1 | BACKGROUND

1.1 | Context

The CalCOFI data set represents the longest (1949-present) and most complete (more than 50,000 sampling stations) time series of oceanographic and larval fish data in the world. It includes abundance data on the larvae of over 250 species of fish; larval length frequency data and egg abundance data on key commercial species; and oceanographic and plankton data. The physical, chemical, and biological data collected at regular time and space intervals quickly became valuable for documenting climatic cycles in the California Current and a range of biological responses to them. CalCOFI research drew world attention to the biological response to the dramatic Pacific-warming event in 1957-58 and introduced the term "El Niño" into the scientific literature.

CalCOFI conducts quarterly cruises off southern & central California, collecting a suite of hydrographic and biological data on station and underway. Data collected at depths down to 500 m include: temperature, salinity, oxygen, phosphate, silicate, nitrate and nitrite, chlorophyll, transmissometer, PAR, C14 primary productivity, phytoplankton biodiversity, zooplankton biomass, and zooplankton biodiversity.

1.2 | Scope

We would like to know if a connection between Salinity and Temperature exists

2 | REFERENCE LINKS

Main Website: https://calcofi.com/

Bottle-Dataset: https://new.data.calcofi.com/index.php/database/calcofi-database/bottle-field-descriptions
Cast-Dataset: https://new.data.calcofi.com/index.php/database/calcofi-database/cast-table-column-descriptions

3 | EDA (EXPLORATION DATA ANALYSIS)

▼ 3.1 | Import Packages and Datasets

```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
import os
import seaborn as sns
import plotly.express as px
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error
from sklearn.tree import DecisionTreeRegressor
from sklearn.tree import plot_tree
from sklearn import tree
from sklearn.model_selection import train_test_split
from sklearn.neighbors import KNeighborsRegressor
     /opt/conda/lib/python3.10/site-packages/scipy/__init__.py:146: UserWarning: A NumPy version >=1.16.5 and <1.23.0 is required for this νε
       warnings.warn(f"A NumPy version >={np_minversion} and <{np_maxversion}"</pre>
bot=pd.read_csv('/content/bottle.csv',low_memory=False)#.to_csv('bottlecsv.csv')
cast=pd.read_csv('/content/cast.csv',low_memory=False)#.to_csv('castcsv.csv')
immagine.png
bot.info()
```

∠0	PU4q	451/80 HOH-HUTT	T10at64				
27	SiO3uM	354091 non-null	float64				
28	SiO3qu	510866 non-null	float64				
29	NO2uM	337576 non-null	float64				
30	NO2q	529474 non-null	float64				
31	NO3uM	337403 non-null	float64				
32	NO3q	529933 non-null	float64				
33	NH3uM	64962 non-null	float64				
34	NH3q	808299 non-null	float64				
35	C14As1	14432 non-null	float64				
36	C14A1p	12760 non-null	float64				
37	C14A1q	848605 non-null	float64				
38	C14As2	14414 non-null	float64				
39	C14A2p	12742 non-null	float64				
40	C14A2q	848623 non-null	float64				
41	DarkAs	22649 non-null	float64				
42	DarkAp	20457 non-null	float64				
43	DarkAq	840440 non-null	float64				
44	MeanAs	22650 non-null	float64				
45	MeanAp	20457 non-null	float64				
46	MeanAq	840439 non-null	float64				
47	IncTim	14437 non-null	object				
48	LightP	18651 non-null	float64				
49	R Depth	864863 non-null	float64				
50	R_TEMP	853900 non-null	float64				
51	R POTEMP	818816 non-null	float64				
52	R SALINITY	817509 non-null	float64				
53	R SIGMA	812007 non-null	float64				
54	R SVA	812092 non-null	float64				
55	R DYNHT	818206 non-null	float64				
56	_ R 02	696201 non-null	float64				
57	R 02Sat	666448 non-null	float64				
58	R SIO3	354099 non-null	float64				
59	R P04	413325 non-null	float64				
60	R NO3	337411 non-null	float64				
61	R NO2	337584 non-null	float64				
62	R NH4	64982 non-null	float64				
63	R CHLA	225276 non-null	float64				
64	R PHAEO	225275 non-null	float64				
65	R PRES	864863 non-null	int64				
66	R SAMP	122006 non-null	float64				
67	DIC1	1999 non-null	float64				
68	DIC2	224 non-null	float64				
69	TA1	2084 non-null	float64				
70	TA2	234 non-null	float64				
71	pH2	10 non-null	float64				
	•	84 non-null	float64				
72 73	pH1 DIC Quality Comment		object				
dtypes: float64(65), int64(5), object(4)							
dtypes: +loat64(65), int64(5), object(4)							

