Missing Values

October 19, 2025

1 Filling Missing Values

The purpose of this notebook is to demonstrate and compare different techniques for filling missing values in a dataset.

From `config.yaml`:

```
temporal_fill:
  target_columns:
    - soil_moisture_5cm
    - soil_moisture_10cm
    - soil_moisture_20cm
    - soil_moisture_50cm
    - soil_moisture_100cm
    - air_temp_mean
    - rh_mean
    - solar_radiation
    - sur_temp_avg
  max_gap_days: 5
  switch_gap: 4
  regression_window: 7
```

Comparing 4 approaches: 1. Linear Interpolation 2. Forward Fill / Backward Fill 3. Regression-based Fill 4. XGBoost-based Fill

[36]:
```
import sys
import pandas as pd
from pathlib import Path
from sklearn.metrics import mean_squared_error, mean_absolute_error, r2_score
import numpy as np
import time
import matplotlib.pyplot as plt

project_root = Path.cwd().parent

if str(project_root) not in sys.path:
    sys.path.insert(0, str(project_root))

from pipes.request_pipe import RequestPipe
```

```
from pipes.parse_pipe import ParsePipe
```

[7]:
```
TARGETS = ["soil_moisture_5cm", "soil_moisture_10cm", "soil_moisture_20cm",
           "soil_moisture_50cm", "soil_moisture_100cm", "air_temp_mean",
           "rh_mean", "solar_radiation", "sur_temp_avg"]

MAX_GAP_DAYS = 5
SWITCH_GAP = 4
REGRESSION_WINDOW = 7
```

[8]:
```
req = RequestPipe()
parser = ParsePipe()
df = parser.run(req.run())

df = df.sort_values(["station_id", "date"])
station_id = df["station_id"].iloc[0]

data = df[df["station_id"] == station_id].copy()
data["date"] = pd.to_datetime(data["date"])
data = data.set_index("date")
```

[9]:
```
df.head()
```

[9]:

	station_id	date	crx_vn	longitude	latitude	air_temp_max	\
0	4136	2007-07-31	1.302	-117.53	47.42	<NA>	
1	4136	2007-08-01	1.302	-117.53	47.42	32.9	
2	4136	2007-08-02	1.302	-117.53	47.42	35.4	
3	4136	2007-08-03	1.302	-117.53	47.42	29.4	
4	4136	2007-08-04	1.302	-117.53	47.42	27.6	

	air_temp_min	air_temp_mean	air_temp_avg	precipitation	…	\
0	<NA>	<NA>	<NA>	<NA>	…	
1	2.4	17.7	19.4	0.0	…	
2	4.0	19.7	22.0	0.0	…	
3	7.5	18.4	21.5	0.0	…	
4	6.5	17.0	18.0	0.0	…	

	soil_moisture_10cm	soil_moisture_20cm	soil_moisture_50cm	\
0	-99.0	-99.0	-99.0	
1	-99.0	-99.0	-99.0	
2	-99.0	-99.0	-99.0	
3	-99.0	-99.0	-99.0	
4	-99.0	-99.0	-99.0	

	soil_moisture_100cm	soil_temp_5cm	soil_temp_10cm	soil_temp_20cm	\
0	-99.0	NaN	NaN	NaN	
1	-99.0	NaN	NaN	NaN	

```
2               -99.0           NaN            NaN            NaN
3               -99.0           NaN            NaN            NaN
4               -99.0           NaN            NaN            NaN

  soil_temp_50cm  soil_temp_100cm                        source_file
0            NaN              NaN  uscrn_WA_Spokane_17_SSW_2007.txt
1            NaN              NaN  uscrn_WA_Spokane_17_SSW_2007.txt
2            NaN              NaN  uscrn_WA_Spokane_17_SSW_2007.txt
3            NaN              NaN  uscrn_WA_Spokane_17_SSW_2007.txt
4            NaN              NaN  uscrn_WA_Spokane_17_SSW_2007.txt

[5 rows x 29 columns]
```

1.1 Candidates

First, we need to check if all of these target columns are good canididates for filling missing values. If all of them are `NULL` for a given station, we can't fill them with anything but `NULL`.

