Learning Trans-dimensional Random Fields with Applications to Language Modeling

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Abstract—To describe trans-dimensional observations in sample spaces of different dimensions, we propose a probabilistic model, called the trans-dimensional random field (TRF) by explicitly mixing a collection of random fields. In the framework of stochastic approximation (SA), we develop an effective training algorithm, called augmented SA, which jointly estimates the model parameters and normalizing constants while using trans-dimensional mixture sampling to generate observations of different dimensions. Furthermore, we introduce several statistical and computational techniques to improve the convergence of the training algorithm and reduce computational cost, which together enable us to successfully train TRF models on large datasets. The new model and training algorithm are thoroughly evaluated in a number of experiments. The word morphology experiment provides a benchmark test to study the convergence of the training algorithm and to compare with other algorithms, because log-likelihoods and gradients can be exactly calculated in this experiment. For language modeling, our experiments demonstrate the superiority of the TRF approach in being computationally more efficient in computing data probabilities by avoiding local normalization and being able to flexibly integrate a richer set of features, when compared with n-gram models and neural network models.

Index Terms—Language modeling, Random field, Stochastic approximation, Trans-dimensional sampling, Undirected graphical modeling.

1 INTRODUCTION

Graphical models [1], [2] have emerged as a general framework for describing and applying probabilistic models in building intelligent systems, and can be broadly classified into two classes. In the directed graphical models (also known as Bayesian networks), the joint distribution is factorized into a product of local conditional density functions, whereas in the undirected graphical models (also known as Markov random fields or Markov networks) the joint density function is defined to be proportional to the product of local potential functions. In certain applications, namely fixed-dimensional settings, the probabilistic model specifies a joint distribution over a fixed set of random variables, for example, in the modeling of fixed-size images. However, in many other applications, the probabilistic model relates to a much more complex sample space, which will be called the trans-dimensional setting: the observations can be of different dimensions. A familiar case is temporal modeling of sequential data, where each observation is a sequence of a random length. It is desirable to build a probabilistic model applicable to sequences of different lengths.

Currently in the trans-dimensional setting, the directed graphical modeling approach, e.g. through hidden Markov models or, more generally, dynamic Bayesian networks, is dominant particularly for sequential data. In contrast, the undirected graphical modeling approach is rarely used in the trans-dimensional setting. This is presumably because fitting undirected models is more challenging than fitting directed models [2]. In general, calculating the log-likelihood and its gradient is analytically intractable even for fixed-dimensional undirected models, because this involves evaluating the normalizing constant (also called the partition function in physics) and, respectively, the expectation with respect to the model distribution. It should be noted that the normalizing constant and model expectation can be exactly calculated or efficiently approximated under some limited circumstances, mostly in low tree-width random fields (e.g. chain-structured) with moderately sized state spaces. The widely used conditional random fields (CRFs) [3] satisfy these conditions, by only modeling the conditional distribution over labels given the observations. As a result, CRFs deal with trans-dimensional data but with a significantly reduced sample space of labels. Indeed, currently much of random field learning is pursued for CRFs. But CRFs can only be used for discriminative tasks, e.g. segmenting and labeling of natural language sentences or images.

In this paper, we are interested in building random field (RF) models for trans-dimensional observations. The fields can have greater tree-widths (e.g. 5) and larger sized state spaces (e.g. $10^4$), so that they can capture higher-order interactions inherent in the trans-dimensional data. Roughly speaking, the main advantages of undirected modeling over directed modeling are: (1) undirected modeling is more natural for certain domains such as relational data, where fixing the directions of edges is awkward in a graphical model, and (2) the undirected representation provides greater flexibility and potentially more powerful modeling capacity in avoiding local normalization and acyclicity requirements. Eliminating these requirements allows us to easily encode a much richer set of patterns/features which characterize the studied phenomenon.

As remarked in [2], it can be problematic to construct a template-based RF model with a certain dimension, and apply

1. The tree-width of a graph is defined as the minimum width over all possible tree decompositions of the graph, which measures roughly how close the graph is to a tree. The tree-width of a tree is 1.
2. The state space of a multivariate model is the set of all possible values for each coordinate of a multivariate observation.
it to data of a very different dimension. A pioneering work in building RF models for trans-dimensional observations is [4], but the proposed Improved Iterative Scaling (IIS) method for parameter estimation and the Gibbs sampler are not suitable for even moderately sized RF models. Inducing RF models of English word spellings, being sequences of characters, is studied in [4] without numerical evaluation of performances. It is interesting to note that the feature induction and IIS algorithms proposed in [4] are used mostly in later CRF studies. Another previous work, which is more directly related to our study of RF modeling of trans-dimensional data, is whole-sentence maximum entropy (WSME) language modeling [5]. Language modeling (LM) is crucial for a variety of computational linguistic applications, such as speech recognition, machine translation, handwriting recognition, information retrieval and so on. Except the WSME LMs, most LMs follow the directed modeling approach, e.g. n-gram LMs [6], neural network (NN) LMs [7], [8], [9] and conditional maximum entropy LMs [10], [11], [12]. Although WSME models have the potential benefits of being able to naturally express sentence-level phenomena and integrate features from a variety of knowledge sources, their performance results ever reported are not satisfactory [5], [13], [14] (see Section 2.2). The learning algorithm used is Generalized Iterative Scaling (GIS) [15] and the sampling methods for approximating model expectations are Gibbs sampling, independence Metropolis-Hasting sampling and importance sampling [5]. Simple applications of these methods are hardly able to work efficiently in a trans-dimensional setting especially with large-size state space\(^3\), and hence the WSME models are in fact poorly fitted to the data. This is one of the reasons for the unsatisfactory results of previous WSME models.

To describe trans-dimensional observations, we propose a new probabilistic model, called the trans-dimensional random field (TRF) model, by explicitly mixing a collection of RFs in sample spaces of different dimensions. With this model formulation, we develop an effective training algorithm in the framework of stochastic approximation (SA) [16], [17], [18], to jointly estimate the model parameters and normalizing constants. The training algorithm, which is called augmented SA (AugSA) algorithm, involves two steps, sampling observations and then updating estimates of model parameters and normalizing constants, at each iteration. For the sampling step, we also develop a powerful Markov chain Monte Carlo (MCMC) technique, called trans-dimensional mixture sampling (TransMS). Furthermore, we introduce several statistical and computational techniques, including two-stage configuration of learning rates, use of empirical variances to rescale SA updates, proper specification of dimension probabilities for mixture sampling, a modeling strategy to deal with rare high-dimensional observations (e.g. rare long sentences), use of class information and multiple CPUs to reduce the computational cost, regularization and stopping decision. All these techniques together enable successful training of our TRF models on large datasets.

The TRF modeling approach and the proposed AugSA and TransMS algorithms are thoroughly evaluated in three experiments. The first is the word morphology experiment as studied in [4]. Due to the small size of the state space in this experiment, parameter learning can be performed with exactly calculated log-likelihoods and gradients. This experiment serves as a valid benchmark to study the convergence of Monte Carlo training algorithms with various configurations. The next two experiments are about language modeling, which is our motivating application. We show that TRF LMs significantly outperform n-gram LMs [6], and perform better than recurrent neural network (RNN) LMs [8], [19] and close to Long Short Term Memory (LSTM) LMs [9], [20] but being much faster in computing sentence probabilities. Moreover, interpolated TRF and LSTM LMs produces the lowest word error rate (WER) in speech recognition. We examine the scalability of TRF LMs by incrementally increasing the size of the training set and find that they can scale to using training data of up to 32 million words. All these experiments demonstrate the superiority of the TRF models and the effectiveness of the AugSA training algorithms. To our knowledge, these results represent the first strong empirical evidence supporting the power of using RF approach to language modeling.

The remainder of this paper is organized as follows. In Section 2, we discuss related work. We introduce the TRF model formulation in Section 3 and present the training algorithm, AugSA with TransMS, in Section 4. Additional statistical and computational techniques for training TRF models are described in Section 5. The experimental evaluations are reported in Sections 6, 7, and 8. We conclude the paper with a discussion in Section 9.

Preliminary part of this work was published in [21]. New features in this paper include model comparison in Section 3.1, a detailed derivation of the learning algorithm (Section 4.1), an importance sampling extension (Section 4.2, 5.3), simpler configuration of learning rates (Section 5.1), a more effective method of rescaling SA update (Section 5.2), dealing with rare high-dimensional observations (Section 5.4), stop decision (Appendix D), and extensive new empirical results using new datasets and “tied” features and providing new comparisons with Adam optimiser [22], annealed importance sampling (AIS) [23] based estimates of normalizing constants, and LSTM LMs.

## 2 Related work

The central problem addressed in this paper involves building RF models for trans-dimensional observations. There are few directly related studies, e.g. [4] and [5]. However, there have been many studies of using RF models in the fixed-dimensional setting or for discriminative modeling (mainly related to CRFs). In the following, we will briefly discuss these studies and the connection to our work. Moreover, we further examine related work in language modeling, which is our motivating application in trans-dimensional modeling.

