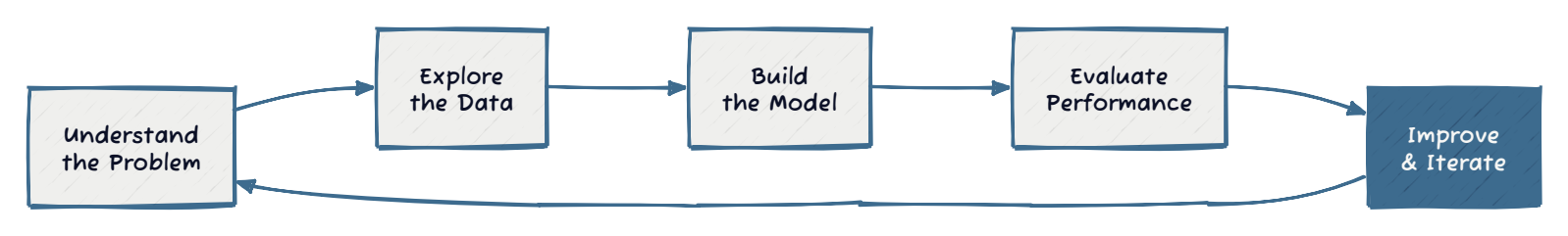
Day 04

The Modeling Project

MSU REU Machine Learning Short Course

The Full ML Loop

Days 1–3: Each piece separately. **Today: You run the entire loop yourself.**

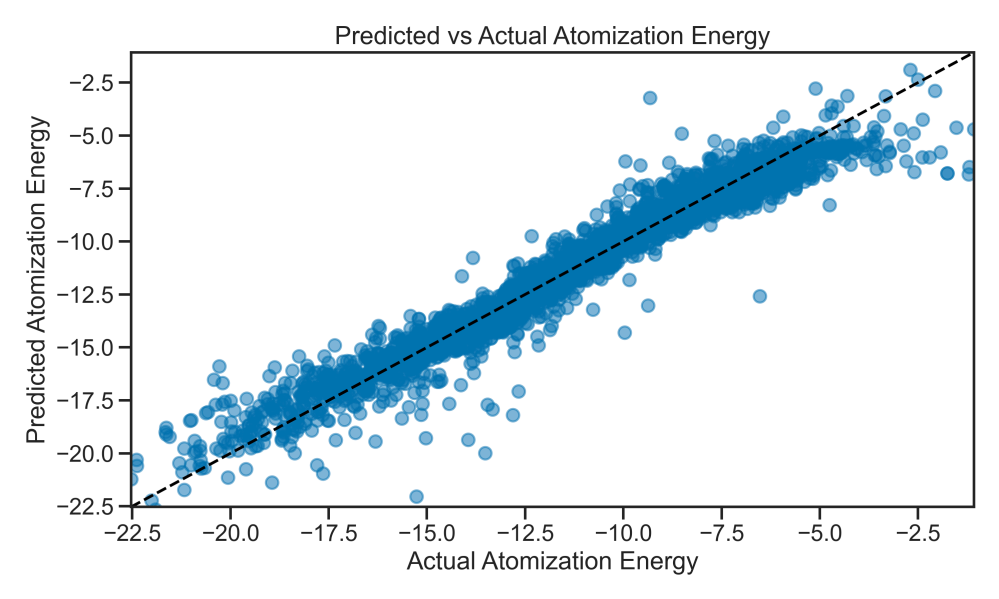


Key insight: There is no single right answer. The goal is a better model, not a perfect one.

Real data science is iteration: try something, measure it, diagnose the bottleneck, try something else.

Today's Dataset: Molecular Atomization Energy

Predict the energy required to pull a molecule apart.



- **1275 features** from the Coulomb matrix representation of each molecule.
- **Real-world challenge:** Most features are noise. Your job: find the signal.

Why This Dataset is Different

	SDSS (Days 1–3)	Molecular Energy (Today)
Size	100k objects	~16k molecules
Features	17 (clean, well-understood)	1275 (mostly noise)
Problem	Which features matter for classification?	How do you even start?

Day 1–3: You could visualize all features, understand relationships.