memory usage: 488.3+ MB

It has been decided to reduce the dataset to the following features:

bottle=bot.iloc[:,[0,4,5,6,7,8]] bottle

	Cst_Cnt	Depthm	T_degC	Salnty	02m1_L	STheta
0	1	0	10.500	33.4400	NaN	25.64900
1	1	8	10.460	33.4400	NaN	25.65600
2	1	10	10.460	33.4370	NaN	25.65400
3	1	19	10.450	33.4200	NaN	25.64300
4	1	20	10.450	33.4210	NaN	25.64300
•••						
864858	34404	0	18.744	33.4083	5.805	23.87055
864859	34404	2	18.744	33.4083	5.805	23.87072
864860	34404	5	18.692	33.4150	5.796	23.88911
864861	34404	10	18.161	33.4062	5.816	24.01426
864862	34404	15	17.533	33.3880	5.774	24.15297

864863 rows × 6 columns

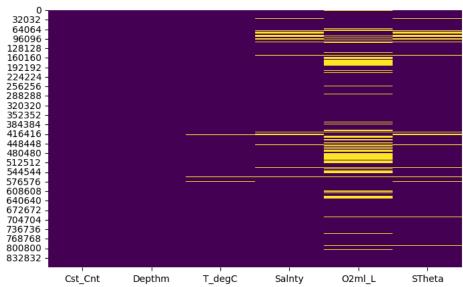
```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 864863 entries, 0 to 864862
Data columns (total 6 columns):
# Column Non-Null Count
                             Dtype
0
    Cst_Cnt 864863 non-null int64
1
    Depthm
             864863 non-null
                             int64
             853900 non-null float64
    T_degC
             817509 non-null float64
    Salnty
    02ml_L
             696201 non-null
                            float64
    STheta
             812174 non-null float64
dtypes: float64(4), int64(2)
memory usage: 39.6 MB
```

▼ 3.2 | NAN VALUES ANALYSIS

Nan Values Visualization

```
plt.rcParams["figure.figsize"] = (8,5)
sns.heatmap(bottle.isna(),cbar=False,cmap='viridis')
```





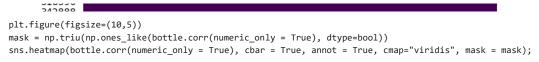
Data cleaning

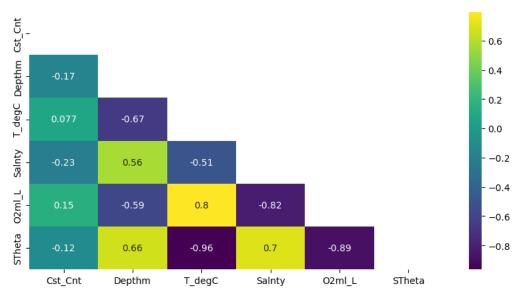
```
cols=bottle.columns

for colonna in cols:
    bottle=bottle[~bottle[colonna].isnull()]

bottle=bottle.reset_index(drop=True)
plt.rcParams["figure.figsize"] = (8,5)
sns.heatmap(bottle.isna(),cbar=False,cmap='viridis')
```

