On the relationship between variational inference and adaptive importance sampling

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The importance weighted autoencoder (IWAE) (Burda et al., 2016) and reweighted wake-sleep (RWS) algorithm (Bornschein and Bengio, 2015) are popular approaches which employ multiple samples to achieve bias reductions compared to standard variational methods. However, their relationship has hitherto been unclear. We introduce a simple, unified framework for multi-sample variational inference termed adaptive importance sampling for learning (AISLE) and show that it admits IWAE and RWS as special cases. Through a principled application of a variance-reduction technique from Tucker et al. (2019), we also show that the sticking-the-landing (STL) gradient from Roeder et al. (2017), which previously lacked theoretical justification, can be recovered as a special case of RWS (and hence of AISLE). In particular, this indicates that the breakdown of RWS – but not of STL – observed in Tucker et al. (2019) may not be attributable to the lack of a joint objective for the generative-model and inference-network parameters as previously conjectured. Finally, we argue that our adaptive-importance-sampling interpretation of variational inference leads to more natural and principled extensions to sequential Monte Carlo methods than the IWAE-type multi-sample objective interpretation.

1 Introduction

1.1 Problem statement

Let $x$ be some observation and let $z$ be some latent variable taking values in some space $Z$. These are modeled via the generative model $p_\theta(z, x) = p_\theta(z)p_\theta(x|z)$ which
gives rise to the marginal likelihood $p_\theta(x) = \int_Z p_\theta(z, x) \, dz$ of the model parameters $\theta$. The latter may also be viewed as the evidence for the model parametrised by a particular value of $\theta$. In this work, we analyse algorithms for variational inference, i.e. algorithms which aim to

1. learn the generative model, i.e. find a value $\theta^*$ which is approximately equal to the maximum-likelihood estimate (MLE) $\theta_{\text{MLE}} := \arg \max_\theta p_\theta(x)$;

2. construct a tractable variational approximation $q_{\phi,x}(z)$ of $p_\theta(z|x) = p_\theta(z, x)/p_\theta(x)$, i.e. find the value $\phi^*$ such that $q_{\phi^*,x}(z)$ is as close as possible to $p_\theta(z|x)$ in some suitable sense.

A few comments about the above setting are in order. Firstly, as is common in the literature, we restrict our presentation to a single latent representation–observation pair $(z, x)$ to avoid notational clutter. However, the extension to multiple independent observations is straightforward and the extension to time-series observations via sequential Monte Carlo methods is briefly discussed in Subsection 3.3. Secondly, we assume that no parameters are shared between the generative model $p_\theta(z, x)$ and the variational approximation $q_{\phi,x}(z)$. This is common in neural-network applications but could be easily relaxed. Thirdly, the above setting is general enough to cover amortised inference which is why we often refer to $\phi$ as the parameters of an inference network.

Both $\theta$ and $\phi$ are typically optimised simultaneously via a stochastic gradient-ascent algorithm. In recent years, several such schemes have been proposed. All of these employ $K \geq 1$ samples to reduce errors.

- **IWAE.** The importance weighted autoencoder (IWAE) from Burda et al. (2016) optimises a joint but biased objective for $\theta$ and $\phi$ (though optimising $\phi$ decreases the bias). This multi-sample objective is expressible as an integral on a $K$-dimensional space. Its gradients can be unbiasedly approximated via the vanilla Monte Carlo method.

- **STL.** The sticking the landing (STL) algorithm from Roeder et al. (2017) coincides with IWAE except that it uses a heuristic modification of the $\phi$-gradient estimator which is biased for the IWAE objective as proved in Tucker et al. (2019). For $K = 1$, STL reduces to the path-derivative variational autoencoder (VAE) gradient from Roeder et al. (2017).

- **RWS.** The reweighted wake-sleep (RWS) algorithm from Bornschein and Bengio (2015) (with only the wake update for the inference network parameters) optimises two separate but unbiased objectives for $\theta$ and $\phi$. Its gradients are approximated by self-normalised importance sampling with $K$ samples which induces bias (though again, optimising $\phi$ decreases this bias). RWS can also be viewed as employing an adaptive importance sampling approach which iteratively improves its proposal distribution while simultaneously employing the optimised importance-sampling scheme to estimate the $\theta$-gradients.

