Probabilistic Inference of NYC Congestion from Taxi Data

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Abstract

- This document describes the expected style, structure, and rough proportions for your final project write-up.
- While you are free to break from this structure, consider it a strong prior for our expectations of the final report.
- Length is a hard constraint. You are only allowed max **8 pages** in this format. While you can include supplementary material, it will not be factored into the grading process. It is your responsibility to convey the main contributions of the work in the length given.

1. Introduction

Example Structure:

- What is the problem of interest and what (high-level) are the current best methods for solving it?
- How do you plan to improve/understand/modify this or related methods?
- Preview your research process, list the contributions you made, and summarize your experimental findings.

2. Background

The NYC Taxi and Limousine Commission (TLC) makes available[1] a dataset of taxi rides taken in the city. For our purposes, each ride is characterized by the time and location (latitude and longitude) of the pickup as well as the corresponding quantities for the drop-off[2]. Moreover, there is an abundance of data. In January of 2009 alone, there were over 14 million taxi rides recorded.

When we aggregate by hour of day (Figure 1), we see some variance with anywhere between a hundred thousand and a million trips per interval. This is reassuring for future bucketing of the data.

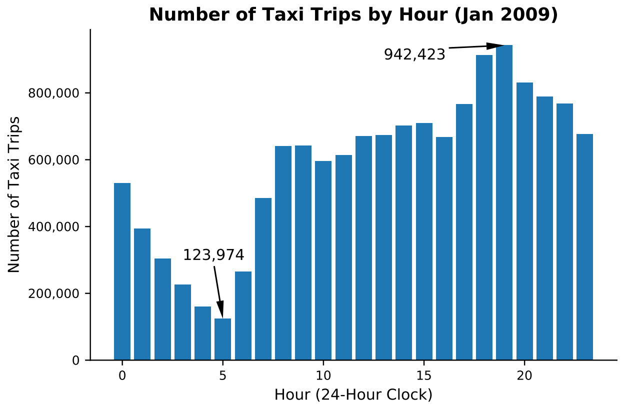


Figure 1. Taxi Trips by Time of Day

While we are not lacking in data volume, two important challenges do appear when working with this dataset. The first is that the data set is not completely clean. Case in point, while most trip durations (Figure 2) are reasonable for a taxi trip, just over 1% of trips have a drop-off time that is before the pick-up time, making for a trip with negative duration. Furthermore, the longest trip has duration of just over 42 days. It is difficult to accurately assess the veracity of the pickup and dropoff coordinates, but we observe that some trips have geographic coordinates that place the start or end of the trip in the ocean.

Additionally, whereas we would like to infer road conditions along the route of a taxi trip, we can only observe the start and end-points. The fact that the route taken is unobservable is primarily responsible for our inference challenges.

3. Related Work

Example Structure:

- What 3-5 papers have been published in this space?
- How do these differ from your approach?
- What data or methodologies do each of these works use?
- How do you plan to compare to these methods?

[1] http://www.nyc.gov/html/tlc/html/about/trip_record_data.shtml

[2] Additional information orthogonal to predicting trip duration—such as passenger counts and tip—is discarded

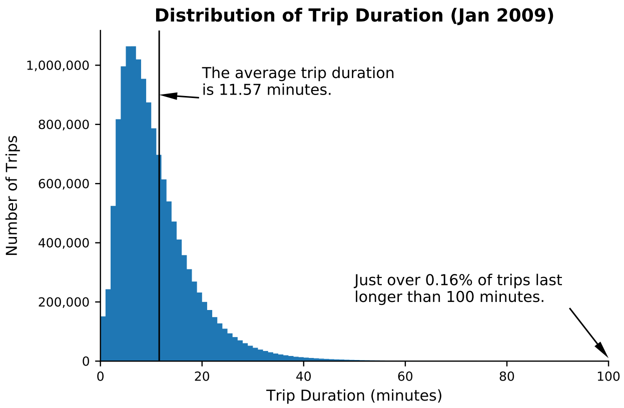
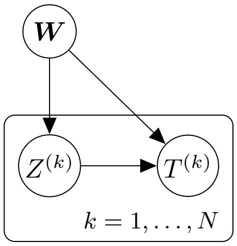


