Project Explanation - Novartis Datathon 2025

> **This document explains EXACTLY what each file does, step-by-step, in simple terms.**
> Based on the competition requirements from `datathon_explanation.md`.

Input/Output Summary Table

Step	Module	Input	Output	Goal
1	`config.py`	None	Constants, paths, params	Central configuration
2	`data_loader.py`	Raw CSVs	Merged DataFrame	Load & combine all data
2a	Data Cleaning 🆕	Merged DataFrame	Cleaned DataFrame	Remove duplicates, validate ranges
3	`bucket_calculator.py`	Merged DataFrame	`aux_bucket_avgvol.csv`	Calculate pre-entry avg & buckets
4	`feature_engineering.py`	Merged DataFrame + aux	DataFrame + **76 features** 🆕	Create ML-ready features
4a	FeatureScaler 🆕	Feature DataFrame	Scaled DataFrame	Standardize/normalize features
4b	Target Encoding 🆕	Categorical columns	Encoded DataFrame	Leakage-safe target encoding
5	`models.py`	Features (X) + Target (y)	Trained model + predictions	Train prediction model
5b	`HybridPhysicsMLModel`	Features + avg_vol + months	Hybrid model + predictions	Physics + ML combined
5c	`ARIHOWModel`	Time-series per brand	ARHOW predictions	SARIMAX + Holt-Winters ensemble
5d	GroupKFold CV 🆕	Features + groups	CV scores	Brand-aware cross-validation
5e	EnsembleBlender 🆕	Multiple model preds	Blended predictions	Learn optimal ensemble weights

Step	Module	Input	Output	Goal
6	`evaluation.py`	Predictions + Actuals	PE Score	Measure prediction quality
7	`submission.py`	Test predictions	CSV + JSON summary	Format for competition
8	`pipeline.py`	All modules	End-to-end execution	Orchestrate workflow

The Big Picture: What Are We Doing?

The Business Problem (In Plain English)

Imagine you're Novartis, a big pharmaceutical company. You sell a drug called "BrandX" for $100.

Then the patent expires.

Now other companies can make **generic copies** that do the same thing but cost only $20.

What happens? Your sales **DROP** (this is called **generic erosion**).

The Question: How much will sales drop over the next 24 months?

Why Does This Matter?

Novartis needs to:

- Plan budgets
- Allocate resources
- Make business decisions

Your job: Build a model that predicts this sales decline accurately.

The Two Scenarios

Scenario	What You Have	What You Predict
Scenario 1	Only BEFORE generic entry	Months 0-23 (all 24 months)
Scenario 2	Before + First 6 months actual	Months 6-23 (remaining 18 months)

Think of it like weather forecasting:

- **Scenario 1** = Predicting next week's weather with only historical data
- **Scenario 2** = Predicting next week's weather knowing today's weather

---

Train vs Test Data: How They're Used

NO, We Don't Merge Train + Test Together

The project keeps them **separate** for different purposes:

🟢 TRAINING Data (`train=True`)

File	Purpose
`df_volume_train.csv`	Historical sales (months -24 to +23)
`df_generics_train.csv`	Competitor info
`df_medicine_info.csv`	Drug characteristics

Used for:

- **Learning patterns** - Train your ML models
- **Feature engineering** - Compute avg_vol baselines
- **Validation** - Split into train/val to tune hyperparameters
- **1,953 brands** with full history (before AND after generic entry)

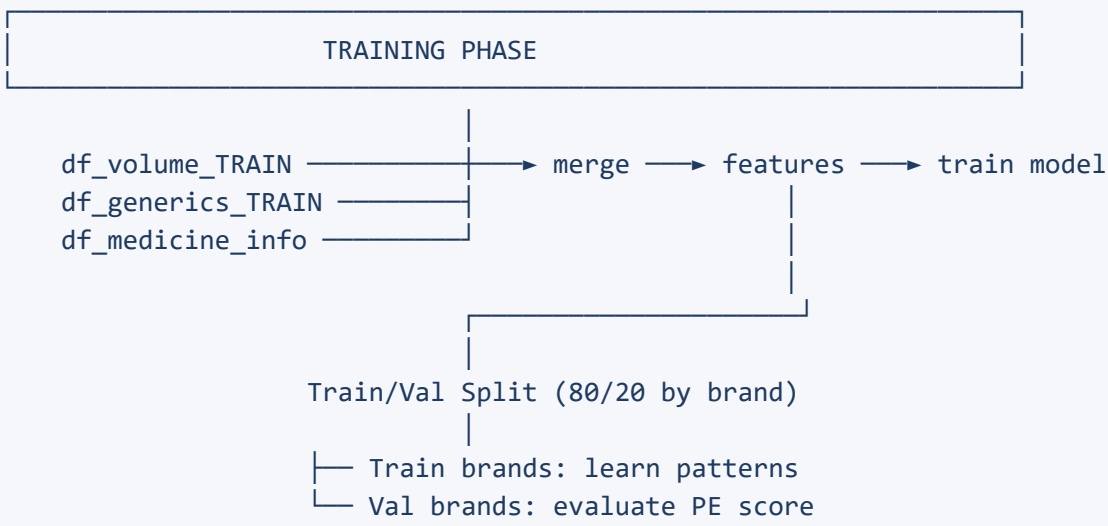
🟢 TEST Data (`train=False`)

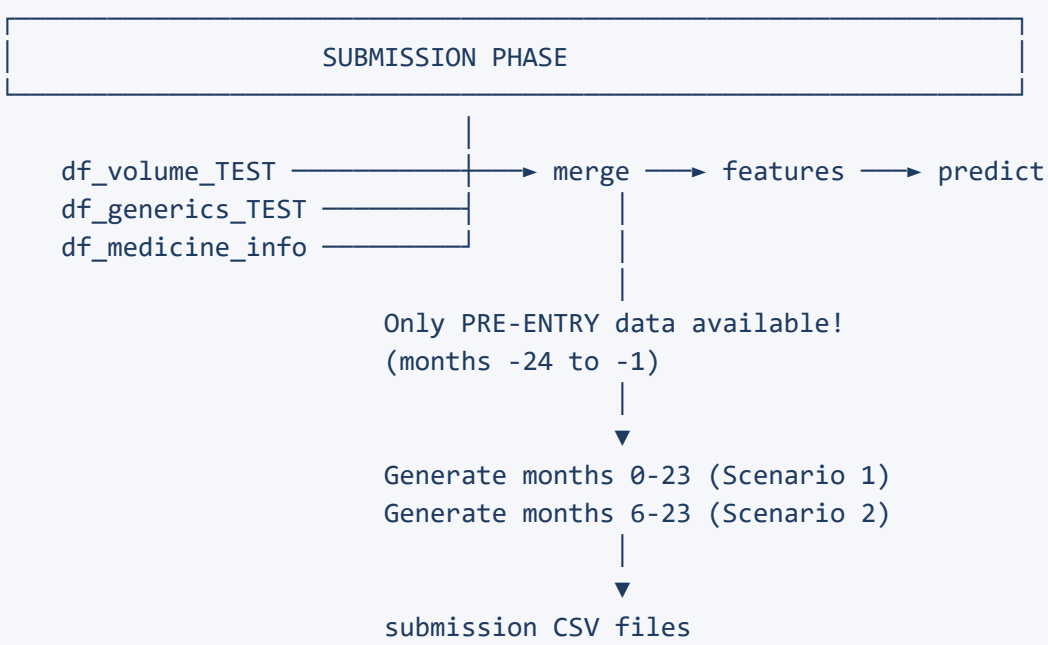
File	Purpose
`df_volume_test.csv`	Pre-entry data ONLY (months -24 to -1)
`df_generics_test.csv`	Competitor info
`df_medicine_info.csv`	Drug characteristics

Used for:

- **Generating predictions** - Apply trained model to new brands
- **Submission** - Create the CSV files you upload
- **340 brands** - NO post-entry actuals (that's what you predict!)

📋 Visual Data Flow





Key Differences

Aspect	Training	Test
Brands	1,953	340
Post-entry data	☑ Has months 0-23	❌ Must predict
Pre-entry data	☑ Has months -24 to -1	☑ Has months -24 to -1
Used for	Learning	Predicting
avg_vol source	Train brands	Test brands (separate calculation)

Important: Each test brand's predictions are normalized by **its own** pre-entry average!

The Bucket System (VERY IMPORTANT!)