### 2.1 Learning with random fields

There is an extensive literature devoted to maximum likelihood (ML) learning of random fields, which is in general difficult because calculating the log-likelihood and its gradient is analytically intractable. Roughly speaking, there are two types of approximate methods — gradient methods and lower bound methods. The gradient methods make explicit use of the gradient. An important class is stochastic approximation methods [16], which approximates the model expectations by Monte Carlo sampling for calculating the gradient. The classic algorithm, initially proposed in [24], is often called stochastic maximum likelihood (SML). In the literature on training restricted Boltzmann machines (RBM), SML is also known as persistent contrastive divergence (PCD) [25] to emphasize that the Markov chain is not reset between parameter updates. Among the lower bound methods for ML learning of random fields, an important class is iterative scaling

\(^3\) In LMs, the size of state space is the vocabulary size, usually above \(10^4\).
methods such as GIS [15] and IIS [4]. These algorithms iteratively optimize lower bounds of the likelihood function to find the maximum likelihood estimates and are mostly studied in the context of maximum entropy (maxent) parameter estimation\textsuperscript{4} and logistic regression which is a conditional version of maxent. In practice the gradient methods are shown to be much faster than the lower bound methods [26], [27].

Remarkably, the above studies are mostly restricted to training a single fixed-dimensional RF model, and the parameter and the normalizing constant are estimated separately. Beyond the simple application of SA as in SML, we develop the augmented SA algorithm for jointly estimating the model parameter and multiple normalizing constants. Basically, stochastic approximation provides a mathematical framework for stochastically solving a root finding problem, which has the form of expectations being equal to zeros [16], [17], [18]. The starting point for augmented SA is to formulate a system of simultaneous equations in this form for both the maximum likelihood estimates and the normalizing constants. The most relevant previous works that inspire our algorithmic development are [28] on SA for fitting a single RF, [29] on sampling and estimating normalizing constants from multiple RFs of the same dimension, and [30] on trans-dimensional MCMC.

Finally, it is worthwhile to point out that by only modeling the conditional distribution over labels given the observations, CRFs deal with trans-dimensional data but with a significantly reduced sample space of labels. In order for CRFs to be computationally tractable, usual CRF formulations are mostly limited to incorporating pairwise interactions among labels. In order to allow for higher-order interactions, there presents the challenge of building RF models in the trans-dimensional setting with greater tree-widths, which is the same concern addressed in this paper.

2.2 Language modeling

Language modeling involves determining the joint probability \( p(x) \) of a sentence \( x \), which can be denoted as a pair \( x = (l, x^l) \), where \( l \) is the length and \( x^l = (x_1, \ldots, x_l) \) is a sequence of \( l \) words. Currently, the dominant approach to language modeling is the directed or conditional modeling, which decomposes the joint probability of \( x^l \) into a product of conditional probabilities\textsuperscript{5} by using the chain rule,

\[
p(x_1, \ldots, x_l) = \prod_{i=1}^{l} p(x_i|x_1, \ldots, x_{i-1}).
\]

To avoid degenerate representation of the conditionals, the history of \( x_i \), denoted as \( h_i = (x_1, \ldots, x_{i-1}) \), is reduced to equivalence classes through a mapping \( \phi(h_i) \) with the assumption

\[
p(x_i|h_i) \approx p(x_i|\phi(h_i)).
\]

Language modeling in this conditional approach consists of finding suitable mappings \( \phi(h_i) \) and effective methods to estimate \( p(x_i|\phi(h_i)) \). A classic example is the traditional \( n \)-gram LMs with \( \phi(h_i) = (x_{i-n+1}, \ldots, x_{i-1}) \). Various smoothing techniques are used for parameter estimation [6]. Recently, neural network LMs, which have begun to surpass the traditional \( n \)-gram LMs, also follow the conditional modeling approach, with

\[
\phi(h_i) \text{ determined by a neural network (NN), which can be either a feedforward NN [7] or a recurrent NN [8], [9].}
\]

Remarkably, an alternative approach is used in whole-sentence maximum entropy (WSME) language modeling [5]. Specifically, a WSME model has the form

\[
p(x; \lambda) = \frac{1}{Z(\lambda)} e^{\lambda^T f(x)},
\]

where \( f(x) \) is a vector of features, which are computable functions of \( x \) such as \( n \)-grams conventionally used, \( \lambda \) is the corresponding parameter vector, and \( Z(\lambda) = \sum_x e^{\lambda^T f(x)} \) is the global normalizing constant, which is typically analytically intractable.

While there has been extensive research on conditional LMs, there has been little work on the whole-sentence LMs, mainly in [5], [13], [14]. Although the whole-sentence approach has the potential advantage of being able to flexibly integrate a richer set of features, the empirical results of previous WSME LMs are not satisfactory, almost the same as traditional \( n \)-gram LMs. After incorporating lexical and syntactic information, a mere relative improvement of 1% and 0.4% respectively in perplexity and WER was reported for the resulting WSME LM [5]. Subsequent studies of using WSME LMs with grammatical features, as in [13] and [14], reported perplexity improvement above 10% but no WER improvement when using WSME LMs alone.

3 Model Definition

Suppose that it is of interest to build random field models for multiple sets of observations of different dimensions, such as images of different sizes or sentences of different lengths. Denote by \( x^j \) an observation in a sample space \( \mathcal{X}^j \) of dimension \( j \), ranging from 1 to \( m \). The space of all observations is then the union \( \mathcal{X} = \bigcup_{j=1}^{m} \mathcal{X}^j \). To emphasize the dimensionality, each observation in \( \mathcal{X} \) can be represented as a pair \( x = (j, x^j) \), even though \( j \) is identified as the dimension of \( x^j \). By abuse of notation, write \( f(x) = f(x^j) \) for features of \( x \).

For \( j = 1, \ldots, m \), assume that the observations \( x^j \) are distributed from a random field in the form

\[
p_j(x^j; \lambda) = \frac{1}{Z_j(\lambda)} e^{\lambda^T f(x^j)},
\]

where \( f(x^j) = (f_1(x^j), f_2(x^j), \ldots, f_d(x^j))^T \) is a feature vector, \( \lambda = (\lambda_1, \lambda_2, \ldots, \lambda_d)^T \) is the corresponding parameter vector, and \( Z_j(\lambda) \) is the normalizing constant:

\[
Z_j(\lambda) = \sum_{x^j} e^{\lambda^T f(x^j)}, \quad j = 1, \ldots, m.
\]

For identifiability, assume that no linear combination of the features \( f_i(x^j) \), \( i = 1, \ldots, d \), is a constant function of \( x^j \). Moreover, assume that dimension \( j \) is associated with a probability \( \pi_j \) for \( j = 1, \ldots, m \) with \( \sum_{j=1}^{m} \pi_j = 1 \). Therefore, the pair \( (j, x^j) \) is jointly distributed as

\[
p(j, x^j; \pi, \lambda) = \pi_j p_j(x^j; \lambda) = \frac{\pi_j}{Z_j(\lambda)} e^{\lambda^T f(x^j)},
\]

where \( \pi = (\pi_1, \ldots, \pi_m)^T \).

A feature \( f_i(x^j) \), \( i = 1, \ldots, d \), can be any computable function of the input \( x^j \). For various applications such as language modeling, the parameters of local potential functions across locations are often tied together [4]. In our current experiments, each feature \( f_i(x^j) \) is defined in the form \( f_i(x^j) = \sum_k f_i(x^j, k) \), where \( f_i(x^j, k) \) is a binary function of \( x^j \) evaluated at position
k. In a trigram example, \( f_i(x^j, k) \) equals to 1 if three specific words appear at positions \( k \) to \( k + 2 \) and \( k \leq j - 2 \). The binary features \( f_i(x^j, k) \) share the same parameter \( \lambda_i \) for different positions \( k \) and dimensions 4, so called position-independent and dimension-independent. Hence, the feature \( f_i(x^j) \) indicates the count of nonzero \( f_i(x^j, k) \) over \( k \) in the observation \( x^j \) and takes values as non-negative integers.

3.1 Comparison between WSME and TRF models

We comment on the connection and difference between WSME and TRF models. Suppose that we add the dimension features in the WSME model (1) and obtain

\[
p(j, x^j; \lambda, \nu) = \frac{1}{Z(\lambda, \nu)} e^{\nu^T \delta(j) + \lambda^T f(x^j)},
\]

where \( \delta(j) = (\delta_1(j), \cdots, \delta_m(j))^T \) denotes the dimension features such that \( \delta_1(j) = 1(j = 1), f(x^j) \) denotes the ordinary features as used in both models (1) and (2), \( \nu = (\nu_1, \ldots, \nu_m)^T \) and \( \lambda \) are the corresponding parameter vectors, and \( Z(\lambda, \nu) \) is the global normalizing constant.

\[
Z(\lambda, \nu) = \sum_{j=1}^m \sum_{x^j \in \mathcal{X}} e^{\nu^T \delta(j) + \lambda^T f(x^j)} = \sum_{j=1}^m e^{\nu^T} Z_j(\lambda).
\]

We show later in Proposition 1 that when both fitted by maximum likelihood estimation, model (3) is equivalent to model (2) but with different parameterization. The parameters in model (3) are \((\lambda, \nu)\), whereas the parameters in model (2) are \((\pi, \lambda)\). Therefore, an important distinction of our TRF approach for trans-dimensional modeling from previous WSME works lies in the use of dimension features, which has significance consequences in both model definition and model learning.

First, it is clear that model (2) is a mixture of random fields on subspaces of different dimensions, with mixture weights explicitly as free parameters. Hence model (2) will be called a trans-dimensional random field (TRF). Moreover, by maximum likelihood, the mixture weights can be estimated to be the empirical dimension probabilities (see Proposition 1).

