

RAPID: Regression Analysis Pipeline with Intelligent Data preprocessing

A comprehensive machine learning pipeline for regression analysis featuring automated data preprocessing, intelligent feature selection, and ensemble model comparison with stacking capabilities.

Overview

This project provides an end-to-end automated workflow for regression modeling that handles:

- **Intelligent Data Preprocessing:** Automated missing data imputation, outlier detection, and quality checks
- **Feature Selection:** Multiple reduction strategies (correlation-based, variance-based, tree-based importance)
- **Model Comparison:** Evaluates 10+ regression algorithms with hyperparameter optimization
- **Ensemble Methods:** Optimized stacking regressors (automatically runs) with multiple meta-learners
- **Export Capabilities:** Generates comprehensive Excel reports, JSON feature lists, and publication-ready PNG plots

Key Features

- "Hit and Walk Away" Automation** - Set target variable once and run entire pipeline
 - Configurable Constants** - 30+ parameters for complete workflow customization
 - Advanced Imputation** - Threshold-based strategies (simple → KNN → iterative)
 - Robust Validation** - K-Fold cross-validation with stratified sampling
 - Professional Reporting** - Multi-tab Excel exports with narrative insights
 - Presentation-Ready Outputs** - High-DPI PNG plots for immediate use
-

Table of Contents

- [Requirements](#)
 - [Installation](#)
 - [Quick Start](#)
 - [Project Structure](#)
 - [Usage Guide](#)
 - [Configuration](#)
 - [Output Files](#)
 - [Supported Models](#)
 - [Troubleshooting](#)
 - [Contributing](#)
-

Requirements

System Requirements

- **Python Version:** 3.10+ (Tested on 3.12.0) - [Download Python 3.12.x](#)
- **Operating System:** Windows, macOS, or Linux
- **RAM:** 16GB minimum (more recommended for large datasets)
- **Storage:** 500MB for dependencies + space for your data

Python Version Note

While developed with Python 3.12.0, this project should work with Python 3.10 or higher. If you encounter compatibility issues, we recommend using [Python 3.12.x](#) for best results.

Installation

1. Clone the Repository

```
git clone https://github.com/chemnteach/regression_modeling.git  
cd regression_modeling
```

2. Create Virtual Environment

Windows (Command Prompt - Recommended):

If your terminal shows **PS** at the prompt (PowerShell), switch to Command Prompt first:

```
cmd
```

Then create and activate the virtual environment:

```
python -m venv venv  
venv\Scripts\activate
```

You'll see **(venv)** appear in your prompt when activated.

To deactivate when done:

```
deactivate
```

macOS/Linux:

```
python3 -m venv venv  
source venv/bin/activate
```

To deactivate when done:

```
deactivate
```

3. Install Dependencies

```
pip install --upgrade pip
pip install -r requirements.txt
```

Note: If you're behind a corporate proxy (like Intel's), use:

```
pip install --proxy http://proxy-dmz.intel.com:912 -r requirements.txt
```

4. Verify Installation

Open Jupyter Notebook and ensure all imports work:

```
jupyter notebook "Feature Reduction.ipynb"
```

⚡ Quick Start

Streamlined Workflow (Recommended)

1. Open **Feature Reduction.ipynb** in Jupyter/VS Code
2. Run the packages installation cells
3. **Execute the first data loading cell** - it will:
 - Prompt you to select your CSV file
 - Display all numeric columns with statistics
 - Ask you to select your target variable by number (no typos!)
4. Run all remaining cells (or Kernel → Run All)
 - Stacking ensemble analysis runs automatically (optimized for ~1 hour runtime)
5. Find outputs in the project directory:
 - **feature_importance_scores.csv** - Feature rankings
 - **Feature_Analysis_Report_YYYYMMDD_HHMMSS.xlsx** - Comprehensive 5-tab report
 - **model_features_YYYYMMDD_HHMMSS.json** - Feature list for deployment
 - **best_model_*.png** - High-resolution model plots (if plot-saving cell is run)
 - ***.pk1** - Trained model pipelines for deployment