[10]:
```
df["date"] = pd.to_datetime(df["date"], errors="coerce")
df = df.sort_values(["station_id", "date"])
```

[11]:
```
station_id = df["station_id"].iloc[0]
data = df[df["station_id"] == station_id].set_index("date")
```

[12]:
```
data = data.replace(-99.0, pd.NA)
```

[13]:
```
candidates = [col for col in TARGETS if data[col].notna().sum() > 0]
print("Candidate columns for interpolation:")
print(candidates)
```

```
Candidate columns for interpolation:
['soil_moisture_5cm', 'soil_moisture_10cm', 'soil_moisture_20cm',
'soil_moisture_50cm', 'soil_moisture_100cm', 'air_temp_mean', 'rh_mean',
'solar_radiation', 'sur_temp_avg']
```

[14]:
```
excluded = set(TARGETS) - set(candidates)
if excluded:
    print("\nExcluded (all null or invalid):", list(excluded))
else:
    print("\nAll target columns are valid candidates.")
```

```
All target columns are valid candidates.
```

Good! :)

1.2 Setup

We're going to use a small subset of the data for demonstration purposes...this can be safely scaled up to the full dataset later (I think).

[15]:
```
valid_counts = data[TARGETS].notna().sum(axis=1)
non_empty_dates = data.index[valid_counts > 0]

print("First valid record:", non_empty_dates.min())
print("Last valid record:", non_empty_dates.max())
```

```
First valid record: 2007-08-01 00:00:00
Last valid record: 2025-10-18 00:00:00
```

[16]:
```
# From Jun 1st 2018 to Sep 30th 2018

subset = data.loc["2018-06-01":"2018-09-30", TARGETS].copy()
subset = subset.replace(-99.0, pd.NA)

# Randomly mask 10%...ish of existing values to simulate gaps (same pattern for␣
 ↪all)
mask = subset.notna() & (pd.DataFrame(np.random.rand(*subset.shape),␣
 ↪index=subset.index, columns=subset.columns) < 0.1)
subset_masked = subset.mask(mask)

df_linear = subset_masked.copy(deep=True)
df_fbfill = subset_masked.copy(deep=True)
df_reg = subset_masked.copy(deep=True)
df_xgb = subset_masked.copy(deep=True)
```

[17]:
```
subset.head()
```

[17]:

date	soil_moisture_5cm	soil_moisture_10cm	soil_moisture_20cm	soil_moisture_50cm	soil_moisture_100cm	air_temp_mean	rh_mean	solar_radiation	sur_temp_avg
2018-06-01	0.153	0.183	0.171	0.138	0.129	10.7	59.7	22.01	14.5
2018-06-02	0.146	0.178	0.166	0.134	0.125	12.6	58.3	28.27	18.0
2018-06-03	0.137	0.172	0.16	0.129	0.12	16.4	51.1	25.82	21.9
2018-06-04	0.129	0.165	0.154	0.125	0.117	12.7	49.0		
2018-06-05	0.122	0.16	0.148	0.121	0.113	10.9	53.7		

```
2018-06-04          22.44         16.7
2018-06-05          27.66         16.1
```

[18]:
```
print((df_linear.isna() == df_fbfill.isna()).all().all())
print((df_fbfill.isna() == df_reg.isna()).all().all())
print((df_reg.isna() == df_xgb.isna()).all().all())
```

```
True
True
True
```

1.3 Evaluation Strategy

Since we dropped some values artificially, we can use those dropped values to evaluate the performance of each filling method. We'll use RMSE, MAE and R^2 as our evaluation metrics.

