

Feature Engineering

Feature engineering involves the selection, manipulation and transformation of raw data into features used in supervised learning. The purpose of feature engineering and selection is to improve the performance of machine-learning algorithms. In consequence, model accuracy on unseen data should be improved.

This notebook includes:

- Outlier and missing analysis: detect (MAD z-score) and missing data.
- Missing-value handling: null impulsion, mean impulsion, median impulsion, multivariate Imputation, K-Nearest Neighbor, interpolation & extrapolation.
- Creating features: residual according to high correlations, golden combination characteristic, target encoding, rolling means, polynomial features
- Feature selection: mutual info, target correlation, correlated features, feature outliers, null importance
- Results evaluation: benchmark model - TabPFN regression

1. Configuration and Preparation

1.1 Parameters

These parameters not only enable parameterization of this Notebook, but also allow us to easily call and execute Jupyter Notebooks in other notebooks via papermill.

In [1]:

```
# parameters
# for function call, please set this cell tag as 'parameters'
parameters = dict(
    input_dir = "../data/", # input dir as parameter, which allows other notebooks to access and call this notebook flexibly.
    missing_outlier_r_threshold = 7, # threshold for the removal of rows with large number of missing and outliers, recommend 6
    missing_outlier_c_threshold = 200, # threshold for the removal of columns with large number of missing and outliers, recommend 10
    impute_method = 'interp', # imputation methods: 'zero', 'mean', 'median', 'mice', 'knn', 'interp'
    corr_method = 'spearman', # 'pearson' or 'spearman'
```

```

corr_threshold = 0.9, # correlation threshold to determine close related feature pairs, recommend 0.8, 0.85 or 0.9
target_corr_threshold = 0.01, # correlation threshold to determine close related feature pairs, recommend 0.01 or 0.02
null_importance_threshold = 90, # threshold for null importance, recommend 80 or 90
OnlyOrigNumFeatures = True, # whether only provide the original numerical features for the Learning
KeepOrigNumFeatures = True, # whether keep original numerical features for the Learning
UseTimeSeries = False, # use the complete time series of trian and test data set
RemoveMissingOutlier = False, # whether remove the rows and columns with a large number of missing and outlier values
)

# assign and organize parameter values
input_dir = parameters['input_dir']
missing_outlier_r_threshold = parameters['missing_outlier_r_threshold']
missing_outlier_c_threshold = parameters['missing_outlier_c_threshold']
impute_method = parameters['impute_method']
corr_method = parameters['corr_method']
corr_threshold = parameters['corr_threshold']
target_corr_threshold = parameters['target_corr_threshold']
null_importance_threshold = parameters['null_importance_threshold']
OnlyOrigNumFeatures = parameters['OnlyOrigNumFeatures']
KeepOrigNumFeatures = parameters['KeepOrigNumFeatures']
UseTimeSeries = parameters['UseTimeSeries']
RemoveMissingOutlier = parameters['RemoveMissingOutlier']

if OnlyOrigNumFeatures:
    KeepOrigNumFeatures = True

```

1.2 Configuration

In [2]:

```

# configuration
# paths
X_TRAIN_PATH = f"{input_dir}X_train_NHkHMNU.csv"
X_TEST_PATH = f"{input_dir}X_test_final.csv"
Y_TRAIN_PATH = f"{input_dir}y_train_ZAN5mwg.csv"

# seed for random number
RANDOM_STATE = 47

```

In [3]:

```

# relevant feature lists
drop_features = ['DE_NET_IMPORT', 'FR_DE_EXCHANGE', 'FR_NET_IMPORT']

```

```
country_features = ["TEMP", "RAIN", "WIND", "GAS", "COAL", "HYDRO", "NUCLEAR", "SOLAR", "WINDPOW", "CONSUMPTION", "RESIDUAL_LC"]
eu_features = ['GAS_RET', 'COAL_RET', 'CARBON_RET']
de_features = ['DE_' + x for x in country_features] + ['DE_LIGNITE']
fr_features = ['FR_' + x for x in country_features]
weather_measures = ['TEMP', 'RAIN', 'WIND']
weather_features = ['DE_' + x for x in weather_measures] + ['FR_' + x for x in weather_measures]
use_measures = ["CONSUMPTION", "RESIDUAL_LOAD", "NET_EXPORT"]
use_features = ['DE_' + x for x in use_measures] + ['FR_' + x for x in use_measures] + ["DE_FR_EXCHANGE"]
renew_energy = ["HYDRO", "SOLAR", "WINDPOW"]
renew_features = ['DE_' + x for x in renew_energy] + ['FR_' + x for x in renew_energy]
nonrenew_energy = ["GAS", "COAL", "NUCLEAR"]
nonrenew_features = ['DE_' + x for x in nonrenew_energy] + ['FR_' + x for x in nonrenew_energy] + ["DE_LIGNITE"]
```

1.3 Imports and load data

In [4]:

```
# imports of libraries and functions
import numpy as np
import pandas as pd
import lightgbm as lgb
import scipy
import seaborn as sns
import scrapbook as sb
import math
import matplotlib.pyplot as plt
import matplotlib.gridspec as gridspec
import warnings

from fancyimpute import IterativeImputer, KNN, SimpleFill
from sklearn.feature_selection import mutual_info_regression
from sklearn.ensemble import HistGradientBoostingRegressor
from sklearn.inspection import permutation_importance
from sklearn.model_selection import train_test_split
from scipy.stats import spearmanr
from sklearn.metrics import mean_squared_error, r2_score
from tabPFN import TabPFNRegressor

warnings.filterwarnings('ignore')
```

```
In [5]: # Load data and preparing
X_train = pd.read_csv(X_TRAIN_PATH)
X_test = pd.read_csv(X_TEST_PATH)
y_train = pd.read_csv(Y_TRAIN_PATH)

assert "ID" in X_train.columns and "ID" in y_train.columns, "ID column must exist in both X_train and y_train"

# dropped due to very high correlation according to EDA
X_y_train = X_train.merge(y_train, on="ID", how="left").drop(drop_features, axis=1)
X_train_test = pd.concat([X_train, X_test], ignore_index=True).drop(drop_features, axis=1)
X_test.drop(drop_features, axis=1, inplace=True)
```

```
In [6]: # country info and simple target encoding on countries
if "COUNTRY" in X_train_test.columns:
    print(X_train_test["COUNTRY"].value_counts(dropna=False))
else:
    print("No COUNTRY column found.")

if KeepOrigNumFeatures :
    orig_num_cols = [x for x in X_train_test.columns if x not in ['DAY_ID', 'COUNTRY']]

target_mean_de = X_y_train.loc[X_y_train['COUNTRY'] == 'DE', 'TARGET'].mean()
target_mean_fr = X_y_train.loc[X_y_train['COUNTRY'] == 'FR', 'TARGET'].mean()
X_y_train['COUNTRY_MEAN'] = X_y_train['COUNTRY'].apply(lambda x: target_mean_de if x == 'DE' else target_mean_fr)
X_train_test['COUNTRY_MEAN'] = X_train_test['COUNTRY'].apply(lambda x: target_mean_de if x == 'DE' else target_mean_fr)

NON_FEATURE = {"ID", "COUNTRY", "TARGET"}
num_cols = [c for c in X_train_test.columns if c not in NON_FEATURE and pd.api.types.is_numeric_dtype(X_train_test[c])]
print("Numeric feature count:", len(num_cols))
```

COUNTRY
 FR 1216
 DE 932
 Name: count, dtype: int64
 Numeric feature count: 31

2. Outlier Treatment

Outlier treatment based on MAD z-score, which is a modified z-score that uses the Median Absolute Deviation (MAD) instead of the standard deviation to detect outliers in a dataset, making it more robust against extreme values. To calculate it, you find the median of the data, then find the median of the absolute deviations from that median, and use that value to scale the differences from the median for each data point. As the target has too many outliers, we do not cap the outliers, but only to remove the noise rows with a large number of missing and outlier values.

```
In [7]: # cap outliers based on MAD z-score
def mad_winsorize(df, cols=None, thresh=3.5, constant=1.4826, eps=1e-9):
    x = df.copy()
    if cols is None:
        cols = x.select_dtypes(include=np.number).columns
    med = x[cols].median()
    mad = (x[cols] - med).abs().median()
    scale = constant * mad + eps
    lo = med - thresh * scale
    hi = med + thresh * scale
    x[cols] = x[cols].clip(lower=lo, upper=hi, axis=1)
    return x
```

```
In [8]: # statistic the missing and outliers in each row of dataframe
def row_missing_and_outliers(
    df: pd.DataFrame,
    cols=None,
    method: str = "mad",
    thresh: float = 3.5,
    constant: float = 1.4826,
    eps: float = 1e-9,
):
    x = df.copy()
    n_missing = x.isna().sum(axis=1)

    if cols is None:
        cols = x.select_dtypes(include=np.number).columns.tolist()
    if not cols:
        outlier_counts = pd.Series(0, index=x.index, name="n_outliers")
    return pd.DataFrame({"n_missing": n_missing, "n_outliers": outlier_counts})

    if method.lower() == "z":
```

```

        mu = x[cols].mean()
        sd = x[cols].std(ddof=0).replace(0, np.nan)
        scale = sd + eps
        z = (x[cols] - mu) / scale

    elif method.lower() == "mad":
        med = x[cols].median()
        mad = (x[cols] - med).abs().median().replace(0, np.nan)
        scale = constant * mad + eps
        z = (x[cols] - med) / scale
    else:
        raise ValueError("method must be 'mad' or 'z'")

    out_mask = z.abs() > thresh
    out_mask = out_mask & x[cols].notna()
    n_outliers = out_mask.sum(axis=1)

    return pd.DataFrame({
        'ID': x.ID,
        "n_missing": n_missing,
        "n_outliers": n_outliers
    })

```

In [9]: # staticic the missing and outliers in each column of dataframe

```

def column_missing_and_outliers(
    df: pd.DataFrame,
    cols=None,
    method: str = "mad",
    thresh: float = 3.5,
    constant: float = 1.4826,
    eps: float = 1e-9
) -> pd.DataFrame:
    x = df.copy()

    n_missing = x.isna().sum(axis=0)
    n_total = len(x)
    frac_missing = n_missing / max(n_total, 1)

    if cols is None:
        num_col = x.select_dtypes(include=np.number).columns.tolist()

```

```
else:
    num_col = list(cols)

n_outliers = pd.Series(np.nan, index=x.columns, dtype=float)
frac_outliers = pd.Series(np.nan, index=x.columns, dtype=float)
center_used = pd.Series(np.nan, index=x.columns, dtype=float)
scale_used = pd.Series(np.nan, index=x.columns, dtype=float)

if len(num_col) > 0:
    if method.lower() == "z":
        center = x[num_col].mean(axis=0)
        scale = x[num_col].std(axis=0, ddof=0)
    elif method.lower() == "mad":
        center = x[num_col].median(axis=0)
        mad = (x[num_col] - center).abs().median(axis=0)
        scale = constant * mad
    else:
        raise ValueError("method must be 'mad' or 'z'")

    scale = scale.replace(0, np.nan)

Z = (x[num_col] - center) / (scale + eps)
valid = x[num_col].notna() & np.isfinite(Z)
out_mask = valid & (Z.abs() > thresh)

n_out = out_mask.sum(axis=0)
denom = valid.sum(axis=0).replace(0, np.nan)

n_outliers.loc[num_col] = n_out
frac_outliers.loc[num_col] = (n_out / denom)
center_used.loc[num_col] = center
scale_used.loc[num_col] = scale

res = pd.DataFrame({
    #'column': num_col,
    "n_missing": n_missing,
    "frac_missing": frac_missing,
    "n_outliers": n_outliers,
    "frac_outliers": frac_outliers,
    "center": center_used,
    "scale": scale_used
})
```

```

    })
return res

```

```
In [10]: # count the rows and columns with a large number of missing and outlier values
r_missing_outlier = row_missing_and_outliers(X_y_train)
drop_rows = list(r_missing_outlier.loc[(r_missing_outlier.n_missing + r_missing_outlier.n_outliers) > missing_outlier_r_thresh])
print(f"The number of rows with a large count of missing and outlier values is {len(drop_rows)}")

c_missing_outlier = column_missing_and_outliers(X_y_train)
drop_columns = list(c_missing_outlier.loc[(c_missing_outlier.n_missing + c_missing_outlier.n_outliers) > missing_outlier_c_thresh])
print(f"The number of columns with a large count of missing and outlier values is {len(drop_columns)}")
if 'TARGET' in drop_columns:
    drop_columns.remove('TARGET')
display(drop_columns)
```

The number of rows with a large count of missing and outlier values is 35
The number of columns with a large count of missing and outlier values is 1
['FR_COAL']

```
In [11]: # remove the rows with a large number of missing and outlier values
display((X_train.shape, y_train.shape, X_train_test.shape, X_y_train.shape))

if RemoveMissingOutlier and len(drop_rows) > 0:
    X_train = X_train[~X_train['ID'].isin(drop_rows)]
    y_train = y_train[~y_train['ID'].isin(drop_rows)]
    X_train_test = X_train_test[~X_train_test['ID'].isin(drop_rows)]
    X_y_train = X_y_train[~X_y_train['ID'].isin(drop_rows)]

    display((X_train.shape, y_train.shape, X_train_test.shape, X_y_train.shape))
```

((1494, 35), (1494, 2), (2148, 33), (1494, 34))

```
In [12]: # plot the outliers for each feature
plots = [(c, X_y_train[c]) for c in X_y_train.columns]

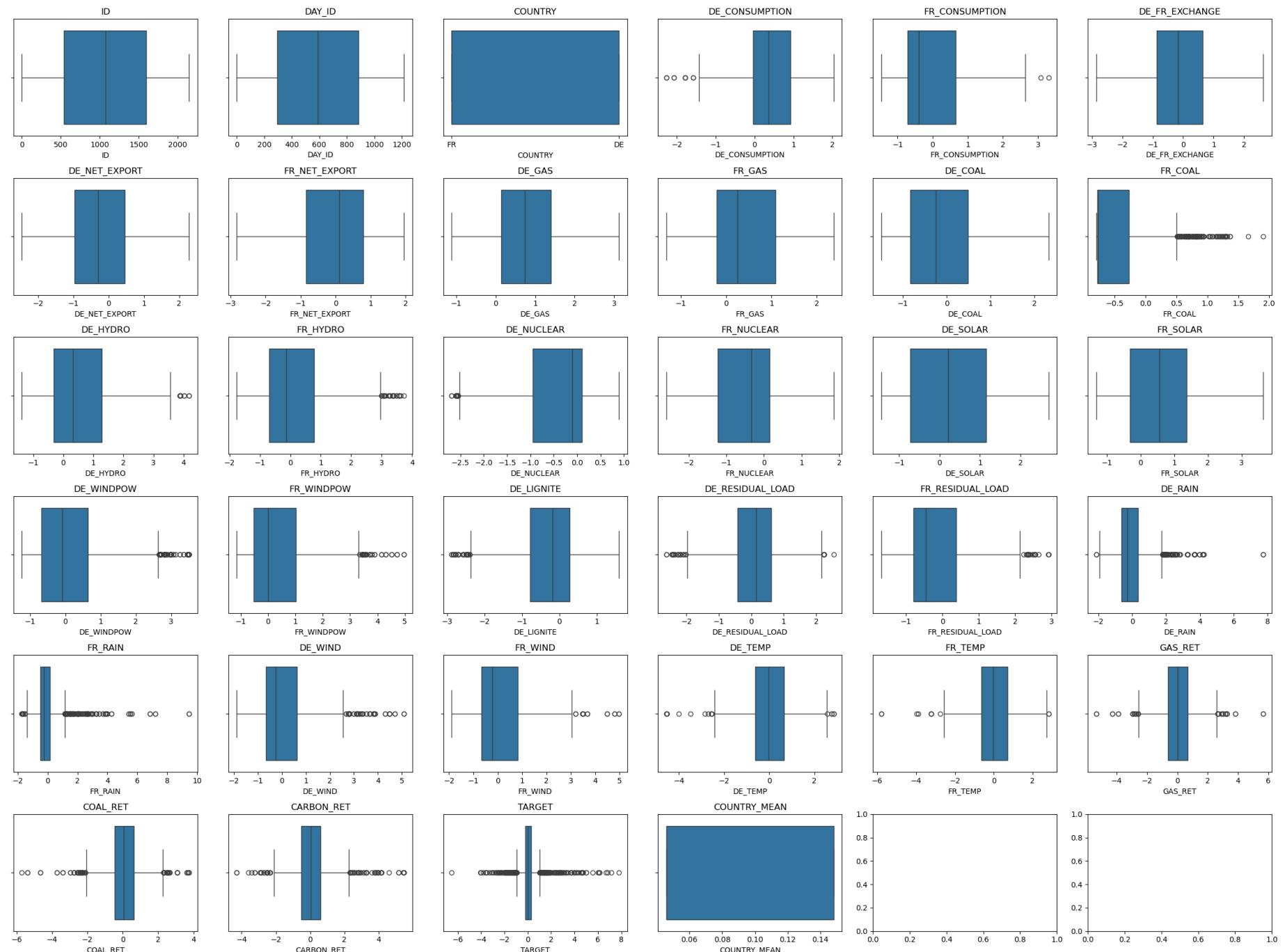
K = len(plots)
N = math.ceil(math.sqrt(K))
M = math.ceil(K / N)

fig, axes = plt.subplots(M, N, figsize=(N*4, M*3), squeeze=False)
axes = axes.ravel()
```

```
for i, (name, s) in enumerate(plots):
    sns.boxplot(x=s, ax=axes[i])
    axes[i].set_title(f"{name}")

plt.tight_layout()
plt.show()
```

feature_engineering



3. Handling Missing Values

3.1 Check Missing Values

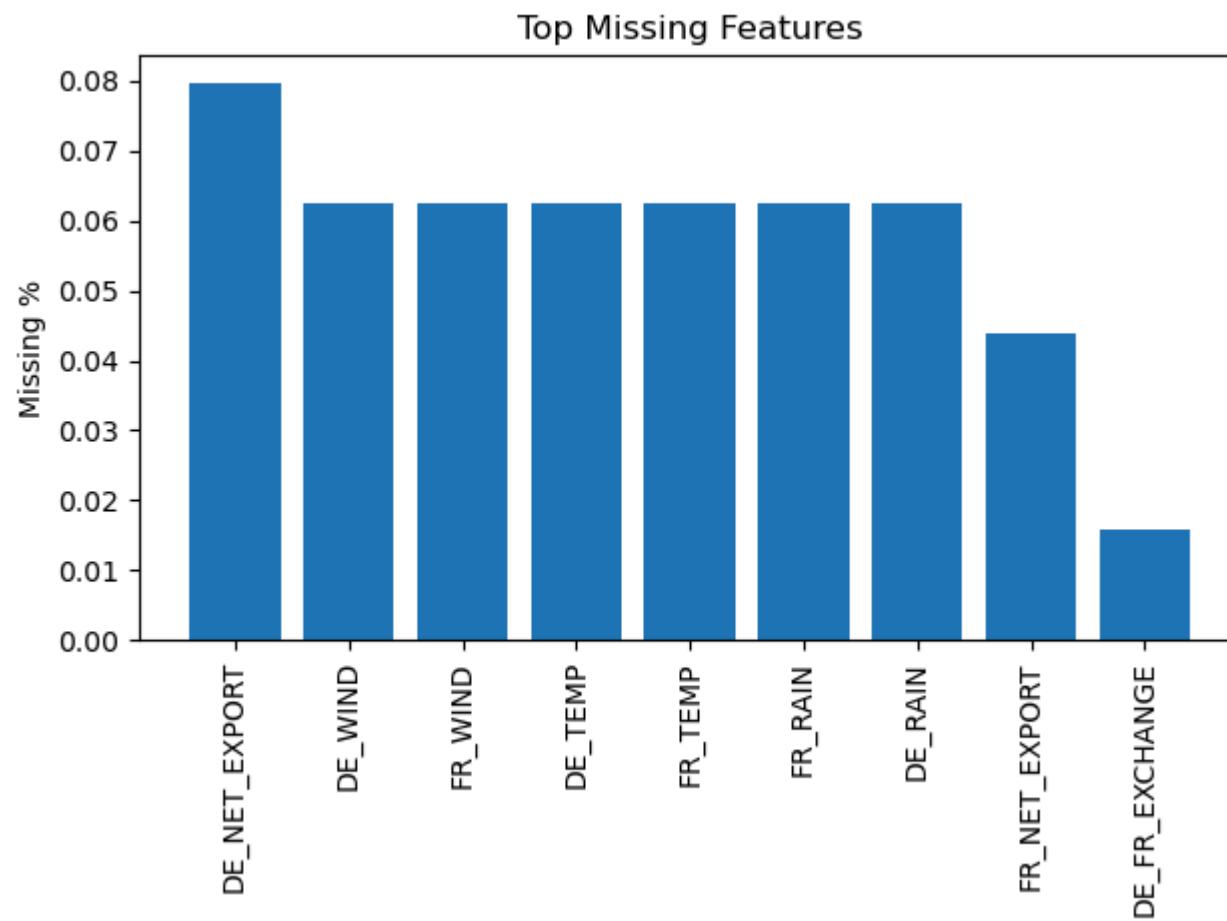
In [13]:

```
# List top missing features
missing_counts = X_train_test.isna().sum().sort_values(ascending=False)
missing_pct = (missing_counts / len(X_train_test)).sort_values(ascending=False)
missing_df = pd.DataFrame({"missing_count": missing_counts, "missing_pct": missing_pct})
print("List features with missing values:")
display(missing_df[missing_df.missing_count      > 0])

# plot top missing features - single figure
top_miss = missing_df.head((missing_df['missing_count'] > 0).sum())
plt.figure()
plt.bar(top_miss.index.astype(str), top_miss["missing_pct"].values)
plt.xticks(rotation=90)
plt.ylabel("Missing %")
plt.title("Top Missing Features")
plt.tight_layout()
plt.show()
```

