Truncated Variational Expectation Maximization

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Abstract

We derive a novel variational expectation maximization approach based on truncated variational distributions. Truncated distributions are proportional to exact posteriors within a subset of a discrete state space and equal zero otherwise. The novel variational approach is realized by first generalizing the standard variational EM framework to include variational distributions with exact (‘hard’) zeros. A fully variational treatment of truncated distributions then allows for deriving novel and mathematically grounded results, which in turn can be used to formulate novel efficient algorithms to optimize the parameters of probabilistic generative models. We find the free energies which correspond to truncated distributions to be given by concise and efficiently computable expressions, while update equations for model parameters (M-steps) remain in their standard form. Furthermore, we obtain generic expressions for expectation values w.r.t. truncated distributions. Based on these observations, we show how efficient and easily applicable meta-algorithms can be formulated that guarantee a monotonic increase of the free energy. Example applications of the here derived framework provide novel theoretical results and learning procedures for latent variable models as well as mixture models including procedures to tightly couple sampling and variational optimization approaches. Furthermore, by considering a special case of truncated variational distributions, we can cleanly and fully embed the well-known ‘hard EM’ approaches into the variational EM framework, and we show that ‘hard EM’ (for models with discrete latents) provably optimizes a lower free energy bound of the data log-likelihood.

1 Introduction

The application of expectation maximization (EM; [Dempster et al., 1977]) is a standard approach to optimize the parameters of probabilistic data models. The EM meta-algorithm hereby seeks parameters that optimize the data likelihood given the data model and given a set of data points. Data models are typically defined based on directed acyclic graphs, which describe the data generation process using probabilistic descriptions of sets of hidden and observed variables and their interactions. EM approaches for most non-trivial such generative data models are intractable, however, and tractable approximations to EM are, therefore, very wide-spread. EM
approaches range from sampling-based approximations of expectation values and related non-parametric approaches (e.g. Ghahramani and Jordan, 1995), over maximum a-posteriori or ‘hard EM’ approaches (e.g. Juang and Rabiner, 1990; Celeux and Govaert, 1992; Olshausen and Field, 1996; Lee et al., 2007; Mairal et al., 2010), Laplace approximations (e.g. Kass and Steffey, 1989; Friston et al., 2007) to variational EM approaches (Saul et al., 1996; Neal and Hinton, 1998; Jordan et al., 1999; Opper and Winther, 2005; Seeger, 2008; and many more).

Instead of aiming at a direct maximization of the data likelihood, variational EM seeks to maximize a lower-bound of the likelihood: the variational free energy. Variational free energies can be formulated such that their optimization becomes tractable by avoiding the summation or integration over intractably large hidden state spaces. Since the framework of variational free energy approximations has first been explicitly introduced in Machine Learning (e.g. Saul et al., 1996; Neal and Hinton, 1998; Jordan et al., 1999), variational approximations for the EM meta-algorithm have been widely applied and were generalized in many different ways. Variational EM is now routinely used to train latent variable models (or multiple-causes) models, to train time-series models or to train complex graphical models including models for deep unsupervised learning (see, e.g. Jaakkola, 2000; Bishop, 2006; Murphy, 2012; Patel et al., 2016 for overviews).

Very prominent examples of variational EM are based on factored variational distributions (Jordan et al., 1999) or Gaussian variational distributions (e.g. Opper and Winther, 2005; Seeger, 2008; Opper and Archambeau, 2009). Truncated distributions were introduced later than factored or Gaussian approaches (Lücke and Sahani, 2008; Lücke and Eggert, 2010), and they used instead of a variational loop a sparsity assumption (Lücke and Sahani, 2008) or preselection of latent states (Lücke and Eggert, 2010; Sheikh et al., 2014; Dai and Lücke, 2014; Shelton et al., 2017).

Among approaches which are not considered variational are sampling based approximations (e.g. Zhou et al., 2009), or approaches which use just one state (the one with the approximate maximal posterior value) for the optimization of model parameters (Juang and Rabiner, 1990; Celeux and Govaert, 1992; Olshausen and Field, 1996; Allahverdyan and Galstyan, 2011; Van den Oord and Schrauwen, 2014). The latter is commonly referred to as ‘MAP training’ (Olshausen and Field, 1996; Allahverdyan and Galstyan, 2011), ‘hard EM’ (Poon and Domingos, 2011; Allahverdyan and Galstyan, 2011; Van den Oord and Schrauwen, 2014), ‘zero temperature EM’ (Turner and Sahani, 2011), as ‘classification EM’ (Celeux and Govaert, 1992) for mixture models, or as ‘Viterbi training’ for hidden Markov Models (Juang and Rabiner, 1990; Cohen and Smith, 2010; Allahverdyan and Galstyan, 2011). In deep learning, ‘hard EM’ was used, for instance, for generative formulations of convolutional neural networks (Patel et al., 2016), deep Gaussian Mixture Models (Van den Oord and Schrauwen, 2014), or Sum-Product Networks (Poon and Domingos, 2011). Note in this respect that also variational approximations (primarily factored ones) have been considered for (deep) graphical models, and deep models have been generalized to fully Bayesian settings (e.g. Attias, 2000; Jaakkola, 2000; Beal and Ghahramani, 2003). For the purposes of this study, we will introduce a novel variational EM approach assuming one set of observed and one set of hidden variables (without distinguishing subsets of these latents). Such a setup may suggest a bipartite graphical models with no further structure, i.e., a data model in which all hidden variables have the same form of influence on the observed variables (compare, e.g., Neal and Hinton, 1998). Such models are presumably best suited to follow the introduction of the basic ideas of the novel approach and to highlight its elementary properties. However, as
we will not make assumptions about the set of hidden variables, we here stress that the derived
results apply for any directed graphical model with discrete latents, i.e., application to more
intricate models including time-series models or deep directed models are straight-forward. The
same does not apply for generalizations to fully Bayesian settings, which would require a major
(and potentially very interesting) future research effort.

This paper summarizes the main result about the novel truncated variational EM (TV-EM)
approach in Sec. 2. The reader interested in applying the approach will find the required infor-
mation there and a partial and explicit form of the algorithm at the end of Sec. 5. In Sec. 3 we
first introduce standard variational EM (and Gaussian and factored variational distributions).
The introduction of the standard framework serves (A) for highlighting the differences between
truncated approaches and standard approaches, and (B) will be required to point out where we
have generalized to non-standard variational distributions. Sec. 4 formally shows that truncated
distributions can be treated as fully variational distributions by generalizing the standard free
energy framework to include distributions with exact zeros. Sec. 5 then derives the theoretical
results which are used to formulate TV-EM as a meta-algorithm. Sec. 6 presents example appli-
cations of the novel variational framework including its application to embed ‘hard EM’ into the
free energy framework. We conclude by discussing the results in Sec. 7.

2 Truncated Variational EM – Summary of the Algorithm

The theoretical results of Secs. 4 and 5 will allow for the formulation of novel variational EM
algorithms applicable to generative models with discrete latents, and for identifying existing
algorithms as variational approaches. All derivations of these later sections are required to obtain
the final results but the final result can be applied without detailed knowledge of the derivations’
details. We therefore summarize the main result in the following, and present the required
derivations and more details and variants later.

2.1 Problem Description and Notation

First we describe the problem addressed and the notation used. Following the framework of
Expectation Maximization (EM; [Dempster et al., 1977], our aim is to maximize the data likeli-
hood defined by a set of \(N\) data points, \(\{\tilde{y}^{(1)}, \ldots, \tilde{y}^{(N)}\}\), where we model the data distribution
by a probabilistic generative model whose distribution \(p(\tilde{y} | \Theta)\) is parameterized by the model
parameters \(\Theta\). We assume generative models with discrete hidden variables \(\tilde{s}\) and (discrete or
continuous) observed variables \(\tilde{y}\) such that the modeled data distribution is given by:

\[
p(\tilde{y} | \Theta) = \sum_{\tilde{s}} p(\tilde{y}, \tilde{s} | \Theta),
\]

where \(\sum_{\tilde{s}}\) goes over all possible values of \(\tilde{s}\). The data log-likelihood is then given by:

\[
\mathcal{L}(\Theta) = \log \left( p(\tilde{y}^{(1)}, \ldots, \tilde{y}^{(N)} | \Theta) \right) = \sum_{n=1}^{N} \log \left( \sum_{\tilde{s}} p(\tilde{y}^{(n)}, \tilde{s} | \Theta) \right).
\]
Expectation Maximization (EM; [Dempster et al., 1977]) is a very popular meta-algorithm that allows for optimizing the likelihood by iterating an E- and an M-step. In its most elementary form, the E-step consists of computing the posterior probability $p(\vec{s} | \vec{y}^{(n)}, \Theta)$ for each data point $\vec{y}^{(n)}$ and latent state $\vec{s}$, while the M-step updates the parameters $\Theta$ to increase the likelihood. The basic EM algorithm was generalized in a number of contributions to provide justification for incremental or online versions and, more importantly for this contribution, to provide the theoretical foundation of variational EM approximations (see, e.g., [Hathaway, 1986] Saul et al., 1996; Neal and Hinton, 1998).

2.2 Truncated Variational EM

The basic idea of truncated EM is the use of truncated posterior distributions as approximations to the full posteriors (e.g., Lücke and Eggert, 2010; Henniges et al., 2014; Dai and Lücke, 2014; Sheikh et al., 2014; Shelton et al., 2017). A truncated approximate posterior distribution is given by:

$$q^{(n)}(\vec{s}) := q^{(n)}(\vec{s}; \mathcal{K}, \Theta) = \frac{p(\vec{s}, \vec{y}^{(n)} | \Theta)}{\sum_{\vec{s}' \in \mathcal{K}^{(n)}} p(\vec{s'}, \vec{y}^{(n)} | \Theta)} \delta(\vec{s} \in \mathcal{K}^{(n)}),$$

where $\delta(\vec{s} \in \mathcal{K}^{(n)})$ is an indicator function, i.e., $\delta(\vec{s} \in \mathcal{K}^{(n)}) = 1$ if $\vec{s} \in \mathcal{K}^{(n)}$ and zero otherwise. Fig. 1 shows an illustration of a truncated posterior approximation. The set $\mathcal{K}^{(n)}$ contains a finite number of hidden states $\vec{s}$. There is one such set for each data point $n$, and we will denote with $\mathcal{K}$ the collection of all sets $\mathcal{K}^{(n)}$, i.e., $\mathcal{K} = \mathcal{K}^{(1:N)} = (\mathcal{K}^{(1)}, \ldots, \mathcal{K}^{(N)})$ (we will use the ‘colon’ notation to denote a range of indices throughout this paper). The expectation values w.r.t. truncated distributions are given by:

$$\langle g(\vec{s}) \rangle_{q^{(n)}} = \frac{\sum_{\vec{s} \in \mathcal{K}^{(n)}} p(\vec{s}, \vec{y}^{(n)} | \Theta) g(\vec{s})}{\sum_{\vec{s}' \in \mathcal{K}^{(n)}} p(\vec{s'}, \vec{y}^{(n)} | \Theta)},$$

where $g(\vec{s})$ can be any (well-behaved) function over latents $\vec{s}$. For sufficiently small sets $\mathcal{K}^{(n)}$, the expectation values (4) are computationally tractable if the joint distribution $p(\vec{s}, \vec{y}^{(n)} | \Theta)$ of a probabilistic generative model is efficiently computable. As for most directed graphical models the joint is indeed computational tractable, we will assume such tractability for the paper (unless stated otherwise).

The variational distributions (3) define, similar to other types of variational distributions, a free energy, which is given by:

$$\mathcal{F}(\mathcal{K}, \Theta^{\text{old}}, \Theta) = \sum_{n=1}^{N} \left[ \sum_{\vec{s}} q^{(n)}(\vec{s}; \mathcal{K}, \Theta^{\text{old}}) \log \left( p(\vec{s}, \vec{y}^{(n)} | \Theta) \right) \right] + H(q(\vec{s}; \mathcal{K}, \Theta^{\text{old}})),$$

where $H(q)$ is an entropy term in which $\Theta$ is held fixed at $\Theta^{\text{old}}$. 
Figure 1: Illustration of a truncated posterior approximation. Consider data in the form of images where each image can contain any combination of four patterns (‘cross’, ‘columns’, ‘triangle’, ‘circle’), see left-hand-side for the patterns. Each combination is denoted by a vector $\vec{s}$ with binary entries. Given a noisy image, the inference task is to assign to all $\vec{s}$ a probability value, with each value representing the probability that the image has been generated by a particular pattern combination. Probabilistic inference can be modeled using a suitable generative model for the data (which we will not further specify here). For the illustration we assume that the right model with the optimal parameters $\Theta$ has already been found. Given a data point $\vec{y}^{(n)}$ (upper right), the full posterior $p(\vec{s} | \vec{y}^{(n)}, \Theta)$ then realizes probabilistic inference using Bayes’ rule and the generative model. In the example, high probabilities are assigned to states $\vec{s}$ containing ‘columns’ and ‘triangle’. The ‘cross’ pattern is the least consistent with the data point, which results in low probabilities for any state containing a ‘cross’. A truncated approximation $q^{(n)}(\vec{s}; K, \Theta)$ is obtained using any subset $K^{(n)}$ of the states. In this example $K^{(n)}$ contains the three states with the highest probabilities (lower right), which is the optimal choice for $K^{(n)}$ given the constraint $|K^{(n)}| = 3$. The approximation quality for other truncated approximations strongly depends on the chosen set $K^{(n)}$. 

\[
\begin{bmatrix}
0 \\
1 \\
0
\end{bmatrix}, \begin{bmatrix}
0 \\
0 \\
1
\end{bmatrix}, \begin{bmatrix}
0 \\
1 \\
1
\end{bmatrix} \}
\]
For $\Theta^{\text{old}} = \Theta$ the free energy can be shown (see Sec. 5, Prop. 3) to take on a simplified form given by:

$$
F(K, \Theta) = F(K, \Theta, \Theta) = \sum_{n=1}^{N} \log \left( \sum_{\vec{s} \in K^{(n)}} p(\vec{s}, \vec{y}^{(n)} | \Theta) \right).
$$

The free energy (6) we will refer to as simplified truncated free energy or just truncated free energy. The truncated free energy is a lower bound of the log-likelihood (2) and it is provably monotonically increased by the following procedure:

$$
K^{\text{new}} = \arg \max_{K} \{ F(K, \Theta^{\text{old}}) \} \quad \text{TV-E-step (7)}
$$

$$
\Theta^{\text{new}} = \arg \max_{\Theta} \{ F(K^{\text{new}}, \Theta^{\text{old}}, \Theta) \} \quad \text{TV-M-step (8)}
$$

$$
\Theta^{\text{old}} = \Theta^{\text{new}} \quad \text{(9)}
$$

We will refer to one iteration of Eqns. (7) to (9) as a truncated variational EM (TV-EM) iteration. The repetition of TV-EM iterations until convergence of $\Theta$ monotonically increases the lower free energy bound (6) of the likelihood to at least local optima.

The optimization of $F(K, \Theta)$ w.r.t. $K$ has hereby to be taken as optimization for sets $K^{(n)}$ with limited size. Small $K^{(n)}$ of constrained size will ensure computational tractability as well as non-trivial solutions of (7). The $K^{(n)}$ can hereby be thought of as being all constraint to the same constant size, $|K^{(n)}| = \text{const}$ for all $n$, although the results which we will derive in this study will allow for other size constraints. For sufficiently small state sets $K^{(n)}$, the TV-E-step (7) is a constraint discrete optimization of a computationally tractable function, Eqn. 6. Furthermore, regarding the TV-M-step, any closed-form or gradient updates of $\Theta$ derived using (8) are in this case computationally tractable because the expectation values w.r.t. $q^{(n)}(\vec{s}; K, \Theta)$ are tractable according to Eqn. 4. For many standard generative models (e.g., sparse coding models, mixture models, hidden Markov models etc.) the M-steps are well-known and often derivable in closed-form. The TV-M-step (8) warrants that such M-step equations remain unchanged if TV-EM is applied – only the expectation values (which the M-steps depend on) have to be replaced by Eqn. 4. Like for other variational EM approximations, the variational E- and M-steps (Eqns. 7 and 8) can also be changed to just partially optimize the free energy, i.e., to increase instead of maximizing the free energy. For partial TV-E- and/or TV-M-steps the guarantee that the free energy monotonically increases does continue to hold (see Eqns. 50).

Eqns. 4 to 9 sufficiently summarize the TV-EM meta-algorithm such that it can directly be applied to a generative model with discrete latents. Sec. 5.3 reiterates the algorithm in a very explicit form which shows that the algorithm is formulated solely in terms of joint $p(\vec{y}, \vec{s} | \Theta)$ given by the generative model. In Sec. 6 we will discuss different realizations of concrete TV-EM algorithms. The reader interested in applying TV-EM may directly be referred to these sections.

We will now proceed and derive TV-EM (Eqns. 7 to 9 with Eqn. 6) step by step. All of the following derivations will be necessary to prove the properties of the TV-EM algorithm, and none of the Eqns. 6 to 9 will turn out to be trivial. This includes Eqns. 8 and 9 although they may seem straight-forward at first sight.
3 Related Work: Variational Approaches to Expectation Maximization

Before we formally introduce and derive truncated variational EM as a novel type of variational EM, we first discuss related work by first reviewing variational approximations in general, and by discussing their most wide-spread special cases and some recent developments. While most of this section reviews well-known as well as some recent results, we will later show that some of the central derivations which allow for using prominent variational approaches (such as Gaussian variational or factored variational approaches) can and have to be generalized for truncated distributions. Furthermore, reviews of the well-known variational approaches will facilitate the introduction of truncated variational EM and will allow to contrast its properties with these and other related approaches.