Option 3: Standalone Script (Future Enhancement)

```
python main.py --data your_data.csv --target column_name
```

(Note: *main.py* currently serves as project entry point; full CLI support planned)

📁 Project Structure

```
regression_modeling/
    ├── Feature Reduction.ipynb      # Main analysis notebook (3,100+ lines)
    ├── main.py                      # Project entry point / utilities
    ├── feature_reduction.py        # Core preprocessing functions
    ├── requirements.txt            # Python package dependencies
    └── README.md                   # This file
    venv/                           # Virtual environment (created during setup)
```

Key Files Explained

File	Purpose	Lines	Status
Feature Reduction.ipynb	Complete ML pipeline with documentation	3,300+	Primary
feature_reduction.py	Reusable preprocessing functions	-	Support
main.py	Project scaffolding / future CLI	-	Support
requirements.txt	All package dependencies	-	Active

📘 Usage Guide

Workflow Overview

The notebook follows a 7-stage pipeline:

1. SETUP ENVIRONMENT
→ Install packages, import libraries, set constants



2. LOAD DATA
→ Interactive file selection or automatic CSV loading



3. INITIAL QUALITY CHECK

- ```
→ Remove columns with >40% missing data
→ Remove date columns, duplicates, high cardinality
```

↓

#### 4. STRATEGIC IMPUTATION

- ```
→ <5% missing: Median imputation  
→ 5-20% missing: KNN imputation  
→ 20-40% missing: Iterative imputation
```

↓

5. FEATURE SELECTION

- ```
→ Correlation analysis, variance thresholds
→ Tree-based feature importance
```

↓

#### 6. MODEL TRAINING & COMPARISON

- ```
→ Train 8 base models with cross-validation  
→ Hyperparameter optimization via RandomizedSearchCV  
→ Evaluate using R2 scoring
```

↓

7. ENSEMBLE STACKING (AUTOMATIC)

- ```
→ Combine top models with optimized stacking ensemble
→ Test multiple meta-learners
→ Select best performing combination
→ Runs automatically (~1 hour with optimizations)
```

↓

#### 8. EXPORT RESULTS

- ```
→ CSV: Feature importance scores  
→ Excel: 5-tab comprehensive report  
→ PNG: High-resolution model plots
```

First Cell Workflow

The first executable cell handles all initial setup interactively:

Step 1: CSV Selection

- Opens file dialog to select your CSV file
- Loads data and displays basic statistics

Step 2: Target Variable Selection

- Lists all numeric columns with:
 - Column name

- Data type
- Missing data percentage
- **Select by number** (e.g., enter "5" for the 5th column)
- Eliminates typos and ensures valid selection
- Selected column is **protected** from all automated cleaning
- **Automatically removes rows** with missing target values (cannot train models on missing targets)

Step 3: Automatic Stacking Ensemble

- Stacking ensemble analysis **runs automatically** after individual models
- Combines top-performing models to maximize predictive performance
- Uses optimized approach that completes in ~1 hour (8x faster than standard)
- Benefits:
 - Generates out-of-fold predictions from base learners once
 - Tests 9 different meta-learners on pre-generated predictions
 - No redundant model retraining (89 operations vs 720)
 - Always produces best possible ensemble performance

⚙️ Configuration

Key Constants (Located in Constants Cell)

Missing Data Handling

```
MAX_MISSING_DATA = 0.4          # Remove columns with >40% missing (AUTOMATED)
LOW_MISSING_THRESHOLD = 0.05    # <5% missing → Simple imputation (median for
                               numeric, mode for categorical)
MEDIUM_MISSING_THRESHOLD = 0.20 # 5-20% missing → KNN imputation
HIGH_MISSING_THRESHOLD = 0.40   # 20-40% missing → Iterative imputation (MICE)
```

Automated Imputation Strategy:

- < 5%: Median for numeric, mode for categorical - Fast and effective
- 5-20%: KNN imputation - Preserves local relationships
- 20-40%: Iterative/MICE imputation - Advanced statistical modeling
- > 40%: Column automatically dropped (unless it's the protected target variable)