List features with missing values:

	missing_count	missing_pct
DE_NET_EXPORT	171	0.079609
DE_WIND	134	0.062384
FR_WIND	134	0.062384
DE_TEMP	134	0.062384
FR_TEMP	134	0.062384
FR_RAIN	134	0.062384
DE_RAIN	134	0.062384
FR_NET_EXPORT	94	0.043762
DE_FR_EXCHANGE	34	0.015829



3.2 Imputation of missing values

In the missing-data imputation section, we implemented and compared the following methods: null impulsion ('zero'), mean impulsion ('mean'), median impulsion ('median'), multivariate Imputation ('mice'), K-Nearest Neighbor ('knn'), interpolation & extrapolation ('interp'). We also distinguished between two impulsion scenarios: (1) the standard approach where the training and test sets are handled separately, and (2) combining the two datasets to form a complete time series and performing impulsion on that series. In the second scenario, we first standardize the time series and then interpolate, finally merging the results back into the original datasets keyed by 'DAY_ID'. This ensures that feature values for the same day are consistent, thereby preserving the original data logic.

```
In [14]: # impute missing values with different methods
imp_cols = num_cols[:-1]

if UseTimeSeries:
    # provide and sort complete time series of train and test data set
    df_timeseries = X_train_test[imp_cols].copy()
    df_timeseries.sort_values("DAY_ID", inplace=True)
    df_timeseries.drop_duplicates(inplace=True)
    print(f"There are {len(df_timeseries[df_timeseries.duplicated(subset=['DAY_ID'])])} duplicates in the time ser

    # impute missing values
    X_filled_zero = SimpleFill(fill_method='zero').fit_transform(df_timeseries)
    X_filled_mean = SimpleFill(fill_method='mean').fit_transform(df_timeseries)
    X_filled_median = SimpleFill(fill_method='median').fit_transform(df_timeseries)
    X_filled_mice = IterativeImputer(max_iter=10, random_state=RANDOM_STATE).fit_transform(df_timeseries)
    X_filled_knn = KNN(k=5).fit_transform(df_timeseries)
    X_filled_interp = df_timeseries.interpolate(method='polynomial', order=2, limit_direction="both")
    X_filled_interp = X_filled_interp.interpolate(method="linear", limit_direction="both")

    X_filled_zero = pd.DataFrame(X_filled_zero, columns=imp_cols)
    X_filled_mean = pd.DataFrame(X_filled_mean, columns=imp_cols)
    X_filled_median = pd.DataFrame(X_filled_median, columns=imp_cols)
    X_filled_mice = pd.DataFrame(X_filled_mice, columns=imp_cols)
    X_filled_knn = pd.DataFrame(X_filled_knn, columns=imp_cols)
else:
    X_train_imp = X_train[['ID']].merge(X_train_test, on='ID', how='left')[imp_cols]
    X_test_imp = X_test[['ID']].merge(X_train_test, on='ID', how='left')[imp_cols]

    X_tr_filled_zero = SimpleFill(fill_method='zero').fit_transform(X_train_imp)
    X_tr_filled_mean = SimpleFill(fill_method='mean').fit_transform(X_train_imp)
    X_tr_filled_median = SimpleFill(fill_method='median').fit_transform(X_train_imp)
    X_tr_filled_mice = IterativeImputer(max_iter=10, random_state=RANDOM_STATE).fit_transform(X_train_imp)
    X_tr_filled_knn = KNN(k=5).fit_transform(X_train_imp)
    X_tr_filled_interp = X_train.interpolate(method='polynomial', order=3).fillna(0.0)

    X_tr_filled_zero = pd.DataFrame(X_tr_filled_zero, columns=imp_cols)
    X_tr_filled_mean = pd.DataFrame(X_tr_filled_mean, columns=imp_cols)
    X_tr_filled_median = pd.DataFrame(X_tr_filled_median, columns=imp_cols)
    X_tr_filled_mice = pd.DataFrame(X_tr_filled_mice, columns=imp_cols)
    X_tr_filled_knn = pd.DataFrame(X_tr_filled_knn, columns=imp_cols)
```

```
X_te_filled_zero = SimpleFill(fill_method='zero').fit_transform(X_test_imp)
X_te_filled_mean = SimpleFill(fill_method='mean').fit_transform(X_test_imp)
X_te_filled_median = SimpleFill(fill_method='median').fit_transform(X_test_imp)
X_te_filled_mice = IterativeImputer(max_iter=10, random_state=RANDOM_STATE).fit_transform(X_test_imp)
X_te_filled_knn = KNN(k=5).fit_transform(X_test_imp)
X_te_filled_interp = X_test.interpolate(method='polynomial',order=3)

X_te_filled_zero = pd.DataFrame(X_te_filled_zero, columns=imp_cols)
X_te_filled_mean = pd.DataFrame(X_te_filled_mean, columns=imp_cols)
X_te_filled_median = pd.DataFrame(X_te_filled_median, columns=imp_cols)
X_te_filled_mice = pd.DataFrame(X_te_filled_mice, columns=imp_cols)
X_te_filled_knn = pd.DataFrame(X_te_filled_knn, columns=imp_cols)

X_filled_zero = pd.concat([X_tr_filled_zero, X_te_filled_zero], ignore_index=True)
X_filled_mean = pd.concat([X_tr_filled_mean, X_te_filled_mean], ignore_index=True)
X_filled_median = pd.concat([X_tr_filled_median, X_te_filled_median], ignore_index=True)
X_filled_mice = pd.concat([X_tr_filled_mice, X_te_filled_mice], ignore_index=True)
X_filled_knn = pd.concat([X_tr_filled_knn, X_te_filled_knn], ignore_index=True)
X_filled_interp = pd.concat([X_tr_filled_interp, X_te_filled_interp], ignore_index=True).fillna(0.0)
```

```
Imputing row 1/1494 with 1 missing, elapsed time: 0.196
Imputing row 101/1494 with 0 missing, elapsed time: 0.198
Imputing row 201/1494 with 0 missing, elapsed time: 0.199
Imputing row 301/1494 with 0 missing, elapsed time: 0.200
Imputing row 401/1494 with 0 missing, elapsed time: 0.201
Imputing row 501/1494 with 0 missing, elapsed time: 0.202
Imputing row 601/1494 with 0 missing, elapsed time: 0.203
Imputing row 701/1494 with 6 missing, elapsed time: 0.204
Imputing row 801/1494 with 2 missing, elapsed time: 0.205
Imputing row 901/1494 with 0 missing, elapsed time: 0.206
Imputing row 1001/1494 with 0 missing, elapsed time: 0.207
Imputing row 1101/1494 with 0 missing, elapsed time: 0.208
Imputing row 1201/1494 with 0 missing, elapsed time: 0.210
Imputing row 1301/1494 with 6 missing, elapsed time: 0.211
Imputing row 1401/1494 with 0 missing, elapsed time: 0.212
Imputing row 1/654 with 0 missing, elapsed time: 0.050
Imputing row 101/654 with 0 missing, elapsed time: 0.051
Imputing row 201/654 with 0 missing, elapsed time: 0.051
Imputing row 301/654 with 0 missing, elapsed time: 0.052
Imputing row 401/654 with 0 missing, elapsed time: 0.053
Imputing row 501/654 with 0 missing, elapsed time: 0.054
Imputing row 601/654 with 0 missing, elapsed time: 0.055
```

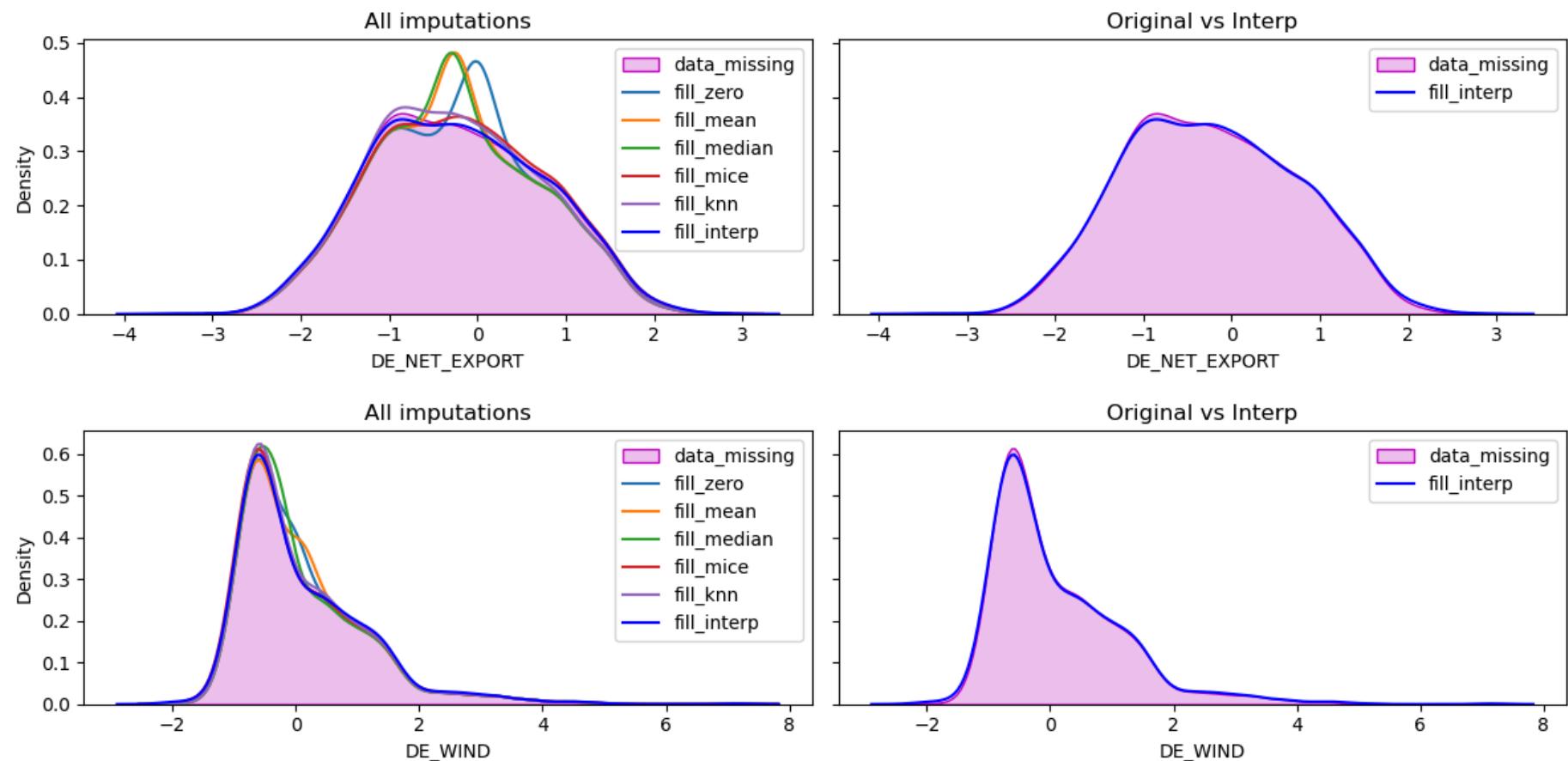
```
In [15]: # plot distribution between features before and after imputation
for c in top_miss.index:
    fig, axes = plt.subplots(1, 2, figsize=(12, 3), sharey=True)
    ax1, ax2 = axes

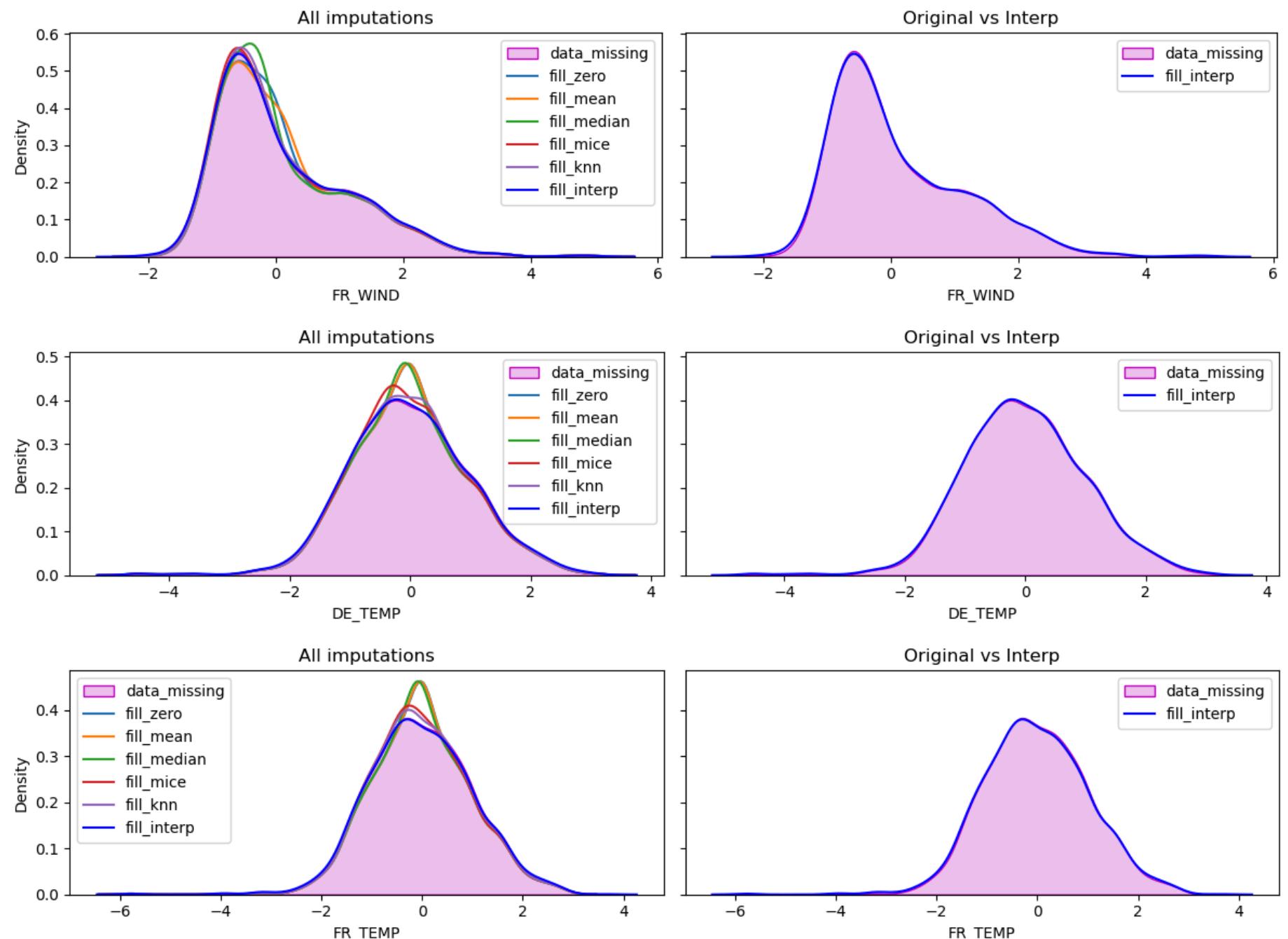
    sns.kdeplot(X_train_test[imp_cols][c], color='m', fill=True, ax=ax1, label='data_missing')
    sns.kdeplot(X_filled_zero[c], ax=ax1, label='fill_zero')
    sns.kdeplot(X_filled_mean[c], ax=ax1, label='fill_mean')
    sns.kdeplot(X_filled_median[c], ax=ax1, label='fill_median')
    sns.kdeplot(X_filled_mice[c], ax=ax1, label='fill_mice')
    sns.kdeplot(X_filled_knn[c], ax=ax1, label='fill_knn')
    sns.kdeplot(X_filled_interp[c], color='b', ax=ax1, label='fill_interp')
    ax1.set_xlabel(c)
    ax1.set_title('All imputations')
    ax1.legend()

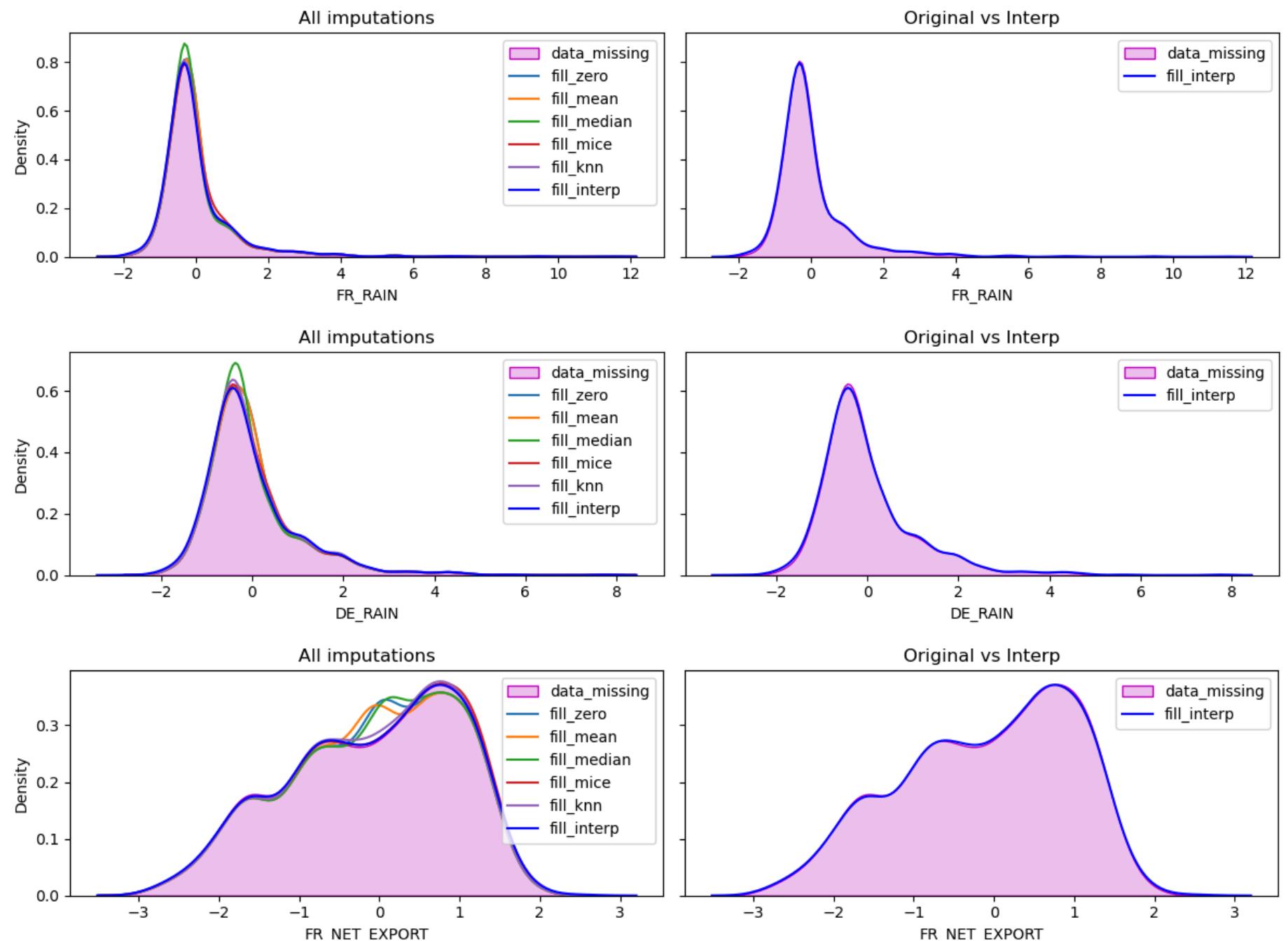
    sns.kdeplot(X_train_test[c], color='m', fill=True, ax=ax2, label='data_missing')
    sns.kdeplot(X_filled_interp[c], color='b', ax=ax2, label='fill_interp')
```