3.1 The Variational Free Energy Formulation

Following the establishment of EM as a standard tool for likelihood maximization (Dempster et al., 1977), its basic form was generalized to provide justification for incremental or online versions and, more importantly, to provide the theoretical foundation of variational EM approximations (see, e.g., Hathaway 1986; Saul et al. 1996; Neal and Hinton 1998). As it will be of importance further below, we here briefly recapitulate the derivation of the free energy in its standard textbook form (see, e.g., Saul et al., 1996; Murphy, 2012; Barber, 2012). For this recall Jensen’s inequality, which can for our purposes be denoted as follows: Let $f$, $g$ and $q$ be real-valued functions such that $g(\vec{s}), f(\vec{s}), q(\vec{s}) \in \mathbb{R}$ and let us denote the functions domain (the set of all possible states $\vec{s}$) by $\Omega$. For all $\vec{s} \in \Omega$ let $q(\vec{s})$ be a non-negative function that sums to one, i.e., $\sum_{\vec{s} \in \Omega} q(\vec{s}) = 1$. Then for any concave function $f$ the following inequality holds:

$$f\left(\sum_{\vec{s}} q(\vec{s}) g(\vec{s})\right) \geq \sum_{\vec{s}} q(\vec{s}) f(g(\vec{s})).$$

(10)

Note that $\sum_{\vec{s}}$ in (10) again denotes a summation over all states $\vec{s}$. Any distribution $q(\vec{s})$ on $\Omega$ satisfies the conditions on $q$ for Jensen’s inequality. If we additionally demand $q(\vec{s})$ to be strictly positive, i.e. $q(\vec{s}) > 0$ for all $\vec{s}$, we can apply Jensen’s inequality to the data likelihood (2) because the logarithm is a concave function. We obtain:

$$L(\Theta) = \sum_{n=1}^{N} \log \left( \sum_{\vec{s}} p(\vec{s}, \vec{y}^{(n)} | \Theta) \right) = \sum_{n=1}^{N} \log \left( \sum_{\vec{s}} q^{(n)}(\vec{s}) \frac{1}{q^{(n)}(\vec{s})} p(\vec{s}, \vec{y}^{(n)} | \Theta) \right) \geq \sum_{n=1}^{N} \sum_{\vec{s}} q^{(n)}(\vec{s}) \log \left( \frac{1}{q^{(n)}(\vec{s})} p(\vec{s}, \vec{y}^{(n)} | \Theta) \right) = \sum_{n=1}^{N} \left( \sum_{\vec{s}} q^{(n)}(\vec{s}) \log \left( p(\vec{s}, \vec{y}^{(n)} | \Theta) \right) - \sum_{\vec{s}} q^{(n)}(\vec{s}) \log \left( q^{(n)}(\vec{s}) \right) \right).$$

(11)

The crucial novel entity that emerges in this derivation is a lower bound of the likelihood which is termed the (variational) free energy (compare Saul and Jordan 1996; Neal and Hinton 1998).
\[ L(\Theta) \geq F(q, \Theta) := \sum_{n=1}^{N} \left( \sum_{\vec{s}} q^{(n)}(\vec{s}) \log p(\vec{s}, \vec{y}^{(n)} | \Theta) \right) + H(q), \]  

where \( H(q) = -\sum_{n} \sum_{\vec{s}} q^{(n)}(\vec{s}) \log q^{(n)}(\vec{s}) \) is a function (the Shannon entropy) that depends on the distribution \( q(\vec{s}) = q^{(1:N)}(\vec{s}) = (q^{(1)}(\vec{s}), \ldots, q^{(N)}(\vec{s})) \) but not on the model parameters \( \Theta \). Given a data point \( \vec{y}^{(n)} \), the distribution \( q^{(n)}(\vec{s}) \) is called a variational distribution. Also the collection of all distributions \( q(\vec{s}) \), with \( q(\vec{s}) = (q^{(1)}(\vec{s}), \ldots, q^{(N)}(\vec{s})) \), is referred to as variational distribution. The name ‘free energy’ was inherited from statistical physics where approximations to the Helmholtz free energy of a physical system take a very similar mathematical form (see, e.g., MacKay 2003).

A basic result for variational EM (e.g. Jordan et al., 1999; Neal and Hinton, 1998; MacKay, 2003; Murphy, 2012) is that the difference between the likelihood (2) and the free energy (12) is given by the Kullback-Leibler divergence between the variational distributions and the posterior distributions:

\[ L(\Theta) - F(q, \Theta) = \sum_{n} D_{\text{KL}}(q^{(n)}(\vec{s}), p(\vec{s} | \vec{y}^{(n)}, \Theta)) \geq 0, \]  

where \( D_{\text{KL}}(q, p) \) denotes the Kullback-Leibler (KL) divergence. Using (13) we observe that the free energy \( F(q, \Theta) \) is maximized if we choose (for all \( n \)) the posterior distribution as variational distribution:

\[ q^{(n)}(\vec{s}) := p(\vec{s} | \vec{y}^{(n)}, \Theta) = L(\Theta) = F(q, \Theta), \]  

which is the subject of Lemma 1 by Neal and Hinton (1998).

In the case of generative models with tractable posterior, Eqn.14 is used to maximize the likelihood (2) by iteratively maximizing the free energy (12) instead. Optimizing the latter is easier, as derivatives of the free energy can be taken while the parameters \( \Theta \) of the posterior distribution are held fixed. After maximizing \( F(q, \Theta) \) w.r.t. \( \Theta \) (the M-step), we can set \( q^{(n)}(\vec{s}) = p(\vec{s} | \vec{y}^{(n)}, \Theta^{\text{old}}) \) with \( \Theta^{\text{old}} = \Theta \) because this choice maximizes the free energy according to (14). Reiterating these well-know results will be of importance for truncated distributions later on.

Choosing \( q^{(n)}(\vec{s}) \) equal to the full posterior is sometimes referred to as exact EM. However, the computation of posterior distributions represents the crucial computational intractability for most generative data models: typically neither the posteriors nor expectation values w.r.t. them are computationally tractable as they require summations over all possible states \( \vec{s} \).

### 3.2 The Variational Approximation of EM

Overcoming the problem of computational intractability while maintaining an as good as possible approximation to the full posterior is the main motivation for variational approximations (and other approximation schemes). For variational EM the basic idea is to maximize the free energy \( F(q, \Theta) \) in (12) for a constrained class of variation distributions \( q \). If we can find variational distributions \( q \) such that
(A) optimization of $F(q, \Theta)$ is tractable, and
(B) such that the lower bound $F(q, \Theta)$ becomes as similar (as tight) as possible to $\mathcal{L}(\Theta)$,

then a tractable approximate optimization of $\mathcal{L}(\Theta)$ is obtained.

By definition of the free energy, almost no restrictions are imposed on the choice of the distributions $q$, such that they can, in principle, be chosen to take any functional form and to be dependent on any set of parameters. To fulfill requirement (A) some choice for a functional form of $q$ has to be made, however. As a consequence, the distributions $q^{(n)}(\mathbf{s})$ become equipped with additional parameters and these parameters are then optimized to make $F(q, \Theta)$ as tight as possible (requirement B). The variational distributions are then typically denoted by $q^{(n)}(\mathbf{s}; \Lambda)$ with the additional parameters $\Lambda$ being referred to as variational parameters. Having chosen a variational distribution, the free energy is often taken to depend on $\Lambda$ rather than on the variational distributions themselves, i.e., $F(\Lambda, \Theta)$.

Without being more specific about the choice of variational distributions and parameters, the iterative procedure to optimize the free energy may then be abstractly denoted by:

Opt 1 : $\Lambda^{\text{new}} = \arg\max_{\Lambda} F(\Lambda, \Theta^{\text{old}})$ while holding $\Theta^{\text{old}}$ fixed (V-E-step)

Opt 2 : $\Theta^{\text{new}} = \arg\max_{\Theta} F(\Lambda^{\text{new}}, \Theta)$ while holding $\Lambda^{\text{new}}$ fixed (V-M-step)

$\Theta^{\text{old}} = \Theta^{\text{new}}$

The two optimization steps are repeated until the parameters $\Theta$ have sufficiently converged.

In principle, many possible choices of variational distributions that fulfill requirements (A) and (B) are conceivable; and any choice would give rise to a variational EM procedure. Still, the application of variational EM has been dominated by two standard types of variational distributions: Gaussian variational distributions and factored variational distributions.

### 3.3 Gaussian and Factored Variational EM

As one of the most basic distributions is the Gaussian distribution, a natural choice for variational distributions (for continuous latents) is a multi-variate Gaussian:

$$q^{(n)}(\mathbf{s}) := q^{(n)}(\mathbf{s}; \Lambda) = q^{(n)}(\mathbf{s}; \mu^{(n)}, \Sigma^{(n)}) = \mathcal{N}(\mathbf{s}; \mu^{(n)}, \Sigma^{(n)}),$$  \hspace{1cm} (15)

where $\Lambda^{(n)} = (\mu^{(n)}, \Sigma^{(n)})$ and where $\Lambda = (\Lambda^{(1)}, \ldots, \Lambda^{(N)})$ is the set of all variational parameters (one mean and one covariance matrix per data point). The Gaussian variational approach approximates each posterior distribution by a Gaussian distribution. The optimization of the variational parameters in (15) results in update equations for mean and variance that maximize the free energy and minimize the KL-divergence between true posteriors and the variational Gaussians. Gaussian distributions are especially well suited for data models with mono-modal posteriors, and are consequently popular, e.g., for optimization of sparse linear models (e.g. Opper and Winther (2005), Seeger (2008), Opper and Archambeau (2009)). Gaussians can capture data correlations and jointly optimize mean and variance in the KL-divergence sense.
The second (and more predominant) standard variant of variational EM builds up on the choice of variational distributions that factor over sets of hidden variables. Most commonly the choice is a fully factored distribution:

$$q^{(n)}(\vec{s}) := q^{(n)}(\vec{s}; \Lambda) = \prod_{h=1}^{H} q_h(s_h; \overrightarrow{\lambda}_h^{(n)})$$

where $\overrightarrow{\lambda}_h^{(n)}$ are parameters associated with one hidden variable $h$ for one data point $n$, and where $\Lambda$ is the collection of all these parameters (all $h$ and $n$ combinations). Using factored distributions in combination with specific choices for the factors $q_h(s_h; \overrightarrow{\lambda}_h^{(n)})$ then results in computationally tractable optimizations. For the usual generative models the factors are often chosen to be identical to the prior distributions of the individual hidden variables (e.g. Jordan et al., 1999; Haft et al., 2004). Because of a mathematical analogy to variational free energy approximations in statistical physics (which initially motivated variational EM), fully factored variational approaches (16) are also frequently termed mean-field approximations.

### 3.4 Further Variational Optimization Approaches

Any variational distributions that contain fully factored or Gaussian distributions as special cases, can potentially improve on these standard distributions because they can make the free energy a tighter lower-bound. Generalizations of fully factored approaches can be defined by allowing for dependencies between small sets of variables (doubles, triples etc) resulting in partially factored approaches. Such approaches can potentially capture more complex posterior interdependencies (correlations and higher-order dependencies), and they are therefore also termed structured variational approaches or structured mean-field to highlight their close relation to fully factored approaches (compare Saul and Jordan, 1996; MacKay, 2003; Bouchard-Côté and Jordan, 2009; Murphy, 2012).

As factorized variational distributions (including structured ones) make potentially harmful assumptions (Ilin and Valpola, 2003; MacKay, 2003; Turner and Sahani, 2011; Sheikh et al., 2014) alternative distributions have continuously been investigated. Examples are ‘normalizing flow’ approaches for continuous latents (Rezende and Mohamed, 2015), or approaches that expand mean-field variational approaches hierarchically to include dependencies (Ranganath et al., 2015), or copula-based approaches (Tran et al., 2015). Such approaches use specific transformations of distributions to allow for modeling complex dependencies among latent variables for improved posterior approximations. We will briefly discuss the relation of these approaches to truncated variational EM in the context of ‘black box’ optimization in Sec. 7. Further work which generated recent attention (Hernandez-Lobato et al., 2016; Ranganath et al., 2016) considers generalizations of the original likelihood and free energy objectives (Eqns. 2 and 5). Also related in this context is work on variational approaches using stochastic variational inference (Hoffman et al., 2013), where auxiliary distributions for Markov chains are defined and used to approximate true posteriors. Generalizations of free energy objectives and stochastic variational inference can both be considered complementary lines of research to the results discussed in this work.
4 Truncated Variational Distributions

The introduction of Gaussian and factored variational distributions now provides the ground for the introduction of a novel class of variational distributions. In contrast to the prominent examples of variational EM, we will here neither assume monomodal variational distributions (like Gaussian variational EM) nor independent factors (like mean-field approaches). Furthermore, we will not choose a specific analytic function such as Gaussians or products of elementary distributions. Instead, we use the posterior distribution itself to define variational distributions. More precisely, we define the variational distributions to be proportional to the full posteriors. However, for any given data point \( \vec{y}^{(n)} \), the proportionality will be constrained to a subspace \( \mathcal{K}^{(n)} \) which will allow for computationally tractable procedures. States \( \vec{s} \) not in \( \mathcal{K}^{(n)} \) are assumed to have zero probability (‘hard’ zeros). Formally, such truncated distributions \( q^{(n)}(\vec{s}) = q^{(n)}(\vec{s}; \mathcal{K}, \Theta) \) are given by Eqn. 3.

Truncated distributions have been suggested previously and have successfully been applied to a number of elementary as well as more complex generative data models (Lücke and Eggert, 2010; Dai et al., 2013; Dai and Lücke, 2014; Sheikh et al., 2014; Sheikh and Lücke, 2016; Shelton et al., 2017). Instead of using a variational optimization of approximation parameters similar to Gaussian or mean-field approaches, truncated approximations have, so far, used preselection mechanisms to reduce the number of states evaluated for a truncated approximation (Lücke and Eggert, 2010). While truncated EM was shown to be very efficient in practice (Sheikh and Lücke, 2016; Hughes and Sudderth, 2016; Shelton et al., 2017), no fully variational treatment was provided, and no convergence guarantees and free energy results as they will be derived in this work, were given. We will later see, however, that preselection based truncated EM can be closely related to the fully variational framework developed here.

Having defined the variational distribution of (3), we can now seek to derive the corresponding free energy. However, by considering the standard derivation (11) which shows that the free energy is a lower bound of the likelihood, recall that we required the values of \( q^{(n)}(\vec{s}) \) to be strictly positive, \( q^{(n)}(\vec{s}) > 0 \) for all \( \vec{s} \). In order to embed truncated distributions (3) into the free energy framework, we therefore first have to generalize the free energy formalism to be applicable without the constraint of strict positivity. Such a generalization, which (to the knowledge of the authors) has not been investigated before, is required for our purposes but may be of more general use. As a fist step, we show that the following holds:

Proposition 1

Let \( q^{(n)}(\vec{s}) \) be variational distributions defined on a set of states \( \Omega \) (with values not necessarily greater zero), then a free energy function \( F(q, \Theta) \) exists and is given by:

\[
F(q, \Theta) := \sum_{n=1}^{N} \left( \sum_{\vec{s}} q^{(n)}(\vec{s}) \log \left( p(\vec{s}, \vec{y}^{(n)} | \Theta) \right) \right) + H(q). \tag{17}
\]

Proof

First let us (as was also done for Eqn. 17) drop the notation of variational parameters to increase readability. Then observe that the standard derivation (11) shows that the proposition is true if \( q^{(n)}(\vec{s}) > 0 \) for all \( \vec{s} \in \Omega \) and all \( n \). To show that (17) is true for any distribution, consider the
case of variational distributions \( q^{(n)}(\vec{s}) \) for which \( q^{(n)}(\vec{s}) > 0 \) is true only in proper subsets \( \mathcal{K}^{(n)} \) of the state space \( \Omega \), and equal to zero for all \( \vec{s} \notin \mathcal{K}^{(n)} \). For a given data point \( n \) a distribution is either \( q^{(n)}(\vec{s}) > 0 \) for all \( \vec{s} \) or there exists a proper subset \( \mathcal{K}^{(n)} \). In the latter case, it is trivial to define such a \( \mathcal{K}^{(n)} \), and as \( q^{(n)}(\vec{s}) \) is a distribution (i.e., sums to one), this implies that \( \mathcal{K}^{(n)} \) is not empty. For the main part of the proof we will now assume that for all \( n \) there exists a proper subset \( \mathcal{K}^{(n)} \) of \( \Omega \). A general \( q \) may consist of distributions \( q^{(n)}(\vec{s}) \) that are strictly positive for some \( n \) and have proper subsets \( \mathcal{K}^{(n)} \) for the other \( n \). However, addressing these mixed cases will turn out to be straightforward, and we will come back to this general case at the end of the proof.

Given a distribution \( q^{(n)}(\vec{s}) \) with set \( \mathcal{K}^{(n)} \), let us define an auxiliary function \( \tilde{q}^{(n)}(\vec{s}) \) as follows:

\[
\tilde{q}^{(n)}(\vec{s}) = \left\{ \begin{array}{ll}
q^{(n)}(\vec{s}) - \epsilon_n^- & \text{for all } \vec{s} \in \mathcal{K}^{(n)} \\
q^{(n)}(\vec{s}) + \epsilon_n^+ & \text{for all } \vec{s} \notin \mathcal{K}^{(n)}
\end{array} \right.
\]  

(18)

Let \( \epsilon_n^- \) be greater zero but smaller than any value of \( q^{(n)}(\vec{s}) \) in \( \mathcal{K}^{(n)} \), i.e.,

\[ 0 < \epsilon_n^- < \min_{\vec{s} \in \mathcal{K}^{(n)}} \{ q^{(n)}(\vec{s}) \} \quad \text{and let} \quad \epsilon_n^+ := \frac{|\mathcal{K}^{(n)}|}{|\Omega| - |\mathcal{K}^{(n)}|} \epsilon_n^- , \]

(19)

where \( |\mathcal{K}^{(n)}| \) is the number of states in \( \mathcal{K}^{(n)} \) and where \( |\Omega| \) is the number of all possible states. As we have defined \( \mathcal{K}^{(n)} \) to contain only values \( q^{(n)}(\vec{s}) > 0 \), the minimum in \( \mathcal{K}^{(n)} \) is greater zero, i.e., we can always find an \( \epsilon_n^- \) satisfying (19). Consequently, \( \epsilon_n^+ \) is also greater zero and finite as we demanded the \( \mathcal{K}^{(n)} \) to be proper subsets of \( \Omega \) (\( |\mathcal{K}^{(n)}| < |\Omega| \)).