▼ 3.3 | CORRELATION MATRIX



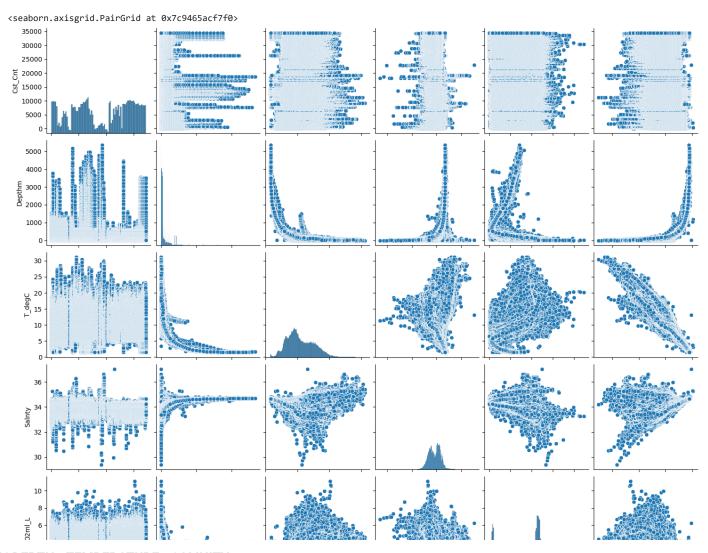


The Pearson's coefficient between Temperature and Salinity is not so high, -0.51

→ 3.4 | FEATURES PLOTS

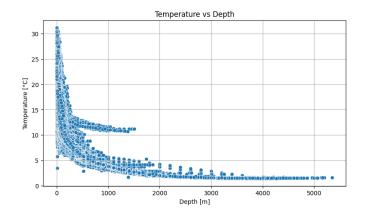
Plot pairwise relationships in the dataset

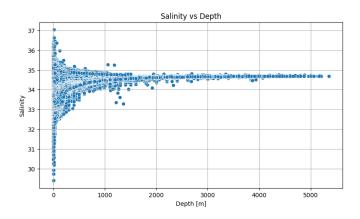
sns.pairplot(bottle)



→ 3.5 | DEPTH - TEMPERATURE - SALINITY

fig, ax = plt.subplots(1,2, figsize=(20,5))
g1=sns.scatterplot(data=bottle,x='Depthm',y='T_degC',ax=ax[0])
ax[0].set(xlabel='Depth [m]',ylabel='Temperature [°C]',title='Temperature vs Depth')
ax[0].grid()
g2=sns.scatterplot(data=bottle,x='Depthm',y='Salnty',ax=ax[1])
ax[1].set(xlabel='Depth [m]',ylabel='Salinity',title='Salinity vs Depth')
ax[1].grid()





- In the first plot some points in the upper part of the image show a different trend from the rest of the graph. It's an unexpected behavior, because, for instance, at around 1000 m depth the expected temperature is around 5°C, but we also find temperatures between 10°C and 15°C (https://www.windows2universe.org/earth/Water/temp.html)
- In the second plot we can notice that the points converge asymptotically from both high and low salinity values. It means that in some areas of the ocean the salinity encreases with the depth, vice versa in other areas it decreases.

Distribution of Measuring Points on Geograph Datamap

Here we show the measuring points on the map using latitude and longitude informations.

```
df_merge=bottle.merge(cast, how='inner',on='Cst_Cnt')
fig = px.scatter_mapbox(df_merge,
                        lat="Lat Dec",
                        lon="Lon_Dec",
                        #hover_name="Address",
                        hover_data=["Depthm"],
                        color="T_degC",
                        #color_continuous_scale=color_scale,
                        #size="Listed",
                        #animation_frame='Year',
                        zoom=3,
                        height=800,
                        width=800)
#fig.update_layout(mapbox_style="open-street-map")
fig.update_layout(
    mapbox_style="white-bg",
   mapbox_layers=[
        {
            "below": 'traces',
            "sourcetype": "raster",
            "sourceattribution": "United States Geological Survey",
            "source": [
                "https://basemap.nationalmap.gov/arcgis/rest/services/USGSImageryOnly/MapServer/tile/\{z\}/\{y\}/\{x\}"
            ]
        }])
fig.show()
```

If we isolate points with salinity values in the range going from 34.85 to 38 we observe our alternative trend highlighted in the Temperature-Depth graph. It came out!

```
fig, ax = plt.subplots(1,2, figsize=(20,5))
bottle_filter=bottle[(bottle['Salnty']>34.85)&(bottle['Salnty']<38)]
gl=sns.scatterplot(data=bottle,x='Depthm',y='T_degC',ax=ax[0])
gl=sns.scatterplot(data=bottle_filter,x='Depthm',y='T_degC',ax=ax[0],legend=None,alpha=0.7)
ax[0].set(xlabel='Depth [m]',ylabel='Temperature [°C]',title='Temperature vs Depth')
ax[0].grid()
g2=sns.scatterplot(data=bottle,x='Depthm',y='Salnty',ax=ax[1])
g2=sns.scatterplot(data=bottle_filter,x='Depthm',y='Salnty',ax=ax[1],alpha=0.7)
ax[1].set(xlabel='Depth [m]',ylabel='Salinity',title='Salinity vs Depth')
ax[1].grid()</pre>
```