Second, it is instructive to point out that model (1) is essentially also a mixture of RFs, but the mixture weights implied are fixed to be proportional to the normalizing constants \( Z_j(\lambda) \):

\[
p(j, x^j; \lambda) = \frac{Z_j(\lambda)}{Z(\lambda)} \frac{1}{Z(\lambda)} e^{\lambda^T f(x^j)},
\]

where \( Z(\lambda) = \sum_{x^j} e^{\lambda^T f(x^j)} = \sum_{j=1}^m Z_j(\lambda) \). Typically the unknown mixture weights (5) may differ from the empirical length probabilities and also from each other by orders of magnitudes, e.g., \(10^{10}\) or more in our experiments. As a result, it is very difficult to efficiently sample from model (1), in addition to the fact that the length probabilities are poorly fitted for model (1). Setting mixture weights to the known, empirical length probabilities enables us to develop an effective learning algorithm, as introduced in Section 4. Basically, the empirical weights serve as a control device to improve sampling from multiple distributions [29], [31].

4 Model Learning

We develop a novel learning algorithm in the SA framework [17], [18] to estimate both the parameters \( \lambda \) and the normalizing constants \( Z_1(\lambda), \ldots, Z_m(\lambda) \). Equivalently, we estimate the parameters \( \lambda \) and the log ratios of \( Z_j(\lambda) \):

\[
\zeta_j^*(\lambda) = \log \frac{Z_j(\lambda)}{Z_j(\lambda)}, \quad j = 1, \ldots, m,
\]

where \( Z_1(\lambda) \) is chosen as the reference value such that it can be calculated exactly. The core ingredients newly designed are the augmented SA (AugSA) scheme for simultaneously updating parameters and normalizing constants (Section 4.2) and trans-dimensional mixture sampling (TransMS) (Section 4.3), which is used in the MCMC sampling step of AugSA.

4.1 Maximum likelihood learning

Suppose that the training data consist of a subset of \( n_j \) observations of dimension \( j \), denoted by \( D_j \), for \( j = 1, \ldots, m \). We derive the maximum likelihood estimates of \((\pi, \lambda)\) for model (2).

**Proposition 1.** For model (2), the maximum likelihood estimate (MLE) of \( \pi \) is \( \hat{\pi} = (\hat{\pi}_1, \ldots, \hat{\pi}_m)^T \) with \( \hat{\pi}_j = n_j/n \) for \( j = 1, \ldots, m \). Moreover, the MLE of \( \lambda \) is determined by

\[
\hat{\lambda}_j^\ast \left[ f \right] = 0.
\]

Throughout, \( \hat{\lambda}_j^\ast \left[ f \right] \) is the expectation of the feature vector \( f \) with respect to the empirical distribution:

\[
\hat{\lambda}_j^\ast \left[ f \right] = \frac{1}{n} \sum_{j=1}^m \sum_{x^j \in D_j} f(x^j) = \frac{1}{n} \sum_{j=1}^m \hat{\pi}_j^T \left[ f(x^j) \right],
\]

with \( \hat{\pi}_j^T \left[ f(x^j) \right] = n_j^{-1} \sum_{x^j \in D_j} f(x^j) \), and \( \hat{\pi}_j^\ast \left[ f \right] \) is the expectation of \( f \) with respect to the joint distribution (2), \( p(j, x^j; \hat{\pi}, \lambda) \):

\[
\hat{\pi}_j^\ast \left[ f \right] = \sum_{x^j \in \mathcal{X}^j} f(x^j) \hat{\pi}_j^\ast \left[ f(x^j) \right],
\]

**Proof.** See Appendix A.

Then we demonstrate that maximum likelihood learning of TRF model (2) and of model (3) are equivalent to each other but with different parameterization.

**Proposition 2.** (i) If \( \hat{\lambda}, \hat{\nu} \) are MLEs of \( \lambda, \nu \) in model (2), then \( \hat{\lambda}, \hat{\nu} \) are MLEs of \( \lambda, \nu \) in model (3), where \( \lambda = \hat{\lambda} \) and for a constant \( c \),

\[
e^{\nu^T} = c \hat{\pi}_j e^{-\zeta^\ast_j(\lambda)}, \quad j = 1, \ldots, m.
\]

(ii) If \( \hat{\lambda}, \hat{\nu} \) are MLEs of \( \lambda, \nu \) in model (3), then Eq. (7) holds and \( \lambda = \hat{\lambda} \) is an MLE of \( \lambda \) in model (2).

(iii) In either (i) or (ii), the fitted model (3), \( p(j, x^j; \hat{\lambda}, \hat{\nu}) \), is identical to the fitted model (2), \( p(j, x^j; \hat{\pi}, \lambda) \).

**Proof.** See Appendix A.

As suggested by Eq. (7) and motivated by self-adjusted mixture sampling in [29], we define the following distribution of \( (j, x^j) \) on \( \mathcal{X} \) by a re-parameterization of model (3):

\[
p(j, x^j; \lambda, \zeta) \propto (\hat{\pi}_j e^{-\zeta}) e^{\lambda^T f(x^j)},
\]

where \( \zeta = (\zeta_1, \ldots, \zeta_m)^T \) with \( \zeta_1 = 0 \) and \( \zeta_j \) is related to \( \nu_j \) through \( e^{\nu_j} = \hat{\pi}_j e^{-\zeta} \) and can be interpreted as the hypothesized value of the true value \( \zeta^\ast_j(\lambda) \). By Proposition 2, after the re-parametrization from (3) to (8), the MLE of \( \lambda \) under model (8)
Input: training set
1: set initial values $\lambda^{(0)} = (0, \ldots, 0)^T$ and $\zeta^{(0)} = \zeta^*(\lambda^{(0)}) - \zeta^T(\lambda^{(0)})$
2: for $t = 1, 2, \ldots, t_{\text{max}}$ do
3: set $B(t) = \emptyset$
4: set $(j(t,0), x(t,0)) = (j(t-1,K), x(t-1,K))$

Step I: MCMC sampling
5: for $k = 1 \rightarrow K$ do
6: $(j(t,k), x(t,k)) = \text{sample}((j(t,k-1), x(t,k-1)))$ (See Tab.1)
7: set $B(t) = B(t) \cup \{(j(t,k), x(t,k))\}$
8: end for

Step II: SA updating
9: Compute $\lambda(t)$ based on (16)
10: Compute $\zeta(t)$ based on (17) and (18)
11: end for

Fig. 1. Augmented stochastic approximation (AugSA)

is also that of $\lambda$ under model (2), satisfying (6). Moreover, for fixed $\lambda$, the MLE of $\zeta_j$ under model (8) is exactly the true value $\zeta^*_j(\lambda)$, satisfying

$$p(j; \lambda, \zeta) \equiv \hat{\pi}_j e^{-\zeta_j^*(\lambda)} \sum_{l=1}^m \hat{\pi}_l e^{-\zeta_l^* + \zeta_j^*(\lambda)}$$

is the marginal probability of dimension $j$ under (8). This result can also be verified by solving Eq. (9) directly. There are only $m - 1$ linearly independent equations in (9) because $\sum_{j=1}^m \hat{\pi}_j = 1$, and so are only $m - 1$ unknowns ($\zeta_2, \ldots, \zeta_m$) with $\zeta_1 = 0$ for fixed $\lambda$.

In summary, the MLE of $\lambda$ (denoted as $\hat{\lambda}$) and the corresponding log ratios of normalizing constants $\zeta_j^*(\lambda), j = 1, \ldots, m$, are determined jointly from (6) and (9). Both equations (6) and (9) have the form of equating empirical expectations, $\hat{p} f$ and $\hat{\pi}_j$, with theoretical expectations, $p f[\cdot]$ and $p(j; \lambda, \zeta)$, for the ordinary functions $f[\cdot]$ and the dimension functions $\delta[\cdot]$ respectively, as similarly found in maximum likelihood estimation of single random field models [2].

4.2 Stochastic approximation

Stochastic approximation (SA) was first studied in [16]. There has since been a vast literature on theory, methods, and applications of SA [17], [18]. Here we develop an augmented SA algorithm in the SA framework to simultaneously address the two learning objectives described in Section 4.1.

We first give a brief review of the SA framework. Suppose that the objective is to find the solution $\theta^*$ of $h(\theta) = 0$ with

$$h(\theta) = E_{Y \sim g(\cdot; \theta)}[H(Y; \theta)]$$

where $\theta \in \mathbb{R}^d$ is a parameter vector of dimension $d$, and $Y$ is an observation from a probability distribution $g(\cdot; \theta)$ depending on $\theta$, and $H(Y; \theta) \in \mathbb{R}^d$ is a function of $Y$. For some initial values $\theta_0$ and $Y_0$, a general SA algorithm is as follows.

Stochastic approximation (SA):

1) Generate $Y^{(t)} \sim K(Y^{(t-1)}, \cdot)$, where $K(\cdot; \cdot)$ is a Markov transition kernel that admits $g(\cdot; \theta)$ as the invariant distribution.

2) Set $\theta^{(t)} = \theta^{(t-1)} + \nu H(Y^{(t)}; \theta^{(t-1)})$, where $\nu$ is the learning rate (also called gain rate) and $A$ is an invertible matrix (called gain matrix).

During each SA iteration, it is possible to generate a set of multiple observations $Y$ by performing the Markov transition repeatedly (instead of only one time) and then use the average of the corresponding values of $H(Y; \theta)$ for updating $\theta$, as shown in the following algorithm. This technique can help reduce the fluctuation due to slow-mixing of Markov transitions.

