
Implicit Reparameterization Gradients

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Abstract

By providing a simple and efficient way of computing low-variance gradients of continuous random variables, the reparameterization trick has become the technique of choice for training a variety of latent variable models. However, it is not applicable to a number of important continuous distributions. We introduce an alternative approach to computing reparameterization gradients based on implicit differentiation and demonstrate its broader applicability by applying it to Gamma, Beta, Dirichlet, and von Mises distributions, which cannot be used with the classic reparameterization trick. Our experiments show that the proposed approach is faster and more accurate than the existing gradient estimators for these distributions.

1 Introduction

Pathwise gradient estimators are a core tool for stochastic estimation in machine learning and statistics [12, 15, 26, 42, 51]. In machine learning, we now commonly introduce these estimators using the “reparameterization trick”, in which we replace a probability distribution with an equivalent parameterization of it, using a deterministic and differentiable transformation of some fixed base distribution. This reparameterization is a powerful tool for learning because it makes backpropagation possible in computation graphs with certain types of continuous random variables, e.g. with Normal, Logistic, or Concrete distributions [23, 30]. Many of the recent advances in machine learning were made possible by this ability to backpropagate through stochastic nodes. They include variational autoencoders (VAEs), automatic variational inference [26, 28, 42], Bayesian learning in neural networks [7, 14], and principled regularization in deep networks [13, 34].

The reparameterization trick is easily used with distributions that have location-scale parameterizations or tractable inverse cumulative distribution functions (CDFs), or are expressible as deterministic transformations of such distributions. These seemingly modest requirements are still fairly restrictive as they preclude a number of standard distributions, such as truncated, mixture, Gamma, Beta, Dirichlet, or von Mises, from being used with reparameterization gradients. This paper provides a general tool for reparameterization in these important cases.

The limited applicability of reparameterization has often been addressed by using a different class of gradient estimators, the score-function estimators [12, 16, 53]. While being more general, they typically result in high-variance gradients which require problem-specific variance reduction techniques to be practical. Generalized reparameterizations involve combining the reparameterization and score-function estimators [36, 44]. Another approach is to approximate the intractable derivative of the inverse CDF [27].

Following Graves [17], we use implicit differentiation to differentiate the CDF rather than its inverse. While the method of Graves [17] is only practical for distributions with analytically tractable CDFs and has been used solely with mixture distributions, we leverage automatic differentiation to handle distributions with *numerically* tractable CDFs, such as Gamma and von Mises. We review the standard reparameterization trick in Section 2 and then make the following contributions:

- We develop *implicit reparameterization gradients* that provide unbiased estimators for continuous distributions with numerically tractable CDFs. This allows many other important distributions to be used as easily as the Normal distribution in stochastic computation graphs.
- We show that the proposed gradients are both faster and more accurate than alternative approaches.
- We demonstrate that our method can outperform existing stochastic variational methods at training the Latent Dirichlet Allocation topic model in a black-box fashion using amortized inference.
- We use implicit reparameterization gradients to train VAEs with Gamma, Beta, and von Mises latent variables instead of the usual Normal variables, leading to latent spaces with interesting alternative topologies.

2 Background

2.1 Explicit reparameterization gradients

We start with a review of the original formulation of reparameterization gradients [26, 42, 51], which we will refer to as *explicit* reparameterization. Suppose we would like to optimize an expectation $\mathbb{E}_{q_\phi(z)} [f(z)]$ of some continuously differentiable function $f(z)$ w.r.t. the parameters ϕ of the distribution. We assume that we can find a standardization function $\mathcal{S}_\phi(z)$ that when applied to a sample from $q_\phi(z)$ removes its dependence on the parameters of the distribution. The standardization function should be continuously differentiable w.r.t. its argument and parameters, and invertible:

$$\mathcal{S}_\phi(z) = \varepsilon \sim q(\varepsilon) \quad z = \mathcal{S}_\phi^{-1}(\varepsilon). \quad (1)$$

For example, for a Gaussian distribution $\mathcal{N}(\mu, \sigma)$ we can use $\mathcal{S}_{\mu, \sigma}(z) = (z - \mu)/\sigma \sim \mathcal{N}(0, 1)$. We can then express the objective as an expectation w.r.t. ε , transferring the dependence on ϕ into f :

$$\mathbb{E}_{q_\phi(z)} [f(z)] = \mathbb{E}_{q(\varepsilon)} [f(\mathcal{S}_\phi^{-1}(\varepsilon))]. \quad (2)$$

This allows us to compute the gradient of the expectation as the expectation of the gradients:

$$\nabla_\phi \mathbb{E}_{q_\phi(z)} [f(z)] = \mathbb{E}_{q(\varepsilon)} [\nabla_\phi f(\mathcal{S}_\phi^{-1}(\varepsilon))] = \mathbb{E}_{q(\varepsilon)} [\nabla_z f(\mathcal{S}_\phi^{-1}(\varepsilon)) \nabla_\phi \mathcal{S}_\phi^{-1}(\varepsilon)]. \quad (3)$$

A standardization function $\mathcal{S}_\phi(z)$ satisfying the requirements exists for a wide range of continuous distributions, but it is not always practical to take advantage of this. For instance, the CDF $F(z|\phi)$ of a univariate distribution provides such a function, mapping samples from it to samples from the uniform distribution over $[0, 1]$. However, inverting the CDF is often complicated and expensive, and computing its derivative is even harder.

