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Adaptive Systems

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Spatial Summarization of Image Collections

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This dissertation is submitted for the degree of *Master of Science ETH in Computer Science*

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Abstract

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Symbols

Symbols

η	Learning rate
κ	Largest subset size
ν	Noise-to-data ratio
θ	Model parameters
σ	Gaussian distribution's standard deviation
$\mathcal{D}$	Set of data samples
K	Latent coherence dimensions
L	Latent diversity dimensions
M	Number of features
$\mathcal{N}$	Set of noise samples
$\mathbb{R}$	Real numbers
S, T	Subset
V	Ground set
Z	Normalization constant

Matrices

$\mathbf{B}$	Feature diversity weights
$\mathbf{E}$	Feature coherence weights
$\mathcal{I}$	Identity
$\mathbf{W}^b$	Coherence weights
$\mathbf{W}^e$	Diversity weights
$\mathbf{X}$	Features

Vectors

$\mathbf{a}$	Utility weights for features
$\mathbf{u}$	Utility weights

Indices

i, j	Element

k	Feature
c	Coherence dimension
d	Diversity dimension

Acronyms and Abbreviations

ETH	Eidgenössische Technische Hochschule
FLID	Facility Location Diversity
FLDC	Facility Location Diversity and Coherence
FFLDC	Featurized Facility Location Diversity and Coherence
MLE	Maximum Likelihood Estimation
NCE	Noise Contrastive Estimation
LAS	Learning & Adaptive Systems
SGD	Stochastic Gradient Descent

Chapter 1

Introduction

Motivation (tourist routes and summarization), and quick idea of the methodology.

1.1 Contributions

Summarization of contributions.

Chapter 2

Related Work

2.1 Probabilistic Sub/super-modular models

Talk about the importance of these models and the recent interest in them, e.g. DPPs, Sampling.

2.2 Image collection summarization

Generally about the problem and the different approaches.

2.3 Tourist routes recommendation

The initial papers I found on this, basically Markov chains and clustering.

Chapter 3

Background

This chapter presents the supporting concepts and methods that will be used throughout this work.

3.1 Submodular Probability Set Functions

As described before, probability models over sets are of great interest and can be applied to diverse settings. In particular, submodular probability set functions have been utilized in multiple domains, such as document summarization and information gathering (Krause and Golovin, 2014).
Probability set functions are a class of distributions P over subsets S of a ground set V, i.e. functions that satisfy $\forall S \subseteq V, P : 2^V \rightarrow \mathbb{R} \mid 0 \leq P(S) \leq 1$ and $\sum_{S \subseteq V} P(S) = 1$. These distributions can also be understood as probabilities over binary sequences $[a_1, \ldots, a_n]$ of fixed size $n = |V|$ (Bruno et al., 1999). Hereby, w.l.o.g., let $V = \{1, \ldots, n\}$.
A set function $F : 2^V \rightarrow \mathbb{R}$ is submodular if it exhibits a "diminishing returns" property (Krause and Golovin, 2014), namely if it satisfies:

$$\forall S, T \subseteq V : S \subseteq T, i \notin T \mid F(S \cup i) - F(S) \geq F(T \cup i) - F(T) \tag{3.1}$$

Intuitively this indicates that adding an element to a smaller set yields a larger effect, i.e. in terms of the set function F value, than adding it to a larger one. This is a natural property in the context of summarization where adding more information to a large summary can be less effective than adding it to a smaller one. This property also makes them good candidates for modeling the concept of diversity (Tschiatschek et al., 2016).

3.2 Supermodularity and Modularity

Analogous to the use of submodular functions to model diversity, supermodular functions can be used to model complementarity or coherence between elements.
A set function is supermodular if it satisfies the condition in (3.1) with the inequality sign reversed, i.e. a set function $F(S)$ is supermodular iff $-F(S)$ is submodular. Supermodularity is used extensively in economics to model complementarity between strategies in games (Amir, 2005).
Finally, if a function F is both submodular and supermodular, i.e. it satisfies condition (3.1) with equality, then it is said to be a modular function. These are the simplest examples of submodular or supermodular functions and are akin to linear functions but in a discrete domain (Krause and Golovin, 2014).

3.3 Probabilistic Log-sub/supermodular Models

This work is interested in a particular class of probability set functions, namely probabilistic log-submodular and log-supermodular models, which are probabilities $P(S)$ of the form (Djolonga and Krause, 2014):

$$P(S) \propto \exp(F(S)) \tag{3.2}$$

Where $F(S)$ is a submodular or supermodular function, respectively. These models encompass many practical probabilistic models such as repulsive Ising models, Deterministic Point Processes (DPPs) and binary pairwise Markov Random Fields (MRFs) (Djolonga and Krause, 2014, 2015).
This model class is of interest because the contributions of this work focus on extensions to a novel probabilistic log-submodular model proposed by Tschiatschek et al. (2016) which will be described in the next section.

3.3.1 Partition Function

In log-submodular models the normalization constant Z is known as the *partition function* (Djolonga and Krause, 2014). Z is necessary to fully determine the normalized model and compute quantities such as marginal probabilities, however its exact computation is known to be #P-complete (Jerrum and Sinclair, 1990). This makes it impossible in practice to perform such computations except for special cases of the model.

3.4 Facility Location Diversity Model (FLID)

Every modular function can be written as a sum of individual weights for each element $i \in V$ assuming a normalization such that $F(\emptyset) = 0$ (Krause and Golovin, 2014), i.e.

$$F(S) = \sum_{i \in S} u(i) \tag{3.3}$$

Where $u(i)$ is some function $u : V \to \mathbb{R}$. For convenience, denote $\mathbf{u}$ as the vector of modular weights where $u_i = u(i)$. Therefore any log-modular function can be written as:

$$P(S) \propto \exp\left(\sum_{i \in S} u_i\right) = \prod_{i \in S} \exp(u_i) \tag{3.4}$$

This is the simplest log-submodular probability function and is the modular part for the FLID model proposed by Tschiatschek et al. (2016). In this model, $\mathbf{u}$ can be thought of as modeling the relevance or utility of each element, for example in the context of spatial summarization this utility could be proportional to the popularity of a location or to how many times it has been photographed.
However, these utilities alone can not capture interactions between the elements in a set. To address this, Tschiatschek et al. (2016) propose an additional term that models set diversity, its objective is to characterize redundant elements and assign lower probabilities to sets that contain them.
This term is based on representing each element i with an L-dimensional vector $\mathbf{w}^b \in \mathbb{R}^L_{\geq 0}$, where each dimension $1 \leq d \leq L$ captures a concept related to set diversity and $w^b_{i,d}$ quantifies the relevance of each element i for each concept d (Tschiatschek et al., 2016). Hereby, define $\mathbf{W}^b \in \mathbb{R}^{|V| \times L}_{\geq 0}$ as the matrix where the i-th row is the representation $\mathbf{w}^b$ of element i.
For each dimension d, the diversity of a set S is quantified by $\max_{i \in S} w^b_{i,d} - \sum_{i \in S} w^b_{i,d}$. This assigns a negative value for sets that contain more than one element with nonzero weight

Table 3.1: FLID probability distribution for the scenario in Example 3.4.2.

