Generative machine learning for discrete-continuous choice data

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Wong, M., & Farooq, B. (2020). A bi-partite generative model framework for analyzing and simulating large scale multiple discrete-continuous travel behaviour data. Transportation Research Part C: Emerging Technologies, 110, 247-268.

https://arxiv.org/abs/1901.06415

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Introduction

Opportunities

- New large scale ubiquitous multidimensional travel data sources (a.k.a. Big Data)
  - Increased size and complexity
  - Representative of the population behaviour
  - Contain rich latent information

Introduction

Challenges

- Necessitates exploring new modelling techniques
  - Flexible in modelling the underlying heterogeneities in rich datasets
  - Improved estimation methods
  - Useful inference and interpretation

Introduction

Generative Modelling

- Construction of model of underlying distribution of the data
  - Using unsupervised learning
  - Generate new data
    With similar stochastic variations as the population

Generative Bi-Partite Framework

Basic notion

- Interested in describing the generation of the data by some unknown stochastic process
- Describe in probabilistic terms, how a set of latent/hidden variables could have generated the data

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Generative Bi-Partite Framework

Observed dataset

- $\mathbf{x} = x_{1:K} \in \mathbb{R}^{\mathcal{D}}$
  - $\mathbf{x}_D = (\underbrace{x_1, \ldots, x_{D_{\text{cont}}}}_{\text{continuous}}, \underbrace{x_{D_{\text{cont}+1}}, \ldots, x_{D_{\text{cont}}+D_{\text{cat}}}}_{\text{discrete}})$

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Generative Bi-Partite Framework

Observed dataset

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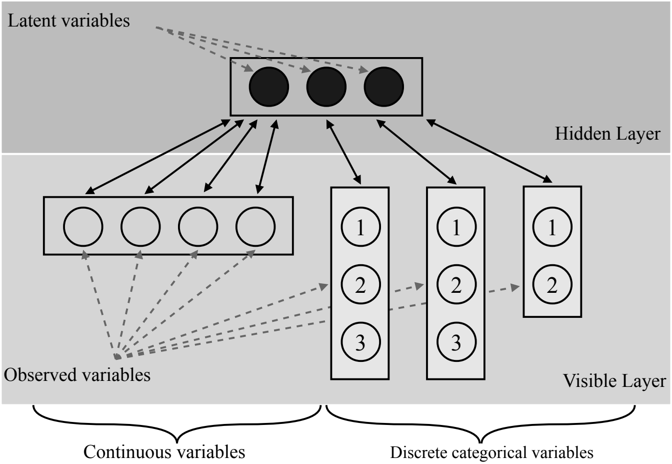
Latent/hidden variables

- $\mathbf{s} = s_{1:J} \in \{0, 1\}$
- Set of binary hidden random variables
- Independent and identically distributed (i.i.d.)

Generative Bi-Partite Framework



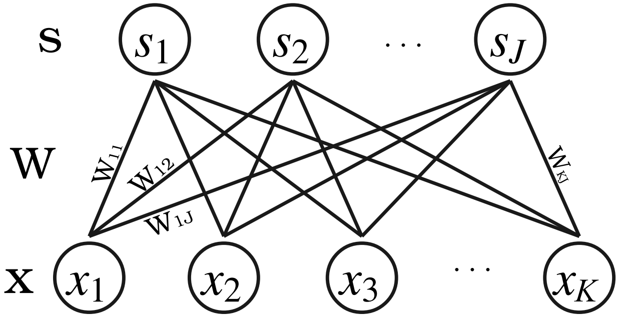
Model Structure

Joint distribution

- $p(\mathbf{x}, \mathbf{s})$ over the set of observed $\mathbf{x} = x_{1:K} \in \mathbb{R}^{\mathcal{D}}$ and *binary* hidden random $\mathbf{s} = s_{1:J} \in \{0, 1\}$
- ~~Restricted~~ Boltzmann probability distribution

$$p(\mathbf{x}, \mathbf{s}) = \frac{e^{-E(\mathbf{x},\mathbf{s})}}{\sum_{x,s} e^{-E(\mathbf{x},\mathbf{s})}} \tag{1}$$

Model Structure



Model Structure

Boltzmann Energy Function

- $p(\mathbf{x}, \mathbf{s})$ as RBM with:

$$E(\mathbf{x}, \mathbf{s}) = -\mathbf{x}^\top \mathbf{W}\mathbf{s} - \mathbf{b}^\top \mathbf{x} - \mathbf{c}^\top \mathbf{s} \tag{2}$$