Not all drugs decline the same way:

Bucket	Mean Erosion	What It Means	Scoring Weight
Bucket 1	≤ 0.25	SEVERE erosion (sales crash to <25% of original)	**2× (double!)**
Bucket 2	> 0.25	Moderate erosion	1× (normal)

Why This Matters:

If you predict Bucket 1 drugs wrong, your score gets **penalized TWICE as much!**

Strategy: Focus extra effort on predicting high-erosion drugs accurately.

File-by-File Explanation

1️⃣ `src/config.py` - The Central Control Panel 🆕

	Description
📥 **INPUT**	None (configuration file)
📤 **OUTPUT**	Python constants, paths, toggles, and parameters importable by other modules
🎯 **GOAL**	Centralize ALL settings so you can change them in ONE place and run the entire pipeline

What it does: Stores ALL settings, toggles, and constants in ONE place. **This is the ONLY file you need to edit to customize the pipeline!**

Configuration Sections:

```
#
================================================================================
# 1. RUN MODE & TOGGLES - Control what runs
#
================================================================================
RUN_SCENARIO = 1              # 1, 2, or [1, 2] for both scenarios
TEST_MODE = True              # True = fast (50 brands), False = full training
TEST_MODE_BRANDS = 50         # Number of brands in test mode
SUBMISSION_MODEL = 'baseline' # Model for final submissions

# Pipeline step toggles
RUN_EDA = False               # Run EDA visualization
RUN_TRAINING = True           # Train models
RUN_SUBMISSION = False        # Generate submission files
RUN_VALIDATION = False        # Validate submissions

#
================================================================================
# 2. MODEL TOGGLES - Enable/disable specific models
#
================================================================================
MODELS_ENABLED = {
    'baseline_no_erosion': True,   # ~1 sec  - Predicts avg_vol (no decline)
    'baseline_exp_decay': True,    # ~2 sec  - Exponential decay (BEST!)
    'lightgbm': True,              # ~5 sec  - LightGBM gradient boosting
    'xgboost': True,               # ~10 sec - XGBoost gradient boosting
    'hybrid_lightgbm': True,       # ~8 sec  - Decay + LightGBM residual
    'hybrid_xgboost': True,        # ~12 sec - Decay + XGBoost residual
    'arihow': True,                # ~30 sec - SARIMAX + Holt-Winters
}

#
================================================================================
# 3. TIME-WINDOW SAMPLE WEIGHTS (NEW!) 🆕
#
================================================================================
USE_TIME_WINDOW_WEIGHTS = True  # Enable time-window based sample weighting
```

```
# Scenario 1: Months 0-5 most important (50% of PE score!)
S1_TIME_WINDOW_WEIGHTS = {
    '0_5': 2.5,        # Months 0-5: 2.5× weight (matches PE formula)
    '6_11': 1.0,       # Months 6-11: normal weight
    '12_23': 0.5,      # Months 12-23: lower weight
    'pre_entry': 0.1   # Pre-entry months: minimal weight
}

# Scenario 2: Months 6-11 most important (50% of PE score!)
S2_TIME_WINDOW_WEIGHTS = {
    '6_11': 2.5,       # Months 6-11: 2.5× weight (matches PE formula)
    '12_23': 1.5,      # Months 12-23: higher weight (30% of PE)
    'pre_entry': 0.1   # Pre-entry months: minimal weight
}

#
================================================================================
# 4-14. Other sections: Paths, Constants, Model Parameters, etc.
#
================================================================================
```

View current config:

```
python src/config.py
```

In simple terms: This is like a "control panel" where you adjust all the knobs in one place instead of hunting through every file.

---

2 `src/data_loader.py` - The Data Reader

	Description
INPUT	3 raw CSV files: `df_volume_[train/test].csv`, `df_generics_[train/test].csv`, `df_medicine_info.csv`
OUTPUT	Single merged DataFrame with all columns from all 3 files
GOAL	Combine scattered data into ONE unified table for analysis

What it does: Loads the 3 CSV files and combines them.

The 3 datasets:

File	Contains	Key Columns

File	Contains	Key Columns
`df_volume`	Sales history	`volume` (units sold each month)
`df_generics`	Competition info	`n_gxs` (number of generic competitors)
`df_medicine_info`	Drug characteristics	`ther_area`, `hospital_rate`, etc.

Key functions:

```
# Load one dataset
volume_df = load_volume_data(train=True)

# Load all 3 datasets
volume, generics, medicine = load_all_data(train=True)

# MERGE them together into ONE table
merged = merge_datasets(volume, generics, medicine)
```

In simple terms: Like gathering ingredients from 3 different shelves and putting them on ONE cutting board.

Output: A single DataFrame with ALL information per (country, brand, month).

2a. Data Cleaning Functions 🆕

New data cleaning utilities to ensure data quality before feature engineering:

```
from data_loader import (
    remove_duplicates,
    verify_months_postgx_range,
    check_multiple_rows_per_month,
    create_time_to_50pct_features,
    impute_avg_vol_regression,
    create_vol_norm_gt1_flag,
    clean_data
)
```

`remove_duplicates(df)` - Drops exact duplicate rows

```
df_clean = remove_duplicates(df)
# Logs: "Removed X duplicate rows (Y% of data)"
```

`verify_months_postgx_range(df, expected_min=-9, expected_max=23)` - Validates month range

```
is_valid = verify_months_postgx_range(df)
# Returns: True if all months_postgx in [-9, 23], else False with warning
```

`check_multiple_rows_per_month(df)` - Detects duplicate (brand, month) pairs

```
duplicates = check_multiple_rows_per_month(df)
# Returns: DataFrame of duplicate entries or empty if clean
```

`create_time_to_50pct_features(df)` - Calculate erosion speed metrics

```
df = create_time_to_50pct_features(df)
# Adds columns: time_to_50pct, reached_50pct, erosion_speed_category
```

`impute_avg_vol_regression(df)` - Fill missing avg_vol using ML regression

```
df = impute_avg_vol_regression(df)
# Uses GBT regressor to predict missing avg_vol from other features
```

`create_vol_norm_gt1_flag(df)` - Flag anomalous volume growth

```
df = create_vol_norm_gt1_flag(df)
# Adds: vol_norm_gt1 (binary flag for volume exceeding pre-entry baseline)
```

`clean_data(df)` - Run all cleaning steps in sequence

```
df_clean = clean_data(df)
# Combines: remove_duplicates → verify_months_postgx_range → etc.
```

---

3 `src/bucket_calculator.py` - The Normalization Engine

	Description

	Description
📥 **INPUT**	Merged DataFrame with `volume` column and `months_pregx` (pre-entry months: -12 to -1)
📤 **OUTPUT**	`aux_bucket_avgvol.csv` file with columns: `country`, `brand_name`, `avg_vol`, `mean_erosion`, `bucket`
🎯 **GOAL**	Calculate the baseline (avg_vol) and bucket assignment for scoring

What it does: Calculates key metrics for evaluation.

Step-by-step:

Step A: Calculate `Avg_j` (Pre-entry Average)

```
For each drug:
    Avg_j = average volume from month -12 to -1
```

Example:

- BrandX sold 1000, 1100, 900, ... units in the 12 months BEFORE generics arrived
- Avg_j = average of these = 1000 units

Why? This is the "baseline" to compare against. If you predict 500 units and Avg_j was 1000, that's 50% of baseline.

Step B: Calculate Normalized Volume

```
Normalized Volume = Actual Volume / Avg_j
```

Example:

- Month 3 actual: 400 units
- Avg_j: 1000 units
- Normalized: 400/1000 = 0.4 (40% of original sales)

Step C: Calculate Mean Erosion

```
Mean Erosion = average(Normalized Volume) over months 0-23
```

Example:

- BrandX normalized volumes: [0.8, 0.6, 0.4, 0.3, 0.2, ...]
- Mean erosion = average = 0.35

Step D: Assign Buckets

```
if Mean Erosion ≤ 0.25:
    Bucket = 1  (HIGH erosion - severe sales crash)
else:
    Bucket = 2  (LOWER erosion - moderate decline)
```

Output file: `aux_bucket_avgvol.csv` containing:

- `country`, `brand_name`
- `avg_vol` (the pre-entry average)
- `mean_erosion`
- `bucket` (1 or 2)

---

4 `src/feature_engineering.py` - The Feature Factory

	Description
📥 **INPUT**	Merged DataFrame + `aux_bucket_avgvol.csv` (for avg_vol baseline)
📤 **OUTPUT**	DataFrame with original columns + **76 NEW feature columns** 🆕
🎯 **GOAL**	Transform raw data into ML-friendly patterns that capture erosion dynamics

What it does: Creates **76 features** for the ML model to learn from.