[19]:
```
class Stopwatch:
    def __init__(self):
        self.start_time = None
        self.elapsed = 0.0

    def start(self):
        self.start_time = time.time()

    def stop(self):
        if self.start_time is None:
            raise RuntimeError("Stopwatch not started.")
        self.elapsed = time.time() - self.start_time
        return self.elapsed

    def reset(self):
        self.start_time = None
        self.elapsed = 0.0

    def __str__(self):
        return f"{self.elapsed:.3f} seconds"

def evaluate_fill(true_df, filled_df, targets):
    metrics = {}
    for col in targets:
        mask = true_df[col].notna()
        y_true = true_df.loc[mask, col]
        y_pred = filled_df.loc[mask, col]

        valid_mask = y_pred.notna()
        y_true = y_true[valid_mask]
        y_pred = y_pred[valid_mask]
```

```
        if len(y_true) == 0:
            metrics[col] = {"RMSE": np.nan, "MAE": np.nan, "R2": np.nan}
            continue

        metrics[col] = {
            "RMSE": np.sqrt(mean_squared_error(y_true, y_pred)),
            "MAE": mean_absolute_error(y_true, y_pred),
            "R2": r2_score(y_true, y_pred),
        }
    return pd.DataFrame(metrics).T

def physical_validity_check(df, targets):
    invalid = {}
    for col in targets:
        s = df[col]
        if "soil_moisture" in col:
            invalid[col] = ((s < 0) | (s > 1)).sum()
        elif "temp" in col:
            invalid[col] = ((s < -60) | (s > 60)).sum()
        elif "radiation" in col:
            invalid[col] = (s < 0).sum()
        elif "rh_mean" in col:
            invalid[col] = ((s < 0) | (s > 100)).sum()
        else:
            invalid[col] = 0
    return pd.DataFrame.from_dict(invalid, orient="index", columns=["Invalid␣
 ↪Count"])

def summarize_results(results_dict):
    records = []
    for method, (metrics_df, runtime) in results_dict.items():
        df_tmp = metrics_df.copy()
        df_tmp["Runtime (s)"] = runtime
        df_tmp["Method"] = method
        records.append(df_tmp)
    summary = pd.concat(records)
    return summary.reset_index(names=["Target"])
```

This means we're perfectly aligned across all 4 dfs.

1.3.1 Linear Interpolation

[20]:
```
df_linear = df_linear.apply(pd.to_numeric, errors="coerce")

timer = Stopwatch()
timer.start()
```

```
linear_filled = df_linear.interpolate(method="linear", limit=MAX_GAP_DAYS)

runtime_linear = timer.stop()
print(f"Linear interpolation completed in {runtime_linear:.3f} seconds")

# Evaluate performance
linear_metrics = evaluate_fill(subset, linear_filled, TARGETS)
invalid_linear = physical_validity_check(linear_filled, TARGETS)

display(linear_metrics)
display(invalid_linear)
```

```
Linear interpolation completed in 0.002 seconds
```

	RMSE	MAE	R2
soil_moisture_5cm	0.001133	0.000204	0.998919
soil_moisture_10cm	0.000144	0.000025	0.999982
soil_moisture_20cm	0.000187	0.000047	0.999964
soil_moisture_50cm	0.000232	0.000058	0.999934
soil_moisture_100cm	0.000234	0.000063	0.999914
air_temp_mean	0.293298	0.073278	0.994720
rh_mean	2.961240	0.731543	0.892900
solar_radiation	2.042213	0.436405	0.868763
sur_temp_avg	0.602990	0.143939	0.987373

	Invalid Count
soil_moisture_5cm	0
soil_moisture_10cm	0
soil_moisture_20cm	0
soil_moisture_50cm	0
soil_moisture_100cm	0
air_temp_mean	0
rh_mean	0
solar_radiation	0
sur_temp_avg	0

1.3.2 Forward Fill / Backward Fill

[21]:
```
df_fbfill = df_fbfill.apply(pd.to_numeric, errors="coerce")

timer.reset()
timer.start()

fb_filled = (
    df_fbfill
    .ffill(limit=MAX_GAP_DAYS)
```

```
    .bfill(limit=MAX_GAP_DAYS)
)

runtime_fb = timer.stop()
print(f"Forward/Backward fill completed in {runtime_fb:.3f} seconds")

fb_metrics = evaluate_fill(subset, fb_filled, TARGETS)
invalid_fb = physical_validity_check(fb_filled, TARGETS)

display(fb_metrics)
display(invalid_fb)
```

```
Forward/Backward fill completed in 0.001 seconds
```