Distribution of Measuring Points for filtered dataset

Then we show the measuring points from the filtered dataset in the specific salinity range: 34.85 - 38.

```
34
df_merge_filter=bottle_filter.merge(cast, how='inner',on='Cst_Cnt')
fig = px.scatter_mapbox(df_merge_filter,
                       lat="Lat_Dec",
                       lon="Lon_Dec",
                       #hover name="Address",
                       hover_data=["Depthm","Salnty","Cst_Cnt"],
                       color="T_degC",
                       #color_continuous_scale=color_scale,
                       #size="Listed",
                       #animation_frame='Year',
                       zoom=5,
                       height=800,
                       width=800)
#fig.update_layout(mapbox_style="open-street-map")
fig.update_layout(
   mapbox_style="white-bg",
   mapbox_layers=[
           "below": 'traces',
           "sourcetype": "raster",
           "sourceattribution": "United States Geological Survey",
           "source": [
               "https://basemap.nationalmap.gov/arcgis/rest/services/USGSImageryOnly/MapServer/tile/\{z\}/\{y\}/\{x\}"
       }])
fig.show()
```

We note that most points with high salinity values are located in the gulf.

▼ 3.6 | SALINITY - TEMPERATURE

```
plt.rcParams['figure.figsize']=10,6
ax=sns.scatterplot(data=bottle,x='Salnty',y='T_degC')
ax.set(xlabel='Salinity',ylabel='Temperature',title='Salinity vs Temperature')
plt.grid()
```

. . . .

Salinity and Temperature don't seem to have a strong relationship.

We can try to use some additional information using the potential density (https://en.wikipedia.org/wiki/Potential_density). Remind that potential density is not a measured but a calculated quantity from Temperature, Pressure and Salinity.

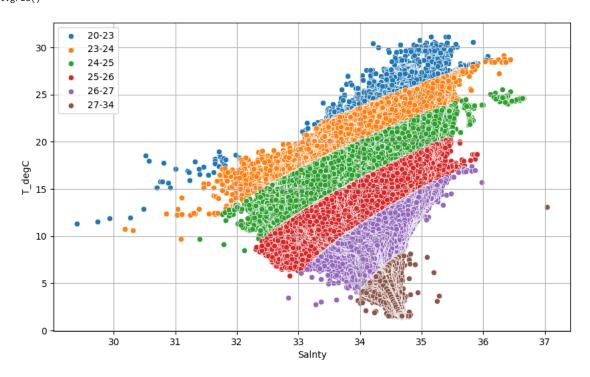
Thanks to proportional link between chlorine and salinity, the last one (difficult to measure) is calculated through the measurement of chlorine, using an electrical conductivity meter.

The technology used to measure Conductivity, Temperature, and Pressure (related to Depth) at the same time in seawater is called CTD (https://en.wikipedia.org/wiki/CTD_(instrument))

```
Salinity-Temperature and potential Density plot

Description

Descript
```



It works! But remind, it's not the real density at the specific depth, it's a potential density.

→ 4 | PREDICTIVE MODELS

Split Train - Test

```
### Split
bottle_train, bottle_test = train_test_split(bottle, test_size=0.2, random_state=1234)
```

```
print("bottle_train: ", bottle_train.shape)
print("bottle_test: ", bottle_test.shape,"\n")

#features =['Salnty','STheta']
features =bottle.columns.drop('T_degC').tolist()
target = 'T_degC'
X_train = bottle_train[features].values
y_train = bottle_train[target].values
X_test = bottle_test[features].values
y_test = bottle_test[target].values

bottle_train: (529014, 6)
bottle_test: (132254, 6)
```

▼ 4.1 | LINEAR REGRESSION

Temperature from Salinity

```
features1=['Salnty'] #only Salinity feature
X_train1 = bottle_train[features1].values
y_train1 = bottle_train[target].values
X_test1 = bottle_test[features1].values
y_test1 = bottle_test[target].values

# creazione modello regressione lineare
model = LinearRegression()
model.fit(X_train1,y_train1)
y_predict1 = model.predict(X_test1)
```

Linear Regression Error

```
#calcolo errore modello di regressione
print(model)
mse_lin=mean_squared_error(y_test1, y_predict1)
RMSE_lin=mse_lin**(1/2.0)
print('RMSE_lin:',RMSE_lin)
    LinearRegression()
    RMSE_lin: 3.6326596110432914
```