Feature Categories:

A. Lag Features (Past Values)

```
volume_lag_1  = volume from 1 month ago
volume_lag_3  = volume from 3 months ago
volume_lag_6  = volume from 6 months ago
volume_lag_12 = volume from 12 months ago
```

Why? Recent sales predict future sales.

B. Rolling Features (Trends)

```
rolling_mean_3  = average of last 3 months
rolling_std_3   = volatility of last 3 months
rolling_mean_6  = average of last 6 months
rolling_mean_12 = average of last 12 months
```

Why? Captures momentum and stability.

C. Competition Features (Generics)

```
n_gxs              = number of generic competitors NOW
n_gxs_cummax       = maximum competitors seen so far
months_with_generics = how long generics have been in market
max_n_gxs_post     = max competitors the brand will ever face (brand-level) 🆕
```

Why? More competitors = more erosion.

D. Pre-Entry Features (CRITICAL for Scenario 1)

```
avg_vol            = pre-entry average (the baseline)
pre_entry_slope    = was sales growing or declining BEFORE generics?
pre_entry_volatility = how stable were sales before?
log_avg_vol        = log transform of avg_vol (reduces skew) 🆕
pre_loe_growth_flag = 1 if pre-entry slope > 0 (growing brand) 🆕
```

Why? In Scenario 1, this is ALL you have to predict with!

E. Time Features

```
months_postgx = months since generic entry (0, 1, 2, ...)
month_sin/cos = capture seasonality
is_early_postgx = is this in first 6 months? (binary)
```

F. Early Post-LOE Features (For Scenario 2) 🆕

```
# Aggregate features from months 0-5 for Scenario 2 predictions
early_vol_mean   = mean volume in months 0-5
```

```
early_vol_min    = minimum volume in months 0-5
early_vol_max    = maximum volume in months 0-5
early_vol_last   = volume at month 5 (last known value)
early_vol_slope  = linear trend in months 0-5
early_erosion_ratio = (avg_vol - early_vol_mean) / avg_vol
early_n_gxs_max  = max competitors seen in months 0-5
early_volatility = std deviation in months 0-5
```

Why? In Scenario 2, we have actual months 0-5 - use them to predict 6-23!

G. Anomaly & Quality Flags 🆕

```
vol_norm_gt1     = binary flag for volume > pre-entry baseline
time_to_50pct    = months until erosion reached 50%
erosion_speed_category = 'fast', 'medium', 'slow', 'none'
```

Output: DataFrame with original data + **76 new feature columns**.

4a. FeatureScaler Class 🆕

New class for standardized feature scaling:

```
from feature_engineering import FeatureScaler, scale_features

# Initialize scaler with different modes
scaler = FeatureScaler(
    mode='standard',      # 'standard', 'minmax', or 'log'
    clip_outliers=True,   # Clip to 3 std deviations before scaling
    epsilon=1e-8          # Smoothing for log transform
)

# Fit on training data
scaler.fit(X_train)

# Transform training and validation data
X_train_scaled = scaler.transform(X_train)
X_val_scaled = scaler.transform(X_val)

# Or use convenience function
X_scaled = scale_features(X_train, mode='standard')
```

Scaling Modes:

- `standard` : Zero mean, unit variance (StandardScaler)

- `minmax` : Scale to [0, 1] range (MinMaxScaler)
- `log` : Log transform (good for skewed distributions like volume)

4b. Target Encoding (Leakage-Safe) 🆕

Cross-validated target encoding to prevent data leakage:

```
from feature_engineering import target_encode_cv,
create_target_encoded_features

# Within CV folds - encodes using only training data in each fold
df_encoded = target_encode_cv(
    df,
    col='ther_area',           # Column to encode
    target='vol_norm',         # Target variable
    cv=5,                      # Number of CV folds
    smoothing=10               # Bayesian smoothing parameter
)
# Adds: ther_area_target_encoded

# Batch encode multiple categorical columns
df = create_target_encoded_features(df, target='vol_norm')
# Encodes: ther_area, country, nfc_code (if present)
```

Why target encoding? Converts high-cardinality categoricals (like country) to meaningful numeric values based on target correlation, without label leakage.

4c. Sample Weighting (Time-Window Based) 🆕

Configurable sample weights that emphasize important time periods:

```
from feature_engineering import (
    compute_time_window_weights,
    compute_combined_sample_weights
)

# Time-window only weights
weights = compute_time_window_weights(df, scenario=1)
# Uses config.S1_TIME_WINDOW_WEIGHTS:
#   months 0-5:   2.5x weight (MOST important for scoring!)
#   months 6-11:  1.0x weight
#   months 12-23: 0.5x weight
#   pre-entry:    0.1x weight

# Combined bucket × time-window weights
weights = compute_combined_sample_weights(df, scenario=1)
# Multiplies bucket weights × time-window weights
```

Why weighting? PE scoring weights months 0-5 at 50% - train model to prioritize these!

4d. Horizon-as-Row Dataset 🆕

Alternative dataset structure for forecasting models:

```
from feature_engineering import create_horizon_as_row_dataset

# Convert time-series to cross-sectional format
df_horizon = create_horizon_as_row_dataset(df, horizons=[0, 6, 12, 18])
# Each row is (brand, horizon) with features from observation point
# Useful for: gradient boosting treating each horizon as independent
prediction
```

Output: DataFrame with original data + **76 new feature columns**.

---

5 `src/models.py` - The Prediction Models

	Description
📥 **INPUT**	Feature matrix X (from feature_engineering), target vector y (actual volumes), avg_vol per brand
📤 **OUTPUT**	Trained model object + predictions array + saved model file (`.joblib`)
🎯 **GOAL**	Learn patterns from historical data to predict future sales volumes

What it does: Implements different prediction strategies.

A. Baseline Models (Simple)

1. No Erosion Baseline:

```
prediction = avg_vol  # (assume sales stay the same forever)
```

This is the WORST case - it ignores erosion completely.

2. Linear Decay:

```
prediction = avg_vol × (1 - 0.03 × month)
```

Sales drop by 3% each month in a straight line.

3. Exponential Decay: ☑ BEST PERFORMER

```
prediction = avg_vol × exp(-0.05 × month)
```

Sales drop quickly at first, then slow down (like real erosion!).

Why exponential works best: Generic erosion follows this pattern naturally:

- Month 0-3: Big drop (generics are new, doctors switch)
- Month 12+: Slower decline (loyal patients stay)

B. ML Models (Complex)

LightGBM / XGBoost:

- Use ALL 40 features
- Learn patterns from historical data
- Can capture non-linear relationships

```
model = GradientBoostingModel(model_type='lightgbm')
model.fit(X_train, y_train)
predictions = model.predict(X_test)
model.save("scenario1_lightgbm")
```

Current Result: Baseline exponential (PE=1.18) beats ML models (PE=2.84+)

Why? The decay pattern is so consistent that a simple formula works better than complex ML on this data.

C. Hybrid Model (Physics + ML) 🆕

The Best of Both Worlds!

```
# Physics-based baseline
base_prediction = avg_vol × exp(-0.05 × month)

# ML learns the residuals (what physics misses)
residual = ML_model.predict(features)

# Combine them
final_prediction = base_prediction + residual
```

Why Hybrid?

- Physics captures the KNOWN decay pattern
- ML corrects systematic deviations
- Best of both worlds!

Class: `HybridPhysicsMLModel`

```
from models import HybridPhysicsMLModel

hybrid = HybridPhysicsMLModel(
    ml_model_type='lightgbm',  # or 'xgboost'
    decay_rate=0.05
)

# Training requires avg_vol and months for physics baseline
hybrid.fit(X_train, y_train, avg_vol_train, months_train,
           X_val, y_val, avg_vol_val, months_val)

# Prediction also needs avg_vol and months
predictions = hybrid.predict(X_test, avg_vol_test, months_test)

# Save/Load
hybrid.save("scenario1_hybrid")
hybrid.load("scenario1_hybrid")
```

Current Results:

Model	Scenario 1 PE	Scenario 2 PE
Hybrid-Physics+LightGBM	**1.08**	29.60
Exponential Decay	1.18	**1.10**
XGBoost	2.84	3.39

Key Insight: Hybrid wins for Scenario 1 (no actuals), Baseline wins for Scenario 2 (has 0-5 actuals).

