# Graph Embeddings for Non-IID Data Feature Representation Learning

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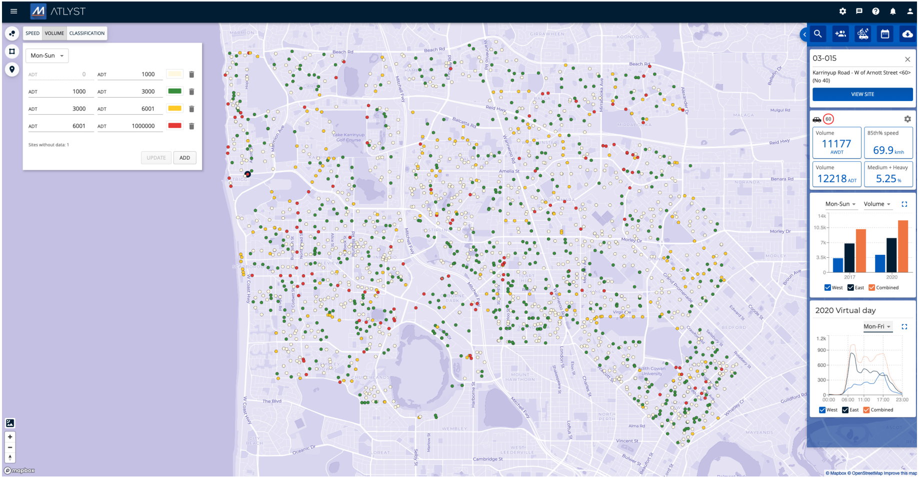
# Motivation: How we handle data now?