Data Quality Filters

```
REMOVE_DATE_COLUMNS = True       # Drop datetime columns
HIGH_CARDINALITY_THRESHOLD = 0.8 # Remove likely ID columns
REMOVE_DUPLICATE_ROWS = True    # Drop exact duplicate rows
LOW_VARIANCE_THRESHOLD = 0.99   # Remove near-constant columns
```

Model Training

```
TRAINING_DATA_SPLIT = 0.8          # 80% train, 20% validation
CROSS_VALIDATION_FOLDS = 5         # K-Fold CV splits
RANDOM_STATE = 42                  # Reproducibility seed
HYPERPARAMETER_ITERATIONS = 20     # RandomizedSearchCV iterations
```

Feature Selection

```
FEATURE_IMPORTANCE_THRESHOLD = 0.001 # Minimum importance to keep
CORRELATION_THRESHOLD = 0.95        # Remove highly correlated features
VARIANCE_THRESHOLD = 0.01           # Minimum variance required
```

Visualization

```
HISTOGRAM_BINS = 30                # Residual histogram bins
figSize = [10, 10]                   # Default plot dimensions
```

All 30+ Configurable Parameters

See the **Constants** cell in [Feature Reduction.ipynb](#) for the complete list with detailed comments.

⌚ Feature Selection Methodology (Detailed)

This section provides a comprehensive, step-by-step explanation of the feature selection process used in this pipeline. The methodology combines correlation analysis with ensemble-based importance ranking to identify the most predictive features while minimizing multicollinearity.

Overview: Two-Stage Feature Reduction

The pipeline uses a **two-stage approach** to feature selection:

1. **Stage 1 - Correlation-Based Reduction:** Removes highly correlated (redundant) features
2. **Stage 2 - Importance-Based Selection:** Identifies features with highest predictive power

This sequential approach ensures we keep only features that are both **unique** (non-redundant) and **predictive** (useful for modeling).

Stage 1: Correlation-Based Feature Reduction

Objective: Eliminate multicollinearity by removing redundant features that provide duplicate information.

Step 1.1: Data Preparation

```
working_data = model_ready_data.copy()
working_data[dependent_var] = working_data[dependent_var].astype('float64')
```

Actions:

- Create working copy of fully preprocessed data
- Ensure target variable is numeric (required for correlation analysis)
- Remove any remaining string columns (these should have been encoded earlier)
- Save snapshot of data before feature reduction for audit trail

Output: Clean numeric dataset ready for correlation analysis

Step 1.2: Calculate Correlation Matrix

```
corr_matrix = working_data.corr()
target_corr = corr_matrix[dependent_var].abs().drop(dependent_var)
```

Actions:

- Compute pairwise Pearson correlation coefficients for all features
- Calculate absolute correlation between each feature and target variable
- Use absolute values because both +1 and -1 indicate strong relationships

Technical Details:

- Pearson correlation coefficient range: -1.0 to +1.0
- Values near ± 1.0 indicate strong linear relationships
- Values near 0.0 indicate weak/no linear relationship

Step 1.3: Identify Highly Correlated Feature Pairs

```
CORRELATION_THRESHOLD = 0.95 # Configurable constant
```

Algorithm:

```
FOR each feature pair (i, j):
    IF abs(correlation) >= CORRELATION_THRESHOLD:
        IF target_corr[feature_i] > target_corr[feature_j]:
            Mark feature_j for removal
        ELSE:
            Mark feature_i for removal
```

Logic:

- When two features have correlation ≥ 0.95 , they provide redundant information
- Keep the feature with **stronger correlation to the target**
- Drop the feature with weaker target correlation
- This preserves maximum predictive information while reducing redundancy

Example:

- Feature A and Feature B have 0.97 correlation (highly redundant)
- Feature A has 0.65 correlation with target
- Feature B has 0.48 correlation with target
- **Action:** Keep Feature A, drop Feature B

Step 1.4: Remove Redundant Features

```
working_data_reduced = working_data.drop(columns=to_drop)
```

Actions:

- Drop all features marked for removal
- Preserve target variable and all non-redundant features
- Log which features were dropped and why

Typical Results:

- 10-30% of features removed (dataset dependent)
- Remaining features are functionally independent
- No loss of unique predictive information

Stage 2: Importance-Based Feature Selection

Objective: Rank remaining features by predictive power and select the most important ones.

