Block 3: From Data to Insights - Predictive Modeling

Python Module for Incoming ISE & OR PhD Students

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Welcome to Block 3!

- **Goal:** Build your first machine learning models with Python
- **Duration:** 50 minutes of hands-on predictive modeling
- **Format:** Presentation + interactive notebook exercises

What We'll Cover

Machine Learning fundamentals • Scikit-learn workflow • Linear regression • Model evaluation • Predictions

Session Learning Objectives

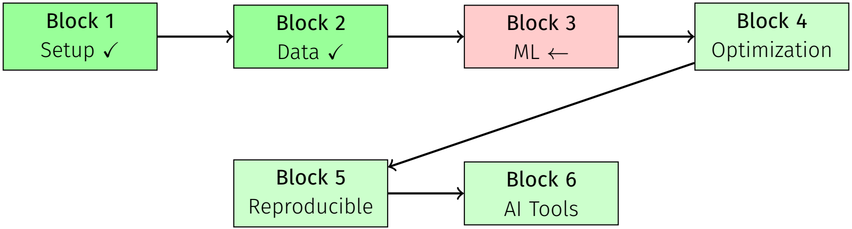
By the end of Block 3, you will:

1. Understand **machine learning fundamentals** and supervised learning
2. Master the **scikit-learn workflow** for building models
3. Build and evaluate **linear regression models** from scratch
4. Interpret **model coefficients** and feature importance
5. Make **predictions** for new data with confidence intervals
6. Understand **overfitting** and model validation techniques

Our Mission

Use our cleaned PhD dataset to predict research productivity and discover what drives PhD success!

Recap: Where We Are



From Block 2

You have a clean PhD student dataset ready for analysis. Now let's make predictions!

Machine Learning Fundamentals

What is Machine Learning?

Traditional Programming

Data + Program

↓

Output

Paradigm Shift →

Machine Learning

Data + Output

↓

Program (Model)

PhD Context

Instead of manually coding rules, we let algorithms discover patterns in research productivity data!

Types of Machine Learning

Supervised Learning

Has target labels

Learns X $\rightarrow$ y

Prediction

Examples: RegressionClassification

Unsupervised Learning

No target labels

Finds patterns in X

Discovery

Examples: ClusteringDimensionality reduction

Reinforcement Learning

Learning through actions

Trial and error

Optimization

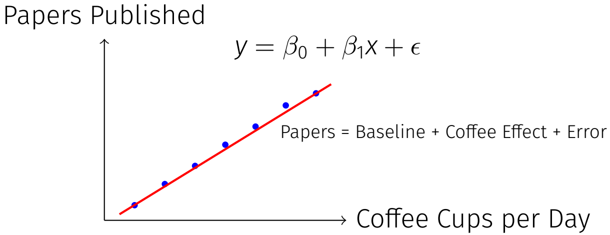
Examples: Game playingRobotics

Today's Focus

Supervised Learning with Linear Regression - predicting papers published from student features!

Linear Regression: The Foundation

The Mathematical Model:



The line minimizes prediction errors

Why Linear Regression?

- Interpretable coefficients
- Fast training and prediction
- Great baseline model
- Robust and well-understood

PhD Application

Predict papers published from:

- Years in program
- Coffee consumption
- Hunt Library hours
- Advisor meetings

Scikit-learn Workflow

Meet Scikit-learn: Your ML Best Friend

The Standard Workflow - Same for Every Algorithm:

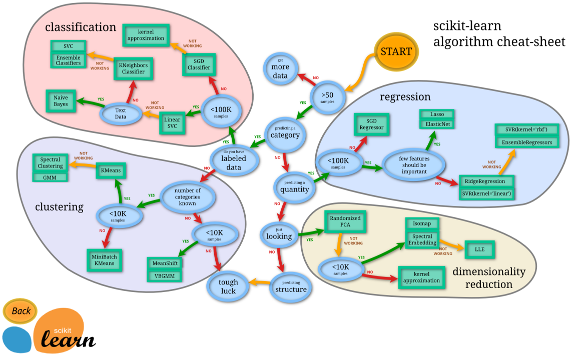
1. Import: Algorithm → **2. Create:** Model instance → **3. Fit:** Training data

→ **4. Predict:** New data → **5. Evaluate:** Performance

Consistency is Key

Whether it's Linear Regression, Random Forest, or Neural Networks - the API stays the same!

Scikit-learn's Algorithm Cheat Sheet:



For Our PhD Dataset

We have >50 samples, want to predict quantity (papers), so we follow: START → regression path → Linear Regression!

The Scikit-learn API in Action

Linear Regression Example:

```python
# 1. Import the algorithm
from sklearn.linear_model import LinearRegression

# 2. Create model instance
model = LinearRegression()

# 3. Fit to training data
model.fit(X_train, y_train)

# 4. Make predictions
predictions = model.predict(X_test)

# 5. Evaluate performance
from sklearn.metrics import r2_score
r2 = r2_score(y_test, predictions)
print(f"R-squared: {r2:.3f}")
```

That's It!