S	$P(S)$
$\{h,s\},\{h,f\}$	≈ 0.41
$\{h\},\{s\},\{f\}$	≈ 0.06
$\{\},\{s,f\},\{h,s,f\}$	≈ 0.00

$w^b_{\cdot,d}$ in that dimension (Tschiatschek et al., 2016). Equation (3.5) shows the complete term, this sums over all L dimensions to account the diversity in each concept.

$$\operatorname{div}(S) = \sum_{d=1}^{L} \left(\max_{i \in S} w^b_{i,d} - \sum_{i \in S} w^b_{i,d} \right) \tag{3.5}$$

Finally, the complete FLID model proposed by Tschiatschek et al. (2016) combines these two terms and is given by:

$$P(S) = \frac{1}{Z} \exp\left(\sum_{i \in S} u_i + \sum_{d=1}^{L} \left(\max_{i \in S} w^b_{i,d} - \sum_{i \in S} w^b_{i,d} \right) \right) \tag{FLID}$$

3.4.1 Partition Function

As mentioned before, the computation of the partition function is generally intractable for log-submodular models. However, for FLID this can be computed in time $O(|V|^{L+1})$ which is polynomial on the size of the ground set and significantly better than the cost of enumerating the powerset of V, i.e. $O(2^{|V|})$ (Tschiatschek et al., 2016). Nevertheless, it is worth noting that this complexity is exponential in L which means that the partition function computation is only pratical for a limited range of FLID models, namely those with $L \ll |V|$.

3.4.2 Example: Two Landmarks

In order to better illustrate the model, consider a town with 3 popular locations: A town hall (h), a statue (s) and a fountain (f). Assume that historic data shows that visitors only take photos at either the town hall and the statue, or at the town hall and the fountain. This can be modeled with FLID by introducing a latent dimension representing some concept that is present in both the statue and the fountain but not in the town hall, e.g. "is not a building".
Concretely, let $V = \{h,s,f\}$ and $\mathbf{u} = (2,2,2)^\intercal$, indicating that all locations are equally popular. A suitable diversity weight matrix would then be $\mathbf{W}^b = (0,20,20)^\intercal$. Table 3.1 shows the resulting probabilities of the subsets, accurately representing the aforementioned problem. Note that the probabilities are not exactly $0.5/0.5$ for the sets of interest but this could be easily fixed by increasing the utilities to ensure that sets of size 2 have a larger unnormalized magnitude compared to individual ones.

3.5 Learning from Data

Much of the interest in log-submodular models is concentrated on performing inference for known functions (Tschiatschek et al., 2016). However, Tschiatschek et al. (2016) explore how to learn such models from data, i.e. estimate the model parameters from observations with an unknown distribution.

Even though Maximum likelihood Estimation (MLE) is the commonly used method for the task of parameter estimation from data, it only works efficiently for normalized models (Gutmann and Hyvärinen, 2012). This makes it intractable for the general class of log-submodular models, and also a wide range of FLID models because the computation of Z is exponential on L. Gutmann and Hyvärinen (2012) propose an alternative method for parameter estimation in unnormalized models known as Noise Contrastive Estimation (NCE) and this is the method used by Tschiatschek et al. (2016) to learn the FLID model.

3.5.1 NCE Learning

The idea behind NCE is to transform the unsupervised learning task of estimating a probability density from data into a supervised classification task. In order to do this, the observed data $\mathcal{D}$, assumed to be drawn from an unknown distribution P_d, is compared to an artificially generated set of noise samples $\mathcal{N}$ drawn from a known distribution P_n that can be efficiently normalized. The classification task is to maximize the likelihood of correctly discriminating each sample as either observed data or artificial noise.
Formally, denote $\mathcal{A}$ as the complete set of labeled samples, i.e. $\mathcal{A} = \{(S, Y_s) : S \in \mathcal{D} \cup \mathcal{N}\}$ where $Y_s = 1$ for $S \in \mathcal{D}$ and $Y_s = 0$ for $S \in \mathcal{N}$. Additionally, let ν be the noise-to-data ratio, i.e. $\nu = {}^{|\mathcal{N}|}/_{|\mathcal{D}|}$.
The goal is to estimate the posterior probabilities $P(Y_s = 1 \mid S; \theta)$ and $P(Y_s = 0 \mid S; \theta)$, in order to discriminate noise from data samples. These probabilities are given by equations (3.6) and (3.7).

$$P(Y_s = 1 \mid S; \theta) = \frac{\hat{P}_d(S; \theta)}{\hat{P}_d(S; \theta) + \nu P_n(S)} \tag{3.6}$$

$$P(Y_s = 0 \mid S; \theta) = \frac{\nu P_n(S)}{\hat{P}_d(S; \theta) + \nu P_n(S)} \tag{3.7}$$

It is worth noting that $\hat{P}_d$ is used instead of P_d, because the real density is not known. As indicated by Gutmann and Hyvärinen (2012), $\hat{P}_d$ can be an unnormalized distribution for NCE where the partition function Z is included in the set of parameters θ as $\hat{Z}$, hence resulting in an approximately normalized distribution after the optimization.
In order to obtain these posterior probabilities, the following conditional log-likelihood objective is maximized (Gutmann and Hyvärinen, 2012):

$$g(\theta) = \sum_{S \in \mathcal{D}} \log P(Y_s = 1 \mid S; \theta) + \sum_{S \in \mathcal{N}} \log P(Y_s = 0 \mid S; \theta) \tag{3.8}$$

This maximization can be performed using a gradient-based optimization method such as Stochastic Gradient Descent (SGD).

Practical Considerations

A couple of considerations are necessary for obtaining good estimates with NCE (Gutmann and Hyvärinen, 2012):

1. The parameterized probability function $\hat{P}_d(S; \theta)$ must be of the same family as the real distribution P_d, i.e. $\exists \theta^* \mid \hat{P}_d(S; \theta^*) = P_d$.