2.2 Stochastic variational inference

Stochastic variational inference [19] for latent variable models is perhaps the most popular use case for reparameterization gradients. Consider a model $p_\theta(\mathbf{x}) = \int p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z}$, where \mathbf{x} is an observation, $\mathbf{z} \in \mathbb{R}^D$ is a vector-valued latent variable, $p_\theta(\mathbf{x}|\mathbf{z})$ is the likelihood function with parameters θ , and $p(\mathbf{z})$ is the prior distribution. Except for a few special cases, maximum likelihood learning in such models is intractable because of the difficulty of the integrals involved. Variational inference [22] provides a tractable alternative by introducing a variational posterior distribution $q_\phi(\mathbf{z}|\mathbf{x})$ and maximizing a lower bound on the marginal log-likelihood:

$$\mathcal{L}(\mathbf{x}, \theta, \phi) = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} [\log p_\theta(\mathbf{x}|\mathbf{z})] - \text{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z})) \leq \log p_\theta(\mathbf{x}). \quad (4)$$

Training models with modern stochastic variational inference [26, 39] involves gradient-based optimization of the bound w.r.t. the model parameters θ and the variational posterior parameters ϕ . While the KL-divergence term and its gradients can often be computed analytically, the remaining term and its gradients are typically intractable and are approximated using samples from the variational posterior. The most general form of this approach involves score-function gradient estimators [33, 39, 41] that handle both discrete and continuous latent variables but have relatively high variance. The reparameterization trick usually provides a lower variance gradient estimator and is easier to use, but due to the limitations discussed above, is not applicable to many important continuous distributions.

3 Implicit reparameterization gradients

We propose an alternative way of computing the reparameterization gradient that avoids the inversion of the standardization function. We start from Eqn. (3) and perform a change of variable $z = \mathcal{S}_\phi^{-1}(\varepsilon)$:

$$\nabla_\phi \mathbb{E}_{q_\phi(z)} [f(z)] = \mathbb{E}_{q_\phi(z)} [\nabla_z f(z) \nabla_\phi z]; \quad \nabla_\phi z = \nabla_\phi \mathcal{S}_\phi^{-1}(\varepsilon)|_{\varepsilon=\mathcal{S}_\phi(z)}. \quad (5)$$

Our key insight is that we can compute $\nabla_\phi z$ by *implicit differentiation*. We apply the *total* gradient ∇_ϕ^{TD} to the equality $\mathcal{S}_\phi(z) = \varepsilon$. Then, we use the chain rule to expand the total gradient in terms of the partial gradients. The standardization function $\mathcal{S}_\phi(z)$ depends on the parameters ϕ directly via the subscript parameters and indirectly via the argument z , while the noise ε is independent of ϕ by the definition of a standardization function. Thus, we have $\nabla_z \mathcal{S}_\phi(z) \nabla_\phi z + \nabla_\phi \mathcal{S}_\phi(z) = \mathbf{0}$, where all the gradients are partial. Solving this equation for $\nabla_\phi z$ yields

$$\nabla_\phi z = -(\nabla_z \mathcal{S}_\phi(z))^{-1} \nabla_\phi \mathcal{S}_\phi(z) \quad (6)$$

This expression for the gradient only requires differentiating the standardization function and not inverting it. Note that its value does not change under any invertible transformation $T(\varepsilon)$ of the standardization function, since the corresponding Jacobian $\nabla_\varepsilon T(\varepsilon)$ cancels out with the inverse.

Example: univariate Normal distribution $\mathcal{N}(\mu, \sigma^2)$. We illustrate that explicit and implicit reparameterizations give identical results. A standardization function is given by $\mathcal{S}_{\mu, \sigma}(z) = (z - \mu)/\sigma = \varepsilon \sim \mathcal{N}(0, 1)$. Explicit reparameterization inverts this function: $z = \mathcal{S}_{\mu, \sigma}^{-1}(\varepsilon) = \mu + \sigma\varepsilon$, $\frac{\partial z}{\partial \mu} = 1$, $\frac{\partial z}{\partial \sigma} = \varepsilon$. The implicit reparameterization, Eqn. (6), gives:

$$\frac{\partial z}{\partial \mu} = -\frac{\frac{\partial \mathcal{S}_{\mu, \sigma}(z)}{\partial \mu}}{\frac{\partial \mathcal{S}_{\mu, \sigma}(z)}{\partial z}} = -\frac{-\frac{1}{\sigma}}{\frac{1}{\sigma}} = 1, \quad \frac{\partial z}{\partial \sigma} = -\frac{\frac{\partial \mathcal{S}_{\mu, \sigma}(z)}{\partial \sigma}}{\frac{\partial \mathcal{S}_{\mu, \sigma}(z)}{\partial z}} = -\frac{-\frac{z-\mu}{\sigma^2}}{\frac{1}{\sigma}} = \frac{z-\mu}{\sigma}. \quad (7)$$

The expressions are equivalent, but the implicit version avoids inverting $\mathcal{S}_{\mu, \sigma}(z)$.