With definitions (19) observe that \( \tilde{q}^{(n)}(\vec{s}) > 0 \) for all \( \vec{s} \) and that \( \sum_{\vec{s}} \tilde{q}(\vec{s}) = 1 \), i.e., \( \tilde{q}^{(n)}(\vec{s}) \) is a distribution on \( \Omega \) which satisfies (other than \( q^{(n)}(\vec{s}) \)) the requirement for the original derivation of the variational free energy (11). We can therefore use the free energy definition for \( \tilde{q}(\vec{s}) = (\tilde{q}^{(1)}(\vec{s}), \ldots, \tilde{q}^{(N)}(\vec{s})) \) and then consider the limit to small \( \epsilon_n^- \). For this, we insert the definition of \( \tilde{q}^{(n)}(\vec{s}) \) into the free energy and find:

\[
\mathcal{L}(\Theta) \geq \mathcal{F}(\tilde{q}, \Theta)
\]

\[
= \sum_n \left( \sum_{\vec{s}} \tilde{q}^{(n)}(\vec{s}) \log (p(\vec{s}, \vec{y}^{(n)}) | \Theta)) - \sum_{\vec{s}} \tilde{q}^{(n)}(\vec{s}) \log (\tilde{q}^{(n)}(\vec{s})) \right)
\]

\[
= \sum_n \left( \sum_{\vec{s} \in \mathcal{K}^{(n)}} \left( q^{(n)}(\vec{s}) - \epsilon_n^- \right) \log (p(\vec{s}, \vec{y}^{(n)}) | \Theta)) - \sum_{\vec{s} \notin \mathcal{K}^{(n)}} \left( q^{(n)}(\vec{s}) - \epsilon_n^- \right) \log (q^{(n)}(\vec{s}) - \epsilon_n^- ) \right)
\]

\[
+ \sum_{\vec{s} \notin \mathcal{K}^{(n)}} \left( q^{(n)}(\vec{s}) + \epsilon_n^+ \right) \log (p(\vec{s}, \vec{y}^{(n)}) | \Theta)) - \sum_{\vec{s} \notin \mathcal{K}^{(n)}} \left( q^{(n)}(\vec{s}) + \epsilon_n^+ \right) \log (q^{(n)}(\vec{s}) + \epsilon_n^+ ) \right)
\]

\[
= \sum_n \left( \sum_{\vec{s}} q^{(n)}(\vec{s}) \log (p(\vec{s}, \vec{y}^{(n)}) | \Theta)) - \epsilon_n^- \sum_{\vec{s} \in \mathcal{K}^{(n)}} \log (p(\vec{s}, \vec{y}^{(n)}) | \Theta)) + \epsilon_n^+ \sum_{\vec{s} \notin \mathcal{K}^{(n)}} \log (p(\vec{s}, \vec{y}^{(n)}) | \Theta))
\]

\[
- \sum_{\vec{s} \in \mathcal{K}^{(n)}} \left( q^{(n)}(\vec{s}) - \epsilon_n^- \right) \log (q^{(n)}(\vec{s}) - \epsilon_n^- ) - \epsilon_n^+ \log (\epsilon_n^+ ) \sum_{\vec{s} \notin \mathcal{K}^{(n)}} 1 \right)
\]
Then observe that the second summand of $F$ observe that in this case all summands of the last line of

Let us now consider infinitesimally small

with exact zeros for the other

where we have used (because of Eqn. 23) the convention

Thus, the limit

This expression applies for any $\epsilon_n$ satisfying (19) and therefore also if we replace:

such that we obtain:

Let us now consider infinitesimally small $\epsilon > 0$, i.e., let us consider the limit when $\epsilon \to 0$. First, observe that in this case all summands of the last line of $F(\bar{q}, \Theta)$ in (21) trivially converge to zero. Then observe that the second summand of $F(\bar{q}, \Theta)$ converges to

as $q^{(n)}(\bar{s})$ is finite and greater zero for all $\bar{s} \in \mathcal{K}^{(n)}$. Finally, the third summand in (21) can be observed to converge (following l'Hôpital) to zero:

Thus, the limit $\epsilon \to 0$ exists and is given by:

where we have used (because of Eqn. 23) the convention $q^{(n)}(\bar{s}) \log (q^{(n)}(\bar{s})) = 0$ for all $q^{(n)}(\bar{s}) = 0$. We will use this convention (which is also commonly used for the KL-divergence) throughout the paper.

Eqn. 24 shows that Proposition 1 holds for any $q$ with distributions $\epsilon^{(n)}(\bar{s})$ with proper subsets $\mathcal{K}^{(n)}$ of $\Omega$. To finally show that Proposition 1 holds for general $q$ (with discrete $\bar{s}$), consider the mixed case that $q$ contains strictly positive distributions $q^{(n)}$ for some $n$ and distributions $\epsilon^{(n)}$ with exact zeros for the other $n$’s. Let us define the set $J \subseteq \{1, \ldots, N\}$ to contain those $n$ with
which finally shows that Proposition 1 holds for any \( q \) that are not strictly positive. Using \( J \) and \( \bar{J} \) we then define an auxiliary function \( \bar{q} \) by using \( \bar{q}^{(n)}(\bar{s}) \) of Eqn. 18 only for \( n \in J \) and by setting \( \bar{q}^{(n)}(\bar{s}) = q^{(n)}(\bar{s}) \) for all \( \bar{s} \) for all \( n \in J \). The functions \( \bar{q}^{(n)} \) are then again strictly positive distributions on \( \Omega \) for all \( n \) and we can again apply the standard result 11:

\[
L(\Theta) \geq \mathcal{F}(\bar{q}, \Theta) = \sum_{n} \left( \sum_{s} \bar{q}^{(n)}(s) \log \left( p(s, \bar{y}^{(n)} | \Theta) \right) - \sum_{s} q^{(n)}(s) \log \left( \bar{q}^{(n)}(s) \right) \right)
\]

\[
= \sum_{n \in J} \left( \sum_{s} q^{(n)}(s) \log \left( p(s, \bar{y}^{(n)} | \Theta) \right) - \sum_{s} q^{(n)}(s) \log \left( q^{(n)}(s) \right) \right) \\
+ \lim_{\epsilon \to 0} \left( \sum_{n \in \bar{J}} \left( \sum_{s} \bar{q}^{(n)}(s) \log \left( p(s, \bar{y}^{(n)} | \Theta) \right) - \sum_{s} \bar{q}^{(n)}(s) \log \left( \bar{q}^{(n)}(s) \right) \right) \right)
\]

Now we apply the same arguments as above but only to the sum over all \( n \in J \), for which everything remains as for the derivation above. Eqn. 24 therefore applies if we only consider sums over \( J \). Thus in the limit \( \epsilon \to 0 \) we obtain in the mixed case:

\[
\mathcal{F}(q, \Theta) = \lim_{\epsilon \to 0} \left( \mathcal{F}(\bar{q}, \Theta) \right)
\]

\[
= \sum_{n \in J} \left( \sum_{s} q^{(n)}(s) \log \left( p(s, \bar{y}^{(n)} | \Theta) \right) - \sum_{s} q^{(n)}(s) \log \left( q^{(n)}(s) \right) \right) \\
+ \lim_{\epsilon \to 0} \left( \sum_{n \in \bar{J}} \left( \sum_{s} \bar{q}^{(n)}(s) \log \left( p(s, \bar{y}^{(n)} | \Theta) \right) - \sum_{s} \bar{q}^{(n)}(s) \log \left( \bar{q}^{(n)}(s) \right) \right) \right)
\]

which finally shows that Proposition 1 holds for any \( q \) with any distributions \( q^{(n)} \) on \( \Omega \).

\( \Box \)

As the free energy 17 for general \( q \) was obtained as a limit, we have to show that it remains a lower bound of \( L(\Theta) \) also in this limit. Using the KL-divergence result 13, this can however be shown using a similar approach as for the proof above.

**Proposition 2**

Let \( q^{(n)}(\bar{s}) \) be variational distributions over a set of states \( \Omega \) (with values not necessarily greater zero), then the corresponding free energy 17 is a lower bound of the likelihood, and the difference between likelihood and free energy is given by the sum over KL-divergences:

\[
L(\Theta) - \mathcal{F}(q, \Theta) = \sum_{n} D_{\text{KL}}(q^{(n)}(\bar{s}), p(\bar{s} | \bar{y}^{(n)}, \Theta)) \geq 0.
\]  \( \text{(25)} \)

**Proof**

Given distributions \( q^{(n)}(\bar{s}) \) let us consider the same auxiliary distributions \( \bar{q}^{(n)}(\bar{s}) \) as for the proof of Prop. 1 (see Eqn. 18). As \( \bar{q}^{(n)}(\bar{s}) \) are strictly positive distributions, Eqn. 13 applies:

\[
L(\Theta) - \mathcal{F}(\bar{q}, \Theta) = \sum_{n} D_{\text{KL}}(\bar{q}^{(n)}(\bar{s}), p(\bar{s} | \bar{y}^{(n)}, \Theta)) \geq 0,
\]  \( \text{(26)} \)

for any collection of \( \epsilon_n \) satisfying 19. If we now consider a sequence \( \epsilon_k = 1/k \), we know that for any \( n \) there exists a finite \( K \) such that for all \( k > K \) applies that \( \epsilon_n = \epsilon_k = 1/k \) fulfills condition
If we now set \( \epsilon_n^- = \epsilon_k = 1/k \) for all \( n \), we know because of finitely many data points \( n \) that there also exists a finite \( K \) such that condition \((19)\) is fulfilled for all \( k > K \). If we now define a sequence of distributions \( \tilde{q}_k(\tilde{s}) = (\tilde{q}_k^{(1)}, \ldots, \tilde{q}_k^{(N)}) \) by choosing \( \epsilon_n^- = \epsilon_k = 1/k \) for all \( n \), we know that for all \( k > K \) applies:

\[
D_k = L(\Theta) - F(\tilde{q}_k, \Theta) = \sum_n D_{KL}(\tilde{q}_k^{(n)}(\tilde{s}), p(\tilde{s} | \tilde{y}^{(n)}, \Theta)) \geq 0. 
\]

The sequence \( D_k \) is hence a sequence in the interval \([0, \infty)\). As the limit \( \lim_{k \to \infty} F(\tilde{q}_k, \Theta) \) is finite, \( D_k \) converges to a finite value within \([0, \infty)\) (which is left-closed). If \( q \) contains some strictly positive \( q^{(n)} \), we only use \( \epsilon_n^- = \epsilon_k = 1/k \) for all \( n \in J \). Finally, by using Proposition 1, the limit \( \lim_{k \to \infty} D_k \) is given by:

\[
0 \leq \lim_{k \to \infty} D_k = L(\Theta) - \lim_{k \to \infty} F(\tilde{q}_k, \Theta)
\]

\[
= L(\Theta) - \sum_n \sum_{\tilde{s}} q^{(n)}(\tilde{s}) \log(p(\tilde{s} | \tilde{y}^{(n)} | \Theta)) + \sum_n \sum_{\tilde{s}} q^{(n)}(\tilde{s}) \log(q^{(n)}(\tilde{s}))
\]

\[
= L(\Theta) - \sum_n \sum_{\tilde{s}} q^{(n)}(\tilde{s}) \log(p(\tilde{y}^{(n)} | \Theta)) - \sum_n \sum_{\tilde{s}} q^{(n)}(\tilde{s}) \log(p(\tilde{s} | \tilde{y}, \Theta)) + \sum_n \sum_{\tilde{s}} q^{(n)}(\tilde{s}) \log(q^{(n)}(\tilde{s}))
\]

\[
= \sum_n D_{KL}(q^{(n)}(\tilde{s}), p(\tilde{s} | \tilde{y}^{(n)}, \Theta))
\]

where the last part follows the lines of the standard derivation for the difference \( L(\Theta) - F(q, \Theta) \). Note that we again used the convention \( q^{(n)}(\tilde{s}) \log(q^{(n)}(\tilde{s})) = 0 \) for all \( q^{(n)}(\tilde{s}) = 0 \).

\( \square \)

Taken together, Propositions 1 and 2 mean that we can generalize the standard free energy framework to any variational distribution – the requirement of strictly positive distributions can be dropped. As a consequence, we can use the (generalized) free energy framework also for the truncated variational distributions in \((3)\).

We can now insert the specific truncated distributions \((3)\) into the free energy \((17)\). As for non-variational EM \((14)\) with exact posterior as variational distributions, \( q^{(n)}(\tilde{s}) = p(\tilde{s} | \tilde{y}^{(n)}, \hat{\Theta}) \), we will distinguish between parameters \( \hat{\Theta} \) of the variational distribution and the parameters \( \Theta \) of the generative data model. Like for the M-step of exact EM, this allows for taking derivatives of the log-joint \( \log(p(\tilde{s}, \tilde{y}^{(n)} | \Theta)) \) while the variational distributions can be treated as constant (we will come back to this point further below). Inserting the truncated distributions \( q^{(n)}(\tilde{s}; K, \hat{\Theta}) \) into the free energy \((17)\) then yields:

\[
F(K, \hat{\Theta}, \Theta) = \sum_{n=1}^N \left[ \sum_{\tilde{s}} q^{(n)}(\tilde{s}; K, \hat{\Theta}) \log(p(\tilde{s}, \tilde{y}^{(n)} | \Theta)) \right] + H(q(\tilde{s}; K, \hat{\Theta})). 
\]

The free energy now depends on three sets of parameters, \( K, \hat{\Theta} \) and \( \Theta \). The Shannon-entropy \( H(q(\tilde{s}; K, \hat{\Theta})) \) is independent of the parameters \( \Theta \).

15
5 Optimization of Truncated Variational Free Energies

The variational parameters of $K$ and $\hat{\Theta}$ that we aim at optimizing are different from the typical variational parameters, e.g., different from those of factored variational approaches or of Gaussian approximations. For each $n$, the set $K^{(n)}$ contains discrete points in latent space; and the parameters $\hat{\Theta}$ are of the same type as those of the generative model but with potentially different values. As the (generalized) variational framework of Sec. 4 does not require strict positivity from the variational distributions, the truncated distributions $q^{(n)}(\vec{s}; K, \hat{\Theta})$ can now be treated within a variational free energy framework.

Following the free energy approach we aim at optimizing the free energy (28) instead of directly optimizing the likelihood. We will do so by optimizing $F(K, \hat{\Theta}, \Theta)$ step-by-step w.r.t. its three sets of parameters:

Opt 1: $K^{\text{new}} = \arg\max_K \{ F(K, \hat{\Theta}^{\text{old}}, \Theta^{\text{old}}) \}$ while holding $\hat{\Theta}^{\text{old}}$ and $\Theta^{\text{old}}$ fixed

Opt 2: $\Theta^{\text{new}} = \arg\max_\Theta \{ F(K^{\text{new}}, \hat{\Theta}^{\text{old}}, \Theta) \}$ while holding $K^{\text{new}}$ and $\hat{\Theta}^{\text{old}}$ fixed

Opt 3: $\hat{\Theta}^{\text{new}} = \arg\max_{\hat{\Theta}} \{ F(K^{\text{new}}, \hat{\Theta}, \Theta^{\text{new}}) \}$ while holding $K^{\text{new}}$ and $\Theta^{\text{new}}$ fixed

set $\hat{\Theta}^{\text{old}} = \hat{\Theta}^{\text{new}}$ and $\Theta^{\text{old}} = \Theta^{\text{new}}$ and start-over with Opt 1

The order of the updates is chosen for later convenience. Each of the three optimization steps by definition increases the free energy $F(K, \hat{\Theta}, \Theta)$ w.r.t. one of its arguments. Opt 2 which updates the model parameters $\Theta$ corresponds to the M-step. Opt 1 and Opt 3 optimize the two sets of variational parameters $K$ and $\hat{\Theta}$, respectively, and correspond to the E-step for truncated variational distributions. One iteration of Eqns. 29 will be referred to as TV-EM iteration (as in introduced in Sec. 2), and by definition the free energy is monotonically increased.

The optimization steps (29) of TV-EM are formal definitions. In order to be applicable in practice, a more concrete procedure for each of the three optimization steps is required.