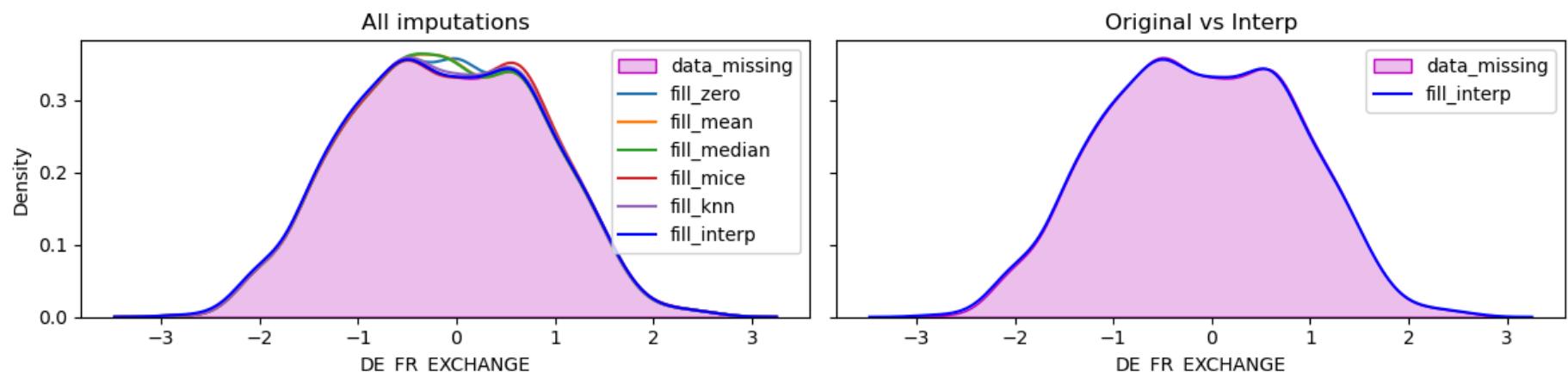
```
ax2.set_xlabel(c)
ax2.set_title('Original vs Interp')
ax2.legend()

plt.tight_layout()
plt.show()
```









```
In [16]: if impute_method == 'interp' and not UseTimeSeries:
    X_train_test_filled = pd.merge(X_train_test[['ID', 'COUNTRY_MEAN']], eval(f"X_filled_{impute_method}"), on='ID', how='left'
else:
    X_train_test_filled = pd.merge(X_train_test[['ID', 'DAY_ID', 'COUNTRY', 'COUNTRY_MEAN']], eval(f"X_filled_{impute_method}"
```

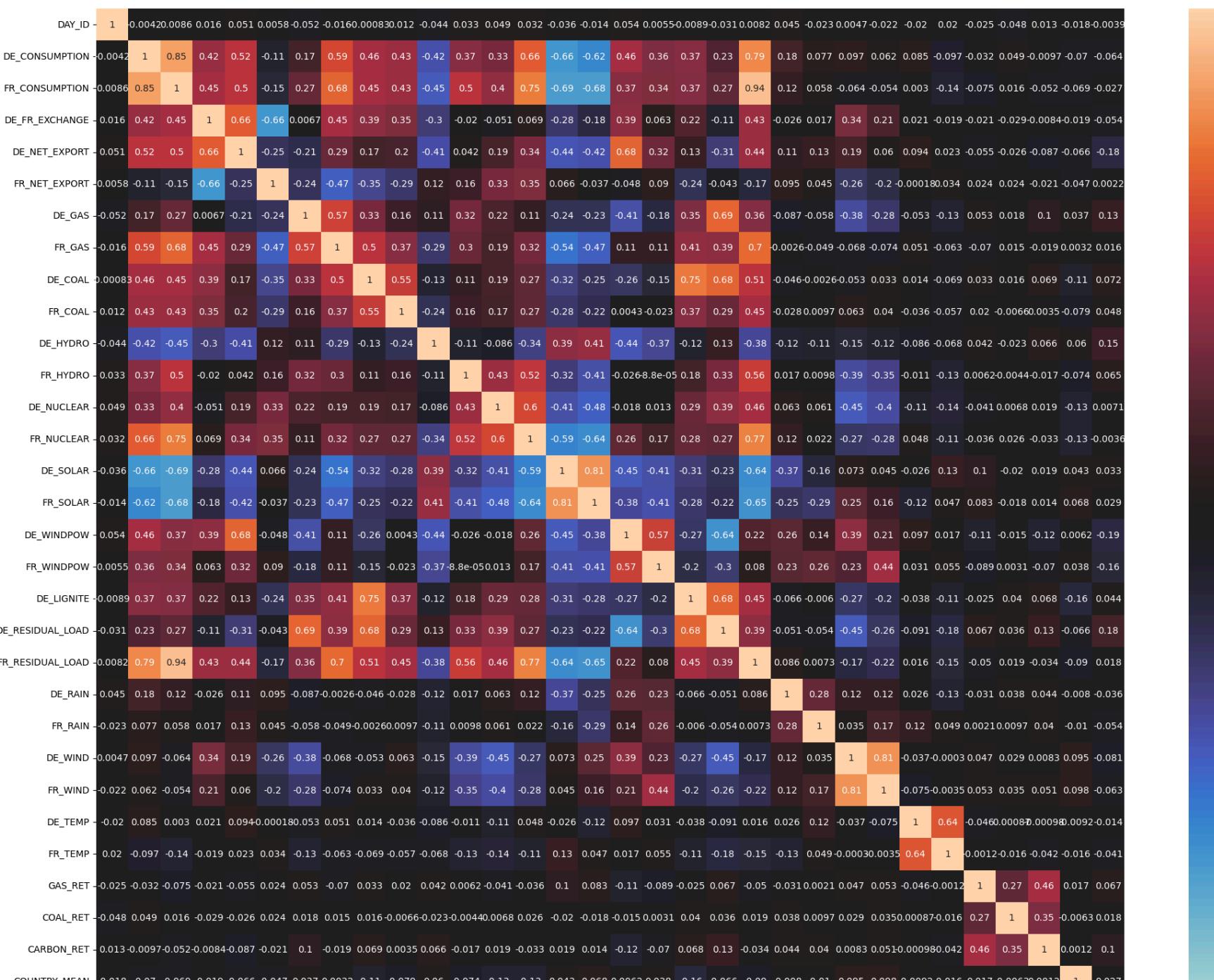
3.3 Statistic after Imputation

```
# plot heatmap of train data with target after imputation
X_y_train_filled = pd.merge(X_train_test_filled, y_train, on='ID', how='right')
print("Missing value count:", X_y_train_filled.isna().sum().sum())

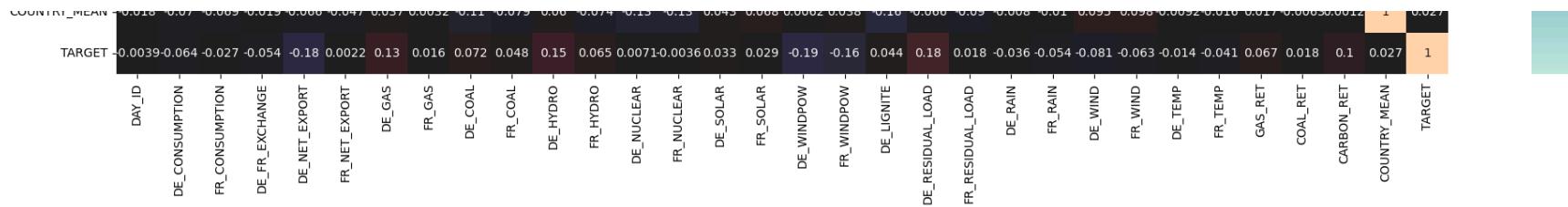
corr = X_y_train_filled[num_cols + ["TARGET"]].corr(method=parameters['corr_method'])
print("Correlation matrix shape:", corr.shape)

plt.figure(figsize=[25,20])
sns.heatmap(corr, annot=True, vmin=-1, vmax=1, center=0)
plt.show()
```

Missing value count: 0
Correlation matrix shape: (32, 32)



feature_engineering



In [18]: # top absolute correlated pairs by |r|

```

pairs = []
cols = corr.columns
for i in range(len(cols)):
    for j in range(i+1, len(cols)):
        r = corr.iloc[i, j]
        pairs.append((cols[i], cols[j], abs(r), r))
pairs_sorted = sorted(pairs, key=lambda x: x[2], reverse=True)[:20]
display(pd.DataFrame(pairs_sorted, columns=["feat1", "feat2", "|r|", "r"]))

```

	feat1	feat2	r	r
0	FR_CONSUMPTION	FR_RESIDUAL_LOAD	0.941636	0.941636
1	DE_CONSUMPTION	FR_CONSUMPTION	0.846620	0.846620
2	DE_WIND	FR_WIND	0.812468	0.812468
3	DE_SOLAR	FR_SOLAR	0.808753	0.808753
4	DE_CONSUMPTION	FR_RESIDUAL_LOAD	0.786134	0.786134
5	FR_NUCLEAR	FR_RESIDUAL_LOAD	0.770119	0.770119
6	FR_CONSUMPTION	FR_NUCLEAR	0.751069	0.751069
7	DE_COAL	DE_LIGNITE	0.749457	0.749457
8	FR_GAS	FR_RESIDUAL_LOAD	0.702212	0.702212
9	DE_GAS	DE_RESIDUAL_LOAD	0.687535	0.687535
10	FR_CONSUMPTION	DE_SOLAR	0.686956	-0.686956
11	FR_CONSUMPTION	FR_SOLAR	0.683373	-0.683373
12	FR_CONSUMPTION	FR_GAS	0.682848	0.682848
13	DE_LIGNITE	DE_RESIDUAL_LOAD	0.682123	0.682123
14	DE_NET_EXPORT	DE_WINDPOW	0.680917	0.680917
15	DE_COAL	DE_RESIDUAL_LOAD	0.680489	0.680489
16	DE_FR_EXCHANGE	DE_NET_EXPORT	0.663661	0.663661
17	DE_CONSUMPTION	DE_SOLAR	0.659928	-0.659928
18	DE_FR_EXCHANGE	FR_NET_EXPORT	0.658739	-0.658739
19	DE_CONSUMPTION	FR_NUCLEAR	0.657896	0.657896

```
In [19]: # calculate correlations between features and target, plot the top target correlations
assert "TARGET" in X_y_train_filled.columns, "TARGET missing after merge"
```

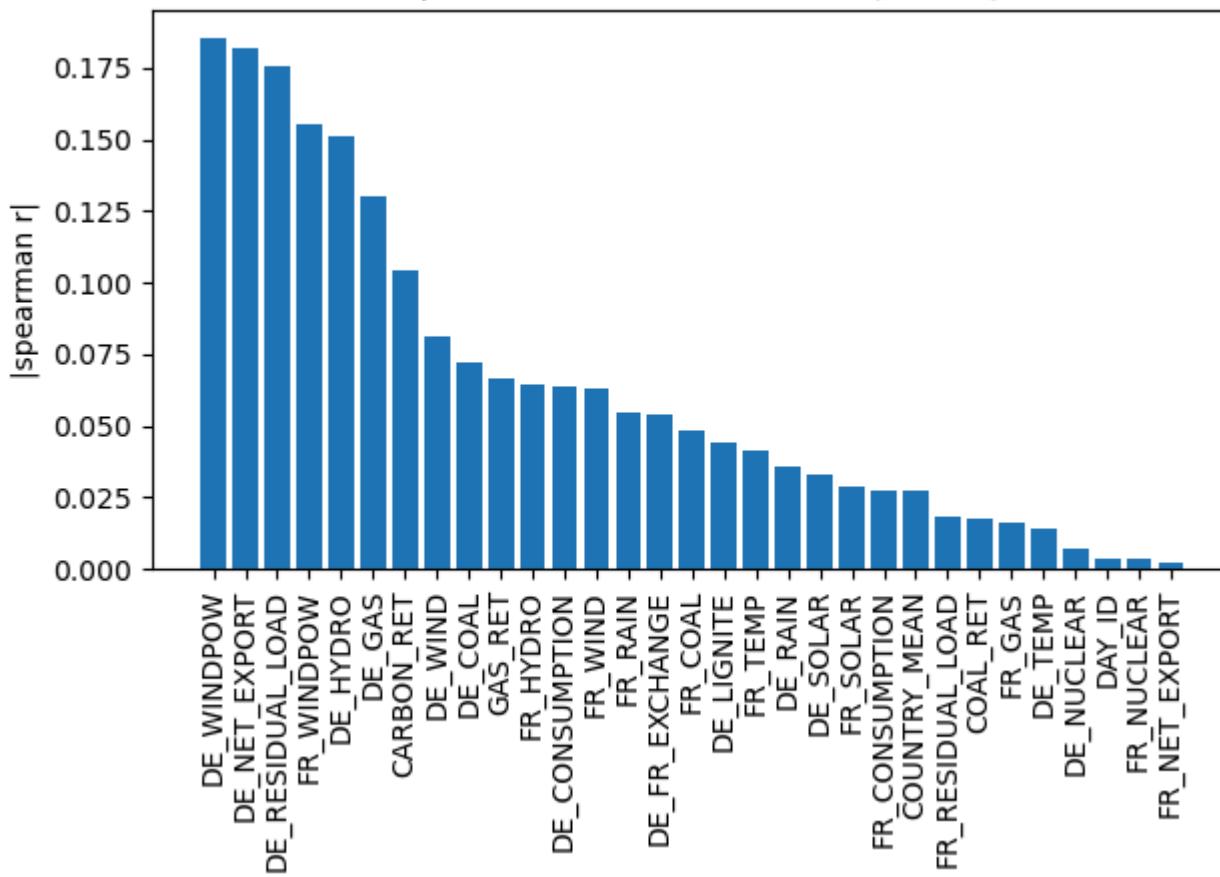
```
target_corr = X_y_train_filled[num_cols + ["TARGET"]].corr(method=parameters['corr_method'])["TARGET"].drop("TARGET").sort_values(ascending=False)

# Bar of absolute correlations (top-k)
tc_abs = target_corr.abs().sort_values(ascending=False)
plt.figure()
plt.bar(tc_abs.index.astype(str), tc_abs.values)
plt.xticks(rotation=90)
plt.ylabel(f"|\{parameters['corr_method']}\|")
plt.title("Top Correlation with TARGET (Global)")
plt.tight_layout()
plt.show()
```

DE_RESIDUAL_LOAD	0.175793
DE_HYDRO	0.151367
DE_GAS	0.129905
CARBON_RET	0.104375
DE_COAL	0.072380
GAS_RET	0.066800
FR_HYDRO	0.064682
FR_COAL	0.048463
DE_LIGNITE	0.044180
DE_SOLAR	0.032740
FR_SOLAR	0.028839
COUNTRY_MEAN	0.027114
FR_RESIDUAL_LOAD	0.018241
COAL_RET	0.017573
FR_GAS	0.016334
DE_NUCLEAR	0.007052
FR_NET_EXPORT	0.002212
FR_NUCLEAR	-0.003619
DAY_ID	-0.003901
DE_TEMP	-0.013885
FR_CONSUMPTION	-0.027242
DE_RAIN	-0.036054
FR_TEMP	-0.041060
DE_FR_EXCHANGE	-0.054010
FR_RAIN	-0.054358
FR_WIND	-0.063296
DE_CONSUMPTION	-0.063617
DE_WIND	-0.081106
FR_WINDPOW	-0.155568
DE_NET_EXPORT	-0.182006
DE_WINDPOW	-0.185688

Name: TARGET, dtype: float64

Top Correlation with TARGET (Global)

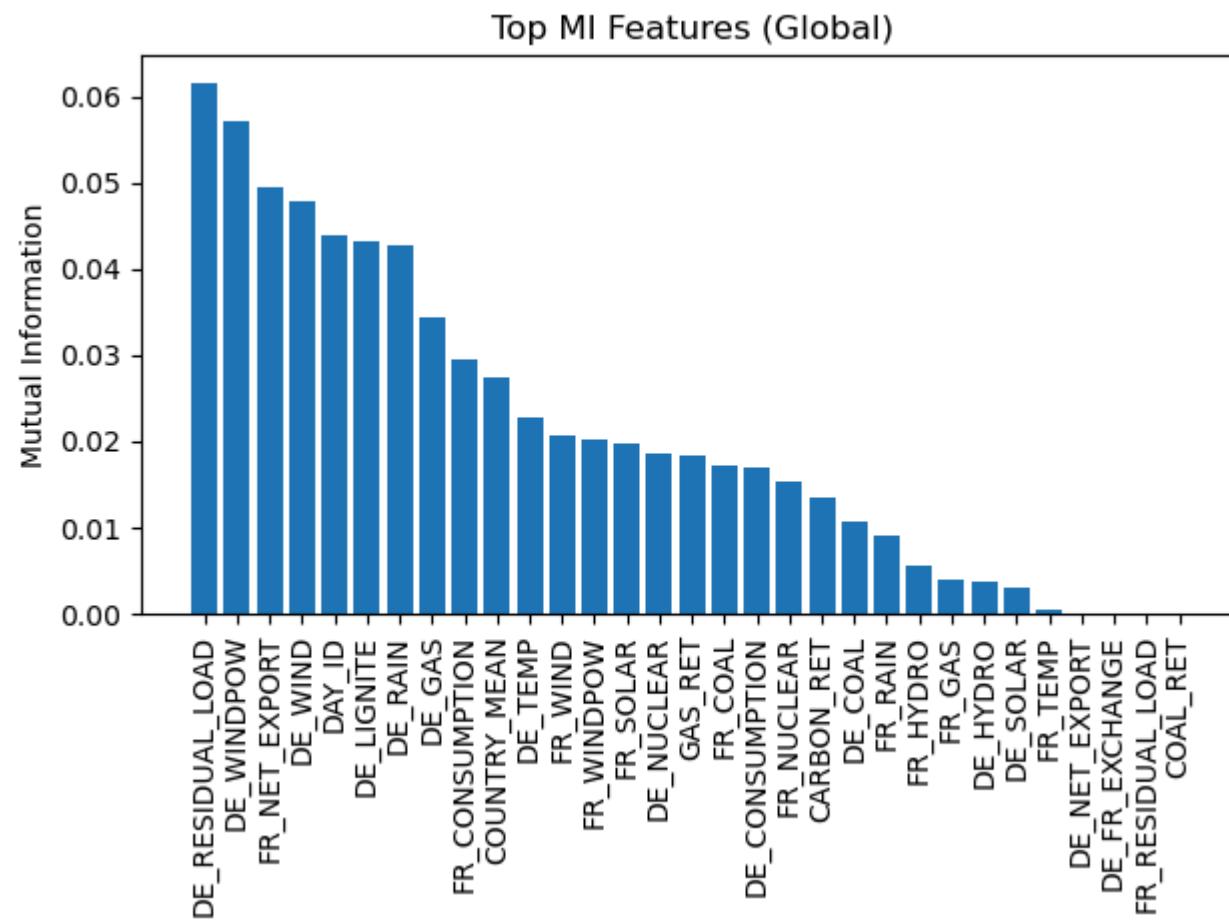


```
In [20]: # mutual Information ranking (top-k) of the train data set after imputation
mi = mutual_info_regression(X_y_train_filled[num_cols], X_y_train_filled['TARGET'], random_state=RANDOM_STATE)
mi_series = pd.Series(mi, index=num_cols).sort_values(ascending=False)
display(mi_series)

plt.figure()
plt.bar(mi_series.index.astype(str), mi_series.values)
plt.xticks(rotation=90)
plt.ylabel("Mutual Information")
plt.title("Top MI Features (Global)")
```

```
plt.tight_layout()  
plt.show()
```

