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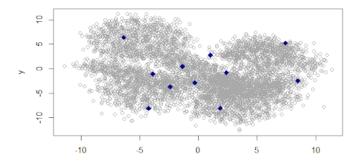
MATH 7560 Statistical Learning II || BGSU

April 24, 2025

K-means: Data & Motivation

Clustering Task

- **Goal**: Partition \mathbb{R}^2 data into k = 11 clusters.
- Comparison: Standard K-means vs K-means++ initialization.
- K-means++ Motivation: Better initial centroids for potentially faster/better clustering.



K-means vs K-means++ Results

Standard K-means:

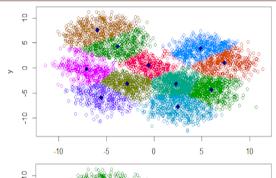
• **Stats**: 5 iterations, WCSS = 22,824.

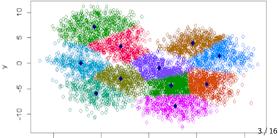
K-means++ Initialization:

• **Stats**: 8 iterations, WCSS = 22.943.

Observat<u>ion</u>

K-means++ offered no clear advantage over standard K-means for this dataset (visually or by WCSS).



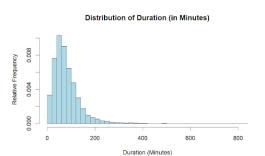


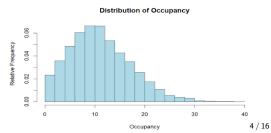
Duration (minutes):

Statistic	Value
Minimum	6.00
1st Quartile	44.00
Median	68.00
Mean	81.78
3rd Quartile	103.00
Maximum	822.00

Occupancy (students):

Statistic	Value
Minimum	1.00
1st Quartile	7.00
Median	11.00
Mean	11.62
3rd Quartile	15.00
Maximum	40.00





Kmeans++

Category	Key Features
Temporal	Time of day, Day of week, Week of semester
Academic	Course level, GPA categories, Credit load
Visit	Duration patterns, Group sizes, Visit frequency
Course	Subject areas, Level progression, Course mix
Student	Major groups, Class standing, Academic progress

External Source	Key Features
R library 'lunar'	Moon phase data
R library 'openmeteo'	Hourly weather metrics (temperature, humidity, pressure, cloud cover, wind, radiation, precipitation, & soil conditions)

Engineered Into

Dropped Raw Features

Raw Feature

Course Name

Course Number

Stuc	dent_l	Ds		Tota	ıl_Visi	ts, S	emester_'	Visits,	Avg_{-}	Week	ly_Vi	sits
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Class_Standing_Self_Reported, Class_Standing_BGSU Class_Standing

Major_Category, Has_Multiple_Majors Major Expected_Graduation Expected_Graduation_Date, Months_Until_Graduation

Course_Name_Category

Course_Type Course_Type_Category Course_Code_by_Thousands Course_Level, Advanced_Course_Ratio

Feature Engineering Strategy

Raw features were transformed into more informative derived features, capturing higher-level patterns and relationships in the data.

Unique_Courses, Course_Level_Mix

Duration Task Models

Occupancy Task Models

			<u> </u>
Model	Hyperparameters	Model	Hyperparameters
MARS	num_terms: [7,15] prod_degree: 1	MARS	num_terms: [120, 130] prod_degree: 1
Random Forest	trees: [300, 325] min_n: [15, 25] mtry: [20, 25]	Random Forest	trees: [250, 350] min_n: [2, 3] mtry: [40, 45]
XGBoost	trees: [75, 100] tree_depth: [15, 21] learn_rate: 0.05 min_n: [10, 15] mtry: [12, 15]	XGBoost	trees: [350, 450] tree_depth: [6, 8] learn_rate: 0.1 min_n: [2, 3] mtry: [30, 35]