Figure 2. Taxi Trips by Duration

4. Model

We represent a city's road network with a connected graph $G = (V, E)$. Assume that each vertex $i \in V$ is associated with a weight w_i, representing the cost of traversing vertex i. A trip is represented by a path in G, and the distribution of the trip's duration depends on the weights w_i of vertices included in the path. Note that the choice of the path can in general depend on the collection of weights $\boldsymbol{W}$. In full generality, the model is represented by Figure 3, where trips in the data are indexed by (k), $T^{(k)}$ is the observed trip duration, and $Z^{(k)}$ is the path taken by trip k, a latent variable. Our primary interest is to perform inference on $\boldsymbol{W}$, so as to learn the levels of congestion associated with each vertex in G.

Figure 3. Representation of model as a directed graph

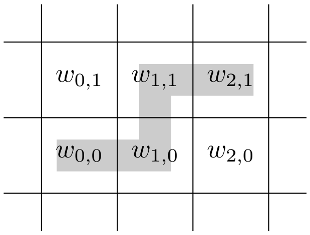


4.1. Parameterization

In principle, in our application to the New York City taxi data, we may take G to be a graph representing the exact road network in New York City, where each vertex is a *road segment* and the directed edge $(i, j) \in E$ if one can drive directly onto road segment j from road segment i; such a parameterization allows w_i to be directly interpretable as a measure of congestion on road segment i. However, such a detailed construction presents serious computational challenges when training on a large dataset, since solving pathfinding problems and computing minimal paths are non-trivially expensive.[3]

To avoid these challenges, we parameterize G as an undirected rectangular grid. Despite not being able to pinpoint weights w_i to congestion of specific road segments, we are nonetheless able to interpret the weights w_i as representative of congestion on a small patch of land. We may now represent a path $Z^{(k)}$ as a set of indices i of grid points traversed by the path. In full generality, there are an infinite number of paths connecting any two points i, j on the grid, but the vast majority of these paths are not sensible. Thus we restrict the set of possible paths for trip k to a *set of reasonable paths* $\boldsymbol{Z}^{(k)}$, where each path in $\boldsymbol{Z}^{(k)}$ travels strictly in the direction of the destination. For instance, if the destination of j is to the northeast of the starting location i, then the set of reasonable paths $\boldsymbol{Z}$ are the set of paths that only involve northward or eastward movements (e.g. Figure 4 shows a reasonable path from $(0, 0)$ to $(2, 1)$). Such a parameterization is more general than many in the literature; Zhan et al. (2013), for instance, uses the K-shortest path algorithm and considers the shortest 20 paths as a set of reasonable paths.

Figure 4. An example of a reasonable path



We parameterize the conditional distribution of $T^{(k)}$ as Normal, in the following reformulation of the directed graphical model:

$$\boldsymbol{W} \sim p(\boldsymbol{W})$$
$$Z^{(k)} \sim p(Z^{(k)} | \boldsymbol{W})$$
$$T^{(k)} | \boldsymbol{W}, Z^{(k)} \sim \mathcal{N}\left(\sum_{i \in Z^{(k)}} w_i, \sigma^2 \right),$$

where $p(Z^{(k)}|\boldsymbol{W})$ is a distribution over $\boldsymbol{Z}^{(k)}$. We consider two different ways to parameterize $p(Z^{(k)}|\boldsymbol{W})$: softmax regression and uniform. In the *softmax regression* model, a type of generalized linear model for discrete choice problems (McFadden et al., 1973), we parameterize the route

[3] Manhattan has on the order of 10^4 road segments, and the dataset contains the order of 10^7 trips for January 2009 alone.

choice such that

$$p(Z^{(k)}|\boldsymbol{W}) \propto \exp\left(-\sum_{i\in Z^{(k)}} w_i\right),$$

in order to encode the fact that drivers avoid routes that take a long period of time. In the *uniform* model, we simply assume that route choice is independent and uniform on the set of reasonable paths:

$$p(Z^{(k)}|\boldsymbol{W}) \propto 1.$$

The uniform model trades off realism in modeling for improvement in computation and training, as we see in Section 5.