| Site name | Year | Description | Asset number | Lat | Lng | ADT | AWDT | AWEDT | 85% speed | Light vehicles(%) | Medium vehicles(%) | Heavy vehicles(%) | Cycle(%) | Motorcycle(%) | Unclassifiable(%) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 05-013 | 2021 | Cobb Street - E of Calais Road <50> (No 77) | | -31.907133 | 115.769148 | 875.00 | 899.00 | 797.00 | 54.11 | 90.66 | 7.56 | 0.11 | 0.91 | 0.69 | 0.07 |
| 05-062 | 2021 | Westview Street - N of Scarborough Beach Road <50> (No 151) | | -31.893093 | 115.774083 | 857.00 | 879.00 | 790.00 | 36.68 | 93.76 | 3.57 | 0.07 | 0.94 | 0.57 | 1.09 |
| 05-014 | 2021 | Cobb Street - E of Cornelian Street <50> (No 122) | | -31.907387 | 115.774543 | 3617.00 | 3838.00 | 2954.00 | 54.50 | 94.53 | 4.00 | 0.12 | 0.70 | 0.62 | 0.03 |
| 07-030 | 2021 | Maree Street - W of Blissett Way <50> (No 26) | | -31.851122 | 115.817148 | 223.00 | 234.00 | 203.00 | 54.40 | 94.95 | 3.51 | 0.23 | 0.84 | 0.47 | 0.00 |
| 08-027 | 2021 | Swiftlet Way - N of Willowbank Entrance <50> (No 4) | | -31.866735 | 115.791622 | 639.00 | 648.00 | 604.00 | 38.02 | 92.95 | 5.42 | 0.12 | 0.60 | 0.91 | 0.00 |
| 06-026 | 2021 | Monyash Road - S of Wessex Street <50> (No 28) | | -31.853747 | 115.790568 | 278.00 | 266.00 | 322.00 | 49.39 | 90.82 | 7.17 | 0.35 | 0.99 | 0.62 | 0.05 |
| 05-054 | 2021 | Stanley Street - N of Ventnor Street <50> (No 100B) | | -31.902667 | 115.762312 | 431.00 | 437.00 | 416.00 | 47.02 | 95.20 | 3.28 | 0.00 | 0.32 | 1.08 | 0.12 |
| 06-006 | 2021 | Camelot Street - E of Duffy Road <50> (No 7) | | -31.853608 | 115.794553 | 1119.00 | 1162.00 | 980.00 | 45.68 | 93.24 | 5.25 | 0.70 | 0.33 | 0.45 | 0.03 |
| 06-001 | 2021 | Almadine Drive - E of Marmion Avenue <50> (No 52) | | -31.853632 | 115.768778 | 2011.00 | 2387.00 | 873.00 | 54.61 | 94.29 | 4.33 | 0.31 | 0.48 | 0.51 | 0.08 |
| 05-028 | 2021 | Duke Street - N of Brighton Road <50> (No 193) | | -31.896198 | 115.771465 | 7359.00 | 7728.00 | 6266.00 | 58.00 | 92.68 | 6.55 | 0.26 | 0.07 | 0.42 | 0.03 |
| 05-022 | 2021 | Dover Road - N of Ventnor Street <50> (No 45) | | -31.902717 | 115.765752 | 407.00 | 416.00 | 367.00 | 53.71 | 94.05 | 3.82 | 0.06 | 0.69 | 1.38 | 0.00 |
| 05-050 | 2021 | Sackville Terrace - W of Abbett Street <60> (No 77 Abbett) | | -31.887698 | 115.768812 | 6965.00 | 6801.00 | 7455.00 | 47.81 | 92.40 | 5.90 | 0.21 | 0.53 | 0.87 | 0.10 |
| 06-043 | 2021 | Whittington Avenue - W of Godecke Rise <50> (No 12) | | -31.847642 | 115.769412 | 1169.00 | 1174.00 | 1151.00 | 55.58 | 95.72 | 2.93 | 0.16 | 0.42 | 0.70 | 0.07 |
| 08-003 | 2021 | Balcatta Road West - E of Careniup Avenue <50> (70m East) | | -31.85932 | 115.796223 | 564.00 | 582.00 | 504.00 | 57.71 | 90.62 | 7.52 | 0.51 | 1.01 | 0.29 | 0.04 |
| 06-042 | 2021 | Whittington Avenue - E of Bradbourne Drive <50> (No 54) | | -31.848895 | 115.765343 | 1015.00 | 1020.00 | 999.00 | 56.30 | 94.49 | 3.89 | 0.25 | 0.46 | 0.88 | 0.02 |
| 18-006 | 2021 | Dolomite Court - E of Silkwood Turn <50> (No 29) | | -31.921695 | 115.79033 | 858.00 | 969.00 | 493.00 | 51.70 | 94.67 | 3.71 | 0.06 | 1.20 | 0.29 | 0.06 |
| 06-014 | 2021 | Edlaston Road - E of Kersey Way E <50> (No 33) | | -31.846663 | 115.775163 | 698.00 | 705.00 | 678.00 | 58.90 | 94.66 | 3.85 | 0.13 | 0.68 | 0.66 | 0.04 |