2. The noise distribution P_n is nonzero whenever P_d is nonzero.

Additionally, the following statements must be considered when choosing the noise distribution P_n (Gutmann and Hyvärinen, 2012):

1. A distribution that can be sampled easily.

2. Noise that is as similar as possible to the data, otherwise the classification problem could be too easy.

3. A noise sample as large as possible.

3.5.2 Learning FLID via NCE and SGD

Stochastic Gradient Descent was used by Tschiatschek et al. (2016) to learn the FLID model through NCE. SGD is a gradient-based method that has proven effective in large-scale learning tasks due to its efficiency when the computation time is a limiting factor (Bottou, 2010; Zhang, 2004), hence making it appropriate for the scale of data sourced from the internet, such as public user photos in Flickr.
In each iteration, the gradient $\nabla \log P(Y_s = y \mid S; \theta)$ must be computed. For FLID, the parameter vector θ is composed by $\mathbf{u}, \mathbf{W}^b$ and $\hat{Z}$, and the corresponding gradients are given by:

$$\nabla \log P(Y_s = y \mid S; \theta) = \left(y - \frac{1}{1 + \nu \frac{P_n(S)}{\hat{P}_d(S;\theta)}} \right) \nabla \log \hat{P}_d(S; \theta) \tag{3.9}$$

$$\hat{P}_d(S; \theta) = \frac{1}{\hat{Z}} P(S; \mathbf{u}, \mathbf{W}^b) \tag{3.10}$$

$$\left(\nabla_{\mathbf{u}} \log \hat{P}_d(S; \hat{Z}, \mathbf{u}, \mathbf{W}^b) \right)_i = \begin{cases} 1 & \text{if } i \in S \\ 0 & \text{otherwise} \end{cases} \tag{3.11}$$

$$\left(\nabla_{\mathbf{W}^b} \log \hat{P}_d(S; \hat{Z}, \mathbf{u}, \mathbf{W}^b) \right)_{i,d} = \begin{cases} -1 & \text{if } i \in S \text{ and } i \neq \operatorname{argmax}_{j \in S} w^b_{j,d} \\ 0 & \text{otherwise} \end{cases} \tag{3.12}$$

$$\nabla_{\hat{Z}} \log \hat{P}_d(S; \hat{Z}, \mathbf{u}, \mathbf{W}^b) = \frac{-1}{\hat{Z}} \tag{3.13}$$

Where $P(S; \mathbf{u}, \mathbf{W}^b)$ is the unnormalized (FLID) equation, $(\nabla_{\mathbf{u}} \cdot)_i$ represents the i-th entry of the gradient with respect to $\mathbf{u}$ and $(\nabla_{\mathbf{W}^b} \cdot)_{i,d}$ represents the (i,d)-th entry of the sub-gradient with respect to $\mathbf{W}^b$ (Tschiatschek et al., 2016).

Computational Complexity

As described by Tschiatschek et al. (2016), the running time requirement for calculating the sub-gradient for FLID is $O(L|S|)$, and for a complete pass over data and noise samples is then $O(|\mathcal{D} \cup \mathcal{N}|\kappa L)$ where $\kappa = \max_{S \in \mathcal{D} \cup \mathcal{N}} |S|$. This shows that learning is efficient as it is only linear on the size of the data and the noise, assuming small values for κ and L.

3.5.3 AdaGrad

A commonly used learning rate function for SGD is $\eta(t) = \eta_0 t^{-p}$, which offers the best convergence speed in theory and also does it often in practice (Bottou, 2012), however it can lead to poor performance due to slow rates of convergence to the solution (Darken and Moody, 1992). By contrast, choosing a larger η_0 may not lead to better results due to the instability in the parameters for small t (Darken and Moody, 1990).
This behavior was observed during the experiments with real data to be presented in later sections, therefore an alternative for the learning rate was sought. In particular, Adaptive Gradient (AdaGrad) was implemented.
AdaGrad was proposed by Duchi et al. (2011), the idea of this method is to adapt the learning rate for each parameter in θ individually in a way that frequently updated parameters have slower learning rates while infrequent parameters have larger ones. The intuition

is that an update to a rare parameter is more informative than one to a parameter that is frequently updated.
Concretely, with AdaGrad the update step for each parameter in θ is given by:

$$\theta_j^{\tau+1} \leftarrow \theta_j^{\tau} - \frac{\eta}{\sqrt{G_{j,j}}} \nabla g(\theta)_j^{\tau} \tag{3.14}$$

Where $G_{j,j}$ contains the information about past gradients for parameter j and is given by:

$$G_{j,j} = \sum_{t=1}^{\tau} \left(\nabla g(\theta)_j^t \right)^2 \tag{3.15}$$

In equation (3.15) $\nabla g(\theta)_j^t$ denotes the j-th entry of the gradient at time step t.
It is worth noting that AdaGrad does not incur in an significant increase in running time or memory requirements for the training which makes it inexpensive to include in the implementation of NCE.

Chapter 4

Extending FLID

4.1 Beyond Diversity: FLDC

Diversity is an important property in the context of summarization (Tschiatschek et al., 2016), however it is not the only one. Coherence is also a desired property of summaries, particularly for structured summaries (Yan et al., 2011). Balancing coherence and diversity is considered a challenge and maxiziming diversity alone may lead to disconnected summaries, while focusing on coherence can hinder the breadth of the resulting summaries (Shahaf et al., 2012).

To better understand why coherence is important, consider the construction of a spatial summary for photos taken in a city. A model based on spatial diversity would create sets containing photos taking at distant locations in the city, however another possibility is to have summaries that contain photos that were taken close to some starting point, in this case the desired property is not spatial diversity but rather coherence.

Therefore, a natural extension to the FLID model is to add the capacity of modeling coherence along with diversity. I propose the addition of a log-supermodular term analogous to the log-submodular term (3.5) in order to model the complementarity between elements. This supermodular term introduces a representation of the elements using K-dimensional vectors $\mathbf{w}^K \in \mathbb{R}^K_{\geq 0}$, where each dimension $1 \leq c \leq K$ captures a concept that relates to set coherence and $w_{i,c}$ quantifies the contribution of each element i to each coherence concept c. The coherence of a set S with respect to each concept c is quantified as $\sum_{i \in S} w^e_{i,c} - \max_{i \in S} w^e_{i,c}$ which is a supermodular term mirroring the submodular term in FLID. Summing over all the concepts results in the proposed coherence term. Hereby, define $\mathbf{W}^e \in \mathbb{R}^{|V| \times K}_{\geq 0}$ as the matrix where the i-th row is the representation $\mathbf{w}^e$ of element i.

Adding the coherence term to FLID results in the extended model, which I refer to as the Facility Location Diversity and Coherence (FLDC) model. Its probability distribution is defined as:

$$P(S) = \frac{1}{Z} \exp\left(\sum_{i \in S} u_i + \operatorname{div}(S) + \sum_{c=1}^{K} \left(\sum_{i \in S} w^e_{i,c} - \max_{i \in S} w^e_{i,c} \right) \right) \tag{FLDC}$$

4.1.1 Partition Function

For the FLDC model, the partition function can be computed in $O(|V|^{L+K+1})$ time. This complexity can be derived using a similar algorithm as the one presented by Tschiatschek et al. (2016) for FLID, the key observation is that the algorithm they present only requires the ordering of weights to determine elegible element for a set given a set of maximum weights per dimension, therefore this can be easily extented to include the the ordering

Table 4.1: Probability distribution for Example 4.1.3.