Deep Learning Hyperparameters **Duration Task Models** Model **Hyperparameters** Model Ir: $[10^{-3}, 5 \times 10^{-3}]$ batch_size: {64, 128}

Occupancy Task Models

gru_dim: {128, 256, 512} num_layers: $\{1,2\}$ $gru_expansion: [0.5, 1.4]$ **dropout_rate**: [0.25, 0.42] weight_decay: $[10^{-6}, 10^{-5}]$ activation_fn: relu

num_layers: 2 **GRU**

Trans-

former

Model Building

Hyperparameters Ir: $[1.2 \times 10^{-3}, 5 \times 10^{-3}]$ batch_size: {64, 128} gru_dim: 512

Ir: $[10^{-3}, 7 \times 10^{-3}]$ weight_decay: $[10^{-6}, 10^{-4}]$ $gru_expansion: [0.6, 1.4]$ **dropout_rate**: [0.25, 0.42] weight_decay: $[10^{-6}, 5 \times 10^{-6}]$ activation fn: relu Ir: $[8 \times 10^{-4}, 1.5 \times 10^{-3}]$ batch_size: {64, 128}

d_hid: 128

d_model: {64, 128, 256} **nhead**: {4,8} nlayers: $\{2,3\}$ dropout: [0.05, 0.20] weight_decay: $[10^{-6}, 10^{-5}]$

GRU

Trans**nhead**: {4,8} nlayers: $\{2,3\}$ former d hid: 128 dropout: [0.05, 0.20]

batch size: 64

d_model: 128

Preprocessing Pipeline Details

R 'recipes' Pipeline Steps

- Define roles (outcome, predictors)
- Remove specified ID/date/unwanted columns
- Convert Check_In_Time to minutes past midnight
- Impute missing numerics (mean)
- Mandle novel factor levels
- Oreate dummy variables (drop first)
- Remove zero-variance predictors
- Normalize numeric predictors

Step 5: Handling Novel Factor Levels

Prepares for unseen categories in new data:

- Adds a special "novel" level to factors.
- Replaces unknown categories with "novel" instead of causing errors.
- Ensures robust predictions, especially before dummy encoding.

Duration Task

Model	RMSE	R²
XGBoost	59.9	0.099
Random Forest	60.1	0.090
Transformer	61.3	0.010
MARS	61.6	0.045
GRU	63.8	0.041

Occupancy Task

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Model	RMSE	R²		
XGBoost	1.83	0.911		
Random Forest	1.93	0.902		
GRU	3.16	0.738		
Transformer	3.26	0.706		
MARS	3.78	0.617		

Key Performance Observations

Based on holdout set metrics:

• Duration Task: XGBoost achieved the lowest RMSE (59.9) and highest R² (0.099).

Duration Prediction:

Component	Value
Model Pipeline CV Method RMSE R ²	PenalizedSplines vanilla kfold 59.47 0.059
Ridge α Spline degree Spline knots Scaler	14.38 3 15 RobustScaler

Occupancy Prediction:

Component	Value
Model	PenalizedSplines
Pipeline	vanilla
CV Method	rolling
RMSE	3.64
R ²	0.303
Ridge α	29.76
Spline degree	3
Spline knots	15
Scaler	RobustScaler

Key Insight

Both tasks achieved best results with PenalizedSplines and vanilla features, though with different CV methods & regularization.

Kmeans++

Kmeans++

Occupancy: Best Model Diagnostics

Sanity Check

Kmeans++

Main Results:

- PenalizedSplines with vanilla features performed best
- Occupancy prediction shows promise ($R^2 = 0.303$)
- Duration prediction remains challenging ($R^2 = 0.059$)

Future Directions:

- Incorporate weather data
- Explore non-linear relationships further
- Investigate time series approaches

Impact

While duration prediction remains difficult, our occupancy model shows strong potential for a victory #CautiousOptimism

Thank You

For Your Attention

Questions & Discussion Welcome