Universal standardization function. For univariate distributions, a standardization function is given by the CDF: $\mathcal{S}_\phi(z) = F(z|\phi) \sim \text{Uniform}(0, 1)$. Assuming that the CDF is strictly monotonic and continuously differentiable w.r.t. z and ϕ , it satisfies the requirements for a standardization function. Plugging this function into (6), we have

$$\nabla_\phi z = -\frac{\nabla_\phi F(z|\phi)}{q_\phi(z)}. \quad (8)$$

Therefore, computing the implicit gradient requires only differentiating the CDF. In the multivariate case, we can perform the multivariate distributional transform [45]:

$$\mathcal{S}_\phi(z) = (F(z_1|\phi), F(z_2|z_1, \phi), \dots, F(z_D|z_1, \dots, z_{D-1}, \phi)) = \varepsilon, \quad (9)$$

where $q(\varepsilon) = \prod_{d=1}^D \text{Uniform}(\varepsilon_d|0, 1)$. Eqn. (6) requires computing the gradient of the (conditional) CDFs and solving a linear system with matrix $\nabla_z \mathcal{S}_\phi(z)$. If the distribution is factorized, the matrix is diagonal and the system can be solved in $O(D)$. Otherwise, the matrix is triangular because each CDF depends only on the preceding elements, and the system is solvable in $O(D^2)$.

Algorithm. We present the comparison between the standard explicit and the proposed implicit reparameterization in Table 1. Samples of z in implicit reparameterization can be obtained with any suitable method, such as rejection sampling [10]. The required gradients of the standardization function can be computed either analytically or using automatic differentiation.

4 Applications of implicit reparameterization gradients

We now demonstrate how implicit reparameterization can be applied to a variety of distributions. Our strategy is to provide a computation method for a standardization function, such as CDF or multivariate distributional transform, and its gradients.

Truncated univariate distribution. A truncated distribution is obtained by restricting a distribution's domain to some range $[a, b]$. Its CDF can be computed from the CDF of the original distribution:

Table 1: Comparison of the two reparameterization types. While they provide the same result, the implicit version is easier to implement for distributions such as Gamma because it does not require inverting the standardization function $\mathcal{S}_\phi(z)$.

	Explicit reparameterization	Implicit reparameterization (proposed)
Forward pass	Sample $\varepsilon \sim q(\varepsilon)$ Set $z \leftarrow \mathcal{S}_\phi^{-1}(\varepsilon)$	Sample $z \sim q_\phi(z)$
Backward pass	Set $\nabla_\phi z \leftarrow \nabla_\phi \mathcal{S}_\phi^{-1}(\varepsilon)$ Set $\nabla_\phi f(z) \leftarrow \nabla_z f(z) \nabla_\phi z$	Set $\nabla_\phi z \leftarrow -(\nabla_z \mathcal{S}_\phi(z))^{-1} \nabla_\phi \mathcal{S}_\phi(z)$ Set $\nabla_\phi f(z) \leftarrow \nabla_z f(z) \nabla_\phi z$

$\hat{F}(z|\phi, a, b) = \frac{F(z|\phi) - F(a|\phi)}{F(b|\phi) - F(a|\phi)}$, $z \in [a, b]$. Assuming that the gradient $\nabla_\phi F(z|\phi)$ is available, we can easily compute the implicit gradient for the truncated distribution.

Mixture distribution $q_\phi(z) = \sum_{i=1}^K w_i q_{\phi_i}(z)$, where $\phi = (\phi_1, \dots, \phi_K, w_1, \dots, w_K)$. In the univariate case, the CDF of the mixture is simply $\sum_{i=1}^K w_i F(z|\phi_i)$. In the multivariate case, the distributional transform is given by $F(z_d|z_1, \dots, z_{d-1}, \phi) = \sum_{i=1}^K w_i^d F(z_d|z_1, \dots, z_{d-1}, \phi_i)$, where $w_i^d = \frac{w_i q_{\phi_i}(z_1, \dots, z_{d-1})}{\sum_{j=1}^K w_j q_{\phi_j}(z_1, \dots, z_{d-1})}$ is the posterior weight for the mixture component after observing the first $d - 1$ dimensions of the sample. The required gradient can be obtained via automatic differentiation. When the mixture components are fully factorized, we obtain the same result as [17], but in a simpler form, due to automatic differentiation and the explicitly specified linear system.