S	$P(S)$
$\{1,2\}$	0.5
$\{3,4\}$	0.5
Otherwise	0.0

for the coherence weights as well. This requires evaluating K more dimensions which results in the added term to the exponent of the complexity expression, which makes the computation of the partition function more impractical than in the FLID case.

4.1.2 Learning FLDC models

As with FLID, the parameters for an FLDC model can be estimated using NCE. For FLDC the vector θ is composed of $[\mathbf{u}, \mathbf{W}^b, \mathbf{W}^e, \hat{Z}]$ and its gradient is the same as in equations (3.9)-(3.13) with the addition of a gradient with respect to the new parameter, $\mathbf{W}^e$, which is given by:

$$\left(\nabla_{\mathbf{W}^e} \log \hat{P}_d(S; \hat{Z}, \mathbf{u}, \mathbf{W}^e, \mathbf{W}^e)\right)_{i,c} = \begin{cases} 1 & \text{if } i \in S \text{ and } i \neq \operatorname{argmax}_{j \in S} w^e_{j,c} \\ 0 & \text{otherwise} \end{cases} \tag{4.1}$$

Where $(\nabla_{\mathbf{W}^e \cdot})_{i,c}$ represents the (i,c)-th entry in the gradient with respect to $\mathbf{W}^e$.
This also affects the overall complexity of the learning algorithm. Computing the gradient takes $O(L+K)|S|$ for FLDC at each step, therefore the running time of a full pass over the data and noise samples takes $O(|\mathcal{D} \cup \mathcal{N}|\kappa(L+K))$. This is not significantly more expensive than learning FLID under the assumption that $K \simeq L$.

4.1.3 Example: Two Non-overlapping Clusters

As an example of the extended model, consider the distribution presented in table 4.1 for $V = \{1,2,3,4\}$, representing a set of two non-overlapping clusters with 2 elements each. Intuitively, this can be modeled by considering that there is diversity between elements in different clusters while inside a cluster there is a coherence component that ties them together.
Concretely, the weight matrices $\mathbf{W}^b, \mathbf{W}^e$ in Figure 4.1 illustrate one possible instance of the model. The corresponding utility vector is $\mathbf{u} = \overrightarrow{0}$, because there is no indication that an individual element is favored over the pairs. This model is easily interpretable and accurately realizes the distribution.

4.2 Generalizing through Features: FFLDC

An important characteristic of the FLID model, and by extension the FLDC one, is that it is agnostic to the type of elements in the ground set, this allows its application to a wide range of problems without prior knowledge. However the downside is that the model has no capability to make use of information about the elements, if available, to improve the modeling of the data. Moreover, if a new element is added to the set there is no way to generalize the existing knowledge about similar elements.
In order to solve these problems, I propose a further extension to the model. Firstly, an element ($i \in V$) is represented as a vector $\mathbf{x}_i \in \mathbb{R}^M$ where each entry is a feature, e.g. for venues one feature could be its aggregated rating while another indicates whether it is

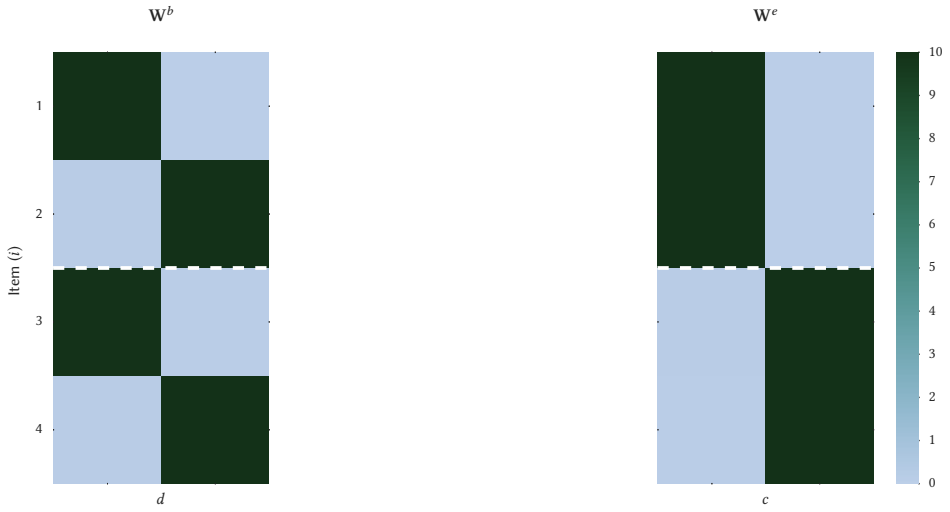

Figure 4.1: Diversity and coherence weights for FLDC model in Example 4.1.3. The dotted line divides the clusters.

indoors or outdoors. The representations of all elements is collected by matrix $\mathbf{X} \in \mathbb{R}^{|V| \times M}$ where each row i corresponds to the repreesntation $\mathbf{x}_i$ of element i.
Then, the utility vector $\mathbf{u}$ and weight matrices $\mathbf{W}^b, \mathbf{W}^e$ are factorized to include this feature matrix $\mathbf{X}$ as follows:

$$\mathbf{u} = \mathbf{X}\mathbf{a} \tag{4.2}$$

$$\mathbf{W}^b = \mathbf{X}\mathbf{B} \tag{4.3}$$

$$\mathbf{W}^e = \mathbf{X}\mathbf{E} \tag{4.4}$$

Where $\mathbf{a} \in \mathbb{R}^M$ represents the contribution of each feature to the total utility of an item, while $\mathbf{B} \in \mathbb{R}^{M \times L}$ and $\mathbf{E} \in \mathbb{R}^{M \times K}$ encode the contribution of each feature to each latent diversity and coherence dimension, respectively. The intuition behind this factorization is that the information about the items can enhance the latent representations, hence producing a richer model. For example if $M < |V|$ and the features are sufficient to represent the items, it is expected that learning will be easier because of the reduced number of parameters with respect to learning the equivalent FLDC model.
I refer to the extended model as the Featurized Facility Location Diversity and Coherence (FFLDC) model and its probability distribution is defined as:

$$P(S) = \frac{1}{Z} \exp\left(\sum_{i \in S} \sum_{k=1}^{M} x_{i,k} a_k + fdiv(S) + fcoh(S) \right) \tag{FFLDC}$$

$$fdiv(S) = \sum_{d=1}^{L} \left(\max_{i \in S} \sum_{k=1}^{M} x_{i,k} b_{k,d} - \sum_{i \in S} \sum_{k=1}^{M} x_{i,k} b_{k,d} \right) \tag{4.5}$$

$$fcoh(S) = \sum_{c=1}^{K} \left(\sum_{i \in S} \sum_{k=1}^{M} x_{i,k} e_{k,c} - \max_{i \in S} \sum_{k=1}^{M} x_{i,k} e_{k,c} \right) \tag{4.6}$$

Where a_i is the i-th entry of $\mathbf{a}$, $b_{k,d}$ is the (k,d)-th entry of $\mathbf{B}$, $e_{k,d}$ is the (k,e)-th entry of $\mathbf{E}$ and $x_{i,k}$ is the (i,k)-th entry of X.