5c. ARHOW Model (SARIMAX + Holt-Winters Ensemble)

Time-Series Based Forecasting!

The ARHOW (ARIMA + Holt-Winters) model uses a sophisticated ensemble approach:

```
# For each brand, fit two time-series models on pre-entry data:
1. SARIMAX - Captures autocorrelation and trend
2. Holt-Winters (ExponentialSmoothing) - Captures level and trend
```

```
# Learn optimal weights via Linear Regression:
y_hat = β₀ × y_SARIMAX + β₁ × y_HW

# The weights are learned from the last N observations
```

Why This Approach?

- SARIMAX captures autoregressive patterns in the data
- Holt-Winters captures exponential smoothing trends
- Learned weights (β_0, β_1) adapt to each brand's characteristics
- No manual weight tuning required

Class: `ARIHOWModel`

```
from models import ARIHOWModel

arhow = ARIHOWModel(
    arima_order=(1, 1, 1),      # ARIMA(p,d,q)
    seasonal_order=(0, 0, 0, 0), # SARIMA seasonal
    hw_trend='add',              # Holt-Winters trend type
    hw_seasonal=None,            # HW seasonality
    hw_seasonal_periods=12,      # Seasonal period
    weight_window=12             # Observations for weight learning
)

# Fit on ALL brands (not just training set)
arhow.fit(df)  # Full dataframe with all brands

# Predict for test brands
predictions = arhow.predict(X_test)

# Inspect learned weights per brand
weights = arhow.get_brand_weights()
# Returns: {(country, brand): {'beta0': 0.6, 'beta1': 0.4, 'method':
'weights'}, ...}
```

Key Features:

- ☑ Fits on ALL brands' pre-entry data (not just training brands)
- ☑ Uses `get_forecast()` with RangeIndex for statsmodels compatibility
- ☑ Falls back to exponential decay if time-series fitting fails
- ☑ Suppresses statsmodels warnings for cleaner output

5d. GroupKFold Cross-Validation NEW

Prevent Brand Leakage in CV!

Standard KFold can split the same brand's months across train/val, causing leakage. GroupKFold ensures all months of a brand stay together:

```
from models import GBTModel

model = GBTModel(model_type='lightgbm')

# GroupKFold CV - brands stay together in folds
cv_results = model.cross_validate_grouped(
    X, y,
    groups=df['brand_id'],  # Brand identifier column
    n_splits=5,             # Number of CV folds
    sample_weight=weights   # Optional sample weights
)

# Returns dict with:
# - 'fold_scores': list of fold validation scores
# - 'mean_score': average across folds
# - 'std_score': standard deviation
# - 'fold_models': trained model per fold (optional)
```

Why GroupKFold?

- Standard CV leaks future information when brand months span train/val
- GroupKFold treats each brand as an atomic unit
- More realistic estimate of generalization to NEW brands

5e. EnsembleBlender Class 🆕

Learn Optimal Model Combination Weights!

Instead of guessing ensemble weights, learn them from validation data:

```
from models import EnsembleBlender, optimize_ensemble_weights

# Get predictions from multiple models
preds_dict = {
    'exp_decay': baseline_model.predict(X_val),
    'lightgbm': lgb_model.predict(X_val),
    'hybrid': hybrid_model.predict(X_val)
}

# Option 1: EnsembleBlender class
blender = EnsembleBlender(method='ridge')  # 'ridge', 'nnls', or 'simple'
blender.fit(preds_dict, y_val, avg_vol=avg_vol_val)

# Get learned weights
```

```
print(blender.weights_)
# {'exp_decay': 0.65, 'lightgbm': 0.25, 'hybrid': 0.10}

# Blend predictions for test set
test_preds_dict = {
    'exp_decay': baseline_model.predict(X_test),
    'lightgbm': lgb_model.predict(X_test),
    'hybrid': hybrid_model.predict(X_test)
}
final_preds = blender.predict(test_preds_dict)

# Option 2: Convenience function
weights, blender = optimize_ensemble_weights(
    preds_dict, y_val,
    method='ridge',
    return_blender=True
)
```

Blending Methods:

- `ridge` : Ridge regression (handles correlated predictions)
- `nnls` : Non-negative least squares (weights ≥ 0)
- `simple` : Equal weights (baseline)

Why Ensemble Blending?

- Different models capture different patterns
- Learned weights adapt to your specific data
- Often beats best single model

---

6 `src/evaluation.py` - The Scoring System

	Description
📥 **INPUT**	Predictions DataFrame, Actuals DataFrame, `aux_bucket_avgvol.csv` (for avg_vol & buckets)
📤 **OUTPUT**	PE score (float) - lower is better
🎯 **GOAL**	Measure prediction accuracy using the EXACT same formula the competition uses

What it does: Calculates the official competition metric (PE = Prediction Error).

Scenario 1 PE Formula:

```
PE = 0.2 × (monthly errors normalized)
   + 0.5 × (error in months 0-5 sum)      ← 50% WEIGHT!
```

```
      + 0.2 × (error in months 6-11 sum)
      + 0.1 × (error in months 12-23 sum)
```

In plain English:

- Getting months 0-5 right is HALF your score
- Monthly individual errors = 20%
- Later months matter less

Scenario 2 PE Formula:

```
PE = 0.2 × (monthly errors normalized)
   + 0.5 × (error in months 6-11 sum)     ← 50% WEIGHT!
   + 0.3 × (error in months 12-23 sum)
```

Final Score Calculation:

```
Final Score = (2 × avg_PE_bucket1 + 1 × avg_PE_bucket2) /
total_weighted_brands
```

The key insight: Bucket 1 errors count DOUBLE.

Example:

- Bucket 1 average PE: 0.5 (10 brands)
- Bucket 2 average PE: 0.3 (100 brands)
- Final = (2×0.5×10 + 1×0.3×100) / (2×10 + 1×100) = (10 + 30) / 120 = 0.33

📊 Detailed PE Calculation Example

Setup: One Brand Example

Let's say you're predicting for **Brand_ABC** in **Country_001**:

Pre-Entry Data (months -12 to -1)	Volume
Month -12	1000
Month -11	1100
...	...
Month -1	1200
Avg_j (pre-entry average)	**1000**

Your Predictions vs Actuals (Scenario 1):

Month	Prediction	Actual	Error
0	800	750	50
1	750	700	50
2-5	...	...	...
6-23	...	...	...

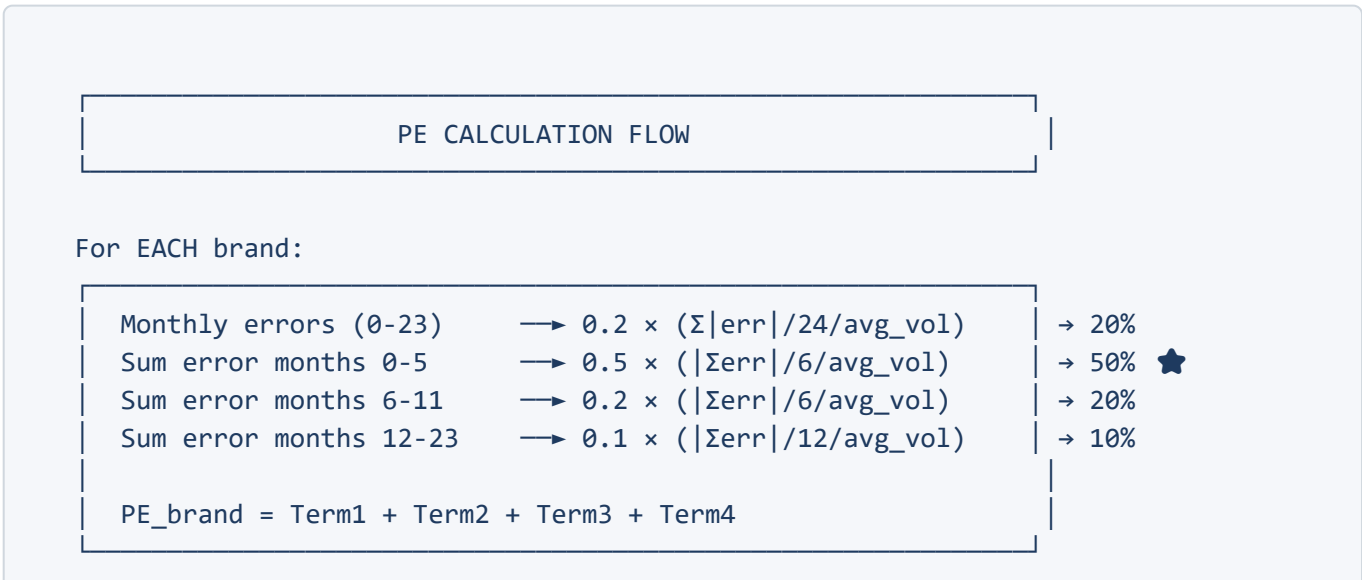
Step 1: Calculate Each PE Term

```
Term 1 (Monthly): 0.2 × (Σ|errors| / 24 / avg_vol) = 0.2 × (600/24/1000) =
0.005
Term 2 (Sum 0-5): 0.5 × (|Σerr| / 6 / avg_vol) = 0.5 × (270/6/1000) = 0.0225
⭐ 50%!
Term 3 (Sum 6-11): 0.2 × (|Σerr| / 6 / avg_vol) = 0.2 × (150/6/1000) = 0.005
Term 4 (Sum 12-23): 0.1 × (|Σerr| / 12 / avg_vol) = 0.1 × (100/12/1000) =
0.00083

PE_brand = 0.005 + 0.0225 + 0.005 + 0.00083 = 0.0333
```