In our application to the Manhattan dataset, we perform MLE inference, or, equivalently, MAP inference with $p(\boldsymbol{W}) \propto 1$. In principle, it is not difficult to parameterize the prior of $\boldsymbol{W}$ as an undirected graphical model, since we need only to supply edge and unary potentials. For instance, to impose a correlated prior on $\boldsymbol{W}$, as suggested by some (Hunter et al., 2009), we simply penalize large differences in neighboring weights in the edge potential, effectively assuming a prior model that is similar to a continuous version of the Ising model.

5. Inference (or Training)

We perform maximum likelihood inference, maximizing

$$\max_{\boldsymbol{W}} \log p(\{T^{(k)}\}_{k=1}^{N}|\boldsymbol{W}) = \max_{\boldsymbol{W}} \sum_{k=1}^{N} \log p(T^{(k)}|\boldsymbol{W}).$$

The log-likelihood is

$$\begin{aligned}
&\log p(T^{(k)}|\boldsymbol{W})\\
&= \log\left(\sum_{Z^{(k)}\in\boldsymbol{Z}^{(k)}} p(T^{(k)}|Z^{(k)},\boldsymbol{W})p(Z^{(k)}|\boldsymbol{W})\right)\\
&= \log\left(\mathbb{E}_{Z^{(k)}}\left[p(T^{(k)}|Z^{(k)},\boldsymbol{W})\right]\right).
\end{aligned}$$

The expectation is a sum of the size $|\boldsymbol{Z}^{(k)}|$, which, for an $m \times n$ trip[4], is of $\binom{m+n}{n} \approx \frac{(n+m)^n}{n^n}e^n$ terms. Computing this expectation is the main inference challenge of our project.

5.1. Inference in the uniform model

By assuming the uniform model $p(Z|\boldsymbol{W}) \propto 1$, we gain the ability to work with an expectation over $\boldsymbol{W}$ instead of an expectation over $\boldsymbol{Z}$, since the probability that a particular weight is included in a path is readily computable from elementary combinatorics. We maximize an approximate lower bound of the log-likelihood by applications of Jensen's inequality:

$$\begin{aligned}
\ell(\boldsymbol{W}) &= \log\left(\mathbb{E}_{Z^{(k)}}\left[p(T^{(k)}|Z^{(k)},\boldsymbol{W})\right]\right)\\
&= \log\left(\mathbb{E}_{Z^{(k)}}\left[\frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{1}{2\sigma^2}(T^{(k)}-\sum w_i)^2}\right]\right)
\end{aligned}$$

Note that the Normal density is concave for $|T^{(k)} - \sum w_i| < \sigma$ and convex otherwise. Applying Jensen's inequality locally, we obtain that

$$B(\boldsymbol{W}) = \frac{1}{2\sigma^2}\left(T^{(k)} - \sum_i w_i\pi_i\right)^2,$$

where π_i is the marginal probability of node i being included in a uniform route,[5] is a local lower bound for the negative log-likelihood for trips that we predict poorly and is a local upper bound for trips that we predict well, up to a constant. Thus $B(\boldsymbol{W})$ is a good approximation of the objective function that is easily computable, involving only mn as opposed to $\binom{m+n}{n}$ terms.