- $\mathbf{W} \in \mathbb{R}^{K \times J}$ is the weight matrix, connecting $\mathbf{s} = (s_1, s_2, ..., s_J)$ and $\mathbf{x} = (x_1, x_2, .., x_K)$
- $\mathbf{b}$ and $\mathbf{c}$ are the parameters for the visible and hidden layer

Model Structure

Observed variables (discrete)

- For $x_{D_{\text{cat}}} = (x_{D_{\text{cat}_1}}, \ldots, x_{D_{\text{cat}_k}})$, with $x_{D_{\text{cat}_k}} = 1$ i.e. k alternative for variable $x_{D_{\text{cat}}}$ is chosen:

$$p(x_{D_{\text{cat}_k}} = 1) = \frac{e^{f_k(\mathbf{s};\theta)}}{\sum_{k'} e^{f_{k'}(\mathbf{s};\theta)}}$$

Model Structure

Observed variables (continuous)

- $x_{D_{\mathrm{cont}}}$ is drawn from a Gaussian $\mathcal{N}(W, \Sigma^2)$
- To accommodate positive values only, stepped sigmoidal is used:

$$\sum_{i=1}^{\infty} \sigma(\mathbf{s} - i) \approx \ln(1 + e^{s})$$

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Model Structure

Latent/Hidden variables

- With prior $p(\mathbf{s})$, we can quantify how $\mathbf{x}$ is related to $\mathbf{s}$ via likelihood function $p(\mathbf{x}|\mathbf{s})$
- Posterier distribution:

$$p(\mathbf{s}|\mathbf{x}) = \frac{p(\mathbf{x}, \mathbf{s})}{p(\mathbf{x})} \propto p(\mathbf{x}|\mathbf{s})p(\mathbf{s})$$

Model Estimation

Estimation problem

- Obtaining the posterior belief $p(\mathbf{s}|\mathbf{x})$
  - $\arg\max_\theta p(\mathbf{x})$ (Max Likelihood of data)
- $p(\mathbf{x}) = \int_{\mathbf{s}} p(\mathbf{x}|\mathbf{s})p(\mathbf{s})d\mathbf{s}$

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Model Estimation

Estimation algorithm

- MCMC algorithms could be a solution
- High computational cost
- Posterior approximation may be difficult with large datasets and complex distributions

Model Estimation

Variational Bayesian Inference

- There exists a tractable distribution $q(\mathbf{s})$ that approximates the exact posterior $p(\mathbf{s}|\mathbf{x})$
- We search over the set of distributions that minimizes the Kullback-Leibler (KL) divergence objective function:

$$\begin{aligned} \arg\min \quad & D_{KL}[q(\mathbf{s})||p(\mathbf{s}|\mathbf{x})] \\ s.t. \quad & \frac{p(\mathbf{s}|\mathbf{x})}{q(\mathbf{s})} > 0, \\ & D_{KL}[q(\mathbf{s})||p(\mathbf{s}|\mathbf{x})] = 0 \iff q(\mathbf{s}) = p(\mathbf{s}|\mathbf{x}) \end{aligned} \tag{3}$$

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Model Estimation

Variational Bayesian Inference

- In our case:

$$(D_{KL}[q(\mathbf{s})||p(\mathbf{s}|\mathbf{x})] = -\int_{\mathbf{s}} q(\mathbf{s}) \ln \frac{p(\mathbf{s}|\mathbf{x})}{q(\mathbf{s})} d\mathbf{s})$$

- Where:

$$q(\mathbf{s}) = \prod_{j=1}^{J} q(s_j) \approx \prod_{j=1}^{J} p(s_j|\mathbf{x}), \quad \mathbf{s} = \{s_1, s_2, ..., s_J\}$$

- Product of Expert Model (PoE), where each expert has tractable closed form solution $q(s_j) = (1 + e^{-Wx-c})^{-1}$.

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Model Estimation

Variational Bayesian Inference

- From Eq 3, using change-of-measure technique, $D_{KL}[q(\mathbf{s})||p(\mathbf{s}|\mathbf{x})]$:

$$= \int q(\mathbf{s}) \ln q(\mathbf{s}) d\mathbf{s} - \int q(\mathbf{s}) \ln p(\mathbf{x}, \mathbf{s}) d\mathbf{s} + \ln p(\mathbf{x}) \int q(\mathbf{s}) d\mathbf{s}$$

$$= -\mathcal{F} + \ln p(\mathbf{x})$$

Model Estimation

Variational Bayesian Inference

- $\mathcal{F}$ is the variational free energy and:

$$\arg\min D_{KL}[q(\mathbf{s})||p(\mathbf{s}|\mathbf{x})] = \arg\max F$$

- Variational free energy objective is the lower bound approximation to log-likelihood of data as $\ln p(\mathbf{x}) \geq \mathcal{F}$