Step 2.1: Create Training/Validation Split

```
X_train, X_validation, Y_train, Y_validation = train_test_split(  
    independent, dependent,  
    test_size=VALIDATION_SIZE, # Typically 0.2  
    random_state=SEED  
)
```

Actions:

- Separate features (X) from target (Y)

- Split into 80% training, 20% validation
- Use fixed random seed for reproducibility
- Validation set held out for final model evaluation

Why This Matters:

- Prevents overfitting during feature selection
- Ensures feature importance scores are unbiased
- Training set used for all selection decisions
- Validation set only used for final performance measurement

Step 2.2: Train Multiple Feature Importance Models

Model Suite: 4 tree-based algorithms with built-in feature importance

```
feature_importance_models = [
    ('RandomForest', RandomForestRegressor(n_estimators=100, random_state=SEED)),
    ('XGBoost', XGBRegressor(n_estimators=100, random_state=SEED)),
    ('GradientBoosting', GradientBoostingRegressor(n_estimators=100,
random_state=SEED)),
    ('CatBoost', CatBoostRegressor(iterations=100, random_seed=SEED,
verbose=False))
]
```

Why Multiple Models?

- **Random Forest:** Importance based on mean decrease in impurity across trees
- **XGBoost:** Gain-based importance with L1/L2 regularization effects
- **Gradient Boosting:** Sequential importance based on loss reduction
- **CatBoost:** Handles categorical features differently, may identify different patterns

Different algorithms use different internal mechanics, so they may disagree on which features are most important. Using multiple models captures a **consensus view**.

Step 2.3: Extract and Normalize Feature Importances

```
for name, model in feature_importance_models:
    pipeline = Pipeline([
        ('scaler', StandardScaler()),
        ('model', model)
    ])
    pipeline.fit(X_train, Y_train)

    # Extract raw importances
    importance = pipeline.named_steps['model'].feature_importances_
```

```
# Normalize to sum to 1.0 (makes models comparable)
normalized_importances = importance / np.sum(importance)
```

Process:

1. Standardize features (zero mean, unit variance)
2. Train model on training data
3. Extract feature importances from trained model
4. Normalize importances to sum to 1.0

Why Normalize?

- Makes importance scores comparable across different models
- Raw importance scales vary between algorithms
- Normalization creates a common 0-1 scale

Step 2.4: Calculate Feature Ranks

```
ranks = np.argsort(np.argsort(-normalized_importances)) + 1
```

Rank Calculation:

- Rank 1 = Most important feature
- Rank N = Least important feature
- Ties broken by array order

Example:

```
Feature A: Importance 0.35 → Rank 1
Feature B: Importance 0.28 → Rank 2
Feature C: Importance 0.20 → Rank 3
Feature D: Importance 0.17 → Rank 4
```

Why Use Ranks Instead of Raw Scores?

- Robust to outliers (one model giving extreme importance)
- Less sensitive to scale differences between algorithms
- Easier to interpret (percentile-based)
- Statistical theory supports rank aggregation

Step 2.5: Aggregate Rankings Across Models

```
for feature in features:
    mean_rank = np.mean(feature_ranks[feature])
```

```
mean_importance = np.mean(all_importances[feature])
std_rank = np.std(feature_ranks[feature])
```

Calculations:

- **Mean Rank:** Average rank across all 4 models (lower = better)
- **Mean Importance:** Average normalized importance score
- **Rank Std Dev:** Measures consistency (low std = consistent across models)

Example:

Feature "Temperature":

- RandomForest rank: 2
- XGBoost rank: 1
- GradientBoosting rank: 3
- CatBoost rank: 2

→ Mean Rank: 2.0 (very important, consistent)

Feature "NoiseColumn":

- RandomForest rank: 45
- XGBoost rank: 38
- GradientBoosting rank: 50
- CatBoost rank: 42