| 06-016 | 2021 | Everingham Street - S of Osmaston Road <50> (No 76) | | -31.851858 | 115.777517 | 2312.00 | 2838.00 | 727.00 | 50.51 | 94.91 | 3.90 | 0.14 | 0.26 | 0.41 | 0.38 |
| 27-028 | 2021 | Fourth Avenue - W of John Street <50> (No 70) | | -31.926933 | 115.880983 | 1314.00 | 1423.00 | 1145.00 | 54.22 | 94.52 | 3.34 | 0.08 | 1.28 | 0.74 | 0.04 |
| 28-025 | 2021 | Harcourt Street -  E of Beaufort Street <50> (No 13) | | -31.92012 | 115.889367 | 211.00 | 180.00 | 214.00 | 46.30 | 90.56 | 5.41 | 0.32 | 2.42 | 1.13 | 0.16 |
| 28-078 | 2021 | Dundas Road -  E of Arthur Street <50> (No 11) | | -31.919552 | 115.886608 | 1505.00 | 1526.00 | 1450.00 | 52.49 | 94.54 | 2.98 | 0.07 | 1.62 | 0.54 | 0.25 |
| 28-050 | 2021 | Wood Street -  W of Beaufort Street <50> (No 14) | | -31.916963 | 115.889622 | 2095.00 | 2195.00 | 1824.00 | 49.00 | 94.90 | 3.03 | 0.17 | 1.14 | 0.62 | 0.13 |
| 06-013 | 2021 | Edlaston Road - W of Alvaston Drive <50> (No 60) | | -31.846517 | 115.779003 | 1045.00 | 1058.00 | 1009.00 | 52.42 | 94.78 | 4.54 | 0.13 | 0.07 | 0.45 | 0.02 |
| 18-046 | 2021 | Campus Way - W of Pearson Street <50> (No 6) | | -31.925042 | 115.793828 | 318.00 | 326.00 | 283.00 | 44.21 | 94.63 | 3.87 | 0.15 | 0.38 | 0.70 | 0.27 |
| 28-074 | 2021 | Beaufort Street -  S of Eighth Avenue <50> (HN 851 (Hair Studio)) | | -31.922678 | 115.8839 | 22457.00 | 22692.00 | 21826.00 | 50.90 | 93.37 | 5.26 | 0.20 | 0.45 | 0.68 | 0.05 |
| 28-080 | 2021 | Normanby Road -  W of Beaufort Street <50> (No 6) | | -31.919038 | 115.887795 | 265.00 | 279.00 | 227.00 | 45.22 | 92.41 | 3.54 | 0.06 | 3.07 | 0.81 | 0.12 |
| 07-027 | 2021 | Hornet Street - S of Eglinton Crescent <50> (No 4) | | -31.853987 | 115.809802 | 619.00 | 630.00 | 577.00 | 44.89 | 92.55 | 6.19 | 0.21 | 0.35 | 0.56 | 0.14 |
| 06-031 | 2021 | Osmaston Road - S of Edlaston Road <50> (No 47) | | -31.849087 | 115.772533 | 1848.00 | 2233.00 | 690.00 | 53.10 | 94.26 | 4.01 | 0.15 | 0.97 | 0.50 | 0.11 |
| 05-006 | 2021 | Brighton Road - E of Hinderwell Street <50> (No 101) | | -31.898005 | 115.767125 | 8918.00 | 8891.00 | 9047.00 | 54.22 | 94.77 | 4.03 | 0.08 | 0.30 | 0.77 | 0.05 |
| 05-009 | 2021 | Burniston Street - N of Scarborough Beach Road <50> (No 145) | | -31.892408 | 115.770427 | 877.00 | 928.00 | 719.00 | 51.01 | 94.28 | 3.98 | 0.36 | 0.41 | 0.89 | 0.09 |
| 07-019 | 2021 | Eglinton Crescent - W of Erindale Road <50> (No 147) | | -31.853707 | 115.8118 | 2432.00 | 2820.00 | 1262.00 | 59.69 | 92.68 | 6.22 | 0.25 | 0.27 | 0.53 | 0.06 |
| 30-073 | 2021 | The Strand - E of McLean Street <50> (No 332) | | -31.896713 | 115.878838 | 2482.00 | 2533.00 | 2320.00 | 59.51 | 94.36 | 4.58 | 0.23 | 0.49 | 0.26 | 0.08 |
| 18-043 | 2021 | Mountainbell Road - N of Cromarty Road <50> (20m North) | | -31.927283 | 115.793548 | 452.00 | 462.00 | 398.00 | 34.60 | 82.49 | 11.26 | 0.03 | 0.97 | 0.57 | 4.69 |
| 18-044 | 2021 | Parrotbush Road - N of Cromarty Road <50> (No 4) | | -31.927255 | 115.792547 | 839.00 | 878.00 | 699.00 | 40.21 | 84.73 | 6.67 | 0.10 | 0.85 | 0.38 | 7.27 |
| 28-075 | 2021 | Nelson Street -  N of York Street <50> (No 20) | | -31.918648 | 115.892252 | 905.00 | 932.00 | 832.00 | 53.10 | 94.32 | 3.63 | 0.02 | 1.38 | 0.63 | 0.02 |
| 28-077 | 2021 | Central Avenue -  W of Beaufort Street <50> (No 145) | | -31.924177 | 115.880942 | 13448.00 | 14180.00 | 11595.00 | 60.52 | 95.61 | 3.33 | 0.17 | 0.25 | 0.60 | 0.04 |