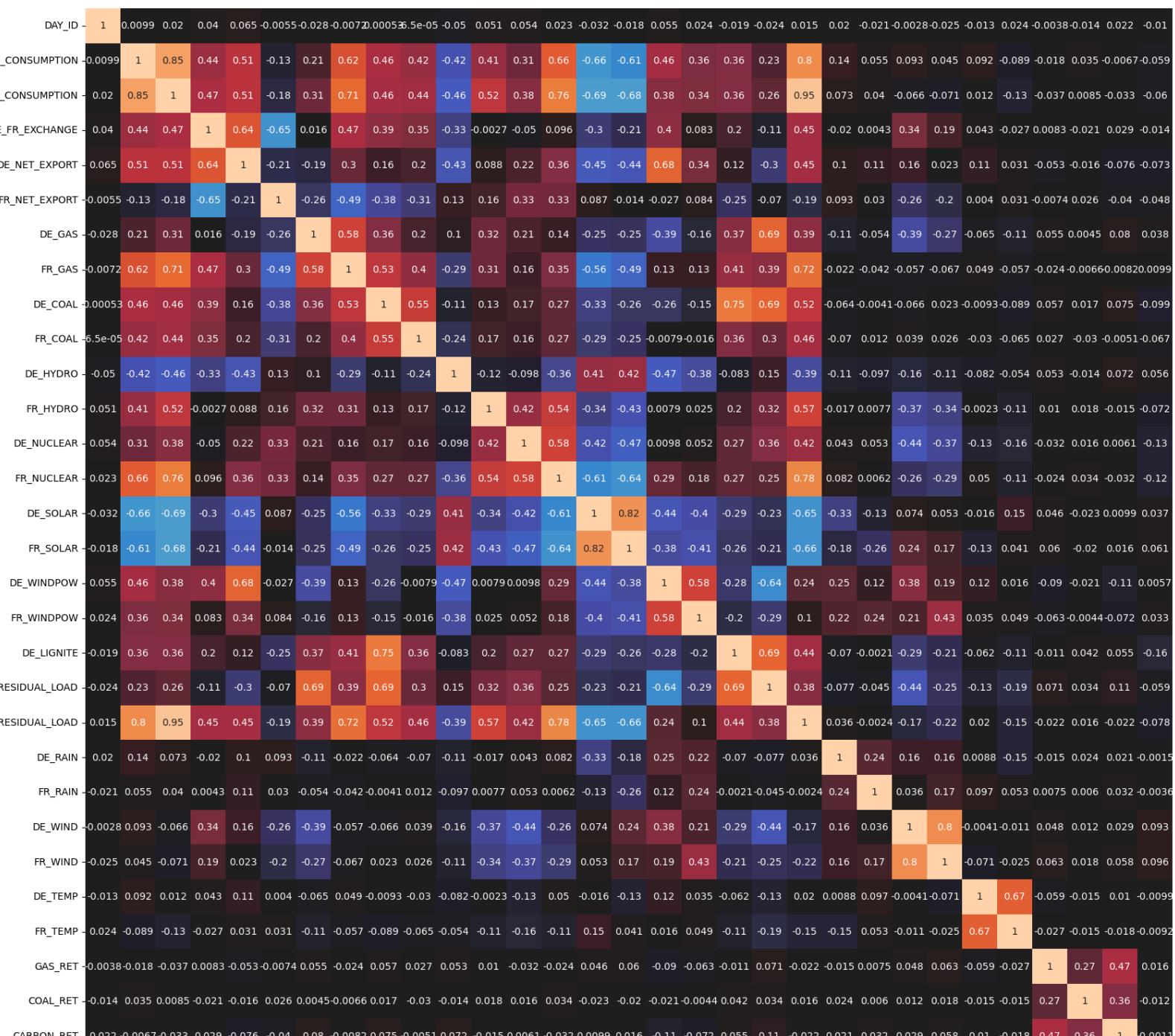
```
DE_RESIDUAL_LOAD      0.061609  
DE_WINDPOW            0.057206  
FR_NET_EXPORT         0.049533  
DE_WIND                0.047792  
DAY_ID                 0.043862  
DE_LIGNITE             0.043258  
DE_RAIN                 0.042631  
DE_GAS                  0.034452  
FR_CONSUMPTION          0.029595  
COUNTRY_MEAN           0.027362  
DE_TEMP                 0.022885  
FR_WIND                 0.020686  
FR_WINDPOW              0.020285  
FR_SOLAR                 0.019679  
DE_NUCLEAR               0.018527  
GAS_RET                  0.018324  
FR_COAL                  0.017179  
DE_CONSUMPTION            0.016898  
FR_NUCLEAR                0.015249  
CARBON_RET                 0.013482  
DE_COAL                  0.010798  
FR_RAIN                  0.008993  
FR_HYDRO                  0.005717  
FR_GAS                   0.003900  
DE_HYDRO                  0.003653  
DE_SOLAR                  0.002997  
FR_TEMP                  0.000545  
DE_NET_EXPORT              0.000000  
DE_FR_EXCHANGE             0.000000  
FR_RESIDUAL_LOAD           0.000000  
COAL_RET                  0.000000  
dtype: float64
```



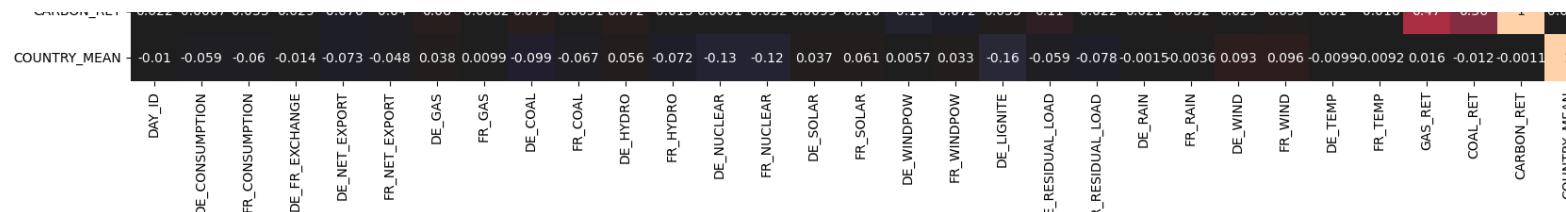
```
In [21]: # plot heatmap of train and test data set after imputation
corr = X_train_test_filled[num_cols].corr(method=parameters['corr_method'])
print("Correlation matrix shape:", corr.shape)

plt.figure(figsize=[25,20])
sns.heatmap(corr, annot=True, vmin=-1, vmax=1, center=0)
plt.show()
```

Correlation matrix shape: (31, 31)



feature_engineering



In [22]: *# Top correlated pairs by |r|*

```

pairs = []
cols = corr.columns
for i in range(len(cols)):
    for j in range(i+1, len(cols)):
        r = corr.iloc[i, j]
        pairs.append((cols[i], cols[j], abs(r), r))
pairs_sorted = sorted(pairs, key=lambda x: x[2], reverse=True)[:20]
display(pd.DataFrame(pairs_sorted, columns=["feat1", "feat2", "|r|", "r"]))

```

	feat1	feat2	r	r
0	FR_CONSUMPTION	FR_RESIDUAL_LOAD	0.948533	0.948533
1	DE_CONSUMPTION	FR_CONSUMPTION	0.850321	0.850321
2	DE_SOLAR	FR_SOLAR	0.815540	0.815540
3	DE_WIND	FR_WIND	0.802614	0.802614
4	DE_CONSUMPTION	FR_RESIDUAL_LOAD	0.796443	0.796443
5	FR_NUCLEAR	FR_RESIDUAL_LOAD	0.778629	0.778629
6	FR_CONSUMPTION	FR_NUCLEAR	0.757543	0.757543
7	DE_COAL	DE_LIGNITE	0.745513	0.745513
8	FR_GAS	FR_RESIDUAL_LOAD	0.720014	0.720014
9	FR_CONSUMPTION	FR_GAS	0.708716	0.708716
10	DE_COAL	DE_RESIDUAL_LOAD	0.691176	0.691176
11	FR_CONSUMPTION	DE_SOLAR	0.690325	-0.690325
12	DE_LIGNITE	DE_RESIDUAL_LOAD	0.689595	0.689595
13	DE_GAS	DE_RESIDUAL_LOAD	0.687199	0.687199
14	FR_CONSUMPTION	FR_SOLAR	0.683123	-0.683123
15	DE_NET_EXPORT	DE_WINDPOW	0.682868	0.682868
16	DE_TEMP	FR_TEMP	0.667540	0.667540
17	DE_CONSUMPTION	FR_NUCLEAR	0.662555	0.662555
18	DE_CONSUMPTION	DE_SOLAR	0.657111	-0.657111
19	FR_SOLAR	FR_RESIDUAL_LOAD	0.655051	-0.655051

4. Creating Features

4.1 Add residual columns according to high correlations

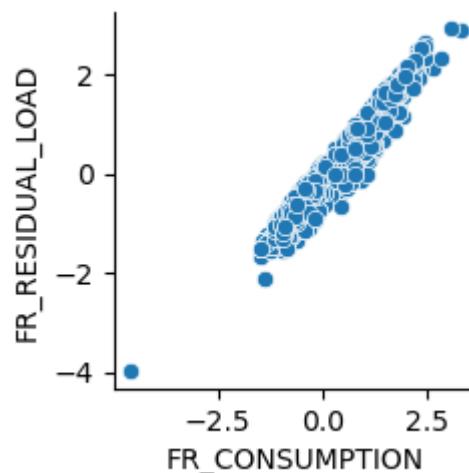
```
In [23]: df_sorted_corr = pd.DataFrame(pairs_sorted, columns=["feat1", "feat2", "|r|", "r"])
df_top_corr = df_sorted_corr[df_sorted_corr["|r|"] > corr_threshold]
df_top_corr
```

```
Out[23]:
```

	feat1	feat2	r	r
0	FR_CONSUMPTION	FR_RESIDUAL_LOAD	0.948533	0.948533

```
In [24]: plt.clf()
plt.figure()
for idx, data in df_top_corr.iterrows():
    sns.pairplot(data=X_train_test_filled, x_vars=data.feat1, y_vars=data.feat2)
plt.show()
```

```
<Figure size 640x480 with 0 Axes>
<Figure size 640x480 with 0 Axes>
```



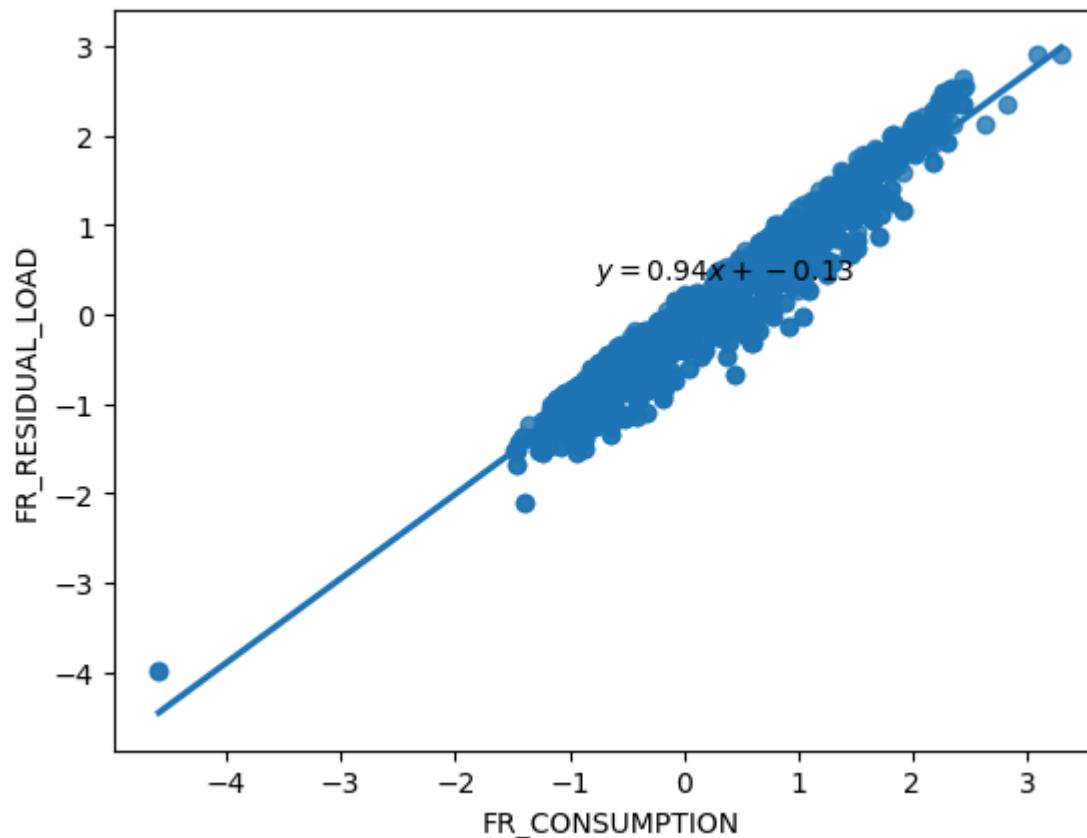
```
In [25]: x_feature = df_top_corr.feat1.values[0]
y_feature = df_top_corr.feat2.values[0]

p = sns.regplot(x=x_feature, y=y_feature, data=X_train_test_filled)
```

```
#calculate slope and intercept of regression equation
slope, intercept, r, p, sterr = scipy.stats.linregress(x=p.get_lines()[0].get_xdata(),
                                                       y=p.get_lines()[0].get_ydata())

#add regression equation to plot
result_string = f"$y = {slope:.2f}x + {intercept:.2f}$"

plt.figtext(0.5, 0.6, result_string)
plt.show()
```



```
In [26]: drop_features.append(y_feature)
if KeepOrigNumFeatures:
    drop_features = [x for x in drop_features if x not in orig_num_cols]
```

```
X_trte_engineered = X_train_test_filled.copy()
X_trte_engineered['RES_' + y_feature] = X_trte_engineered[y_feature] - (slope * X_trte_engineered[y_feature] + intercept)
```

4.2 Create features with golden combination characteristic

```
In [27]: # create gold characteristics
for f in (de_features + fr_features + eu_features):
    if UseTimeSeries:
        f_mean_de = X_trte_engineered.loc[X_trte_engineered['COUNTRY'] == 'DE', f].mean()
        f_mean_fr = X_trte_engineered.loc[X_trte_engineered['COUNTRY'] == 'FR', f].mean()
        f_std_de = X_trte_engineered.loc[X_trte_engineered['COUNTRY'] == 'DE', f].std()
        f_std_fr = X_trte_engineered.loc[X_trte_engineered['COUNTRY'] == 'FR', f].std()
    else:
        df_temp = X_train[['ID']].merge(X_trte_engineered, on='ID', how='left')
        f_mean_de = df_temp.loc[df_temp['COUNTRY'] == 'DE', f].mean()
        f_mean_fr = df_temp.loc[df_temp['COUNTRY'] == 'FR', f].mean()
        f_std_de = df_temp.loc[df_temp['COUNTRY'] == 'DE', f].std()
        f_std_fr = df_temp.loc[df_temp['COUNTRY'] == 'FR', f].std()

    X_trte_engineered['GOLD_' + f] = X_trte_engineered.apply(lambda row: (row[f] - f_mean_de) / f_std_de if row.COUNTRY == 'DE' else (row[f] - f_mean_fr) / f_std_fr)
```

4.3 Create features regarding target encoding

Group sum with target correlations as coefficient. There are five groups that need to be considered. They are EU commodity price variations, weather measures, electricity use metrics, renewable energy measures and non-renewable energy measures.

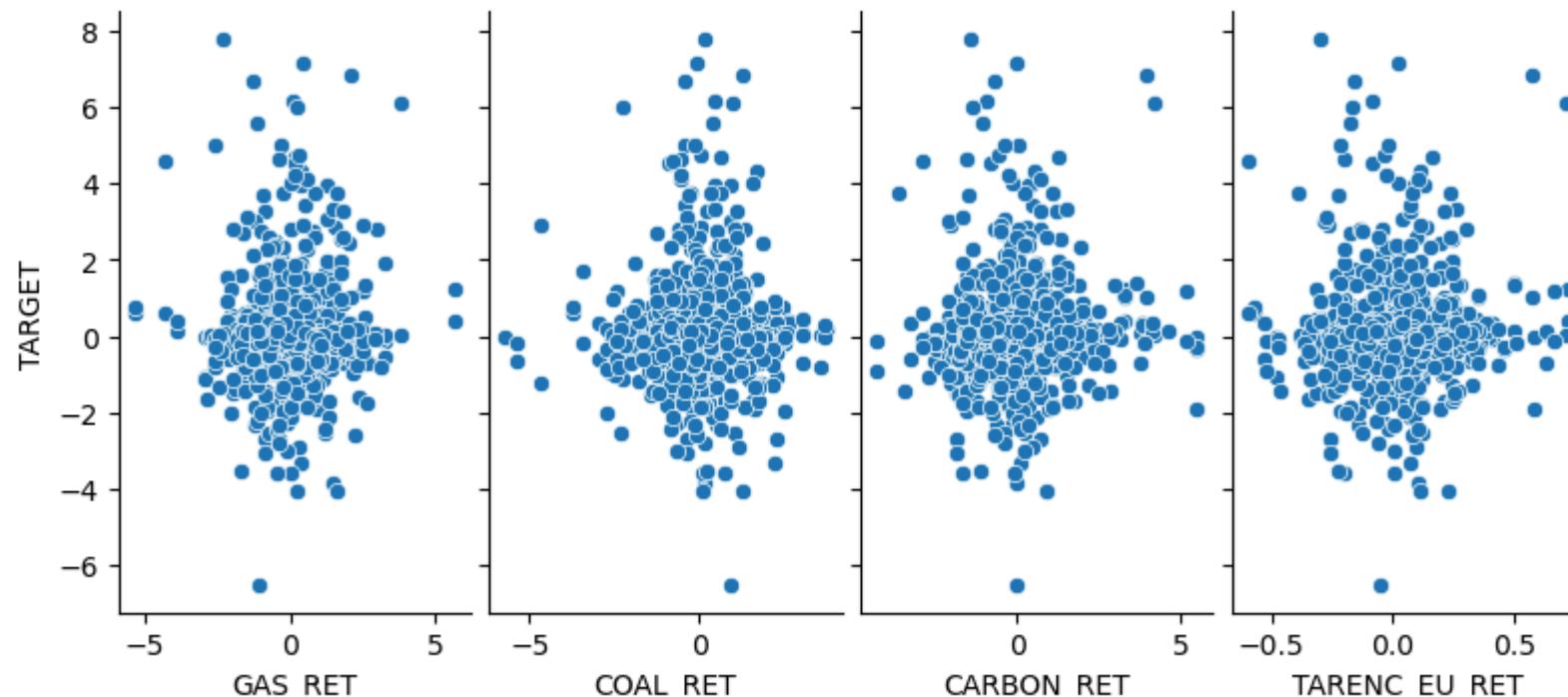
4.3.1 Target encoding on EU commodity price variations

```
In [28]: # target encoding
X_trte_engineered['TARENC_EU_RET'] = 0.0
for f in eu_features:
    X_trte_engineered['TARENC_EU_RET'] += target_corr[f] * X_trte_engineered[f]
```

```
In [29]: # plot features regarding EU commodity price variations
Xy_tr_teengineered = pd.merge(X_trte_engineered, y_train, on='ID', how='right')
display(X_trte_engineered.shape)
display(Xy_tr_teengineered.shape)
```

```
plt.clf()
diag = sns.pairplot(data=Xy_tr_engineered, x_vars=eu_features+[ 'TARENC_EU_RET'], y_vars='TARGET')
diag.fig.set_size_inches(8, 4)
diag.set(xlim=(None, None))
plt.show()
```

(2148, 66)
(1494, 67)
<Figure size 640x480 with 0 Axes>



4.3.2 Target encoding on weather measures

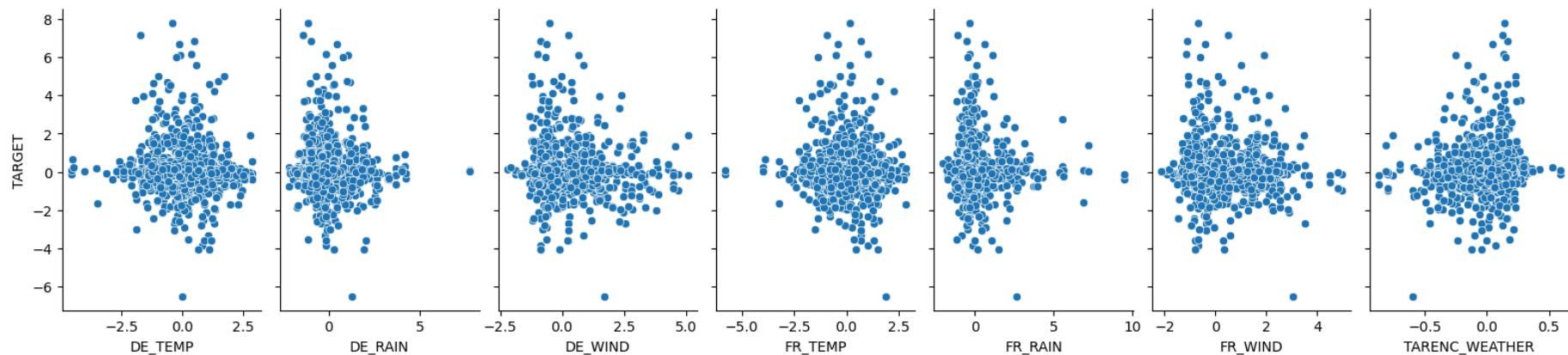
In [30]:

```
# target encoding
X_trte_engineered[ 'TARENC_WEATHER' ] = 0.0
for f in weather_features:
    X_trte_engineered[ 'TARENC_WEATHER' ] += target_corr[f] * X_trte_engineered[f]
```

```
In [31]: # plot features regarding weather measures
Xy_tr_engineered = pd.merge(X_trte_engineered, y_train, on='ID', how='right')
display(X_trte_engineered.shape)
display(Xy_tr_engineered.shape)

plt.clf()
diag = sns.pairplot(data=Xy_tr_engineered, x_vars=weather_features+['TARENC_WEATHER'], y_vars='TARGET')
diag.fig.set_size_inches(16, 4)
diag.set(xlim=(None, None))
plt.show()
```