5.2. Inference in the softmax regression model

We now consider a more realistic but more complex model, where we parameterize $Z|\boldsymbol{W}$ as a GLM, namely as a softmax regression where $p(Z|\boldsymbol{W}) \propto \exp\left(-\sum_{i\in Z} w_i\right)$, encoding drivers' preferences for shorter trips. The log-likelihood in this model is

$$\begin{aligned}
&\ell(\boldsymbol{W})\\
&= \log\left(\mathbb{E}_{Z^{(k)}}\left[\frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{1}{2\sigma^2}(T^{(k)}-\sum_i w_i)^2}\right]\right)\\
&= \log\left(\sum_{Z^{(k)}\in\boldsymbol{Z}^{(k)}} \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{1}{2\sigma^2}(T^{(k)}-\sum_i w_i)^2}p(Z^{(k)}|\boldsymbol{W})\right)
\end{aligned}$$

Before we discuss our inference strategy, we first discuss a few difficulties of the model. At first glance, the latent variable structure seems lend well to the Expectation-Maximization algorithm (Dempster et al., 1977). However, the EM algorithm requires computing the term

$$Q(\boldsymbol{W}|\boldsymbol{W}^{(t)}) = \mathbb{E}\left(\log(T^{(k)}, Z^{(k)}|\boldsymbol{W})|T^{(k)}, \boldsymbol{W}^{(t)}\right),$$

[4] By an $m \times n$ trip, we mean a trip with east-west distance n and north-south distance m

[5] π_i can be computed analytically. Suppose the source and destination of the trip are (n, m) apart and vertex i is (a, b) away from the source. Then, by elementary combinatorics,

$$\pi_i = \frac{\binom{a+b}{a}\binom{n+m-a-b}{n-a}}{\binom{n+m}{n}}$$

and computing the expectation requires the conditional distribution $p(Z|T,\boldsymbol{W}) = \frac{p(T|Z,\boldsymbol{W})p(Z|\boldsymbol{W})}{p(T|\boldsymbol{W})}$, where the denominator is intractable to compute. We might also consider techniques in variational inference (Blei et al., 2017). However, the latent variable $Z^{(k)}$ is a random set of indices with the property that the indices form a path on the grid, and thus cannot be reasonably decomposed into independent components, ruling out the mean-field algorithm. Another promising option is stochastic gradient variational Bayes (SGVB) and variational autoencoders (Kingma & Welling, 2013), which is designed for large datasets for which the EM algorithm fails. However, SGVB requires a reparameterization of the latent variable drawn from an approximate distribution, in order for the gradients to be properly computed. In SGVB, one independently draws some ϵ from a distribution and obtains z via $z = g(\epsilon)$ for some continuous function g.[6] This is difficult to do in our context, since Z is not continuous nor scalar-valued. Thus it is difficult to find an ϵ and a continuous transformation to approximate samples from the distribution of Z.

Our inference strategy is based on a sampling-based approximating to the expectation over $\boldsymbol{Z}$. The key trick we use is that

$$\mathbb{E}_Z\left[f(Z^{(k)})\right] = |\boldsymbol{Z}^{(k)}|\mathbb{E}_{\tilde{Z}}\left[f(\tilde{Z}^{(k)})p_Z(\tilde{Z}^{(k)}|\boldsymbol{W})\right], \quad (1)$$

where $\tilde{Z}$ is drawn uniformly from $\boldsymbol{Z}$. This is the same technique as in importance sampling, except here the objective is to derive computationally tractable approximations, rather than maximizing the efficiency of the approximations. Exchanging $\log$ and expectation operator and applying (1) yields the following upper bound for negative log-likelihood, up to a constant,

$$\frac{1}{2L\sigma^2}\sum_{j=1}^{L}\left[T^{(k)} + \sum_{i\in\tilde{Z}_j^{(k)}} w_i\right]^2 + \frac{1}{L}\sum_{i=1}^{L}\sum_{i\in\tilde{Z}_j^{(k)}} w_i \quad (2)$$
$$+ \operatorname*{logsumexp}_{i=1,\dots,L}\left(-\sum_{\tilde{Z}_i} w_i\right),$$

where we sample uniformly and independently $\{\tilde{Z}_j^{(k)}\}_{j=1}^{L}$. The pseudocode of the implementation is detailed in Algorithm 1.