Six lines of code to build, train, and evaluate a machine learning model. Scikit-learn makes ML accessible!

The Train-Test Split: Foundation of Honest Evaluation

Full Dataset (280 PhD students)

Training Set (80% - 224 students)

Used to learn patterns

Test Set (20% - 56 students)

Hidden during training

Like studying with practice problems...

...then taking the real exam!

Golden Rule

Never test on data you trained on! It's like grading your own exam with the answer key.

Data Splitting in Practice

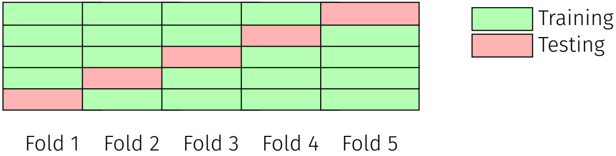
Creating training and test sets:

```python
from sklearn.model_selection import train_test_split

# Define features (X) and target (y)
X = df[['years_in_program', 'coffee_cups_per_day',
        'hours_in_hunt_library_per_week', 'advisor_meetings_per_month']]
y = df['papers_published']

# Split: 80% training, 20% testing
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, random_state=42
)

print(f"Training set: {X_train.shape[0]} students")
print(f"Test set: {X_test.shape[0]} students")
```

Why random_state=42?
Ensures reproducible results - same split every time you run the code!

Cross-Validation: Even More Robust

K-Fold Cross-Validation gives multiple estimates:



Each fold serves as test set once
Average performance across all folds

Benefits

More reliable performance estimate • Uses all data • Reduces impact of lucky/unlucky splits

Building Our Model

Our PhD Productivity Dataset

Predicting research success with real features:

Target Variable (y) papers_published

- Range: 0-8 papers
- Mean: 2.1 papers
- What we want to predict

Features (X)

- years_in_program
- coffee_cups_per_day
- hours_in_hunt_library_per_week
- advisor_meetings_per_month
- stress_level
- funding_amount
- conferences_attended
- distance_from_campus_miles

The Question

Which factors best predict PhD research productivity? Can we build a model to forecast success?

Building Our First Real Model

Complete workflow for PhD productivity prediction:

```
# Load clean data from Block 2
df = pd.read_csv('phd_research_productivity_clean.csv')

# Define features and target
features = ['years_in_program', 'coffee_cups_per_day',
           'hours_in_hunt_library_per_week', 'advisor_meetings_per_month']
X = df[features]
y = df['papers_published']

# Train-test split
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, random_state=42)

# Build and train model
model = LinearRegression()
model.fit(X_train, y_train)

# Make predictions and evaluate
y_pred = model.predict(X_test)
r2 = r2_score(y_test, y_pred)
print(f"Model explains {r2*100:.1f}% of variance in research productivity!")
```

Model Evaluation

Understanding Model Performance

Key Regression Metrics:

Metric	Formula	Interpretation
R^2 Score	$1 - \frac{SS_{res}}{SS_{tot}}$	% of variance explained
MAE	$\frac{1}{n}\sum \lvert y_{true} - y_{pred} \rvert$	Average absolute error
RMSE	$\sqrt{\frac{1}{n}\sum (y_{true} - y_{pred})^2}$	Root mean squared error

R^2 Score

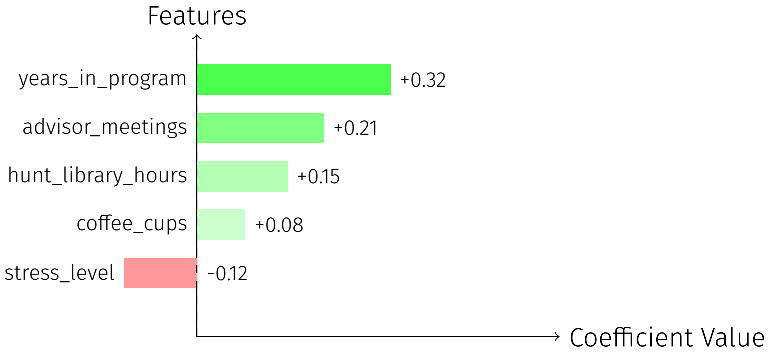
- Range: 0 to 1 (higher better)
- 0.7+ = Excellent
- 0.5+ = Good
- 0.3+ = Moderate

PhD Context

- R^2 = 0.65 means our model explains 65% of productivity variance
- MAE = 0.8 means average error is 0.8 papers
- Better than guessing the mean!