Step 2: Aggregate with Bucket Weighting

```
Bucket 1 (40 brands): avg PE = 0.04  →  weighted: 2 × 0.04 = 0.08
Bucket 2 (300 brands): avg PE = 0.025 → weighted: 1 × 0.025 = 0.025

Final Score = 0.08 + 0.025 = 0.105
```

Visual Summary:



```
                                    │
                                    ▼
    ┌─────────────────────────────────────────────────────────────┐
    │  BUCKET WEIGHTING                                           │
    │                                                             │
    │  Bucket 1 (high erosion):  2× weight  ← FOCUS HERE!         │
    │  Bucket 2 (normal erosion): 1× weight                       │
    │                                                             │
    │  Final = (2/n_B1)×Σ(PE_B1) + (1/n_B2)×Σ(PE_B2)              │
    └─────────────────────────────────────────────────────────────┘
                                    │
                                    ▼
                          🎯 LOWER = BETTER 🎯

              0.0 = Perfect    |    3.0+ = Very Bad
```

Key Takeaways for Winning:

Priority	Focus Area	Why
#1	Months 0-5 accuracy	50% of your PE score!
#2	Bucket 1 brands	Errors count 2×
#3	Early erosion pattern	Get the "cliff" shape right
#4	Months 6-11	20% of score
#5	Months 12-23	Only 10% of score

---

7 `src/submission.py` - The Output Generator

	Description
INPUT	Predictions DataFrame with columns: `country`, `brand_name`, `months_postgx`, `volume`
OUTPUT	CSV file formatted for competition upload (e.g., `scenario1_baseline_final.csv`)
GOAL	Format predictions into the EXACT structure required by the competition

What it does: Creates the CSV file you upload to the competition.

Required Format:

country	brand_name	months_postgx	volume
COUNTRY_001	BRAND_ABC	0	1234.56
COUNTRY_001	BRAND_ABC	1	1100.23

country	brand_name	months_postgx	volume
...	...	...	...
COUNTRY_001	BRAND_ABC	23	456.78

Validation Checks:

```
☑ All required columns present
☑ No missing values
☑ No negative volumes
☑ Correct months for scenario (0-23 or 6-23)
☑ Every brand has all required months
☑ Total rows = brands × months
```

Example output:

- Scenario 1: 340 brands × 24 months = 8,160 rows
- Scenario 2: 340 brands × 18 months = 6,120 rows

📤 Files to Upload (Competition Submission)

You need to upload **2 CSV files**:

File	Predicts	For
`scenario1_[model]_final.csv`	Months **0-23** (24 months)	228 test brands
`scenario2_[model]_final.csv`	Months **6-23** (18 months)	112 test brands

Expected Row Counts:

Submission	Brands	Months	Total Rows
Scenario 1	228	24 (0-23)	**5,472 rows**
Scenario 2	112	18 (6-23)	**2,016 rows**

Generate & Validate:

```
python scripts/generate_final_submissions.py  # Generate both files
python scripts/validate_submissions.py        # Validate before upload
```

---

8 `src/pipeline.py` - The Orchestrator

	Description
📥 **INPUT**	Command-line arguments: `--scenario` (1 or 2), `--model` (baseline/lightgbm/xgboost)
📤 **OUTPUT**	Trained model files, submission CSVs, performance reports
🎯 **GOAL**	Run the ENTIRE workflow from raw data to final submission in ONE command

What it does: Runs EVERYTHING in the correct order.

The Pipeline Steps:

```
STEP 1: Load Data
    ↓
STEP 2: Create Auxiliary File (avg_vol, buckets)
    ↓
STEP 3: Feature Engineering (create 40 features)
    ↓
STEP 4: Split Train/Validation
    ↓
STEP 5: Prepare X (features) and y (target)
    ↓
STEP 6: Train Model
    ↓
STEP 7: Evaluate on Validation Set
    ↓
STEP 8: Generate Submission File
```

Usage:

```
python src/pipeline.py --scenario 1 --model lightgbm
```

---

9 `src/eda_analysis.py` - The Data Explorer

	Description
📥 **INPUT**	Merged DataFrame from data_loader
📤 **OUTPUT**	Dictionary of statistics, DataFrames with aggregated insights
🎯 **GOAL**	Understand data patterns BEFORE modeling to inform feature engineering

What it does: Analyzes and understands the data BEFORE modeling.

Key analyses:

```
# Data quality
- Missing values per column
- Duplicate records
- Negative volumes

# Distribution analysis
- Volume distribution (heavily right-skewed)
- Brands per country
- Brands per therapeutic area

# Erosion analysis
- Average erosion curve over 24 months
- Erosion by bucket
- Impact of competition on erosion

# Bucket analysis
- How many Bucket 1 vs Bucket 2?
- Characteristics of high-erosion drugs
```

Scripts Explained

`scripts/run_demo.py`

	Description
INPUT	Raw data files
OUTPUT	Console output showing pipeline works
GOAL	Quick sanity check that all code works

Purpose: Quick test to make sure everything works.

```
python scripts/run_demo.py
```

What it does:

1. Loads small sample of data
2. Creates features
3. Trains baseline model
4. Evaluates predictions
5. Generates sample submission

Use when: You want to quickly verify the code works.

`scripts/train_models.py`

	Description
📥 **INPUT**	Raw data files, `--scenario` argument (1 or 2)
📤 **OUTPUT**	Model files in `models/`, comparison CSV in `reports/`
🎯 **GOAL**	Train ALL models and find the best one for each scenario

Purpose: Train and compare ALL models.

```
python scripts/train_models.py --scenario 1
python scripts/train_models.py --scenario 2
```

What it does:

1. Trains No Erosion baseline
2. Trains Exponential Decay baseline (tunes λ)
3. Trains LightGBM
4. Trains XGBoost
5. Compares all models
6. Saves best models to `models/`
7. Saves comparison to `reports/model_comparison_scenarioX.csv`

`scripts/generate_final_submissions.py`

	Description
📥 **INPUT**	Test data, trained models, `--model` argument
📤 **OUTPUT**	`submissions/scenario1_*_final.csv`, `submissions/scenario2_*_final.csv`
🎯 **GOAL**	Create the final CSV files ready for competition upload

Purpose: Create the final competition submission files.

```
python scripts/generate_final_submissions.py --model baseline
```

Output:

- `submissions/scenario1_baseline_final.csv`
- `submissions/scenario2_baseline_final.csv`

`scripts/validate_submissions.py`

	Description
📥 **INPUT**	Submission CSV files in `submissions/` folder
📤 **OUTPUT**	Console output with pass/fail for each check
🎯 **GOAL**	Verify submission files meet ALL competition requirements BEFORE upload

Purpose: Check submissions BEFORE uploading.

```
python scripts/validate_submissions.py
```

Checks:

- ☑ Correct column names
- ☑ No missing values
- ☑ No negative volumes
- ☑ Correct months per scenario
- ☑ All brands present
- ☑ Correct total row count

📓 Notebooks Explained

Notebook	Input	Output	Goal
`01_eda_visualization.ipynb`	Raw data	Visualizations + insights	Understand data before modeling
`02_feature_exploration.ipynb`	Feature DataFrame	Feature correlation heatmaps, importance charts	Validate feature engineering
`03_model_results.ipynb`	Model comparison CSVs	Performance charts	Compare models, analyze predictions

Notebook	Purpose
`01_eda_visualization.ipynb`	See data distributions, erosion curves, bucket breakdown
`02_feature_exploration.ipynb`	Visualize features, correlations, importances
`03_model_results.ipynb`	Compare model performance, analyze submissions

These are for VISUALIZATION only - all logic is in `src/` files.