Remark. If $\mathbf{X} = \mathcal{I}$, then FFLDC is equivalent to FLDC, with $\mathbf{a} = \mathbf{u}$, $\mathbf{W}^b = \mathbf{B}$ and $\mathbf{W}^e = \mathbf{E}$.

The use of features also allows the application of the model to previously unseen elements, hence solving the aforementioned problem of generalization. This is possible because the model is defined on the space of features and not items, and for a previously unseen element j only its representation $\mathbf{x}_j$ is required in order to evaluate the probability of sets containing this element.

4.2.1 Partition Function

The computation of the partition function for this model can be done using the fact that any FFLDC model can be transformed into an equivalent FLDC model through the factorizations in equations (4.2)-(4.4). This transformation requires $O(|V|M(L+K))$ time for the matrix multiplications, therefore the overall complexity of calculating the partition function for an FFLDC model is $O(|V|M(L+K)+|V|^{L+K+1})$. This expression can be simplified to $O(|V|^{L+K+1})$ because the exponential term is significantly larger assuming sensible values for M. Given that the complexity of computing the partition function for FFLDC is equivalent to the FLDC model, it is also intractable in practice.

4.2.2 Learning FFLDC models

For FFLDC, the parameter vector θ is different from the previous models, it is composed by $[\mathbf{a}, \mathbf{B}, \mathbf{C}, \hat{Z}]$ and the gradient of the NCE objective $g(\theta)$ is given by:

$$\left(\nabla_{\mathbf{a}} \log \hat{P}_d(S; \hat{Z}, \mathbf{a}, \mathbf{B}, \mathbf{E})\right)_m = \sum_{i \in S} x_{i,m} \tag{4.7}$$

$$\left(\nabla_{\mathbf{B}} \log \hat{P}_d(S; \hat{Z}, \mathbf{a}, \mathbf{B}, \mathbf{E})\right)_{m,d} = x_{i^d,m} - \sum_{i \in S} x_{i,m} \tag{4.8}$$

$$\left(\nabla_{\mathbf{E}} \log \hat{P}_d(S; \hat{Z}, \mathbf{a}, \mathbf{B}, \mathbf{E})\right)_{m,c} = x_{i^c,m} - \sum_{i \in S} x_{i,m} \tag{4.9}$$

Where $i^d = \operatorname{argmax}_{i \in S} \sum_{k=1}^{M} x_{i,k} b_{k,d}$ and $i^c = \operatorname{argmax}_{i \in S} \sum_{k=1}^{M} x_{i,k} e_{k,c}$. $(\nabla_{\mathbf{a}} \cdot)_m$ represents the m-th entry of the sub-gradient with respect to a, $(\nabla_{\mathbf{B}} \cdot)_{m,d}$ represents the (m,d)-th entry of the sub-gradient with respect to B and $(\nabla_{\mathbf{E}} \cdot)_{m,c}$ represents the (m,c)-th entry of the sub-gradient with respect to E.

Remark. For $\mathbf{X} = \mathcal{I}$, the sub-gradients in 4.7-4.9 are equivalent to the FLDC sub-gradients. Because $x_{i,m} = 1$ only when $i = m$.

Regarding running time complexity, the FFLDC model requires more computations for the gradient due to the inclusion of features. Concretely, computing the gradient for a set S takes $O(|S|M(L+K))$ which makes the running time of a single pass over data and noise samples equal to $O(|\mathcal{D} \cup \mathcal{N}|M(L+K)\kappa)$. Even though this is larger than the complexity of FLID or FLDC, it is efficient because it is still linear on the data.

4.2.3 Example: Rated locations

A small town has 6 popular locations, each of them has been rated from 0 to 5, where 0 represents a bad review and 5 an excellent review. Collected data shows that a typical visitor is more likely to visit and take photos at places with high ratings, however this is not the only factor driving their behavior. For example, an average visitor does not visit two places that serve food on the same day instead the data shows that visitors usually go to one place that serves food and then to an outdoor one, or they just visit one that has both characteristics. This data is summarized in Table 4.2, the task is to model this behavior using the FFLDC model.
In this example there is knowledge about the items and what features are relevant for the data. These features are summarized in equation (4.10). The first column corresponds to

Table 4.2: Synthetic data for Example 4.2.3.

Locations visited (S)	$P(S)$
$\{1,3\}$	0.30
$\{3,4\}$	0.25
$\{3,6\}$	0.15
$\{2\}$	0.10
$\{1\}$	0.06
$\{3\},\{4\}$	0.04
$\{5\},\{6\}$	0.03
Otherwise	0.00

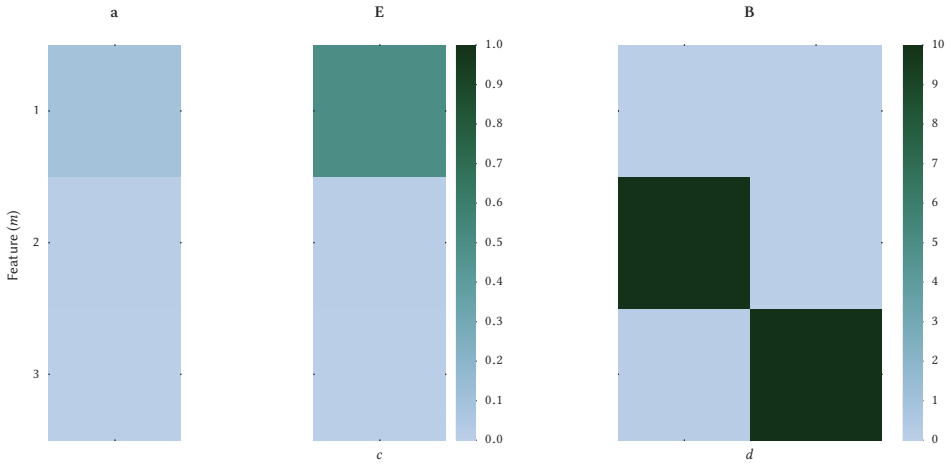

Figure 4.2: FFLDC sample model for Example 4.2.3.

the aforementioned rating, the second and third are binary features indicating whether the location is an outdoor one and whether it serves food, respectively.

$$\mathbf{X} = \begin{pmatrix} 4 & 1 & 0 \\ 4 & 1 & 1 \\ 3 & 0 & 1 \\ 3 & 1 & 0 \\ 2 & 1 & 1 \\ 2 & 1 & 0 \end{pmatrix} \tag{4.10}$$

A possiblity is an FFLDC model that encourages diversity on the second a third feature, i.e. models the idea that visitors do not go to more than one place that serves food or is outdoor, while assigning a positive utility and coherence value to the first feature, i.e. modeling the preference for places with high ratings. One such model is presented in Figure 4.2, this approximates distribution from Table 4.2 and illustrates the type of model that is useful in this example.