Gamma distribution $\text{Gamma}(\alpha, \beta)$ with shape $\alpha > 0$ and rate $\beta > 0$. The rate can be standardized using the scaling property: if $z \sim \text{Gamma}(\alpha, 1)$, then $z/\beta \sim \text{Gamma}(\alpha, \beta)$. For the shape parameter, the CDF of the Gamma distribution with shape α and unit rate is the regularized incomplete Gamma function $\gamma(z, \alpha)$ that does not have an analytic expression. Following Moore [35], we propose to apply forward-mode automatic differentiation [2] to a numerical method [3] that computes its value. This provides the derivative $\frac{\partial \gamma(z, \alpha)}{\partial \alpha}$ for roughly twice the cost of computing the CDF.

Student’s t -distribution samples can be derived from samples of Gamma. Indeed, if $\sigma \sim \text{Gamma}(\frac{\nu}{2}, \frac{\nu}{2})$, then $z \sim \mathcal{N}(0, \sigma^2)$ is t -distributed with ν degrees of freedom.

Beta and Dirichlet distribution samples can also be obtained from samples of Gamma. If $z_1 \sim \text{Gamma}(\alpha, 1)$ and $z_2 \sim \text{Gamma}(\beta, 1)$, then $\frac{z_1}{z_1 + z_2} \sim \text{Beta}(\alpha, \beta)$. Similarly, if $z_i \sim \text{Gamma}(\alpha_i, 1)$, then $\left(\frac{z_1}{\sum_{j=1}^D z_j}, \dots, \frac{z_D}{\sum_{j=1}^D z_j} \right) \sim \text{Dirichlet}(\alpha_1, \dots, \alpha_D)$.

Von Mises distribution [31, 32] is a maximum entropy distribution on a circle with the density function $\text{vonMises}(z|\mu, \kappa) = \frac{\exp(\kappa \cos(z - \mu))}{2\pi I_0(\kappa)}$, where μ is the location parameter, $\kappa > 0$ is the concentration, and $I_0(\kappa)$ is the modified Bessel function of the first kind. The location parameter μ can be standardized by noting that if $z \sim \text{vonMises}(0, \kappa)$, then $z + \mu \sim \text{vonMises}(\mu, \kappa)$. For the concentration parameter κ , we propose to use implicit reparameterization by performing forward-mode automatic differentiation of an efficient numerical method [18] for computation of the CDF.

4.1 Accuracy and speed of reparameterization gradient estimators

Implicit reparameterization requires differentiating the CDF w.r.t. its parameters. When this operation is analytically intractable, e.g. for Gamma and von Mises distributions, we estimate it via forward-mode differentiation of the code that numerically evaluates the CDF. We implement this approach by manually performing the required modifications of the C++ code (see Appendix B). An alternative is to use a central finite difference approximation of the derivative: $\frac{\partial F(z|\phi)}{\partial \phi} \approx \frac{F(z|\phi(1+\delta)) - F(z|\phi(1-\delta))}{2\delta}$, where $0 < \delta < 1$ is the *relative* step size that we choose via grid search. For the Gamma distribution, we also compare with two alternatives: (1) the estimator of Knowles [27] that performs explicit reparameterization by approximately computing the derivative of the inverse CDF; (2) the concurrently developed method of Jankowiak and Obermeyer [25] that computes implicit reparameterization using a closed-form approximation of the CDF derivative. We use the reference PyTorch Paszke et al. [40] implementation of the method of Jankowiak and Obermeyer [25]. The ground truth value of the CDF

Table 2: Average error and time (measured in seconds per element) of the reparameterization gradient computation methods. Automatic differentiation achieves the lowest error and the highest speed.

Method	Precision	Gamma		Von Mises	
		Mean abs. error	Time (s)	Mean abs. error	Time (s)
Automatic differentiation	float32	2.3×10^{-6}	1.9×10^{-8}	1.9×10^{-7}	3.1×10^{-8}
Finite difference		1.9×10^{-3}	3.8×10^{-8}	9.6×10^{-5}	3.8×10^{-8}
Jankowiak and Obermeyer [25]		4.1×10^{-5}	9.0×10^{-8}	–	–
Automatic differentiation	float64	5.4×10^{-13}	3.2×10^{-8}	1.3×10^{-13}	3.7×10^{-8}
Finite difference		3.2×10^{-9}	7.1×10^{-8}	1.1×10^{-10}	5.9×10^{-8}
Knowles [27]		6.5×10^{-3}	1.2×10^{-6}	–	–

derivative is computed in a computationally expensive but accurate way (see Appendix C). The results in Table 2 suggest that the automatic differentiation approach provides the highest accuracy and speed. The finite difference method can be easier to implement if a CDF computation method is available, but requires computation in float64 to obtain the float32 precision. This can be problematic for devices such as GPUs and other accelerators that do not support fast high-precision computation. The approach of Knowles is slower and significantly less accurate due to the approximations of the inverse CDF derivative computation method. The method of Jankowiak and Obermeyer is $4.5\times$ slower and $3\times$ less accurate than the automatic differentiation approach, which reflects the complexity of obtaining fast and accurate closed-form approximations to the CDF derivative. In the remaining experiments we use automatic differentiation and float32 precision.