5.3. Prediction

We conclude this section by briefly discussing prediction in our models. In the uniform model, prediction is straightforward. We calculate the expected time $\widehat{T} = \sum_i w_i\pi_i$, where π_i is the marginal probability that node i is included in a uniformly randomly chosen path. Computing prediction is slightly more subtle in the softmax regression model. In the softmax regression model, we sample L_{pred} uniformly chosen paths and take the weighted average of the sums of w_i in each path, where the weights are proportional to $\exp(-\sum_{i\in Z} w_i)$ for path Z.

Algorithm 1 Training algorithm for softmax path selection

```
{Optimizing using torch.optim.Adam}
for trip $k$ in $1,\dots,N$ do
    Sample $L$ random paths uniformly.
    Compute the objective function as in (2) for observation $k$.
    Compute the gradients of the objective function with respect to $\boldsymbol{W}$.
    Update $\boldsymbol{W}$.
end for
```

6. Methods

6.1. Data Processing

For our dataset, we started with the TLC dataset of all NYC taxi trips taken in January 2009. From the raw data, we added several computed columns. We one-hot-encoded columns for hour of day (24 columns) as well as for day of the week (7 columns). We also explicitly computed the duration of the trip in seconds as the dependent variable to predict.

In addition to adding columns, we filtered the original dataset. We only consider trips whose start- and end-locations that falls inside a rectangle that bounds Manhattan. We also removed trips with duration less than two minutes or more than two hours.

We performed a principal component analysis on all demeaned and standardized geographic coordinates (both start and end locations) from the filtered data. We thus transform the coordinates into the first and second principal components. This allowed us to compute the rotational matrix so that Manhattan lies approximately orthogonal to the x-axis. For the discrete grid models, these coordinates were further discretized into a 20×70 grid. Each node in the grid approximately corresponds to a $400\text{ft} \times 400\text{ft}$ area. We chose the grid size as a compromise between computational tractability and model expressiveness.

We saved the dataset as a whole, and we also partitioned into (day of week, hour) groups, using the one-hot encoded vectors. Some models were trained on the entire dataset (e.g. Neural Network), and some were trained individually on the partioned datasets (e.g. Structural Models).

[6] Here we are using the notation in (Kingma & Welling, 2013).

6.2. Baselines

We calculated three baselines. The first was a linear regression predicting trip duration from trip distance (calculated using the Pythagorean Theorem and the start and end coordinates), and trained on a partitioned data set.

The second was a neural network trained on the entire dataset taking as input the start and end coordinates as well as the day of week and hour one-hot encoded vectors. The neural network had one hidden layer with 50 neurons and a $\tanh$ activation function.

The third baseline was constructed by querying the Google Maps Distance Matrix API.[7] While there was no need to train this baseline, there was a rate limit constraint on how many test data points it could be tested on. We assess its performance on 2,500 data points in a representative partioned test dataset.

6.3. Training

Training implementations varied from model to model. In training the neural network baseline, SGD was used with a learning rate of 10^{-7} run for 12 epochs on the full data set. This took between 30 minutes and an hour. The uniform paths structural model was similarly trained with SGD, with a learning rate of 10^{-4}.

The uniform model was only trained on a subset of the dataset corresponding to all trips on a given day of the week and on a given hour. Convergence appeared after roughly two epochs, and the model was run for 5 epochs taking just under ten minutes.

The softmax regression model was trained using the Adam optimizer (Kingma & Ba, 2014) with learning rate 10^{-2} for 10 epochs, taking approximately an hour. Additionally, the softmax regression model take hyperparameters L (sample size in each stochastic draw) and σ^2 (variance of trip time). We chose $L = 20$ and $\sigma^2 = 100$. These values are again chosen to strike a bargain between realism and computation feasibility. The model appears to converge by the second epoch.