With this model, if a new location j is considered then it is straightforward to estimate the probability of sets that include it. For example, consider a seventh location with the following feature representation $\mathbf{x}_7 = [5,1,0]$, using the same model a new distribution can be computed without changing the model parameters, as it would be the case with

Table 4.3: Synthetic data for Example 4.2.3 after adding a new item.

Locations visited (S)	$P(S)$
$\{3,7\}$	0.24
$\{1,3\}$	0.21
$\{3,4\}$	0.19
$\{3,6\}$	0.10
$\{7\}$	0.06
$\{1\},\{2\}$	0.04
$\{3\},\{4\}$	0.03
$\{5\},\{6\}$	0.02
Otherwise	0.00

FLID or FLDC. The updated distribution is shown in Table 4.3 and it can be considered a sensible distribution given to the problem description and the high rating of the new location, hence showing the ability of the model to generalize.

Chapter 5

Synthetic Experiments

5.0.4 Example datasets

This section presents the results obtained after learning the datasets introduced in the examples for each model. In every instance 1000 samples were generated from the specific distribution, along with 2000 noise samples ($\nu = 2$). This shows the ability of NCE to learn models that incorporate diversity and coherence between items and features.

FLID: Two landmarks

Firstly, recall the following characteristics about the dataset in the example:

- There are 3 elements, h, s, f.
- There are only 2 possible sets, $\{h, s\}$ and $\{h, f\}$. Both equally likely, i.e. $P(S) = 0.5$.
- The model can be realized with a single diversity dimension, i.e. $L = 1$.

The resulting utility vector and weight matrix are:

$$\mathbf{u} = (5.42, 2.82, 2.79)^\intercal$$
$$\mathbf{W}^b = (0.02, 6.10, 6.10)^\intercal$$

This is a slightly different model from the one suggested in section 3.4.2, however the normalized probability distribution for this model shown in table 5.1 proves that it closely approximates the distribution.

FLDC: Disjoint pairs

Firstly, recall the following characteristics about the dataset in the example:

Table 5.1: Learned distribution for example 4.2.3

S	$P(S)$
$\{h, s\}$	0.48
$\{h, f\}$	0.47
$\{h\}$	0.03
$\{h, s, f\}$	0.02

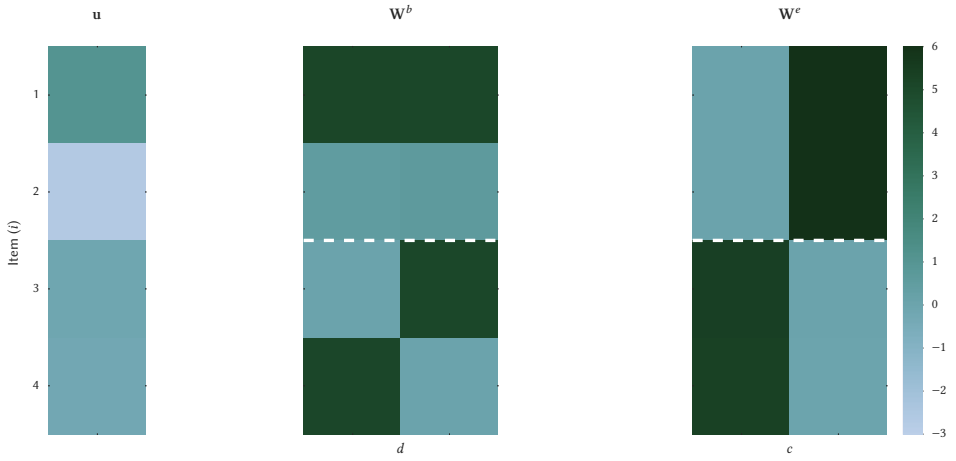

Figure 5.1: Learned model for example 4.1.3. The white line divides the disjoint pairs described in the example.

- There are 4 items, i.e. $V = \{1, 2, 3, 4\}$.
- There are only 2 possible sets, $\{1, 2\}$ and $\{3, 4\}$. Both equally likely, i.e. $P(S) = 0.5$.
- The model can be realized with a 2 diversity and 2 coherence dimensions.

Figure 5.1 shows the resulting utility vector $\mathbf{u}$ and weight matrices $\mathbf{W}^b, \mathbf{W}^e$ after learning. The model shown in the figure displays the desired properties of diversity between the disjoint pairs whilist having coherence between the items in each pair. Despite being different from the proposed model in section 4.1.3 it approximately realizes the desired distribution.

FFLDC: Rated locations

Firstly, recall the following characteristics about the dataset in the example:

- There are 6 items, i.e. $V = \{1, 2, 3, 4, 5, 6\}$.
- The full distribution is related to the features and is given in table 4.2.
- The proposed model has 2 diversity dimensions and one coherence dimension.

Figure 5.2 shows the resulting model after learning. Unfortunately, this model can be not as easily interpreted as the one proposed in figure 4.2, nevertheless it accurately models the distribution from the example. This result demonstrates the ability of the learning algorithm to represent a distribution using features.
It is important to note that the presented results for these experiments correspond to the best of multiple runs. It was observed that the learning algorithm does not always arrive to a good solution. This is explained by the fact that $g(\theta)$ is not a convex function which means that there exists the risk of reaching a local minima in some cases. Due to this, most of the experiments in the following sections are executed over several data folds to account for the randomness.

5.0.5 Learning rate sensitivity

This section expands on the discussion about the learning rate and explores its effect on the learning of the synthetic data from the FFLDC example in section 4.2.3, as well as the effect of implementing AdaGrad.

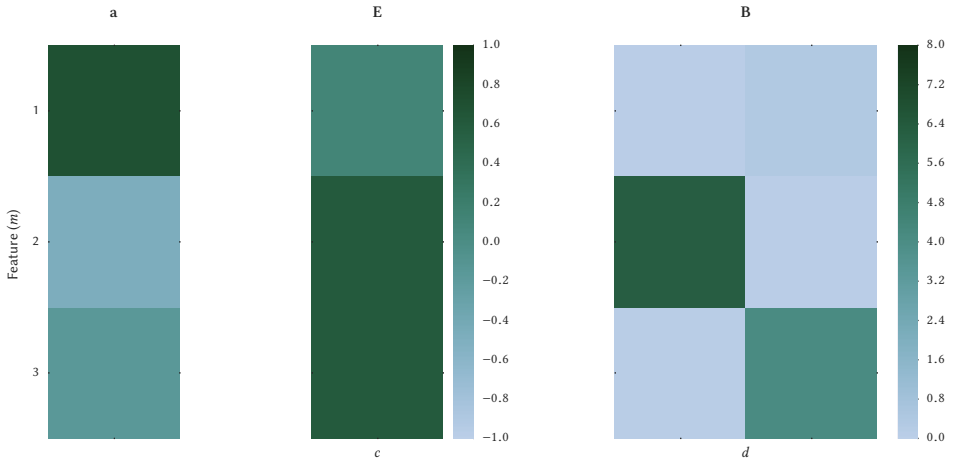

Figure 5.2: Learned model for example 4.2.3

The first experiment considers the stability of the optimization without AdaGrad. In the experiments presented in this section the following configuration of the learning algorithm is used:

- 1000 data samples from the distribution in table 4.2 are used, along with 2000 noise samples, i.e. $\nu = 2$.
- Each run does 100 passes over the data and noise samples.
- The algorithm is executed 8 times to obtain statistics about the results.