Of these three methods, the IWAE is the most popular. Though without a further reparametrisation from Tucker et al. (2019), its $\phi$-gradients can be poorly behaved.
and this becomes a particular problem when the approach is extended to sequential Monte Carlo methods for which such reparametrisations are not fully applicable. Furthermore, [88x759]Le et al. (2018b) recently showed that RWS outperforms IWAE in some scenarios. However, [89x730]Tucker et al. (2019) demonstrated empirically that RWS can break down and conjectured that this is due to the fact that RWS does not optimise a joint objective (for \( \theta \) and \( \phi \)). Meanwhile, STL performed consistently well despite lacking a firm theoretical footing. Thus, it is not clear which of these algorithms is preferable.

In this work, we argue that directly optimising the proposal distribution used in importance sampling (as in RWS) yields a more principled approach to variational inference than optimising multi-sample objectives (as in IWAEs). This is because in contrast to the latter, the objectives of the former are expressible as integrals over a space whose dimension does not grow with \( K \) and are therefore easier to optimise. Furthermore, the \( \phi \)-gradients of the former not suffer from the breakdown highlighted in Rainforth et al. (2018) and are also better at dealing with discrete latent variables Le et al. (2018b). Finally, adaptive importance sampling strategies much more naturally extend to the use of sequential Monte Carlo methods.

To formalise these arguments, we slightly generalise the RWS algorithm to obtain a generic adaptive importance sampling framework for variational inference which we term adaptive importance sampling for learning (AISLE) for ease of reference. We then show that AISLE admits IWAE, STL and RWS as special cases.

1.2 Contributions

Importance sampling as well as the IWAE, STL and RWS algorithms are reviewed in Section 2. Novel material is presented in Section 3 where we introduce the AISLE algorithm:

- In Subsection 3.3, we show that AISLE admits RWS as a special case. In addition, we prove that STL is in turn recovered as a special case of RWS (and hence of AISLE) via a principled and novel application of the variance-reduction technique from [89x715]Tucker et al. (2019). This indicates that the breakdown of RWS observed in Tucker et al. (2019) may not be due to its lack of a joint objective as previously conjectured (because STL avoided this breakdown). Our derivation also provides a theoretical foundation for STL which was hitherto only heuristically justified.

- In Subsection 3.4, we prove that AISLE also admits the IWAE as a special case (if the latter uses the variance-reduction technique from [89x701]Tucker et al. 2019 which is necessary to circumvent the breakdown highlighted in [89x730]Rainforth et al. 2018). This makes it clear that the bias-reduction potential of IWAE (over standard variational inference) comes at the price of gradient approximations which are based on importance-sampling and which therefore typically scale poorly with dimension.

- In Subsection 3.5, we briefly explain that AISLE extends more naturally to a sequential Monte Carlo setting than IWAE-type multi-sample objective approaches.
In the supplementary materials available with this paper, we also compare all
algorithms discussed in this work empirically on Gaussian models.

1.3 Notation

We assume that all (probability) measures $p$ used in this work are absolutely
continuous w.r.t. some suitable dominating measure $dz$ and with some abuse
of notation, we use the same symbol for the measure and the density, i.e. we
write $p(dz) = p(z)dz$. With this convention, we often employ the shorthand
$p(f) := \int_Z f(z)p(z)\,dz$ for the integral of some $p$-integrable test function $f$; note
that if $p$ is a probability measure then $p(f) = \mathbb{E}_{z \sim p}[f(z)]$.

Furthermore, to keep the notation concise, we hereafter suppress dependence on
the observation $x$, i.e. we write $q_\phi(z) := q_{\phi,x}(z)$ as well as
$$
\pi_\theta(z) := p_\theta(z|x) = \frac{p_\theta(z,x)}{p_\theta(x)} = \frac{\gamma_\theta(z)}{Z_\theta},
$$
where $\gamma_\theta(z) := p_\theta(z,x)$ and where $Z_\theta := p_\theta(x) = \int_Z \gamma_\theta(z)\,dz = \gamma_\theta(1)$. Here, $1 \equiv 1$
is the function that takes value 1 everywhere on its domain.

