400, C, 'Pearson r(ANN)='+str(Pearson_lr), fontsize = 14, color='tomato') #plt.text(B-400, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') #plt.xlabel('Last 200 hours of testing period',fontsize=18) #plt.title('Artificial Neural Network(ANN) Calibration vs Laboratory Calibration',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

[484]:
```
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),␣
 ↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),␣
 ↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
 ↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
 ↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))

MBE_ANN_SO2=MBE(pred,y_test)/np.std(y_test)
CRMSE_ANN_SO2=CRMSE(y_test,pred)/np.std(y_test)
pred_ann=pred
```

```
Regressor model performance:
Mean absolute error(MAE) = 0.5
Mean squared error(MSE) = 0.45
Median absolute error = 0.37
Explain variance score = 0.06
R2 score = 0.04
```

[485]:

```python
import random
alpha=1.4
LV=max(y_test)
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=y_test[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/(LV))*100
Random=(2*(P1+P2)**0.5/(LV))*100


import random
alpha=1.4
LV=12.5
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
```

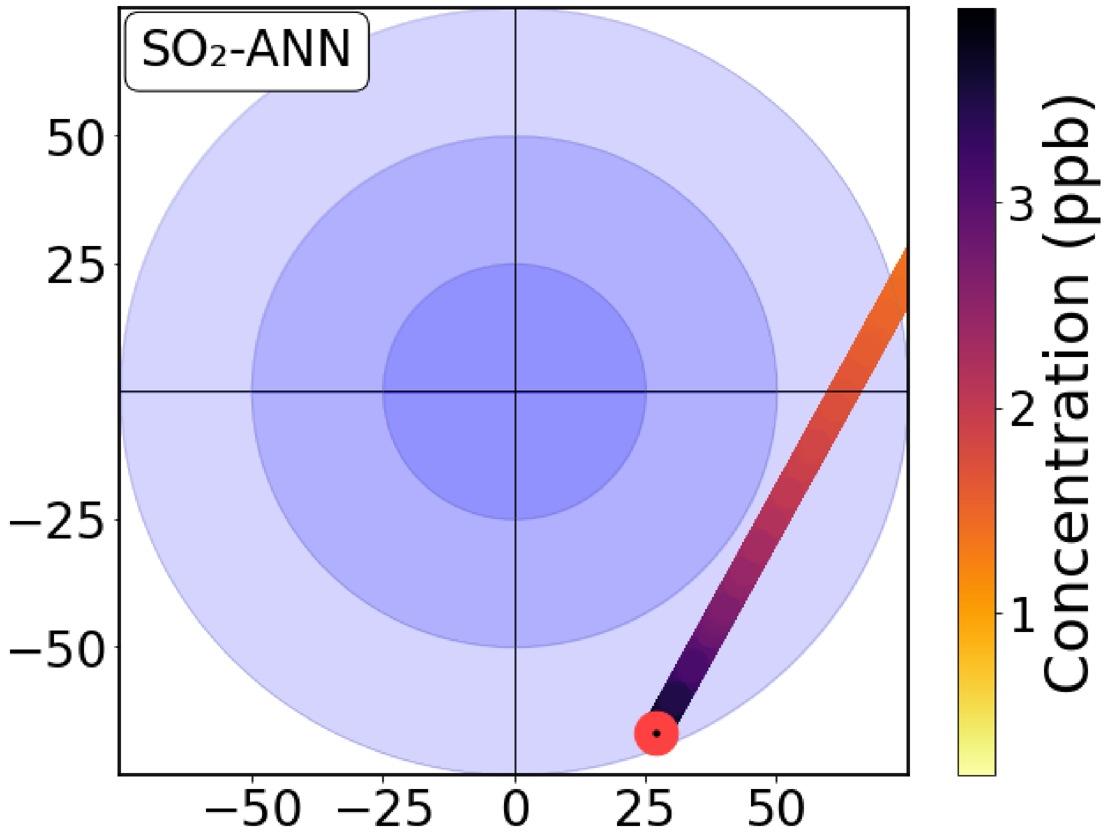
```
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=17.5
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
```

```
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[486]:
```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
```

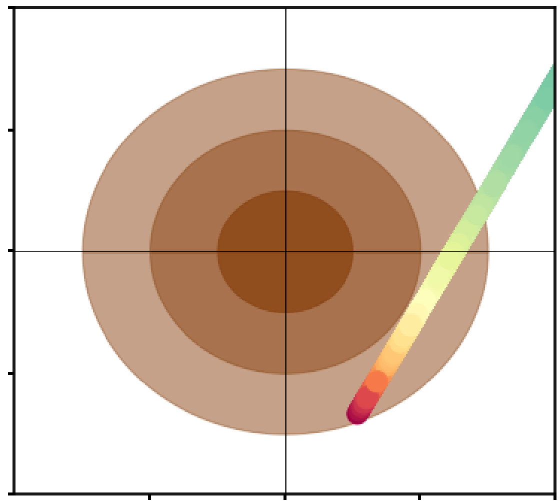
```
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$_{0}$'+'/'+r'$ref_{i}$,␣
↪'+r'$(_{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.
↪array(A4[2]),cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
```

```python
plt.xticks([-50,-25,0,25,50],fontsize=28)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=28)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,1,2,3,4,5])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = textstr = 'SO2-ANN'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
 ↪rotation_mode='anchor')
#plt.text(-25,-7, 'T25'.translate(subscript),fontsize=24)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
#plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_SO2_ANN.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[487]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=25
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 25, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
```

```python
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_SO2_ANN1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



11 Model 5 : XGBoost

[488]:
```
from xgboost import  XGBRegressor
from numpy import absolute
from pandas import read_csv
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import RepeatedKFold
# create an xgboost regression model
#n_estimators=10000, max_depth=5, eta=0.01, subsample=0.9,colsample_bytree=0.
↪4,alpha=10
model = XGBRegressor(n_estimators=10000, max_depth=5, eta=0.01, subsample=0.9,
                     colsample_bytree=0.4,alpha=10)

model.fit(X_train,y_train)
```

[488]:
```
XGBRegressor(alpha=10, base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=0.4, eta=0.01, gamma=0,
             gpu_id=-1, importance_type='gain', interaction_constraints='',
             learning_rate=0.00999999978, max_delta_step=0, max_depth=5,
             min_child_weight=1, missing=nan, monotone_constraints='()',
             n_estimators=10000, n_jobs=0, num_parallel_tree=1, random_state=0,
             reg_alpha=10, reg_lambda=1, scale_pos_weight=1, subsample=0.9,
             tree_method='exact', validate_parameters=1, verbosity=None)
```

[489]:
```
pred = model.predict(X_test)
pred_xgb_so2=pred
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_xgb_SO2=sMAPE_lr
RMSE_xgb_SO2=RMSE_lr/np.mean(np.array(y_test))
Pearson_xgb_SO2=Pearson_lr
R2_xgb_SO2=round(sm.r2_score(y_test, pred), 2)
RMSE_Xgb_SO2=RMSE_lr
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

fig= plt.figure(figsize=(8,6)) ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) plt.plot(index,y_test[A:], color='limegreen',linewidth=3) plt.plot(index,pred[A:], color='darkgoldenrod',linewidth=3) plt.plot(index,LAB1[A:], color='#426eff',linewidth=3) plt.legend(['Ref', 'XGBoost-Calibrated', 'LAB-Calibrated(scaled)'], loc = 2, bbox_to_anchor = (0.65,1)) plt.ylabel('SO2 Concentration(ppb)'.translate(subscript),fontsize=18) #plt.text(B-200, C,r'$R^2(XGB)$ ='+str(R2_xgb_SO2) , fontsize = 14, color='darkgoldenrod') #plt.text(B-200, D,r'$R^2(Lab)$ ='+str(R2_lab_SO2), fontsize = 14, color='#426eff') #plt.text(B-400, C, 'Pearson r(XGB)='+str(Pearson_lr), fontsize = 14, color='darkgoldenrod') #plt.text(B-400, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') #plt.xlabel('Last 200 hours of testing period',fontsize=18) #plt.title('XGBoost Calibration vs Laboratory Calibration',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

[490]:
```
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),␣
↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),␣
↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))

MBE_XGB_SO2=MBE(pred,y_test)/np.std(y_test)
CRMSE_XGB_SO2=CRMSE(y_test,pred)/np.std(y_test)
pred_xgb=pred
```

```
Regressor model performance:
Mean absolute error(MAE) = 0.48
Mean squared error(MSE) = 0.4
Median absolute error = 0.37
Explain variance score = 0.19
R2 score = 0.15
```

[491]:
```
import random
alpha=1.4
LV=max(y_test)
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=y_test[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
```

```python
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/(LV))*100
Random=(2*(P1+P2)**0.5/(LV))*100

import random
alpha=1.4
LV=12.5
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=17.5
```