Figure 5.3 shows the behavior of $g(\theta)$ during learning, each point corresponds to the average value of $g(\theta)$ after each pass over the data and noise samples with its corresponding 95% confidence interval.
The results in figure 5.3 display what was mentioned in section 3.5.3, they show that for small values of η_0 the learning can be significantly slow and that large values of η_0 may lead to instability. Concretely, the first row displays slow but stable learning rates while the last row displays learning rates that are too high, the middle row displays the ideal learning rates. Fortunately, in the particular case of this synthetic dataset there exists a learning rate for which the objective function converges however, as it will be seen on real data, this is not always the case. An interesting characteristic shown in this figure is the behavior of the confidence intervals for $\eta_0 = 0.005$, even though the learning is considerably slow there is also a large variation, in this instance the initialization has a larger influence because the learned model doesn't change much from it.
In contrast, figure 5.4 shows the objective function for various values of η_0 after incorporating AdaGrad to the implementations. These results show that training with AdaGrad is stable for a larger range of eta_0, although slower for small values of η_0 which were good for the learning without AdaGrad. For large enough η_0 values, it can be clearly seen from the figure that SGD with AdaGrad reaches convergence significantly faster, often in the first few iterations.
Finally, figure 5.5 shows a direct comparison between training with and without AdaGrad using the best values of η_0 for each configuration. In this figure both algorithms converge to an optimal value, however it also shows that training with AdaGrad converges significantly faster and its average appears slightly more stable.
These combined results indicate that using AdaGrad is the best strategy for learning the models.

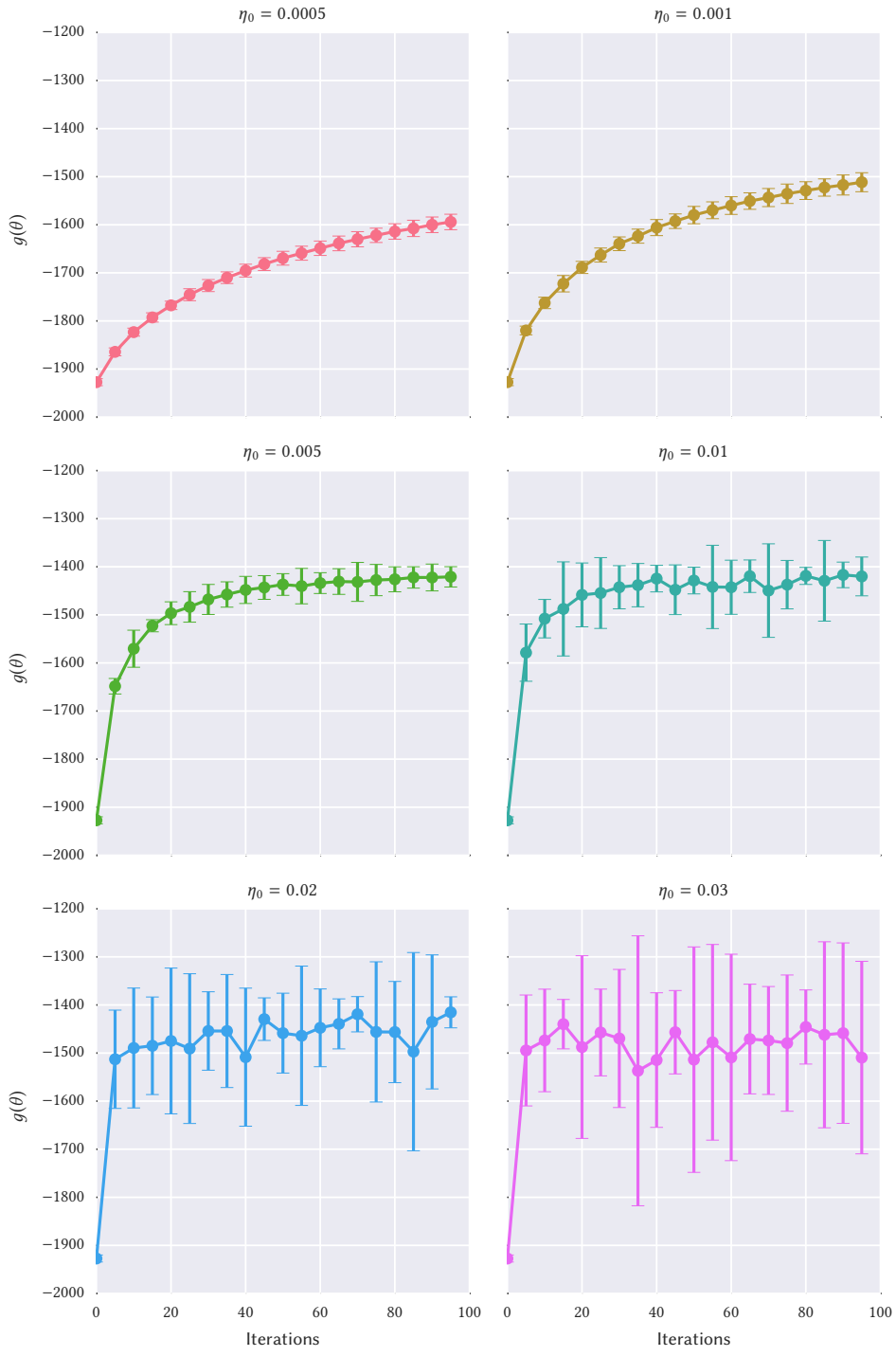

Figure 5.3: Objective function during learning for various values of η_0 without AdaGrad.