2 Background

2.1 Importance sampling

**Basic idea.** We hereafter assume that the support of $q_\phi$ includes the support of
$\pi_\theta$. Write $\psi := (\theta,\phi)$ then the following importance weight function is well defined:
$$
w_\psi(z) := \frac{\gamma_\theta(z)}{q_\phi(z)}.
$$

For $\pi_\theta$-integrable test functions $f : Z \to \mathbb{R}$, we can unbiasedly approximate integrals
of the form
$$
\gamma_\theta(f) := \int_Z f(z)\gamma_\theta(z)\,dz = \int_Z f(z)w_\psi(z)q_\phi(z)\,dz = q_\phi(fw_\psi), \quad (1)
$$
via importance sampling – note that this is just an application of the vanilla Monte
Carlo method to the expectation from the r.h.s. of (1) – using $K$ independent and
identically distributed (IID) samples $z^1, \ldots, z^K \sim q_\phi$, as
$$
\hat{\gamma}_\theta(\phi, z^{1:K})(f) := \frac{1}{K} \sum_{k=1}^K w_\psi(z^k)f(z^k),
$$
where the notation $\langle \phi, z^{1:K} \rangle$ stresses the estimator’s dependence on $\phi$ and $z^{1:K} := (z^1, \ldots, z^K)$. 


Self-normalised importance sampling. Approximating integrals of the form
\[
\pi_{\theta}(f) := \int_{\mathbb{Z}} f(z) \pi_{\theta}(z) \, dz = \frac{\gamma_{\theta}(f)}{\gamma_{\theta}(1)},
\]
is slightly more complicated due to the fact that the marginal likelihood \(Z_{\theta} = \gamma_{\theta}(1) = p_{\theta}(x)\) is typically intractable. Plugging in importance-sampling approximations for both the numerator and denominator leads to the following self-normalised importance sampling estimate:
\[
\hat{\pi}_{\theta}(\phi, z^{1:K})(f) := \frac{\hat{\gamma}_{\theta}(\phi, z^{1:K})(f)}{\hat{\gamma}_{\theta}(\phi, z^{1:K})(1)} = \sum_{k=1}^{K} \frac{w_{\psi}(z^k)}{\sum_{l=1}^{K} w_{\psi}(z^l)} f(z^k).
\]

Properties. Proposition 1 summarises some well-known properties of importance-sampling approximations (see, e.g., Geweke, 1989) used throughout this work.

**Proposition 1.** Let \(f : \mathbb{Z} \to \mathbb{R}\) be some \(\pi_{\theta}\)-integrable test function and \(z^1, \ldots, z^K \sim q_{\phi}\).

Then if \(\sup w_{\psi} < \infty\),

1. \(\mathbb{E}[\hat{\gamma}_{\theta}(\phi, z^{1:K})(f)] = \gamma_{\theta}(f), \) for any \(K \in \mathbb{N}\),
2. \(\mathbb{E}[\hat{\pi}_{\theta}(\phi, z^{1:K})(f)] = \pi_{\theta}(f) + \mathcal{O}(K^{-1})\) and \(\text{var}[\hat{\pi}_{\theta}(\phi, z^{1:K})(f)] = \mathcal{O}(K^{-2})\),
3. \(\hat{\gamma}_{\theta}(\phi, z^{1:K})(f) \to \gamma_{\theta}(f)\) and \(\hat{\pi}_{\theta}(\phi, z^{1:K})(f) \to \pi_{\theta}(f)\), almost surely, as \(K \to \infty\).

**Proof.** Part 1 is immediate; Part 2 is proved, e.g. in Liu (2001, p. 35); Part 3 is a direct consequence of the strong law of large numbers.

Part 1 of Proposition 1 shows that (non self-normalised) importance-sampling approximations \(\hat{\gamma}_{\theta}(\phi, z^{1:K})(f)\) are unbiased. In particular,
\[
\hat{Z}_{\theta}(\phi, z^{1:K}) := \hat{\gamma}_{\theta}(\phi, z^{1:K})(1) = \frac{1}{K} \sum_{k=1}^{K} w_{\psi}(z^k),
\]
is an unbiased estimate of the normalising constant \(Z_{\theta} = \gamma_{\theta}(1) = p_{\theta}(x)\). In contrast, the self-normalised importance-sampling approximation \(\hat{\pi}_{\theta}(\phi, z^{1:K})(f)\) is typically not unbiased. However, Part 3 shows that it is still consistent and Part 2 ensures that the bias decays quickly in \(K\).