5 Related work

Surrogate distributions. When explicit reparameterization is not feasible, it is often possible to modify the model to use alternative distributions that are reparameterizable. This is a popular approach due to its simplicity. Kucukelbir et al. [28] approximate posterior distributions by a deterministic transformation of Normal samples; Nalisnick et al. [37] and Nalisnick and Smyth [38] replace Beta distributions with Kumaraswamy distributions in the Dirichlet Process stick-breaking construction; Zhang et al. [54] substitute the Gamma distribution for a Weibull distribution; Srivastava and Sutton [47, 48] replace the Dirichlet distribution with a Logistic Normal. Surrogate distributions however do not always have all the desirable properties of the distributions they replace. For example, as noted by Ruiz et al. [44], such surrogate distributions struggle to capture sparsity, which is achievable with Gamma and Dirichlet distributions.

Integrating out the nuisance variables. In some cases it is possible to trade computation for simplicity of reparameterization. Roeder et al. [43] consider a mixture of reparameterizable distributions and analytically sum out the discrete mixture component id variable. For a mixture with K components, this results in a K -fold increase of computation, compared to direct reparameterization of the mixture. This approach becomes prohibitively expensive for a chain of mixture distributions, where the amount of computation grows exponentially with the length of the chain. On the other hand, we can always estimate the gradients with just one sample by directly reparameterizing the mixture.

Implicit reparameterization gradients. Reparameterization gradients have been known in the operations research community since the late 1980s under the name of pathwise, or stochastic, gradients [12, 49]. There the “explicit” and “implicit” versions were usually introduced side-by-side, but they were applied only to univariate distributions and simple computational graphs that do not require backpropagation. In the machine learning community, the implicit reparameterization gradients for univariate distributions were introduced by Salimans and Knowles [46]. That work, as well as Hoffman and Blei [21], used the implicit gradients to perform backpropagation through the Gamma distribution using a finite difference approximation of the CDF derivative. Graves [17] independently introduced the implicit reparameterization gradients for multivariate distributions with analytically tractable CDFs, such as mixtures. We add to this rich literature by generalizing the technique to handle arbitrary standardization functions, deriving a simpler expression than that of Graves [17] for the multivariate case, showing the connection to explicit reparameterization gradients, and providing an efficient automatic differentiation method to compute the intractable CDF derivatives.

Reparameterization gradients as differential equation solutions. The concurrent works [24, 25] provide a complementary view of the reparameterization gradients as solutions of a differential equation called the transport equation. For univariate distributions, the unique solution is Eqn. (8). However, for the non-factorial multivariate distributions, there are multiple solutions. By choosing an appropriate one, the variance of the gradient estimator may be reduced. Unfortunately, there does not seem to be a general way to obtain these solutions, so distribution-specific derivations are required. We hypothesize that the transport equation solutions correspond to the implicit reparameterization gradients for different standardization functions.

Generalized reparameterizations. The limitations of standard reparameterization was recently tackled by several other works. Ruiz et al. [44] introduced generalized reparameterization gradients (GRG) that expand the applicability of the reparameterization trick by using a standardization function that allows the underlying base distribution to depend weakly on the parameter vector (e.g. only through the higher moments). The resulting gradient estimator, which in addition to the reparameterized gradients term includes a score-function gradient term that takes into account the dependence of the base distribution on the parameter vector, was applied to the Gamma, Beta, and log-Normal distributions. The challenge of using this approach lies in finding an effective approximate standardization function, which is nontrivial yet essential for obtaining low-variance gradients.

Rejection sampling variational inference (RSVI) [36] is a closely-related approach that combines the reparameterization gradients from the proposal distribution of a rejection sampler with a score-function gradient term that takes into account the effect of the accept/reject step. When applied to the gamma distribution the RSVI gradients can have lower variance gradients than those computed using GRG [36]. Davidson et al. [9] have recently demonstrated the use of RSVI with the von Mises-Fisher distribution.

6 Experiments

We apply implicit reparameterization for two distributions with analytically intractable CDFs (Gamma and von Mises) to three problems: a toy setting of stochastic cross-entropy estimation, training a Latent Dirichlet Allocation [6] (LDA) topic model, and training VAEs [26, 42] with non-Normal latent distributions. We use the RSVI gradient estimator [36] as our main baseline. For Gamma distributions, RSVI provides a *shape augmentation* parameter B that decreases the magnitude of the score-function correction term by using additional B samples from a uniform distribution. As $B \rightarrow \infty$, the term vanishes and the RSVI gradient becomes equivalent to ours, but with a higher computational cost. Von Mises distribution does not have such an augmentation parameter. For LDA, we also compare with a surrogate distribution approach [47] and a classic stochastic variational inference method [19]. The experimental details are given in Appendix D. We use TensorFlow [1] for our experiments. Implicit reparameterization for Gamma, Student’s t , Beta, Dirichlet and von Mises distributions is available in TensorFlow Probability [11]. This library also contains an implementation of the LDA model from section 6.2