```
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

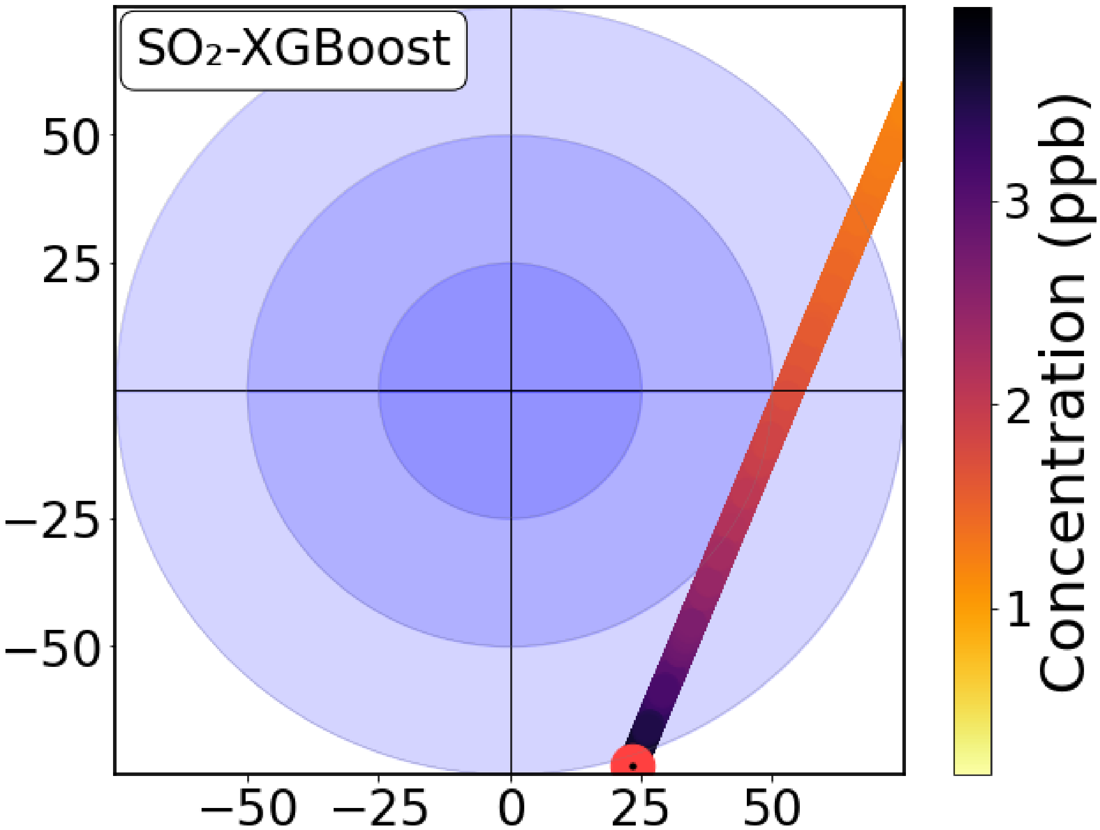
[492]:

```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =25
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
```

```python
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,25.1,0.1)
r1=25
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
```

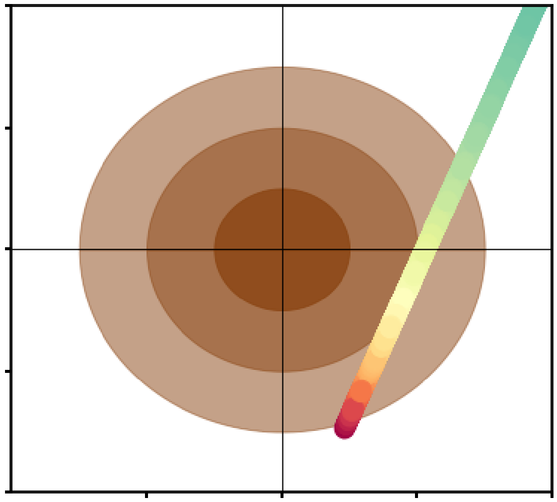
```python
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$ _{0}$'+'/'+r'$ref_{i}$,'+r'$( _{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.array(A4[2]),cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=28)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=28)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,1,2,3,4,5])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = textstr = 'SO2-XGBoost'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,rotation_mode='anchor')
#plt.text(-25,-7, 'T25'.translate(subscript),fontsize=24)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
```

```
#plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_SO2_XGB.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[493]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=25
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )
```

```
fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 25, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_SO2_XGB1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



12 O3 CALIBRATION

[494]:
```
import pandas as pd
import scipy.io
import numpy as np
data = pd.read_csv('O3.txt', header = None,low_memory=False)
data.columns=['AE','WE','Temp','RH','Time']
Time=data['Time'].to_list()
time=[]
for i in range(len(Time)):
    time.append(float(abs(Time[i])))
Time=np.array(time)
Date=pd.to_datetime(Time-719529,unit='d').round('s')
data['Date'] = Date.tolist()
data=data.set_index('Date')
data.drop('Time',axis = 1, inplace = True)
data=data.resample('5min').mean()
Data_O3=data
Data_O3['Ref']=Ref_O3
WE=Data_O3['WE'].to_list()
AE=Data_O3['AE'].to_list()
signal=np.array(WE)-np.array(AE)
Data_O3['Net Signal']=signal
```

```
Data_03['Month']=Data_03.index.month
Data_03['Day_of_week']=Data_03.index.dayofweek
Data_03['Day']=Data_03.index.day
Data_03['Hour']=Data_03.index.hour
03_Data=Data_03
03_Data=03_Data[(03_Data[03_Data.columns] >= 0).all(axis=1)]
03_Data=03_Data.dropna()
data = pd.read_csv('Conc_03.txt', header = None,low_memory=False)
data.columns=['Lab1','Temp','RH','Time','Ref']
Time=data['Time'].to_list()
time=[]
for i in range(len(Time)):
    time.append(float(abs(Time[i])))
Time=np.array(time)
Date=pd.to_datetime(Time-719529,unit='d').round('s')
data['Date'] = Date.tolist()
data=data.set_index('Date')
data.drop('Time',axis = 1, inplace = True)
data=data.resample('5min').mean()
Data_03=data
signal=np.array(WE)-np.array(AE)
Data_03['Net Signal']=signal
Data_03['Month']=Data_03.index.month
Data_03['Day_of_week']=Data_03.index.dayofweek
Data_03['Day']=Data_03.index.day
Data_03['Hour']=Data_03.index.hour
ref_NO2=Data_NO2['Ref'].to_list()
Data_03['Ref_NO2']=ref_NO2
03_Data=Data_03
03_Data=03_Data[(03_Data[03_Data.columns] >= 0).all(axis=1)]
03_Data=03_Data.dropna()
03_Data=03_Data.resample('5min').mean()
03_Data=03_Data.dropna()
03_Data.head()
```

[494]:

```
                            Lab1       Temp         RH        Ref  Net Signal  \
Date
2019-10-02 11:55:00   621.625704  26.378438  58.063437  46.094860    3.605625
2019-10-02 12:10:00  1788.609900  25.500000  48.612609  55.810810    3.528696
2019-10-02 12:15:00   287.254970  25.765087  48.441408  57.907075   17.781453
2019-10-02 12:20:00    99.598353  26.120078  47.716553  58.880540   20.285180
2019-10-07 10:50:00   105.723457  32.399528  37.143389  48.533490   11.862076

                     Month  Day_of_week  Day  Hour    Ref_NO2
Date
2019-10-02 11:55:00   10.0          2.0  2.0  11.0  15.230400
2019-10-02 12:10:00   10.0          2.0  2.0  12.0   6.665136
```

```
2019-10-02 12:15:00   10.0          2.0  2.0  12.0   6.642805
2019-10-02 12:20:00   10.0          2.0  2.0  12.0   2.844210
2019-10-07 10:50:00   10.0          0.0  7.0  10.0   4.344894
```

[495]:
```
#Ref=O3_Data['Ref'].to_list()
#O3_Data=O3_Data[O3_Data.Ref.between(np.mean(Ref)-1*np.std(Ref), np.
 ↪mean(Ref)+1*np.std(Ref))]
#O3_Data.shape
```

12.1 Model 1: LR

[496]:
```
df1=[x for _, x in O3_Data.groupby('Month')]
data_oct=df1[4]
#data_oct=data_oct.sample(frac=1)
data_nov=df1[5]
#data_nov=data_nov.sample(frac=1)
data_dec=df1[6]
#data_dec=data_dec.sample(frac=1)
data_jan=df1[0]
#data_jan=data_jan.sample(frac=1)
data_feb=df1[1]
#data_feb=data_feb.sample(frac=1)
data_mar=df1[2]

data_Oct=data_oct.resample('15min').mean()
data_Oct=data_Oct.dropna()
data_Oct1=data_Oct[:int(0.8*data_Oct.shape[0])]
data_Oct2=data_Oct[int(0.8*data_Oct.shape[0]):]
data_Nov=data_nov.resample('15min').mean()
data_Nov=data_Nov.dropna()
data_Nov1=data_Nov[:int(0.8*data_Nov.shape[0])]
data_Nov2=data_Nov[int(0.8*data_Nov.shape[0]):]
data_Dec=data_dec.resample('15min').mean()
data_Dec=data_Dec.dropna()
data_Dec1=data_Dec[:int(0.8*data_Dec.shape[0])]
data_Dec2=data_Dec[int(0.8*data_Dec.shape[0]):]
data_Jan=data_jan.resample('15min').mean()
data_Jan=data_Jan.dropna()
data_Jan1=data_Jan[:int(0.8*data_Jan.shape[0])]
data_Jan2=data_Jan[int(0.8*data_Jan.shape[0]):]
data_Feb=data_feb.resample('15min').mean()
data_Feb=data_Feb.dropna()
data_Feb1=data_Feb[:int(0.8*data_Feb.shape[0])]
data_Feb2=data_Feb[int(0.8*data_Feb.shape[0]):]
data_Mar=data_mar.resample('15min').mean()
data_Mar=data_Mar.dropna()
data_Mar1=data_Mar[:int(0.8*data_Mar.shape[0])]
```

```
data_Mar2=data_Mar[int(0.8*data_Mar.shape[0]):]
frame1=[data_Oct1,data_Nov1,data_Dec1,data_Jan1,data_Feb1,data_Mar1]
frame2=[data_Oct2,data_Nov2,data_Dec2,data_Jan2,data_Feb2,data_Mar2]
O3_data1=pd.concat(frame1)
O3_data2=pd.concat(frame2)
O3_data=pd.concat([O3_data1,O3_data2])
O3_data.shape
```

[496]: (12041, 10)

[497]:
```
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_absolute_error as mae
import sklearn.metrics as sm
import matplotlib.pyplot as plt
#,'Ref_CO','Ref_NO2','Ref_SO2'
X=O3_data[['Net␣
↪Signal','Lab1','Temp','RH','Month','Day_of_week','Hour','Ref_NO2']]#,'Ref_NO2'
y=O3_data['Ref']
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.
↪2,shuffle=False)
len(X_test)
```

[497]: 2409

[498]:
```
lr = LinearRegression()
model = lr.fit(X_train, y_train)
pred = model.predict(X_test)
lab1=X_test['Lab1'].to_list()
for i in range(len(lab1)):
    if lab1[i]>370:
        lab1[i]=np.mean(lab1)
Index=[i for i in range(len(y_test))]
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_lr_O3=sMAPE_lr
RMSE_lr_O3=RMSE_lr/np.mean(np.array(y_test))
Pearson_lr_O3=Pearson_lr
```

