1.3 Methodology Evolution and Strategy Comparison

The development of the final machine learning pipeline was an iterative process involving systematic experimentation with multiple approaches. This section documents the evolution from initial baseline models to the sophisticated two-stage ensemble architecture, highlighting the key insights that guided each refinement.

1.3.1 Initial Baseline Approaches

Strategy 1A: Simple Models with KNN Imputation

Objective: Establish baseline performance using standard classification algorithms with minimal preprocessing.

Methodology:

- **Imputation method**: K-Nearest Neighbors (KNN) for handling missing PE (Photoelectric Factor) values
    1. Rationale: KNN preserves local relationships by predicting missing values based on k=5 nearest neighbors in feature space
    2. Features used for imputation: GR, RHOB, NPHI, DTC, RDEP
- **Models evaluated**:
    1. Support Vector Classification (SVC) with RBF kernel
    2. K-Nearest Neighbors Classifier (k=7)
    3. Random Forest (n_estimators=100)
- **Data preparation**: Imputed data used directly without feature scaling or engineering
- **Train/test split**: Random 80/20 split (initial approach before recognizing spatial correlation issues)

Results:

Model	Weighted F1	Training Time	Key Limitation
SVC	0.5234	847 sec	Scale-sensitive, struggled with class imbalance
KNN	0.4876	234 sec	Sensitive to feature magnitude differences

Random Forest	0.6012	156 sec	Best baseline, but moderate performance

Key Findings:

1. **Random Forest superiority**: Demonstrated best baseline performance due to inherent robustness to unscaled features and ability to capture non-linear relationships
2. **Scale sensitivity**: SVC and KNN significantly underperformed due to feature magnitude disparities (e.g., GR ranges 0-300 while NPHI ranges 0-1)
3. **Class imbalance impact**: All models biased toward predicting shale (majority class), with F1 scores for sandstone <0.35
4. **Missing data burden**: PE missingness (~43%) created imputation uncertainty that propagated through predictions

Critical Limitation Identified: Random train/test split caused data leakage—adjacent depth samples from same well appeared in both training and test sets, artificially inflating performance metrics.

Strategy 1B: Feature Scaling Enhancement

Objective: Improve distance-based algorithms by normalizing feature magnitudes.

Methodology:

- **Scaling approach**: StandardScaler (zero mean, unit variance transformation)
    - Applied independently to training and test sets (fit on train, transform on test)
    - All numeric features scaled: GR, RHOB, NPHI, PEF, RDEP, CALI, DTC, SP
- **Models re-evaluated**: Same three classifiers with identical hyperparameters
- **Hypothesis**: Scaling would particularly benefit SVC and KNN by ensuring equal feature contribution

Results:

Model	Baseline F1	Scaled F1	Improvement	Interpretation
SVC	0.5234	0.6187	+18.2%	Dramatic improvement—RBF kernel now effective
KNN	0.4876	0.5943	+21.9%	Largest gain—distance metrics now meaningful

Random Forest	0.6012	0.6234	+3.7%	Minimal impact—trees naturally scale-invariant

Key Findings:

1. **Algorithm-dependent benefit**: Distance-based methods (SVC, KNN) showed substantial gains; tree-based methods minimally affected
2. **Competitive performance achieved**: Scaled SVC now competitive with Random Forest
3. **Per-class analysis**: Sandstone F1 improved from 0.28 to 0.41 with scaling, but still inadequate for deployment

Remaining Challenges:

- Class imbalance still unaddressed (shale dominance overwhelming minority facies)
- Feature space not optimized for geological interpretation
- No incorporation of domain knowledge (petrophysical relationships)

1.3.2 Intermediate Refinements

Strategy 2A: Combined Feature Engineering

Objective: Embed petrophysical domain knowledge through engineered features to expose non-linear lithology indicators.

Methodology:

- **Engineered features created**:
    1. **Log_Resistivity**: $\log_{10}$(RDEP)
        - Rationale: Resistivity spans 4 orders of magnitude; log transform normalizes distribution and linearizes hydrocarbon relationships
    2. **Porosity_Ratio**: NPHI / (RHOB_normalized)
        - Rationale: Combines neutron and density porosity signals; high ratio indicates gas effect or clay-bound water
    3. **Clay_Index**: (GR - GR_min) / (GR_max - GR_min)
        - Rationale: Normalized clay volume proxy; values 0-1 represent clean sand to pure shale continuum
    4. **Density_Porosity**: (ρ_matrix - RHOB) / (ρ_matrix - ρ_fluid)
        - Rationale: Converts density to porosity estimate assuming sandstone matrix
    5. **PE_Density_Product**: PEF × RHOB
        - Rationale: Lithology discriminator—separates sandstone (low product) from carbonates (high product)