Linear Regression Plot

```
g2=sns.regplot(x='Salnty',y="T_degC",data=bottle, color="red")
sns.scatterplot(data=bottle,x='Salnty',y='T_degC')
g2.set(xlabel='Salinity', ylabel='Temperature',title='Linear Regression')
```

```
[Text(0.5, 0, 'Salinity'),
Text(0, 0.5, 'Temperature'),
Text(0.5, 1.0, 'Linear Regression')]
Linear Regression
30 -
```

It doesn't seem to exist a clear trend. It's consistently with the -0.5 Pearson's coefficient got from the confusion matrix. The linear regression is inversely proportional, but it doesn't seem a strong correlation. Of course we isolated the feature of Salinity from the others. We could try to use it with other phisical quantities that we've maintained in this work

```
Multiple Linear Regression

# creazione modello regressione lineare
model = LinearRegression()
model.fit(X_train,y_train)
print(model)
y_predict2 = model.predict(X_test)

#calcolo errore modello di regressione
mse_multilin=mean_squared_error(y_test, y_predict2)
RMSE_multilin=mse_multilin**(1/2.0)

print('RMSE_multilin:',RMSE_multilin)

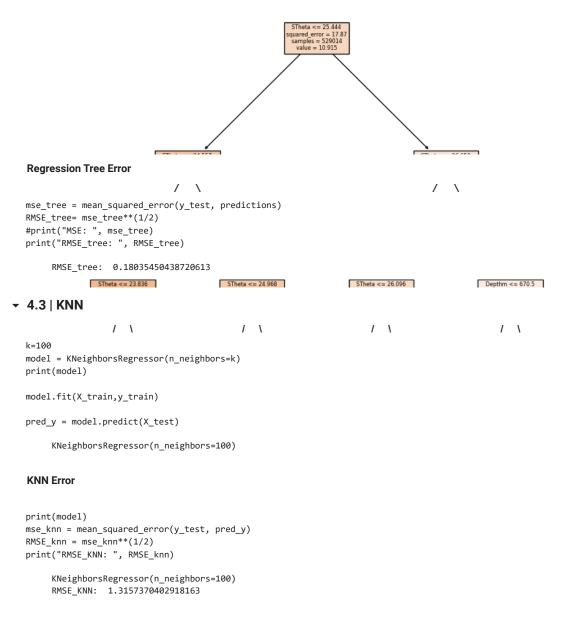
LinearRegression()
RMSE_multilin: 0.3323601966453793
```

Much better

▼ 4.2 | REGRESSION TREE

```
model_tree = DecisionTreeRegressor(random_state=44,max_depth=10)
model_tree.fit(X_train, y_train)
predictions = model_tree.predict(X_test)

plt.figure(figsize=(10,10))
#plot decision tree depth=4
tree.plot_tree(model_tree,feature_names=features,filled=True,max_depth=2);
```



KNN alghoritm is worse than multilinear regressor and decision tree regressor.

▼ 4.4 | FEATURE IMPORTANCE ANALYSIS

for i,feature in enumerate(features):

We can get a feature importance analysis through the decision tree model used above

```
print('',feature,'=', model_tree.feature_importances_[i])

    Cst_Cnt = 8.900949273136677e-06
    Depthm = 0.019813619791390027
    Salnty = 0.06121591882241469
    02ml_L = 4.917424923116525e-05
    STheta = 0.9189123861876909

pd.Series(model_tree.feature_importances_[1:5] , index=['Depth','Salinity','Oxygen','Density']).nlargest(4).plot(kind='barh',figsize=(10,4))
```



Density (STheta=0.919) and Salinity (Salnty=0.061) have the higher feature importance as shown in the theoretical model

immagine.png

So, we can try to repeat our predictions using only these forementioned two features