5.1 The Truncated Free Energy

Instead of investigating and applying the three optimization steps individually, we will carefully analyze each optimization in a theoretically grounded way. For this purpose, let us first introduce a free energy defined by setting the values of the variational parameters $\hat{\Theta}$ equal to the model parameters $\Theta$:

$$F(K, \Theta) := F(K, \Theta, \Theta) = \sum_{n=1}^{N} \left[ \sum_{\vec{s}} q^{(n)}(\vec{s}; K, \Theta) \log \left( p(\vec{s}, \vec{y}^{(n)} | \Theta) \right) \right] + H(q^{(n)}(\vec{s}; K, \Theta)) \quad (30)$$

Given the definition of the truncated variational distribution $q^{(n)}(\vec{s}; K, \Theta)$ in (3), it can then be shown that the free energy $F(K, \Theta)$ can be decisively simplified as follows:
Proposition 3
Given a generative model defined by the joint distribution \( p(\mathbf{s}, \mathbf{y} | \Theta) \). If \( \mathcal{F}(\mathcal{K}, \Theta) \) is the free energy defined by [30] with truncated distributions given by [3], then it follows that
\[
\mathcal{F}(\mathcal{K}, \Theta) = \sum_{n=1}^{N} \log \left( \sum_{\mathbf{s} \in \mathcal{K}^{(n)}} p(\mathbf{s}, \mathbf{y}^{(n)} | \Theta) \right).
\]

Proof
Following Propositions 1 and 2, \( \mathcal{F}(\mathcal{K}, \Theta) \) is a lower bound of \( \mathcal{L}(\Theta) \), which satisfies:
\[
\mathcal{L}(\Theta) - \mathcal{F}(\mathcal{K}, \Theta) = \sum_{n} D_{KL} \left( q^{(n)}(\mathbf{s}; \mathcal{K}, \Theta), p(\mathbf{s} | \mathbf{y}^{(n)}, \Theta) \right)
\]

For notational purposes let us introduce the normalizer \( Z^{(n)} = \sum_{\mathbf{s} \in \mathcal{K}^{(n)}} p(\mathbf{s} | \mathbf{y}^{(n)}, \Theta) \) such that:
\[
q^{(n)}(\mathbf{s}; \mathcal{K}, \Theta) = \frac{1}{Z^{(n)}} p(\mathbf{s} | \mathbf{y}^{(n)}, \Theta) \delta(\mathbf{s} \in \mathcal{K}^{(n)})
\]

From the above it follows that:
\[
\mathcal{F}(\mathcal{K}, \Theta)
= \mathcal{L}(\Theta) - \sum_{n} D_{KL} \left( q^{(n)}(\mathbf{s}; \mathcal{K}, \Theta), p(\mathbf{s} | \mathbf{y}^{(n)}, \Theta) \right)
= \sum_{n} \log(p(\mathbf{y}^{(n)} | \Theta)) + \sum_{n} \sum_{\mathbf{s}} q^{(n)}(\mathbf{s}; \mathcal{K}, \Theta) \log \left( \frac{p(\mathbf{s} | \mathbf{y}^{(n)}, \Theta)}{q^{(n)}(\mathbf{s}; \mathcal{K}, \Theta)} \right)
= \sum_{n} \log(p(\mathbf{y}^{(n)} | \Theta)) + \sum_{n} \sum_{\mathbf{s}} \frac{1}{Z^{(n)}} p(\mathbf{s} | \mathbf{y}^{(n)}, \Theta) \delta(\mathbf{s} \in \mathcal{K}^{(n)}) \log \left( \frac{p(\mathbf{s} | \mathbf{y}^{(n)}, \Theta)}{\frac{1}{Z^{(n)}} p(\mathbf{s} | \mathbf{y}^{(n)}, \Theta) \delta(\mathbf{s} \in \mathcal{K}^{(n)})} \right)
= \sum_{n} \log(p(\mathbf{y}^{(n)} | \Theta)) + \sum_{n} \sum_{\mathbf{s} \in \mathcal{K}^{(n)}} \frac{1}{Z^{(n)}} p(\mathbf{s} | \mathbf{y}^{(n)}, \Theta) \log \left( \frac{p(\mathbf{s} | \mathbf{y}^{(n)}, \Theta)}{Z^{(n)} p(\mathbf{s} | \mathbf{y}^{(n)}, \Theta) } \right)
= \sum_{n} \log(p(\mathbf{y}^{(n)} | \Theta)) + \sum_{n} \sum_{\mathbf{s} \in \mathcal{K}^{(n)}} \frac{1}{Z^{(n)}} p(\mathbf{s} | \mathbf{y}^{(n)}, \Theta) \log(Z^{(n)}).
\]

Again we used the convention \( q^{(n)}(\mathbf{s}) \log(q^{(n)}(\mathbf{s})) = 0 \) for all \( q^{(n)}(\mathbf{s}) = 0 \). Observing the intermediate result above, note that \( Z^{(n)} \) is independent of \( \mathbf{s} \). We can therefore continue as follows:
\[
\mathcal{F}(\mathcal{K}, \Theta) = \sum_{n} \log(p(\mathbf{y}^{(n)} | \Theta)) + \sum_{n} \log \left( \frac{Z^{(n)}}{Z^{(n)}} \sum_{\mathbf{s} \in \mathcal{K}^{(n)}} p(\mathbf{s} | \mathbf{y}^{(n)}, \Theta) \right)
= \sum_{n} \log(p(\mathbf{y}^{(n)} | \Theta)) + \sum_{n} \log \left( Z^{(n)} \right)
= \sum_{n} \log(p(\mathbf{y}^{(n)} | \Theta)) + \sum_{n} \log \left( \sum_{\mathbf{s} \in \mathcal{K}^{(n)}} p(\mathbf{s} | \mathbf{y}^{(n)}, \Theta) \right)
= \sum_{n} \log(p(\mathbf{y}^{(n)} | \Theta)) + \sum_{n} \log \left( \frac{\sum_{\mathbf{s} \in \mathcal{K}^{(n)}} p(\mathbf{s}, \mathbf{y}^{(n)} | \Theta)}{p(\mathbf{y}^{(n)} | \Theta)} \right)
= \sum_{n} \log \left( \sum_{\mathbf{s} \in \mathcal{K}^{(n)}} p(\mathbf{s}, \mathbf{y}^{(n)} | \Theta) \right)
\]
Considering Eqn. 31 we instantly observe that \( \mathcal{F}(\mathcal{K}, \Theta) \) is computationally tractable if \( \mathcal{K} \) is sufficiently small. Also the fact that \( \mathcal{F}(\mathcal{K}, \Theta) \) lower-bounds the log-likelihood can instantly be observed. Importantly, however, Prop. 3 shows that Eqn. 31 is a variational free energy which corresponds to the truncated variational distributions [3]. Furthermore, Prop. 3 directly relates [31] to the free energy [28]. As \( \mathcal{F}(\mathcal{K}, \Theta) \) is a special case of \( \mathcal{F}(\mathcal{K}, \hat{\Theta}, \Theta) \) both free energies are lower bounds of the likelihood \( \mathcal{L}(\Theta) \). Furthermore, it can be shown that \( \mathcal{F}(\mathcal{K}, \Theta) \) can be obtained as a variational lower bound of \( \mathcal{F}(\mathcal{K}, \Theta) \) and that the following holds.

**Proposition 4**

Given a generative model defined by the joint \( p(\tilde{s}, \tilde{y}|\Theta) \), let \( \mathcal{L}(\Theta) \) be the likelihood in Eqn. 2 and let \( \mathcal{F}(\mathcal{K}, \hat{\Theta}, \Theta) \) and \( \mathcal{F}(\mathcal{K}, \Theta) \) be the free energies defined by Eqn. 28 and 31 respectively. Then, for all values of \( \mathcal{K}, \hat{\Theta}, \) and \( \Theta \) the following applies:

\[
\mathcal{L}(\Theta) \geq \mathcal{F}(\mathcal{K}, \Theta) \geq \mathcal{F}(\mathcal{K}, \hat{\Theta}, \Theta).
\]

**Proof**

\( \mathcal{F}(\mathcal{K}, \Theta) \) is a special case of \( \mathcal{F}(\mathcal{K}, \hat{\Theta}, \Theta) \) by definition (Eqn. 30), and as such a lower bound of \( \mathcal{L}(\Theta) \). To show that \( \mathcal{F}(\mathcal{K}, \Theta) \geq \mathcal{F}(\mathcal{K}, \hat{\Theta}, \Theta) \), we use Proposition 3 and apply Jensen’s inequality:

\[
\mathcal{F}(\mathcal{K}, \Theta) = \sum_n \sum_{\tilde{s} \in \mathcal{K}(n)} \log \left( p(\tilde{s}, \tilde{y}^{(n)} | \Theta) \right)
\]

\[
= \sum_n \sum_{\tilde{s} \in \mathcal{K}(n)} \log \left( \hat{q}^{(n)}(\tilde{s}) p(\tilde{s}, \tilde{y}^{(n)} | \Theta) \hat{q}^{(n)}(\tilde{s}) \right)
\]

\[
\geq \sum_n \sum_{\tilde{s} \in \mathcal{K}(n)} \hat{q}^{(n)}(\tilde{s}) \log \left( \frac{p(\tilde{s}, \tilde{y}^{(n)} | \Theta)}{\hat{q}^{(n)}(\tilde{s})} \right)
\]

if \( \sum_{\tilde{s} \in \mathcal{K}(n)} \hat{q}^{(n)}(\tilde{s}) = 1 \) and \( \hat{q}^{(n)}(\tilde{s}) \geq 0 \) for all \( \tilde{s} \in \mathcal{K}(n) \). We now define:

\[
\hat{q}^{(n)}(\tilde{s}) = \frac{p(\tilde{s} | \tilde{y}^{(n)}, \hat{\Theta})}{\sum_{\tilde{s} \in \mathcal{K}(n)} p(\tilde{s} | \tilde{y}^{(n)}, \hat{\Theta})}.
\]

The choice of \( \hat{q}^{(n)}(\tilde{s}) \) fulfills the conditions for Jensen’s inequality but note that it is not a probability density on the whole state space \( \Omega \) of \( \tilde{s} \). Inserting \( \hat{q}^{(n)}(\tilde{s}) \) into (38) we obtain:

\[
\mathcal{F}(\mathcal{K}, \Theta) \geq \sum_n \sum_{\tilde{s} \in \mathcal{K}(n)} \frac{p(\tilde{s} | \tilde{y}^{(n)}, \hat{\Theta})}{\sum_{\tilde{s} \in \mathcal{K}(n)} p(\tilde{s} | \tilde{y}^{(n)}, \hat{\Theta})} \log \left( \frac{p(\tilde{s}, \tilde{y}^{(n)} | \Theta)}{\sum_{\tilde{s} \in \mathcal{K}(n)} p(\tilde{s} | \tilde{y}^{(n)}, \hat{\Theta})} \right)
\]

\[
= \sum_n \sum_{\tilde{s}} q^{(n)}(\tilde{s}; \mathcal{K}, \hat{\Theta}) \log \left( \frac{p(\tilde{s}, \tilde{y}^{(n)} | \Theta)}{q^{(n)}(\tilde{s}; \mathcal{K}, \Theta)} \right)
\]

\[
= \sum_n \sum_{\tilde{s}} q^{(n)}(\tilde{s}; \mathcal{K}, \hat{\Theta}) \log \left( p(\tilde{s}, \tilde{y}^{(n)} | \Theta) \right) + H(q^{(n)}(\tilde{s}; \mathcal{K}, \hat{\Theta}))
\]

\[
= \mathcal{F}(\mathcal{K}, \hat{\Theta}, \Theta),
\]
where \( q^{(n)}(\hat{s}; \hat{\kappa}, \hat{\Theta}) \) is the truncated variational distribution in (3) and where \( F(\kappa, \hat{\Theta}, \Theta) \) is the corresponding free energy in (28).

Having established that \( F(\kappa, \hat{\Theta}, \Theta) \) is a lower bound of \( F(\kappa, \Theta) \) for all \( \hat{\Theta} \), the following applies for the differences between \( L(\Theta) \), \( F(\kappa, \Theta) \), and \( F(\kappa, \hat{\Theta}, \Theta) \):

**Corollary 1**

All as above.

\[
L(\Theta) - F(\kappa, \Theta) = \sum_n D_{KL}(q^{(n)}(\hat{s}; \kappa, \Theta), p(\hat{s}| y^{(n)}, \Theta)) \geq 0, \\
F(\kappa, \Theta) - F(\hat{\kappa}, \hat{\Theta}, \Theta) = \sum_n D_{KL}(q^{(n)}(\hat{s}; \hat{\kappa}, \hat{\Theta}), p(\hat{s}| \hat{y}^{(n)}, \Theta)) - \sum_n D_{KL}(q^{(n)}(\hat{s}; \kappa, \Theta), p(\hat{s}| \hat{y}^{(n)}, \Theta)) \geq 0, \\
L(\Theta) - F(\hat{\kappa}, \hat{\Theta}, \Theta) = \sum_n D_{KL}(q^{(n)}(\hat{s}; \hat{\kappa}, \hat{\Theta}), p(\hat{s}| \hat{y}^{(n)}, \Theta)) \geq 0.
\]

**Proof**

The first and the last equation are a direct consequence of Propositions 2 and 4 and of the fact that \( F(\kappa, \Theta) \) and \( F(\hat{\kappa}, \hat{\Theta}, \Theta) \) are both variational lower bounds of \( L(\Theta) \). The second equation is obtained by taking the difference of the first and the last equation. The fact that the difference of the KL-divergences of the second equation is greater zero follows from Proposition 4.

By considering Corollary 1, we can now solve the last optimization step (Opt 3) in (29) analytically. Indeed, it can be shown that \( F(\kappa, \hat{\Theta}, \Theta) \) is optimized w.r.t. \( \hat{\Theta} \) if the values of the variational parameters \( \hat{\Theta} \) are set equal to model parameters \( \Theta \):

**Proposition 5**

If \( F(\kappa, \hat{\Theta}, \Theta) \) is the truncated free energy of Eqn. 28, then it applies for fixed \( \kappa \) and \( \Theta \) that

\[
\text{argmax}_{\hat{\Theta}} \{ F(\kappa, \hat{\Theta}, \Theta) \} = \Theta. \tag{44}
\]

**Proof**

Let us first re-express \( F(\kappa, \hat{\Theta}, \Theta) \) using Corollary 1:

\[
F(\kappa, \hat{\Theta}, \Theta) = F(\kappa, \Theta) + \sum_n D_{KL}(q^{(n)}(\hat{s}; \kappa, \Theta), p(\hat{s}| \hat{y}^{(n)}, \Theta)) - \sum_n D_{KL}(q^{(n)}(\hat{s}; \kappa, \hat{\Theta}), p(\hat{s}| \hat{y}^{(n)}, \Theta)) \\
= F(\kappa, \Theta) + \sum_n D_{KL}(q^{(n)}(\hat{s}), p^{(n)}(\Theta)) - \sum_n D_{KL}(q^{(n)}(\hat{s}; \hat{\Theta}), p^{(n)}(\Theta)), \tag{45}
\]

where the last line abbreviates the distributions for readability. As only the last summand depends on \( \Theta \), \( F(\kappa, \hat{\Theta}, \Theta) \) is maximized if \( \sum_n D_{KL}(q^{(n)}(\hat{\Theta}), p^{(n)}(\Theta)) \) is minimized. Now we also know from Corollary 1 that \( \sum_n D_{KL}(q^{(n)}(\hat{\Theta}), p^{(n)}(\Theta)) \geq \sum_n D_{KL}(q^{(n)}(\Theta), p^{(n)}(\Theta)) \), where only the left-hand-side depends on \( \Theta \). Hence, the most minimal value for \( \sum_n D_{KL}(q^{(n)}(\hat{\Theta}), p^{(n)}(\Theta)) \) achievable is

\[
\sum_n D_{KL}(q^{(n)}(\hat{\Theta}), p^{(n)}(\Theta)) = \sum_n D_{KL}(q^{(n)}(\hat{\Theta}), p^{(n)}(\Theta)). \tag{46}
\]
By choosing $\hat{\Theta} = \Theta$ we can indeed satisfy the equality, and therefore know that $\sum_n D_{KL}(q^{(n)}(\hat{\Theta}), p^{(n)}(\Theta))$ takes on a global minimum for this choice. This global minimum then implies (because of Eqn. 45) a global maximum of $F(K, \hat{\Theta}, \Theta)$ w.r.t. $\hat{\Theta}$.

□

Note that there can potentially be other global maxima, e.g., due to permutations of the parameters without effect on $q^{(n)}(\vec{s}; K, \hat{\Theta})$. Using the KL-divergences of Corollary 1 makes it salient that it is sufficient to equate $q^{(n)}(\vec{s}; K, \hat{\Theta})$ and $q^{(n)}(\vec{s}; K, \Theta)$, which is a weaker condition than equating $\Theta$ and $\hat{\Theta}$. To show that $\hat{\Theta} = \Theta$ is maximizing $F(K, \hat{\Theta}, \Theta)$ we can, alternatively, also use Proposition 4 directly, i.e., $F(K, \Theta) \geq F(K, \hat{\Theta}, \Theta)$. Either way, we can conclude that $F(K, \hat{\Theta}, \Theta)$ is maximized for $\hat{\Theta} = \Theta$, in which case $F(K, \hat{\Theta}, \Theta)$ becomes equal to $F(K, \Theta)$.

Using Proposition 5 solves the third optimization step of Eqs. 29 and one TV-EM iteration reduces to two optimizations: by applying (44) the third optimization (Opt 3 of Eqs. 29), is simply given by $\hat{\Theta}_{new} = \Theta_{new}$. After combining this update with the last line of Eqs. 29 we obtain:

\[
\text{Opt 1 : } K_{new} = \arg\max_K \{ F(K, \hat{\Theta}_{old}, \Theta_{old}) \} \\
\text{Opt 2 : } \Theta_{new} = \arg\max_{\Theta} \{ F(K_{new}, \hat{\Theta}_{old}, \Theta) \}
\]

\[\hat{\Theta}_{old} = \Theta_{new} \quad \text{and} \quad \Theta_{old} = \Theta_{new} \tag{47}\]

As the variational parameters $\hat{\Theta}_{old}$ and the model parameters $\Theta_{old}$ are now both set to the same values in the last line of (47), we can now for Opt 1 use (without loss of generality) the simplified form of free energy $F(K, \Theta)$ as given by Eqn. 31. As a consequence, we can replace the two resets of the parameters $\Theta$ in the last line by the single reset $\Theta_{old} = \Theta_{new}$ and finally obtain the TV-EM formulation of Eqs. 7 to 9 as stated in the beginning.

To recapitulate, we have thus finally proven that iterating the TV-EM steps of Eqs. 7 to 9 monotonically increases the free energy (5), which is a lower bound of the log-likelihood (2). The proof follows from the updates (29), which monotonically increase the free energy by definition. Using Propositions 1 to 5 and Corollary 1, Eqs. 7 to 9 result in the same updates as (29) but represent a strong simplification. Note, in this respect, that it is important for the TV-M-step (8) to be of the same form as for exact EM and other types of variational EM approximations because this form means that any M-step equations derived for any previously considered generative model can be reused for truncated variational EM. Maintaining the standard M-step update is non-trivial for truncated distributions and required the application of the theoretical results derived above:

First, we needed to start with a three-stage optimization for $F(K, \hat{\Theta}, \Theta)$. A direct optimization of the simplified free energy $F(K, \Theta)$ in a two-stage procedure would change the M-step to a non-standard form. This is because the truncated distributions do also depend on $\Theta$ (and derivatives w.r.t. to all $\Theta$’s would be required). By treating $\hat{\Theta}$ as variational parameters, derivatives exclusively w.r.t. the log-joint probability of the generative model can be taken, and this results, e.g., in the well-known closed-form updates of Gaussian Mixture Models, Hidden Markov Models, Factor Analysis etc. All these M-step results and similar such results for many other models can thus directly be used for TV-EM.