	RMSE	MAE	R2
soil_moisture_5cm	0.002126	0.000504	0.996190
soil_moisture_10cm	0.000315	0.000050	0.999915
soil_moisture_20cm	0.000436	0.000107	0.999802
soil_moisture_50cm	0.000375	0.000091	0.999827
soil_moisture_100cm	0.000766	0.000190	0.999073
air_temp_mean	0.630033	0.152893	0.975638
rh_mean	3.537403	0.842975	0.847168
solar_radiation	2.906263	0.586364	0.734220
sur_temp_avg	0.685324	0.182645	0.983689

	Invalid Count
soil_moisture_5cm	0
soil_moisture_10cm	0
soil_moisture_20cm	0
soil_moisture_50cm	0
soil_moisture_100cm	0
air_temp_mean	0
rh_mean	0
solar_radiation	0
sur_temp_avg	0

1.3.3 Regression-based Fill

[22]:
```
def rolling_regression_fill(df, targets, window=REGRESSION_WINDOW):
    df = df.copy()
    for col in targets:
        series = df[col].astype(float)
        for i in range(window, len(series)):
            if pd.isna(series.iloc[i]):

                y = series.iloc[i - window:i].dropna()
                if len(y) >= 2:
```

```
                    try:
                        x = np.arange(len(y))
                        coeffs = np.polyfit(x, y.values, deg=1)
                        series.iloc[i] = coeffs[1] + coeffs[0] * len(y)
                    except Exception as e:
                        print(f"[WARN] Regression failed for {col} at index {i}:
 ↪ {e}")
        df[col] = series
    return df

df_reg = df_reg.apply(pd.to_numeric, errors="coerce")

timer.reset()
timer.start()

reg_filled = rolling_regression_fill(df_reg, TARGETS, window=REGRESSION_WINDOW)

runtime_reg = timer.stop()
print(f"Regression-based fill completed in {runtime_reg:.3f} seconds")

reg_metrics = evaluate_fill(subset, reg_filled, TARGETS)
invalid_reg = physical_validity_check(reg_filled, TARGETS)

display(reg_metrics)
display(invalid_reg)
```

```
Regression-based fill completed in 0.021 seconds
```

	RMSE	MAE	R2
soil_moisture_5cm	0.001154	0.000284	0.998721
soil_moisture_10cm	0.000250	0.000057	0.999947
soil_moisture_20cm	0.000466	0.000113	0.999773
soil_moisture_50cm	0.000410	0.000104	0.999793
soil_moisture_100cm	0.000768	0.000181	0.999029
air_temp_mean	0.702757	0.158290	0.969689
rh_mean	3.851396	0.945484	0.820244
solar_radiation	2.910917	0.607831	0.731422
sur_temp_avg	0.963324	0.227867	0.968011

	Invalid Count
soil_moisture_5cm	0
soil_moisture_10cm	0
soil_moisture_20cm	0
soil_moisture_50cm	0
soil_moisture_100cm	0
air_temp_mean	0
rh_mean	0
solar_radiation	0
sur_temp_avg	0

1.3.4 XGBoost-based Fill

[32]:
```
from xgboost import XGBRegressor

# I fucked up somewhere up top, this is just to patch it on the spot...doesn't␣
 ↪matter since this is not production level stuff
def add_lag_features(df, targets, lags=[1, 2, 3]):
    df = df.copy()
    for col in targets:
        for lag in lags:
            df[f"{col}_lag{lag}"] = df[col].shift(lag)
    return df

def xgboost_fill(df, targets, window=REGRESSION_WINDOW):
    df = df.copy()
    df = df.apply(pd.to_numeric, errors="coerce")

    feature_cols = [
        c for c in df.columns
        if c not in targets
        and df[c].notna().sum() > 0
        and c != "station_id"
        and c != "source_file"
    ]
    if not feature_cols:
        print("[WARN] No valid feature columns found for XGBoost.")
        return df

    for col in targets:
        y = df[col]
        X = df[feature_cols]

        mask_train = y.notna()
        mask_pred = y.isna()

        if mask_train.sum() < 20:
            print(f"[WARN] Skipping {col} ... not enough non-null samples.")
            continue

        try:
            model = XGBRegressor(
                n_estimators=200,
                max_depth=4,
                learning_rate=0.05,
                subsample=0.8,
```

```
                colsample_bytree=0.8,
                random_state=42,
                n_jobs=-1,
                verbosity=0
            )

            model.fit(X[mask_train], y[mask_train])

            if mask_pred.sum() > 0:
                preds = model.predict(X[mask_pred])
                df.loc[mask_pred, col] = preds

        except Exception as e:
            print(f"[ERROR] XGBoost failed for {col}: {e}")

    return df

df_xgb = add_lag_features(df_xgb, TARGETS, lags=[1, 2, 3])

timer.reset()
timer.start()

xgb_filled = xgboost_fill(df_xgb, TARGETS, window=REGRESSION_WINDOW)

runtime_xgb = timer.stop()
print(f"XGBoost-based fill completed in {runtime_xgb:.3f} seconds")

xgb_metrics = evaluate_fill(subset, xgb_filled, TARGETS)
invalid_xgb = physical_validity_check(xgb_filled, TARGETS)

display(xgb_metrics)
display(invalid_xgb)
```

```
XGBoost-based fill completed in 1.568 seconds
```