6.1 Gradient of the cross-entropy

We compare the variance of the implicit and RSVI gradient estimators on a toy problem of stochastic estimation of the cross-entropy gradient, $\frac{\partial}{\partial \phi} \mathbb{E}_{q_\phi(\mathbf{z})}[-\log p(\mathbf{z})]$. It was introduced by Naesseth et al. [36] as minimization of the KL-divergence; however, since they analytically compute the entropy, the only source of variance is the cross-entropy term. We use their setting for the Dirichlet distribution: $p(\mathbf{z}) = \text{Dirichlet}(\mathbf{z}|\alpha_1, \alpha_2, \dots, \alpha_{100})$, $q_\phi(\mathbf{z}) = \text{Dirichlet}(\mathbf{z}|\phi, \alpha_2, \dots, \alpha_{100})$, where α are the posterior parameters for a Dirichlet with a uniform prior after observing 100 samples from a Categorical distribution. The Dirichlet samples are obtained by transforming samples from Gamma. Additionally, we construct a similar problem with the von Mises distribution: $p(\mathbf{z}) = \prod_{d=1}^{10} \text{vonMises}(z_d|0, 2)$ and $q_\phi(\mathbf{z}) = \text{vonMises}(z_1|0, \phi) \prod_{d=2}^{10} \text{vonMises}(z_d|0, 2)$.

The results presented on Fig. 1 show that the implicit gradient is faster and has lower variance than RSVI. For the Dirichlet distribution, increasing the shape augmentation parameter B allows RSVI to asymptotically approach the variance of the implicit gradient. However, this comes at an additional

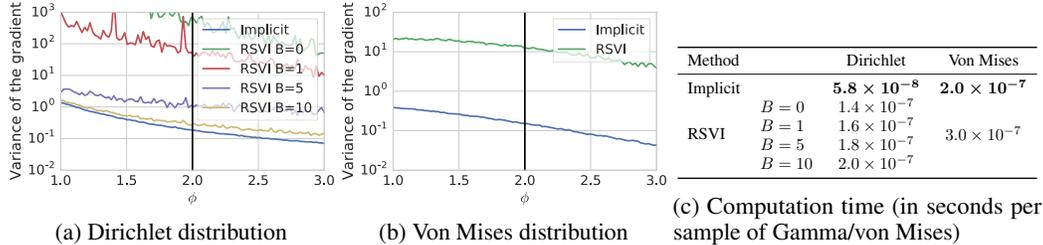


Figure 1: Variance of the gradient and computation time for the cross-entropy optimization problem. The vertical line denotes the optimal value for the parameter. Implicit gradient is faster and has lower variance than RSVI [36].

computational cost and requires tuning this parameter. Furthermore, such a parameter is not available for other distributions, including von Mises.

6.2 Latent Dirichlet Allocation

LDA [6] is a popular topic model that represents each document as a bag-of-words and finds a set of topics so that each document is well-described by a few topics. It has been extended in various ways, e.g. [4, 5], and often serves as a testbed for approximate inference methods [19, 20, 50]. LDA is a latent variable model with a likelihood $p_{\Phi}(\mathbf{w}|\mathbf{z}) = \prod_{i=1}^K \text{Categorical}(w_i|\Phi\mathbf{z})$, and the prior $p_{\alpha}(\mathbf{z}) = \text{Dirichlet}(\mathbf{z}|\alpha)$, where \mathbf{w} is the observed document represented as a vector of word counts, \mathbf{z} is a distribution of topics, $\Phi \in \mathbb{R}^{\#\text{words} \times \#\text{topics}}$ is a matrix that specifies the categorical distribution of words in each topic, and α parameterizes the prior distribution over the topics. We perform amortized variational inference by using a neural network to parameterize the Dirichlet variational posterior over the topics \mathbf{z} as a function of the observation.

We use the 20 Newsgroups (11,200 documents, 2,000-word vocabulary) and RCV1 [29] (800,000 documents, 10,000-word vocabulary) datasets with the same preprocessing as in [47]. We report the test perplexity of the models, $\exp\left(-\frac{1}{N} \sum_{n=1}^N \frac{1}{L_n} \log p(\mathbf{w}_n)\right)$, where L_n is the number of words in the document and the marginal log-likelihood is approximated with a single-sample estimate of the evidence lower bound. Following [52], we optimize the prior parameters α during training.

We compare amortized variational inference in LDA using implicit reparameterization to several alternatives: (i) training the LDA model with the RSVI gradients; (ii) stochastic variational inference (SVI) [19] training method for LDA; (iii) the method of Srivastava and Sutton [47], which we refer to as LN-LDA, that uses a Logistic Normal approximation in place of the Dirichlet prior and performs amortized variational inference using a Logistic Normal variational posterior.

The results in Table 3 and Fig. 3(a-b) show that RSVI matches the implicit gradient results only at $B = 20$, as opposed to $B = 10$ for the previous problem. Lower gradient variance leads to faster training objective convergence. Interestingly, amortized inference can achieve better perplexity than SVI. Finally, we see that LDA trained with implicit gradients performs as well or better than LN-LDA. The learned topics and the prior weights shown on Fig. 2 demonstrate that LDA automatically determines the number of topics in the corpus by setting some of the prior weights to 0; this does not occur in LN-LDA model. Additionally, LN-LDA is prone to representing the same topic several times, perhaps due to a non-sparse variational posterior distribution.