```
sMAPE_lab_O3=sMAPE_lab
RMSE_lab_O3=RMSE_lab/np.mean(np.array(lab1))
Pearson_lab_O3=Pearson_lab
R2_lr_O3=round(sm.r2_score(y_test, pred), 2)
R2_lab_O3=round(sm.r2_score(y_test, lab1), 2)
RMSE_Lr_O3=RMSE_lr
RMSE_Lab_O3=RMSE_lab

A=len(y_test)
D=max(lab1)-0.10*max(lab1)
C=max(lab1)-0.03*max(lab1)
B=A

Pearson_lr_O3,R2_lr_O3,RMSE_Lr_O3
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

[498]: (0.96, 0.92, 4.3)

fig= plt.figure(figsize=(8,6)) index=[i for i in range(1,len(y_test)+1)] ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) plt.plot(index,y_test, color='limegreen',linewidth=3) plt.plot(index,pred, color='#513e00',linewidth=3) plt.plot(index,lab1, color='#426eff',linewidth=3) plt.legend(['Ref', 'LR-Calibrated', 'LAB-Calibrated'], loc = 2, bbox_to_anchor = (0.75,1)) plt.ylabel('O3 Concentration(ppb)'.translate(subscript),fontsize=18) #plt.text(B-5, C,r'$R^2(LR)$ ='+str(R2_lr_O3) , fontsize = 14, color='#513e00') #plt.text(B-5, D,r'$R^2(Lab)$ ='+str(R2_lab_O3) , fontsize = 14, color='#426eff') #plt.text(B-70, C, 'Pearson r(LR)='+str(Pearson_lr), fontsize = 14, color='#513e00') #plt.text(B-70, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') plt.xlabel('Testing period(hours)',fontsize=18) #plt.title('Linear Regression Calibration vs Laboratory Calibration',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

[499]:
```
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),
 ↪2))
```

```
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),␣
↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))

MBE_LR_03=MBE(pred,y_test)/np.std(y_test)
CRMSE_LR_03=CRMSE(y_test,pred)/np.std(y_test)
MBE_LAB_03=MBE(lab1,y_test)/(3.6*np.std(y_test))
CRMSE_LAB_03=CRMSE(y_test,lab1)/(3.6*np.std(y_test))
pred_lr=pred
```

```
Regressor model performance:
Mean absolute error(MAE) = 3.49
Mean squared error(MSE) = 18.62
Median absolute error = 3.05
Explain variance score = 0.92
R2 score = 0.92
```

[500]:
```
import random
alpha=1.4
LV=max(y_test)
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(lab1)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([1 for i in range(len(ref))])
u=prec
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
```

```
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=25
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(lab1)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=35
Cal=0
for i in range(len(y_test)):
```

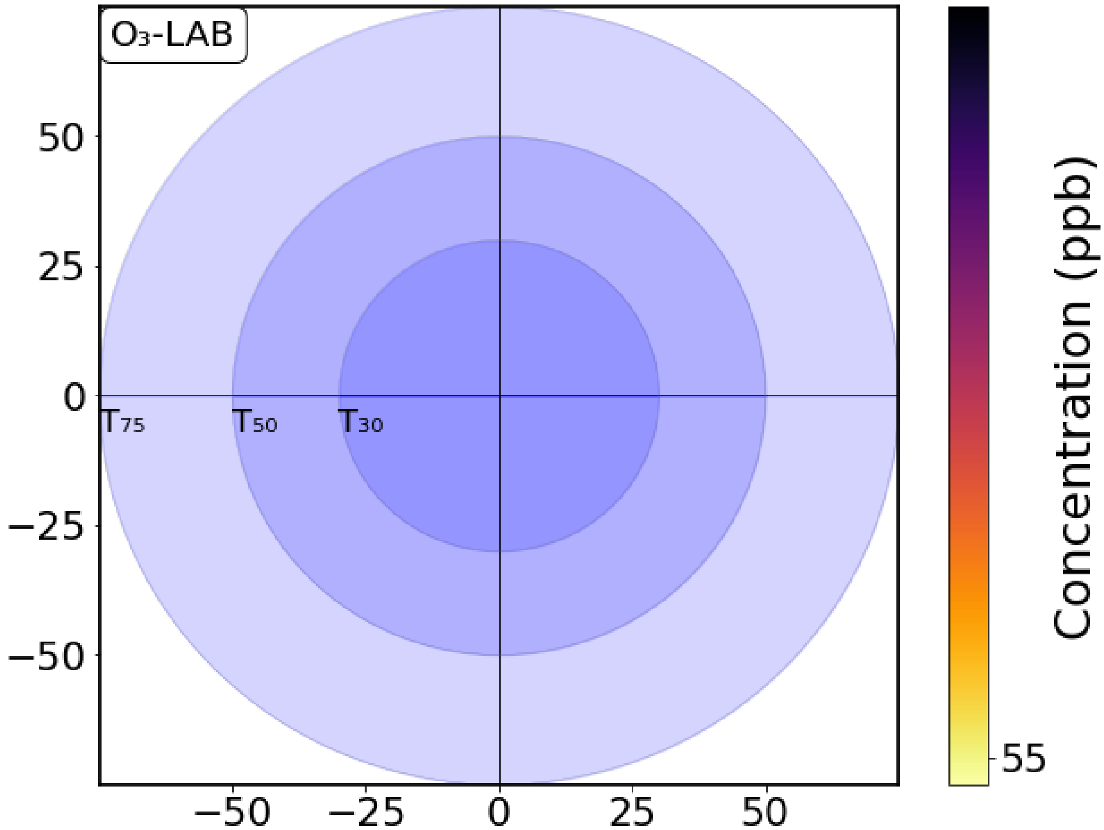
```
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(lab1)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[501]:
```
A4=target(lab1,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =30
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
```

```python
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.15)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,30.1,0.1)
r1=30
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')
```

```
#plt.xlabel('Relative random effect (RR), ' + r'$_{0}$'+'/'+r'$ref_{i}$,␣
↪'+r'$(_{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.
↪array(A4[2]),cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.
↪array(A4[2]),cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.
↪array(A4[2]),cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,75),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=22)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,0,25,50],fontsize=22)
#plt.colorbar()
cbar = plt.colorbar(ticks=[55,60,65])
cbar.ax.tick_params(labelsize=22)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=27)
plt.scatter(Random,Bias+0.2,marker="*",s=600, color='teal')
textstr = 'O3-LAB'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.015, 0.985, textstr, transform=ax.transAxes, fontsize=20,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
↪rotation_mode='anchor')
plt.text(-30,-7, 'T30'.translate(subscript),fontsize=18)
plt.text(-50,-7, 'T50'.translate(subscript),fontsize=18)
plt.text(-75,-7, 'T75'.translate(subscript),fontsize=18)
#plt.text(-140,140, 'T=200%',fontsize=14)
```

```
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_O3_LAB.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[502]:
```
import random
alpha=1.4
LV=max(y_test)
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([1 for i in range(len(ref))])
u=prec
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
```

```
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=25
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
```

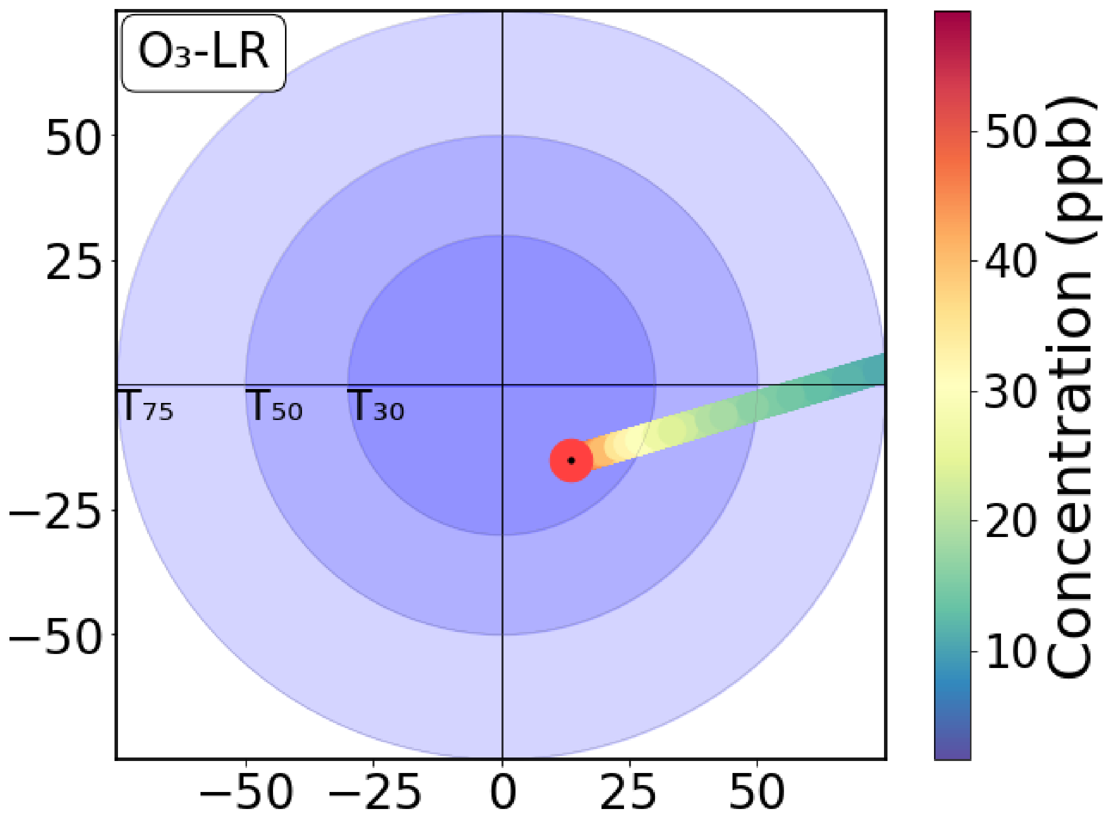
```
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=35
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[503]:
```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =30
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
```