### 2.2 Importance weighted autoencoder (IWAE)

**Objective.** The importance weighted autoencoder (IWAE), introduced by Burda et al. (2016), seeks to find a value \(\theta^*\) of the generative-model parameters \(\theta\) which maximises a lower bound \(\mathcal{L}_{\psi}^K\) on the log-marginal likelihood (log-evidence) which depends on the inference-network parameters \(\phi\) and the number of samples, \(K \geq 1\).

\[
\psi^* := (\theta^*, \phi^*) := \arg \max_{\psi} \mathcal{L}_{\psi}^K, \\
\mathcal{L}_{\psi}^K := \mathbb{E}_{z^1, \ldots, z^K \sim q_{\phi}} \left[ \log \hat{Z}_{\theta}(\phi, z^{1:K}) \right].
\]
For any finite $K$, optimisation of the inference-network parameters $\phi$ tightens the evidence bound. \cite{Burda et al. (2016)} prove the following properties. Firstly, $\mathcal{L}_\psi^K \leq \log Z_\theta$ follows from Jensen’s inequality and Part 1 of Proposition 1. Secondly, again by Jensen’s inequality, $\mathcal{L}_\psi^K \leq \mathcal{L}_\psi^{K+1}$. These inequalities are strict unless $\pi_\theta = q_\phi$. Finally, Part 3 of Proposition 1 (along with the dominated convergence theorem) shows that for any $\phi$, $\mathcal{L}_\psi^K \uparrow \log Z_\theta$ as $K \to \infty$. If $K = 1$, the IWAE reduces to the variational autoencoder (VAE) from Kingma and Welling \cite{2014}. However, for $K > 1$, as pointed out in Cremer et al. \cite{2017}; Domke and Sheldon \cite{2018}, the IWAE also constitutes another VAE on an extended space based on an auxiliary-variable construction developed in Andrieu and Roberts \cite{2009}; Andrieu et al. \cite{2010}; Lee \cite{2011} (see, e.g. Finke \cite{2015} for a review). By casting sequential Monte Carlo (SMC) methods as a special case of importance sampling on a larger space, this construction also immediately yields the evidence bounds of the SMC extensions of \cite{2017} proposed in Maddison et al. \cite{2017}; Le et al. \cite{2018a}; Naesseth et al. \cite{2018}.

**Gradients.** The $\theta$-gradient

$$\nabla_\theta \mathcal{L}_\psi^K = \mathbb{E}_{z^1,\ldots,z^K \sim q_\phi} \left[ \hat{\pi}_\theta(\phi, z^{1:K}) (\nabla_\theta \log \gamma_\theta) \right],$$

is typically intractable. However, it can be approximated via a vanilla Monte Carlo approximation using a single sample point $z^{1:K}$ (whose components are drawn IID from $q_\phi$), i.e. by

$$\nabla_{\text{IWAE}} \langle \phi, z^{1:K} \rangle := \hat{\pi}_\theta(\phi, z^{1:K}) (\nabla_\theta \log \gamma_\theta) = \sum_{k=1}^{K} \frac{w_\psi(z^k)}{\sum_{l=1}^{K} w_\psi(z^l)} \nabla_\theta \log \gamma_\theta(z^k).$$

The $\phi$-gradient

$$\nabla_\phi \mathcal{L}_\psi^K = \mathbb{E}_{z^1,\ldots,z^K \sim q_\phi} \left[ \nabla_\phi \log \hat{Z}_\theta(\phi, z^{1:K}) + \log \hat{Z}_\theta(\phi, z^{1:K}) \sum_{k=1}^{K} \nabla_\phi \log q_\phi(z^k) \right],$$

is also typically intractable. However, the term inside the second expectation in \cite{3} often has such a large variance that a vanilla Monte Carlo approximation using a single sample point $z^{1:K}$ becomes impractically noisy \cite{Paisley et al. 2012}. To remove the high-variance term in \cite{3}, a well known reparametrisation trick \cite{2014} is typically employed. It requires that there exists a distribution $q$ on some space $\mathcal{E}$ and a diffeomorphism $h_\phi : \mathcal{E} \to \mathcal{Z}$ such that

$$\varepsilon \sim q \iff h_\phi(\varepsilon) \sim q_\phi.$$ 

Then using this reparametrisation, the IWAE objective from \cite{2} may be written as

$$\mathcal{L}_\psi^K = \mathbb{E}_{\varepsilon^1,\ldots,\varepsilon^K \sim q} \left[ \log \hat{Z}_\theta(\phi, \{h_\phi(\varepsilon^k)\}_{k=1}^{K}) \right].$$