# Motivation: Visualization of the structural information



# Motivation: What's Next?

It looks cool, but:

- How to make machines represent, interpret and leverage structured information effectively?

# Problem definition

- How to encode structural information of a network into a machine learning problem?
- Whether the structural enhanced feature space improve classification performance?
- Knowledge graph embedding compares with homogenous network embedding in feature encoding?
- We use a traffic network where spatial information is naturally present.

# Methodology: The I.I.D (Independent Identical Distribution) Assumption

| Models | Rows/Observations | Columns/Features |
|---|---|---|
| Logistic Regression | Assume independent | Assume independent |
| Naïve Bayes | Assume independent | Assume independent |
| SVM | Assume independent | Assume independent |
| DT/RF | Assume independent | Assume independent |
| kNN | No assumption | No assumption |

Liu et al, IJCNN 2014

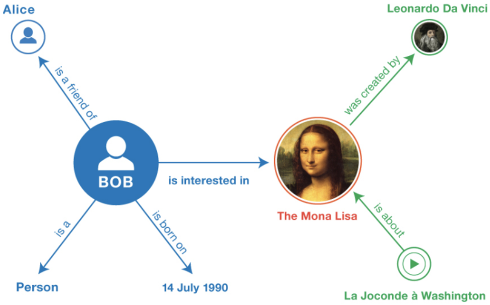
# Methodology: Graph


A simple graph

- Nodes are of the same type.
- Edges can be directed or weighted.

https://web.stanford.edu/class/cs520/2020/notes/What_is_a_Knowledge_Graph.html

# Methodology: Knowledge Graph (KG)

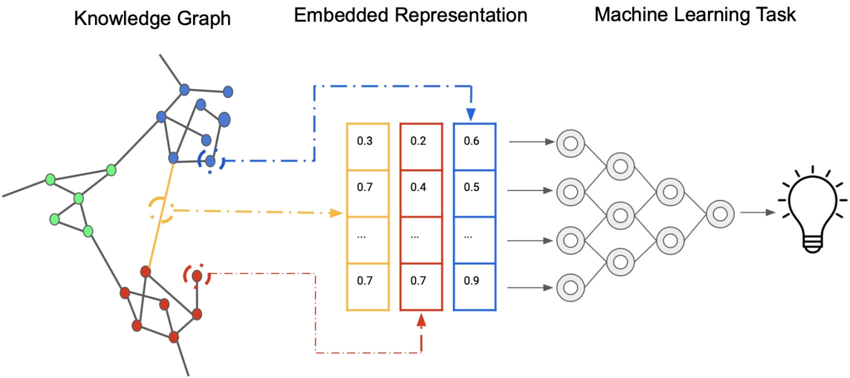



A simple knowledge graph

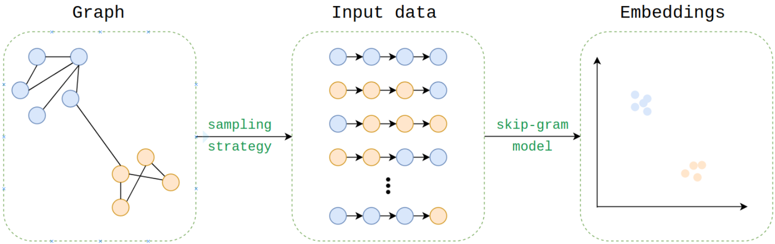
- Nodes and edges all have types.
- Ontology required.

# Methodology: Graph and Knowledge Graph

## Embedding Workflow



# Methodology: Graph Embedding with Node2vec

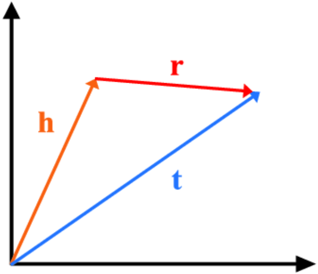



node2vec embedding process

- Biased random walk, which explores neighborhoods in BFS as well as DFS fashion, generate sequences as input.
- Capture homophily and structural equivalence.

https://snap.stanford.edu/node2vec/

# Methodology: Knowledge Graph Embedding with TransE




$$h + r = t$$

https://en.wikipedia.org/wiki/Knowledge_graph_embedding
Bordes et al, Advances in Neural Information Processing Systems, 2013

# Methodology: How we handle spatial datasets?

1. **Graph and Knowledge Graph Construction**: A road network graph and a traffic knowledge graph.
2. **Representation learning**: Compute the embeddings by node2vec, TransE respectively.
3. **Machine Learning Tasks**: Use embeddings as input, apply SVM, kNN and RF.