```
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,30.1,0.1)
r1=30
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')
```

```
plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$_{0}$'+'/'+r'$ref_{i}$,␣
↪'+r'$(_{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.
↪array(A4[2]),cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=28)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=28)
#plt.colorbar()
cbar = plt.colorbar(ticks=[10,20,30,40,50,60])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = textstr = 'O3-LR'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')
```

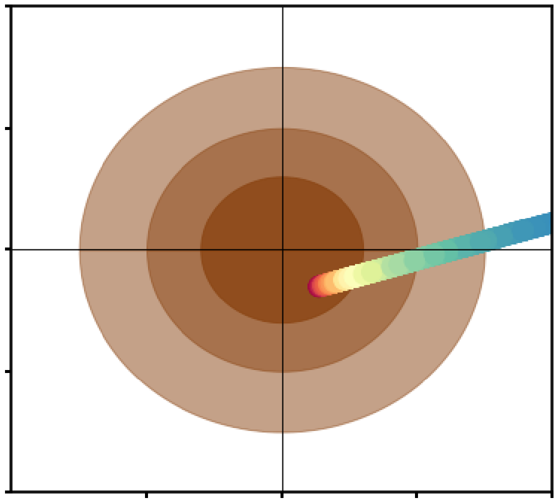
```
plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
↪rotation_mode='anchor')
plt.text(-30,-7, 'T30'.translate(subscript),fontsize=24)
plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_O3_LR.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[504]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=30
radius2=50
radius3=75
```

```
a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 30, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
```

```
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_03_LR1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



12.2 Model 2: SVR

[505]:
```
from sklearn.svm import SVR
from sklearn.preprocessing import StandardScaler
regressor = SVR(kernel = 'rbf')
regressor.fit(X_train, y_train)
pred = regressor.predict(X_test)
```

[506]:
```
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
```

```
sMAPE_svr_O3=sMAPE_lr
RMSE_svr_O3=RMSE_lr/np.mean(np.array(y_test))
Pearson_svr_O3=Pearson_lr
R2_svr_O3=round(sm.r2_score(y_test, pred), 2)
RMSE_Svr_O3=RMSE_lr
Pearson_svr_O3,R2_svr_O3,RMSE_Svr_O3
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

[506]: (0.97, 0.94, 3.7)

fig= plt.figure(figsize=(8,6)) ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) plt.plot(index,y_test, color='limegreen',linewidth=3) plt.plot(index,pred, color='brown',linewidth=3) plt.plot(index,lab1, color='#426eff',linewidth=3) plt.legend(['Ref', 'SVR-Calibrated', 'LAB-Calibrated'], loc = 2, bbox_to_anchor = (0.75,1)) plt.ylabel('O3 Concentration(ppb)'.translate(subscript),fontsize=18) #plt.text(B-5, C,r'$R^2(SVR)$ ='+str(R2_svr_O3) , fontsize = 14, color='brown') #plt.text(B-5, D,r'$R^2(Lab)$ ='+str(R2_lab_O3) , fontsize = 14, color='#426eff') #plt.text(B-70, C, 'Pearson r(SVR)='+str(Pearson_lr), fontsize = 14, color='brown') #plt.text(B-70, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') plt.xlabel('Testing period(hours)',fontsize=18) #plt.xlabel('Last 200 hours of testing period',fontsize=18) #plt.title('Support Vector Regression(SVR) vs Laboratory Calibration',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

[507]:
```
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),␣
 ↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),␣
 ↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
 ↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
 ↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))
```

```
MBE_SVR_03=MBE(pred,y_test)/np.std(y_test)
CRMSE_SVR_03=CRMSE(y_test,pred)/np.std(y_test)
pred_svr=pred
```

```
Regressor model performance:
Mean absolute error(MAE) = 2.93
Mean squared error(MSE) = 13.91
Median absolute error = 2.4
Explain variance score = 0.94
R2 score = 0.94
```

[508]:

```
import random
alpha=1.4
LV=max(y_test)
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([1 for i in range(len(ref))])
u=prec
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
```

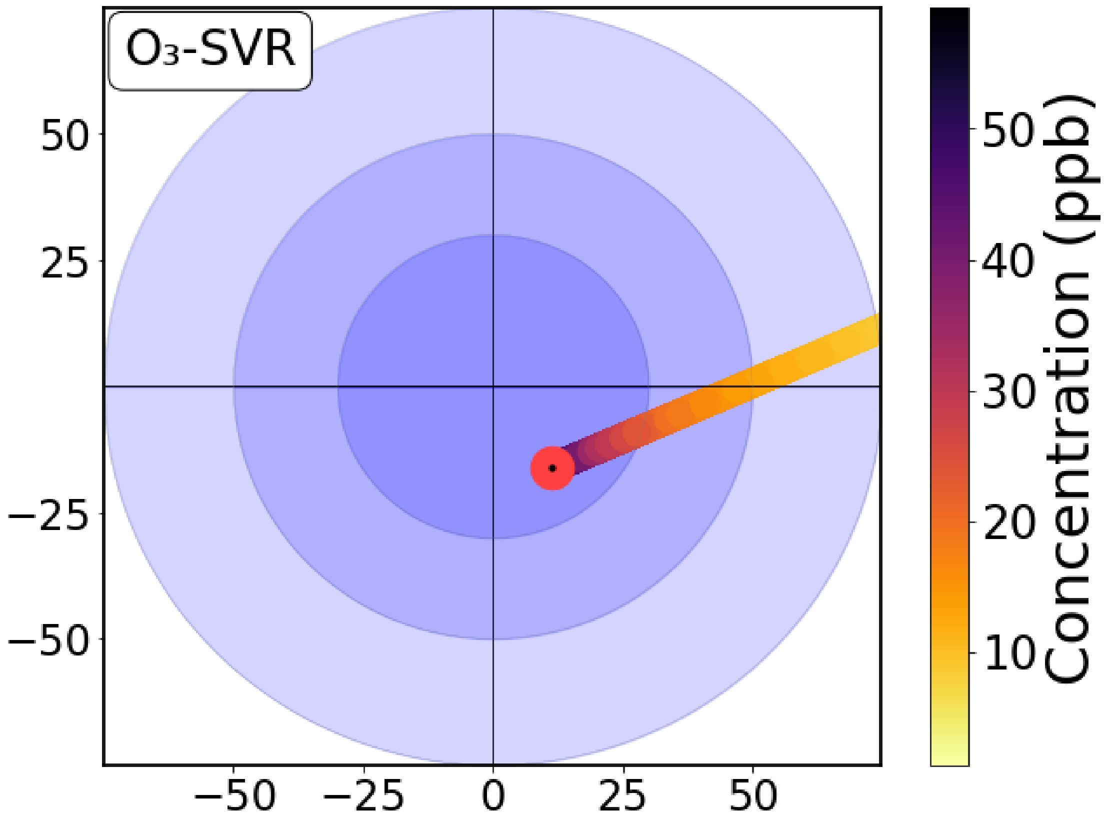
```
LV=25
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=35
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
```

```
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[509]:
```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =30
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
```

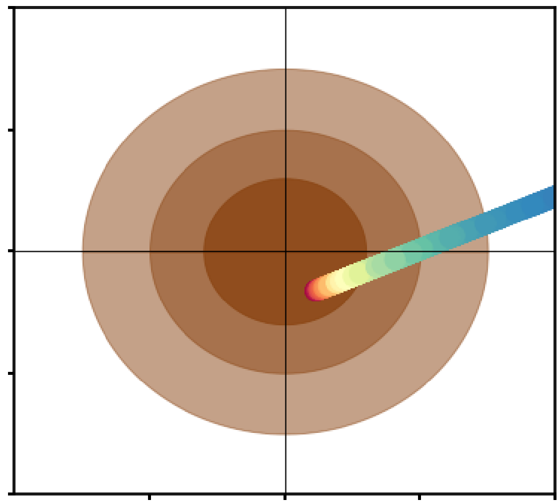
```
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,30.1,0.1)
r1=30
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$_{0}$'+'/'+r'$ref_{i}$,␣
↪'+r'$(_{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.
↪array(A4[2]),cmap=reversed_color_map )
```

```
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=24)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=24)
#plt.colorbar()
cbar = plt.colorbar(ticks=[10,20,30,40,50,60])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = textstr = 'O3-SVR'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
↪rotation_mode='anchor')
#plt.text(-30,-7, 'T30'.translate(subscript),fontsize=24)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
#plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_O3_SVR.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[510]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=30
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 30, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
```

```python
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_O3_SVR1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



12.3 Model 3 : Random Forest

[511]:
```
from sklearn.ensemble import RandomForestRegressor

 # create regressor object
regressor =RandomForestRegressor(max_features=0.4920275171813018,␣
 ↪max_leaf_nodes=1267,
                              n_estimators=318, n_jobs=-1)
# fit the regressor with x and y data
regressor.fit(X_train, y_train)
```

[511]:
```
RandomForestRegressor(max_features=0.4920275171813018, max_leaf_nodes=1267,
                      n_estimators=318, n_jobs=-1)
```

[512]:
```
Index=[i for i in range(len(y_test))]
features_O3=regressor.feature_importances_
pred = regressor.predict(X_test)
pred_rf_o3=pred
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
```

```
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_rf_O3=sMAPE_lr
RMSE_rf_O3=RMSE_lr/np.mean(np.array(y_test))
Pearson_rf_O3=Pearson_lr
R2_rf_O3=round(sm.r2_score(y_test, pred), 2)
RMSE_Rf_O3=RMSE_lr
Pearson_rf_O3,R2_rf_O3,RMSE_Rf_O3
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