This implies the following representation for the $\phi$-gradient,

$$\nabla_\phi \mathcal{L}_\psi^K = \mathbb{E}_{\varepsilon^1,\ldots,\varepsilon^K \sim q} \left[ \sum_{k=1}^{K} \frac{w_\psi(h_\phi(\varepsilon^k))}{\sum_{l=1}^{K} w_\psi(h_\phi(\varepsilon^l))} \nabla_\phi \log w_\psi(h_\phi(\varepsilon^k)) \right]
\n= \mathbb{E}_{\varepsilon^1,\ldots,\varepsilon^K \sim q} \left[ \hat{\pi}_\theta(\phi, z^{1:K}) (\nabla_\phi \log \circ w_\psi \circ h_\phi) \circ h_\phi^{-1} \right].$$
which is unbiasedly approximated via a vanilla Monte Carlo approximation (again using a single sample point $z^{1:K}$ whose components are drawn from $q_\phi$) as

$$
\nabla_{\phi}^{\text{IWAE}} \langle \theta, z^{1:K} \rangle := \pi_\theta(\phi, z^{1:K}) (\nabla_\phi [\log o w_\psi o h_\phi] o h_\phi^{-1})
= \sum_{k=1}^K \frac{w_\psi(z^k)}{\sum_{l=1}^K w_\psi(z^l)} \nabla_\phi [\log o w_\psi o h_\phi] (h_\phi^{-1}(z^k)).
$$

(4)

**Reparametrised $\phi$-gradient from Tucker et al. (2019).** As pointed out in Rainforth et al. (2018), the $\phi$-gradient from (4) breaks down as $K$ is increased in the sense that its mean decays to zero too quickly relative to its variance. More formally, Rainforth et al. (2018) show that this is because (4) constitutes a self-normalised importance-sampling approximation of

$$
\pi_\theta(\nabla_\phi [\log o w_\psi o h_\phi] o h_\phi^{-1}) = q_\phi (Z_\phi^{-1} w_\psi \nabla_\phi [\log o w_\psi o h_\phi] o h_\phi^{-1})
= Z_\phi^{-1} q ([w_\psi o h_\phi] \nabla_\phi [\log o w_\psi o h_\phi])
= Z_\phi^{-1} \nabla_\phi q_\phi (w_\psi)
= Z_\phi^{-1} \nabla_\phi Z_\phi
= 0.
$$

Hence, by Part 2 of Proposition 1, the signal-to-noise ratio of the $\phi$-gradient decays as

$$
\frac{\mathbb{E}_{z^{1:K} \sim q_\phi} [\nabla_{\phi}^{\text{IWAE}} \langle \theta, z^{1:K} \rangle]}{\sqrt{\text{var}_{z^{1:K} \sim q_\phi} [\nabla_{\phi}^{\text{IWAE}} \langle \theta, z^{1:K} \rangle]}} = \mathcal{O}(K^{-1/2}).
$$

To circumvent this breakdown, Tucker et al. (2019) recently proposed the alternative estimator

$$
\nabla_{\phi}^{\text{IWAE}} \langle \theta, z^{1:K} \rangle := \sum_{k=1}^K \frac{w_\psi(z^k)}{\sum_{l=1}^K w_\psi(z^l)} \nabla_\phi [\log o w_{\psi'} o h_\phi] \vert_{\psi'=\psi} (h_\phi^{-1}(z^k)).
$$

(5)

They also showed that this estimator is equal to $\nabla_{\phi}^{\text{IWAE}} \langle \theta, z^{1:K} \rangle$ in expectation and hence also unbiased for $\nabla_{\phi} L^K_\psi$. This is a consequence of the following identity proved in Tucker et al. (2019) Section 8.1): for any $\phi$ and suitably regular function $f_\phi : Z \to \mathbb{R}$,

$$
q_\phi (f_\phi \nabla_\phi \log q_\phi) = q (\nabla_\phi [f_{\phi'} o h_\phi] \vert_{\phi'=\phi})
= q_\phi (\nabla_\phi [f_{\phi'} o h_\phi] \vert_{\phi'=\phi} o h_\phi^{-1})
= q_\phi (f_\phi \nabla_\phi [\log o f_{\phi'} o h_\phi] \vert_{\phi'=\phi} o h_\phi^{-1}),
$$