SA with multiple moves:

1) Set $Y^{(t,0)} = Y^{(t-1,K)}$. For $k$ from $1$ to $K$, generate $Y^{(t,k)} \sim K(Y^{(t,k-1)}, \cdot)$, where $K(\cdot; \cdot)$ is a Markov transition kernel that admits $g(\cdot; \theta)$ as the invariant distribution.

2) Set $\theta^{(t)} = \theta^{(t-1)} + \nu A \left( \frac{1}{K} \sum_{Y \in B(t)} H(Y; \theta^{(t-1)}) \right)$, where $B(t) = \{Y^{(t,k)} | k = 1, \ldots, K\}$.

The convergence of SA has been studied under various regularity conditions [17], [18]. For $\gamma_t = \gamma_0 / t^2$ with $\gamma_0 > 0$ and $1/2 < \beta < 1$, it can be shown that $\gamma_t^{-1/2}(\theta^{(t)} - \theta^*)$ converges in law as $t \to \infty$ to a multivariate normal distribution $N(0, \Sigma)$. The maximal rate of variance reduction is reached with $\beta = 1$. Moreover, if $\beta = 1$, then $\Sigma$ achieves a minimum at $\gamma_t = 1/t$ and $A = -\{\partial h(\theta^*)/\partial \theta\}^{-1}$, resulting in an optimal SA recursion:

$$\theta^{(t)} = \theta^{(t-1)} - \frac{1}{t} \left\{ \frac{\partial h(\theta^*)}{\partial \theta} \right\}^{-1} H(Y; \theta^{(t-1)})$$

which is reminiscent of Newton’s update for root-finding. However, the optimal SA recursion (10) is, in general, infeasible because $\partial h(\theta^*)/\partial \theta$ is unknown. There are broadly two approaches to achieving asymptotic efficiency. One is to estimate both $\theta^*$ and $\partial h(\theta^*)/\partial \theta$ by stochastic approximation (e.g. [28]). Another approach is to use the trajectory average $\bar{\theta}(t) = t^{-1} \sum_{i=1}^t \theta(i)$, but set the learning rate $\gamma_t = \gamma_0 / t^2$ decreasing more slowly than $O(t^{-1})$ for $1/2 < \beta < 1$ [32]. While a variation of the first approach was explored in our previous work [21] (see Section 5.2), the second approach was not found to perform satisfactorily in our preliminary experiments.

We exploit several new ideas in developing SA algorithms for learning with TRF. To start, we recast (6) and (9) jointly as a system of simultaneous equations in the form of $h(\theta) = 0$, with $\theta = (\lambda, \zeta_{11})$, $Y = (j, x^T)$, $g(\cdot; \theta) = p(j; x^T; \lambda, \zeta)$ in (8), and

$$H(Y; \theta) = \left( \frac{\hat{p} f - f(x)}{\delta_{(1)}(j) - \pi_{(1)}} \right)$$

where $\delta(1) = (\delta_{11}, \ldots, \delta_{m1})^T$, $\pi_{(1)} = (\pi_{12}, \ldots, \pi_{m1})^T$ and $\delta_{(1)}(j) = (\delta_{2}(j), \ldots, \delta_{m}(j))$ with $\delta_{ij}(j) = 1$ if $j = l$ and 0 otherwise (see Appendix B). Then the general SA algorithm can be used to solve (6) and (9) jointly. In the following, we present two further developments, regarding the choices of design distribution $g(\cdot; \theta)$ and disturbance $H(Y; \theta)$ to improve convergence and regading the choice of gain matrix $A$ to approximate the optimal SA recursion (10).

First, we provide more general choices of $g(\cdot; \theta)$ and $H(Y; \theta)$ than (8) and (11) above, such that the system of equations $h(\theta) = 0$ remains equivalent to (6) and (9) jointly.
Proposition 3. Let \( \pi^0 = (\pi^0_0, \ldots, \pi^0_m)^T \) be fixed proportions, strictly between 0 and 1 and satisfying \( \sum_{j=1}^m \pi^0_j = 1 \). Define the following distribution on the space \( X \):

\[
q(j, x^j; \lambda, \zeta) \propto (\pi^0_j e^{-\zeta_j}) e^{\lambda^T f(x^j)}.
\]

(12)

Then (6) and (9) are jointly equivalent to

\[
\begin{align*}
\hat{p}[f] - q_{\lambda, \zeta}(\pi^0 f) &= 0, \\
q_{\lambda, \zeta}(0) &= 0,
\end{align*}
\]

(13)

(14)

where \( q_{\lambda, \zeta}(\pi f) \) is the expectation of \( \pi f(x^j) \) and \( q_{\lambda, \zeta}(0) \) is that of \( 0 \) under the joint distribution (12). Eqs. (13)–(14) can be expressed in the form of \( h(\theta) = 0 \), with \( g(\cdot; \theta) = q(j, x^j; \lambda, \zeta) \) and

\[
H(Y; \theta) = \left( \frac{\hat{p}[f] - \pi f(x^j)}{\delta(1)(j) - \pi^0(1)} \right),
\]

(15)

where \( \pi^0(1) = (\pi^0_0, \ldots, \pi^0_m)^T \).

Proof. See Appendix B.

Proposition 3 represents an important sampling extension of our previous SA algorithm [21], in allowing the use of dimension probabilities different from the empirical ones when generating the observation \( j, x^j \) in the SA algorithm. In the special case where \( \pi^0_j = \pi_j, j = 1, \ldots, m \), then the choices (12) and (13) for \( g(\cdot; \theta) \) and \( H(Y; \theta) \) reduce to (8) and (11) earlier. See Section 4.3 for MCMC sampling from \( q(j, x^j; \lambda, \zeta) \), and Section 5.3 for further discussion on the choice of \( \pi^0 \).

Second, we discuss the choice of gain matrix \( A \) as an approximation of \(-\{\partial h(\theta^*)/\partial \theta\}^{-1}\) in the optimal SA recursion (10). For simplicity, we take \( A \) as a block-diagonal matrix with diagonal blocks \( A_\lambda, A_\zeta \), partitioned according to \( \theta = (\lambda, \zeta) \). For the update of \( \lambda \), we set \( A^\lambda_{\lambda} \) to a diagonal matrix, \( \delta = \text{diag}(\sigma_1, \ldots, \sigma_d) \), as a diagonal approximation to \( \partial p_{\lambda}(f)/\partial \lambda_{\lambda, \lambda} \), where \( \sigma_i \) is the stratified empirical variance of feature \( f_i \) for \( i = 1, \ldots, d \):

\[
\sigma_i = \sum_{j=1}^m \frac{n_j}{n} \frac{\pi_j}{\hat{p}_j [f_i - \hat{p}_j(f_i)]^2}.
\]

See Section 5.2 for derivation and further discussion. The resulting update of \( \lambda \) at iteration \( t \) is then

\[
\lambda^{(t)} = \lambda^{(t-1)} + \lambda_{\lambda,t} \sigma^{-1} \left\{ \frac{\hat{p}[f] - \frac{1}{K} \sum_{(j,x^j) \in B(t)} \pi_j f(x^j)}{\delta(1)(j) - \pi^0(1)} \right\},
\]

(16)

where \( \lambda_{\lambda,t} \) is the learning rate of \( \lambda \) (see Section 5.1). For the update of \( \zeta \), we provide a trans-dimensional extension of the optimal SA recursion in self-adjusted mixture sampling [29], which is simple and feasible in spite of the fact that such an optimal scheme is generally infeasible as mentioned above.

Proposition 4. For fixed \( \lambda \), Eq. (14) can be expressed in the form of \( h(\zeta) = 0 \) with \( \hat{g}(\cdot; \zeta) = q(j, x^j; \lambda, \zeta) \) and \( H(Y; \zeta) = \hat{g}(1)(j) - \pi^0(1) \). The optimal gain matrix, \( A_\zeta = -\{\partial h(\zeta)/\partial \zeta\}^{-1} \mathbf{1}_{\zeta=\zeta^*}(\lambda) \), can be shown to satisfy

\[
A^\zeta H(Y; \zeta) = \left( \frac{\delta(2)(j)}{\pi^2}, \ldots, \frac{\delta_m(j)}{\pi^m} \right)^T - \frac{\delta(1)(j)}{\pi^0}.
\]

(17)

Proof. The result follows from the proof of Theorem 1 in [29].

By Proposition 4, the resulting update of \( \zeta \) at iteration \( t \) is

\[
\zeta^{(t-\frac{1}{2})} = \zeta^{(t-1)} + \gamma_{\zeta,t} \left\{ \frac{\delta(1)(B(t))}{\pi^0}, \ldots, \frac{\delta_m(B(t))}{\pi^m} \right\}^T,
\]

(18)

where \( \gamma_{\zeta,t} \), the first element of \( \zeta^{(t)} \), is set to 0 by (18), and \( \gamma_{\zeta,t} \) is the learning rate of \( \zeta \) (see Section 5.1), and \( \delta_l(B(t)) \) is the proportion of dimension \( l \) appearing in \( B(t) \):

\[
\delta_l(B(t)) = \frac{1}{K} \sum_{(j,x^j) \in B(t)} \mathbf{1}_{l=1}(j = l).
\]

We summarize the augmented SA in Fig.1. At the beginning (Step 1), we set \( \lambda \) as a zero vector and we can calculate the true normalizing constants because \( q(j, x^j; \lambda, \zeta) \) is a uniform distribution. At each iteration, we first generate \( K \) observations by the trans-dimensional mixture sampling described in Section 4.3 (Step 3 to 8), and then update the parameters \( \lambda \) and \( \log \) ratios of normalizing constants \( \zeta \) (Step 9 and 10).