7. Results

- What were the results comparing previous work / baseline systems / your systems on the main task?
- What were the secondary results comparing the variants of your system?
- This section should be fact based and relatively dry. What happened, what was significant?

We train our model and test the model on an out-of-sample test-set using the methods discussed in Section 5.3. Table 1 contains the main prediction results of our model relative to some benchmark predictions such as the Google Maps Distance Matrix API, neural network, and linear regression. We note that, in terms of predictive metrics, our models were able to outperform Google Maps and linear regression, but were not able to outperform the neural network, even though the difference is not very large. Despite the disappointing outcome, the advantage of our framework is that the parameters have structural interpretations, whereas the neural network is a black box.

In terms of prediction, the uniform model and the softmax model appear very similar, whereas the uniform model performs slightly better. We suspect that, due to computational constraints, L is too small for the softmax model to really be expressive, as the number of weights updated by the softmax model is much fewer than that of the uniform model. Curiously, both the uniform and softmax models have a nontrivial bias in $\widehat{\mathbb{E}}(\epsilon)$. We suspect that the bias is generated by the approximate nature of our inference procedures, where our objective functions are approximations to the likelihood.

8. Discussion

- What conclusions can you draw from the results section?
- Is there further analysis you can do into the results of the system? Here is a good place to include visualizations, graphs, qualitative analysis of your results.

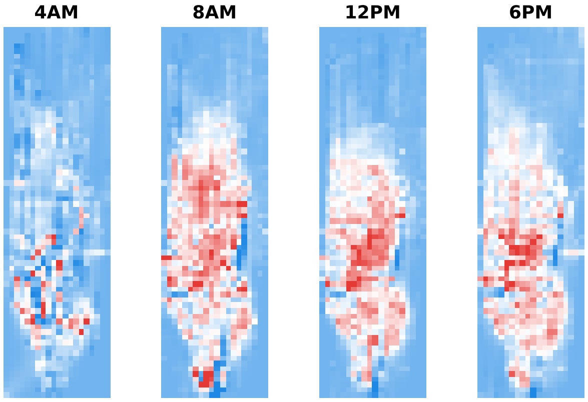


Figure 5. Learned Weights of Uniform Model, Various Times Tuesday

- What questions remain open? What did you think might work, but did not?

[7] https://developers.google.com/maps/documentation/distance-matrix/

	Baseline			Model	
	Google Maps	Neural Network[2]	Linear Regression[3]	Uniform Model	Softmax Model
$\mathrm{SD}(T)$	7.40	6.85	6.13	6.22	6.22
$\widehat{\mathbb{E}}[\epsilon]$[1]	-0.83	-0.07	-0.05	0.61	0.99
$\mathrm{SD}(\epsilon)$	4.98	3.88	5.01	4.28	4.28
$\widehat{\mathbb{E}}[\lvert\epsilon\rvert]$	3.42	2.44	3.60	2.82	2.86
Median($\lvert\epsilon\rvert$)	2.55	1.67	2.93	1.92	1.92
Percentile($\lvert\epsilon\rvert, 99$)	16.54	12.79	16.62	14.72	15.24
Test-set[4] R^2	0.54	0.68	0.33	0.53	0.53

Table 1. Prediction results on test set

[1] Here $\epsilon = (\text{Actual trip duration}) - (\text{Predicted duration})$ in minutes. $\widehat{\mathbb{E}}$ denotes the sample mean.

[2] We restrict the test-set to 8:00–9:00 AM on Tuesdays in January 2009 for all models *except* the neural network, for which we use an out-of-sample test set on the *entire* range of trip times, since the neural network encodes time-of-day and day-of-week data.

[3] In linear regression, we simply regress T on straight-line distance between the source and the destination.

[4] Test-set R^2 is calculated as $1 - \frac{\mathrm{Var}(\epsilon)}{\mathrm{Var}(T)}$ on the underlying dataset being tested on. Note that the test-set R^2 is an out-of-sample R^2.

9. Conclusion

- What happened?
- What next?

References

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