(2148, 67)
(1494, 68)
<Figure size 640x480 with 0 Axes>



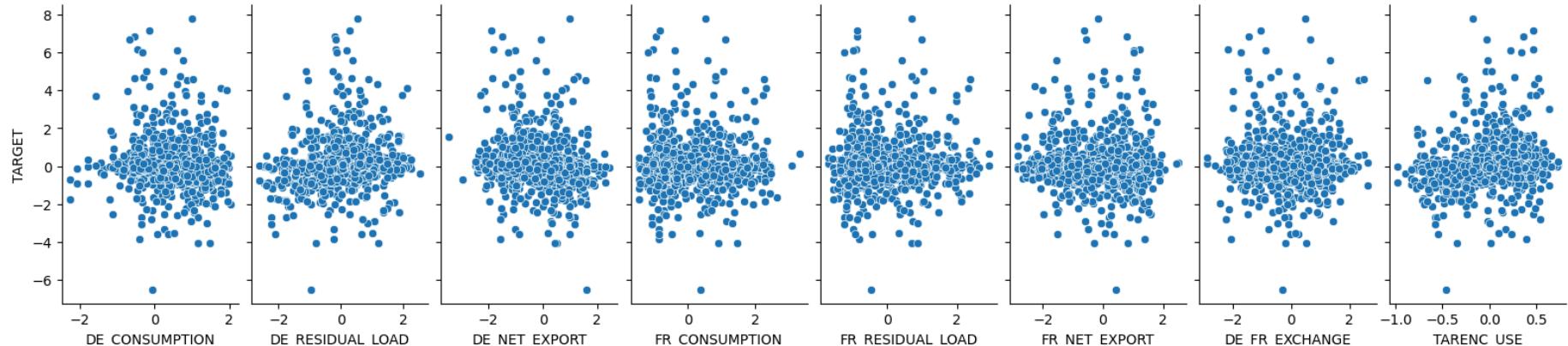
4.3.3 Target encoding on electricity use metrics

```
In [32]: # target encoding
X_trte_engineered['TARENC_USE'] = 0.0
for f in use_features:
    X_trte_engineered['TARENC_USE'] += target_corr[f] * X_trte_engineered[f]
```

```
In [33]: # plot features regarding electricity use metrics
Xy_tr_engineered = pd.merge(X_trte_engineered, y_train, on='ID', how='right')
display(X_trte_engineered.shape)
display(Xy_tr_engineered.shape)
```

```
plt.clf()
diag = sns.pairplot(data=Xy_tr_engineered, x_vars=use_features+['TARENC_USE'], y_vars='TARGET')
diag.fig.set_size_inches(16, 4)
diag.set(xlim=(None, None))
plt.show()
```

(2148, 68)
(1494, 69)
<Figure size 640x480 with 0 Axes>



4.3.4 Target encoding on renewable energy measures

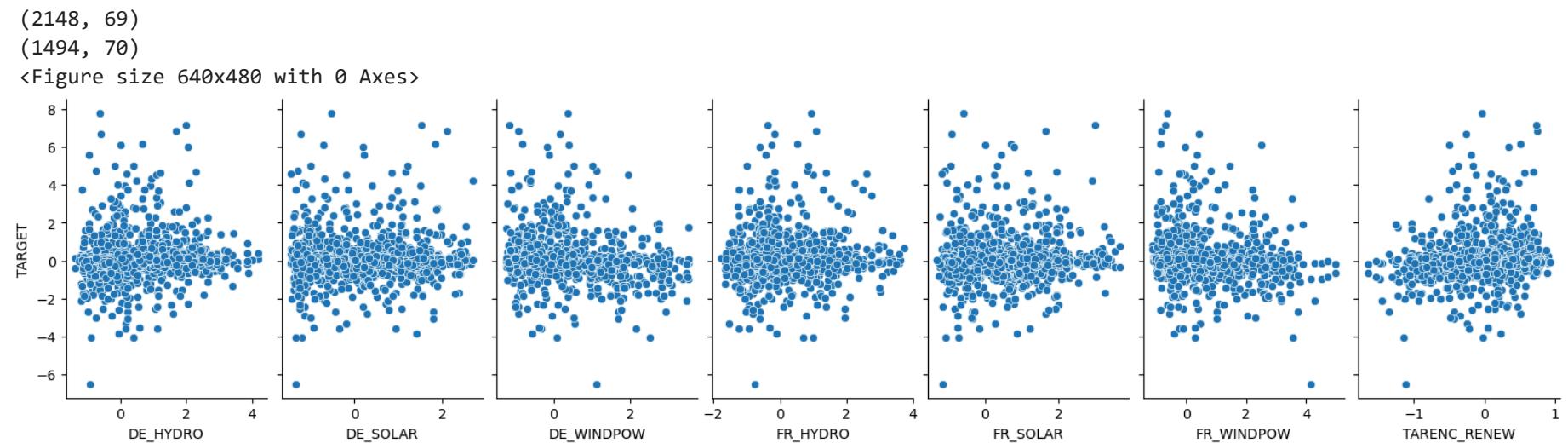
In [34]:

```
# target encoding
X_trte_engineered['TARENC_RENEW'] = 0.0
for f in renew_features:
    X_trte_engineered['TARENC_RENEW'] += target_corr[f] * X_trte_engineered[f]
```

In [35]:

```
# plot features regarding renewable energy measures
Xy_tr_engineered = pd.merge(X_trte_engineered, y_train, on='ID', how='right')
display(X_trte_engineered.shape)
display(Xy_tr_engineered.shape)

plt.clf()
diag = sns.pairplot(data=Xy_tr_engineered, x_vars=renew_features+['TARENC_RENEW'], y_vars='TARGET')
diag.fig.set_size_inches(16, 4)
diag.set(xlim=(None, None))
plt.show()
```



4.3.5 Target encoding on non-renewable energy measures

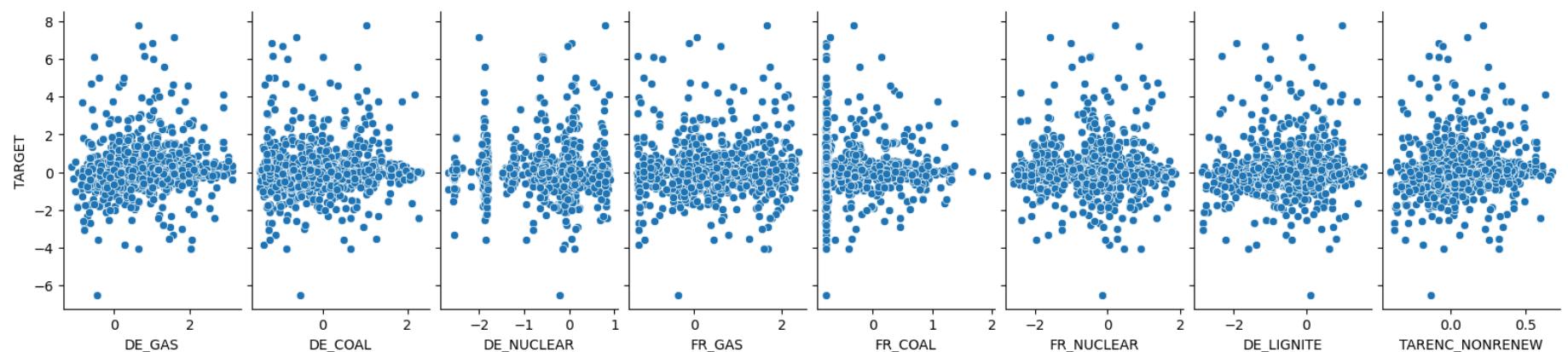
```
In [36]: # target encoding
X_trte_engineered['TARENC_NONRENEW'] = 0.0
for f in nonrenew_features:
    X_trte_engineered['TARENC_NONRENEW'] += target_corr[f] * X_trte_engineered[f]
```

```
In [37]: # plot features regarding non-renewable energy measures
Xy_tr_engineered = pd.merge(X_trte_engineered, y_train, on='ID', how='right')
display(X_trte_engineered.shape)
display(Xy_tr_engineered.shape)

plt.clf()
diag = sns.pairplot(data=Xy_tr_engineered, x_vars=nonrenew_features+[ 'TARENC_NONRENEW'], y_vars='TARGET')
diag.fig.set_size_inches(16, 4)
diag.set(xlim=(None, None))
plt.show()
```

(2148, 70)
(1494, 71)
<Figure size 640x480 with 0 Axes>

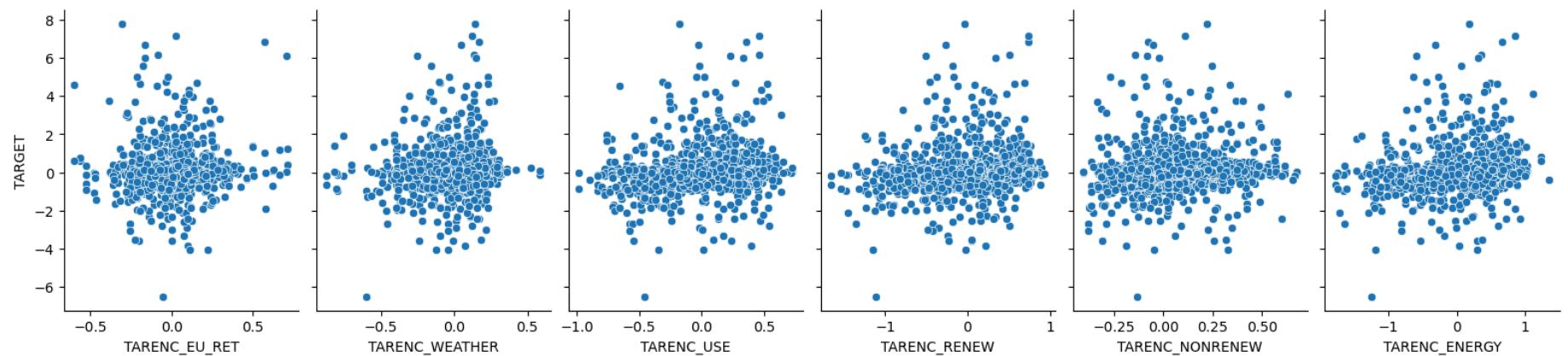
feature_engineering



```
In [38]: # plot all target encoding features
X_trte_engineered['TARENC_ENERGY'] = X_trte_engineered['TARENC_RENEW'] + X_trte_engineered['TARENC_NONRENEW']
Xy_tr_engineered = pd.merge(X_trte_engineered, y_train, on='ID', how='right')
display(Xy_tr_engineered.shape)
display(Xy_tr_engineered.shape)
target_encoding_list = [x for x in X_trte_engineered if 'TARENC_' in x]

plt.clf()
diag = sns.pairplot(data=Xy_tr_engineered, x_vars=target_encoding_list, y_vars='TARGET')
diag.fig.set_size_inches(16, 4)
diag.set(xlim=(None, None))
plt.show()

(2148, 71)
(1494, 72)
<Figure size 640x480 with 0 Axes>
```



4.4 Add features based on 7-day-rolling

```
In [39]: # check rolling duplicates
if UseTimeSeries:
    df_rolling = X_train_test_filled[num_cols[:-1]].copy()
    df_rolling.sort_values("DAY_ID", inplace=True)
    df_rolling.drop_duplicates(inplace=True)
    df_rolling[df_rolling.duplicated(subset=['DAY_ID'], keep=False)]
```

```
In [40]: # carry out 7-day-rolling
if UseTimeSeries:
    for fea in num_cols[1:-1]:
        if fea in df_rolling.columns:
            df_rolling[f"ROLL_{fea}"] = df_rolling[fea].rolling(7, min_periods=1).mean()
            df_rolling.drop(fea, axis=1, inplace=True)

    X_trte_engineered = pd.merge(X_trte_engineered, df_rolling, on='DAY_ID', how='left')
```

4.5 Create polynomial features for DE and FR data

```
In [41]: # Split train and test data set by DE and FR
X_trte_engineered_de = X_trte_engineered[X_trte_engineered['COUNTRY'] == 'DE']
X_trte_engineered_de.sort_values("DAY_ID", inplace=True)
X_trte_engineered_fr = X_trte_engineered[X_trte_engineered['COUNTRY'] == 'FR']
```

```
X_trte_engineered_fr.sort_values("DAY_ID", inplace=True)

y_train_de = Xy_tr_engineered.loc[Xy_tr_engineered['COUNTRY'] == 'DE', ['ID', 'TARGET']]
y_train_fr = Xy_tr_engineered.loc[Xy_tr_engineered['COUNTRY'] == 'FR', ['ID', 'TARGET']]
```

In [42]:

```
# polynomial features combined on DE and FR features
for fea in country_features:
    de = f"DE_{fea}"; fr = f"FR_{fea}"

    if de in X_trte_engineered_de.columns and fr in X_trte_engineered_de.columns:
        X_trte_engineered_de[f"DIFF_{fea}"] = X_trte_engineered_de[de] - X_trte_engineered_de[fr]
        X_trte_engineered_de[f"SUM_{fea}"] = X_trte_engineered_de[de] + X_trte_engineered_de[fr]

    if de in X_trte_engineered_fr.columns and fr in X_trte_engineered_fr.columns:
        X_trte_engineered_fr[f"DIFF_{fea}"] = X_trte_engineered_fr[fr] - X_trte_engineered_fr[de]
        X_trte_engineered_fr[f"SUM_{fea}"] = X_trte_engineered_fr[de] + X_trte_engineered_fr[fr]
```

In [43]:

```
# results obtained by merging DE and FR feature/target data and drop the
X_trte_finished = pd.concat([X_trte_engineered_de, X_trte_engineered_fr], ignore_index=True).drop('COUNTRY', axis=1, inplace=False)

to_drop = [x for x in drop_features if x in X_trte_finished.columns]
if all(item in X_trte_finished.columns for item in to_drop):
    X_trte_finished.drop(to_drop, axis=1, inplace=True)

Xy_tr_finished = pd.merge(X_trte_finished, y_train, on='ID', how='right')
```

5. Feature selection

5.1 Remove features with low mutual info and high target correlation

In [44]:

```
# mutual information ranking (top-k)
mi = mutual_info_regression(Xy_tr_finished.drop('TARGET', axis=1), Xy_tr_finished['TARGET'], random_state=RANDOM_STATE)
mi_series = pd.Series(mi, index=Xy_tr_finished.columns[:-1]).sort_values(ascending=False)
df_mi = mi_series.to_frame('MI')
df_mi_zero = df_mi[df_mi.MI <= 0.0]
display(df_mi_zero)
```

MI	
DE_NET_EXPORT	0.0
FR_RESIDUAL_LOAD	0.0
DE_FR_EXCHANGE	0.0
GOLD_FR_RESIDUAL_LOAD	0.0
GOLD_FR_HYDRO	0.0
GOLD_FR_WIND	0.0
GOLD_DE_NET_EXPORT	0.0
GOLD_FR_COAL	0.0
GOLD_DE_COAL	0.0
RES_FR_RESIDUAL_LOAD	0.0
COAL_RET	0.0
GOLD_FR_NUCLEAR	0.0
GOLD_FR_WINDPOW	0.0
DIFF_RAIN	0.0
GOLD_COAL_RET	0.0
SUM_SOLAR	0.0
SUM_COAL	0.0

In [45]:

```
# high target correlations
assert "TARGET" in Xy_tr_finished.columns, "TARGET missing after merge"
target_corr = np.abs(Xy_tr_finished.corr(method=parameters['corr_method'])["TARGET"].drop("TARGET")).sort_values(ascending=False)
df_target_corr = target_corr.to_frame()
df_low_corr = df_target_corr[df_target_corr.TARGET <= target_corr_threshold]
display(df_low_corr)
```

TARGET
GOLD_DE_NUCLEAR 0.009531
DIFF_TEMP 0.009030
DE_NUCLEAR 0.007052
SUM_NUCLEAR 0.006183
DAY_ID 0.003901
FR_NUCLEAR 0.003619
GOLD_FR_NET_EXPORT 0.002950
FR_NET_EXPORT 0.002212
GOLD_FR_NUCLEAR 0.001109

```
In [46]: # determine drop list according to low mutual info and high target correlation
mi_zero_or_low_corr = list(set(df_low_corr.index).union(set(df_mi_zero.index)))
display(mi_zero_or_low_corr)
```

```
[ 'RES_FR_RESIDUAL_LOAD',
  'GOLD_FR_NET_EXPORT',
  'DE_NUCLEAR',
  'FR_RESIDUAL_LOAD',
  'GOLD_FR_WIND',
  'GOLD_FR_WINDPOW',
  'GOLD_COAL_RET',
  'GOLD_DE_NET_EXPORT',
  'SUM_COAL',
  'DIFF_RAIN',
  'DIFF_TEMP',
  'GOLD_DE_NUCLEAR',
  'GOLD_FR_COAL',
  'GOLD_DE_COAL',
  'GOLD_FR_RESIDUAL_LOAD',
  'SUM_NUCLEAR',
  'GOLD_FR_NUCLEAR',
  'FR_NET_EXPORT',
  'GOLD_FR_HYDRO',
  'DE_FR_EXCHANGE',
  'DAY_ID',
  'FR_NUCLEAR',
  'COAL_RET',
  'SUM_SOLAR',
  'DE_NET_EXPORT']
```

```
In [47]: # remove the selected features
drop_features += mi_zero_or_low_corr
if KeepOrigNumFeatures:
    drop_features = [x for x in drop_features if x not in orig_num_cols]

to_drop = [x for x in drop_features if x in X_trte_finished.columns]
if all(item in X_trte_finished.columns for item in to_drop):
    X_trte_finished.drop(to_drop, axis=1, inplace=True)

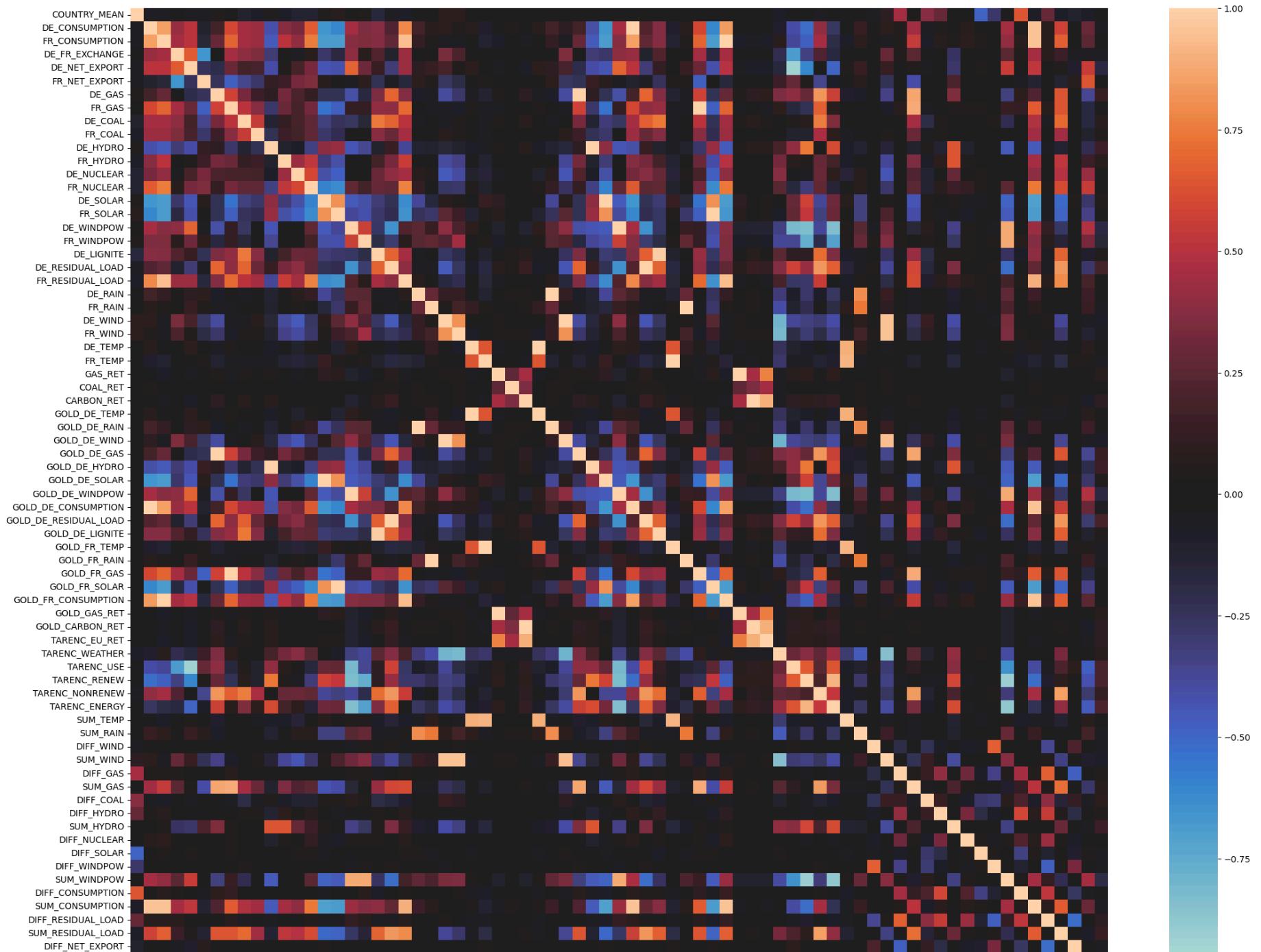
Xy_tr_finished = pd.merge(X_trte_finished, y_train, on='ID', how='right')
```

5.2 Processing selection of highly correlated features

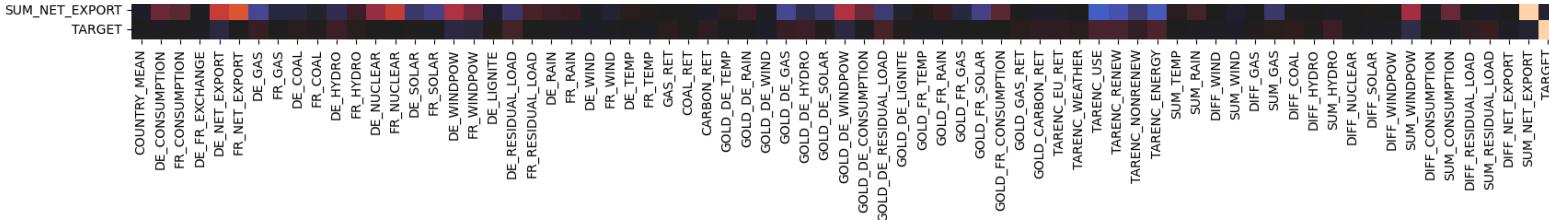
```
In [48]: # plot heatmap of train data with target after feature creating
if not UseTimeSeries:
    corr = Xy_tr_finished.drop('ID', axis=1).corr(method=parameters['corr_method'])
    print("Correlation matrix shape:", corr.shape)

    plt.figure(figsize=[25,20])
    sns.heatmap(corr, annot=False, vmin=-1, vmax=1, center=0)
    plt.show()
```