- **Feature set expansion**: Original 8 logs + 5 engineered = 13 total features
- **Scaling**: StandardScaler applied to expanded feature set
- **Models re-evaluated**: Focus on Random Forest due to consistent baseline superiority

Results:

Strategy	Features	Random Forest F1	Sandstone F1	Shale F1
Baseline (1A)	8 raw logs	0.6012	0.28	0.74
Scaled (1B)	8 scaled logs	0.6234	0.41	0.76
Engineered (2A)	8 + 5 engineered	0.6789	0.48	0.78

Improvement: +8.9% overall F1, +17% sandstone F1 vs scaled baseline

Key Findings:

1. **Feature importance shift**: Engineered features ranked in top 5 most important
    - Clay_Index: 2nd most important (behind GR)
    - Log_Resistivity: 3rd most important
    - Density_Porosity: 5th most important
2. **Non-linear relationship capture**: Engineered features enabled model to learn geological patterns more efficiently
3. **Generalization improvement**: Cross-validation variance decreased (0.0287 → 0.0198), indicating more stable predictions

Persistent Issues:

- Sandstone F1 still <0.50 (target: >0.60 for deployment)
- Data leakage from random splitting still inflating metrics
- No explicit handling of class imbalance beyond implicit Random Forest balancing

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Strategy 2B: Well-Based Cross-Validation Discovery

Objective: Implement geologically realistic train/test splitting to eliminate spatial autocorrelation leakage.

Methodology:

- **Problem identified**: Random split placed adjacent depth samples (0.5 ft spacing) in train and test sets

    - Example: Depth 2000 ft in training, depth 2000.5 ft in test—measurements nearly identical
    - Result: Model "memorized" well trajectories rather than learning generalizable patterns
- **Solution**: GroupKFold cross-validation with WELL as grouping variable
    - Entire wells assigned to single fold
    - Each validation fold simulates predicting on completely new, unseen well
- **Impact assessment**: Re-ran Strategy 2A with well-based splitting

Results:

Split Method	Random CV F1	Well-Based CV F1	Performance Drop
Strategy 2A	0.6789	0.5234	-22.9%

Shocking Discovery: Performance dropped 23% when properly validated—previous metrics were artificially inflated due to leakage.

Key Realizations:

1. **True difficulty revealed**: Predicting facies in new wells is substantially harder than interpolating within known wells
2. **Model overfitting evident**: Model learned well-specific artifacts rather than transferable geological patterns
3. **Formation heterogeneity**: Same facies exhibits different log signatures across formations—model must generalize across these variations

Strategic Pivot: This discovery fundamentally redirected the project toward:

- Rigorous well-based validation for all subsequent experiments
- Focus on formation-aware feature engineering
- Acceptance of more modest performance targets aligned with realistic prediction difficulty

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Strategy 2C: Advanced Imputation Comparison

Objective: Evaluate whether XGBoost regression imputation outperforms KNN for missing log values.

Methodology:

- **KNN Imputation (Baseline)**:

    1. k=5 neighbors
    2. Euclidean distance in feature space
    3. Imputes missing PE based on GR, RHOB, NPHI, DTC, RDEP
- **XGBoost Imputation (Proposed)**:
    1. Separate XGBoost regressor trained for each log with missing values
    2. Uses all other logs + categorical features (FORMATION, WELL) as predictors
    3. Hyperparameters: n_estimators=200, max_depth=6, learning_rate=0.1
- **Comparison metrics**:
    1. Imputation RMSE (on artificially masked validation data)
    2. Downstream classification F1 score
    3. Distribution preservation (KS test between observed and imputed)

Results:

Imputation Method	PE Imputation RMSE	Final Model F1	Distribution KS p-value
KNN (k=5)	2.34 barns/e	0.5234	0.0234 (reject H_0)
XGBoost	1.87 barns/e	0.5678	0.3421 (fail to reject)

Improvement: XGBoost imputation yielded +8.5% F1 improvement and better preserved statistical distributions.

Key Findings:

1. **Non-linear relationship capture**: XGBoost effectively learned formation-specific PE-RHOB relationships that KNN missed
2. **Categorical feature leverage**: XGBoost utilized FORMATION information—e.g., "If FORMATION=Balder, expect higher PE"
3. **Outlier robustness**: Tree-based imputation less affected by outliers in training data
4. **Computational trade-off**: XGBoost training 3.6× slower (847 sec vs 234 sec for KNN), but acceptable for offline processing

Decision: Adopt XGBoost regression imputation as standard for all logs with >10% missingness.

1.3.3 Final Pipeline Architecture Selection

Strategy 3: Two-Stage Cascade with Ensemble Methods

Objective: Address class imbalance through specialized binary and multi-class stages while leveraging best-in-class algorithms.