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Learning Algorithm

Learning $q(s)$ using $\mathcal{F}$

$$
\begin{aligned}
\nabla_{q(\mathbf{s};\theta)} F &= \nabla_{q(\mathbf{s};\theta)} \ln \sum_{s} p(\mathbf{x}, \mathbf{s}; \theta) && (4)\\
&= \nabla_{q(\mathbf{s};\theta)} \ln \frac{\sum_{s} e^{-E(\mathbf{x},\mathbf{s};\theta)}}{\sum_{x,s} e^{-E(\mathbf{x},\mathbf{s}\theta)}} && (5)\\
&= \nabla_{q(\mathbf{s};\theta)} \Bigg(\underbrace{\ln \sum_{s} e^{-E(\mathbf{x},\mathbf{s};\theta)}}_{\text{utility } U} - \underbrace{\ln \sum_{x,s} e^{-E(\mathbf{x},\mathbf{s};\theta)}}_{\text{entropy } \mathcal{H}} \Bigg) && (6)
\end{aligned}
$$

Learning Algorithm

Learning $q(s)$ using $\mathcal{F}$

Using stochastic gradient descent

$$\theta_t \leftarrow \theta_{t-1} - \frac{1}{A_\tau}\eta \sum_{A_\tau} \nabla_{q(\mathbf{s};\theta)} - \mathcal{F}_{A_\tau} \qquad \forall A_\tau \in \mathcal{D}, \tau = 1, \ldots T$$

Learning Algorithm

Input : RBM data sample $\mathcal{D} = \{\mathbf{x}_1, ..., \mathbf{x}_n\}$, batch sample $A_i \subset \mathcal{D}, i = 1, ..., d$, learning rate η, iteration steps T
Output: gradient approximation $\theta = (\mathbf{W}, \mathbf{c}, \mathbf{b})$.

init: $\theta = 0$, $\tau = 1$;
forall $A_\tau \in \mathcal{D}, \tau = 1, ..., T$ **do**
  forall $(\mathbf{x}_n) \in A_\tau$ **do**
    for $t = 1$ **to** N **do**
      CD_t: iterate over Gibbs chain
      positive phase
      $\mathbf{x}^0 \leftarrow \mathbf{x}_n$
      $\mathbf{s}^0 \sim \prod_{j=1}^{H} p(s_j|\mathbf{x}^0)$
      negative phase
      $\mathbf{x}^t \sim \prod_{i=1}^{I} p(x_i|\mathbf{s}^0)$
      $\mathbf{s}^t \sim \prod_{j=1}^{H} p(s_j|\mathbf{x}^t)$
    end
  end
  % Variational free energy term
  $\nabla_{q(\mathbf{s};\theta)}(-\mathcal{F})_{A_\tau} \approx (\langle \mathbf{x}^t \mathbf{s}^t \rangle - \langle \mathbf{x}^0 \mathbf{s}^0 \rangle)$
  % parameter update step
  for $\theta \in \theta$ **do**
    $\theta_{\tau+1} \leftarrow \theta_\tau - \eta \nabla_{q(\mathbf{s};\theta)}(-\mathcal{F})_{A_\tau}$;
  end
end

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Inference Using RBM

Simple Example

- Two observed variables $[x, y]$ connected by a single hidden unit s_j
- Boltzmann Energy:
  $E(x, y, s) = -\sum_{s_j} xW_{1,j}s_j - \sum_{s_j} yW_{1,j}s_j - b_1x - \sum_{s_j} c_js_j - b_2y$

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Inference Using RBM

Simple Example

- Then for $P(y|x) = \dfrac{e^{-F(x,y)}}{\sum_{y'} e^{-F(x,y')}}$

$$
\begin{aligned}
F(x,y) &= -\ln \sum_{s_j \in \{0,1\}} e^{-E(x,y,s_j)} \\
&= -b_1 x - d_2 y - \ln(1 + e^{-xW_{1,j} - yW_{1,j} - c_j})
\end{aligned}
$$

Inference Using RBM

Simple Example

- Suppose $y = \{y^1, y^2, y^3\}$

$$
\begin{aligned}
F(x_1, y_1^1) &= -\Big(b_1 x_1 + d_2^1 \cdot (y_1^1 = 1) + d_2^2 \cdot (y_1^2 = 0) \\
&+ d_2^3 \cdot (y_1^3 = 0) + \ln(1 + e^{-x_1 W_{1,j} - y_1 W_{1,j} - c_j})\Big) \\
&= -\Big(b_1 x_1 + d_2^1 + \underbrace{\ln(1 + e^{-x_1 W_{1,j} - y_1 W_{1,j} - c_j})}_{\text{single correction term}}\Big)
\end{aligned}
$$