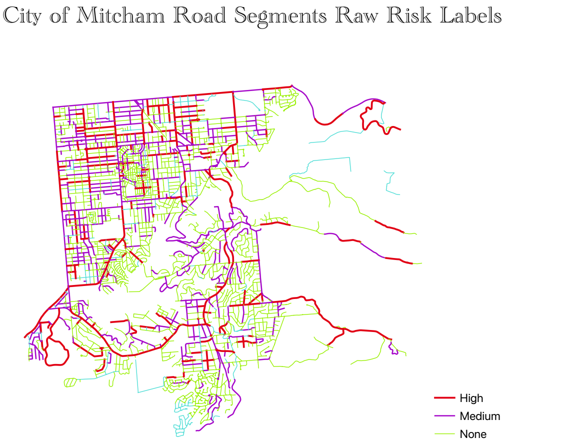
# Dataset

The road network is composed of 2287 road segments, for each road segment, we selected the following 8 features:

- a unique *asset id* to identify road segments
- *speed limit*, eg: 40km/h, 50km/h, 60km/h
- difference between speed limit and 85*th* %*ile* speed
- average daily *AM peak hour traffic volume*
- average daily *PM peak hour traffic volume*
- total *number of rear end hit* accidents since 2016
- total *number of crashes* since 2016
- total *number of casualties* since 2016

1 for asset management, 2 for speed, 2 for volume, 3 for risk

# Dataset: Overview



# Graph and Knowledge Graph Construction

1. **Graph and Knowledge Graph Construction**: A road network graph and a traffic knowledge graph.
2. **Representation learning**: Compute the embeddings by node2vec, TransE respectively.
3. **Machine Learning Tasks**: Use embeddings as input, apply SVM, kNN and RF.

# Graph and Knowledge Graph Construction (cont.)

With the help of Neo4j[1], we build a simple road network graph, which contains the following:

| Name | Type | Comments | Numbers |
|---|---|---|---|
| **RoadSegment** | Node | Use asset id to distinguish nodes | 2287 |
| **Link** | Edge | Link connected RoadSegment | 3772 |

To build a knowledge graph upon this:

- Keep the road segment nodes.
- Discrete attributes to obtain nodes for *speed/volume/risk*.

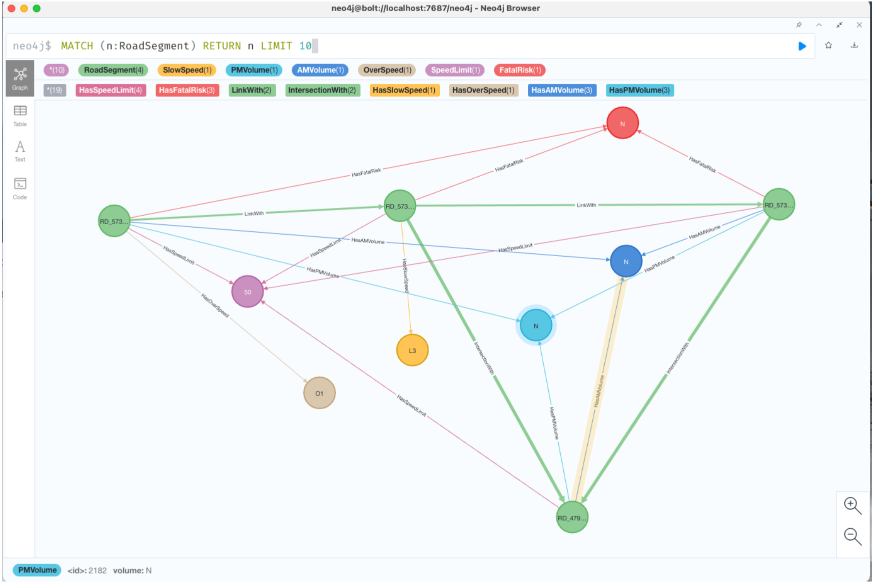
[1] https://neo4j.com/

# Graph and Knowledge Graph Construction (cont.)

Same, with Neo4j, the summary of traffic knowledge graph we built as following:

| Name | Type | Explain | Numbers |
|---|---|---|---|
| **RoadSegment** | Node | Use ASSET_ID to distinguish nodes | 2287 |
| **FatalRisk** | Node | Enumerate, H/M/N, stands for risk level | 3 |
| **RearEndHit** | Node | RearEndHit occurred | 1 |
| **OverSpeed** | Node | Enumerate, $O_1/O_2/O_3/O_4/O_5$ | 5 |
| **SlowSpeed** | Node | Enumerate, $L_1/L_2/L_3/L_4/L_5$ | 5 |
| **SpeedLimit** | Node | Enumerate, 15/25/40/50/60/70 (km/h) | 6 |
| **AMVolume** | Node | Enumerate, H/M/L/N | 4 |
| **PMVolume** | Node | Enumerate, H/M/L/N | 4 |
| **LinkWith** | Edge | Link connected RoadSegment | 1086 |
| **IntersectionWith** | Edge | The link between roadsegments is intersection | 2686 |
| **HasFatalRisk** | Edge | Link RoadSegment with FatalRisk nodes | 2287 |
| **HasRearEndHit** | Edge | Link RearEndHit with RoadSegment | 117 |
| **HasOverSpeed** | Edge | Link OverSpeed nodes with RoadSegment | 423 |
| **HasSlowSpeed** | Edge | Link SlowSpeed nodes with RoadSegment | 548 |
| **HasSpeedLimit** | Edge | Link SpeedLimit nodes with RoadSegment | 2287 |
| **HasAMVolume** | Edge | Link AMVolume nodes with RoadSegment | 974 |
| **HasPMVolume** | Edge | Link PMVolume nodes with RoadSegment | 974 |

# Graph and Knowledge Graph Construction (cont.)



# Representation Learning

1. **Graph and Knowledge Graph Construction**: A road network graph and a traffic knowledge graph.
2. **Representation learning**: Compute the embeddings by node2vec, TransE respectively.
3. **Machine Learning Tasks**: Use embeddings as input, apply SVM, kNN and RF.

# Representation Learning: Summary of Results

Using *NetworkX*[2], *node2vec*[3], *pykg2vec*[4], we managed to train and compute the embeddings for both the traffic knowledge graph and the road network graph.

- a 50-dimensions vector for each road segment in the road network graph via node2vec.
- a 58-dimensions vector for each road segment in the traffic KG via TransE.

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[2] https://networkx.org/

[3] https://snap.stanford.edu/node2vec/

[4] https://pykg2vec.readthedocs.io/

# Machine Learning Tasks (cont.)

1. **Graph and Knowledge Graph Construction**: A road network graph and a traffic knowledge graph.
2. **Representation learning**: Compute the embeddings by node2vec, TransE respectively.
3. **Machine Learning Tasks**: Use embeddings as input, apply SVM, kNN and RF.

# Machine Learning Tasks (cont.)

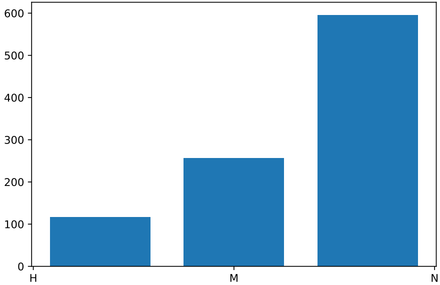
- For our classification task, our target variable is the *risk level*.
- We used SVM, kNN and RF to train the classification models.
- For traditional models, we have 5 input features: *speed limit*, *difference between speed limit and 85th %ile*, *AM peak volume*, *PM peak volume*, *rear end hit number*.
- Only 969 road segments without any missing features, having all the 5 features.
- 1316 have no speed data, and 1313 have no traffic volume data, due to traffic survey limitation.

# Machine Learning Tasks: Input sets for models

We want to see the performance differences when we feed different input sets into models.