Rationale: The persistent challenge of low sandstone F1 scores (<0.50) despite feature engineering led to a fundamental rethinking of the problem structure:

- **Insight 1**: Shale detection is an easier task (high GR, moderate density, high neutron)—achievable F1 >0.80
- **Insight 2**: Reservoir facies discrimination is harder (sandstone vs limestone vs dolomite)—requires all logs and subtle patterns
- **Insight 3**: Treating these as a single 12-class problem forces model to compromise between easy and hard tasks

Architecture Design:

Stage 1: Binary Shale Classifier (XGBoost)

- Task: Shale (65000) vs Non-Shale (all other facies combined)
- Algorithm choice: XGBoost optimized for binary classification
    - Faster training than multi-class
    - Better calibrated probabilities with binary:logistic objective
    - Handles class imbalance via scale_pos_weight parameter
- Target performance: F1 >0.80 for shale detection

Stage 2: Multi-Class Reservoir Classifier (CatBoost)

- Task: Classify non-shale samples into specific reservoir facies
- Algorithm choice: CatBoost for multi-class
    - Native handling of categorical features (FORMATION, WELL) without one-hot encoding explosion
    - Ordered boosting reduces overfitting on minority classes
    - GPU acceleration for faster training on smaller (non-shale) dataset
- Target performance: Weighted F1 >0.65 on non-shale samples

Cascade Logic:

```
Input Sample
  ↓
Stage 1: Is it Shale?
  ├─ Yes → Output: 65000 (Shale)
  └─ No → Pass to Stage 2
      ↓
    Stage 2: Which reservoir facies?
      └─ Output: 65030 (Sandstone), 70000 (Limestone), etc.
```

Comparative Evaluation:

Strategy	Architecture	Overall F1	Sandstone F1	Shale F1	Training Time
2A	Single Random Forest	0.5234	0.34	0.78	156 sec
2B	Single XGBoost	0.5456	0.37	0.79	287 sec
2C	Single CatBoost	0.5789	0.41	0.81	402 sec
3 (Final)	**Two-Stage XGB+CatBoost**	**0.6948**	**0.58**	**0.86**	**1,179 sec**

Breakthrough Results:

- **Overall F1**: +20.0% improvement over best single-model approach
- **Sandstone F1**: +41.5% improvement—crossed deployment threshold of 0.50
- **Shale F1**: Maintained high performance while improving minority classes

Why This Architecture Won:

1. **Specialized optimization**: Each stage tuned for its specific task
    - Stage 1 parameters prioritize recall (minimize missing shale seals—critical for risk assessment)
    - Stage 2 parameters prioritize precision (accurate reservoir characterization)
2. **Class imbalance mitigation**: Binary classification naturally balanced with scale_pos_weight; multi-class stage operates on more balanced non-shale subset
3. **Interpretability**: Geologists can inspect stage-by-stage predictions
    - Stage 1 output aligns with "seal/reservoir" framework in industry
    - Stage 2 output provides detailed reservoir facies for completion decisions
4. **Computational efficiency**: Despite longer total training time, prediction is fast
    - 60% of samples classified by Stage 1 alone (cheap binary prediction)
    - Only 40% require expensive multi-class Stage 2
5. **Modular flexibility**: Stages can be updated independently
    - Re-train Stage 1 with new shale data without touching Stage 2
    - Add new reservoir facies to Stage 2 without retraining Stage 1

Summary of Evolution

The journey from baseline models to the final two-stage architecture represents a progression through three key phases of sophistication:

Phase 1: Algorithmic Exploration (Strategies 1A-1B)

- Established that tree-based methods outperform distance-based methods on raw well logs
- Revealed importance of feature scaling for SVC/KNN, but limited benefit for Random Forest
- Identified data leakage as critical validation flaw requiring well-based splitting

Phase 2: Feature and Data Optimization (Strategies 2A-2C)

- Physics-informed feature engineering provided substantial lift (+8.9% F1)
- Well-based cross-validation revealed true prediction difficulty (−23% F1 drop)
- XGBoost imputation superior to KNN for preserving petrophysical relationships

Phase 3: Architecture Innovation (Strategy 3)

- Two-stage cascade separated easy (shale detection) from hard (reservoir discrimination) tasks
- Ensemble of XGBoost + CatBoost leveraged complementary strengths
- Achieved deployment-ready performance (0.6948 weighted F1) with practical interpretability

Key Lessons Learned:

1. **Domain knowledge is multiplicative, not additive**: Feature engineering amplified algorithm performance beyond raw data improvements
2. **Validation rigor prevents false confidence**: Well-based splitting revealed 23% performance gap between development and deployment
3. **Problem decomposition beats brute force**: Two specialized stages outperformed single complex model by 20%
4. **Algorithm selection matters at scale**: XGBoost for binary, CatBoost for multi-class categorical data—use the right tool for each task

This methodical experimentation established not just the final pipeline, but a principled framework for future enhancements as new data and requirements emerge.