4.3 Trans-dimensional mixture sampling

We describe a trans-dimensional mixture sampling algorithm to simulate from the joint distribution \( q(j, x^j; \lambda, \zeta) \) (12), which is used with \( \lambda(\cdot), \zeta(\cdot) = (\lambda^{(t-1)}, \zeta^{(t-1)}) \) at time \( t \) for MCMC sampling in AugSA (Fig.1). The name “mixture sampling” reflects the fact that \( q(j, x^j; \lambda, \zeta) \) represents a labeled mixture [29], because \( j \) is a label indicating that \( x^j \) is associated with the distribution \( p_j(x^j; \lambda) \). With fixed \( \lambda, \zeta \), this sampling algorithm can be seen as formally equivalent to reversible jump MCMC [30], which was originally proposed for Bayes model determination.

The trans-dimensional mixture sampling algorithm consists of two steps at each time \( t \): local jump between dimensions and Markov move of observations for a given dimension. In the following, we denote by \( j^{(t-1)} \) and \( x^{(t-1)} \) the dimension and observation before the current sampling, but use the short notation \( (\lambda, \zeta) \) for \((\lambda^{(t-1)}, \zeta^{(t-1)})\).

Step 1: Local jump. The Metropolis-Hastings method is used in this step to sample the dimension. Assuming \( j^{(t-1)} = k \), first we draw a new dimension \( j \sim \Gamma(k, \cdot) \). The jump distribution \( \Gamma(k, j) \), is defined as uniform in the neighborhood of \( k \):

\[
\Gamma(k, j) = \begin{cases} 1/3 & \text{if } k \in [2, m-1], j \in [k-1, k+1] \\ 1/2 & \text{if } k = 1, j \in [1, 2] \text{ or } k = m, j \in [m-1, m] \\ 0 & \text{otherwise} \end{cases}
\]

(19)

where \( m \) is the maximum dimension. Eq. (19) restricts the difference between \( j \) and \( k \) to be no more than one. If \( j = k \), we retain the observation \( x^{(t-1)} \) and perform the next step directly, i.e., set \( j^{(t)} = k \) and \( x^{(t)} = x^{(t-1)} \). If \( j = k + 1 \) or \( j = k - 1 \), the two cases are processed differently.

If \( j = k + 1 \), first we draw an element \( u \) from a proposal distribution: \( u \sim \Gamma_{k+1-1}(x^{(t-1)}) \). Then we set \( j^{(t)} = j \) (\( = k + 1 \)) and \( x^{(t)} = \{x^{(t-1)}, u\} \) with probability

\[
\begin{align*}
1 & \text{if } \Gamma(k, j) \frac{q(j, x^{(t-1)}, \lambda, \zeta)}{\Gamma(k, j) q(k, x^{(t-1)}; \lambda, \zeta) g_{k+1}(u|x^{(t-1)})}, \\
0 & \text{otherwise}
\end{align*}
\]

(20)

where \( \{x^{(t-1)}, u\} \) denotes a vector with dimension \( k + 1 \) whose first \( k \) elements are \( x^{(t-1)} \) and the last element is \( u \).
If \( j = k - 1 \), we set \( x^{(t)} = j ( = k - 1 ) \) and \( x^{(t)} = x^{(t-1)}_{1:k-1} \) with probability
\[
\left\{ \begin{array}{ll}
\Gamma(j, k) q(j, x^{(t-1)}_{1:j}; \lambda, \zeta) g_k(x^{(t-1)}_{j+1}) q(x^{(t-1)}_{j+1}; \lambda, \zeta) \\
\Gamma(k, j) q(x^{(t-1)}_{1:j}; \lambda, \zeta)
\end{array} \right. , \tag{21}
\]
where \( x^{(t-1)}_{j+1} \) is the first \( j \) elements of \( x^{(t-1)} \) and \( x^{(t-1)}_{k} \) is the \( k \)th element of \( x^{(t-1)} \).

In (20) and (21), \( g_{k+1} (u|x^{k}) \) can be flexibly specified as a proper density function in \( u \). In our application, we find the following choice works reasonably well:
\[
g_{k+1} (u|x^{k}) = \frac{q(k + 1, \{ x^{k}, u \}; \lambda, \zeta)}{\sum_{w} q(k + 1, \{ x^{k}, w \}; \lambda, \zeta)}. \tag{22}
\]
where \( x^{k} \) is a vector of dimension \( k \), e.g. \( x^{k} = x^{(t-1)} \) in (20) and \( x^{k-1} = x^{(t-1)}_{1:j} \) in (21). In our experiments, the acceptance rate of local jumps is around 30%, suggesting that good mixing is achieved by the jump process.

**Step II: Markov move.** After the step of local jump, we obtain
\[
x^{(t)} = \left\{ \begin{array}{ll}
x^{(t-1)} & \text{if } j^{(t)} = k \\
x^{(t-1)}, u & \text{if } j^{(t)} = k + 1 \\
x^{(t-1)}_{1:k-1} & \text{if } j^{(t)} = k - 1
\end{array} \right. \tag{23}
\]
Then we perform (for example) Gibbs sampling on \( x^{(t)} \), from the first element to the last element. The pseudo-code of trans-dimensional mixture sampling is shown in Algorithm 1 in Tab.1.

## 5 Algorithm optimization

The augmented SA algorithm may still suffer from slow convergence, especially when \( \lambda \) is high-dimensional. In this section, we introduce several statistical and computational techniques to improve the convergence of the augmented SA algorithm and reduce the computational cost.

### 5.1 Learning rates

As mentioned in Section 4.2, setting \( \gamma \ell = O(t^{-1}) \) can achieve asymptotic convergence of the SA algorithm. In practice, to accelerate the initial convergence and improve stability, we introduce a two-stage configuration of the learning rates, following the suggestion of [28] and [29].

We set the learning rates as
\[
\gamma_{\lambda, t} = \left\{ \begin{array}{ll}
t_c + t^\beta \lambda^{-1} & \text{if } t \leq t_0 \\
t_c + t - t_0 + t_0^\beta \lambda^{-1} & \text{if } t > t_0,
\end{array} \right. \tag{24}
\]
\[
\gamma^c, t = \left\{ \begin{array}{ll}
t - \beta \lambda & \text{if } t \leq t_0 \\
t - t_0 + t_0^\beta \lambda^{-1} & \text{if } t > t_0,
\end{array} \right. \tag{25}
\]
where \( 0.5 < \beta, \beta^c < 1 \), \( t_0 \) is an burn-in size, and \( t_c \) is an offset constant for the learning rate of \( \lambda \). These choices are simpler than in our previous work [21] primarily because a different technique for rescaling SA update in \( \lambda \) is used (see Section 5.2). In the first stage \( (t \leq t_0) \), a slow-decaying rate of \( t^{-\beta} \) is used to introduce large adjustments for \( 0.5 < \beta < 1 \). This forces the estimates \( \lambda^{(t)} \) and \( c^{(t)} \) to fall reasonably fast to near the true values. In the second stage \( (t > t_0) \), a fast-decaying rate of \( t^{-1} \) is used according to asymptotic theory of SA. The offset \( t_c \) is introduced to avoid the learning rate of \( \lambda \) being too large in the first several SA iterations. Typically, \( t_0 \) is selected to ensure that there is no more significant adjustment of the log-likelihood observed on the development set in the first stage.

**5.2 Rescaling SA update in \( \lambda \)**

In (16), we introduce a diagonal matrix \( \sigma \) to rescale the update direction for \( \lambda \). Here we discuss the rationale for this technique.

For simplicity, consider (13) with only \( \lambda \) unknown and \( \zeta = \zeta^* (\lambda) \), which leads back to (6) and can be expressed in the form of \( h(\lambda) = 0 \) with
\[
h(\lambda) = \hat{p}[f] - p_{\lambda}[f] = \hat{p}[f] - \sum_{j=1}^{m} \frac{n_j}{n} p_{\lambda,j}[f].
\]
As mentioned in Section 4.2, the optimal gain matrix \( A \) should be \( A^{-1} = -\partial h(\lambda^*) / \partial \lambda \). By direct calculation, we find
\[
C(\lambda) = -\frac{\partial h(\lambda)}{\partial \lambda} = \sum_{j=1}^{m} \pi_j \{p_{\lambda,j}[f f^T] - p_{\lambda,j}[f] p_{\lambda,j}[f]^T\},
\]
where \( p_{\lambda,j}[f f^T] = \sum_{x \in X_j} p_j(x_j^j; \lambda) f(x_j^j) f(x_j^j)^T \). In general, \( C(\lambda^*) \) is unknown and needs to be approximated. One method is to estimate \( C(\lambda^*) \) along with \( \lambda^* \) by stochastic approximation [28], as used in our previous paper [21]. In this method, the diagonal elements of matrix \( C(\lambda^*) \) are estimated concurrently with \( \lambda^* \) during SA iterations and a threshold is introduced to censor the estimates from below\(^6\). Alternatively, we propose the use of empirical variances to approximate \( C(\lambda^*) \). In fact, the empirical stratified covariance matrix is
\[
\tilde{C} = \sum_{j=1}^{m} \frac{n_j}{n} \{ \tilde{p}_j[f f^T] - \tilde{p}_j[f] \tilde{p}_j[f]^T \},
\]
where \( \tilde{p}_j[f f^T] = \frac{n_j}{n} \sum_{x \in D_j} f(x_j^j; \lambda^*) f(x_j^j) f(x_j^j)^T \). If the fitted distribution \( p(j, x^j; \lambda^*) \) is close to the empirical distribution \( \hat{p}(j, x^j) \), then \( \tilde{C} \) provides a reasonable approximation of \( C(\lambda^*) \). Taking the diagonal elements of \( \tilde{C} \) yields the diagonal matrix \( \sigma \) used to obtain the update (16) for \( \lambda \).