(6)

where we use the notation $\phi'$ to indicate that $f_{\phi'}$ is not differentiated w.r.t. the parameters in the subscript. Using this identity, Tucker et al. (2019) also established
that another \[ \text{IWAE} \] \( \phi \)-gradient estimator, heuristically derived in Roeder et al. (2017) and given by

\[
\tilde{\nabla}^{\text{STL}}_{\phi} (\theta, z^{1:K}) := \sum_{k=1}^{K} \frac{w_{\psi}(z^k)}{\sum_{l=1}^{K} w_{\psi}(z^l)} \nabla_{\phi} \left[ \log \circ w_{\psi} \circ h_{\phi} \right]_{\psi = \psi(h_{\phi}^{-1}(z^k))},
\]

is in fact biased for \( \nabla_{\phi} \mathcal{L}^K_{\psi} \). Nonetheless this \( \phi \)-gradient, termed sticking the landing (STL), performed consistently better than or at least on par with state-of-the-art alternatives in Tucker et al. (2019).

### 2.3 Reweighted wake-sleep (RWS)

**Objective.** The reweighted wake-sleep (RWS) algorithm was proposed in Bornschein and Bengio (2015). The RWS algorithm again uses \( K \geq 1 \) samples to optimise \( \psi = (\theta, \phi) \) as

\[
\theta^* := \theta^{\text{ML}} = \arg \max_{\theta} \log Z_{\theta},
\]

\[
\phi^* := \arg \min_{\phi} \text{KL}(\pi_{\theta^{\text{ml}}} || q_{\phi}).
\]

Here, \( \text{KL}(p||q) := \int_Z \log(p(z)/q(z))q(z)dz \) is the Kullback–Leibler (KL)-divergence from \( p \) to \( q \).

**Gradients.** The \( \theta \)- and \( \phi \)-gradients

\[
\begin{bmatrix}
\nabla_{\theta} \log Z_{\theta} \\
-\nabla_{\phi} \text{KL}(\pi_{\theta} || q_{\phi})
\end{bmatrix} = \hat{\pi}_{\theta} \begin{bmatrix}
\nabla_{\theta} \log \gamma_{\theta} \\
\nabla_{\phi} \log q_{\phi}
\end{bmatrix},
\]

are usually intractable and therefore approximated via self-normalised importance sampling:

\[
\begin{bmatrix}
\nabla^{\text{RWS}}_{\theta} (\phi, z^{1:K}) \\
\nabla^{\text{RWS}}_{\phi} (\theta, z^{1:K})
\end{bmatrix} := \hat{\pi}_{\theta} (\phi, z^{1:K}) \begin{bmatrix}
\nabla_{\theta} \log \gamma_{\theta} \\
\nabla_{\phi} \log q_{\phi}
\end{bmatrix}
\]

\[
= \sum_{k=1}^{K} \frac{w_{\psi}(z^k)}{\sum_{l=1}^{K} w_{\psi}(z^l)} \begin{bmatrix}
\nabla_{\theta} \log \gamma_{\theta}(z^k) \\
\nabla_{\phi} \log q_{\phi}(z^k)
\end{bmatrix},
\]

for \( z^1, \ldots, z^K \sim q_{\phi} \). Note that since (9) relies on self-normalised importance sampling, it is not unbiased relative to (8).

The optimisation of \( \theta \) and \( \phi \) is carried out simultaneously. This is because (a) a better proposal \( q_{\phi} \) reduces both bias and variance of (self-normalised) importance-sampling approximations and can therefore be leveraged for reducing the bias and variance of the \( \theta \)-gradients and (b) this strategy reduces the computational cost because the same samples \( z^{1:K} \) and weights \( \{w_{\psi}(z^k)\}_{k=1}^{K} \) are shared by both gradients. However, this simultaneous optimisation is often viewed as the main drawback of RWS because it is not clear which joint objective function (for both \( \theta \) and \( \phi \)) is being optimised.

\(^1\)Following Le et al. (2018b), we restrict our attention to the RWS variant which only uses the “wake-phase” \( \phi \)-updates.
Reparametrised φ-gradient from Tucker et al. (2019). Tucker et al. (2019, Section 4) also apply the identity from (6) to $\nabla_{\phi}^{\text{RWS}}(\theta, z^{1:K})$ to obtain the alternative φ-gradient estimator for RWS:

$$\nabla_{\phi}^{\text{RWS}}(\theta, z^{1:K}) := \sum_{k=1}^{K} \left[ \frac{w_\psi(z^k)}{\sum_{l=1}^{K} w_\psi(z^l)} - \left( \frac{w_\psi(z^k)}{\sum_{l=1}^{K} w_\psi(z^l)} \right)^2 \right] \times \nabla_\phi \log \circ w_\psi \circ h_\phi |_{\psi'=\psi(h_\phi^{-1}(z^k))}. \quad (10)$$

Again, (6) shows that this estimator is equal to $\nabla_{\phi}^{\text{RWS}}(\theta, z^{1:K})$ from (9) in expectation.