Correlation matrix shape: (73, 73)



feature_engineering



-1.00

In [49]: # plot heatmap of train and test data after feature creating

```
if UseTimeSeries:
    corr = X_trte_finished.drop('ID', axis=1).corr(method=parameters['corr_method'])
    print("Correlation matrix shape:", corr.shape)

    plt.figure(figsize=[25,20])
    sns.heatmap(corr, annot=False, vmin=-1, vmax=1, center=0)
    plt.show()
```

In [50]: # top correlated pairs by |r|

```
pairs = []
cols = corr.columns
for i in range(len(cols)):
    for j in range(i+1, len(cols)):
        r = corr.iloc[i, j]
        pairs.append((cols[i], cols[j], abs(r), r))
pairs_sorted = sorted(pairs, key=lambda x: x[2], reverse=True)[:60]
pd_pairs_corr = pd.DataFrame(pairs_sorted, columns=["feat1", "feat2", "|r|", "r"])
pd_pairs_high_corr = pd_pairs_corr[pd_pairs_corr['|r|'] >= corr_threshold]
display(pd_pairs_high_corr)
```

	feat1	feat2	r	r
0	DE_WINDPOW	GOLD_DE_WINDPOW	0.999968	0.999968
1	CARBON_RET	GOLD_CARBON_RET	0.999951	0.999951
2	DE_RAIN	GOLD_DE_RAIN	0.999950	0.999950
3	FR_TEMP	GOLD_FR_TEMP	0.999940	0.999940
4	FR_GAS	GOLD_FR_GAS	0.999828	0.999828
5	DE_TEMP	GOLD_DE_TEMP	0.999791	0.999791
6	GAS_RET	GOLD_GAS_RET	0.999723	0.999723
7	FR_RAIN	GOLD_FR_RAIN	0.999716	0.999716
8	DE_GAS	GOLD_DE_GAS	0.999359	0.999359
9	DE_SOLAR	GOLD_DE_SOLAR	0.998920	0.998920
10	DE_HYDRO	GOLD_DE_HYDRO	0.998081	0.998081
11	DE_CONSUMPTION	GOLD_DE_CONSUMPTION	0.997565	0.997565
12	FR_SOLAR	GOLD_FR_SOLAR	0.997557	0.997557
13	DE_RESIDUAL_LOAD	GOLD_DE_RESIDUAL_LOAD	0.997431	0.997431
14	FR_CONSUMPTION	GOLD_FR_CONSUMPTION	0.995941	0.995941
15	DE_WIND	GOLD_DE_WIND	0.993400	0.993400
16	DE_LIGNITE	GOLD_DE_LIGNITE	0.981081	0.981081
17	FR_CONSUMPTION	SUM_CONSUMPTION	0.959291	0.959291
18	GOLD_FR_CONSUMPTION	SUM_CONSUMPTION	0.955112	0.955112
19	DE_CONSUMPTION	SUM_CONSUMPTION	0.952950	0.952950
20	FR_WIND	SUM_WIND	0.951897	0.951897
21	GOLD_DE_CONSUMPTION	SUM_CONSUMPTION	0.950420	0.950420

	feat1	feat2	r	r
22	DE_WIND	SUM_WIND	0.946841	0.946841
23	FR_CONSUMPTION	FR_RESIDUAL_LOAD	0.941636	0.941636
24	GOLD_DE_WIND	SUM_WIND	0.939552	0.939552
25	FR_RESIDUAL_LOAD	GOLD_FR_CONSUMPTION	0.935795	0.935795
26	DE_NET_EXPORT	TARENC_USE	0.925902	-0.925902
27	TARENC_RENEW	TARENC_ENERGY	0.913896	0.913896
28	FR_TEMP	SUM_TEMP	0.906696	0.906696
29	GOLD_FR_TEMP	SUM_TEMP	0.906653	0.906653
30	TARENC_RENEW	SUM_WINDPOW	0.904811	-0.904811
31	FR_RESIDUAL_LOAD	SUM_CONSUMPTION	0.900091	0.900091

In [51]: `# determine drop list according to highly correlated features`
`drop_pairs = []`

```
for idx, data in pd_pairs_high_corr.iterrows():
    drop_fea = ''

    if (data.feat1 not in drop_pairs) and (data.feat2 not in drop_pairs):
        if (data.feat1 not in num_cols) and (data.feat2 in num_cols):
            drop_fea = data.feat1
        elif (data.feat1 in num_cols) and (data.feat2 not in num_cols):
            drop_fea = data.feat2
        elif (data.feat1 not in num_cols) and (data.feat2 not in num_cols):
            if target_corr[data.feat1] < target_corr[data.feat2]:
                drop_fea = data.feat1
            elif target_corr[data.feat1] > target_corr[data.feat2]:
                drop_fea = data.feat2
            elif mi_series[data.feat1] < mi_series[data.feat2]:
                drop_fea = data.feat1
            else:
                drop_fea = data.feat2
```

```
if dropfea != '':
    drop_pairs.append(dropfea)

display(drop_pairs)

['GOLD_DE_WINDPOW',
 'GOLD_CARBON_RET',
 'GOLD_DE_RAIN',
 'GOLD_FR_TEMP',
 'GOLD_FR_GAS',
 'GOLD_DE_TEMP',
 'GOLD_GAS_RET',
 'GOLD_FR_RAIN',
 'GOLD_DE_GAS',
 'GOLD_DE_SOLAR',
 'GOLD_DE_HYDRO',
 'GOLD_DE_CONSUMPTION',
 'GOLD_FR_SOLAR',
 'GOLD_DE_RESIDUAL_LOAD',
 'GOLD_FR_CONSUMPTION',
 'GOLD_DE_WIND',
 'GOLD_DE_LIGNITE',
 'SUM_CONSUMPTION',
 'SUM_WIND',
 'TARENC_USE',
 'TARENC_RENEW',
 'SUM_TEMP']
```

```
In [52]: # remove the selected features
drop_features += drop_pairs
if KeepOrigNumFeatures:
    drop_features = [x for x in drop_features if x not in orig_num_cols]

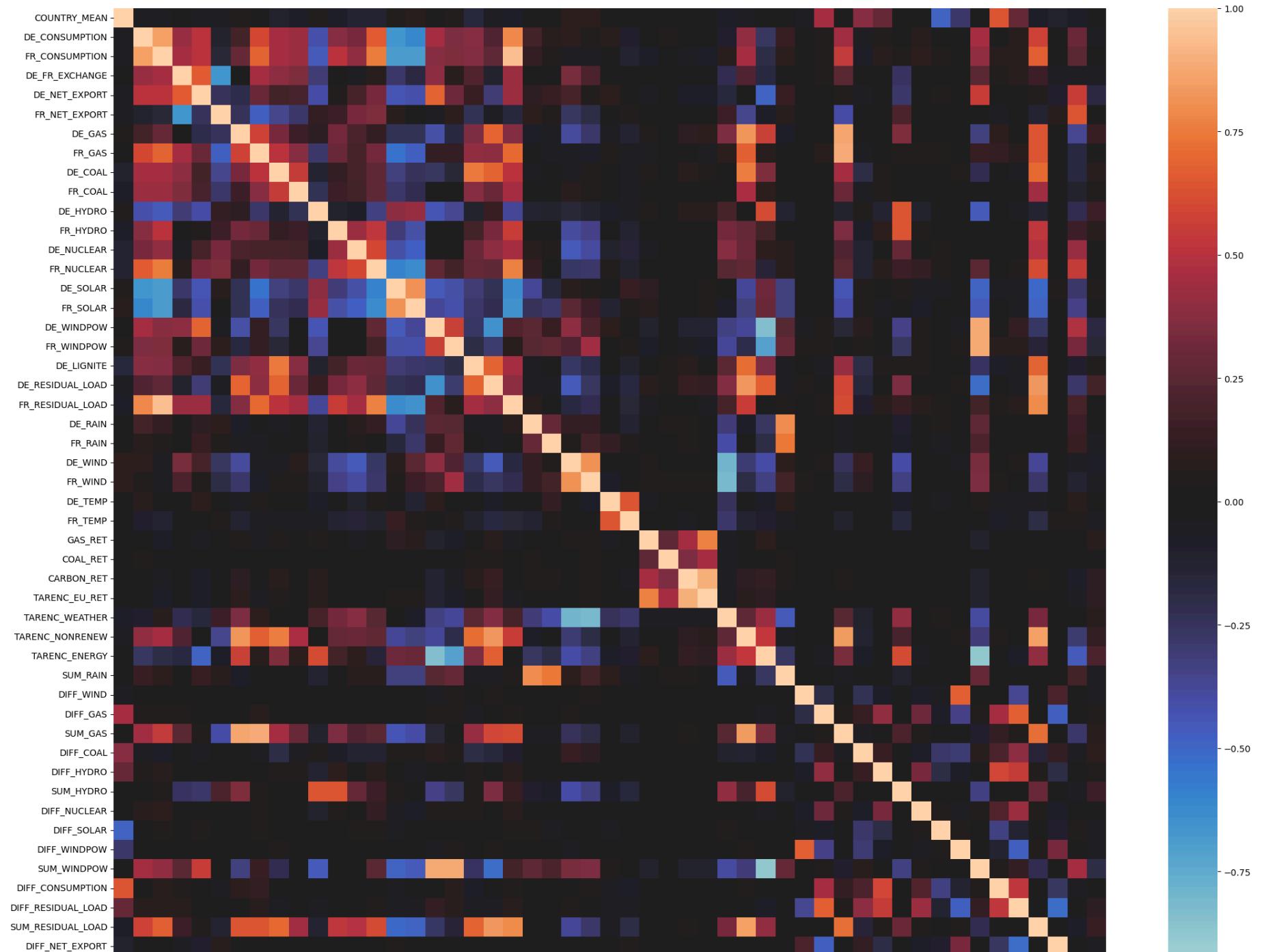
to_drop = [x for x in drop_features if x in X_trte_finished.columns]
if all(item in X_trte_finished.columns for item in to_drop):
    X_trte_finished.drop(to_drop, axis=1, inplace=True)

Xy_tr_finished = pd.merge(X_trte_finished, y_train, on='ID', how='right')
```

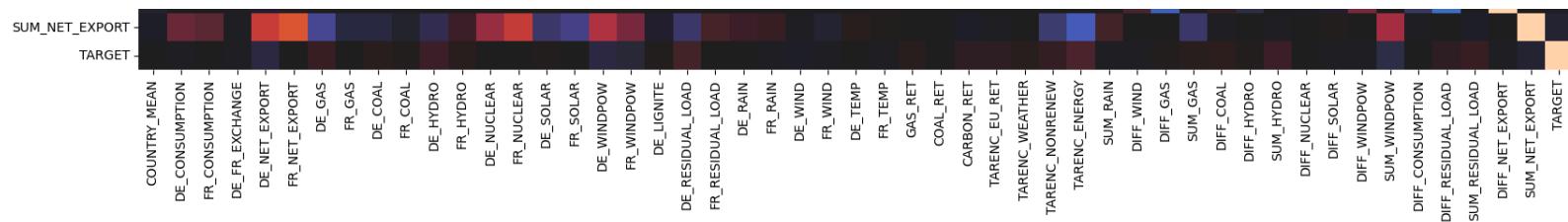
```
In [53]: # plot heatmap of train data with target
if not UseTimeSeries:
    corr = Xy_tr_finished.drop('ID', axis=1).corr(method=parameters['corr_method'])
    print("Correlation matrix shape:", corr.shape)

    plt.figure(figsize=[25,20])
    sns.heatmap(corr, annot=False, vmin=-1, vmax=1, center=0)
    plt.show()
```

Correlation matrix shape: (51, 51)



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In [54]: # plot heatmap of train and test data after feature creating

```
if UseTimeSeries:
    corr = X_trte_finished.drop('ID', axis=1).corr(method=parameters['corr_method'])
    print("Correlation matrix shape:", corr.shape)

    plt.figure(figsize=[25,20])
    sns.heatmap(corr, annot=False, vmin=-1, vmax=1, center=0)
    plt.show()
```

In [55]: # check if there are still highly correlated pairs

```
pairs = []
cols = corr.columns
for i in range(len(cols)):
    for j in range(i+1, len(cols)):
        r = corr.iloc[i, j]
        pairs.append((cols[i], cols[j], abs(r), r))
pairs_sorted = sorted(pairs, key=lambda x: x[2], reverse=True)[:60]
pd_pairs_corr = pd.DataFrame(pairs_sorted, columns=["feat1", "feat2", "|r|", "r"])
pd_pairs_high_corr = pd_pairs_corr[pd_pairs_corr['|r|'] >= corr_threshold]
print(f"there are {len(pd_pairs_high_corr)} highly correlated pairs.")
```

there are 1 highly correlated pairs.

5.3 Selection according to feature outliers

In [56]: # count the columns with a large number of missing and outlier values

```
c_outlier = column_missing_and_outliers(Xy_tr_finished)
drop_c_outlier = list(c_outlier.loc[(c_outlier.n_missing + c_outlier.n_outliers) > missing_outlier_c_threshold].index)
print(f"The number of columns with a large count of outlier values is {len(drop_c_outlier)}")
if 'TARGET' in drop_c_outlier:
    drop_c_outlier.remove('TARGET')
drop_columns += drop_c_outlier
```

```
drop_columns = list(set(drop_columns))
display(drop_columns)
```

The number of columns with a large count of outlier values is 1
['FR_COAL']

```
In [57]: # remove the columns with a large number of missing and outlier values
display((X_train.shape, X_test.shape, X_trte_finished.shape, Xy_tr_finished.shape))
drop_columns_large = [x for x in drop_columns if x in X_trte_finished.columns]
drop_columns_small = [x for x in drop_columns if x in X_train.columns]

if RemoveMissingOutlier and len(drop_columns_small) > 0:
    X_train = X_train.drop(drop_columns_small, axis=1)
    X_test = X_test.drop(drop_columns_small, axis=1)

if RemoveMissingOutlier and len(drop_columns_large) > 0:
    X_trte_finished = X_trte_finished.drop(drop_columns_large, axis=1)
    Xy_tr_finished = Xy_tr_finished.drop(drop_columns_large, axis=1)
    num_cols = [x for x in num_cols if x not in drop_columns]

display((X_train.shape, X_test.shape, X_trte_finished.shape, Xy_tr_finished.shape))

((1494, 35), (654, 32), (2148, 51), (1494, 52))
((1494, 35), (654, 32), (2148, 51), (1494, 52))
```

```
In [58]: # plot the outliers for each feature
plots = [(c, Xy_tr_finished[c]) for c in Xy_tr_finished.columns]

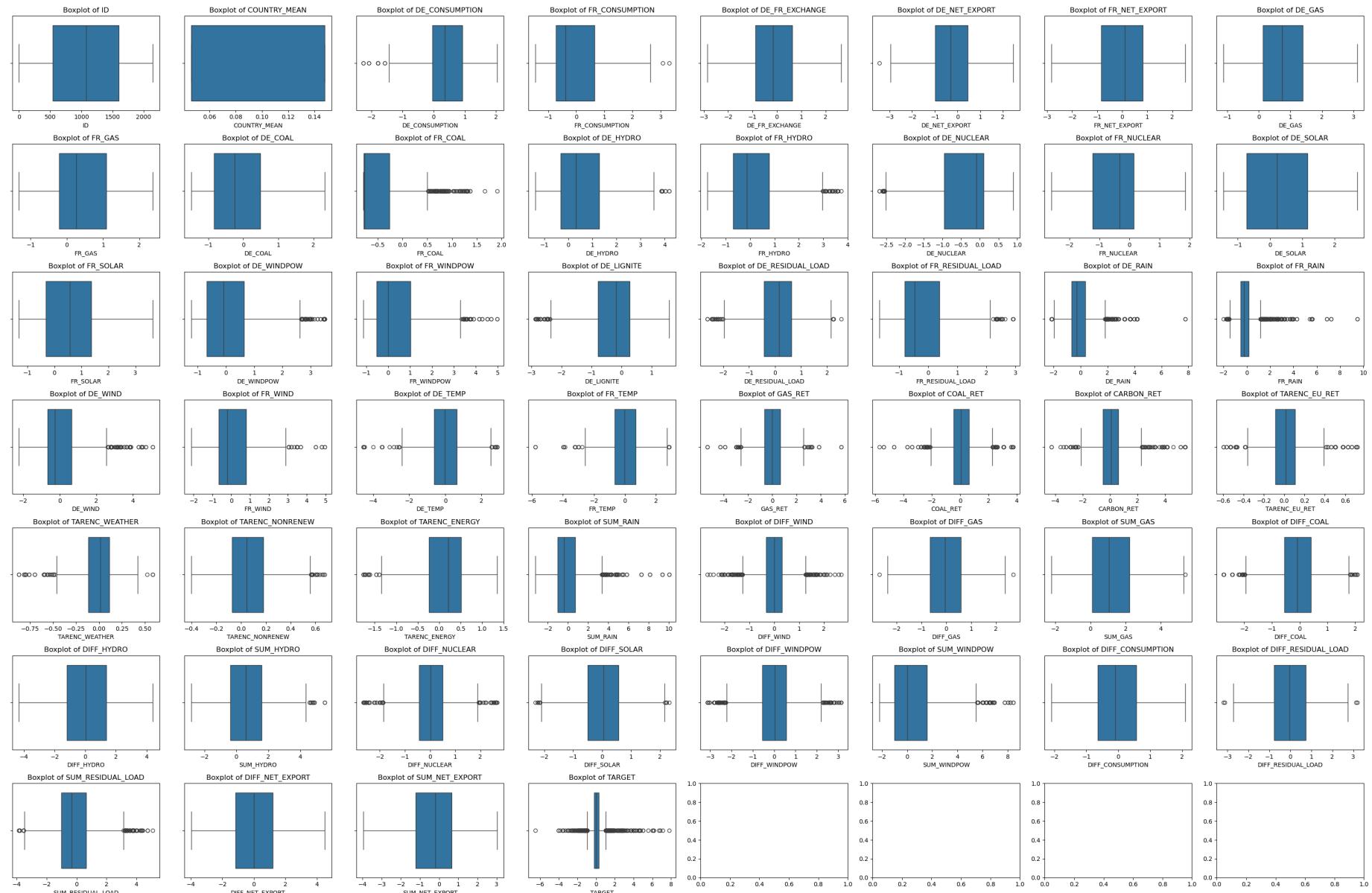
K = len(plots)
N = math.ceil(math.sqrt(K))
M = math.ceil(K / N)

fig, axes = plt.subplots(M, N, figsize=(N*4, M*3), squeeze=False)
axes = axes.ravel()

for i, (name, s) in enumerate(plots):
    sns.boxplot(x=s, ax=axes[i])
    axes[i].set_title(f"Boxplot of {name}")

plt.tight_layout()
plt.show()
```

feature_engineering



5.4 Future selection with null importance

Feature selection process using target permutation tests actual importance significance against the distribution of feature importances when fitted to noise.

```
In [59]: # create scoring function
def get_feature_importances(data, shuffle, seed=None):
    # Gather real features
    train_features = [f for f in data if f not in ['TARGET']]
    # Go over fold and keep track of CV score (train and valid) and feature importances

    # Shuffle target if required
    y = data['TARGET'].copy()
    if shuffle:
        # Here you could as well use a binomial distribution
        y = data['TARGET'].copy().sample(frac=1.0)

        # Fit LightGBM in RF mode, yes it's quicker than sklearn RandomForest
    dtrain = lgb.Dataset(data[train_features], y, free_raw_data=False)
    lgb_params = {
        'objective': 'binary',
        'boosting_type': 'rf',
        'subsample': 0.623,
        'colsample_bytree': 0.7,
        'num_leaves': 127,
        'max_depth': 8,
        'seed': seed,
        'bagging_freq': 1,
        'verbose': -1,
        'n_jobs': 4
    }

    # Fit the model
    clf = lgb.train(params=lgb_params, train_set=dtrain, num_boost_round=200)

    # Get feature importances
    imp_df = pd.DataFrame()
    imp_df["feature"] = list(train_features)
    imp_df["importance_gain"] = clf.feature_importance(importance_type='gain')
    imp_df["importance_split"] = clf.feature_importance(importance_type='split')
    imp_df['trn_score'] = mean_squared_error(y, clf.predict(data[train_features]))
```

```
    return imp_df
```

```
In [60]: # build the benchmark for feature importance
data = Xy_tr_finished
actual_imp_df = get_feature_importances(data=data, shuffle=False)

null_imp_df = pd.DataFrame()
nb_runs = 80
for i in range(nb_runs):
    # Get current run importances
    imp_df = get_feature_importances(data=data, shuffle=True)
    # Concat the latest importances with the old ones
    null_imp_df = pd.concat([null_imp_df, imp_df], axis=0)
```