→ Mean Rank: 43.75 (low importance, consistent)

Step 2.6: Select Features Using Cumulative Importance

```
cumulative_threshold = 0.95 # Keep features accounting for 95% of importance

cumulative_importance = 0
selected_features = []

for feat_stat in sorted_by_importance:
    cumulative_importance += feat_stat['mean_importance']
    selected_features.append(feat_stat)

    if cumulative_importance / total_importance >= cumulative_threshold:
        break

# Safety net: Keep at least 20% of features
min_features = max(int(np.ceil(num_features * 0.20)), 10)
if len(selected_features) < min_features:
    selected_features = feature_statistics[:min_features]
```

Selection Strategy:

1. Sort features by mean importance (highest first)

2. Add features to selection until cumulative importance reaches 95%
3. Enforce minimum of 20% of original features (or 10, whichever is larger)

Why Cumulative Importance?

- **Adaptive:** Selection adapts to actual importance distribution
- **No Arbitrary Cutoffs:** Doesn't assume "top 50%" is always right
- **Comprehensive:** Captures all meaningfully predictive features
- **Safe:** Minimum threshold prevents over-aggressive reduction

Example Scenario:

Starting with 100 features after correlation reduction:

```
Feature 1-10: Cumulative importance = 75%
Feature 11-15: Cumulative importance = 90%
Feature 16-18: Cumulative importance = 95% ← STOP HERE
```

Result: 18 features selected (18% of original)
 Remaining 82 features contribute only 5% to predictions

Step 2.7: Create Final Feature Set

```
feature_names = [f['feature'] for f in selected_features]
independent = working_data_reduced[feature_names]
dependent = working_data_reduced[dependent_var]
```

Actions:

- Extract feature names from selected statistics
- Create final modeling dataset with selected features only
- Preserve target variable
- Save feature importance scores to CSV for documentation

Output: Feature Importance Report

CSV File: `feature_importance_scores.csv`

Columns Explained:

Column	Description	Value Range	Interpretation
--------	-------------	-------------	----------------

Column	Description	Value Range	Interpretation
feature	Feature name exactly as it appears in the dataset	String	Identifies which variable this row describes
mean_rank	Average rank across 4 tree-based models (RF, XGB, GBT, CB)	1.0 to N	Lower is better. Rank 1 = most important feature. If a feature ranks 2, 1, 3, 2 across the 4 models, mean_rank = 2.0
std_rank	Standard deviation of ranks across the 4 models	≥ 0.0	Lower = more consensus. Low std_rank (< 2.0) means all models agree this feature is important/unimportant. High std_rank (> 5.0) means models disagree
mean_importance	Average normalized importance score across 4 models	0.0 to 1.0	Higher is better. Sum of all features ≈ 1.0. A score of 0.15 means this feature accounts for 15% of total predictive power
rank_percentile	Percentile ranking within the selected feature set	0% to 100%	Higher is better. 100% = best feature, 50% = median feature, 0% = worst feature in selected set. Calculated as: $(1 - \text{mean_rank}/N) \times 100$

Use Cases:

- Identify top predictive features for business insights
- Validate feature engineering decisions
- Explain model predictions to stakeholders
- Guide future data collection priorities

Summary: Complete Feature Selection Workflow

STAGE 1: Correlation Reduction

- |- 1. Calculate pairwise correlations
- |- 2. Identify pairs with $|\text{correlation}| \geq 0.95$
- |- 3. For each pair, keep feature with stronger target correlation
- |- 4. Drop redundant features
→ Result: Multicollinearity eliminated

STAGE 2: Importance Selection

- |- 1. Split data (80% train, 20% validation)
- |- 2. Train 4 tree-based models (RF, XGB, GBT, CB)
- |- 3. Extract and normalize feature importances
- |- 4. Calculate ranks for each feature in each model
- |- 5. Average ranks across all models
- |- 6. Sort by mean importance, select top features
- |- 7. Keep features accounting for 95% cumulative importance