Inference Using RBM

Simple Example

- Suppose that $y = \{y^1, y^2, y^3\}$

$$\begin{aligned} F(x_1, y_1^1) &= -\Big(b_1 x_1 + b_2^1 \cdot (y_1^1 = 1) + b_2^2 \cdot (y_1^2 = 0) \\ &+ b_2^3 \cdot (y_1^3 = 0) + \ln(1 + e^{-x_1 W_{1,j} - y_1 W_{1,j} - c_j})\Big) \\ &= -\Big(b_1 x_1 + b_2^1 + \underbrace{\ln(1 + e^{-x_1 W_{1,j} - y_1 W_{1,j} - c_j})}_{\text{single correction term}}\Big) \end{aligned}$$

Inference Using RBM

Simple Example

- Suppose that weights to hidden connections are zero, $W_1 = W_2 = c_j = 0$, then $F(x_1, y_1^1) = -\Big(b_1 x_1 + d_2^1 + \ln(1 + e^0)\Big) = -\underbrace{(b_1 x_1 + d_2^1)}_{\text{MNL utility}}$

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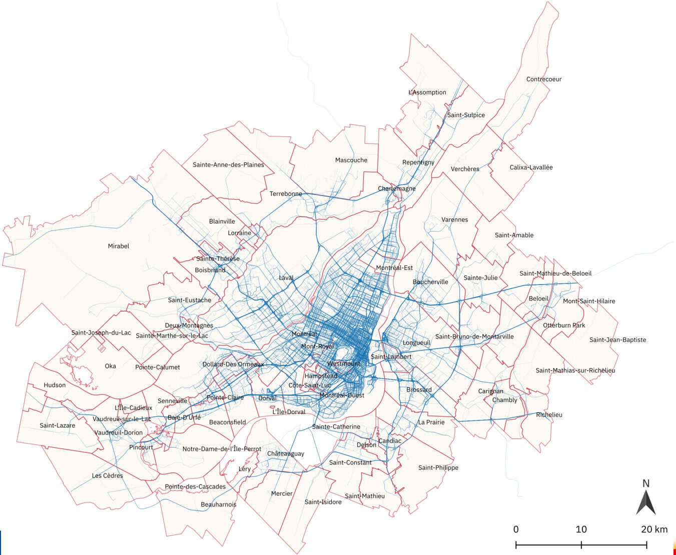
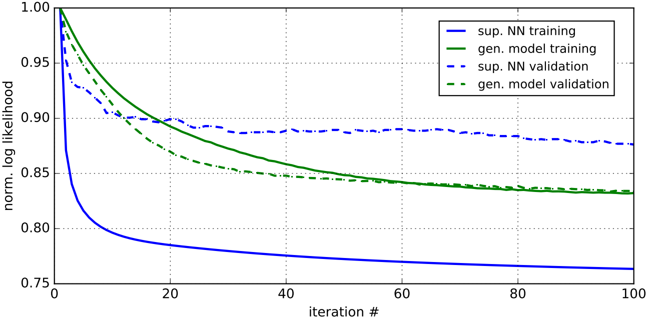
Montreal GPS Dataset

- 2016 MTL Trajet GPS data from the Greater Montréal Region
- Open datset with 293,330 trip observations
- Variables considered:
  - Mode choice
  - Trip purpose
  - Trip distance
  - Origin/destination point
  - Departure/arrival time