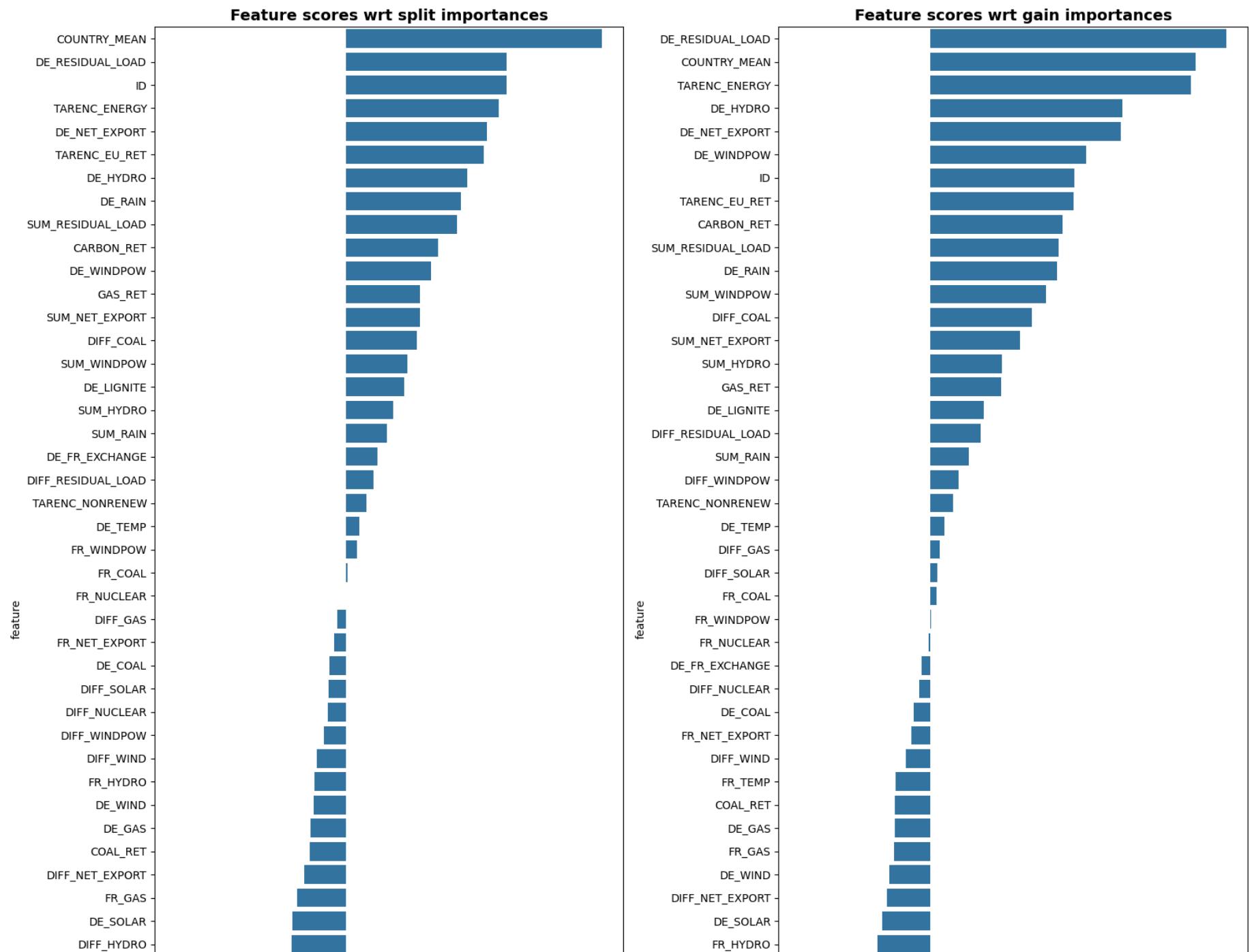
```
In [61]: # compute importance scores
feature_scores = []

for _f in actual_imp_df['feature'].unique():
    f_null_imps_gain = null_imp_df.loc[null_imp_df['feature'] == _f, 'importance_gain'].values
    f_act_imps_gain = actual_imp_df.loc[actual_imp_df['feature'] == _f, 'importance_gain'].mean()
    gain_score = np.log(1e-10 + f_act_imps_gain / (1 + np.percentile(f_null_imps_gain, 75))) # Avoid didvide by zero
    f_null_imps_split = null_imp_df.loc[null_imp_df['feature'] == _f, 'importance_split'].values
    f_act_imps_split = actual_imp_df.loc[actual_imp_df['feature'] == _f, 'importance_split'].mean()
    split_score = np.log(1e-10 + f_act_imps_split / (1 + np.percentile(f_null_imps_split, 75))) # Avoid didvide by zero
    feature_scores.append((_f, split_score, gain_score))

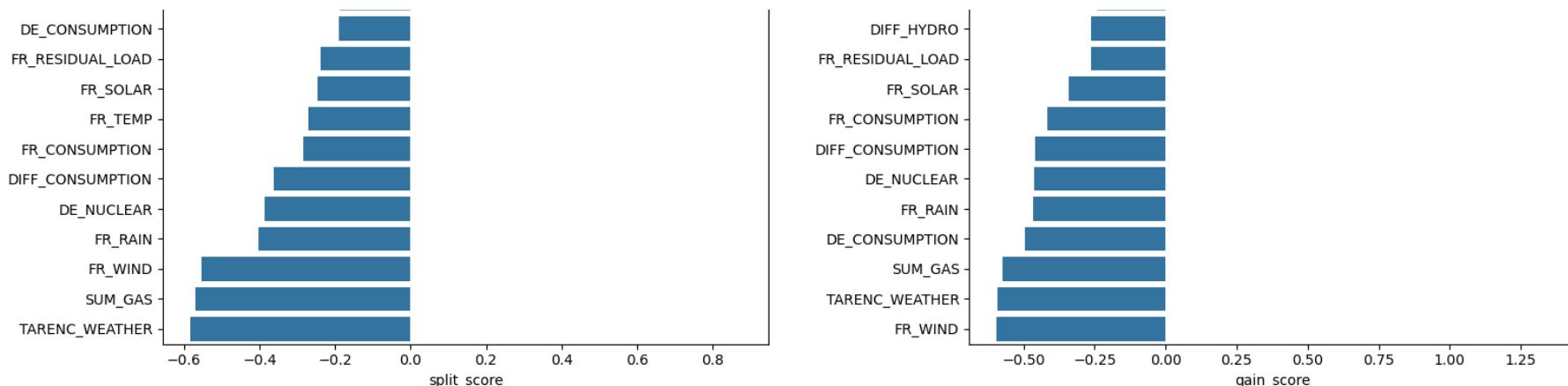
scores_df = pd.DataFrame(feature_scores, columns=['feature', 'split_score', 'gain_score'])
scores_df = scores_df.sort_values('split_score', ascending=False)
```

```
In [62]: # plot null importances distribution
plt.figure(figsize=(16, 16))
gs = gridspec.GridSpec(1, 2)
# Plot Split importances
ax = plt.subplot(gs[0, 0])
sns.barplot(x='split_score', y='feature', data=scores_df.sort_values('split_score', ascending=False).iloc[0:70], ax=ax)
ax.set_title('Feature scores wrt split importances', fontweight='bold', fontsize=14)
# Plot Gain importances
ax = plt.subplot(gs[0, 1])
sns.barplot(x='gain_score', y='feature', data=scores_df.sort_values('gain_score', ascending=False).iloc[0:70], ax=ax)
```

```
ax.set_title('Feature scores wrt gain importances', fontweight='bold', fontsize=14)
plt.tight_layout()
```



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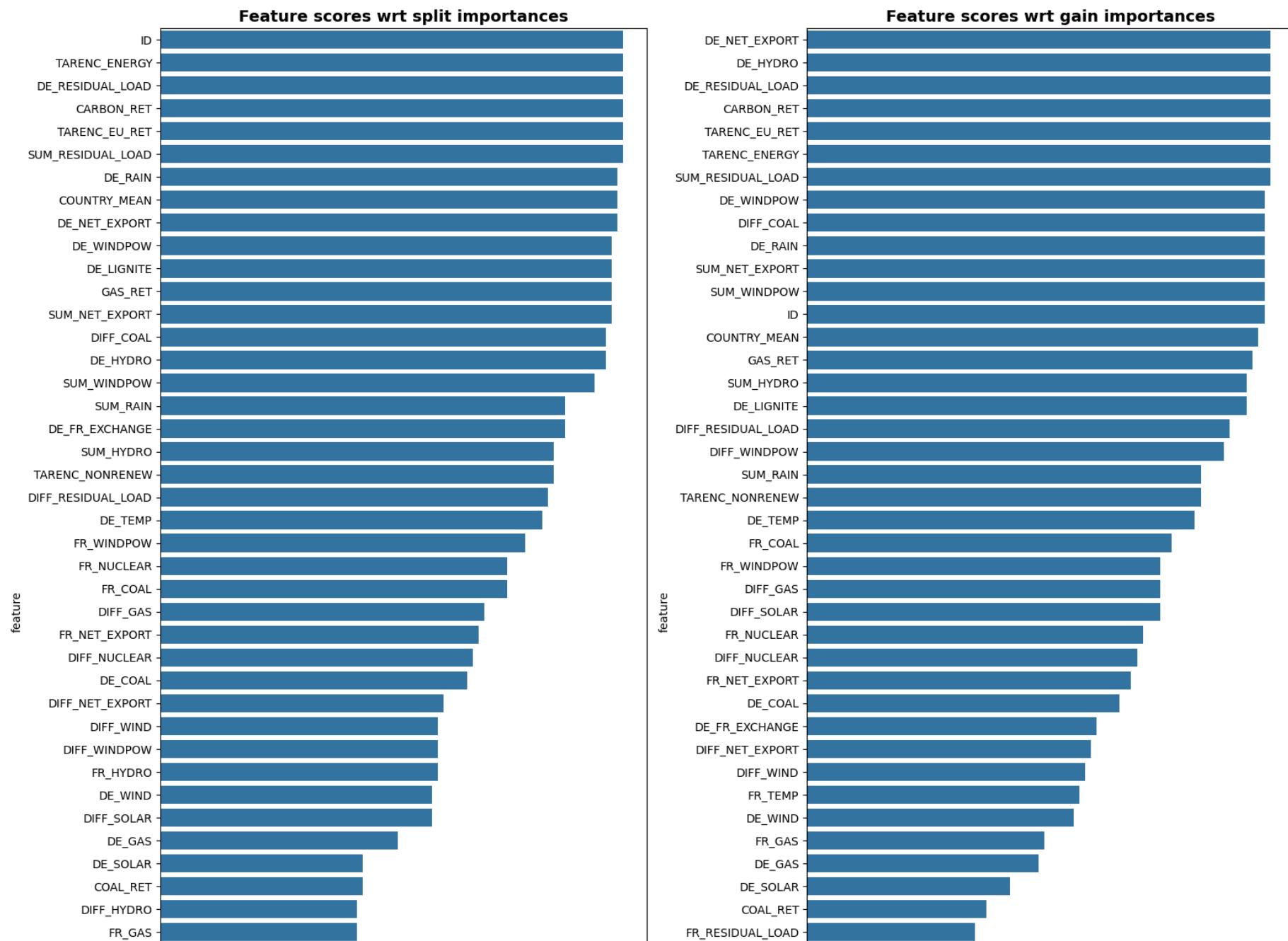


```
In [63]: # compute correlation scores
correlation_scores = []
for _f in actual_imp_df['feature'].unique():
    f_null_imps = null_imp_df.loc[null_imp_df['feature'] == _f, 'importance_gain'].values
    f_act_imps = actual_imp_df.loc[actual_imp_df['feature'] == _f, 'importance_gain'].values
    gain_score = 100 * (f_null_imps < np.percentile(f_act_imps, 25)).sum() / f_null_imps.size
    f_null_imps = null_imp_df.loc[null_imp_df['feature'] == _f, 'importance_split'].values
    f_act_imps = actual_imp_df.loc[actual_imp_df['feature'] == _f, 'importance_split'].values
    split_score = 100 * (f_null_imps < np.percentile(f_act_imps, 25)).sum() / f_null_imps.size
    correlation_scores.append((_f, split_score, gain_score))

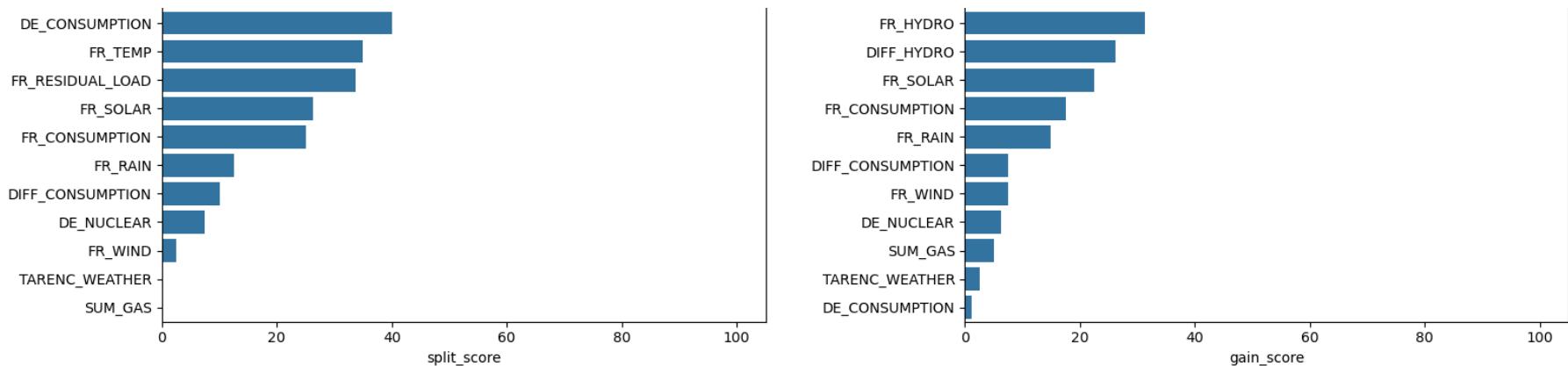
corr_scores_df = pd.DataFrame(correlation_scores, columns=['feature', 'split_score', 'gain_score'])
```

```
In [64]: # plot features' split and gain scores
fig = plt.figure(figsize=(16, 16))
gs = gridspec.GridSpec(1, 2)
# Plot Split importances
ax = plt.subplot(gs[0, 0])
sns.barplot(x='split_score', y='feature', data=corr_scores_df.sort_values('split_score', ascending=False).iloc[0:70], ax=ax)
ax.set_title('Feature scores wrt split importances', fontweight='bold', fontsize=14)
# Plot Gain importances
ax = plt.subplot(gs[0, 1])
sns.barplot(x='gain_score', y='feature', data=corr_scores_df.sort_values('gain_score', ascending=False).iloc[0:70], ax=ax)
ax.set_title('Feature scores wrt gain importances', fontweight='bold', fontsize=14)
plt.tight_layout()
```

```
plt.suptitle("Features' split and gain scores", fontweight='bold', fontsize=16)
fig.subplots_adjust(top=0.93)
```

Features' split and gain scores

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```
In [65]: # determine the drop list based on null importance
split_feats = [_f for _f, _, _score in correlation_scores if _score >= null_importance_threshold]
gain_feats = [_f for _, _, _score in correlation_scores if _score >= null_importance_threshold]
drop_null_importance = [x for x in split_feats if x in gain_feats]
display(drop_null_importance)
```

```
['ID',
 'COUNTRY_MEAN',
 'DE_NET_EXPORT',
 'DE_HYDRO',
 'DE_WINDPOW',
 'DE_LIGNITE',
 'DE_RESIDUAL_LOAD',
 'DE_RAIN',
 'GAS_RET',
 'CARBON_RET',
 'TARENC_EU_RET',
 'TARENC_ENERGY',
 'DIFF_COAL',
 'SUM_WINDPOW',
 'SUM_RESIDUAL_LOAD',
 'SUM_NET_EXPORT']
```

```
In [66]: # remove selected fea
drop_features += drop_null_importance[1:]
if KeepOrigNumFeatures:
    drop_features = [x for x in drop_features if x not in orig_num_cols]
```

```
to_drop = [x for x in drop_features if x in X_trte_finished.columns]
if all(item in X_trte_finished.columns for item in to_drop):
    X_trte_finished.drop(to_drop, axis=1, inplace=True)

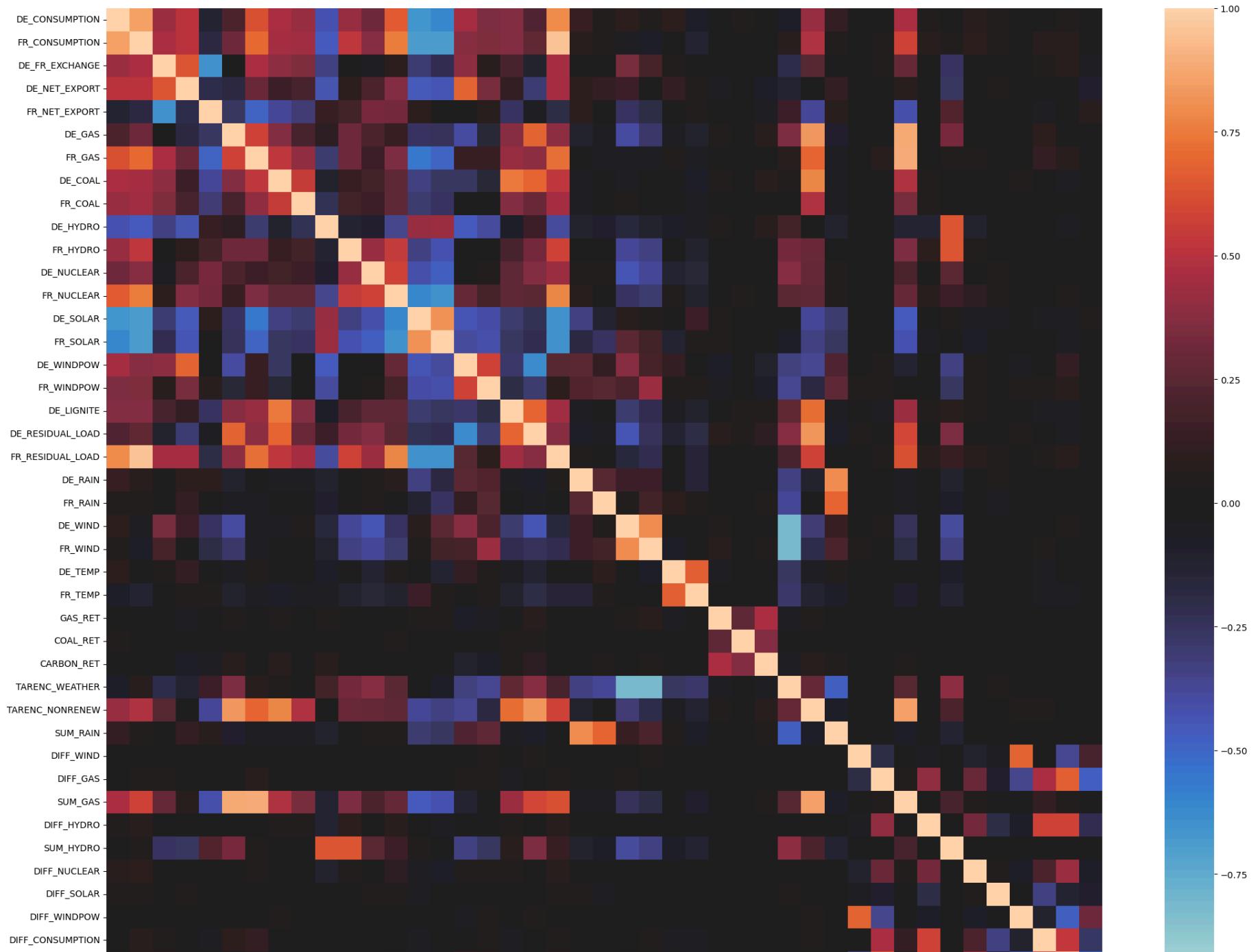
Xy_tr_finished = pd.merge(X_trte_finished, y_train, on='ID', how='right')
```

6. Finalize and check the results of feature engineering

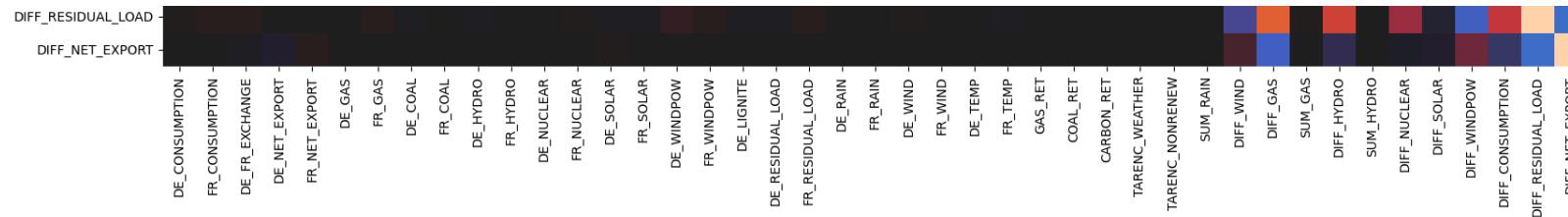
```
In [67]: # plot heatmap of train and test data set after feature selection
corr = X_trte_finished.drop('ID', axis=1).corr(parameters['corr_method'])
print("Correlation matrix shape:", corr.shape)

plt.figure(figsize=[25,20])
sns.heatmap(corr, annot=False, vmin=-1, vmax=1, center=0)
plt.show()
```

Correlation matrix shape: (43, 43)



feature_engineering