	RMSE	MAE	R2
soil_moisture_5cm	0.004325	0.000842	0.984238
soil_moisture_10cm	0.001267	0.000283	0.998627
soil_moisture_20cm	0.003730	0.000655	0.985470
soil_moisture_50cm	0.000880	0.000211	0.999047
soil_moisture_100cm	0.002028	0.000508	0.993502
air_temp_mean	0.553114	0.138197	0.981224
rh_mean	2.975361	0.722806	0.891876
solar_radiation	2.292547	0.524345	0.834618
sur_temp_avg	0.838270	0.184362	0.975596

	Invalid Count
soil_moisture_5cm	0
soil_moisture_10cm	0

```
soil_moisture_20cm              0
soil_moisture_50cm              0
soil_moisture_100cm             0
air_temp_mean                   0
rh_mean                         0
solar_radiation                 0
sur_temp_avg                    0
```

1.4 Results

[34]:
```
summary_metrics = pd.concat(
    [
        linear_metrics.assign(Method="Linear Interpolation"),
        fb_metrics.assign(Method="Forward/Backward Fill"),
        reg_metrics.assign(Method="Regression-based Fill"),
        xgb_metrics.assign(Method="XGBoost-based Fill"),
    ]
).set_index("Method")

summary_metrics = summary_metrics[["RMSE", "MAE", "R2"]]

print("\n=== Quantitative Evaluation Summary ===\n")
pd.options.display.float_format = "{:.4f}".format
display(summary_metrics.round(4))

invalid_summary = pd.DataFrame({
    "Linear": invalid_linear.sum(),
    "Ffill": invalid_fb.sum(),
    "Regression": invalid_reg.sum(),
    "XGBoost": invalid_xgb.sum(),
}).T

print("\n=== Physical Validity Check (Out-of-Range Counts) ===\n")
display(invalid_summary)
```

```
=== Quantitative Evaluation Summary ===
```