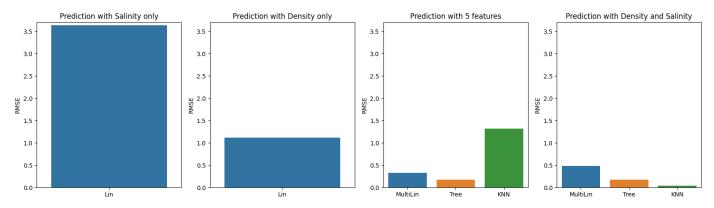
```
features2=['Salnty','STheta'] #only Salinity and Density features
X_train2 = bottle_train[features2].values
y_train2 = bottle_train[target].values
X_test2 = bottle_test[features2].values
y_test2 = bottle_test[target].values
# MULTIPLE LINEAR REGRESSION
model = LinearRegression()
model.fit(X_train2,y_train2)
y_predict2 = model.predict(X_test2)
#print(model)
#calcolo errore modello di regressione
mse_multilin=mean_squared_error(y_test2, y_predict2)
RMSE_multilin_2f=mse_multilin**(1/2.0)
print('RMSE_multilin_2f:',RMSE_multilin_2f)
#DECISION TREE
model = DecisionTreeRegressor(random state=44,max depth=10)
model.fit(X_train2, y_train2)
#print(model)
predictions = model.predict(X_test2)
mse_tree = mean_squared_error(y_test2, predictions)
RMSE_tree_2f= mse_tree**(1/2)
#print("MSE: ", mse_tree)
print("RMSE_tree_2f: ", RMSE_tree_2f)
#KNN
k=100
model = KNeighborsRegressor(n_neighbors=k)
model.fit(X train2,y train2)
pred_y = model.predict(X_test2)
#print(model)
mse_knn = mean_squared_error(y_test2, pred_y)
RMSE_knn_2f = mse_knn^{**}(1/2)
print("RMSE_KNN_2f: ", RMSE_knn_2f)
#linear regression with density
features3=['STheta'] #only Salinity and Density features
X_train3 = bottle_train[features3].values
y_train3 = bottle_train[target].values
X_test3 = bottle_test[features3].values
y_test3 = bottle_test[target].values
# LINEAR REGRESSION with density
model = LinearRegression()
model.fit(X_train3,y_train3)
y_predict3 = model.predict(X_test3)
#calcolo errore modello di regressione per densità
mse_lin_dens=mean_squared_error(y_test3, y_predict3)
```

```
RMSE_lin_dens=mse_lin_dens**(1/2.0)
print("RMSE_dens: ", RMSE_lin_dens)

RMSE_multilin_2f: 0.4813688121553125
RMSE_tree_2f: 0.1778336794244693
RMSE_KNN_2f: 0.04434452522132766
RMSE_dens: 1.1215289238624324
```

RMSE Plot

```
Metodo_g1 = ['MultiLin','Tree','KNN']
Metodo_g2 = ['MultiLin', 'Tree','KNN']
Metodo_g3 = ['Lin']
Metodo_g4 = ['Lin']
RMSE_g1 = [RMSE_multilin_2f,RMSE_tree_2f,RMSE_knn_2f ]
RMSE_g2 = [RMSE_multilin, RMSE_tree,RMSE_knn]
RMSE_g3 = [RMSE_lin]
RMSE_g4 = [RMSE_lin_dens]
#setup figure
fig, ax = plt.subplots(1,4, figsize=(20,5))
g1=sns.barplot(x=Metodo_g1, y=RMSE_g1,ax=ax[3])
g2=sns.barplot(x=Metodo_g2, y=RMSE_g2,ax=ax[2])
{\tt g3=sns.barplot(x=Metodo\_g3, y=RMSE\_g3,ax=ax[0])}
g4=sns.barplot(x=Metodo_g4, y=RMSE_g4,ax=ax[1])
g1.set_title('Prediction with Density and Salinity')
g2.set_title('Prediction with 5 features')
g3.set_title('Prediction with Salinity only')
g4.set_title('Prediction with Density only')
g1.set_ylim(0, 3.7)
g1.set_ylabel('RMSE')
g2.set_ylim(0, 3.7)
g2.set_ylabel('RMSE')
g3.set_ylim(0, 3.7)
g3.set_ylabel('RMSE')
g4.set_ylim(0, 3.7)
g4.set_ylabel('RMSE')
#g2.set_title('Boxplot della Densità')
plt.show()
```



→ 5 | CONCLUSION

- 1. Apparently there isn't a strong relationship between Temperature and Salinity as shown in the picture on the right ('Prediction with Salinity only')
- 2. In order to enhance the temperature prediction with the linear regression model we need to use more features (the picture in the middle): Salinity, Density, Oxygen Saturation, Depth
- 3. KNN model shows better results when we use the only features with a higher importance: Density and Salinity. The same features introduced from the theoretical model on Temperature-Salinity-Density

Last but not least...

Below some plots to give a graphic explanation of why by adding the density feature we are able to improve the error.