The obtained results suggest that the advantage of implicit gradients compared to RSVI increases with the complexity of the problem. When the original distributions are replaced by surrogates, some desirable properties of the solution, such as sparsity, might be lost.

6.3 Variational Autoencoders

VAE [26, 42] is a generative latent variable model trained using amortized variational inference. Both the variational posterior and the generative distributions (also known as the encoder and decoder) are parameterized using neural networks. VAEs typically use the standard Normal distribution as the prior and a factorized Normal as the variational posterior. The form of the likelihood depends on

Table 3: Test perplexity (lower is better) for the topic modeling task. Mean \pm standard deviation over 5 runs. LN-LDA uses Logistic Normal distributions instead of Dirichlet.

Model	Training method	20 Newsgroups	RCV1
LDA [6]	Implicit reparameterization	876 \pm 7	896 \pm 6
	RSVI $B = 1$	1066 \pm 7	1505 \pm 33
	RSVI $B = 5$	968 \pm 18	1075 \pm 15
	RSVI $B = 10$	887 \pm 10	953 \pm 16
	RSVI $B = 20$	865 \pm 11	907 \pm 13
	SVI	964 \pm 4	1330 \pm 4
LN-LDA [47]	Explicit reparameterization	875 \pm 6	951 \pm 10

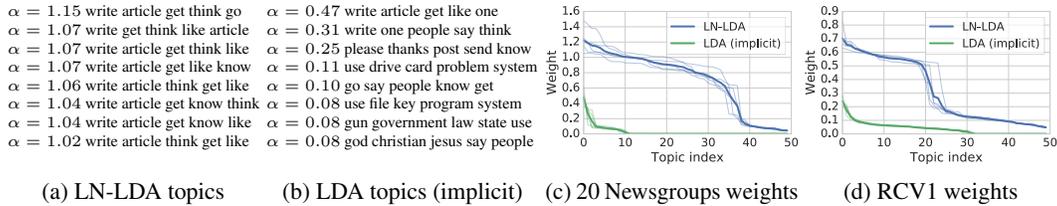


Figure 2: Left: topics with the highest weight for the 20 Newsgroups dataset; Right: prior topic weights α . LDA learns sparse prior weights, while LN-LDA does not.

the data, with factorized Bernoulli or Normal distributions being popular choices for images. In this section, we experiment with using distributions other than Normal for the prior and the variational posterior. The use of alternative distributions allows incorporating different prior assumptions about the latent factors of the data, such as bounded support or periodicity.

We use fully factorized priors and variational posteriors. For the variational posterior we explore Gamma, Beta, and von Mises distributions. For Gamma, we use a sparse Gamma(0.3, 0.3) prior and a bell-shaped prior Gamma(10, 10). For Beta and von Mises, instead of a sparse prior we choose a uniform prior over the corresponding domain.

We train the models on the dynamically binarized MNIST dataset [8] using the fully-connected encoder and decoder architectures from [9], so our results are comparable. The results in Table 4 show that a uniform prior and cyclic latent space of von Mises is advantageous for low-dimensional latent spaces, consistent with the findings of [9]. For a uniform prior, the factorized von Mises distribution outperforms the multivariate von Mises-Fisher distribution in low dimensions, perhaps due to the more flexible concentration parameterization (von Mises-Fisher uses shared concentration across dimensions). The results obtained with bell-shaped priors are similar to the Normal prior/posterior

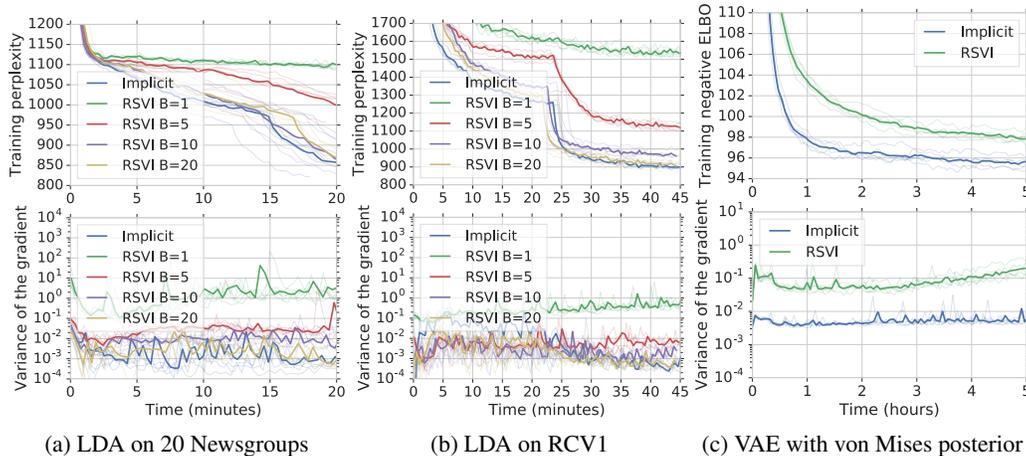


Figure 3: The training objective (top) and the variance of the gradient (bottom) during training. The sharp drop in perplexity on RCV1 dataset occurs at the end of the α burn-in period.