[512]:

```
(0.98, 0.96, 3.2)
```

fig= plt.figure(figsize=(10,5)) ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) ax.plot(index,y__test, color='limegreen',linewidth=3) ax.plot(index,pred, color='indigo',linewidth=3) ax.plot(index,lab1, color='#426eff',linewidth=3) plt.legend(['Ref', 'RF-Calibrated', 'LAB-Calibrated'], loc = 2, bbox_to_anchor = (0.79,1)) plt.ylabel('O3 Concentration(ppb)'.translate(subscript),fontsize=18) plt.text(B-22, C,r'$R^2(RF)$ ='+str(R2_rf_O3) , fontsize = 14, color='indigo') plt.text(B-22, D,r'$R^2(Lab)$ ='+str(R2_lab_O3) , fontsize = 14, color='#426eff') plt.text(B-72, C, 'Pearson r(RF)='+str(Pearson_lr), fontsize = 14, color='indigo') plt.text(B-72, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') plt.xlabel('Last 100 hours of testing period',fontsize=18) #plt.xlabel('Last 200 hours of testing period',fontsize=18) #plt.title('Random Forest(RF) vs Laboratory Calibration',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

[513]:

```
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),␣
 ↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),␣
 ↪2))
```

```
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
 ↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
 ↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))
MBE_RF_03=MBE(pred,y_test)/np.std(y_test)
CRMSE_RF_03=CRMSE(y_test,pred)/np.std(y_test)
pred_rf=pred
```

```
Regressor model performance:
Mean absolute error(MAE) = 2.35
Mean squared error(MSE) = 10.01
Median absolute error = 1.74
Explain variance score = 0.96
R2 score = 0.96
```

[514]:

```
import random
alpha=1.4
LV=max(y_test)
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([1 for i in range(len(ref))])
u=prec
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
```

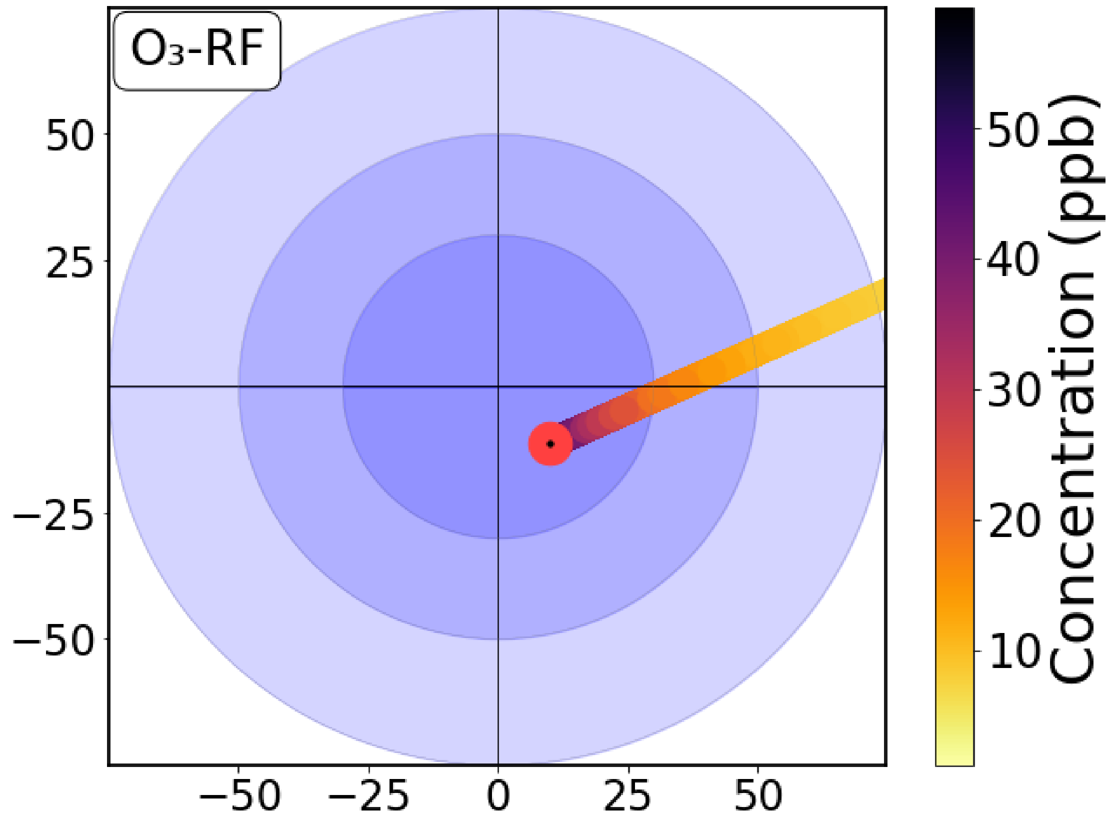
```
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=25
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=35
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
```

```python
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[515]:
```python
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =30
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)
```

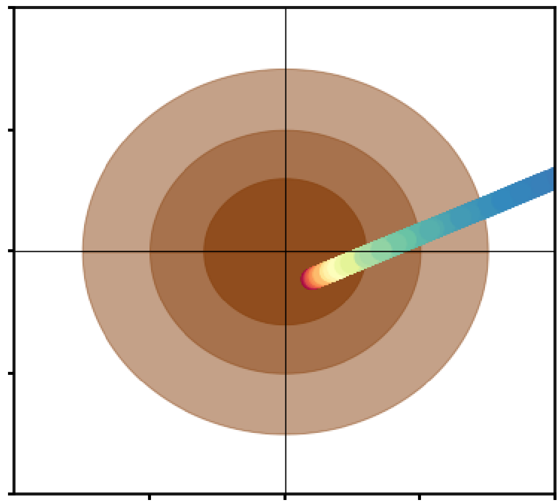
```python
plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,30.1,0.1)
r1=30
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$_{0}$'+'/'+r'$ref_{i}$,
 ↪'+r'$(_{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
```

```
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.
↪array(A4[2]),cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/
↪1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=24)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=24)
#plt.colorbar()
cbar = plt.colorbar(ticks=[10,20,30,40,50,60])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = textstr = 'O3-RF'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
↪rotation_mode='anchor')
#plt.text(-30,-7, 'T30'.translate(subscript),fontsize=24)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
#plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_O3_RF.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[516]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=30
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 30, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
```

```
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_O3_RF1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



12.4 Model 4: ANN

[517]:
```
from keras.models import Sequential
from keras.layers import Dense
from keras import optimizers
from sklearn.preprocessing import StandardScaler
model = Sequential()
model.add(Dense(6, input_shape = (8,),kernel_initializer='normal', activation=␣
↪'linear'))
model.add(Dense(128,kernel_initializer='normal', activation= 'relu'))
model.add(Dense(128, kernel_initializer='normal',activation= 'relu'))
model.add(Dense(100, kernel_initializer='normal',activation= 'relu'))
model.add(Dense(1,kernel_initializer='normal',activation='linear',))
sgd = optimizers.Adam(learning_rate=0.01)

model.compile(optimizer = sgd, loss = 'mean_squared_error', metrics= ['mse',␣
↪'mae'])
model.summary()
```

```
Model: "sequential_11"

_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense_52 (Dense)             (None, 6)                 54
```

```
_________________________________________________________________
dense_53 (Dense)             (None, 128)               896
_________________________________________________________________
dense_54 (Dense)             (None, 128)               16512
_________________________________________________________________
dense_55 (Dense)             (None, 100)               12900
_________________________________________________________________
dense_56 (Dense)             (None, 1)                 101
=================================================================
Total params: 30,463
Trainable params: 30,463
Non-trainable params: 0
_________________________________________________________________
```

[518]:
```
scaler = StandardScaler()
scaler.fit(X_train)
X_train_scaled=scaler.transform(X_train)
X_test_scaled=scaler.transform(X_test)
model.fit(X_train_scaled, y_train, batch_size= 100, epochs=200, verbose= 0)
```

[518]: <tensorflow.python.keras.callbacks.History at 0x138e1c1c0>

[519]:
```
train_pred = model.predict(X_train_scaled)
test_pred = model.predict(X_test_scaled)
pred=[]
for i in range(len(test_pred)):
    pred.append(sum(list(test_pred[i])))
len(y_test)
```

[519]: 2409

[520]:
```
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_ann_03=sMAPE_lr
RMSE_ann_03=RMSE_lr/np.mean(np.array(y_test))
Pearson_ann_03=Pearson_lr
R2_ann_03=round(sm.r2_score(y_test, pred), 2)
RMSE_Ann_03=RMSE_lr
Pearson_ann_03,R2_ann_03,RMSE_Ann_03
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

[520]:
```
(0.98, 0.95, 3.2)
```

fig= plt.figure(figsize=(8,6)) ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) ax.plot(index,y_test, color='limegreen',linewidth=3) ax.plot(index,pred, color='tomato',linewidth=3) ax.plot(index,lab1, color='#426eff',linewidth=3) plt.legend(['Ref', 'ANN-Calibrated', 'LAB-Calibrated'], loc = 2, bbox_to_anchor = (0.75,1)) plt.ylabel('O3 Concentration(ppm)'.translate(subscript),fontsize=18) #plt.text(B-5, C,r'$R^2(ANN)$ ='+str(R2_ann_O3) , fontsize = 14, color='tomato') #plt.text(B-5, D, r'$R^2(Lab)$ ='+str(R2_lab_O3), fontsize = 14, color='#426eff') #plt.text(B-70, C, 'Pearson r(ANN)='+str(Pearson_lr), fontsize = 14, color='tomato') #plt.text(B-70, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') plt.xlabel('Testing period(hours)',fontsize=18) #plt.xlabel('Last 200 hours of testing period',fontsize=18) #plt.title('Artificial Neural Network(ANN) vs Laboratory Calibration',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

[521]:
```python
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),␣
 ↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),␣
 ↪2))
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
 ↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
 ↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))

MBE_ANN_O3=MBE(pred,y_test)/np.std(y_test)
CRMSE_ANN_O3=CRMSE(y_test,pred)/np.std(y_test)
pred_ann=pred
```