Second, when we take derivatives w.r.t. $\Theta$ in the TV-M-step, it may feel straight-forward to hold the parameters $\Theta$ of the variational distributions fixed at their old values $\Theta_{old}$; and
to only afterwards set $\Theta^{\text{old}} = \Theta^{\text{new}}$ as in (9). We are very used to this procedure for exact EM. Note, however, that for exact EM, it is required to prove that such a procedure never decreases the free energy. A possible such proof for exact EM would use Eqn. 13 and full posteriors $p(\vec{s} | \vec{y}^{(n)}, \Theta)$ as variational distributions (using $\Theta$ as variational parameters). The KL-divergence $D_{KL}(p(\vec{s} | \vec{y}^{(n)}, \Theta), p(\vec{s} | \vec{y}^{(n)}, \Theta))$ can then be set to zero by choosing $\Theta = \Theta$, which according to Eqn. 13 globally maximize the free energy (also see Lemma 1 of Neal and Hinton, 1998). For general variational distributions with $\Theta$ as variational parameters, the same does not apply. For truncated variational distributions, it is Prop. 5 which shows that we can proceed with truncated distributions in the same way as we are used to for full posteriors in exact EM. Indeed, Prop. 5 contains Lemma 1 of Neal and Hinton (1998) as a special case: If we set all $K$ distributions in the same way as we are used to for full posteriors in exact EM. Moreover, Prop. 5 then shows that this free energy is maximized if we set $\Theta^{\text{old}}$ of the posteriors $p(\vec{s} | \vec{y}^{(n)}, \Theta^{\text{old}})$ equal to the $\Theta$ obtained in the M-step. Also note that for $\Theta^{(n)} = \Omega$, the TV-EM algorithm reduces to exact EM as the TV-E-step (7) becomes trivial and as the truncated distributions (3) become equal to the exact posteriors.

5.2 Partial Truncated E- and M-Steps

So far, we have considered with Eqns. 29 full maximizations of truncated free energies, for which we derived the TV-EM algorithm given by Eqns. 7 to 9. However, for many generative models such full maximizations are analytically and/or computationally intractable. In order to also address these important cases, we here apply Props. 1 to 5 to partial TV-E- and partial TV-M-steps (which is analogous but not equal to the full maximization). Let us start with a three-stage optimization as before but instead we now consider a partial TV-EM procedure:

\begin{align}
\text{Opt 1 : } & \text{ choose } K^{\text{new}} \text{ such that } F(K^{\text{new}}, \hat{\Theta}^{\text{old}}, \Theta^{\text{old}}) \geq F(K^{\text{old}}, \hat{\Theta}^{\text{old}}, \Theta^{\text{old}}) \\
\text{Opt 2 : } & \text{ choose } \Theta^{\text{new}} \text{ such that } F(K^{\text{new}}, \hat{\Theta}^{\text{old}}, \Theta^{\text{new}}) \geq F(K^{\text{new}}, \hat{\Theta}^{\text{old}}, \Theta^{\text{old}}) \\
\text{Opt 3 : } & \hat{\Theta}^{\text{new}} = \text{argmax} \{ F(K^{\text{new}}, \hat{\Theta}, \Theta^{\text{new}}) \}
\end{align}

(48)

An iteration using (48) monotonically increases the free energy $F(K, \hat{\Theta}, \Theta)$ as each individual optimization by definition never decreases $F(K, \hat{\Theta}, \Theta)$. Opt 1 and Opt 2 are now partial optimizations ($F(K, \hat{\Theta}, \Theta)$ is increased, not maximized), while we maintain for Opt 3 a full maximization. By applying Prop. 5 we can now, as before, replace the maximization of Opt 3 by setting $\hat{\Theta}^{\text{new}} = \Theta^{\text{new}}$. Also as before, we then obtain by combining the analytical solution of Opt 3 with the last line of (48) a two-stage optimization procedure:

\begin{align}
\text{Opt 1 : } & \text{ choose } K^{\text{new}} \text{ such that } F(K^{\text{new}}, \hat{\Theta}^{\text{old}}, \Theta^{\text{old}}) \geq F(K^{\text{old}}, \hat{\Theta}^{\text{old}}, \Theta^{\text{old}}) \\
\text{Opt 2 : } & \text{ choose } \Theta^{\text{new}} \text{ such that } F(K^{\text{new}}, \hat{\Theta}^{\text{old}}, \Theta^{\text{new}}) \geq F(K^{\text{new}}, \hat{\Theta}^{\text{old}}, \Theta^{\text{old}})
\end{align}

(49)

As $\Theta^{\text{old}}$ and $\hat{\Theta}^{\text{old}}$ are now set to the same values, we can replace the free energy $F(K, \hat{\Theta}, \Theta)$ of Opt 1 in (49) by the simplified free energy (31) derived for Proposition 3. By further simplifying...
the last line of (49) we finally arrive at:

\begin{align*}
\text{Opt 1 :} & \text{ choose } K^{\text{new}} \text{ such that } \mathcal{F}(K^{\text{new}}, \Theta^{\text{old}}) \geq \mathcal{F}(K^{\text{old}}, \Theta^{\text{old}}) \\
\text{Opt 2 :} & \text{ choose } \Theta^{\text{new}} \text{ such that } \mathcal{F}(K^{\text{new}}, \Theta^{\text{old}}, \Theta^{\text{new}}) \geq \mathcal{F}(K^{\text{new}}, \Theta^{\text{old}}, \Theta^{\text{old}})
\end{align*}

(50)

Eqns. 50 will be referred to as a partial TV-EM iteration. Like non-partial TV-EM (i.e., Eqns. 7 to 9), a partial TV-EM step monotonically increases the truncated free energy (31). While the derivation of partial TV-EM used the same theoretical results as non-partial TV-EM, note that a main difference is that the variational parameters \(K\) have to be memorized across partial TV-EM iterations. A full optimization does not necessarily require such a memorization. Furthermore, we require initial values of \(K\) for partial TV-EM. Finally, observe that we can, in the same way as above, define TV-EM algorithms with only the TV-E-step being a partial optimization or with only the TV-M-step being a partial optimization.

5.3 Explicit Form

Before we consider applications of the theoretical results for TV-EM, let us formulate the algorithm given in the previous section more explicitly. Obtaining an explicit form for the TV-E-step is straight-forward by just inserting the simplified truncated free energy (31) into the first optimization of Eqns. 50 (see further below). Regarding the TV-M-step, consider the second optimization of Eqns. 50 and let us insert the (non-simplified) truncated free energy (28). After noting that (as usual for variational approaches) the entropy term is not relevant for the optimization of model parameters \(\Theta\), the relevant function to optimize is given by:

\[ Q(\Theta) = \sum_{n=1}^{N} \sum_{\tilde{s}} q^{(n)}(\tilde{s}; \mathcal{K}, \Theta^{\text{old}}) \log \left( p(\tilde{s}, \tilde{y}^{(n)} | \Theta) \right) = \sum_{n=1}^{N} \left\langle \log \left( p(\tilde{s}, \tilde{y}^{(n)} | \Theta) \right) \right\rangle_{q^{(n)}(\tilde{s}; \mathcal{K}, \Theta^{\text{old}})} \]

(51)

If we now insert Eqn. 4 for the expectation value w.r.t. \(q^{(n)}(\tilde{s}; \mathcal{K}, \Theta^{\text{old}})\) in (51), we obtain (together with the TV-E-step) an explicit form of one TV-EM iteration given by:

**TV-E-step:**

change \(K\) from \(K^{\text{old}}\) to \(K^{\text{new}}\) such that \(\sum_{n} \sum_{\tilde{s} \in \mathcal{K}^{(n)}} \log \left( p(\tilde{s}, \tilde{y}^{(n)} | \Theta^{\text{old}}) \right)\) increases.

**TV-M-step:**

change \(\Theta\) from \(\Theta^{\text{old}}\) to \(\Theta^{\text{new}}\) such that \(\sum_{n} \frac{\sum_{\tilde{s} \in \mathcal{K}^{(n)}_{\text{new}}} p(\tilde{s}, \tilde{y}^{(n)} | \Theta^{\text{old}}) \log \left( p(\tilde{s}, \tilde{y}^{(n)} | \Theta) \right)}{\sum_{\tilde{s}' \in \mathcal{K}^{(n)}_{\text{new}}} p(\tilde{s}', \tilde{y}^{(n)} | \Theta^{\text{old}})}\) increases.

**Reset:**

\[ K^{\text{old}} = K^{\text{new}}, \quad \Theta^{\text{old}} = \Theta^{\text{new}} \]

(52)

The form (52) of one TV-EM iteration makes the following explicit: (A) The procedure is fully defined by the joint probability of the considered generative model; and (B) all entities that have
to be computed are computationally tractable given sufficiently small sets $K^{(n)}$ and efficiently computable joint probabilities. Eqns. 52 also highlight the very concise form of the procedure.

If TV-EM is applied to a given generative model, the M-step typically relies on derivatives of the log-joint probability (be it either to derive closed-form update equations or gradient equations for more intricate models). The E-step will ultimately reduce to a pair-wise comparison of joint probabilities, which can be realized efficiently (we will provide more details of such procedures in the following).

6 Applications of Theoretical Results

Our theoretical results and the TV-EM meta-algorithm can now be applied to provide novel theoretical insights, and to point to novel ways to develop learning algorithms for generative models. We will consider three applications of our results: First, we will consider multiple-cause or latent variable generative models, i.e., models for which the values of multiple latent variables combine to generate the data. Second, we consider applications to mixture models, i.e., models for which an observation is always generated by one latent variable. Finally, in the third application we investigate the relation between TV-EM and ‘hard EM’, which is a very widely applied and in practice very successful form of parameter optimization in generative models.

6.1 TV-EM for Multiple-Cause Models

Multiple-cause models or latent variable models are generative models in which a set of latent variables (latent causes) combine to generate an observation. Common examples are sparse coding models (e.g. Olshausen and Field, 1996), noisy-OR Bayes nets (e.g. Singliar and Hauskrecht, 2006) or sigmoid belief networks (Saul et al., 1996; Jordan et al., 1999). The interaction of multiple hidden variables typically gives rise to large latent spaces because of the combinatorics of individual latents. For any larger models, full posteriors over the latent space are not computationally tractable anymore, and variational EM is a standard technique to address such intractabilities.

For our application to multiple-cause models let us consider partial TV-EM (Eqns. 50). Similar to exact EM, the M-step of TV-EM requires the computation of derivatives of the log-joint probability of the considered generative model (compare Eqns. 52). Computing any such derivations is standard except of the expectation values w.r.t. $q^{(n)}(s; \mathcal{K}, \Theta)$ which are for TV-EM computed using (4). The crucial difference to previous variational approaches is hence the truncated variational E-step. Instead of solving fixed-point equations for the variational parameters as, e.g., for mean-field approaches, we have to find variational parameters that take the form of finite sets of hidden states. We will term these states variational states. A (partial) TV-E-step can now be implemented by suggesting new variational states $\tilde{\mathcal{K}}$ and to compare the free energy (31) of these new states with the free energy of the old variational states. The set $\mathcal{K}$ is then replaced by a new set $\tilde{\mathcal{K}}$ if the free energy increases. The efficiency of this procedure will, of course, depend crucially on the way how new variational states are suggested or how new sets $\mathcal{K}$ are defined. Before we consider more concrete examples of TV-E-steps, let us formulate the above described procedure (which directly follows form Eqns. 50) as a meta-algorithm (see Alg. 1). The inner loop of Alg. 1 repeatedly changes the states in $\mathcal{K}$ and its if-clause warrants that $F(\mathcal{K}, \Theta)$
Algorithm 1: Application to Multiple-Cause Models.

init model parameters $\Theta^{\text{old}}$;
init variational states $\mathcal{K}^{\text{old}}$;
repeat
  repeat
    suggest new set of states $\tilde{\mathcal{K}}$;
    if $\mathcal{F}(\tilde{\mathcal{K}}, \Theta^{\text{old}}) > \mathcal{F}(\mathcal{K}^{\text{old}}, \Theta^{\text{old}})$ then
      $\mathcal{K}^{\text{new}} = \tilde{\mathcal{K}}$
    until $\mathcal{F}(\mathcal{K}^{\text{new}}, \Theta^{\text{old}})$ has sufficiently increased;
  compute $\Theta^{\text{new}}$ that optimizes $Q(\Theta) = \sum_{n=1}^{N} \left\langle \log \left(p(\tilde{s}^{(n)} | \Theta)\right) \right\rangle_{q(\mathcal{K}^{\text{new}}, \Theta^{\text{old}})}$;
  $\mathcal{K}^{\text{old}} = \mathcal{K}^{\text{new}}$;
  $\Theta^{\text{old}} = \Theta^{\text{new}}$;
until parameters $\Theta$ have sufficiently converged;

is increased w.r.t. $\mathcal{K}$. The successive optimization of $\mathcal{F}(\mathcal{K}, \Theta)$ w.r.t. $\Theta$ can be accomplished using standard M-step update equations with expectation values estimated by (4). Together with setting $\mathcal{K}^{\text{old}} = \mathcal{K}^{\text{new}}$ and $\Theta^{\text{old}} = \Theta^{\text{new}}$, one iteration thus realizes one partial TV-EM step. The outer loop of Alg. 1 iterates over individual TV-EM steps such that Alg. 1 provably monotonically increases the free energy $\mathcal{F}(\mathcal{K}, \Theta)$. As it is the case for the parameters $\Theta$ of the outer loop, we can terminate the inner loop (the TV-E-step) after one iteration (if the free energy increased) or once there are no or no significant changes of $\mathcal{K}$ observed anymore, or at any intermediate step.

Considering Alg. 1, the computation and comparison of free energies may seem computationally demanding. However, thanks to the specific functional form of the simplified free energy (31), it is sufficient to pair-wise compare the joint probabilities instead of the free energies. That is, for a given data point $\tilde{y}^{(n)}$ and any newly suggested state, it is sufficient to compare the joint probability of the new state with those of the variational states in $\mathcal{K}^{(n)}$:

Proposition 6
Consider the application of TV-EM to a generative model given by the joint $p(\tilde{s}, \tilde{y} | \Theta)$ and let $\mathcal{K}^{(n)}$ be the set of variational states for a data point $\tilde{y}^{(n)}$. If we now replace a state $\tilde{s}^{\text{old}}$ in $\mathcal{K}^{(n)}$ by a new state $\tilde{s}^{\text{new}}$ so far not in $\mathcal{K}^{(n)}$ then the free energy $\mathcal{F}(\mathcal{K}, \Theta)$ of (31) is increased if and only if

$$p(\tilde{s}^{\text{new}}, \tilde{y}^{(n)} | \Theta) > p(\tilde{s}^{\text{old}}, \tilde{y}^{(n)} | \Theta).$$

Proof
For a given data point $n$ let us consider $\mathcal{K}^{(n)}$ and let $\mathcal{K}^{(n)}_{\text{new}}$ be the set defined by replacing the latent state $\tilde{s}^{\text{old}} \in \mathcal{K}^{(n)}$ with $\tilde{s}^{\text{new}} \notin \mathcal{K}^{(n)}$, i.e., $\mathcal{K}^{(n)}_{\text{new}} = \mathcal{K}^{(n)} \setminus \{\tilde{s}^{\text{old}}\} \cup \{\tilde{s}^{\text{new}}\}$. Let us further define $\mathcal{K}^{(n)}_{\text{new}}$ by replacing $\mathcal{K}^{(n)}$ with the set $\mathcal{K}^{(n)}_{\text{new}}$, i.e., $\mathcal{K}^{(n)}_{\text{new}} = \{\mathcal{K}^{(1)}, \ldots, \mathcal{K}^{(n-1)}, \mathcal{K}^{(n)}_{\text{new}}, \mathcal{K}^{(n+1)}, \ldots, \mathcal{K}^{(N)}\}$. 

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Then it follows:

\[
\mathcal{F}(\mathcal{K}^{\text{new}}, \Theta) > \mathcal{F}(\mathcal{K}, \Theta)
\]

\[\iff\]
\[
\sum_{m=1}^{N} \log \left( \sum_{\tilde{s} \in \mathcal{K}^{(n)}} p(\tilde{s}, \tilde{y}^{(n)} | \Theta) \right) + \log \left( \sum_{\tilde{s} \in \mathcal{K}^{\text{new}} \setminus \mathcal{K}^{(n)}} p(\tilde{s}, \tilde{y}^{(n)} | \Theta) \right) > \sum_{m=1}^{N} \log \left( \sum_{\tilde{s} \in \mathcal{K}^{(n)}} p(\tilde{s}, \tilde{y}^{(n)} | \Theta) \right) + \log \left( \sum_{\tilde{s} \in \mathcal{K}^{\text{new}} \setminus \mathcal{K}^{(n)}} p(\tilde{s}, \tilde{y}^{(n)} | \Theta) \right)
\]

\[\iff\]
\[
\log \left( \sum_{\tilde{s} \in \mathcal{K}^{\text{new}} \setminus \mathcal{K}^{(n)}} p(\tilde{s}, \tilde{y}^{(n)} | \Theta) \right) > \log \left( \sum_{\tilde{s} \in \mathcal{K}^{(n)}} p(\tilde{s}, \tilde{y}^{(n)} | \Theta) \right)
\]

\[\iff\]
\[
\sum_{\tilde{s} \in \mathcal{K}^{(n)}} p(\tilde{s}, \tilde{y}^{(n)} | \Theta) + p(\tilde{s}^{\text{new}}, \tilde{y}^{(n)} | \Theta) > \sum_{\tilde{s} \in \mathcal{K}^{\text{new}} \setminus \mathcal{K}^{(n)}} p(\tilde{s}, \tilde{y}^{(n)} | \Theta) + p(\tilde{s}^{\text{old}}, \tilde{y}^{(n)} | \Theta)
\]

\[\iff\]
\[
p(\tilde{s}^{\text{new}}, \tilde{y}^{(n)} | \Theta) > p(\tilde{s}^{\text{old}}, \tilde{y}^{(n)} | \Theta)
\]

\[\square\]

The criterion \[\text{53}\] can not be derived for arbitrary functions \(f(\tilde{s}, \tilde{y}^{(n)})\) nor does it become obvious by considering the original definition of \(\mathcal{F}(\mathcal{K}, \Theta)\) in Eqn. \[\text{30}\]. Only thanks to the simplified form of \(\mathcal{F}(\mathcal{K}, \Theta)\) derived for Prop. 3, the proof of Prop. 6 becomes a straight-forward derivation (and the proof could be regarded as a formal, technical verification of what may have been seen directly by considering the specific functional form of Eqn. \[\text{31}\]).