Today: 1275-dimensional space. You can't visualize it. You need systematic methods.

> How do you determine which features matter? How do you build a model that generalizes?

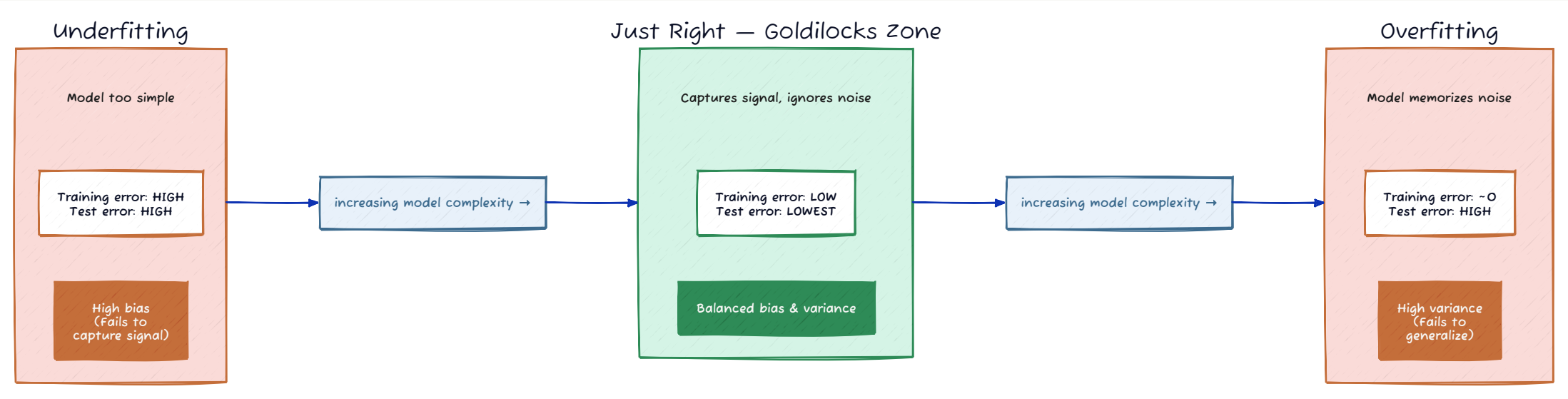
The Curse of Dimensionality

What happens when you have many features?

- **More features = more parameters** — easier to fit noise, not just signal
- **Overfitting risk increases** — with 1275 features, a linear model can fit random data perfectly
- **Computational cost** — training takes longer
- **Interpretability collapse** — what do 1275 learned weights mean?

The goal: Remove noise, keep signal. Go from 1275 → much smaller number of features that actually matter.

Overfitting vs Underfitting: The Goldilocks Problem



Underfitting: Model too simple. Misses real patterns. High bias.

Overfitting: Model memorizes noise. Fails on new data. High variance.

Goldilocks zone: Model is complex enough to capture signal, but simple enough to generalize.

Why Start with a Terrible Model?

Build the simplest possible model first. Expect it to fail.

This is your **diagnostic baseline**. Failure teaches you where to improve.

A bad R^2 tells you: "Something's wrong. What?"

> Then explore: Are features useful? Noisy? Redundant? That's your improvement direction.

Why Start with a Terrible Model?