Reports Structure 🆕 (Updated)

All three notebooks export figures with corresponding JSON summaries and CSV data files in organized subfolders:

```
reports/
├── 01_eda_data/                        # EDA visualization data
│   ├── figures/                        # PNG figures
│   │   ├── fig01_bucket_distribution.png
│   │   ├── fig02_erosion_curves.png
│   │   ├── fig03_sample_trajectories.png
│   │   ├── fig04_competition_impact.png
│   │   ├── fig05_therapeutic_areas.png
│   │   ├── fig06_biological_vs_small.png
│   │   ├── fig07_hospital_rate.png
│   │   └── fig08_erosion_speed.png
│   ├── fig01_bucket_distribution.json/csv
│   ├── fig02_erosion_curves.json/csv
│   ├── fig03_sample_trajectories.json/csv
│   ├── fig04_competition_impact.json + n_gxs_impact.csv
│   ├── fig05_therapeutic_areas.json/csv
│   ├── fig06_biological_vs_small.json/csv
│   ├── fig07_hospital_rate.json/csv
│   ├── fig08_erosion_speed.json + erosion_speed_full.csv
│   └── eda_complete_summary.json
│
├── 02_feature_data/                    # Feature exploration data
│   ├── figures/                        # PNG figures
│   │   ├── fig01_feature_correlation.png
│   │   ├── fig02_target_correlation.png
│   │   ├── fig03_feature_distributions.png
│   │   ├── fig04_lag_features.png
│   │   ├── fig05_rolling_features.png
│   │   ├── fig06_competition_features.png
│   │   └── fig07_time_features.png
│   ├── fig01_feature_correlation.json/csv
│   ├── fig02_target_correlation.json/csv
│   ├── fig03_feature_distributions.json/csv
│   ├── fig04_lag_features.json/csv
│   ├── fig05_rolling_features.json/csv
│   ├── fig06_competition_features.json/csv
│   ├── fig07_time_features.json/csv
│   └── feature_exploration_complete_summary.json
│
├── 03_model_data/                      # Model results data
│   ├── figures/                        # PNG figures
│   │   ├── fig01_model_comparison.png
│   │   ├── fig02_bucket_performance.png
│   │   ├── fig03_feature_importance.png
│   │   ├── fig04_submission_predictions.png
│   │   └── fig05_prediction_distribution.png
│   ├── fig01_model_comparison.json + s1.csv + s2.csv
│   ├── fig02_bucket_performance.json
│   ├── fig03_feature_importance.json + s1.csv + s2.csv
```

```
│   ├── fig04_submission_analysis.json + by_month_s1.csv + by_month_s2.csv
│   ├── fig05_prediction_distribution.json
│   └── model_results_complete_summary.json
│
├── model_comparison_scenario1.csv      # Training results
├── model_comparison_scenario2.csv
├── run_summary_scenario1_*.json        # Run summaries with full config
└── run_summary_scenario2_*.json
```

JSON File Contents:

- Metadata (filename, description, generated timestamp)
- Summary statistics for the visualization
- Interpretations and key insights
- References to corresponding figure files

CSV File Contents:

- Raw data used to generate each figure
- Can be used for custom visualizations or further analysis
- Full data tables for deeper analysis

Running the notebooks:

```
python notebooks/01_eda_visualization.py      # Generates 01_eda_data/
python notebooks/02_feature_exploration.py    # Generates 02_feature_data/
python notebooks/03_model_results.py          # Generates 03_model_data/
```

🔄 Complete Workflow

Option 1: Config-Based (Recommended) 🆕

Just edit `src/config.py` toggles and run ONE command:

```
# 1. Edit config.py to set your preferences:
#    RUN_SCENARIO = 1          # or 2, or [1, 2]
#    TEST_MODE = True          # False for full training
#    MODELS_ENABLED = {...}    # Enable/disable models
#    RUN_TRAINING = True
#    RUN_SUBMISSION = True

# 2. Run the master pipeline
python scripts/run_pipeline.py
```

Option 2: Individual Scripts (CLI Override)

```
# Uses config.py settings by default, CLI can override
python scripts/train_models.py                    # Uses config settings
python scripts/train_models.py --scenario 2       # Override scenario
python scripts/train_models.py --full             # Override to full mode
python scripts/generate_final_submissions.py      # Uses SUBMISSION_MODEL from
config
```

Option 3: Step-by-Step Manual

```
┌──────────────────────────────────────────────────────────────┐
│                    MANUAL WORKFLOW                           │
└──────────────────────────────────────────────────────────────┘

1. SETUP
   pip install -r requirements.txt

2. VIEW CONFIG
   python src/config.py

3. EXPLORE DATA (optional)
   python notebooks/01_eda_visualization.py

4. TRAIN MODELS
   python scripts/train_models.py

5. CHECK RESULTS
   Look at reports/model_comparison_scenario1.csv

6. GENERATE SUBMISSIONS
   python scripts/generate_final_submissions.py

7. VALIDATE
   python scripts/validate_submissions.py

8. SUBMIT
   Upload submissions/*.csv to competition
```

📈 Current Results (Updated November 2025) 🆕

Latest Model Comparison (Test Mode)

Scenario 1: (Predict months 0-23 with only pre-entry data)

Model	Final PE Score
Baseline-ExpDecay(0.020)	**0.1483**
Hybrid-Physics+LightGBM	0.2294
Baseline-NoErosion	0.2470
Hybrid-Physics+XGBoost	0.2716
ARHOW-SARIMAX+HW	0.2995
LightGBM	0.3432
XGBoost	0.6738

Scenario 2: (Predict months 6-23 with actual months 0-5)

Model	Final PE Score
Baseline-ExpDecay(0.020)	**0.1580**
Hybrid-Physics+LightGBM	0.2086
Hybrid-Physics+XGBoost	0.3258
Baseline-NoErosion	0.3289
LightGBM	0.3316
ARHOW-SARIMAX+HW	0.4062
XGBoost	0.6445

Key Findings:

1. **Exponential Decay Baseline wins both scenarios** - Simple physics-based approach outperforms complex ML
2. **Hybrid models are strong second place** - Physics + ML correction works well
3. **ARHOW model** - Time-series approach shows promise but needs tuning
4. **Pure ML models struggle** - XGBoost/LightGBM alone don't capture erosion patterns well

Recommendations:

- **Scenario 1:** Use Exponential Decay (PE=0.1483) or Hybrid-LightGBM (PE=0.2294)
- **Scenario 2:** Use Exponential Decay (PE=0.1580) or Hybrid-LightGBM (PE=0.2086)

Output Files with Timestamps

All training runs and submissions now save with timestamps and JSON summaries.