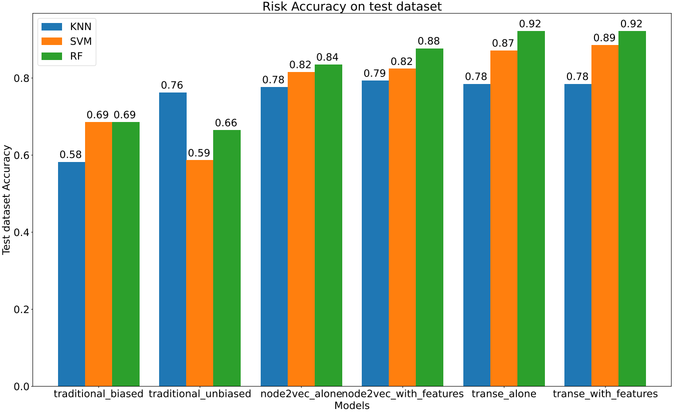
| Input | Reference ID |
|---|---:|
| five features | traditional_biased/unbiased |
| 50-dim vectors (node2vec) | node2vec_alone |
| 50-dim vectors (node2vec) + five features | node2vec_with_features |
| 58-dim vectors (TransE) | transe_alone |
| 58-dim vectors (TransE) + five features | transe_with_features |

# Machine Learning Tasks: Oversampling for highly imbalanced data



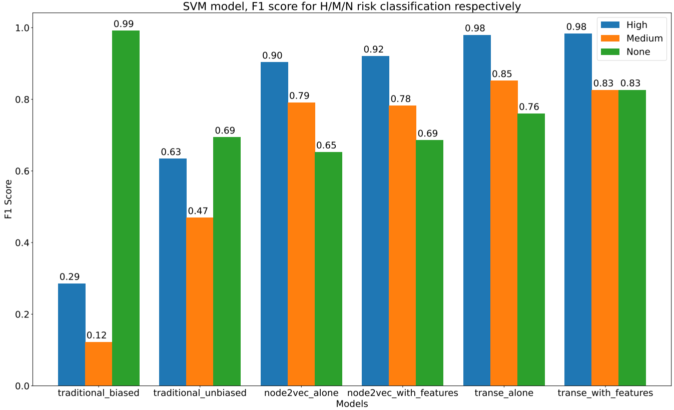

Imbalanced risk level distribution

# Results: Risk classification



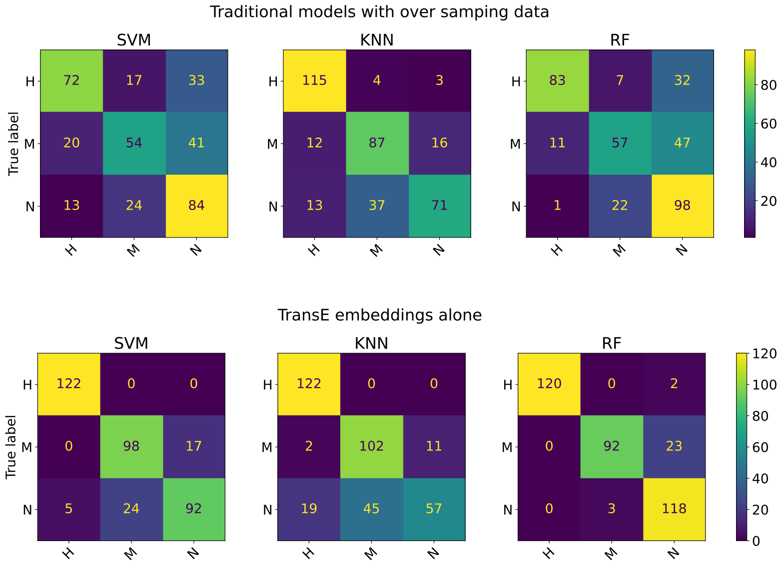

Risk classification accuracy for train and test datasets, per input set, per model