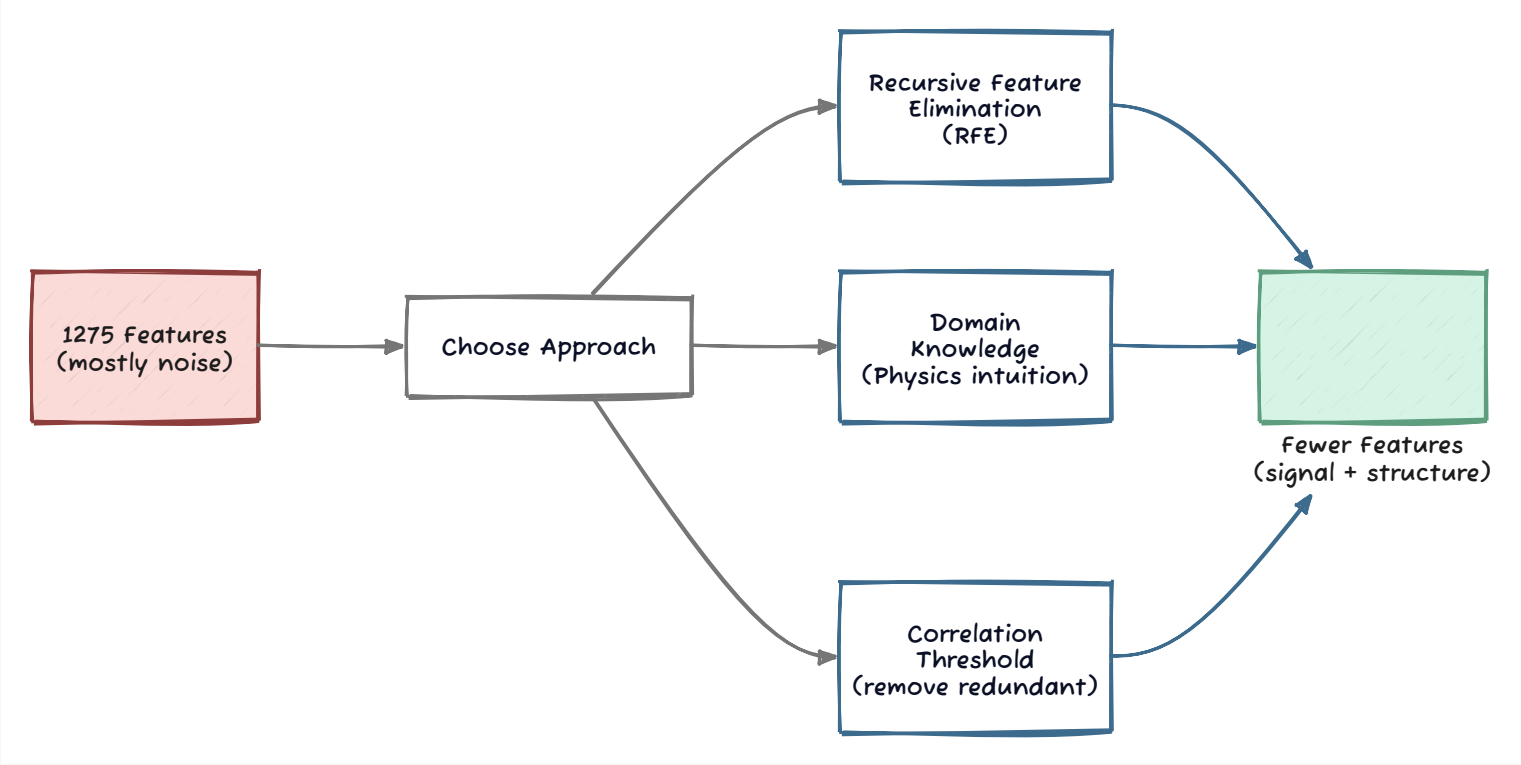
```
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import train_test_split
from sklearn.metrics import r2_score

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2)

model = LinearRegression()
model.fit(X_train, y_train)
r2 = r2_score(y_test, model.predict(X_test))
print(f"R² = {r2:.3f}")  # probably terrible (e.g., 0.15)
```

Feature Selection: Art and Science

Not all 1275 features carry signal. Systematic methods find which ones to keep.



Feature Selection: Art and Science

Not all 1275 features carry signal. Systematic methods find which ones to keep.

Approaches:

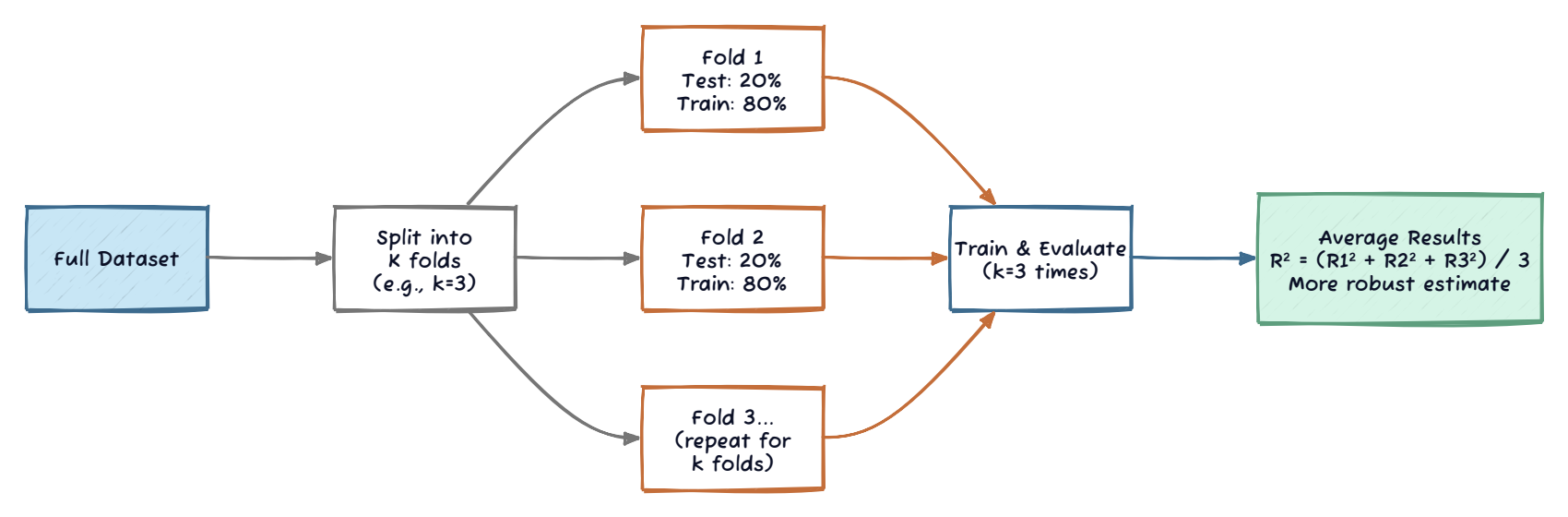
- **Recursive Feature Elimination (RFE):** Iteratively remove least important features
- **Domain knowledge:** Use physics intuition (some features are obviously useless)
- **Correlation threshold:** Remove redundant features (e.g., if two features are 99% correlated, keep one)

> See: Recursive Feature Elimination Notebook

Cross-Validation: More Robust Confidence

One train/test split = one number = could be lucky or unlucky.

K-fold cross-validation: Run the model k times, get k scores, average them.



> See: Cross-Validation

Cross-Validation: More Robust Confidence

Example with k=5:

- Fold 1: Train on 80%, test on 20%
- Fold 2: Train on different 80%, test on different 20%
- ... (repeats 5 times)