Comparison with IWAE. As discussed in Burda et al. (2016), there is a philosophical difference between the IWAE and RWS. Assume that $K$ is finite and that $\pi_\theta \neq q_\phi$ for any $\phi$. In this case, we have the following regarding the optimisation of $\theta$:

- **IWAE** seeks to optimise a biased objective in the sense that $L^K_\phi < \log Z_\theta$; yet, for this biased objective, **IWAE** is able to use vanilla-Monte Carlo based – and hence unbiased – gradients.
- **RWS** seeks to optimise an unbiased objective in the sense that the objective is the true marginal log-likelihood $\log Z_\theta = \log p_\theta(x)$; yet, for this unbiased objective, **RWS** needs to resort to self-normalised importance-sampling based – and hence biased – gradients.

Despite the different paradigms, both approaches lead to the same $\theta$-gradient:

$$\nabla_\theta^{\text{IWAE}}(\phi, z^{1:K}) = \nabla_\theta^{\text{RWS}}(\phi, z^{1:K}),$$

whose bias relative to $\nabla_\theta \log Z_\theta$ decays as $O(K^{-1})$ by Part 2 of Proposition 1. Though, of course, for any given $K$, the distribution of this estimator also depends on the inference-network parameters $\phi$. Further connections between **IWAE** and **RWS** will be formally established in Section 3 in which we show that both methods can be viewed as special cases of a unified adaptive importance-sampling framework.

### 3 AISLE: A unified adaptive importance-sampling framework

#### 3.1 Objective

Note that if $\theta$ is fixed, the **RWS** algorithm reduces to an adaptive importance-sampling scheme which optimises the proposal distribution by minimising the Kullback–Leibler divergence from the target distribution $\pi_\theta$ to the proposal $q_\phi$ (see, e.g., Douc et al., 2007, Cappé et al., 2008, for other adaptive importance-sampling schemes taking this approach). If instead $\phi$ is fixed, the approach reduces to a standard stochastic approximation of the MLE of the generative-model parameters $\theta$. The advantage of optimising $\theta$ and $\phi$ simultaneously is that (a) Monte Carlo samples used to approximate the $\theta$-gradient can be re-used to approximate the $\phi$-gradient
and (b) optimising $\phi$ typically reduces the error (both in terms of bias and variance) of the $\theta$-gradient approximation. However, adapting the proposal distribution $q_\phi$ in importance-sampling schemes need not necessarily be based on minimising the KL-divergence. Numerous other techniques exist in the literature (e.g., Geweke [1989], Evans [1991], Oh and Berger [1992], Richard and Zhang [2007], Cornebise et al. [2008]) and may be preferable in some settings. Indeed, another popular approach with strong theoretical support is based on minimising the $\chi^2$-divergence (see, e.g., Deniz Akyildiz and Míguez [2019]). Based on this insight, we slightly generalise the objective of the RWS algorithm as follows.

$$\theta^* := \theta_{\text{ML}} = \arg \max_\theta \log Z_\theta,$$

$$\phi^* := \arg \min_\phi D_f(\pi_{\theta_{\text{ML}}} \parallel q_\phi). \quad (11)$$

Here, $D_f(p \parallel q) := \int Z_f(\pi_{\theta_{\text{ML}}}(z)/q(z))q(z)dz$ is some $f$-divergence from $p$ to $q$. We reiterate that alternative approaches for optimising $\phi$ (which do not involve the minimisation of some $f$-divergence) could be used. However, (11) suffices for the analysis in the remainder of this work and is therefore stated for concreteness. For easier reference, we hereafter refer to the resulting optimisation algorithm as adaptive importance sampling for learning (AISLE).