By virtue of Prop. 6, the free energy increase for the inner loop of Alg. 1 can be ensured if we, for a new state \(\tilde{s}^{\text{new}}\), find one state in \(\mathcal{K}^{(n)}\) with a lower joint probability than for \(\tilde{s}^{\text{new}}\). Also large numbers of new states, generated in parallel, can be compared in a bunch to the states in \(\mathcal{K}^{(n)}\). The set of states that increases the free energy most, can then be obtained through efficient partial sorting (e.g. Blum et al. 1973). Alternatively, efficient data structures such as heaps or soft heaps (Chazelle, 2000) to store the states of \(\mathcal{K}^{(n)}\) according to their joint probabilities can be used. Any new set of states can then efficiently be compared with the states in \(\mathcal{K}^{(n)}\) using inequality \[\text{53}\].

Given efficient updates of sets \(\mathcal{K}^{(n)}\) using Prop. 6 and the methods discussed above, the efficiency of the whole TV-E-step remains to depend on efficiently finding new states \(\tilde{\mathcal{K}}\) that are indeed sufficiently effective in increasing the free energy.

**Blind search.** The easiest way to suggest new states \(\tilde{\mathcal{K}}\) in Alg. 1 is blind search. Such a search could be realized by randomly (e.g. uniformly) sampling new states of the latent state, and then to use Prop. 6 to compare these sampled states to those in \(\mathcal{K}^{\text{old}}\). Alternatively, one could use random (blind) variations of the old states to generate new states. Applying Prop. 6 would then realize a basic stochastic gradient ascent procedure which improves the free energy. However, especially for large hidden spaces the probability of newly generated states to increase the free energy will be small – any blind search procedure will thus presumably be inefficient in general.
Deterministic construction. Instead of blindly and randomly searching new sets $\mathcal{K}$ in Alg. 1, an alternative would be to deterministically construct newly suggested sets $\tilde{\mathcal{K}}$. Such a construction could use procedures already developed previously (Lücke and Eggert, 2010; Shelton et al., 2011; Dai et al., 2013; Dai and Lücke, 2014), and Alg. 1 would combine these constructions with the theoretical results derived for TV-EM. For instance, most previous work used oracle (or selection) functions to construct sets $\tilde{\mathcal{K}}$. A selection function could take the form of a scalar product (Shelton et al., 2011), of approximations or upper-bounds of marginal probabilities (Lücke and Eggert, 2010), it could be hand-crafted for specific (possibly relatively complex) generative models (Dai et al., 2013; Dai and Lücke, 2014), or a selection function which is itself learned from data could be used (Shelton et al., 2017). Typically, a selection function is first used to determine for each data point $\vec{y}(n)$ a set $I(n)$ of the most relevant latent variables (the other variables are assumed with $s_h = 0$ to not contribute to the generation of $\vec{y}(n)$). Given the set $I(n)$, the set of states $\tilde{\mathcal{K}}(n)$ can then be constructed, for instance, by assuming a sparse combinatorics of the relevant latent variables:

$$\tilde{\mathcal{K}}(n) = \{ \vec{s} | \sum_h s_h \leq \gamma \text{ and } \forall h \notin I(n) : s_h = 0 \} ,$$

where $\gamma$ parameterizes the considered sparsity level. For more details and for a visualization of such a constructed set $\tilde{\mathcal{K}}(n)$ see, e.g., (Lücke and Eggert, 2010, Fig. 2) or (Sheikh et al., 2014). The sets $\tilde{\mathcal{K}}(n)$ were then directly used for the estimation of expectation values (4).

Instead of this previous direct use of $\tilde{\mathcal{K}}(n)$ to define truncated posteriors, we can based on the results obtained here, use $\tilde{\mathcal{K}}(n)$ as newly suggested states of Alg. 1, and combine its elements with the old states $\mathcal{K}_{\text{old}}(n)$ to maximally increase the free energy. Such a procedure would profit from well methods to construct sets $\tilde{\mathcal{K}}$ for the different generative models of previous work. On the downside, any new generative model would require the definition of new construction procedures, and such constructions often make use of ad hoc assumptions such as sparsity (Henniges et al., 2010; Dai et al., 2013; Henniges et al., 2014). On the other hand, novel approaches to automate the construction of sets $\mathcal{K}$ (see Shelton et al., 2017) can directly be applied in this context. In any case, deterministic construction closely links TV-EM to a series of previous pre-selection based EM approximations (Lücke and Eggert, 2010), which have motivated this work initially. Importantly, these previous approaches can now be interpreted as TV-EM with an estimated, one-step partial TV-E-step. ‘Estimated’ because any direct definition of the states to define an approximation does not guarantee the free energy to increase; and the previous procedures are ‘one-step’ because the variational loop of Alg. 1 is replaced by one construction step.

Combination with sampling. A further alternative to blind search would be a stochastic search for new states $\tilde{\mathcal{K}}$ in Alg. 1 using knowledge given by the generative model. Already using the prior distribution of the generative model under consideration would be more efficient than to blindly sample hidden states, e.g., using a uniform distribution. Samples from the prior would lie in areas of the latent space where at least the average over all posteriors has a high probability mass. The space of high prior mass can still be very large, however, and for any given data point, large posterior mass may be located in areas of the latent space very different from areas of high average posterior mass.

Procedures that generate $\tilde{\mathcal{K}}$ by sampling new variational states in a data-driven way promise to be much more efficient. For instance, if samples for newly suggested $\tilde{\mathcal{K}}(n)$ are drawn from the
posterior distribution \( p(\vec{s} | \vec{y}^{(n)}, \Theta) \), their joint probabilities can be expected to be relatively high (and with them the free energy \( F(\mathcal{K}, \Theta) \)). As the relative values of the joints are the crucial criterion to find good sets \( \mathcal{K}^{(n)} \), the common normalizer \( p(\vec{y} | \Theta) \) is not relevant. This observation together with the existence of a well established research field on efficient procedures to generate posterior samples, would represent the advantages of such an approach. Potential disadvantages are that the highest posterior states will quickly be represented by the sets \( \mathcal{K}^{(n)} \) and that many new samples of \( p(\vec{s} | \vec{y}, \Theta) \) may therefore already be contained in \( \mathcal{K} \). Furthermore, posterior sampling is known to be challenging in high-dimensional latent spaces especially for discrete latents. Many of these challenges may potentially carry over to TV-EM if samples from the posterior are used.

Preliminary work by Lücke et al. (2017) investigates such sampling procedures using TV-EM for two concrete models, Binary Sparse Coding (BSC; Haft et al., 2004; Henniges et al., 2010) and sigmoid belief networks (Saul et al., 1996; Jordan et al., 1999). The approach emphasizes scalability and autonomous ‘black-box’ optimization procedures. Both is achieved using a combination of prior sampling and approximate marginal sampling, as both these sampling procedures can be defined without additional derivations.

6.2 TV-EM for Mixture Models

Mixture models can be regarded as complementary to multiple-cause generative models. In their different versions, they are among the most widely applied generative data models and very successful in many tasks of image or sound processing as well as for general pattern analysis tasks (e.g. McLachlan and Peel, 2004; Duda et al., 2001; Zoran and Weiss, 2011; Povey et al., 2011). In contrast to multiple-cause models, any observed variable \( \vec{y} \) is in mixture models assumed to be generated by exactly one cause, i.e., one class. In their most standard version, a discrete hidden variable \( c \) is taken to represent one of \( C \) causes or clusters and to generate data via a noise distribution \( p(\vec{y} | c, \Theta) \). The data distribution assumed by a mixture model is thus given by:

\[
p(\vec{y} | \Theta) = \sum_{c=1}^{C} \pi_c p(\vec{y} | c, \Theta) \quad \text{with} \quad \sum_{c=1}^{C} \pi_c = 1,
\]

where the prior parameters \( \pi_c = p(c | \Theta) \in [0, 1] \) are model parameters commonly referred to as mixing proportions.

As the hidden variable is discrete, TV-EM can directly be applied. We here only change the notation slightly to be more consistent with the conventional mixture model notation, i.e., we replace \( \vec{s} \) for the hidden variable by the integer \( c \in \{1, \ldots, C\} \). The sets \( \mathcal{K}^{(n)} \) then consequently contain subsets of class indices, \( \mathcal{K}^{(n)} \subseteq \{1, \ldots, C\} \).

Mixture models may not be considered as the typical application domain of variational EM procedures, but they were used as example applications already early on. Neal and Hinton (1998), for instance, motivated the application of variational EM by its increased efficiency for mixture models, and we will see below that the same motivation applies for the application of TV-EM.

For this example we consider TV-EM with a full E-step (Eqns. 7 to 9). Based on Eqn. 7 the TV-E-step for mixture models corresponds to finding those states \( c \) that globally maximize the simplified free energy \( F(\mathcal{K}, \Theta) \) of Prop. 3 w.r.t. \( \mathcal{K} \). Let us again constrain all sets \( \mathcal{K}^{(n)} \) to be of the same size, i.e., \( |\mathcal{K}^{(n)}| = C' \leq C \) in this case. Because of the form of the free energy in Eqn. 31,
we can now show that it is sufficient and efficient to pair-wise compare all joint probabilities in order to find optimal $K^{(n)}$.

**Proposition 7**
Consider the application of TV-EM to a mixture model given by (55) with $C$ clusters, and let $K^{(n)}$ (with $|K^{(n)}| = C'$) be the set of variational states for a data point $\tilde{y}^{(n)}$.

Then the free energy is maximized in the TV-E-step (7) if for all $n = 1, \ldots, N$ the sets $K^{(n)}$ contain the $C'$ clusters with the largest joint probabilities, i.e., if

$$\text{for all } c \in K^{(n)} \text{ and } c' \notin K^{(n)} : p(c, \tilde{y}^{(n)} | \Theta) \geq p(c', \tilde{y}^{(n)} | \Theta).$$

(56)

Such a maximum can be found using $O(NC)$ comparisons of joint probabilities.

**Proof**
Let us consider the set $K = (K^{(1)}, \ldots, K^{(N)})$ for which each $K^{(n)}$ fulfills criterion (56). If we now replace for a specific but arbitrary $n$ an arbitrary $c \in K^{(n)}$ by a $c' \notin K^{(n)}$ then by our definition of $K$: $p(c', \tilde{y}^{(n)} | \Theta) \leq p(c, \tilde{y}^{(n)} | \Theta)$. According to Prop. 6, the free energy is then decreased or remains constant. As for any $n$ a change of any cluster $c \in K^{(n)}$ results in a decreased or constant free energy, the set $K$ must represent a global maximum of $F(K, \Theta)$ (no better set can be found).

Regarding the complexity of finding the maximum, let $C^{(n)}$ be a list of all joint probabilities $p(c, \tilde{y}^{(n)} | \Theta)$ for a fixed data point $\tilde{y}^{(n)}$. All such lists $C^{(n)}$ are of size $C$. Let us first suppose that all elements in $C^{(n)}$ have different values. Finding the set $K^{(n)}$ which fulfills (56) is then the problem of finding the $|K^{(n)}|$ largest elements in a list of $C$ elements. This partial sorting problem is according to [Blum et al., 1973] solvable using $O(C)$ comparisons of the elements. In case of two or more identical elements in $C^{(n)}$, the same partial sorting procedure returns a list (i.e., a set $K^{(n)}$) which also fulfills (56) (but there may now be more than one such $K^{(n)}$ satisfying the criterion). By repeating the procedure $N$ times (once for each data point $n$), we can define a set $K = (K^{(1)}, \ldots, K^{(N)})$ for which each $K^{(n)}$ fulfills (56). The set $K$ is therefore (A) computable using $O(NC)$ comparisons of joint probabilities, and (B) it maximizes the free energy because all its $K^{(n)}$ satisfy (56).

Prop. 7 defines a concrete deterministic and efficient procedure applicable to any mixture model of the form (55). In practice, the procedure requires to actually compute all the joint probabilities first (at least up to a common factor) in order to realize the required comparison. The computational demand for computing the joints is $O(NC)$ times the computations required for the evaluation of each joint (which is usually proportional to the number data space dimensions $D$), e.g., $O(NC\times D)$ for Gaussian Mixture Models (GMMs).

As mixture models have latent state spaces of size linear in $C$, it may not be considered surprising that TV-EM is applicable using $O(NC)$ comparisons of joint probabilities. After all, an exact E-step of standard EM, e.g., for GMMs, also only requires $O(NC\times D)$ computations. However, TV-EM can reduce the required computations for the M-step because it uses exact zeros, i.e., M-steps with expectation values (4) can be shown to be less complex. The price to pay
Algorithm 2: Application to Mixture Models.

```
init model parameters \( \Theta^{old} \);
repeat
  for \( n = 1 : N \) do
    for \( c = 1 : C \) do
      compute \( p(c, \tilde{y}^{(n)} | \Theta^{old}) \);
    define \( K^{(n)} \) to contain the \( C' \) indices \( c \) with largest \( p(c, \tilde{y}^{(n)} | \Theta^{old}) \);
    compute \( \Theta^{new} \) that maximizes \( Q(\Theta) = \sum_{n=1}^{N} \left\langle \log \left( p(c, \tilde{y}^{(n)} | \Theta) \right) \right\rangle_{q^{(n)}(c;K,\Theta^{old})} \);
    \( \Theta^{old} = \Theta^{new} \);
  until parameters \( \Theta \) have sufficiently converged;
```

for this reduction is that the formal optimization problem of the TV-E-step (Eqn. 7) considers an optimization problem on a space larger than the state space. For the here (and throughout the paper) assumed equally sized sets \( K^{(n)} \) (here \(|K^{(n)}| = C'\)), the number of all possible subsets \( K^{(n)} \subseteq \{1, \ldots, C\} \) is \( \binom{C}{C'} \). Prop. 7 ensures that we do not have to exhaustively visit all these subsets but can find the maximizing set for each \( n \) efficiently. Again, this efficiency result is ultimately due to the simplified form of the free energy (31).

The application of TV-EM to mixture models (as summarized by Alg. 2) now allows for interpreting earlier applications to mixture models within the derived free energy framework. Truncated approximations were previously applied to mixture models, e.g., to GMMs in work by Shelton et al. (2014) and later by Hughes and Sudderth (2016). The cluster finding procedure used by Shelton et al. (2014) can in the light of this study be recognized as an estimated TV-E-step (using Gaussian Processes to construct the sets \( K^{(n)} \)), while the constrained likelihood optimization for exponential family mixtures as used by Hughes and Sudderth (2016) can be recognized as a full TV-E-step. For Poisson mixtures, Forster and Lücke (2017b) directly applied the TV-EM algorithm (Alg. 2) suggested by Prop. 7. For all the above applications, our theoretical results show that the free energy (31) is the underlying objective function which is maximized. For the algorithms Hughes and Sudderth (2016) and Forster and Lücke (2017b) the TV-EM application to mixture models, furthermore, warrants that the free energy is provably monotonically increased, which follows from Prop. 5 and has not been shown previously. Furthermore, our results apply for any mixture model of the form (55) and for Alg. 2 as well as for corresponding partial EM versions.

The main motivation and focus of the previous truncated approximations for mixture models Hughes and Sudderth (2016) Forster and Lücke (2017b) was the increase of efficiency. The source for the reduction of computational efforts were hereby the hard zeros introduced by truncated posteriors, which significantly reduced the required number of numerical operations in the M-step. The work by Hughes and Sudderth (2016) focuses on this M-step complexity reduction, and they empirically find that the whole EM optimization only requires about half the operations compared
to exact EM. Also, Forster and Lücke (2017b) focus on the complexity reduction provided by the M-step and observe a similar efficiency increase for Poisson mixtures. Notably, TV-EM does not negatively effect the final likelihood values that were reported in these studies. On the contrary, faster convergence and higher final likelihoods for different datasets were observed empirically (Hughes and Sudderth, 2016; Forster and Lücke, 2017b; Lücke and Forster, 2017). This is due to TV-EM avoiding local likelihood optima more efficiently than exact EM – an effect that has also been observed for sparse coding models and (preselection-based) truncated approximations (Exarchakis et al., 2012).

Except of reducing the M-step complexity by TV-EM (Hughes and Sudderth, 2016; Forster and Lücke, 2017b), the here derived results point to a further possibility for complexity reduction. In deriving partial TV-EM (Eqns. 50) we have shown that the free energy (31) also monotonically increases for partial TV-E-steps. A full maximization is, hence, not required to obtain an algorithm that provably increases (31). As efficient criteria to verify increased free energies are available, very efficient partial E-steps were investigated in work parallel to this study. Forster and Lücke (2017a) have thus shown that clustering algorithms in which each EM iteration scales sublinearly with $C$ can be derived. Numerical experiments then show that the free energy (and likelihood) objective is still efficiently increased, which provides evidence for clustering being scalable sublinearly with $C$ (for details see Forster and Lücke, 2017a).