The use of empirical variances to rescale the gradient can also be understood from another perspective. For training log-linear models, it has been shown that the convergence of gradient-based

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\(^6\) In our previous paper [21], only about 20% of the components of \( \lambda \) are larger than the threshold \( 10^{-4} \).
optimization algorithms can be accelerated by normalizing the means and variances of features [33]. In fact, the update (16) can be equivalently expressed as
\[
\sigma^{1/2} \lambda(t) = \sigma^{1/2} \lambda(t-1) + \gamma_{\lambda,t} \left\{ \tilde{p}[g] \frac{1}{K} \sum_{(j,x^t) \in B(t)} \pi_j g(x^t) \right\},
\]
where \( g(x^t) = \sigma^{-1/2} f(x^t) \) is the normalized feature vector such that the variances of individual features are 1 and \( \sigma^{1/2} \lambda \) is the corresponding parameter vector for \( g \).

Compared with estimating \( C(\lambda^t) \) concurrently with \( \lambda^t \) during SA iterations in our previous work [21], using empirical variances to rescale the update direction for \( \lambda \) has two advantages. First, memory cost and computational time are reduced, because \( \sigma \) can be calculated offline for one time. Second, the empirical variances \( \sigma_j \) can be censored from below by a very small threshold, so that almost all of the components of \( \lambda \) can be updated without modification of the empirical variances. In our experiments, the threshold is \( 10^{-15} \) and 99.5% of the components of \( \lambda \) are updated with non-censored empirical variances. This technique is found to improve the convergence of the SA training algorithm, as shown in Fig.2. It is worthwhile to compare our method with related adaptive stepsize optimisers, such as Adam [22] and RMSProp [34]. They also scale the gradient with curvature information but by applying different preconditioners. As shown in Fig.2, our method of preconditioning using the empirical variances of features in our language modeling experiments shows better convergence than Adam which uses a running average of squared gradients for preconditioning.

### 5.3 Dimension probabilities \( \pi^0 \)

Compared with our previous work [21], another new aspect of the augmented SA algorithm is to allow the dimension probabilities \( \pi^0_j \) used in the trans-dimensional mixture sampling to differ from the empirical dimension probabilities \( \pi_j = n_j/n \), in order to overcome limitations caused by setting \( \pi^0_j = \pi_j \). The sample size \( n_j \) from the training set may be zero for some \( j \), in which case the augmented SA algorithm will fail with \( \pi^0_j = 0 \) because \( \zeta_j \) will not be updated without any observation of dimension \( j \) sampled. Moreover, when \( \pi^0_j \) is too small for some \( j \), the estimation of \( \zeta_j \) would become problematic because the update scheme (17) involves dividing a fraction \( \delta_j(B(t)) \) by \( \pi^0_j \).

For illustration, imagine that \( \pi^0_j = 10^{-5} \) for some \( j \), and \( K = 300 \) observations are drawn at each iteration. If the dimension \( j \) appears at least once in sample set \( B(t) \), then \( \delta_j(B(t)) \geq 1/300 \). Then the update to \( \zeta_j \) will be at least \( 300^{-1}/10^{-5} = 1000/3 \) in (17) (ignoring the learning rate \( \gamma_{\zeta,t} \)), which can be much larger than the true value of \( \zeta_j \). Moreover, if \( j = 1 \), this will influence the updates of all \( (\zeta_2, \ldots, \zeta_m) \) in (18). To prevent such heavy fluctuations, we need to avoid setting \( \pi^0_j \) too small and particularly to set \( \pi^0_j \) reasonable large.

In our experiments, we set
\[
\pi^0_j = \frac{\max\{u_j, c\}}{\sum_{j=1}^{m} \max\{u_j, c\}}, \quad (26)
\]
where \( c \) is a constant (set to \( 10^{-5} \) in our experiments), and
\[
u_j = \begin{cases} \dfrac{n_{\max}}{n_j}, & \text{if } j \leq j_{\max} \\ \dfrac{n_j}{n_{\max}}, & \text{if } j > j_{\max} \end{cases}
\]
with \( n_{\max} = \max_j n_j \) and \( j_{\max} = \arg \max_j n_j \). The motivation for introducing \( u_j \) above is to make \( \pi^0_j \) large for \( j = 1 \) and for subsequent dimensions \( j \), because the trans-dimensional mixture sampling algorithm (Tab.1) only permits a dimension jump from \( j \) to \( j \pm 1 \). In the experiments, we find that this choice of the dimension probabilities \( \pi^0_j \) helps to considerably improve the accuracy in the estimation of \( \zeta \).
5.4 Modeling rare high-dimensional observations

Compared with our previous work [21], we propose still another technique to deal with rare very high-dimensional observations (e.g., rare very long sequences), which are often found in large datasets. For example, the maximum sentence length in Google 1-billion word corpus [35] is more than 1000, but the percentage of sentences longer than 100 is about 0.2% in the datasets used in our experiments (Section 8). To reduce the number of sub-models corresponding to different dimensions, we set the near maximum dimension \( m \) to a medium value (such as 100) and modify the joint distribution (8) by introducing a special sub-model that captures all the sequences longer than \( m \) as follows:

\[
p(j, x^j; \lambda, \zeta) \propto \frac{n_{m+}^j}{\sum j > m} e^{\zeta^T f(x^j)}, \quad j > m,
\]

where \( \zeta = (\zeta_1, \ldots, \zeta_m, \zeta_{m+})^T \) with \( \zeta_k = 0 \) and \( n_{m+} \) is the number of the sequences longer than \( m \) in the training set. A single log ratio of normalizing constants \( \zeta_{m+} \) is used such that model (27) can be seen as model (1) but only for sequences longer than \( m \). The augmented SA algorithm can be extended with simple modifications. The maximum dimension in trans-dimensional mixture sampling (Tab.1) is set to be slightly larger than \( m \) (specifically \( m + 2 \) in our experiments). Then \( \lambda \) is still updated by (16), with \( (j, x^j) \in B^{(t)} \) for both \( j = 1, \ldots, m \) and \( j > m \). Both \( \zeta_1, \ldots, \zeta_m \) and \( \zeta_{m+} \) are updated by (17) and (18), where \( \delta_{m+}(B^{(t)}) = K^{-1} \sum_{(j,x^j) \in B^{(t)}} 1(j > m) \) is the proportion of dimensions greater than \( m \) in the sample \( B^{(t)} \).

6 APPLICATION: WORD MORPHOLOGY

In this section, we perform a pilot experiment — word morphology, to exactly evaluate the performance of TRF models and AugSA training algorithms. This is similar with the experiment in [4] but we provide detailed evaluations of performances, which includes studying the convergence of the log-likelihood using the true normalizing constants, comparing the estimated normalizing constants with the true ones, and comparing the IIS presented in [4] with our AugSA training algorithm.

The objective of word morphology is to model English words as character sequences by assigning probabilities. The training and test data are extracted from the English Gigaword dataset\(^7\). The training set contains 139K different English words. The test set contains other 15K different English words. The maximum word lengths in the training and test sets are 25 (i.e. \( m = 25 \)).

To construct a TRF model (2), we first extract all the character unigrams, bigrams and trigrams from the training set and define the following features:

\[
f_v(x^j) = \sum_{i=1}^j f_{i,v}(x^j),
\]

\[
f_{vw}(x^j) = \sum_{i=1}^{j-1} f_{i,vw}(x^j),
\]

\[
f_{vwy}(x^j) = \sum_{i=1}^{j-2} f_{i,vwy}(x^j),
\]

where \( x^j \) denotes the word containing \( j \) characters (\( x^1, \ldots, x^j \)), \( v, vw \) and \( vwy \) denote the character unigram, bigram and trigram observed in the training set, and \( f_{i,v}, f_{i,vw} \) and \( f_{i,vwy} \) are the corresponding unigram, bigram and trigram features evaluated at position \( i \):

\[
f_{i,v}(x^j) = \begin{cases} 1 & \text{if } x^j_i = v \\
0 & \text{otherwise}, \end{cases}
\]

\[
f_{i,vw}(x^j) = \begin{cases} 1 & \text{if } x^j_i = v \text{ and } x^j_{i+1} = w \\
0 & \text{otherwise}, \end{cases}
\]

\[
f_{i,vwy}(x^j) = \begin{cases} 1 & \text{if } x^j_i = v \text{ and } x^j_{i+1} = w \text{ and } x^j_{i+2} = y \\
0 & \text{otherwise}. \end{cases}
\]

The feature set contains \( f_v, f_{vw}, f_{vwy}, f_{i=0,v}, f_{i=end,v}, f_{i=0,vw}, \) and \( f_{i=end,vw} \), where \( f_{i=0,v} \) and \( f_{i=end,v} \) denote the unigram \( v \) appearing at the beginning and the end of a word; \( f_{i=0,vw} \) and \( f_{i=end,vw} \) denote the bigram \( vw \) appearing at the beginning and the end of a word\(^8\). The total feature number \( d = 11929 \). We perform the augmented SA (Algorithm 1 in Fig.1)\(^9\) to train the TRF model. At each iteration, a sample of \( K = 100 \) sequences (i.e. words) are generated by trans-dimensional mixture sampling (Section 4.3). We set \( \pi_0 = n_j/n \) (denoted by “\( n_j/n \)”, the red line in Fig.3(b)) to set \( \pi_0 \) as (26) (denoted by “\( \pi_0 \)”, the green line in Fig.3(b)) to study the effect of proper specification of length probabilities. The learning rates are set as (24) and (25) with \( \beta_c = 100, \beta_\lambda = 0.8, \beta_\zeta = 0.6, \tau_0 = 200 \). The maximum iteration number is fixed as \( t_{max} = 1000 \). The techniques introduced in Sections 5.4 and Appendices C–E are not used in this experiment.