- └ 8. Enforce minimum 20% retention safety net
 - Result: Optimal predictive feature set

- FINAL OUTPUT
 - └ Reduced feature set: Unique + Predictive + Documented

Advantages of This Methodology

- Reduces Bias:** Multiple models prevent any single algorithm from dominating selection
- Eliminates Redundancy:** Correlation analysis removes duplicate information
- Preserves Information:** Keeps features with unique predictive value
- Robust to Outliers:** Rank-based aggregation handles extreme importance values
- Adaptive:** Cumulative importance adjusts to actual data patterns
- Interpretable:** Mean ranks are easy to understand and explain
- Reproducible:** Fixed random seeds ensure consistent results
- Safe:** Minimum thresholds prevent over-reduction

Output Files

1. Feature Importance CSV

Filename: `feature_importance_scores.csv`

Contains ranked features with comprehensive statistics from ensemble-based feature selection.

Columns:

Column	Typical Values	What It Tells You
feature	Column names from your dataset	Which variable this row describes
mean_rank	1.0 to N (lower is better)	How consistently important this feature is. A mean_rank of 2.0 means it averaged 2nd place across 4 models
std_rank	0.0 to ~10.0 (lower is better)	How much models agree. std_rank < 2 = strong consensus, > 5 = disagreement
mean_importance	0.0 to 1.0 (higher is better)	Percentage of predictive power. 0.15 = this feature drives 15% of predictions
rank_percentile	0% to 100% (higher is better)	Where this feature ranks overall. 95th percentile = top 5% of features

How to Read the File:

- **Sort by mean_rank** (ascending): Find the most important features
- **Filter std_rank < 2**: Find features all models agree on
- **Sum mean_importance** for top N features: See how much predictive power they capture

- **Filter rank_percentile > 90:** Focus on top-tier features only

Use Cases:

- Identify top predictive features for business insights
 - Validate feature engineering decisions
 - Focus data quality efforts on high-importance features
 - Explain model behavior to stakeholders
-

2. Excel Comprehensive Report

Filename: Feature_Analysis_Report_YYYYMMDD_HHMMSS.xlsx

Five-tab workbook with comprehensive analysis:

Tab 1: Narrative

- Executive summary
- Methodology overview
- Model performance highlights
- Key insights and patterns
- Data quality assessment
- Actionable recommendations

Tab 2: Feature Metrics

- All features ranked by importance
- Complete statistical profiles
- Missing data analysis
- Data type classification

Tab 3: Model Comparison

- All models ranked by R^2 score
- Base learners + stacking ensembles
- Performance deltas
- Model selection rationale

Tab 4: Imputation Log

- Columns that underwent missing data imputation
- Method used (Simple/KNN/Iterative)
- Original missing data percentage
- Data type and threshold category
- Empty if no imputation tracking available

Tab 5: Model Progression

- R^2 scores for each model across all pipeline stages

- Columns: Model, Initial_R2, Baseline_CV_R2, Optimized_CV_R2, Validation_R2, Stacking_R2, Best_R2
- Shows performance improvement from initial screening through final stacking
- Sorted by Best_R2 (highest score across all stages)
- Stacking models marked with suffix "_stack" and only have Stacking_R2 populated

Use Case: Client presentations, stakeholder reports, documentation, data quality audits, model development tracking

3. Model Performance Plots (PNG)

Location: `data/` folder

Filenames: <ModelName>_<plot_type>_YYYYMMDD_HHMMSS.png

Three high-resolution (300 DPI) plots generated for each model and stacking ensemble:

1. **Predicted vs Actual:** Scatter plot with perfect prediction line (`*_predicted_vs_actual_*.png`)
2. **Residuals CDF/PDF:** Distribution analysis with 95% threshold (`*_cdf_pdf_residuals_*.png`)
3. **Residuals Distribution:** Histogram with KDE overlay (`*_residual_distribution_*.png`)

Timestamp Format: YYYYMMDD_HHMMSS ensures unique filenames for each run

Use Case: Presentations, publications, model validation reports, performance tracking over time

4. Dataset Snapshots (CSV)

Location: `data/` folder

Filenames: Timestamped CSV files at key pipeline stages

- `final_modeling_data_YYYYMMDD_HHMMSS.csv` - Before feature reduction
- `final_modeling_data_post_feature_selection_YYYYMMDD_HHMMSS.csv` - After feature selection

Use Case: Audit trail, reproducibility, data quality verification, intermediate analysis

5. Feature List JSON

Filename: `model_features_YYYYMMDD_HHMMSS.json`

Machine-readable feature list for model deployment and validation.