One feature as Salinity is not enough to find a link with Temperature. A simple straight line is not able to describe a trend of a dependent variable (Temperature) function of two indipendent variables (Density and Salinity).

Instead adding one or more degrees of freedoms (i.e. Density) we give useful informations to our predictive model.

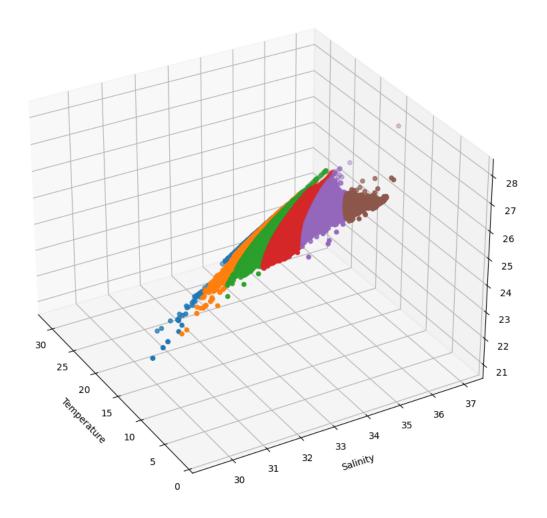
Temperature - Salinity- Density

```
theta_step=[20,23,24,25,26,27,34]
fig = plt.figure(figsize=[10,12])
ax = fig.add_subplot(projection='3d')

# set axis labels
ax.set_xlabel('\nTemperature')
ax.set_ylabel('\nSalinity')
ax.set_zlabel('\nDensity', linespacing=3.4)

for theta1, theta2 in zip(theta_step, theta_step[1:]):
    bottle_stheta=bottle[(bottle['STheta']>=theta1) & (bottle['STheta']<theta2)]
    ax.scatter(bottle_stheta['T_degC'], bottle_stheta['Salnty'], bottle_stheta['STheta'].values.reshape(-1,1))

plt.grid()
plt.gca().invert_zaxis()
plt.gca().view_init(-150, 30)</pre>
```



```
features3=['Salnty','STheta']
X_train3 = bottle_train[features3].values
y_train3 = bottle_train[target].values
model = LinearRegression()
model.fit(X_train3,y_train3)
#interpolazione dei punti del piano
x_mesh = np.linspace(30, 37, N) # intervalli sull'asse della salinità
y_mesh = np.linspace(20, 30,N) # intervalli sull'asse della densità
xx_pred, yy_pred = np.meshgrid(x_mesh, y_mesh)
model_viz = np.array([xx_pred.flatten(), yy_pred.flatten()]).T
predicted = model.predict(model_viz) # Valori di temperatura
The result of the linear regression is no longer a straight line, but a plane
fig = plt.figure(figsize=(10,12))
ax = fig.add_subplot(projection='3d') #crea immagine 3D
# set axis labels
ax.set_xlabel('\nTemperature')
ax.set_ylabel('\nSalinity')
ax.set_zlabel('\nDensity', linespacing=3.4)
ax.plot_trisurf(predicted, xx_pred.flatten(), yy_pred.flatten(), linewidth=0,alpha=0.6) # plot piano di regressione
ax.set_xlim(0,30)
ax.set_ylim(30,37)
ax.set_zlim(21,28)
#Visualizzazione con view: -170,40
plt.gca().view_init(-170, 40)
plt.gca().invert_zaxis()
# plot punti del dataframe Bottle
for theta1, theta2 in zip(theta_step, theta_step[1:]):
   bottle_stheta=bottle[(bottle['STheta']>=theta1) & (bottle['STheta']<theta2)]</pre>
   ax.scatter(bottle\_stheta['T\_degC'],\ bottle\_stheta['Salnty'],\ bottle\_stheta['STheta'].values.reshape(-1,1))
```

```
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ax = fig.add_subplot(projection='3d')
# set axis labels
ax.set_xlabel('\nTemperature')
ax.set_ylabel('\nSalinity')
ax.set_zlabel('\nDensity', linespacing=3.4)
ax.plot\_trisurf(predicted, \ xx\_pred.flatten(), \ yy\_pred.flatten(), \ linewidth=0, alpha=0.3) \ \ \# \ plot \ piano \ di \ regressione
ax.set_xlim(0,30)
ax.set_ylim(30,37)
ax.set_zlim(21,28)
#Visualizzazione con view: -170,30
plt.gca().view_init(-170, 30)
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