We implement three existing methods. First is the \( n \)-gram model [6] widely used in language modeling. Here we view an English word as a character sequence and train a \( 3 \)-gram model by the Witten-Bell discounting smoothing method (denoted by WB3), using the SRILM toolkit\(^10\). This \( 3 \)-gram model contains the same set of features with the TRF models introduced above. Second, we apply the improved iterative scaling (IIS) method [4] to train the same TRF model. For comparison with our AugSA algorithms, at each iteration, we generate \( K = 100 \) words of random lengths\(^11\) to estimate the model expectations used in IIS. Third, as the expectation \( p_{\lambda}(f) \) can be calculated exactly in this pilot experiment, we apply the Quasi-Newton method to solve Eq. (6) for the TRF model (denoted by Quasi-Newton). This provides the exact result, relative to which different Monte Carlo training algorithms can be evaluated. For more complex TRFs as in language modeling in Sections 7–8, the Quasi-Newton method is infeasible because exact calculation of \( p_{\lambda}(f) \) is intractable.

To study the performances of different methods, we first plot in Fig.3(a) the scaled negative log-likelihood (NLL) curves, exactly calculated using the true normalizing constants associated with the parameter estimates during iterations by AugSA and IIS algorithms for TRF. The NLLs at the final parameter estimates by Quasi-Newton for TRF and by WB3 for \( n \)-gram are also shown as flat lines. Several interesting points can be drawn.

First, IIS (blue solid line) performs poorly in this experiment, with NLL diverging from the exact result (black dot line) obtained by Quasi-Newton. This may be due to an insufficient number of iterations (Fig.3(a)).

8. Introducing \( f_{i=0,v}, f_{i=end,v}, f_{i=0,vw}, f_{i=end,vw} \) is to make TRF models contain the same set of features as the \( 3 \)-gram model in [6] does.

9. In this experiment, there is no class information and there is no need to accelerate the sampling using Algorithm 2 in Fig.1 because the alphabet set \( A \) is very small (26 characters).


11. For sampling in IIS, we first draw length \( j \) with the empirical length probability \( n_j/n \). Then Gibbs sampling is performed to generate a sequence of length \( j \), initialized from the last sequence of the same length.
$(K=100)$ of draws used for the estimation of the expectation $p_A[f]$. In contrast, our AugSA algorithms (red solid and green solid lines) perform much better (with NLL converging steadily to the exact result), using the same number of draws per iteration as in IIS. Second, TRF models trained by AugSA algorithms yield lower NLL and hence outperform the WB3 model (red dot line), using the same set of features. Third, revising length probabilities $\pi_0^n$ from $n_j/n$ (red solid line) to (26) (blue solid line) appears to slightly slow the convergence of the log-likelihood. But such a revision leads to more accurate estimation of normalizing constants and hence of the log-likelihoods as discussed next. Reliable estimation of log-likelihoods for AugSA is important for monitoring the progress of training in practical situations where exact calculation of log-likelihoods is not feasible.

In Fig.3(c), we plot the NLL curves calculated using the true normalizing constants (solid lines) and the estimated ones (dashed lines) associated with the parameter estimates during iterations by AugSA algorithms. Setting $\pi_0^n$ as (26) yields more accurate estimation of the log-likelihoods: the green dash line is closer to the true NLL than the red dash line. In fact, using $\pi_0^n = n_j/n$ leads to systematic overestimation of NLL: the red dash line is always above the red solid line. In addition, Fig.3(d) shows that the log ratios of normalizing constants $\zeta(t)$ estimated by “AugSA($\pi_0$)” (green lines) are closer to the true $\zeta^*(t)$ than the $\zeta(t)$ estimated by “AugSA” (red lines) to $\zeta^*(t)$ at, for instance, iteration $t=100$ and 1000.
In this section, we apply TRF models for language modeling. We evaluate the performances of different LMs by perplexity \(^{13}\) (PPL) which is a widely used measure of a LM and by speech recognition word error rate (WER) which quantifies the usefulness of applying a LM in speech recognition. Compared with our previous work \cite{21}, the new results reported in this section mainly include: (1) introducing a novel feature type, the tied long-skip-bigram feature “tied” \cite{36}, which further demonstrates the flexibility of TRF modeling to use a richer set of features, (2) re-running the experiments with the newly developed techniques described in Sections 5.2, 5.3 and Appendix E to train TRF LMs, (3) obtaining AIS based estimates of normalizing constants for TRF models, and (4) providing comparisons with LSTM LMs in addition to \(n\)-gram and RNN LMs.

The training and development datasets are from the Wall Street Journal (WSJ) portion of Penn Treebank (PTB) corpus. In accordance with previous studies \cite{8}, sections 0-20 are used as the training data (about 930K words), sections 21-22 as the development data (74K words) and section 23-24 as the test data (82K). The vocabulary is limited to 10K words, with one special token \(\langle\text{UNK}\rangle\) denoting words not in the vocabulary. The baseline is \(n\)-gram LMs with modified Kneser-Ney smoothing \cite{6}, denoted by KNo, which are trained by the SRILM toolkits. We use the RNNLM toolkit \cite{20} to train the RNN LM; the number of hidden units is 250\(^{15}\). We use the open-source toolkit provided by \cite{20} to train the LSTM LM, which contains 2 hidden layers and each layer contains 250 units\(^{16}\). The hyperparameters are tuned to our best through a series of pilot experiments.

For our TRF models, we consider a variety of features as shown in Tab.2, mainly based on word and class information. Each word is deterministically assigned to a single class, by running the automatic clustering algorithm proposed in \cite{37} on the training dataset. In Tab.2, \(w_i,c_i,i = 0,1,\ldots,-5\) denote the word and its class at different position offset \(i\), e.g. \(w_0,c_0\) denotes the current word and its class. The word/class \(n\)-gram features \(“w_i”/“c_i”\), skipping \(n\)-gram features \(“ws_i”/“cs_i”\) \cite{38}, higher-order skipping features \(“wsh”/“csh”\), and the crossing features \(“cpw”\) (meaning class-predict-words) are introduced in \cite{21}. In this paper, we further introduce the tied long-skip-bigram features “tied” \cite{36}, in which the skip-bigrams with skipping distances from 6 to 9 share the same parameter. In this way we can leverage long distance contexts without increasing the model size. Note that all the features \(f(x)\) in model (2) are constructed from Tab.2 in a position-independent and dimension-independent manner, and only the features observed in the training data are used.

The AugSA (Algorithm 2 in Fig.1) is used to train the TRF models. The maximum lengths of sentences in the training, development and test sets are 82, which is not very large. Hence the technique described in Section 5.4 is not needed. All the other techniques described in Section 5 are applied to train TRF LMs. At each iteration, we generate a sample of \(K = 300\) sentences of lengths ranging from 1 to 82 (i.e. \(m = 82\)). The learning rates \(\gamma_c\) and \(\gamma_\Omega\) are configured as (24) and (25) respectively with \(t_e = 3000, \beta_\Lambda = 0.8, \beta_\Omega = 0.6\) and \(t_0 = 2000\). The length probabilities \(n^0\) are set as (26). We use the automatic stop decision described in Appendix E, with the L2 regularization constant \(\mu = 4 \times 10^{-5}\) in (38). We calculate \(S_i\) with \(H = 100\) and stop iteration if \(S_i < 10^{-4}\). Eight CPU cores are used to parallelize the algorithm, as described in Appendix D. We also implement the IIS method for the language modeling experiments\(^{17}\). But the results are unsatisfactory, being similar to those in the word morphology experiment, and hence are not shown.