```
Regressor model performance:
Mean absolute error(MAE) = 2.34
```

```
Mean squared error(MSE) = 10.5
Median absolute error = 1.6
Explain variance score = 0.95
R2 score = 0.95
```

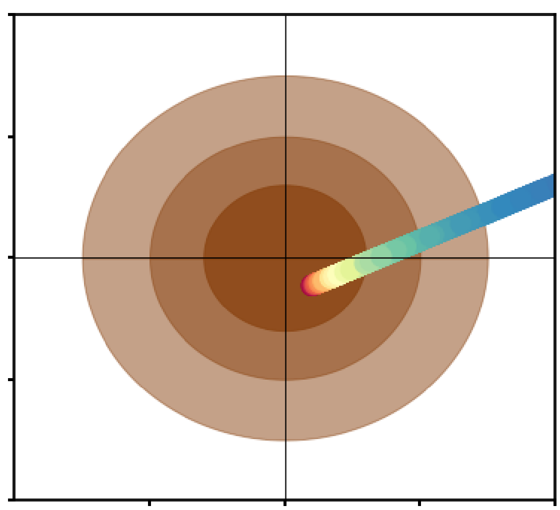
[522]:
```
import random
alpha=1.4
LV=max(y_test)
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([1 for i in range(len(ref))])
u=prec
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=25
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
```

```
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=35
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
```

```
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[523]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=30
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 30, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
 ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias,marker="o",s=350, color='#A2CD5A')
#plt.scatter(Random,Bias,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
```

```
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_03_ANN1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



13 Model 5: XGBoost

[524]:
```python
from xgboost import  XGBRegressor
from numpy import absolute
from pandas import read_csv
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import RepeatedKFold
# create an xgboost regression model
#n_estimators=10000, max_depth=5, eta=0.01, subsample=0.9,colsample_bytree=0.
↪4,alpha=10
model = XGBRegressor(base_score=0.5, booster='gbtree',
             colsample_bylevel=0.9653704353298734, colsample_bynode=1,
             colsample_bytree=0.7225699606707784, gamma=0, gpu_id=-1,
             grow_policy='lossguide', importance_type='gain',
             interaction_constraints='', learning_rate=0.025578608080118973,
             max_delta_step=0, max_depth=0, max_leaves=55,
             min_child_weight=0.9411716091772624,
             monotone_constraints='()', n_estimators=1917, n_jobs=-1,
             num_parallel_tree=1, random_state=0, reg_alpha=0.17587838916410176,
             reg_lambda=15.748976687207163, scale_pos_weight=1,
             subsample=0.9933923477413587, tree_method='hist',
             use_label_encoder=False, validate_parameters=1, verbosity=0)

model.fit(X_train,y_train)
```

[524]:
```
XGBRegressor(base_score=0.5, booster='gbtree',
             colsample_bylevel=0.9653704353298734, colsample_bynode=1,
             colsample_bytree=0.7225699606707784, gamma=0, gpu_id=-1,
             grow_policy='lossguide', importance_type='gain',
             interaction_constraints='', learning_rate=0.025578608080118973,
             max_delta_step=0, max_depth=0, max_leaves=55,
             min_child_weight=0.9411716091772624, missing=nan,
             monotone_constraints='()', n_estimators=1917, n_jobs=-1,
             num_parallel_tree=1, random_state=0, reg_alpha=0.17587838916410176,
             reg_lambda=15.748976687207163, scale_pos_weight=1,
             subsample=0.9933923477413587, tree_method='hist',
             use_label_encoder=False, validate_parameters=1, verbosity=0)
```

[525]:
```python
pred = model.predict(X_test)
pred_xgb_o3=pred
Y_test=y_test.to_list()
Y_test=pd.Series(Y_test,index =Index)
Y_test
Pred=pd.Series(pred,index =Index)
Lab1=pd.Series(lab1,index =Index)
sMAPE_lr=round(smape_loss(Y_test,Pred),2)
sMAPE_lab=round (smape_loss(Y_test,Lab1),2)
```

```
RMSE_lr=round(np.sqrt(sm.mean_squared_error(y_test, pred)),1)
RMSE_lab=round(np.sqrt(sm.mean_squared_error(y_test, lab1)),1)
Pearson_lr=round(np.corrcoef(y_test, pred)[0, 1],2)
Pearson_lab=round(np.corrcoef(y_test, lab1)[0, 1],2)
sMAPE_xgb_O3=sMAPE_lr
RMSE_xgb_O3=RMSE_lr/np.mean(np.array(y_test))
Pearson_xgb_O3=Pearson_lr
R2_xgb_O3=round(sm.r2_score(y_test, pred), 2)
RMSE_Xgb_O3=RMSE_lr
Pearson_xgb_O3,R2_xgb_O3,RMSE_Xgb_O3
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.Int64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:120: FutureWarning:
pandas.UInt64Index is deprecated and will be removed from pandas in a future
version. Use pandas.Index with the appropriate dtype instead.
  supported_index_types = (pd.RangeIndex, pd.Int64Index, pd.UInt64Index)
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/sktime/utils/validation/forecasting.py:126: FutureWarning: is_monotonic
is deprecated and will be removed in a future version. Use
is_monotonic_increasing instead.
  if not time_index.is_monotonic:
```

[525]: (0.98, 0.96, 2.9)

fig= plt.figure(figsize=(8,6)) ax = fig.add_subplot(111) ax.patch.set_facecolor('lightblue') ax.patch.set_alpha(0.3) ax.plot(index,y_test, color='limegreen',linewidth=3) ax.plot(index,pred, color='darkgoldenrod',linewidth=3) ax.plot(index,lab1, color='#426eff',linewidth=3) plt.legend(['Ref', 'XGBoost-Calibrated', 'LAB-Calibrated'], loc = 2, bbox_to_anchor = (0.75,1)) plt.ylabel('O3 Concentration(ppb)'.translate(subscript),fontsize=18) #plt.text(B-5, C,r'$R^2(XGB)$ ='+str(R2_xgb_O3) , fontsize = 14, color='darkgoldenrod') #plt.text(B-5, D,r'$R^2(Lab)$ ='+str(R2_lab_O3) , fontsize = 14, color='#426eff') #plt.text(B-70, C, 'Pearson r(XGB)='+str(Pearson_lr), fontsize = 14, color='darkgoldenrod') #plt.text(B-70, D, 'Pearson r(Lab)='+str(Pearson_lab), fontsize = 14, color='#426eff') plt.xlabel('Testing period(hours)',fontsize=18) #plt.xlabel('Last 200 hours of testing period',fontsize=18) #plt.title('XGBoost vs Laboratory Calibration',fontsize=18) plt.grid(linestyle='-.',linewidth=0.3) plt.show()

[526]:
```
print("Regressor model performance:")
print("Mean absolute error(MAE) =", round(sm.mean_absolute_error(y_test, pred),
 ↪2))
print("Mean squared error(MSE) =", round(sm.mean_squared_error(y_test, pred),
 ↪2))
```

```
print("Median absolute error =", round(sm.median_absolute_error(y_test, pred),␣
↪2))
print("Explain variance score =", round(sm.explained_variance_score(y_test,␣
↪pred), 2))
print("R2 score =", round(sm.r2_score(y_test, pred), 2))
MBE_XGB_03=MBE(pred,y_test)/np.std(y_test)
CRMSE_XGB_03=CRMSE(y_test,pred)/np.std(y_test)
pred_xgb=pred
```

```
Regressor model performance:
Mean absolute error(MAE) = 2.15
Mean squared error(MSE) = 8.45
Median absolute error = 1.6
Explain variance score = 0.96
R2 score = 0.96
```

[527]:

```
import random
alpha=1.4
LV=max(y_test)
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([1 for i in range(len(ref))])
u=prec
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
```

```
Bias=(2*(P3)/LV)*100
Random=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=25
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias1=(2*(P3)/LV)*100
Random1=(2*(P1+P2)**0.5/LV)*100

import random
alpha=1.4
LV=35
Cal=0
for i in range(len(y_test)):
    if y_test[i]==LV:
        Cal=pred[i]
cal=np.array(pred)
ref=np.array(y_test)
ref_mean=np.mean(ref)
```