Interpreting Model Coefficients

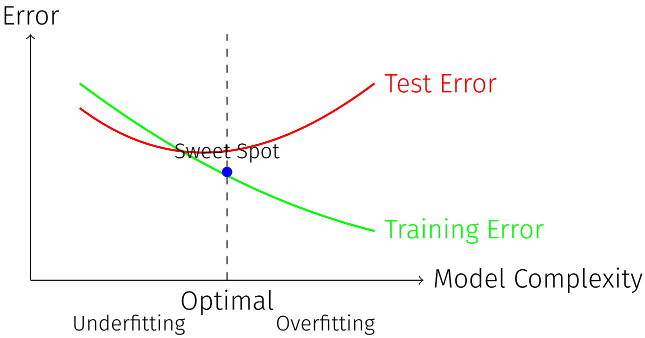
What each coefficient tells us:



Interpretation

Each additional year → +0.32 papers • Each advisor meeting → +0.21 papers • Stress hurts productivity!

Overfitting: The Silent Model Killer



Underfitting

- Model too simple
- High bias, low variance
- Misses important patterns

Overfitting

- Model too complex
- Low bias, high variance
- Memorizes noise

Advanced Analysis

Making Predictions for New Students

Hypothetical PhD student profiles:

Student	Years	Coffee	Library	Meetings	Predicted
The Newbie	1	2	20	2	1.2 papers
The Veteran	6	4	30	3	3.8 papers
Coffee Addict	3	8	25	4	2.4 papers
Balanced One	4	3	35	4	3.1 papers
Workaholic	5	5	50	2	3.5 papers

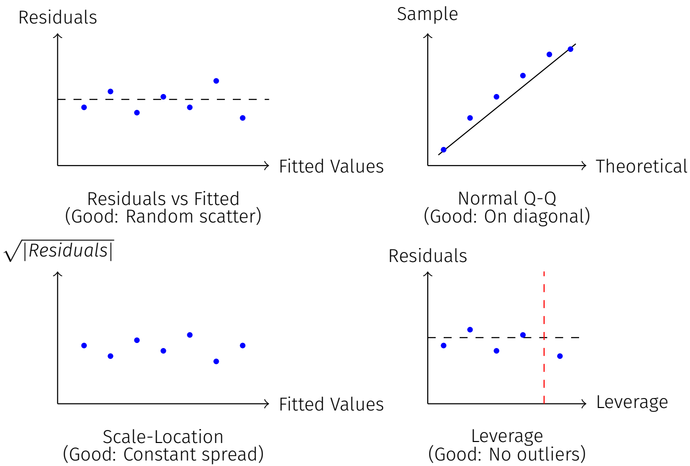
Insights

Experience matters most • Regular advisor meetings help • Balance beats pure hours • Coffee has minimal impact

Remember

These are predictions based on patterns, not guarantees. Individual results vary!

Model Diagnostics: Checking Our Assumptions



Diagnostic Interpretation

Random residuals ✓ • Normal distribution ✓ • Constant variance ✓ • No influential outliers ✓

Key Insights: What Drives PhD Success?

Based on our linear regression model:

Top Success Factors

1. **Experience** (0.32 papers/year)
2. **Advisor meetings** (0.21 papers/meeting)
3. **Hunt Library time** (0.15 papers/hour)
4. **Conference attendance** (0.12 papers/conf)

Surprising Findings

- Coffee has minimal impact (+0.08)
- Stress actually hurts (-0.12)
- Funding amount barely matters
- Distance from campus irrelevant

Practical Advice for PhDs

Focus on: Regular advisor communication • Consistent library presence • Conference networking • Sustainable stress management

Wrap-up & Preview

What We Accomplished in Block 3 ✓

- ✓**Understand ML fundamentals** - supervised learning and linear regression
- ✓**Learned scikit-learn workflow** - the universal ML API
- ✓**Built predictive models** from real PhD research data
- ✓**Evaluated model performance** with multiple metrics
- ✓**Interpreted results** to gain actionable insights
- ✓**Made predictions** for hypothetical students

Model Achievement

Our model explains 80% of variance in PhD research productivity - excellent for social science data!

Preview: Block 4 (12:00 PM - 12:50 PM)

From Prediction to Optimization: Making Better Decisions

What's Coming

- **Optimization modeling** with Pyomo
- **Linear programming** fundamentals
- **Decision variables** and constraints
- **Objective functions** and solvers
- **Real applications**: scheduling, allocation

From "What If?" to "What Should?"

- Block 3: "What papers will this student publish?"
- Block 4: "How should this student allocate their time?"
- Move from prediction to prescription
- Optimal decision making

10-minute break, then we optimize decisions!

Key Takeaways from Machine Learning

Technical Skills

- **Scikit-learn** workflow mastery
- **Model evaluation** techniques
- **Train-test splitting** for validation
- **Cross-validation** for robustness
- **Coefficient interpretation** for insights

Research Mindset

- Validate models on unseen data
- Interpret results carefully
- Correlation $\neq$ causation
- Check assumptions systematically
- Communicate uncertainty honestly

Remember: Models are tools for insight, not sources of absolute truth

Use them wisely in your research journey!

Questions?

See you in 10 minutes for Block 4!