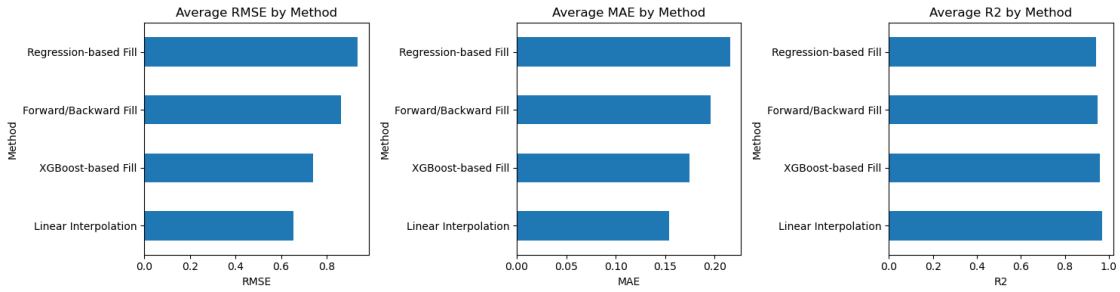
Method	RMSE	MAE	R2
Linear Interpolation	0.0011	0.0002	0.9989
Linear Interpolation	0.0001	0.0000	1.0000
Linear Interpolation	0.0002	0.0000	1.0000
Linear Interpolation	0.0002	0.0001	0.9999
Linear Interpolation	0.0002	0.0001	0.9999
Linear Interpolation	0.2933	0.0733	0.9947

```
Linear Interpolation  2.9612 0.7315 0.8929
Linear Interpolation  2.0422 0.4364 0.8688
Linear Interpolation  0.6030 0.1439 0.9874
Forward/Backward Fill 0.0021 0.0005 0.9962
Forward/Backward Fill 0.0003 0.0000 0.9999
Forward/Backward Fill 0.0004 0.0001 0.9998
Forward/Backward Fill 0.0004 0.0001 0.9998
Forward/Backward Fill 0.0008 0.0002 0.9991
Forward/Backward Fill 0.6300 0.1529 0.9756
Forward/Backward Fill 3.5374 0.8430 0.8472
Forward/Backward Fill 2.9063 0.5864 0.7342
Forward/Backward Fill 0.6853 0.1826 0.9837
Regression-based Fill 0.0012 0.0003 0.9987
Regression-based Fill 0.0003 0.0001 0.9999
Regression-based Fill 0.0005 0.0001 0.9998
Regression-based Fill 0.0004 0.0001 0.9998
Regression-based Fill 0.0008 0.0002 0.9990
Regression-based Fill 0.7028 0.1583 0.9697
Regression-based Fill 3.8514 0.9455 0.8202
Regression-based Fill 2.9109 0.6078 0.7314
Regression-based Fill 0.9633 0.2279 0.9680
XGBoost-based Fill    0.0043 0.0008 0.9842
XGBoost-based Fill    0.0013 0.0003 0.9986
XGBoost-based Fill    0.0037 0.0007 0.9855
XGBoost-based Fill    0.0009 0.0002 0.9990
XGBoost-based Fill    0.0020 0.0005 0.9935
XGBoost-based Fill    0.5531 0.1382 0.9812
XGBoost-based Fill    2.9754 0.7228 0.8919
XGBoost-based Fill    2.2925 0.5243 0.8346
XGBoost-based Fill    0.8383 0.1844 0.9756


=== Physical Validity Check (Out-of-Range Counts) ===


            Invalid Count
Linear                  0
Ffill                   0
Regression              0
XGBoost                 0
```

1.5 Plots

[37]:
```
avg_scores = summary_metrics.groupby("Method")[["RMSE", "MAE", "R2"]].mean()

fig, axes = plt.subplots(1, 3, figsize=(15, 4))
for i, metric in enumerate(["RMSE", "MAE", "R2"]):
    avg_scores[metric].sort_values(ascending=(metric != "R2")).plot(
```

```
        kind="barh", ax=axes[i], title=f"Average {metric} by Method"
    )
    axes[i].set_xlabel(metric)
plt.tight_layout()
plt.show()
```