```
In [68]: # top correlated pairs by |r|
pairs = []
cols = corr.columns
for i in range(len(cols)):
    for j in range(i+1, len(cols)):
        r = corr.iloc[i, j]
        pairs.append((cols[i], cols[j], abs(r), r))
pairs_sorted = sorted(pairs, key=lambda x: x[2], reverse=True)[:60]
pd_pairs_corr = pd.DataFrame(pairs_sorted, columns=["feat1", "feat2", "|r|", "r"])
pd_pairs_high_corr = pd_pairs_corr[pd_pairs_corr['|r|'] >= 0.80]
pd_pairs_high_corr
```

Out[68]:

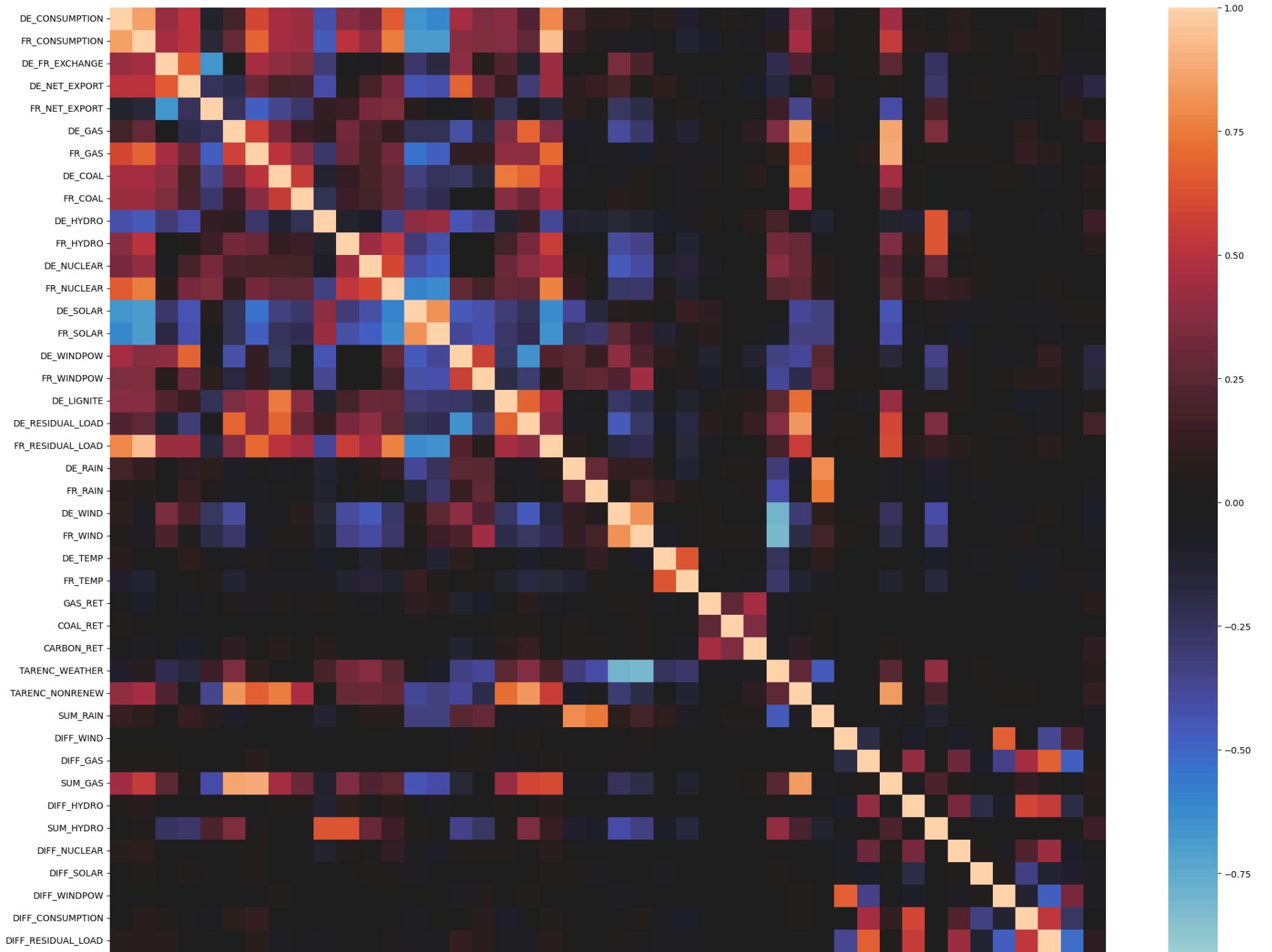
	feat1	feat2	r	r
0	FR_CONSUMPTION	FR_RESIDUAL_LOAD	0.948533	0.948533
1	FR_GAS	SUM_GAS	0.890381	0.890381
2	DE_GAS	SUM_GAS	0.876269	0.876269
3	TARENC_NONRENEW	SUM_GAS	0.853580	0.853580
4	DE_CONSUMPTION	FR_CONSUMPTION	0.850321	0.850321
5	DE_GAS	TARENC_NONRENEW	0.833975	0.833975
6	DE_RESIDUAL_LOAD	TARENC_NONRENEW	0.822407	0.822407
7	DE_SOLAR	FR_SOLAR	0.815540	0.815540
8	FR_WIND	TARENC_WEATHER	0.810122	-0.810122
9	DE_WIND	TARENC_WEATHER	0.805946	-0.805946
10	DE_RAIN	SUM_RAIN	0.803826	0.803826
11	DE_WIND	FR_WIND	0.802614	0.802614

In [69]:

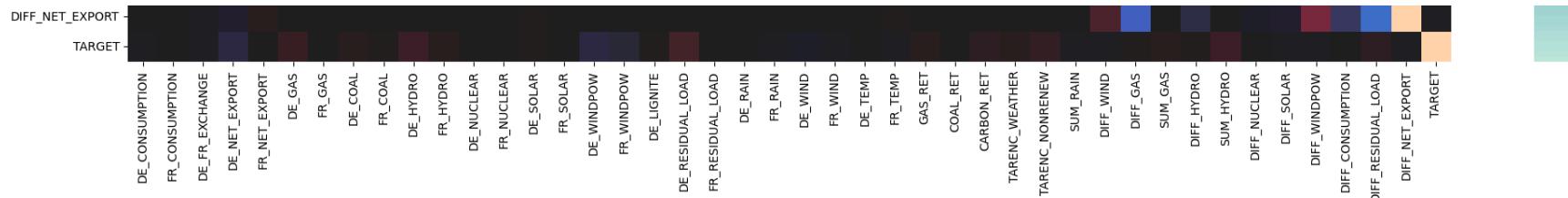
```
# plot heatmap of train data set with target after feature selection
corr = Xy_tr_finished.drop('ID', axis=1).corr(parameters['corr_method'])
print("Correlation matrix shape:", corr.shape)

plt.figure(figsize=[25,20])
sns.heatmap(corr, annot=False, vmin=-1, vmax=1, center=0)
plt.show()
```

Correlation matrix shape: (44, 44)



feature_engineering



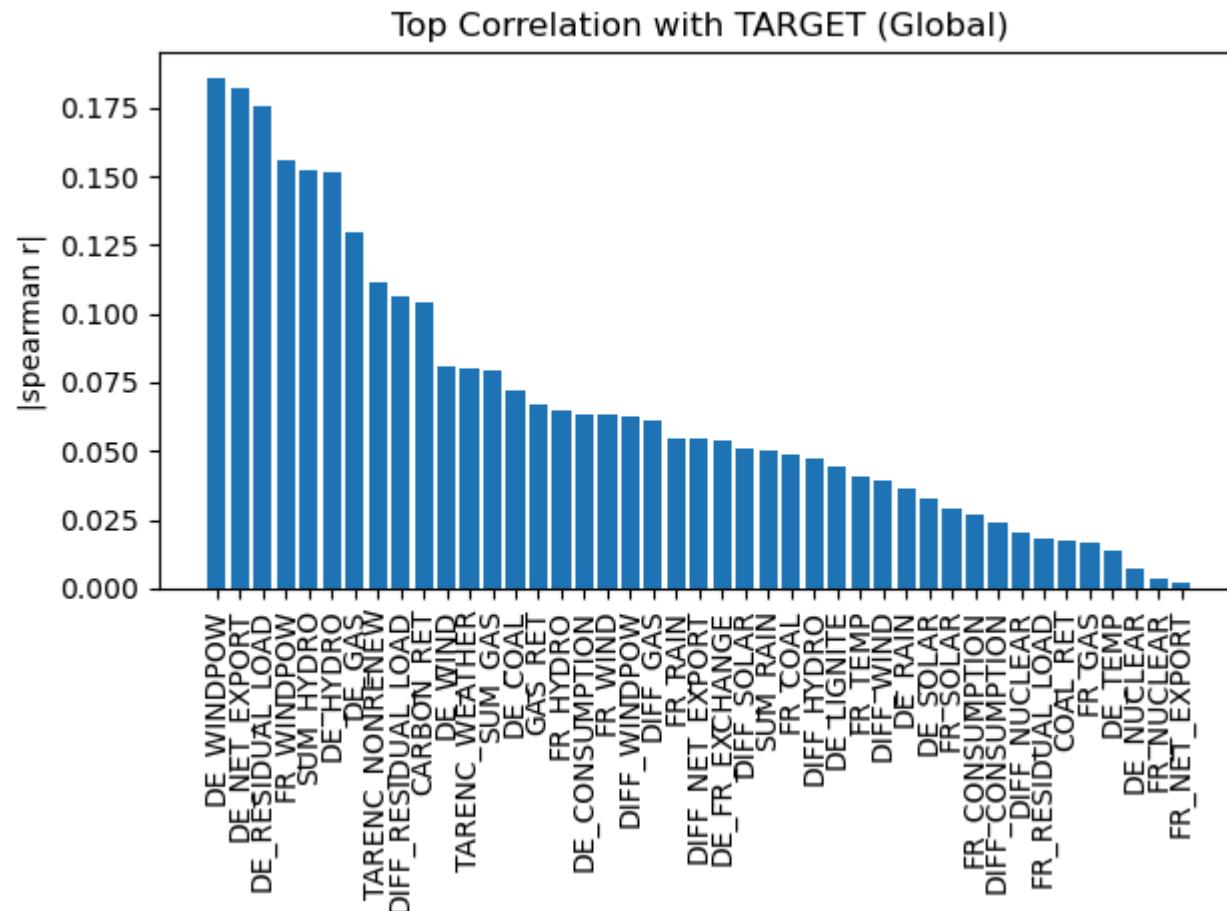
In [70]:

```
# plot high correlation with target
assert "TARGET" in Xy_tr_finished.columns, "TARGET missing after merge"
target_corr = Xy_tr_finished.drop('ID', axis=1).corr(method=parameters['corr_method'])["TARGET"].drop("TARGET").sort_values(ascending=False)
display(target_corr)

# bar of absolute correlations (top-k)
tc_abs = target_corr.abs().sort_values(ascending=False)
plt.figure()
plt.bar(tc_abs.index.astype(str), tc_abs.values)
plt.xticks(rotation=90)
plt.ylabel(f"|\{parameters['corr_method']}\|")
plt.title("Top Correlation with TARGET (Global)")
plt.tight_layout()
plt.show()
```

DE_RESIDUAL_LOAD	0.175793
SUM_HYDRO	0.152320
DE_HYDRO	0.151367
DE_GAS	0.129905
TARENC_NONRENEW	0.111437
DIFF_RESIDUAL_LOAD	0.106547
CARBON_RET	0.104375
TARENC_WEATHER	0.080359
SUM_GAS	0.079039
DE_COAL	0.072380
GAS_RET	0.066800
FR_HYDRO	0.064682
DIFF_GAS	0.060776
FR_COAL	0.048463
DIFF_HYDRO	0.047350
DE_LIGNITE	0.044180
DE_SOLAR	0.032740
FR_SOLAR	0.028839
DIFF_CONSUMPTION	0.024143
FR_RESIDUAL_LOAD	0.018241
COAL_RET	0.017573
FR_GAS	0.016334
DE_NUCLEAR	0.007052
FR_NET_EXPORT	0.002212
FR_NUCLEAR	-0.003619
DE_TEMP	-0.013885
DIFF_NUCLEAR	-0.020674
FR_CONSUMPTION	-0.027242
DE_RAIN	-0.036054
DIFF_WIND	-0.039104
FR_TEMP	-0.041060
SUM_RAIN	-0.050081
DIFF_SOLAR	-0.051146
DE_FR_EXCHANGE	-0.054010
DIFF_NET_EXPORT	-0.054347
FR_RAIN	-0.054358
DIFF_WINDPOW	-0.062525
FR_WIND	-0.063296
DE_CONSUMPTION	-0.063617
DE_WIND	-0.081106
FR_WINDPOW	-0.155568

```
DE_NET_EXPORT      -0.182006
DE_WINDPOW        -0.185688
Name: TARGET, dtype: float64
```



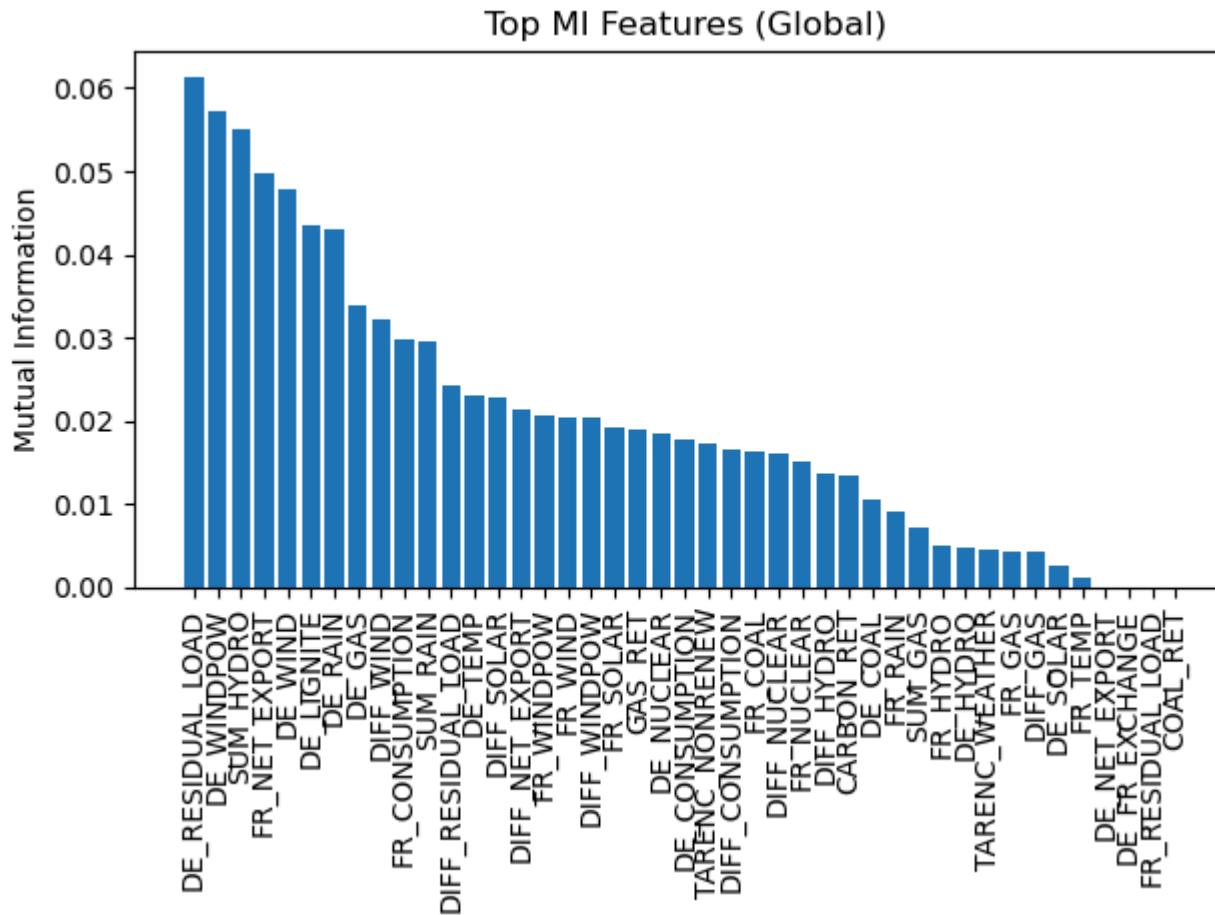
```
In [71]: # plot mutual information ranking (top-k)
mi = mutual_info_regression(Xy_tr_finished.drop(['ID', 'TARGET'], axis=1), Xy_tr_finished['TARGET'], random_state=RANDOM_STATE)
mi_series = pd.Series(mi, index=Xy_tr_finished.columns[1:-1]).sort_values(ascending=False)
display(mi_series)

plt.figure()
plt.bar(mi_series.index.astype(str), mi_series.values)
plt.xticks(rotation=90)
plt.ylabel("Mutual Information")
```

```
plt.title("Top MI Features (Global)")  
plt.tight_layout()  
plt.show()
```

DE_RESIDUAL_LOAD	0.061287
DE_WINDPOW	0.057267
SUM_HYDRO	0.055135
FR_NET_EXPORT	0.049652
DE_WIND	0.047819
DE_LIGNITE	0.043404
DE_RAIN	0.042970
DE_GAS	0.033928
DIFF_WIND	0.032239
FR_CONSUMPTION	0.029868
SUM_RAIN	0.029496
DIFF_RESIDUAL_LOAD	0.024380
DE_TEMP	0.023047
DIFF_SOLAR	0.022829
DIFF_NET_EXPORT	0.021277
FR_WINDPOW	0.020668
FR_WIND	0.020436
DIFF_WINDPOW	0.020376
FR_SOLAR	0.019102
GAS_RET	0.018954
DE_NUCLEAR	0.018599
DE_CONSUMPTION	0.017685
TARENC_NONRENEW	0.017232
DIFF_CONSUMPTION	0.016604
FR_COAL	0.016442
DIFF_NUCLEAR	0.016105
FR_NUCLEAR	0.015078
DIFF_HYDRO	0.013604
CARBON_RET	0.013371
DE_COAL	0.010477
FR_RAIN	0.009210
SUM_GAS	0.007126
FR_HYDRO	0.005136
DE_HYDRO	0.004713
TARENC_WEATHER	0.004582
FR_GAS	0.004252
DIFF_GAS	0.004206
DE_SOLAR	0.002624
FR_TEMP	0.001195
DE_NET_EXPORT	0.000000
DE_FR_EXCHANGE	0.000000

```
FR_RESIDUAL_LOAD      0.000000
COAL_RET              0.000000
dtype: float64
```



```
In [72]: # finalize the engineered data set
if OnlyOrigNumFeatures:
    remain_features = [x for x in X_trte_finished.columns if x in orig_num_cols]
    X_trte_finished = X_trte_finished[remain_features]
    X_trte_finished['DE_NET_IMPORT'] = -1 * X_trte_finished['DE_NET_EXPORT']
    X_trte_finished['FR_NET_IMPORT'] = -1 * X_trte_finished['FR_NET_EXPORT']
    X_trte_finished['FR_DE_EXCHANGE'] = -1 * X_trte_finished['DE_FR_EXCHANGE']

X_train_clean = X_train[['ID']].merge(X_trte_finished, on='ID', how='left')
```

```
X_test_clean = X_test[['ID']].merge(X_trte_finished, on='ID', how='left')

print("Missing value count:", X_train_clean.isna().sum().sum() + X_test_clean.isna().sum().sum())
display(X_train_clean.shape)
display(X_test_clean.shape)
display(y_train.shape)

Missing value count: 0
(1494, 33)
(654, 33)
(1494, 2)
```

7. Evaluate the feature engineering result with ML prediction

```
In [73]: # TabPFN regression
X_train_, X_test_, y_train_, y_test_ = train_test_split(X_train_clean, y_train['TARGET'], test_size=0.15, random_state=RANDOM_

tabPFN_regressor = TabPFNRegressor(random_state=42, device="cuda")
tabPFN_regressor.fit(X_train_.to_numpy(), y_train_.to_numpy())
test_pred = tabPFN_regressor.predict(X_test_)

mse = mean_squared_error(y_test_, test_pred)
spearman = spearmanr(y_test_, test_pred).correlation
r2 = r2_score(y_test_, test_pred)

print(f"RMSE on test set: {mse:.4f}")
print(f"Spearmanon correlation on test set: {spearmanr(y_test_, test_pred).correlation}")

sb.glue("spearman", spearman)
sb.glue("r2", r2)
sb.glue("X_train", X_train_clean)
sb.glue("y_train", y_train)
sb.glue("X_test", X_test_clean)

RMSE on test set: 1.0145
Spearmanon correlation on test set: 0.3475189633375475
```