6.3 TV-EM and ‘hard EM’

A very wide-spread approach to optimize parameters of a given generative model is ‘hard EM’ also known as zero-temperature EM, MAP approximation, Viterbi training, classification EM, etc (see introduction). As the name suggests, ‘hard EM’ is typically introduced as an EM-like algorithm in which the computation of the full posterior in the E-step is replaced by the computation of the state $\vec{s}$ with maximum a-posterior (MAP) probability. In the M-step, the model parameters are then updated by only considering this maximum a-posterior state. Alg. 3 shows a standard form of the ‘hard EM’ algorithm.

‘Hard EM’ is often regarded as an ad hoc procedure, which replaces a computationally intractable full posterior in the E-step by a maximization. Such a maximization is easier because it can be reformulated as the maximization of a computationally tractable objective, the joint $p(\vec{s}, \vec{y}^{(n)} | \Theta)$ (as the normalizer $p(\vec{y}^{(n)} | \Theta)$ does not depend on $\vec{s}$). ‘Hard EM’ can, however, also be derived from annealed versions of EM. Annealed EM is a procedure usually introduced in order to avoid local optima (e.g. Ueda and Nakano 1998; Sahani 1999). A temperature parameter is introduced which forces the probability values of the posterior to become more equal. While

---

**Algorithm 3: The ‘Hard EM’ algorithm.**

init model parameters $\Theta^{old}$;

repeat

for $n = 1 : N$ do

$\vec{s}^{(n)} = \arg\max_{\vec{s}} \{ p(\vec{s}, \vec{y}^{(n)} | \Theta^{old}) \}$; \hspace{1cm} (hard E-step)

$\Theta^{new} = \arg\max_{\Theta} \{ \sum_n \log \{ p(\vec{s}^{(n)}, \vec{y}^{(n)} | \Theta) \} \}$; \hspace{1cm} (M-step)

$\Theta^{old} = \Theta^{new}$;

until parameters $\Theta$ have sufficiently converged;
annealed EM algorithms are obtained for high temperatures, ‘hard EM’ is obtained if instead the limit to zero temperature is considered (see Appendix for details). In any case, ‘hard EM’ remains rather an heuristic approach; it requires to take a limit (temperature zero), and it implicitly assumes that states that maximize the posteriors can actually be found.

By considering Alg. 3, ‘hard EM’ can be formulated by replacing the posterior by a $\delta$-function centered at the MAP state (often termed Dirac-$\delta$ in the continuous and Kronecker-$\delta$ in the discrete case). So far, $\delta$-functions have merely been considered in this context as a way to explicitly formulate the function which replaces the full posterior in the MAP approximation. Following the introduction of truncated posteriors for TV-EM, and in virtue of Props. 1 and 2, we can now treat the $\delta$-functions fully variationally. For this, we consider the states for which the $\delta$-functions are non-zero as variational parameters of truncated distributions. Such a formulation then corresponds to a TV-EM algorithm with sets $\mathcal{K}^{(n)}$ which each contain just one element, i.e. $\mathcal{K}^{(n)} = \{ \tilde{s}^{(n)} \}$ for all $n$. More precisely, we can for this boundary case of TV-EM show the following:

**Proposition 8**
Consider a generative model $p(\tilde{s}, \tilde{y} | \Theta)$ with discrete latents $\tilde{s}$. Then ‘hard EM’ for this model (Alg. 3) is equivalent to a TV-EM algorithm which uses sets $\mathcal{K}^{(n)}$ with just one element each.

**Proof**
Note that all results derived for truncated variational distributions, so far, apply for arbitrary (non-empty) sets $\mathcal{K}^{(n)}$. For a TV-EM algorithm with sets $\mathcal{K}^{(n)}$ that contain just one element each, we can denote these elements by $\tilde{s}^{(n)}$, i.e., $\mathcal{K}^{(n)} = \{ \tilde{s}^{(n)} \}$. Let us first consider the simplified truncated free energy (31) derived in Prop. 3. For $\mathcal{K}^{(n)} = \{ \tilde{s}^{(n)} \}$ we then obtain:

$$
\mathcal{F}(\mathcal{K}, \Theta^{\text{old}}) = \sum_{n=1}^{N} \log \left( \sum_{\tilde{s} \in \mathcal{K}^{(n)}} p(\tilde{s}, \tilde{y}^{(n)} | \Theta^{\text{old}}) \right) = \sum_{n=1}^{N} \log \left( p(\tilde{s}^{(n)}, \tilde{y}^{(n)} | \Theta^{\text{old}}) \right).
$$

(57)

The maximum of $\mathcal{F}(\mathcal{K}, \Theta^{\text{old}})$ w.r.t. $\mathcal{K} = (\mathcal{K}^{(1)}, \ldots, \mathcal{K}^{(N)})$ can be found by individually maximizing each summand $\log \left( p(\tilde{s}^{(n)}, \tilde{y}^{(n)} | \Theta^{\text{old}}) \right)$ w.r.t. $\tilde{s}^{(n)}$. The states $\tilde{s}^{(n)}$ that maximize the summands are then the same as those computed in the hard E-step of Alg. 3 because:

$$
\tilde{s}^{(n)} = \arg\max_{\tilde{s}} \{ \log \left( p(\tilde{s}, \tilde{y}^{(n)} | \Theta^{\text{old}}) \right) \} = \arg\max_{\tilde{s}} \{ \log \left( p(\tilde{s}^{(n)}, \tilde{y}^{(n)} | \Theta^{\text{old}}) \right) \}.
$$

(58)

The new set $\mathcal{K}^{\text{new}}$ which is computed by the TV-E-step is consequently given by $\mathcal{K}^{\text{new}} = \{ \tilde{s}^{(1)} \}, \ldots, \{ \tilde{s}^{(N)} \}$. In the TV-M-step the truncated free energy $\mathcal{F}(\mathcal{K}^{\text{new}}, \Theta^{\text{old}}, \Theta)$ is then optimized w.r.t. $\Theta$. When $\mathcal{K}^{(n)} = \{ \tilde{s}^{(n)} \}$, a truncated distribution $q^{(n)}(\tilde{s}^{(n)} | \mathcal{K}^{\text{new}}, \Theta^{\text{old}})$ is unequal zero only for the state $\tilde{s} = \tilde{s}^{(n)}$, i.e., $q^{(n)}(\tilde{s}^{(n)} | \mathcal{K}^{\text{new}}, \Theta^{\text{old}}) = \delta(\tilde{s} = \tilde{s}^{(n)})$. As, additionally, the entropy term of the free energy vanishes for such $q^{(n)}$, the free energy $\mathcal{F}(\mathcal{K}, \Theta^{\text{old}}, \Theta)$ reduces to:

$$
\mathcal{F}(\mathcal{K}^{\text{new}}, \Theta^{\text{old}}, \Theta) = \sum_{n=1}^{N} \left[ \sum_{\tilde{s}} q^{(n)}(\tilde{s}^{(n)} ; \mathcal{K}^{\text{new}}, \Theta^{\text{old}}) \log \left( p(\tilde{s}^{(n)}, \tilde{y}^{(n)} | \Theta) \right) \right] + H(q(\tilde{s}^{(n)} ; \mathcal{K}^{\text{new}}, \Theta^{\text{old}}))
$$

$$
= \sum_{n=1}^{N} \left[ \sum_{\tilde{s}} \delta(\tilde{s} = \tilde{s}^{(n)}) \log \left( p(\tilde{s}^{(n)}, \tilde{y}^{(n)} | \Theta) \right) \right] = \sum_{n=1}^{N} \log \left( p(\tilde{s}^{(n)}, \tilde{y}^{(n)} | \Theta) \right).
$$
Maximization of the free energy $\mathcal{F}(K, \Theta^{\text{old}}, \Theta)$ w.r.t. $\Theta$ is thus equivalent to the ‘hard’ M-step of Alg. 3. As the $\vec{s}^{(n)}$ used in the hard M-step are precisely those computed in the ‘hard’ E-step, TV-EM with just one element for each $K^{(n)}$ is equivalent to ‘hard EM’ (Alg. 3).

In practice, the maximization in the hard E-step is often difficult to accomplish, such that states $\vec{s}$ are computed that only approximately maximize the posteriors $p(\vec{s} \mid \vec{y}^{(n)}, \Theta)$. Such a partial ‘hard EM’ approach can then be shown to correspond to TV-EM with a partial E-step (Eqns. 50), and the proof follows along the same line as the proof for Prop. 8.

The equivalence of ‘hard EM’ and TV-EM with one state per $K^{(n)}$ (as provided by Prop. 8) applies for any generative model with discrete latents. Based on this equivalence we can instantly conclude that ‘hard EM’ optimizes a truncated free energy.

**Corollary 2**

Consider a generative model $p(\vec{s}, \vec{y} \mid \Theta)$ with discrete latents $\vec{s}$. Then ‘hard EM’ monotonically increases a lower free energy bound of the log-likelihood given by:

$$
\mathcal{F}(\vec{s}^{(1:N)}, \Theta) = \sum_{n=1}^{N} \log \left( p(\vec{s}^{(n)}, \vec{y}^{(n)} \mid \Theta) \right) \leq \mathcal{L}(\Theta),
$$

where $\vec{s}^{(n)}$ are the states computed in the ‘hard’ E-step and the $\Theta$ are the parameters computed by the hard M-step of Alg. 3. The free energy (59) is also monotonically increased if each ‘hard’ E-step in Alg. 3 just monotonically increases (instead of maximizes) the posteriors, i.e. if $\vec{s}^{(n)}$ are found such that for all $n$ applies:

$$
p(\vec{s}^{(n)} \mid \vec{y}^{(n)}, \Theta^{\text{old}}) \geq p(\vec{s}^{(n)}_{\text{old}} \mid \vec{y}^{(n)}, \Theta^{\text{old}}),
$$

where $\vec{s}^{(n)}_{\text{old}}$ are the states found in the previous ‘hard’ E-step.

After each ‘hard EM’ iteration or partial ‘hard EM’ iteration, the difference between log-likelihood (2) and free energy (59) is given by:

$$
\mathcal{L}(\Theta) - \mathcal{F}(\vec{s}^{(1:N)}, \Theta) = -\sum_{n=1}^{N} \log \left( p(\vec{s}^{(n)} \mid \vec{y}^{(n)}, \Theta) \right).
$$

**Proof**

According to Prop. 8, ‘hard’ EM is equivalent to TV-EM (with sets $K^{(n)} = \{ \vec{s}^{(n)} \}$), which implies that results of Props. 1 to 5 are applicable to ‘hard’ EM, including a guaranteed monotonic increase of the simplified truncated free energy (31). For $K^{(n)} = \{ \vec{s}^{(n)} \}$ the truncated free energy $\mathcal{F}(K, \Theta)$ is given by (59), where we replaced $K = \{ \{ \vec{s}^{(1)} \}, \ldots, \{ \vec{s}^{(N)} \} \}$ by $\vec{s}^{(1:N)}$, which proves the first claim.

According to the results for partial TV-EM (Sec. 5.2), the free energy (59) also monotonically increases for a partial TV-E-step (Optimization 1 of Eqns. 50). For $K^{(n)} = \{ \vec{s}^{(n)} \}$, the free energy (59) is monotonically increased if for all $n$ applies $p(\vec{s}^{(n)} \mid \vec{y}^{(n)} \mid \Theta^{\text{old}}) \geq p(\vec{s}^{(n)}_{\text{old}} \mid \vec{y}^{(n)} \mid \Theta^{\text{old}})$ (compare Prop. 6). As the data points are constant, this condition is equivalent to condition (60).
which proves the claim, i.e., it is sufficient to monotonically increase $p(\tilde{\mathbf{s}} | \tilde{g}^{(n)}, \Theta^{\text{old}})$ for all $n$ given the current parameters $\Theta^{\text{old}}$, and starting from the previous MAP states $\tilde{s}_n^{(n)}$.

According to Props. 1 to 3, $\mathcal{F}(\tilde{s}^{1:N}, \Theta)$ is, as a special case of $\mathcal{F}(\tilde{s}^{1:N}, \Theta^{\text{old}}, \Theta)$, a lower bound of the log-likelihood. Furthermore, the difference $\mathcal{L}(\Theta) - \mathcal{F}(\tilde{s}^{1:N}, \Theta)$ is given by the KL-divergence $\sum_n D_{\text{KL}}(q^{(n)}(\tilde{s}; \mathcal{K}, \Theta), p(\tilde{s} | \tilde{g}^{(n)}, \Theta))$ (Corollary 1). As the truncated variational distributions are here given by $q^{(n)}(\tilde{s}; \mathcal{K}^{\text{new}}, \Theta^{\text{old}}) = \delta(\tilde{s} = \tilde{s}^{(n)})$, we obtain (61). The relation between $\mathcal{L}(\Theta) - \mathcal{F}(\tilde{s}^{1:N}, \Theta)$ and the KL-divergence also applies for partial TV-EM and consequently for partial ‘hard EM’ as a special case.

Algorithmically, Prop. 8 does not represent much novelty: optimizations by ‘hard EM’ or (non-partial) TV-EM with $|\mathcal{K}^{(n)}| = 1$ are the same. Importantly, however, Prop. 8 and Corollary 2 for the first time fully embed the frequently used ‘hard EM’ approaches into the theoretical framework of variational free energy optimization. Importantly, this embedding includes the in practice frequently used ‘hard EM’ algorithms which use a partial E-step as a full maximization is computationally more expensive or even NP-hard (see, e.g., Cohen and Smith, 2010). In these cases, Corollary 2 provides the directly applicable result of monotonically increasing free energies, and it provides the theoretical justification for memorizing previous (approximate) MAP states as starting values for the next MAP optimization. The embedding of ‘hard EM’ into the free energy framework is made possible, first, by Prop. 1 and 2, and, second, by the further theoretical results specific to truncated distributions (Props. 3 to 5) which allow to interpret the MAP states $\tilde{s}^{(n)}$ as variational parameters. Note that annealed EM (see Appendix) does not provide such an embedding. Using a rigorous treatment similar to the one for truncated distributions considered in this work, results similar to Props. 4 and 5 may be derivable, and for the limit to zero temperature, results similar to those of Props. 1 and 2 would have to be derived.

Considering the free energy (59), note that objective functions optimized by ‘hard EM’ have already previously been discussed. However, they were usually defined as a tool to interpret the heuristically introduced ‘hard EM’ algorithm. Instead, we have here shown that ‘hard EM’ and its optimization objective can be derived in the same mathematically grounded way as other variational EM procedures such as mean-field or Gaussian variational EM. That is, we considered a constrained set of functions for the approximation of full posteriors, and then canonically derived a variational EM algorithm and a provably increasing free energy objective.

In addition to embedding ‘hard EM’ into the free energy framework, Prop. 8 shows that ‘hard EM’ is a special case of TV-EM. We can, therefore, now also interpret TV-EM as a generalization of ‘hard EM’. TV-EM algorithms using sets $\mathcal{K}^{(n)}$ with more than one element do maintain ‘hard’ (i.e., exact) zeros but they do allow for more than one hidden state with non-zero probability. Such TV-EM generalization of ‘hard EM’ are notably non-trivial. For ‘hard EM’ we do not necessarily require Prop. 5 in order to show that the free energy monotonically increases. This is because the free energy and its simplified version given by Prop. 3 coincide for one element per $\mathcal{K}^{(n)}$. In this case TV-EM (i.e., ‘hard EM’) becomes a straight-forward coordinate-wise ascent approach w.r.t. to this objective. However, any generalization to more than one state with non-
zero probability changes the free energy objective $\mathcal{F}(\mathcal{K}, \Theta)$ to the more general form given by Prop. 3. Taking derivatives of $\mathcal{F}(\mathcal{K}, \Theta)$ in (31) w.r.t. $\Theta$ is now different from taking derivatives of the free energy $\mathcal{F}(\mathcal{K}, \Theta^{old}, \Theta)$ in (28). If the standard M-step equations for a given generative model are maintained (which optimize $\mathcal{F}(\mathcal{K}, \Theta^{old}, \Theta)$) then we require Prop. 5 to show that TV-EM indeed monotonically increases the free energy.

For mixture models, truncated approximations which maintain two, three or other low numbers of states have in empirical studies been found to work very well in practice. Such ‘almost hard EM’ approaches have been applied to invariant multiple-causes models (Dai and Lüdecke 2012; Dai et al., 2013), invariant mixture models (Dai and Lüdecke 2014), standard Gaussian mixture models (Shelton et al., 2014; Hughes and Sudderth, 2016; Lüdecke and Forster, 2017), Poisson mixtures (Forster and Lüdecke, 2017b) and topic models (Hughes and Sudderth, 2016). Already maintaining very low numbers of states per data point was in many experiments shown to efficiently and effectively recover ground-truth parameters, e.g., for GMMs (Shelton et al., 2014; Hughes and Sudderth, 2016), and to very efficiently improve the likelihood objective (Hughes and Sudderth, 2016; Forster and Lüdecke, 2017b; Lüdecke and Forster, 2017; Forster and Lüdecke, 2017a). Earlier applications of truncated approximations (e.g. Dai et al., 2013; Dai and Lüdecke, 2014; Shelton et al., 2014) do not use the theoretical framework derived here but their E-steps can (according to Sec. 6.1) be interpreted as estimated TV-E-steps.

7 Discussion

We have defined and analyzed a novel variational approximation of expectation maximization (EM). Our approach is based on truncated a-posteriori distributions with latent states as variational parameters. Our first set of results (Props. 1 and 2) generalize the variational free energy approach as introduced, e.g., by Saul et al. (1996); Neal and Hinton (1998); Jordan et al. (1999) by including discrete variational distributions with exact zeros. While this generalization is required in order to study truncated variational distributions, Props. 1 and 2 also apply for any other discrete distributions with exact ‘hard’ zeros, i.e., these results are not restricted to the specific truncated distributions of Eqn. 3. As such, Props. 1 and 2 generalize the standard textbook derivation of variational free energies (e.g. Bishop, 2006; Murphy, 2012; Barber, 2012), i.e., the standard additional demand of $q(\hat{s}) > 0$ can be dropped for the discrete case. Props. 3, 4, 5 and Corollary 1 then represent results specific to variational distributions in the form of truncated posteriors (Eqn. 3). Props. 6, 7 and 8 and Corollary 2, finally, represent example applications of the theoretical results.