Average the 5 R^2 scores

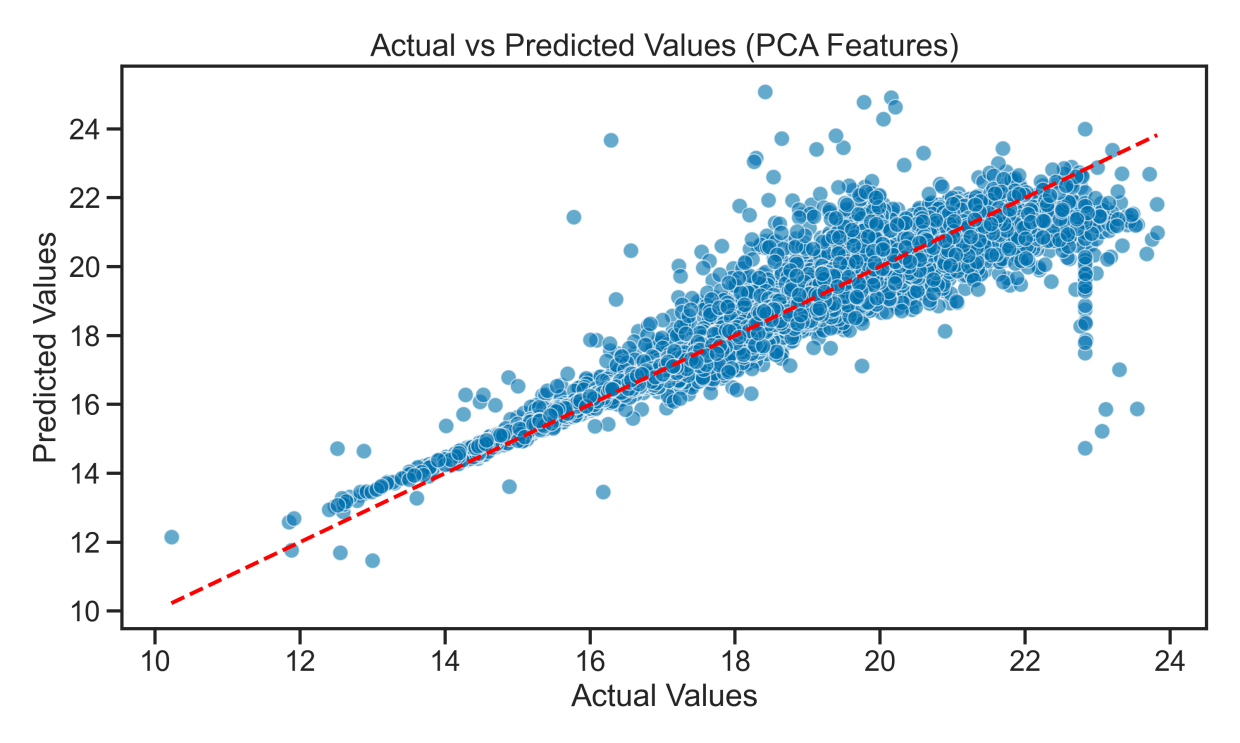
```
from sklearn.model_selection import cross_val_score


scores = cross_val_score(model, X, y, cv=5, scoring='r2')
print(f"R² = {scores.mean():.3f} ± {scores.std():.3f}")  # mean and confidence
```

Dimensionality Reduction: PCA

The problem: 1275 correlated features. Many measure the same thing.

The solution: Find directions of maximum variance. Compress 1275 → much fewer components.



Dimensionality Reduction: PCA

What's happening? PCA finds new axes (components) where data spreads out most. First 50 PCs often capture 95% of variance.

Trade-off:

- Lose interpretability (what does "PC17" mean?)
- Gain efficiency (fewer numbers to work with)
- Often improves generalization (noise gets compressed out)

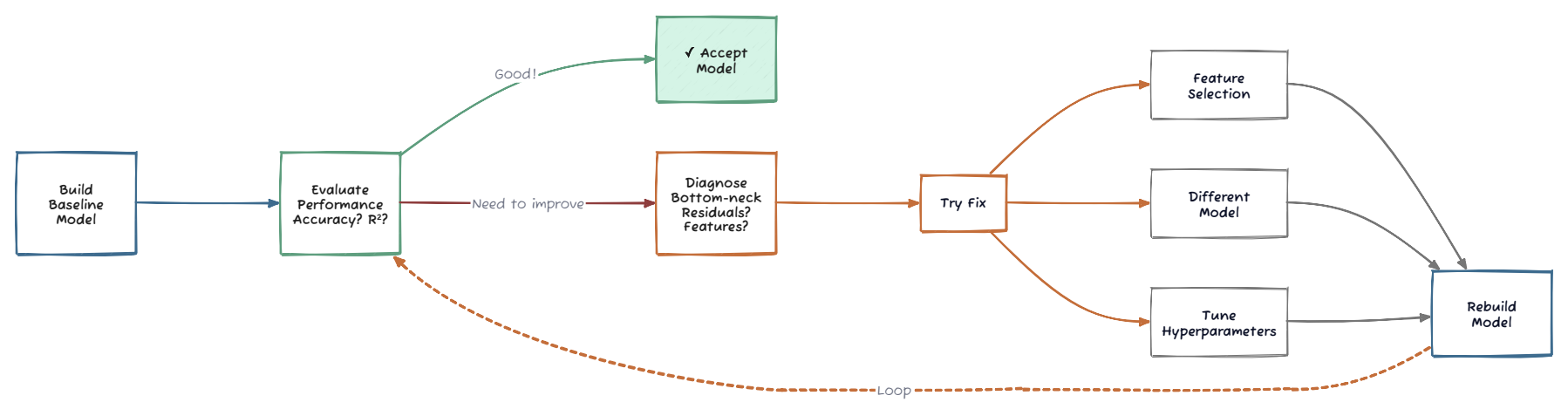
Dimensionality Reduction: PCA

```
from sklearn.decomposition import PCA


pca = PCA(n_components=50)
X_pca = pca.fit_transform(X_train)
print(pca.explained_variance_ratio_.cumsum())  # how much variance explained?
```