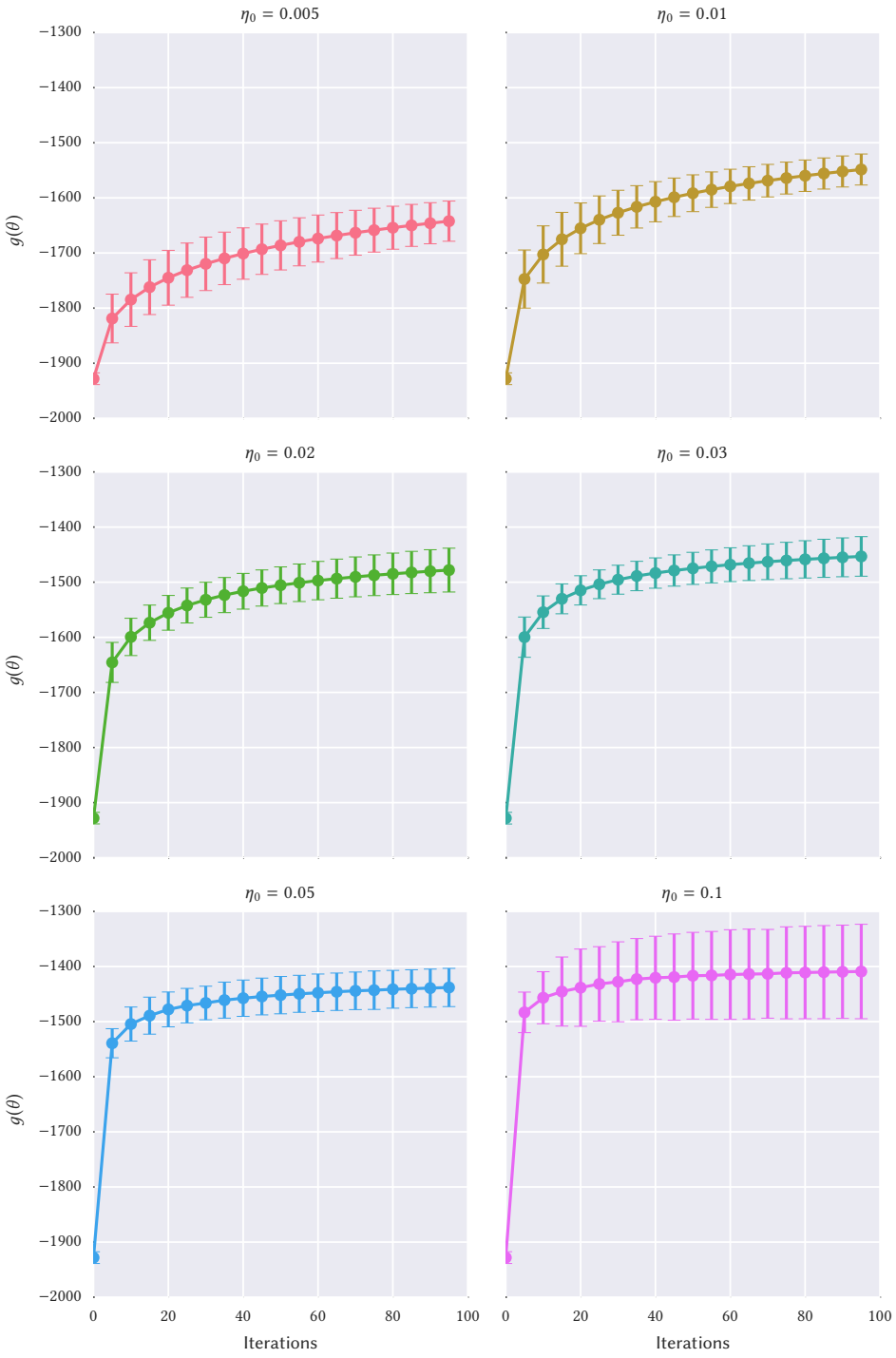

Figure 5.4: Objective function during learning for various values of η_0 with AdaGrad.

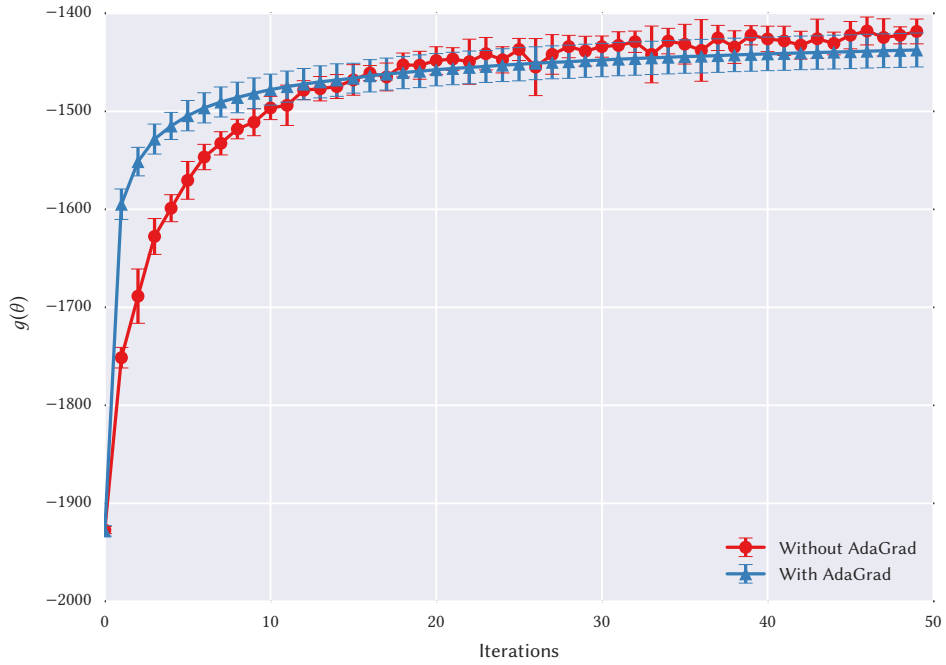

Figure 5.5: Comparison of learning performance with and without AdaGrad. Initial learning rates are $\eta_0 = 0.05$ with AdaGrad and $\eta_0 = 0.005$ without AdaGrad.

Following the first two suggestions, the noise distribution is sampled from a modular model as the one from equation 3.4. This distribution is constructed from estimated marginals, i.e. $\hat{P}(i \in S)$, which are computed using the maximum likelihood estimator, i.e. $\hat{P}(i \in S) = {}^{\#N(i \in S)}/_{|\mathcal{D}|}$. Then the utilities for the modular model are given by:

$$u_i = \log\left(\frac{1}{\hat{P}(i \in S)} - 1\right) \tag{5.1}$$

This model is easy to sample from, hence allowing an efficient generation of large noise samples.

Chapter 6

Experimental Setup

6.1 Flickr Dataset

Dataset description and how it was collected.

6.2 Path finding

How the actual sets (paths) are built from the data, and the 2 sets of data to be explore 10 items (small) and 100 items (big).

6.3 NCE learning

Details on the implementation of NCE, noise generation.

6.4 Baselines

The baseline models (Markov, distance).

6.5 Evaluation

10 fold evaluation, accuracy and MRR.

Chapter 7

Results

7.1 Small dataset

Results on the small dataset. Difference between FLID, FLDC, FFLDC models. Different feature sets.

7.2 Large dataset

Results on the large dataset. Difference between FLID, FLDC, FFLDC models. Different feature sets.

Chapter 8

Conclusion

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