Relation to Preselection-Based Truncated Approximations. Previous algorithms based on truncated approximations of expectation values (Lüdecke and Sahani, 2008; Lüdecke and Eggert, 2010; Henniges et al., 2014; Dai and Lüdecke, 2014; Sheikh et al., 2014; Sheikh and Lüdecke, 2016; Shelton et al., 2017) have motivated this work. These contributions have directly approximated expectation values by exploiting sparsity of latent activities (Lüdecke and Sahani, 2008) and by additionally using a preselection procedure in what was termed Expectation Truncation (ET; Lüdecke and Eggert, 2010). Based on the theoretical framework derived in this work and Sec. 6.1 all previous selection-based approaches can be considered as approximations of TV-EM. Expectation
Truncation can thus be embedded into the framework of variational approaches. While estimated E-steps using ET may potentially decrease the truncated free energy of Prop. 3, the general effectiveness and efficiency of previous ET applications may be taken as evidence for the efficiency and effectiveness of truncated approximations in general. Such efficiency and effectiveness can now be generalized and theoretical guarantees for tractable free energies are available. Furthermore, and maybe most importantly, TV-EM can now provide (A) a straight-forward generalization and applicability to very advanced (including deep) data models, and (B) it avoids any additional effort to define model specific selection functions (compare discussion of ‘black box’ procedures below).

In one aspects, ET provides a result that has not been addressed here, however: it can be shown that preselection allows for the definition of smaller generative models defined per data point, and that optimizing parameters of such smaller models approximately optimizes the parameters of the original larger generative model. This result, valid for a large class of generative models (but not for all), has been used in select-and-sample approaches (Shelton et al., 2012, 2015), was formally proven in (Sheikh and Lücke, 2016), and carries over to recent work using selection functions that are themselves learned from data (Shelton et al., 2017).

Relation to mean-field and ‘sparse EM’. Truncated variational EM is a variational approximation for models with discrete latents. Gaussian variational EM is not applicable to discrete hidden variables. The main standard class of variational approaches for comparison with TV-EM is therefore given by factored variational (i.e. mean-field) approaches (Saul and Jordan, 1996; Jordan et al., 1999). Compared to fully factored approaches (Eqn. 16), a main difference to TV-EM is that truncated approaches do not assume posterior independence. Assuming independence (i.e., neglecting explaining-away effects) has been observed to negatively impact likelihood optimization for different types of generative models (Ilin and Valpola, 2003; MacKay, 2003; Turner and Sahani, 2011; Sheikh et al., 2014). To address such potentially harmful consequences of posterior independence, partly factored approaches (sometimes called structured variational or structured mean-field approaches) have been studied (Saul and Jordan, 1996; MacKay, 2003; Bouchard-Côté and Jordan, 2009). Any deviation from fully factored approaches does, however, often go along with increased analytical and computational effort, and may even provide only limited improvements compared to mean-field (e.g. Turner and Sahani, 2011, for a discussion). In comparison, TV-EM does not assume independence. Computational tractability is instead achieved by approximating posteriors by considering only small subsets of the latent space.

Other than mean-field variational approximations, ‘sparse EM’ is another (less frequently applied) alternative which was discussed early on in the very influential work by Neal and Hinton (1998). Notably, Neal and Hinton (1998) never explicitly mentioned factored variational distributions in their work. Instead the paper discussed with ‘sparse EM’ a variational approach that shares more similarities with TV-EM than with mean-field. In their ‘sparse algorithm’, Neal and Hinton (1998) suggested a variational distribution defined on a subset of the state space which only contains ‘plausible’ values of the latents (their Sec. 5). The probabilities outside of this set were ‘frozen’ to values of an earlier iteration but updated once in a while during learning. The procedure there described is not efficient, e.g. for latent variable models with large state spaces, because ‘sparse EM’ still requires an occasional evaluation of all latent states. As Neal and Hinton (1998) discuss an application to a mixture model, this shortcoming is not very relevant for their
paper. In contrast to ‘sparse EM’, truncated approximations assume exact zeros and can thus realize approximations without ever having to evaluate all hidden states while they are still able to find subsets of the latent space with high posterior mass. However, despite these differences, the results obtained for TV-EM in this work may be regarded as connecting back to an initial (and never followed up) train of thoughts expressed in the work by Neal and Hinton (1998).

### Relation to ‘hard EM’.

A further, very influential class of approximate EM algorithms is ‘hard EM’ (alias ‘zero temperature EM’, ‘classification EM’ or EM using MAP approximations). ‘Hard EM’ approaches have been used for many types of data models including deep models, and they were often observed to work very well in practice. Because of their wide-spread use, e.g., in domains such as sparse coding (Olshausen and Field, 1996; Mairal et al., 2010), compressive sensing (Donoho, 2006; Baraniuk, 2007) but also for relating generative modeling and deep learning (Patel et al., 2016), ‘hard EM’ may even be considered more wide-spread than any conventional or novel variational EM approach. As shown in Sec. 6.3, we here identified ‘hard EM’ as a TV-EM algorithm with sets of variational parameters $\mathcal{K}^{(n)}$ just containing one state (Prop. 8 and Corollary 2). ‘Hard EM’ (including versions with partial posterior optimization) can consequently be cleanly embedded into the variational EM framework and monotonically increasing free energies can be provided. Furthermore, TV-EM provides concrete procedures to generalize any ‘hard EM’ algorithm to algorithms with multiple ‘winning’ states.

For instance, for training of deep networks with ‘hard EM’ (e.g. Poon and Domingos, 2011; Van den Oord and Schrauwen, 2014; Patel et al., 2016), generalizations with more than one non-zero state maybe considered very interesting (especially considering the effectiveness of such approaches for mixture models; e.g. Hughes and Sudderth, 2016; Forster and Lücke, 2017b). Similarly, time-series models such as Hidden Markov Models (HMMs) and their many variants are often trained using ‘hard EM’ (Juang and Rabiner, 1990; Cohen and Smith, 2010; Allahverdyan and Galstyan, 2011). TV-EM generalizations would thus provide promising future generalizations especially when noting that algorithms estimating multiple winning states are sometimes readily available (e.g. Foreman, 1992; Huang et al., 2012). Again, TV-EM may also serve to interpret earlier combinations of ‘hard EM’ and standard EM for HMMs (e.g. Allahverdyan and Galstyan, 2011; Spitkovsky et al., 2011) on the ground of a variational EM framework.

But also for long-standing standard tasks such as clustering, the here obtained results are of direct theoretical and practical relevance. By applying TV-EM to a special case of GMMs (isotropic and equally weighted Gaussians), Lücke and Forster (2017) have shown, for instance, that the optimization of cluster centers decouples from the optimization of cluster variance for $\mathcal{K}^{(n)}$ with just one element (while the same is not true for $|\mathcal{K}^{(n)}| > 1$). The optimization of cluster centers is then observed to be equivalent to $k$-means. The equivalence is notably obtained without the requirement of taking the limit to zero cluster variances (which is the standard textbook procedure to relate GMMs and $k$-means, e.g., MacKay, 2003; Barber, 2012). Furthermore, TV-EM for GMMs provides a free energy objective which is provably (and in this case strictly) increased by $k$-means. The objective bounds the GMM log-likelihood from below and is a function of the $k$-means objective, i.e., of the quantization error (see Lücke and Forster, 2017 for details).

Finally, note that Prop. 8 and Corollary 2 apply in general for any generative model, which (A) implies that TV-EM generalizations of any previous ‘hard EM’ approach are possible, and which (B) suggests that free energy results as for $k$-means and GMMs (Lücke and Forster, 2017)
may be obtained also for other generative models with discrete latents.

**Relation to Sampling.** While standard variational EM procedures are typically regarded as being deterministic, TV-EM shares many properties with stochastic (i.e., sampling based) EM approaches. Like sampling approaches, TV-EM approximates probabilities (in our case posteriors) by a set of states in hidden space, and these states are then used to compute expectation values. Indeed, one option to realize concrete TV-EM optimizations is to suggest new states for $K$ by sampling from appropriate distributions (Sec. 6.1). TV-EM also shares with sampling that the accuracy of the approximation is only limited by computational demand. In the limit of infinite computational resources both sampling and TV-EM converge to EM with exact E-steps. The same can not be said about standard variational approaches like mean-field or Gaussian. TV-EM distinguishes itself from sampling, however, by being a variational approach that optimizes a free energy using variational distributions. While truncated approximations can make use of sampling as part of their optimization, sampling is just one option and other procedures like selection functions or other deterministic procedure (compare Sec. 6.2) can be applied. Also the distributions that are used to suggest states for $K$ are not limited to posterior distributions as also other (potentially easier to use) distributions can be sufficiently efficient in providing samples which increase the truncated free energy. While these are all points of difference, the fact that both TV-EM and sampling are approximating posteriors based on finite sets of hidden states, makes TV-EM the variational approximation that is most closely related to sampling. Also other combinations of variational approaches and sampling have been investigated (see discussion of ‘black box’ approaches below) but none directly treats samples as variational parameters.

** Autonomous and General Purpose (‘Black Box’) Inference and Learning.** Other than providing a general procedure to develop a learning algorithm for a specific generative model of interest, TV-EM is also of relevance for the field of autonomous machine learning, which recently attracted a lot of attention ([Rezende and Mohamed, 2015](#), [Tran et al., 2015](#), [Ranganath et al., 2015](#), [Hernandez-Lobato et al., 2016](#)). The goal of this field of study is to provide procedures that minimize expert intervention in the generation and application of learning and inference algorithms. Typically, user intervention is required for a number of steps in the process of developing a concrete learning algorithm for a given model. Both standard variational approaches and standard sampling have to overcome different analytical and practical computational challenges. A factored variational EM approach, for instance, first has to choose a specific form for the variational distributions, and then requires a potentially significant effort to derive update equations for their variational parameters. Instead, TV-EM does not require additional analytical steps for variational E-step equations, expectation values are computed directly based on the variational states. Also in case of sampling, deriving, e.g., an efficient sampler requires additional and potentially highly non-trivial analytical work. On the other hand, the optimization of $K$ for TV-EM may require additional efforts. For previous truncated approximations, the construction of $K$ using preselection was model dependent (see Sec 6.1). However, given the novel results of this work, previous model specific constructions can be replaced by a general purpose optimization of $K$. If such an optimization is provided, then TV-E-steps are obtained which just use the joint probability of the generative model under consideration. For the M-step, a similar model
independence can be achieved, e.g., by using automatic differentiation techniques, which are continuously further developed. The explicit form of TV-EM in Sec. 5.3 makes all the requirements of the algorithms very explicit and salient.

The formulation in terms of joint probabilities \[52\] also relates TV-EM to research on un-normalized statistical models (e.g., Gutmann and Hyvärinen 2012, and references therein). The basic idea of the approach, e.g., by Gutmann and Hyvärinen (2012), is the use of classifiers to discriminate between observed and generated data, which is not used by TV-EM. Further differences are our focus on discrete latents, and our requirement for computationally tractable joint probabilities. This latter requirement was for classifier-based training dropped in later extensions, e.g., by Gutmann and Corander (2016). On the other hand, classifier-based training (also compare Goodfellow et al. 2014) usually requires the definition of comparison metrics in observed space which is not used by TV-EM.

By considering one TV-EM iteration in its explicit form \[52\], also note that TV-EM is very different, e.g., (A) from Rezende and Mohamed (2015) who use normalizing flows and consider continuous latents, (B) from Ranganath et al. (2015) who successively apply mean-field approach to realize latent dependencies, or (C) from work by Tran et al. (2015) based on copulas. Further related studies are work by Salimans et al. (2015) who use Markov Chain Monte Carlo (MCMC) samplers and treat the samples as auxiliary variables within a standard variational free energy framework as well as studies using stochastic variational inference [Hoffman et al., 2013; Hoffman and Blei 2015], where auxiliary distributions for Markov chains are defined and used to approximate true posteriors. Moreover, Gu et al. (2015) use variational distributions as proposal distributions to realize flexible and efficient MCMC sampling. All these approaches are more indirect than the direct treatment of latent states as variational parameters as done by TV-EM. Salimans et al. (2015), for instance, also make a number of choices to define appropriate MCMC samplers (and they focus on models with continuous latents), Hoffman and Blei (2015) do require sampling to estimate analytical intractabilities for their variational lower bound, and Gu et al. (2015) use variational distributions as a means to improve approximations by of MCMC sampling. For TV-EM, sampling is one option to vary the variational parameters, the procedure is by definition tractable for sufficiently small \(K^{(n)}\), and lower bounds are provably monotonically increased. On the other hand, TV-EM is constrained to discrete latents, and (as a novel approach) the performance for many concrete applications (which has been demonstrated for the other approaches discussed) remains to be explored.

In any case, the very active research on such and other very recent methods for a ‘black-box’ optimization framework highlight (A) the requirement for powerful and efficient approaches for advanced data models, and (B) the short-comings of previous mean-field or Gaussian approximations. The use of collections of hidden states within variational approaches, e.g., as done by Salimans et al. (2015); Hoffman and Blei (2015); Gu et al. (2015) or with truncated approaches [Lücke and Eggert 2010; Shelton et al. 2011; Sheikh et al. 2014; Sheikh and Lücke 2016], seems to be a promising general strategy in this respect.

Outlook and Conclusion. The theoretical framework of free energy optimization (e.g. Saul et al. 1996; Neal and Hinton 1998; Jordan et al. 1999) has been and is of exceptional significance for the development of Machine Learning algorithms. In this work we extend the framework to include variational distributions with ‘hard’ zeros and latent states as variational parameters.
The theoretical results derived from these initial assumptions provided us with concise and easily applicable variational EM algorithms as well as concise and tractable forms of free energies. The derived results, consequently, (A) allow for developing novel algorithms, and (B) allow for embedding recent approaches as well as very established approaches into the framework of free energy optimization. Examples for the development of novel algorithms are combinations of variational EM with sampling or preselection methods (Sec. 6.1), or novel algorithms for mixture models (Sec. 6.2). Approaches that the here derived results embed into a variational free energy framework are relatively recent algorithms based on constrained likelihood optimizations by Hughes and Sudderth (2016), and earlier truncated approximations (Lücke and Sahani 2008, Lücke and Eggert 2010, Henniges et al. 2010, Dai and Lücke 2014, Sheikh et al. 2014). Furthermore, the very popular ‘hard EM’ approaches can cleanly be embedded into the general free energy framework (Sec. 6.3). This embedding deepens the insights into the functioning and capabilities of ‘hard EM’, and it allows for its generalizations (Prop. 8, Corollary 2). Still, Secs. 6.1, 6.2 and 6.3 are example applications of the main theoretical results. Further applications may include future derivations of algorithms other than Alg. 1 and 2, or the embedding of further approaches into the free energy framework. The relation between k-means and Gaussian mixtures as studied by Lücke and Forster (2017) may serve as an example for such an application. Future examples may include generalizations of Viterbi training for HMMs (Juang and Rabiner 1990, Cohen and Smith 2010, Allahverdyan and Galstyan 2011) or applications to train deep networks (Poon and Domingos 2011, Van den Oord and Schrauwen 2014, Patel et al. 2016).

Appendix. ‘Hard EM’ and Annealed EM

‘Hard EM’ can be obtained from exact EM by considering annealed versions of EM (compare Sahani 1999, Mackay 2001). For this we use the original posteriors $p(⃗s | ⃗y, Θ)$ to define annealed posteriors $p_T(⃗s | ⃗y, Θ)$ as follows (also compare Ueda and Nakano 1998, Ghahramani and Hinton 2000, Mandt et al. 2016):

First we define a non-negative energy $E(⃗s, ⃗y; Θ)$ given by:

$$E(⃗s, ⃗y; Θ) = − \log \left( p(⃗y, ⃗s | Θ) \right).$$

We then define the annealed posteriors using the Boltzmann distribution:

$$p_T(⃗s | ⃗y, Θ) = \frac{1}{Z_T(⃗y; Θ)} \exp \left( - T E(⃗s, ⃗y; Θ) \right) = \frac{\exp \left( - T E(⃗s, ⃗y; Θ) \right)}{\sum_{⃗s} \exp \left( - T E(⃗s', ⃗y; Θ) \right)},$$

where $T > 0$ is a ‘temperature’ parameter (often $β = \frac{1}{T}$ is used but for our purposes we remain with $T$). For temperatures $T > 1$, the values of annealed posteriors become increasingly similar, and such posteriors are used for annealed EM. For $T = 1$, we obtain the original posteriors. Finally, in the limit of $T \to 0$ we obtain:

$$\lim_{T \to 0} p_T(⃗s(n) | ⃗y(n), Θ) = \lim_{T \to 0} \frac{\exp \left( - T E(⃗s, ⃗y; Θ) \right)}{\sum_{⃗s} \exp \left( - T E(⃗s', ⃗y; Θ) \right)} = \begin{cases} 1 & \text{if } ⃗s = \text{argmin}_{⃗s'} \{ E(⃗s', ⃗y; Θ) \} \\ 0 & \text{otherwise} \end{cases}$$

$$= \begin{cases} 1 & \text{if } ⃗s = \text{argmax}_{⃗s'} \{ p(⃗s' | ⃗y, Θ) \} \\ 0 & \text{otherwise} \end{cases}$$
As for this limit for $p_T(\tilde{y}^{(n)}, \tilde{y}^{(n)}, \Theta)$ coincides with maximum a-posteriori (MAP) estimates, it is sometimes referred to as ‘zero-temperature EM’ (e.g. Turner and Sahani, 2011).

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