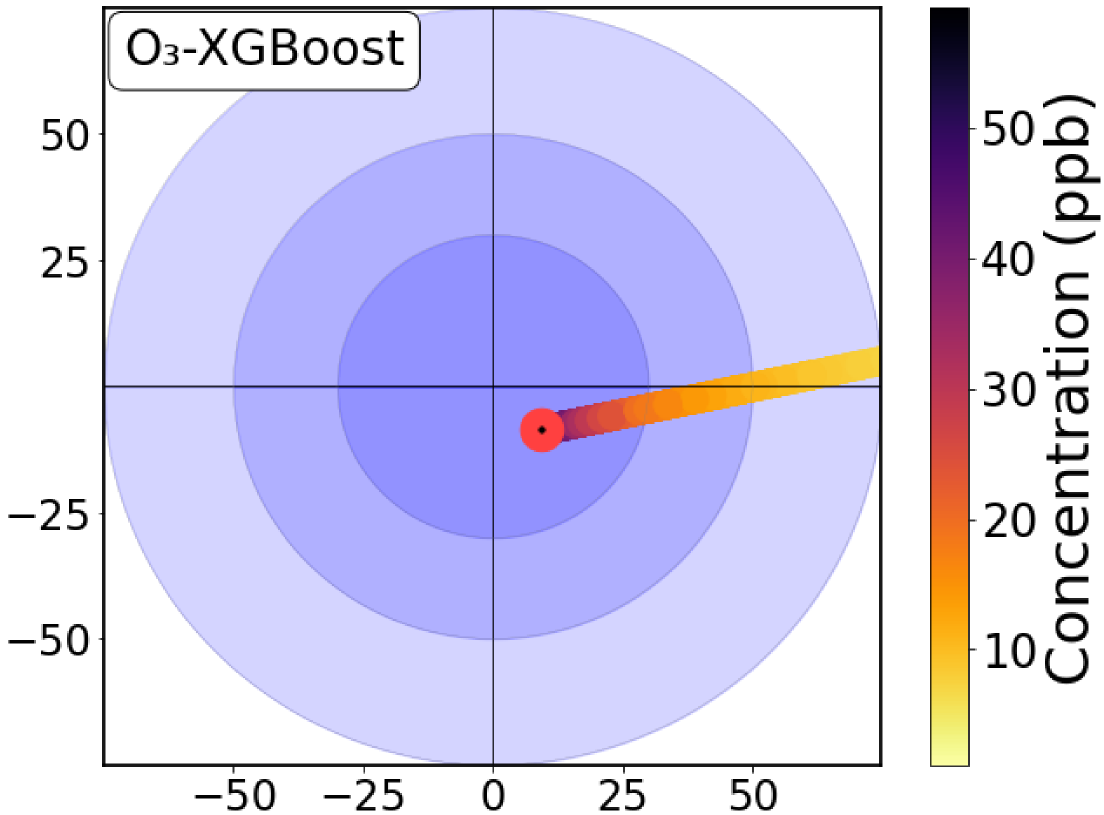
```
cal_mean=np.mean(cal)
prec=np.array([20 for i in range(len(ref))])
u=0.001*ref
#cal=np.log(cal)
#ref=np.log(ref)
sx_s=(1/len(ref))*sum((ref-ref_mean)**2)
sy_s=(1/len(cal))*sum((cal-cal_mean)**2)
sxy=(1/len(cal))*sum((cal-cal_mean)*(ref-ref_mean))
#beta_1=((sy_s-sx_s)+np.sqrt((sy_s-sx_s)**2+4*sxy**2))/(2*sxy)
beta_1=((sy_s-alpha*sx_s)+np.sqrt((sy_s-sx_s)**2+4*alpha*sxy**2))/(2*sxy)
beta_0=cal_mean-beta_1*ref_mean
RSS=sum((cal-beta_0-beta_1*ref)**2-(beta_1**2+alpha)*(0.001*LV)**2)
du_s=RSS/(len(cal)-2)
    #Beta_1=((sy_s-sx_s-du_s)+np.sqrt((sy_s-sx_s-du_s)**2+4*sxy**2))/(2*sxy)
Beta_1=((sy_s-alpha*sx_s-du_s)+np.
 ↪sqrt((sy_s-alpha*sx_s-du_s)**2+4*alpha*sxy**2))/(2*sxy)
Beta_0=cal_mean-Beta_1*ref_mean
P1=(RSS/(len(cal)-2))
P2=(Beta_1**2+alpha)*(0.001*LV)**2+(-2*Beta_1**2+2*Beta_1-1)*(0.001*LV)**2
P3=(Beta_0+(Beta_1-1)*LV)
P=P1+P2+P3
Bias2=(2*(P3)/LV)*100
Random2=(2*(P1+P2)**0.5/LV)*100
```

[528]:

```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =30
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)
```

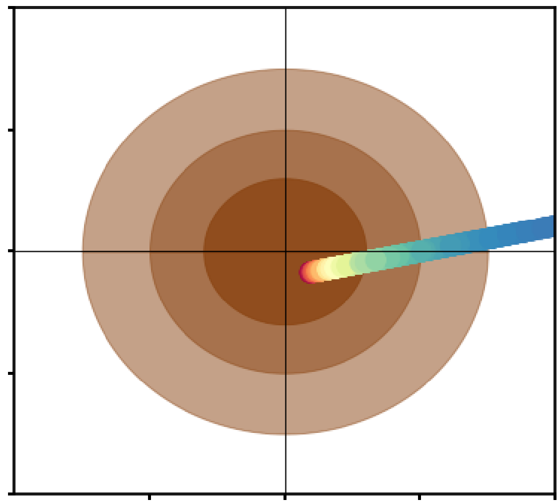
```
plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,30.1,0.1)
r1=30
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$_{0}$'+'/'+r'$ref_{i}$, 
↪'+r'$(_{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
```

```
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.
 ↪array(A4[2]),cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=24)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=24)
#plt.colorbar()
cbar = plt.colorbar(ticks=[10,20,30,40,50,60])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = textstr = 'O3-XGBoost'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
 ↪rotation_mode='anchor')
#plt.text(-30,-7, 'T30'.translate(subscript),fontsize=24)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
#plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_O3_XGB.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



[529]:
```
theta = np.linspace( 0 , 2 * np.pi , 150 )

radius1=30
radius2=50
radius3=75

a1 = radius1 * np.cos( theta )
b1 = radius1 * np.sin( theta )
a2 = radius2 * np.cos( theta )
b2 = radius2 * np.sin( theta )
a3 = radius3 * np.cos( theta )
b3 = radius3 * np.sin( theta )


fig= plt.figure(figsize=(6.5,6))
ax = fig.add_subplot(111)
plt.Circle((0, 0), 30, color='wheat')
plt.Circle((0, 0), 50, color='wheat')
plt.Circle((0, 0), 75, color='wheat')
plt.fill_between(a1, b1, color='#8B4513', alpha=0.8)
plt.fill_between(a2, b2, color='#8B4513', alpha=0.5)
```

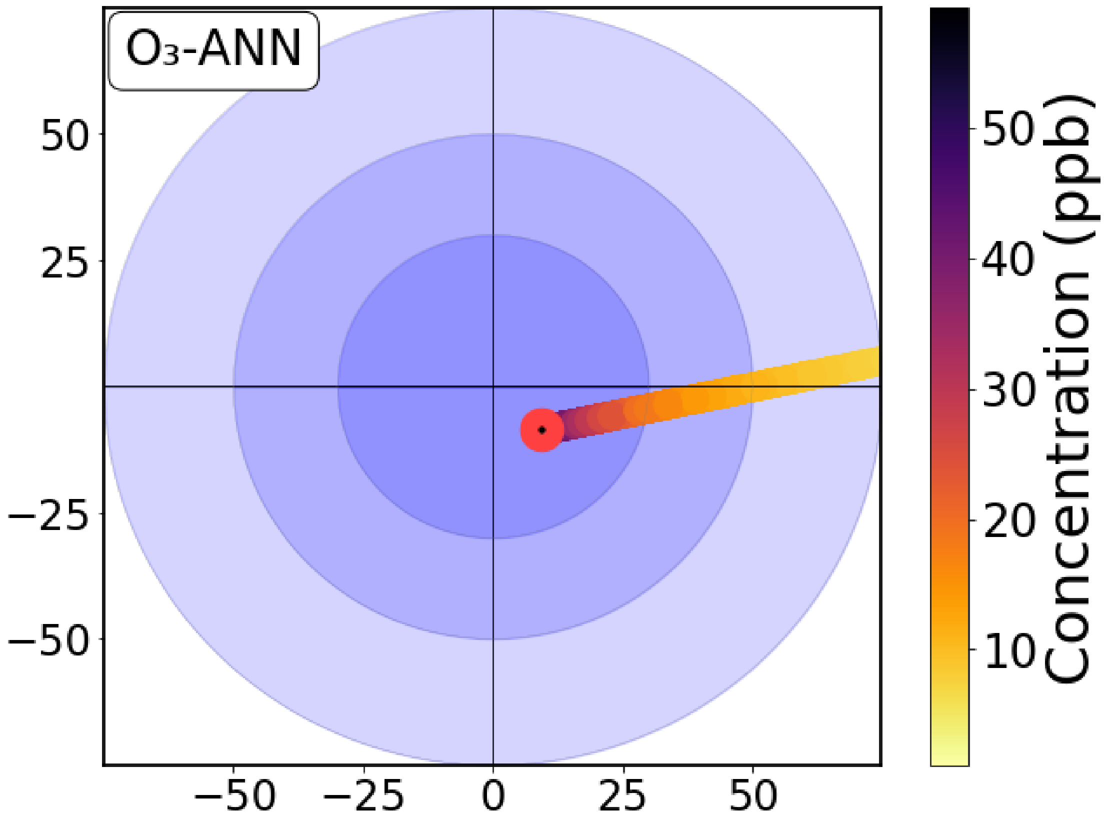
```
plt.fill_between(a3, b3, color='#8B4513', alpha=0.5)
color_map = plt.cm.get_cmap('Spectral')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/
    ↪1000,cmap=reversed_color_map )
#plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor =␣
    ↪(0,1), fontsize=20)
#plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#EE3B3B',alpha=0.5)
#plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
#plt.xlabel('Relative random effect, RR (%)' ,fontsize=20)
#plt.ylabel('Relative bias, RB (%)',fontsize=20)
plt.xticks(fontsize=100)
plt.yticks(fontsize=100)
#plt.xticks(color='w')
plt.vlines([0], -100, 100, linewidth=0.8,color='black')
plt.hlines([0], -100, 100, linewidth=0.8,color='black')
ax.set_ylim(bottom=-100)
ax.set_ylim(top=100)
ax.set_xlim(left=-100)
ax.set_xlim(right=100)
ax.tick_params(direction='out', length=4, width=2, colors='black')
plt.xticks([-50,0,50,100],color='white')
plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75])
#cbar.ax.tick_params(labelsize=20)
#cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR'
#props = dict(boxstyle='round', facecolor='white', alpha=1)
#plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18,
        #verticalalignment='top', bbox=props)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_O3_XGB1.pdf", format="pdf", bbox_inches="tight",dpi=1000)
plt.show()
```



[530]:
```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =30
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =50
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =75
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
```

```
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.17)
plt.fill_between(a2, b2, color='blue',alpha=0.17)
plt.fill_between(a3, b3, color='blue',alpha=0.17)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,30.1,0.1)
r1=30
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,50.1,0.1)
r2=50
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,75.1,0.1)
r3=75
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

#plt.xlabel('Relative random effect (RR), ' + r'$_{0}$'+'/'+r'$ref_{i}$,
 ↪'+r'$(_{1}-1)$'+' in (%)' ,fontsize=22)
#plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
ticks = np.linspace(0, pred.max(), 20, endpoint=True)
color_map = plt.cm.get_cmap('inferno')
```