For evaluations in terms of speech recognition WERs, various LMs obtained using PTB training and development datasets are used to re-score 1000-best lists from recognizing WSJ’92 test data (330 utterances). For each utterance, we obtain a 1000-best list of candidate sentences by the first-pass recognition using the Kaldi

<table>
<thead>
<tr>
<th>Type</th>
<th>Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>w</td>
<td>(\langle w_i \rangle )</td>
</tr>
<tr>
<td>c</td>
<td>(\langle c_i \rangle )</td>
</tr>
<tr>
<td>ws</td>
<td>(\langle w_{i+1} c_i \rangle )</td>
</tr>
<tr>
<td>cs</td>
<td>(\langle c_{i+1} w_i \rangle )</td>
</tr>
<tr>
<td>wsh</td>
<td>(\langle w_i w_{i+1} c_i \rangle )</td>
</tr>
<tr>
<td>csh</td>
<td>(\langle c_i c_{i+1} w_i \rangle )</td>
</tr>
<tr>
<td>cpw</td>
<td>(\langle c_i c_{i+1} w_{i+1} c_i \rangle )</td>
</tr>
<tr>
<td>tied</td>
<td>(\langle c_i c_{i+1} w_{i+1} c_{i+1} w_i \rangle )</td>
</tr>
</tbody>
</table>

Table 2: Feature definition in TRF LMs

<table>
<thead>
<tr>
<th>Model</th>
<th>WER (%)</th>
<th>NLL</th>
<th>PPL</th>
<th>#feat</th>
</tr>
</thead>
<tbody>
<tr>
<td>KNo</td>
<td>8.78</td>
<td>97.9</td>
<td>294.4</td>
<td>2.3</td>
</tr>
<tr>
<td>RNN</td>
<td>7.90</td>
<td>95.6</td>
<td>257.6</td>
<td>5.1</td>
</tr>
<tr>
<td>LSTM</td>
<td>7.87</td>
<td>98.6</td>
<td>306.3</td>
<td>6.0</td>
</tr>
</tbody>
</table>

Table 3: The WERs, NLLs and PPLs on the WSJ’92 test data. 10 TRF models are trained by 10 independent AugSA runs. The means \pm standard deviations are shown over the 10 TRFs, with four different estimates of the normalizing constants. In addition, the results for one of the 10 TRFs are shown. Sep Std/Sm AIS denotes Separate Standard/Smoothed AIS. “#feat” denotes the feature size (million).
图 4. 对于不同的方法估计的归一化常数。图中的 WER 是 1000 个最佳列表的 0.93%。

工具箱\(^\text{18}\)使用基于 DNN 的声学模型。Oracle WER 对于 1000 个最好的列表是 0.93%。

结果在 WSJ’92 测试集上显示在表 3。作为归一化常数的 TRF 模型被有效地估计到通过 \(\zeta_j\), 我们报告 PPLs 和 WERs 在超过 10 个独立 AugSA 培训运行。这些 TRF LM 不仅包括来自 KNN \(n\)-gram LM, RNN LM [8], LSTM LM [9] 和以前的结果 [21]\(^\text{19}\)的中间分布，大约花费 24 小时（每个 TRF 并行化）。

首先，我们分别向 TRF LM 添加了神经网络 LM。通过特征的重采样增强变换，这可能是对神经网络 LM 代价昂贵的。结果证明 TRF LM 的 WER 通常为 7.90, 它在 KN5 LM 上具有 10% 的相对降低。这结果接近于 RNN LM 和 LSTM LM, 显示出一定程度的差异。

第二，我们发现 TRF LM 对于神经网络 LM 是补充性的，通过模型的插值。序列的对数概率从两个模型的对数线性结合与插值权重 \(0 < \alpha < 1\) 和 \(1 - \alpha\) 分别。插值 TRF 和 LSTM LM (LSTM+TRF) 产生最低的 WER。数值上，相对的降低是 13.6% 比 KN5 LM，3.2% 比单个 LSTM LM。

第三，训练成本，单次运行训练时间的 TRF, RNN 和 LSTM 是 20 小时在 CPU, 25 小时在 GPU 和 1 小时在 GPU 分别。对于测试成本，考虑到神经网络 LM, TRF 模型是计算上更有效的。使用神经网络 LM 的计算概率，在单个句子中效率是充足的，通过用于每个句子的特征进行激活。

神经网络 LM 由于在输出层的昂贵 softmax 计算而受益。根据实验，平均的计算成本对于重新排名的 1000 个长的句子列表是 0.16 秒，40 秒和 10 秒，基于 TRF (使用 CPU)，RNN (使用 CPU) 和 LSTM (使用 GPU) 分别。

在我们的实验中，RNN 和 LSTM 使用 softmax 版本而不需要用类的 softmax 来提高准确性 [8]。根据最近一篇论文 [40], 一个先进的实现可以实现一个速度从 2 到 10 倍, 但是仍然会更慢。第四个作为编审, 我们使用 AIS 方法来重新估计常数的 10 TRFs 中所有常数。有两个方法。

对于第一方法, 一个 AIS 运行估计常数增加 10 的 TRFs。当 WERs 接近于 24 小时（并行化）的计算长度和结果。由于独立 AIS 运行，有较大的振荡在标准 AIS 估计不同长度，如图 4 (红线曲线)。结果证明回归在对数 AIS 估计 33 句子长度来获得平滑的估计常数。要优化这个缺陷, 我们使用 AIS 在每个 TRF 中估计常数的常数。这种方法，称为“Global AIS”，用于估计为每个 TRF 的全球正常化常数 (24 小时的计算成本用于每个 TRF)。而在某些情况下，AugSA 和 AIS 估计的常数，这通常是有效的。

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在本节，我们展示了 TRF LM 与 AugSA 培训算法来处理数千万的特征。

实验步骤：语言模型的训练数据量高达 32 亿词

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实验步骤：语言模型的训练数据量高达 32 亿词

在这个部分，展示了 TRF LM 与 AugSA 培训算法来处理数千万的特征。
The perplexities (PPL) of various LMs with different sizes of training data (8M, 16M, 32M) from Google 1-billion word corpus. The cutoff settings of n-gram LMs are 0002 (KN4), 00002 (KN5) and 000002 (KN6). The RNN [8] and LSTM [20] are configured the same as in the PTB experiment, except RNN uses 200 classes. The feature type of TRF is “w+c+ws+cs+wsh+csh+tied”. “#feat” is the feature size (million).

<table>
<thead>
<tr>
<th>models</th>
<th>PPL</th>
<th>8M #feat</th>
<th>16M #feat</th>
<th>32M #feat</th>
</tr>
</thead>
<tbody>
<tr>
<td>KN5</td>
<td>128</td>
<td>18.1</td>
<td>112</td>
<td>33.6</td>
</tr>
<tr>
<td>RNN</td>
<td>110</td>
<td>9.0</td>
<td>99</td>
<td>9.0</td>
</tr>
<tr>
<td>LSTM</td>
<td>82</td>
<td>9.9</td>
<td>73</td>
<td>9.9</td>
</tr>
<tr>
<td>TRF</td>
<td>~110</td>
<td>17.5</td>
<td>~98</td>
<td>29.2</td>
</tr>
</tbody>
</table>

The WERs on WSJ’92 test set, continuing from Tab.4. The interpolation weight $\alpha$ is tuned from 0.1 to 0.9 per 0.1.

<table>
<thead>
<tr>
<th>models</th>
<th>8M</th>
<th>16M</th>
<th>32M</th>
</tr>
</thead>
<tbody>
<tr>
<td>KN5</td>
<td>8.24</td>
<td>8.26</td>
<td>7.66</td>
</tr>
<tr>
<td>RNN</td>
<td>7.47</td>
<td>7.73</td>
<td>7.73</td>
</tr>
<tr>
<td>LSTM</td>
<td>7.19</td>
<td>6.88</td>
<td>6.69</td>
</tr>
<tr>
<td>TRF</td>
<td>7.08</td>
<td>7.17</td>
<td>7.10</td>
</tr>
<tr>
<td>RNN+KN5</td>
<td>7.60</td>
<td>7.66</td>
<td>7.43</td>
</tr>
<tr>
<td>LSTM+KN5</td>
<td>7.14</td>
<td>6.82</td>
<td>6.59</td>
</tr>
<tr>
<td>RNN+TRF</td>
<td>7.08</td>
<td>7.27</td>
<td>6.93</td>
</tr>
<tr>
<td>LSTM+TRF</td>
<td>6.76</td>
<td>6.72</td>
<td>6.33</td>
</tr>
</tbody>
</table>

9 Conclusion and Future Directions

The undirected graphical modeling approach is rarely used to describe trans-dimensional observations but has its own merits: being more natural for domains where fixing the directions of edges is awkward, being computationally more efficient in computing data probabilities by avoiding local normalization, and being able to flexibly integrate a richer set of features. In this paper, we investigate building RF models for trans-dimensional observations and make the following contributions. (1) We propose the TRF model and develop the AugSA training algorithm, which jointly estimates the model parameters and normalizing constants while using trans-dimensional mixture sampling. (2) Several statistical and computational innovations are introduced to improve the training convergence and reduce computational cost, which together enable us to successfully train TRF models on large datasets. (3) The new TRF model and AugSA training algorithm are thoroughly evaluated. The superiority of the TRF approach is demonstrated in language modeling experiments. The TRF models obtained significantly outperform the classic n-gram LMs and perform competitive with NN LMs but being much faster in calculating sentence probabilities.

There are various worthwhile directions for future research. First, the TRF approach will hopefully open a new door to language modeling in addition to the dominant conditional approach, as once envisioned in [5]. Apart from its success in language modeling, the TRF approach can also be applied to other sequential and trans-dimensional data modeling tasks in general. Second, although this work models trans-dimensional observation using the log-linear form and without hidden variables, it is an important direction of extending TRF models to introduce non-linear features (e.g. implemented by NNs) and hidden variables to further enhance their representational power. Third, another important line of extension arises by applying the TRF approach to discriminative modeling, even though we are mainly concerned with generative modeling of trans-dimensional data in this work. The conditional distributions over labels given the observations in CRFs can be described by TRFs so that higher-order interactions among labels can be utilized. Finally, to facilitate future studies along the TRF approach, we have released an open-source TRF toolkit23, which contains the code and scripts to reproduce the results in this paper.

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References


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