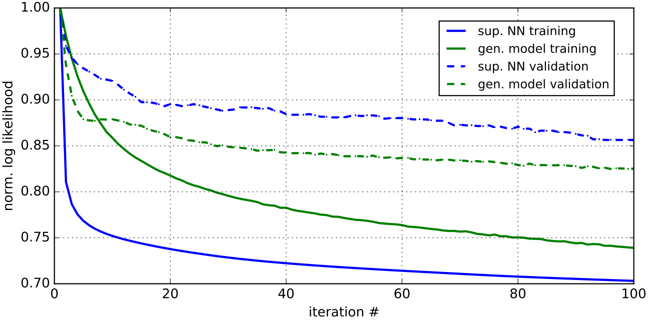
Montreal GPS Dataset



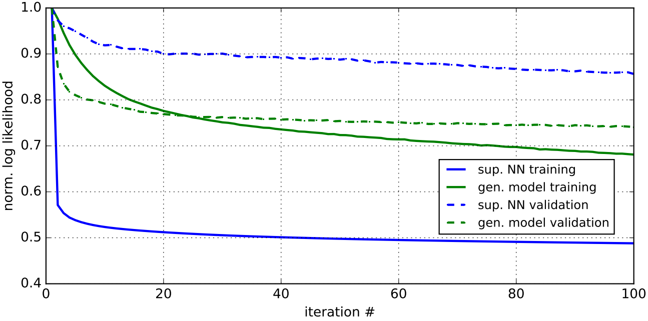
Benchmarkingwith Supervised NN



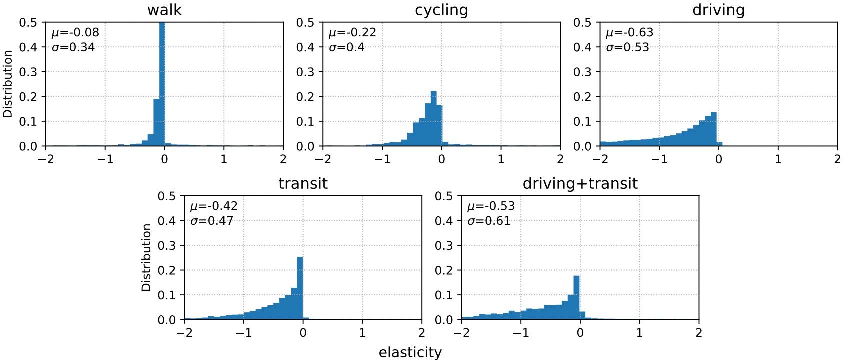
Benchmarkingwith Supervised NN



Benchmarkingwith Supervised NN



Elasticities



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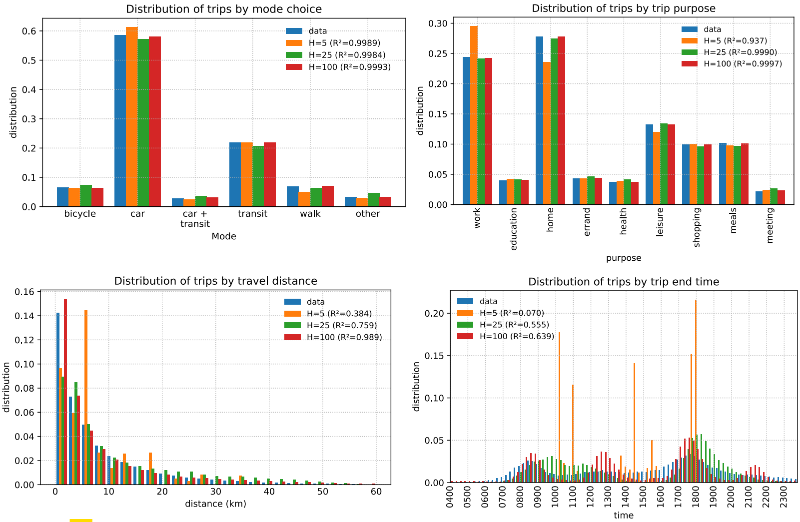
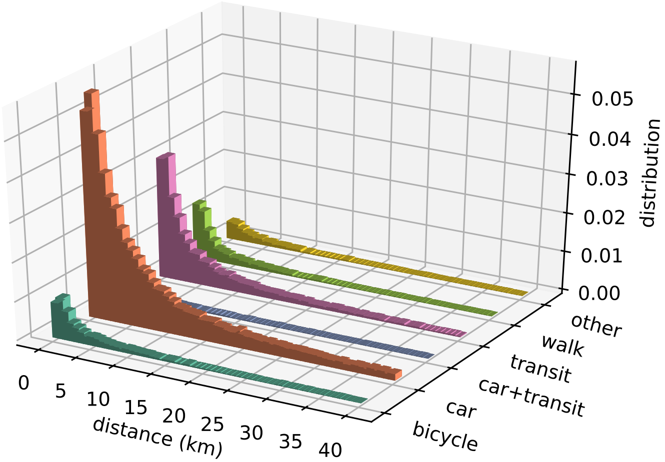
Forecasting



Forecasting



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Concluding Remarks

- RBM based generative model for discrete-continuous travel behaviour data
  - VBI based estimation process
  - Generation of conditional probabilities and economic analysis
- Performed better in forecasting, when compared to supervised feed-forward neural networks

Concluding Remarks

- Increase in latent variables, may cause overfitting
  - Regularization techniques can be used
- Explore the use in population synthesis
- Explore the use of other generative models
  - Variational Autoencorders (VAE)
  - Generative Adversarial Networks (GANs)