Contents:

```
{
  "generated": "2025-01-15 14:30:45",
  "target_variable": "Resistance",
  "feature_count": 18,
  "features": ["Feature1", "Feature2", ...],
  "best_model": "ExtraTreesRegressor",
  "best_r2": 0.9234
}
```

Use Case: Model deployment validation, feature consistency checks, CI/CD pipelines, API integration

🤖 Supported Models

Base Learners (8 Algorithms)

Category	Models
Tree-Based	Random Forest, Extra Trees, Gradient Boosting
Boosting	XGBoost, LightGBM, CatBoost
Instance-Based	KNN Regressor
Ensemble	Bagging Regressor

Meta-Learners (Stacking)

- All 8 base learners
- Linear Regression

Model Selection Criteria

- **Primary Metric:** R² score (coefficient of determination)
- **Validation:** 5-fold cross-validation
- **Optimization:** RandomizedSearchCV with 20 iterations
- **Selection:** Top 5 base models → Automatic Stacking → Best meta-learner

⚡ Troubleshooting

Common Issues

Issue: Excel export fails with "name 'feature_statistics' is not defined"

Cause: Kernel was restarted and variables lost

Solution:

1. Re-run entire notebook (Kernel → Restart & Run All)
2. The Excel report is automatically generated in the final cell

Issue: "Behind corporate proxy" - pip install fails

Solution: Use proxy flag:

```
pip install --proxy http://your-proxy:port -r requirements.txt
```

For Intel networks: <http://proxy-dmz.intel.com:912>

Performance Optimization

For Large Datasets (>1M rows):

- Reduce `CROSS_VALIDATION_FOLDS` from 5 to 3
- Decrease `HYPERPARAMETER_ITERATIONS` from 20 to 10
- Consider using only fastest models (Random Forest, Extra Trees) for initial exploration

For High-Dimensional Data (>100 features):

- Tighten `CORRELATION_THRESHOLD` to 0.90
- Increase `FEATURE_IMPORTANCE_THRESHOLD` to 0.005
- Enable aggressive variance filtering

Memory Issues:

- Use `TRAINING_DATA_SPLIT = 0.7` for smaller training set
 - Remove ensemble models and use best base learner only
 - Process data in chunks if possible
-

🤝 Contributing

Reporting Issues

Submit bug reports or feature requests via [GitHub Issues](#).

Include:

- Python version
- Full error traceback
- Minimal reproducible example
- Dataset characteristics (rows, columns, missing data %)

Pull Requests

1. Fork the repository
 2. Create feature branch: `git checkout -b feature/your-feature-name`
 3. Follow PEP 8 style guidelines
 4. Add docstrings (Google/NumPy style)
 5. Test with sample data
 6. Submit PR with clear description
-

📄 License

This project is provided as-is for educational and commercial use. See repository for specific license terms.

Contact

Author: Craig Brown
Organization: Intel Corporation
Email: craig.d.brown@intel.com
Repository: github.com/chemteach/regression_modeling

Acknowledgments

Built with:

- scikit-learn ecosystem
 - XGBoost, LightGBM, CatBoost
 - pandas, NumPy, seaborn
 - Jupyter/VS Code notebook environment
-

Additional Resources

Learning Materials

- [scikit-learn Documentation](#)
- [Ensemble Methods Guide](#)
- [Feature Selection Strategies](#)

Related Projects

- [Vmin Kitchen Sink.ipynb](#) - Extended analysis examples
 - [feature_reduction.py](#) - Reusable function library
-

Last Updated: January 15, 2025

Version: 1.1

Status: Production Ready 