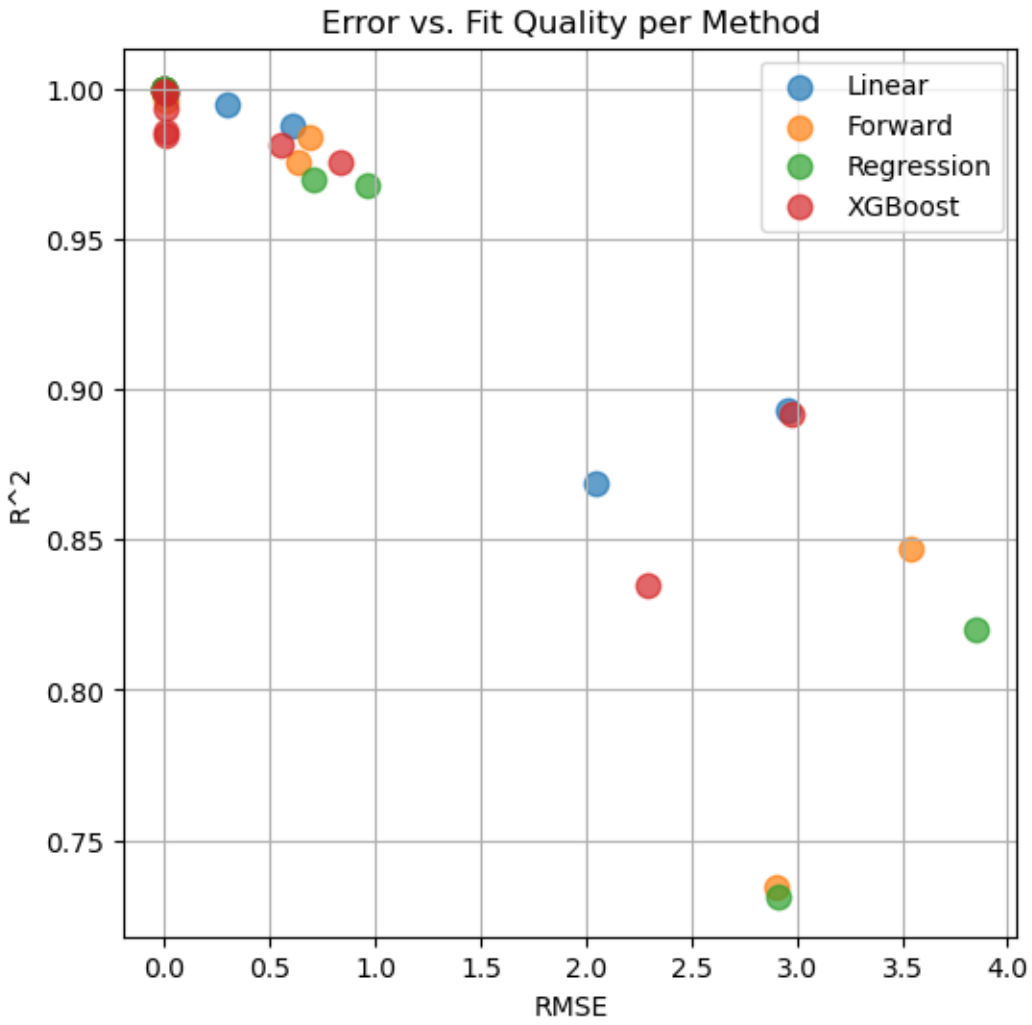


Lower RMSE/MAE is better, higher R^2 is better. Knowing that, we can clearly see that Linear Interpolation and XGBoost-based filling are the best methods overall, with Forward/Backward filling being a close third. Regression-based filling clearly the worst method here.

With that being said, I think our approach moving forward should be:

use Linear Interpolation for small gaps (<= 2 days) use XGBoost-based filling for larger gaps (> 2 days)

[40]:
```
fig, ax = plt.subplots(figsize=(6, 6))

for method, df_metrics in [
    ("Linear", linear_metrics),
    ("Forward", fb_metrics),
    ("Regression", reg_metrics),
    ("XGBoost", xgb_metrics),
]:
    ax.scatter(
        df_metrics["RMSE"], df_metrics["R2"],
        label=method, s=80, alpha=0.7
    )

ax.set_xlabel("RMSE")
ax.set_ylabel("R^2")
ax.set_title("Error vs. Fit Quality per Method")
ax.legend()
plt.grid(True)
plt.show()
```



[47]:
```python
def rank_methods(df):
    means = df.groupby("Method")[["RMSE", "MAE", "R2"]].mean()
    ranks = means.rank(ascending={"RMSE": True, "MAE": True, "R2": False})
    ranks["Overall_Score"] = ranks.mean(axis=1)
    ranks = ranks.round(0).astype(int)

    return ranks.sort_values("Overall_Score")

ranked = rank_methods(summary_metrics)

print("\n=== Method Ranking (Lower = Better) ===\n")
display(ranked)
```

```
=== Method Ranking (Lower = Better) ===
```

Method	RMSE	MAE	R2	Overall_Score
Linear Interpolation	1	1	4	2
XGBoost-based Fill	2	2	3	2
Forward/Backward Fill	3	3	2	3
Regression-based Fill	4	4	1	3