Training Output Files:

```
reports/
├── model_comparison_scenario1_20251128_210310.csv    ← Timestamped CSV
├── model_comparison_scenario1.csv                     ← Latest (easy access)
├── run_summary_scenario1_20251128_210310.json        ← Full JSON summary
├── model_comparison_scenario2_20251128_210433.csv
├── model_comparison_scenario2.csv
└── run_summary_scenario2_20251128_210433.json
```

EDA Data Files: 🆕

```
reports/eda_data/
├── fig01_volume_distribution.json + .csv
├── fig02_erosion_curves.json + .csv
├── fig03_bucket_distribution.json + .csv
├── fig04_generic_impact.json + .csv
├── fig05_therapeutic_area.json + .csv
├── fig06_monthly_patterns.json + .csv
├── fig07_correlation_matrix.json + .csv
└── fig08_country_analysis.json + .csv
```

Submission Output Files:

```
submissions/
├── scenario1_baseline_20251128_185734.csv           ← Timestamped CSV
├── scenario1_baseline_20251128_185734.json          ← Summary JSON
└── scenario1_baseline_final.csv                      ← Latest (easy access)
```

JSON Summary Contents:

Training Run Summary (`run_summary_*.json`):

```
{
  "run_info": {
    "run_id": "20251128_185725",
    "timestamp": "20251128_185725",
    "scenario": 1,
    "date": "2025-11-28",
    "time": "18:57:25"
  },
  "best_model": {
    "name": "Hybrid-Physics+LightGBM",
```

```
    "final_score": 1.0758
  },
  "all_results": [...],
  "config": {
    "paths": {...},
    "constants": {...},
    "metric_weights": {...},
    "model_params": {...}
  },
  "data_info": {
    "train_rows": 75024,
    "val_rows": 18720,
    "n_features": 40,
    "feature_cols": [...]
  },
  "feature_importance": [...]
}
```


Submission Summary (`scenario*_*.json`):


```
{
  "submission_info": {
    "scenario": 1,
    "model_type": "baseline",
    "timestamp": "20251128_185734",
    "date": "2025-11-28",
    "time": "18:57:34"
  },
  "data_stats": {
    "n_brands": 340,
    "n_rows": 8160,
    "months_predicted": [0, 1, ..., 23]
  },
  "volume_predictions": {
    "min": 25.84,
    "max": 126466938.0,
    "mean": 1909240.94,
    "median": 110694.60,
    "std": 7035711.05
  },
  "model_config": {
    "decay_rate": 0.05,
    "model_type": "baseline"
  },
  "full_config": {...}
}
```

🎯 Key Takeaways

1. **Bucket 1 is CRITICAL** - Double weighted, focus on high-erosion drugs
2. **Early months matter most** - 50% of score from first 6 months
3. **Simple models can win** - Exponential decay captures the physics
4. **Normalize everything** - All errors divided by pre-entry average
5. **Validate before submit** - One wrong format = rejected submission

---

📚 Quick Reference

🆕 Config-Based Commands (Recommended)

Task	Command	Config Toggle
Show current config	`python src/config.py`	-
Run full pipeline	`python scripts/run_pipeline.py`	All `RUN_*` toggles
Train models only	`python scripts/train_models.py`	`RUN_SCENARIO`, `TEST_MODE`, `MODELS_ENABLED`
Generate submissions	`python scripts/generate_final_submissions.py`	`RUN_SCENARIO`, `SUBMISSION_MODEL`
Run EDA	`python notebooks/01_eda_visualization.py`	-
Validate submissions	`python scripts/validate_submissions.py`	-

CLI Override Commands (Legacy)

Task	Command
Train specific scenario	`python scripts/train_models.py --scenario 1`
Train in test mode	`python scripts/train_models.py --test`
Force full mode	`python scripts/train_models.py --no-test`

Available Model Types:

- `baseline_no_erosion` - No generic erosion (naive baseline)
- `baseline_exp_decay` - Exponential decay (best for both scenarios) 🏆
- `hybrid_lightgbm` - Physics + LightGBM hybrid (strong second place)
- `hybrid_xgboost` - Physics + XGBoost hybrid
- `arihow` - SARIMAX + Holt-Winters time-series ensemble 🆕
- `lightgbm` - LightGBM gradient boosting
- `xgboost` - XGBoost gradient boosting

🚀 Complete Pipeline: From Zero to Submission (Step-by-Step) 🆕

This section provides a **complete, copy-paste ready** guide to run the entire pipeline from scratch.

Prerequisites

```
# 1. Navigate to project directory
cd D:\Datathon\novartis_datathon_2025\Main_project

# 2. Create virtual environment (first time only)
python -m venv saeed_venv

# 3. Activate virtual environment
.\saeed_venv\Scripts\Activate.ps1

# 4. Install dependencies (first time only)
pip install -r requirements.txt
```

Step 1: Verify Data Files

Ensure raw data files exist in `data/raw/`:

```
data/raw/
├── df_volume_train.csv
├── df_volume_test.csv
├── df_generics_train.csv
├── df_generics_test.csv
└── df_medicine_info.csv
```

Step 2: Configure Pipeline in `src/config.py`

Edit `src/config.py` to set your desired options:

```
# ═══════════════════════════════════════════════════════════════════════
# SECTION 1: RUN MODE SETTINGS (Most frequently changed)
# ═══════════════════════════════════════════════════════════════════════
RUN_SCENARIO = 1              # 1, 2, or [1, 2] for both
TEST_MODE = True              # True = fast (50 brands), False = full
TEST_MODE_BRANDS = 50         # Number of brands in test mode

# ═══════════════════════════════════════════════════════════════════════
# SECTION 2: MODEL ENABLE/DISABLE TOGGLES
# ═══════════════════════════════════════════════════════════════════════
MODELS_ENABLED = {
    'baseline_no_erosion': True,    # No erosion baseline
```

```
    'baseline_exp_decay': True,    # Exponential decay baseline 🏆
    'lightgbm': True,              # LightGBM
    'xgboost': True,               # XGBoost
    'hybrid_lightgbm': True,       # Physics + LightGBM
    'hybrid_xgboost': True,        # Physics + XGBoost
    'arihow': True,                # Time-series ensemble
}

# ═══════════════════════════════════════════════════════════════════════
# SECTION 3: PIPELINE STEP TOGGLES (for run_pipeline.py)
# ═══════════════════════════════════════════════════════════════════════
RUN_EDA = False                # Run EDA visualization
RUN_TRAINING = True            # Run model training
RUN_SUBMISSION = True          # Generate submissions
RUN_VALIDATION = True          # Validate submissions
```

Step 3: Verify Configuration

```
# Check your current configuration
python src/config.py
```

Step 4: Run Complete Pipeline

Option A: Master Pipeline Script (Recommended)

```
# Runs all enabled steps based on config
python scripts/run_pipeline.py
```

Option B: Individual Steps

```
# Step 4a: Run EDA (optional)
python notebooks/01_eda_visualization.py

# Step 4b: Train models
python scripts/train_models.py

# Step 4c: Generate submissions
python scripts/generate_final_submissions.py

# Step 4d: Validate submissions
python scripts/validate_submissions.py
```

Step 5: Review Results

```
# Check model comparison results
type reports\model_comparison_scenario1.csv
```

Or open `notebooks/03_model_results.ipynb` for visualizations.

📋 Quick Reference Commands (Copy-Paste Ready)

```
# ============================================
# COMPLETE PIPELINE - CONFIG-BASED (RECOMMENDED)
# ============================================

# Activate environment
cd D:\Datathon\novartis_datathon_2025\Main_project
.\saeed_venv\Scripts\Activate.ps1

# 1. Check/edit config first
python src/config.py                    # View current settings

# 2. Run master pipeline (uses config toggles)
python scripts/run_pipeline.py          # Runs EDA→Train→Submit→Validate

# Done! Files ready in submissions/ folder

# ============================================
# INDIVIDUAL STEPS (When you need more control)
# ============================================

# Run EDA only
python notebooks/01_eda_visualization.py

# Train models only (uses config.RUN_SCENARIO, TEST_MODE, MODELS_ENABLED)
python scripts/train_models.py

# Generate submissions only (uses config.RUN_SCENARIO, SUBMISSION_MODEL)
python scripts/generate_final_submissions.py

# Validate submissions only
python scripts/validate_submissions.py

# ============================================
# CLI OVERRIDE (For quick tests)
# ============================================

# Override scenario (ignores config.RUN_SCENARIO)
python scripts/train_models.py --scenario 2
```

```
# Override test mode
python scripts/train_models.py --test      # Force test mode
python scripts/train_models.py --no-test   # Force full mode
```

Common Configuration Presets

Edit `src/config.py` with these presets:

```
# === QUICK TEST (Before full run) ===
RUN_SCENARIO = 1
TEST_MODE = True
MODELS_ENABLED = {
    'baseline_no_erosion': False,
    'baseline_exp_decay': True,  # Test best model only
    'lightgbm': False,
    'xgboost': False,
    'hybrid_lightgbm': False,
    'hybrid_xgboost': False,
    'arihow': False,
}
RUN_TRAINING = True
RUN_SUBMISSION = False
RUN_VALIDATION = False

# === FULL PRODUCTION RUN ===
RUN_SCENARIO = [1, 2]    # Both scenarios
TEST_MODE = False        # All brands
MODELS_ENABLED = {all_models: True}  # Enable all
RUN_EDA = True
RUN_TRAINING = True
RUN_SUBMISSION = True
RUN_VALIDATION = True

# === SUBMISSION GENERATION ONLY (Models already trained) ===
RUN_SCENARIO = [1, 2]
RUN_TRAINING = False
RUN_SUBMISSION = True
RUN_VALIDATION = True
```