> See: Principal Component Analysis

The Iteration Loop: How Real Data Science Works



This is not a linear process. You build, evaluate, diagnose, fix, repeat.

The Iteration Loop: How Real Data Science Works

Each iteration teaches you:

- Where your model fails (residuals)
- Which features matter (coefficients, feature importance)
- How confident you should be (cross-validation scores)

When to stop? When you understand your model and its limitations, even if it's not perfect.

Common Pitfalls: What Will Bite You

1. **Using all features** — Linear Regression with 1275 features will overfit
2. **Tuning hyperparameters on test data** — Data leakage! Breaks your honest evaluation
3. **Trusting training accuracy** — Always check test performance
4. **Forgetting to scale** — Feature scaling matters here too
5. **No visualization** — Plot residuals, feature distributions, correlations

Prevention: Follow the pipeline. One step at a time. Visualize everything.

Today's Activity: Modeling Project

Work through **Activity 04: Modeling Project** — open-ended by design.

Step 1: Baseline (Expect Failure)

- Load the molecular energy dataset (1275 features)
- Build a simple Linear Regression with all features
- Check R^2 on test data. Probably bad (~0.2). That's fine — it's diagnostic.

Step 2: Explore & Diagnose

- Plot feature distributions: what's normal? What's skewed?
- Check feature correlations: are some redundant?
- Diagnose: where is your model failing?

Today's Activity: Modeling Project

Step 3: Try an Improvement

- **Option A:** Remove useless features (RFE or correlation threshold)
- **Option B:** Use PCA to compress 1275 → 50 components
- **Option C:** Try a different model (Random Forest, Ridge regression)
- **Pick one and go deep.** Don't try everything.

Step 4: Evaluate with Confidence

- Use **cross-validation** (not just train/test split)
- Report: Mean ± Std of cross-validation scores
- Compare before/after. Did you improve?

Today's Activity: Modeling Project

Step 5: Iterate (If Time)

- What did you learn? What's still broken?
- Try another fix
- Can you push R^2 higher?

> **The goal:** Understand the full loop. Build something, measure it, improve it.
> You don't need a perfect model — you need to understand why it works or fails.

> **Notes:** Cross-Validation · RFE · PCA
>
> **Real tip:** Ask questions. Discuss with neighbors. This is research.

Supervised ML in Physics & Astro

It's one loop, repeated. Same five steps whether you classify spectra or predict energies.

Step	What you did	Days
1. Understand & explore	Load real data, clean it, plot it before modeling	1
2. Prepare	Train/test split, scale features (fit on train only)	2–4
3. Build	`fit → predict` — same `scikit-learn` API for every model	2–4
4. Evaluate	Right metric for the question; read residuals & confusion matrices	2–4
5. Improve	Add/select features, tune, try another model — then loop back	3–4

Classification vs regression = "what is it?" vs "how much?" — same pipeline, different target and metric.

Takeaways: What Transfers to Your Research

1. **Plot before you model, and plot your errors.** Anscombe's quartet, residuals, and class histograms all say the same thing: numbers alone lie.
2. **A feature can dominate everything.** Redshift turned 86% → 99% accuracy. Always ask: is my model learning the physics or memorizing one shortcut?
3. **More features ≠ better.** 1275 noisy features overfit; finding the ~50 that carry signal is the real work.
4. **Honest evaluation is sacred.** Never tune on the test set. Cross-validation gives you a distribution, not a lucky number.
5. **Start simple and expect to fail.** A bad baseline is a diagnostic, not a defeat — failure points to the next move.
6. **There is no single right answer.** The goal is a model you understand, including where and why it breaks.

> This is the workflow. The dataset changes; the loop doesn't.