Table 4: Test negative log-likelihood (lower is better) for VAE on MNIST. Mean \pm standard deviation over 5 runs. The von Mises-Fisher results are from [9].

Prior	Variational posterior	$D = 2$	$D = 5$	$D = 10$	$D = 20$	$D = 40$
$\mathcal{N}(0, 1)$	$\mathcal{N}(\mu, \sigma^2)$	131.1 \pm 0.6	107.9 \pm 0.4	92.5 \pm 0.2	88.1 \pm 0.2	88.1 \pm 0.0
Gamma(0.3, 0.3)	Gamma(α, β)	132.4 \pm 0.3	108.0 \pm 0.3	94.0 \pm 0.3	90.3 \pm 0.2	90.6 \pm 0.2
Gamma(10, 10)	Gamma(α, β)	135.0 \pm 0.2	107.0 \pm 0.2	92.3 \pm 0.2	88.3 \pm 0.2	88.3 \pm 0.1
Uniform(0, 1)	Beta(α, β)	128.3 \pm 0.2	107.4 \pm 0.2	94.1 \pm 0.1	88.9 \pm 0.1	88.6 \pm 0.1
Beta(10, 10)	Beta(α, β)	131.1 \pm 0.4	106.7 \pm 0.1	92.1 \pm 0.2	87.8 \pm 0.1	87.7 \pm 0.1
Uniform($-\pi, \pi$)	vonMises(μ, κ)	127.6 \pm 0.4	107.5 \pm 0.4	94.4 \pm 0.5	90.9 \pm 0.1	91.5 \pm 0.4
vonMises(0, 10)	vonMises(μ, κ)	130.7 \pm 0.8	107.5 \pm 0.5	92.3 \pm 0.2	87.8 \pm 0.2	87.9 \pm 0.3
Uniform(S^D)	vonMisesFisher(μ, κ)	132.5 \pm 0.7	108.4 \pm 0.1	93.2 \pm 0.1	89.0 \pm 0.3	90.9 \pm 0.3

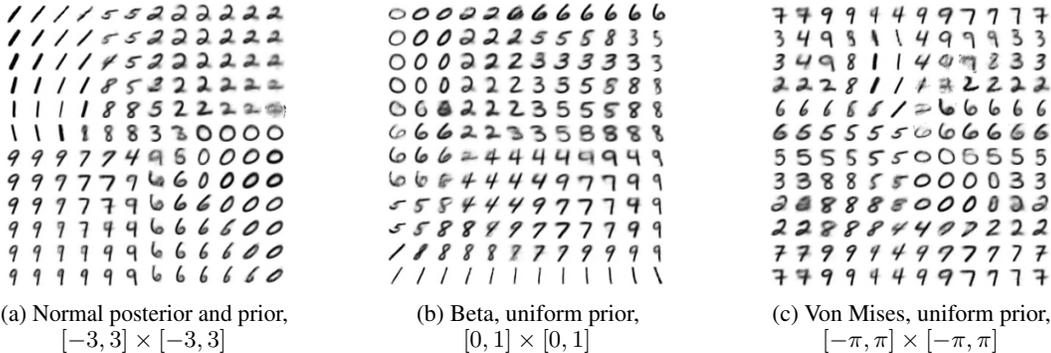


Figure 4: 2D latent spaces learned by a VAE on the MNIST dataset. Normal distribution exhibits a strong pull to the center, while Beta and Von Mises latents are tiling the entire available space.

pair, as expected. The latent spaces learned by models with 2 latents shown on Fig. 4 demonstrate the differences in topology.

We provide a detailed comparison between implicit gradients and RSVI in Table 7 of the supplementary material. For Gamma and Beta distributions, RSVI with $B = 20$ performs similarly to implicit gradients. However, for the von Mises distribution implicit gradients usually perform better than RSVI. For example, for a uniform prior and $D = 40$, implicit gradients yield a 1.3 nat advantage in the test log-likelihood due to lower gradient variance (Fig. 3c).

7 Conclusion

Reparameterization gradients have become established as a central tool underlying many of the recent advances in machine learning. In this paper, we strengthened this tool by extending its applicability to distributions, such as truncated, Gamma, and von Mises, that are often encountered in probabilistic modelling. The proposed implicit reparameterization gradients offer a simple and practical approach to stochastic gradient estimation which has the properties we expect from such a new type of estimator: it is faster than the existing methods and simultaneously provides lower gradient variance. These new estimators allow us to move away from making model choices for reasons of computational convenience. Applying these estimators requires a numerically tractable CDF or some other standardization function. When one is not available, it should be possible to use an approximate standardization function to augment implicit reparameterization with a score function correction term, along the lines of generalized reparameterization. We intend to explore this direction in future work.

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