# Results: Risk classification

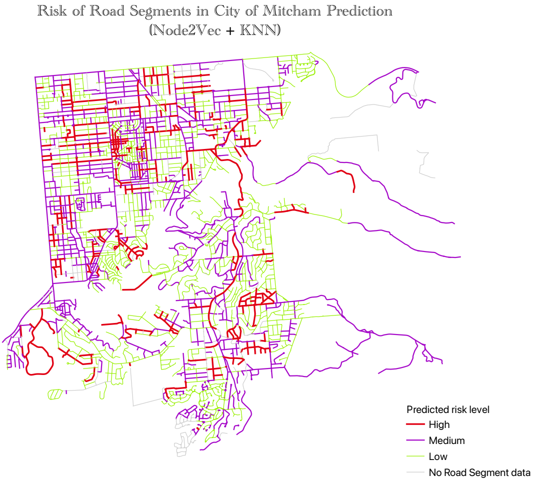



Risk classification f1 score for each input set, per risk level

# Results: Risk classification confusion matrix

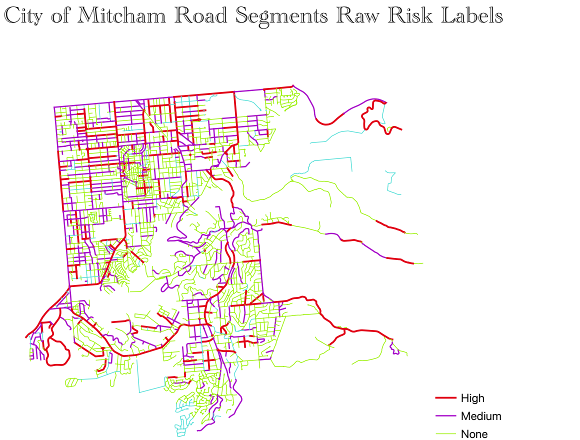


# Results: Risk classification

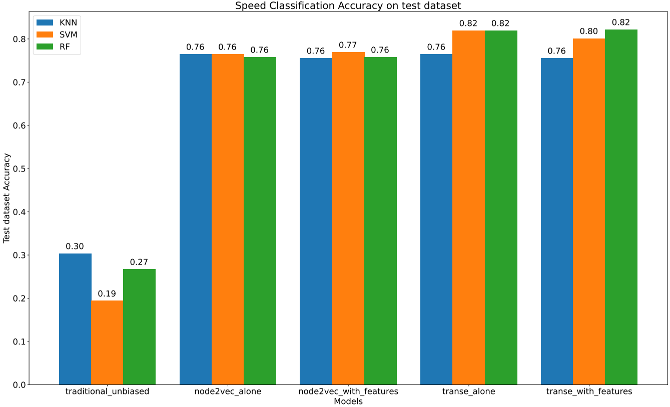



Map visualisation of road segments risk levels predicted by node2vec + kNN

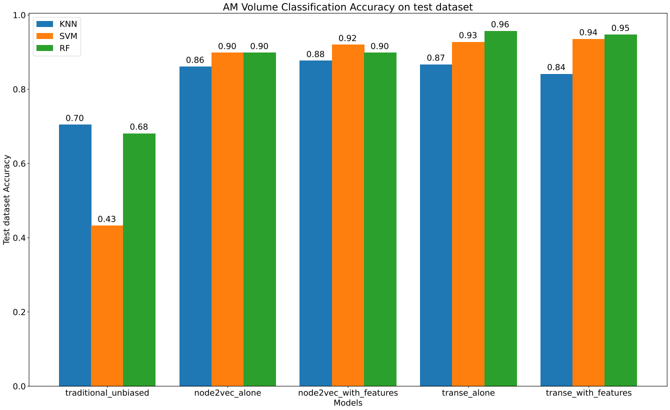
# Results: Risk classification



# Results: Speed classification



# Results: AM Volume classification



# Conclusion: Traffic

- Speed, volume and accidents are seem to be mainly determined by the road network structure.
- Road networks are not the whole story, with help of traffic knowledge graphs, classification accuracy can further improve.
- *node2vec_alone* and *transe_alone* models can handle missing data

# Conclusion: Spatial datasets

- Represent information with graphs or knowledge graphs, can encode structural information. Furthermore, it can handle missing data problem.
- Effective use of the spatial information in the dataset can effectively improve the accuracy of the classification tasks.
- Knowledge graph embeddings can preseve more information, so perform slightly better than homogenous network embeddings.
- Graph and Knowledge Graph embeddings perform well for Non-I.I.D Data feature extraction.

# Future work

- Traffic related
  - Apply on additional traffic related datasets to validate findings.
  - Build more complex traffic knowledge graphs, evaluate the performance.
- Spatial datasets related
  - Build more diverse spatial knowledge graphs.
  - Apply knowledge graph embedding models other than TransE.
- Other
  - Make use of the edge embeddings.
  - Explore how to represent and interpretate temporal information.

THANK YOU

Q & A