Expected Final Output Structure

```
Main_project/
├── models/
│   ├── scenario1_lightgbm.joblib                    # Latest model (always
updated)
```

```
    │   ├── scenario1_lightgbm_20251128_220910.joblib    # Timestamped backup
    │   ├── scenario1_xgboost.joblib
    │   ├── scenario1_xgboost_20251128_220911.joblib
    │   ├── scenario1_hybrid_hybrid.joblib
    │   ├── scenario1_arihow_arihow.joblib
    │   ├── scenario2_lightgbm.joblib
    │   ├── scenario2_xgboost.joblib
    │   ├── scenario2_hybrid_hybrid.joblib
    │   └── scenario2_arihow_arihow.joblib
    ├── reports/
    │   ├── model_comparison_scenario1.csv
    │   ├── model_comparison_scenario1_20251128_220915.csv  # Timestamped
    │   ├── model_comparison_scenario2.csv
    │   ├── run_summary_scenario1_*.json
    │   ├── run_summary_scenario2_*.json
    │   └── eda_data/
    │       ├── fig01-08_*.json
    │       └── fig01-08_*.csv
    └── submissions/
        ├── scenario1_baseline_final.csv  ← UPLOAD THIS
        ├── scenario2_baseline_final.csv  ← UPLOAD THIS
        └── scenario*_*.json
```

🔧 Recent Updates (November 2025) 🆕

1. **Config-Based Pipeline System** 🆕 🔥

- **Centralized configuration in `src/config.py`** - All settings in one place
- **13 well-documented sections** covering run modes, model params, paths, etc.
- **Model enable/disable toggles** - Select which models to train via `MODELS_ENABLED` dict
- **Pipeline step toggles** - `RUN_EDA`, `RUN_TRAINING`, `RUN_SUBMISSION`, `RUN_VALIDATION`
- **Master orchestrator script** - `scripts/run_pipeline.py` runs complete pipeline based on config
- **CLI override still available** - Use `--scenario`, `--test` flags for quick overrides

2. **Timestamped Model Saving** 🆕

- Models now save with timestamps: `scenario1_lightgbm_20251128_220910.joblib`
- Also saves a "latest" copy: `scenario1_lightgbm.joblib` (always updated)
- Reports also timestamped: `model_comparison_scenario1_20251128_220915.csv`
- Prevents accidental overwrites during experiments

3. **ARHOW Model Improvements**

- **Upgraded from basic ARIMA to SARIMAX** - Better handling of seasonal patterns
- **Added Holt-Winters (ExponentialSmoothing)** - Captures level and trend
- **Learned weights via Linear Regression** - Optimal combination: $y\_hat = \beta_0 \times ARIMA + \beta_1 \times HW$
- **Fixed training on ALL brands** - Previously only trained on training brands
- **Added RangeIndex for statsmodels compatibility** - Prevents datetime index errors

4. **Warning Suppression**

- Added `warnings.catch_warnings()` context managers to suppress statsmodels convergence warnings
- Cleaner console output during training

5. **Organized Reports Structure** 🆕

- **Three subfolders**: `01_eda_data/`, `02_feature_data/`, `03_model_data/`
- **Each figure has**: PNG image + JSON summary + CSV raw data
- **Figures subfolder**: Each notebook saves figures to its own `figures/` subfolder
- **Complete summaries**: Each notebook generates a `*_complete_summary.json`

6. **Pandas FutureWarning Fix**

- Updated `feature_engineering.py` to use `include_groups=False` in groupby operations
- Prevents deprecation warnings in newer pandas versions

7. **Data Cleaning Functions** 🆕 💧

- **`remove_duplicates()`** - Removes exact duplicate rows
- **`verify_months_postgx_range()`** - Validates months_postgx values are in expected range
- **`check_multiple_rows_per_month()`** - Detects duplicate (brand, month) combinations
- **`create_time_to_50pct_features()`** - Calculates time to 50% erosion and speed category
- **`impute_avg_vol_regression()`** - ML-based imputation for missing avg_vol
- **`create_vol_norm_gt1_flag()`** - Flags anomalous volume growth above baseline

8. **Full Config in Submission JSON** 🆕

- Submission JSON files now include ALL configuration parameters
- Enables complete reproducibility of any submission
- All 13 config sections saved: run_mode, models_enabled, paths, weights, model params, etc.

⚠️ Important Notes & Gotchas

TEST_MODE Warning

Problem: When `TEST_MODE = True`, only 50 random brands are used for training. Since Bucket 1 brands (high-erosion) are rare (~6.7% of total), there's a high chance **no Bucket 1 brands** will be selected.

Symptom: `bucket1_pe = NaN` in model comparison results

Solution: Set `TEST_MODE = False` in `src/config.py` for full training with all 1,953 brands:

```
# In src/config.py
TEST_MODE = False  # Use all brands for proper Bucket 1 evaluation
```

Bucket Distribution

- **Bucket 1 (high erosion)**: ~130 brands (6.7%) - **2× weight in scoring!**
- **Bucket 2 (lower erosion)**: ~1,823 brands (93.3%)

Focus extra effort on Bucket 1 predictions since they count double in the final PE score.

9. **Feature Engineering Enhancements** 🆕 🔥

- **Feature count increased from 40 to 76 features!**
- `FeatureScaler` **class** - StandardScaler, MinMaxScaler, and log transforms with outlier clipping
- `target_encode_cv()` - Leakage-safe target encoding within CV folds
- `create_log_avg_vol()` - Log transform of avg_vol (reduces skew)
- `create_pre_loe_growth_flag()` - Binary flag for brands with positive pre-LOE growth
- `create_max_n_gxs_post_feature()` - Brand-level max competitors post-LOE
- `create_early_postloe_features()` - 8 new features from months 0-5 for Scenario 2
- `compute_time_window_weights()` - Sample weights aligned with PE scoring formula
- `create_horizon_as_row_dataset()` - Alternative dataset structure for forecasting

10. **Time-Window Sample Weighting** 🆕 🔥

- New config parameters: `USE_TIME_WINDOW_WEIGHTS`, `S1_TIME_WINDOW_WEIGHTS`, `S2_TIME_WINDOW_WEIGHTS`
- Weights align with PE scoring formula:
  - **Scenario 1:** months 0-5 get 2.5× weight (50% of PE score)
  - **Scenario 2:** months 6-11 get 2.5× weight (50% of PE score)
- Trains models to focus on time periods that matter most for competition scoring

11. **GroupKFold Cross-Validation** 🆕

- `cross_validate_grouped()` method in `GBTModel` class
- Ensures all months of a brand stay together in CV folds
- Prevents data leakage from brand months spanning train/val splits
- More realistic estimate of generalization to new brands

12. **EnsembleBlender Class** 🆕

- `EnsembleBlender` - Learns optimal ensemble weights from validation data
- `optimize_ensemble_weights()` - Convenience function for weight optimization
- Three blending methods: `ridge`, `nnls` (non-negative), `simple` (equal)
- Replaces manual weight tuning with data-driven optimization

---

📊 Feature Summary (76 Total)

Category	Count	Examples
Lag Features	4	volume_lag_1, volume_lag_3, volume_lag_6, volume_lag_12
Rolling Features	8	rolling_mean_3, rolling_std_3, rolling_mean_6, rolling_mean_12

Category	Count	Examples
Competition Features	5	n_gxs, n_gxs_cummax, months_with_generics, max_n_gxs_post
Pre-Entry Features	6	avg_vol, log_avg_vol, pre_entry_slope, pre_entry_volatility, pre_loe_growth_flag
Time Features	5	months_postgx, month_sin, month_cos, is_early_postgx
Early Post-LOE Features	8	early_vol_mean, early_vol_min, early_vol_max, early_erosion_ratio
Categorical Encodings	12	ther_area_encoded, country_encoded, nfc_code_encoded
Interaction Features	15	avg_vol_x_n_gxs, pre_slope_x_months, bucket_x_time
Normalized Features	8	vol_norm, vol_norm_diff, vol_norm_pct_change
Quality Flags	5	vol_norm_gt1, reached_50pct, erosion_speed_category

Good luck with the competition! ⏳