```
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.
 ↪array(A4[2]),cmap=reversed_color_map )
#plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map)
#plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.array(A4[2])/
 ↪1000,cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-75)
plt.ylim(ymax=75)
plt.xlim(xmax=75)
plt.xlim(xmin=-75)
plt.xticks(np.arange(-75,76),fontsize=22)
plt.xticks([-50,-25,0,25,50],fontsize=24)

plt.yticks(np.arange(-75,75),fontsize=22)
plt.yticks([-50,-25,25,50],fontsize=24)
#plt.colorbar()
cbar = plt.colorbar(ticks=[10,20,30,40,50,60])
cbar.ax.tick_params(labelsize=26)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=34)
plt.scatter(Random,Bias+0.2,marker="o",s=600, color='#FF4040')
textstr = textstr = 'O3-ANN'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.025, 0.975, textstr, transform=ax.transAxes, fontsize=28,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
 ↪rotation_mode='anchor')
#plt.text(-30,-7, 'T30'.translate(subscript),fontsize=24)
#plt.text(-50,-7, 'T50'.translate(subscript),fontsize=24)
#plt.text(-75,-7, 'T75'.translate(subscript),fontsize=24)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_O3_ANN.pdf", format="pdf", bbox_inches="tight")
plt.show()
```



theta = np.linspace(0 , 2 * np.pi , 150)

radius1=30 radius2=50 radius3=75

a1 = radius1 * np.cos(theta) b1 = radius1 * np.sin(theta) a2 = radius2 * np.cos(theta) b2 = radius2 * np.sin(theta) a3 = radius3 * np.cos(theta) b3 = radius3 * np.sin(theta)

fig= plt.figure(figsize=(6.5,6)) ax = fig.add_subplot(111) plt.Circle((0, 0), 30, color='wheat') plt.Circle((0, 0), 50, color='wheat') plt.Circle((0, 0), 75, color='wheat') plt.fill_between(a1, b1, color='blue', alpha=0.25) plt.fill_between(a2, b2, color='blue', alpha=0.25) plt.fill_between(a3, b3, color='blue', alpha=0.25) #plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor = (0,1), fontsize=20) color_map = plt.cm.get_cmap('inferno') reversed_color_map = color_map.reversed() plt.scatter(A4[0],A4[1],marker='.',s=700,c=np.array(A4[2])/1000,cmap=reversed_color_map) #plt.legend(['LAB','LR','SVR','RF','ANN','XGBoost'],loc = 2, bbox_to_anchor = (0,1), fontsize=20) plt.scatter(Random,Bias+0.2,marker="o",s=350, color='#A2CD5A') plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black') #plt.xlabel('Relative random effect, RR (%)' ,fontsize=20) #plt.ylabel('Relative bias, RB (%)',fontsize=20) plt.xticks(fontsize=100) plt.yticks(fontsize=100) #plt.xticks(color='w') plt.vlines([0], -100, 100, linewidth=0.8,color='black') plt.hlines([0], -100, 100, linewidth=0.8,color='black') ax.set_ylim(bottom=-100) ax.set_ylim(top=100) ax.set_xlim(left=-100) ax.set_xlim(right=100) ax.tick_params(direction='out', length=4, width=2, colors='black') plt.xticks([-50,0,50,100],color='white') plt.yticks([-100,-50,0,50,100], color='white')

#cbar = plt.colorbar(ticks=[0,0.25,0.5,0.75]) #cbar.ax.tick_params(labelsize=20) #cbar.set_label('Concentration (ppm)', rotation=90,fontsize=22)

#textstr = 'CO-LR' #props = dict(boxstyle='round', facecolor='white', alpha=1) #plt.text(0.029, 0.97, textstr, transform=ax.transAxes, fontsize=18, #verticalalignment='top', bbox=props) plt.setp(ax.spines.values(), linewidth=1.8) plt.savefig("dqo_O3_ANN1.pdf", format="pdf", bbox_inches="tight",dpi=1000) plt.show()

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```
A4=target(pred,y_test,1.4)
theta = np.linspace( 0 , 2 * np.pi , 150 )
r1 =30
a1= r1 * np.cos( theta )
b1= r1 * np.sin( theta )
r2 =60
a2=r2* np.cos( theta )
b2=r2* np.sin( theta )
r3 =90
a3=r3* np.cos( theta )
b3=r3* np.sin( theta )

#r4 =150
#a4=r4* np.cos( theta )
#b4=r4* np.sin( theta )
fig= plt.figure(figsize=(10,8))
ax = fig.add_subplot(111)
plt.scatter(1000,1000,marker="*",s=500, color='#00008B')
plt.scatter(1000,1000, marker="*",s=500, color='#8B2323')
plt.scatter(1000,1000,marker="*",s=500, color='#00688B')
#plt.legend(['LUT','UAT','LV'],loc =2, bbox_to_anchor = (0,0.2), fontsize=15)


plt.Circle((0, 0), 1, color='wheat')
#plt.vlines([0], -130, 130, linestyles='dashed',color='violet')
#plt.hlines([0], -130, 130, linestyles='dashed', color='violet')

plt.fill_between(a1, b1, color='blue', alpha=0.15)
plt.fill_between(a2, b2, color='blue',alpha=0.15)
plt.fill_between(a3, b3, color='blue',alpha=0.15)
#plt.fill_between(a4, b4, color='blue',alpha=0.17)

x1=np.arange(0,30.1,0.1)
r1=30
y1=np.sqrt(r1**2-x1**2)
x2=np.arange(0,60.1,0.1)
r2=60
y2=np.sqrt(r2**2-x2**2)

x3=np.arange(0,90.1,0.1)
```

```
r3=90
y3=np.sqrt(r3**2-x3**2)

#x4=np.arange(0,150.1,0.1)
#r4=150
#y4=np.sqrt(r4**2-x4**2)

plt.plot(x1,y1, linewidth=0.2, color='grey')
plt.plot(x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(x2,y2, linewidth=0.2, color='grey')
plt.plot(x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(x3,y3, linewidth=0.2, color='grey')
plt.plot(x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(x4,y4, linewidth=0.2, color='grey')
#plt.plot(x4,-1*y4, linewidth=0.2, color='grey')

plt.plot(-1*x1,y1, linewidth=0.2, color='grey')
plt.plot(-1*x1,-1*y1, linewidth=0.2, color='grey')
plt.plot(-1*x2,y2, linewidth=0.2, color='grey')
plt.plot(-1*x2,-1*y2, linewidth=0.2, color='grey')
plt.plot(-1*x3,y3, linewidth=0.2, color='grey')
plt.plot(-1*x3,-1*y3, linewidth=0.2, color='grey')
#plt.plot(-1*x4,y4, linewidth=0.2, color='grey')
#plt.plot(-1*x4,-1*y4, linewidth=0.2, color='grey')

plt.xlabel('Relative random effect (RR), ' + r'$ _{0}$'+'/'+r'$ref_{i}$,␣
 ↪'+r'$( _{1}-1)$'+' in (%)' ,fontsize=22)
plt.ylabel('Relative bias, RB (%)',fontsize=22)
#plt.title('CO',fontsize=18)
color_map = plt.cm.get_cmap('inferno')
reversed_color_map = color_map.reversed()
plt.scatter(A4[0],A4[1],marker='.',s=1000,c=np.
 ↪array(A4[2]),cmap=reversed_color_map )
plt.scatter(A4[3],A4[1],marker='.',s=300,c=np.
 ↪array(A4[2]),cmap=reversed_color_map)
plt.scatter(A4[4],A4[1],marker='.',s=100,c=np.
 ↪array(A4[2]),cmap=reversed_color_map)
plt.vlines([0], -230, 230,color='black',linewidth=0.8)
plt.hlines([0], -230, 230, color='black',linewidth=0.8)
plt.ylim(ymin=-90)
plt.ylim(ymax=90)
plt.xlim(xmax=90)
plt.xlim(xmin=-90)
plt.xticks(np.arange(-90,90),fontsize=22)
plt.xticks([-60,-30,0,30,60],fontsize=22)

plt.yticks(np.arange(-90,90),fontsize=22)
```

```
plt.yticks([-60,-30,0,30,60],fontsize=22)
#plt.colorbar()
cbar = plt.colorbar(ticks=[0,10,20,30,40,50,60])
cbar.ax.tick_params(labelsize=22)
cbar.set_label('Concentration (ppb)', rotation=90,fontsize=27)
plt.scatter(Random,Bias+0.2,marker="*",s=600, color='teal')
textstr = 'O3-ANN'.translate(subscript)
props = dict(boxstyle='round', facecolor='white', alpha=1)
plt.text(0.015, 0.985, textstr, transform=ax.transAxes, fontsize=20,
        verticalalignment='top', bbox=props)
#plt.scatter(Random1,Bias1,marker="*",s=500, color='#00008B')
#plt.scatter(Random2,Bias2,marker="*",s=500, color='#8B2323')
#plt.scatter(Random1,Bias1,marker=".",s=40, color='black')
#plt.scatter(Random2,Bias2,marker=".",s=40, color='black')

plt.scatter(Random,Bias+0.2,marker=".",s=40, color='black')
U=np.round(np.sqrt(Bias**2+Random**2),1)
#if U<200:
    #plt.text(Random+3,Bias+16,'REU (LV)='+str(U)+'%',fontsize=16,rotation=90,␣
 ↪rotation_mode='anchor')
plt.text(-30,-7, 'T30'.translate(subscript),fontsize=18)
plt.text(-60,-7, 'T60'.translate(subscript),fontsize=18)
plt.text(-90,-7, 'T90'.translate(subscript),fontsize=18)
#plt.text(-140,140, 'T=200%',fontsize=14)
plt.setp(ax.spines.values(), linewidth=1.8)
plt.savefig("dqo_O3_Test.pdf", format="pdf", bbox_inches="tight")
plt.show()
```

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