3.2 Gradients

As for RWS, we perform the optimisation via a stochastic gradient-ascent approach. In particular, the intractable $\theta$-gradient $\nabla_\theta \log Z_\theta = \pi_\theta(\nabla_\theta \log \gamma_\theta)$ is approximated by the self-normalised importance-sampling estimate

$$\nabla_\theta \text{AISLE}(\phi, z^{1:K}) := \hat{\pi}_\theta(\phi, z^{1:K}) \nabla_\theta \log \gamma_\theta$$

$$= \sum_{k=1}^K \frac{w_\phi(z_k)}{\sum_{l=1}^K w_\phi(z_l)} \nabla_\theta \log \gamma_\theta(z_k), \quad (12)$$

for $z^1, \ldots, z^K \overset{iid}{\sim} q_\phi$. As noted at the end of the previous section, this $\theta$-gradient is thus the same for all algorithms discussed in this work. However, the $\phi$-gradients depend on the particular choice of $f$-divergence in (11).

3.3 Special case I: RWS and STL

We recover RWS as a special case of AISLE if we define the $f$-divergence through $f(y) := y \log y$ because in this case $D_f(p \parallel q) = \text{KL}(p \parallel q)$ reduces to the KL-divergence. Our main contribution in this subsection is to show that a more principled application of the identity from [6] to RWS leads to the STL estimator from [7] proposed in Roeder et al. [2017].

Recall that Tucker et al. [2019, Section 4] obtained an alternative $\phi$-gradient estimator $\nabla_\phi \text{RWS}(\theta, z^{1:K})$ given in (10). Specifically, in order to derive (10) they first replaced the exact (but intractable) $\phi$-gradient $-\nabla_\phi \text{KL}(\pi_\theta \parallel q_\phi) = \pi_\theta(\nabla_\phi \log q_\phi)$ by the self-normalised importance-sampling approximation $\nabla_\phi \text{RWS}(\theta, z^{1:K})$ and then applied the identity from [6]. Note that this may result in a variance reduction but
does not change the bias of the gradient estimator. Therefore, in order to potentially reduce both bias and variance, we argue here that a more principled approach is to \textit{first} apply the identity from (6) to the exact \( \phi \)-gradient and \textit{then} approximate the resulting expression via self-normalised importance sampling. Specifically, applying (6) with \( f_\phi = w_\psi \) yields

\[
\pi_\theta(\nabla_\phi \log q_\phi) = q_\phi(w_\psi \nabla_\phi \log q_\phi)/Z_\theta = \pi_\theta(\nabla_\phi \log q_\phi)\big|_{\psi' = \psi \circ h_\phi^{-1}}
\]

whose self-normalised importance-sampling approximation, for \( z^1, \ldots, z^K \sim q_\phi \), is

\[
\nabla^{\text{AISLE}}(\phi, z^{1:K}) := \pi_\theta(\phi, z^{1:K})(\nabla_\phi \log q_\phi)\big|_{\psi' = \psi \circ h_\phi^{-1}}
= \sum_{k=1}^{K} \frac{w_\phi(z^k)}{\sum_{l=1}^{K} w_\phi(z^l)} \nabla_\phi \log q_\phi \big|_{\psi' = \psi \circ h_\phi^{-1}(z^k)}
= \nabla^{\text{STL}}(\phi, z^{1:K}). \tag{13}
\]

The identity from (13) is notable because the \text{STL} estimator from Roeder et al. (2017) has hitherto been viewed as an alternative gradient for IWAE for which it is biased and only heuristically justified even though it performed very well empirically in Tucker et al. (2019). The fact that STL exhibited good performance even in an example in which plain RWS breaks down, suggests that this breakdown may not be due to RWS lack of optimising a joint objective as previously conjectured.

### 3.4 Special case II: IWAE

We now demonstrate that the \text{IWAE} can be recovered as a special case of \text{AISLE}. To establish this relationship, we take \( f(y) := (y - 1)^2 \) so that

\[
D_f(p||q) = \chi^2(p||q) := \int_Z \left( \frac{p(z)}{q(z)} - 1 \right)^2 q(z) \, dz = \int_Z \frac{p(z)}{q(z)} p(z) \, dz - 1,
\]

is the \( \chi^2 \)-divergence. Minimising this divergence is natural in importance sampling since \( \chi^2(\pi_\theta||q_\phi) = \text{var}_{z \sim q_\phi}[\phi(z)/Z_\theta] \) is the variance of the importance weights and the sampling approximation of its reciprocal is proportional to the effective sample size introduced in Kong et al. (1994); Liu (1996) which is widely used in practice to assess and improve the efficiency of importance-sampling schemes. In this case, the \( \phi \)-gradient is

\[
-\nabla_\phi \chi^2(\pi_\theta||q_\phi) = -\pi_\theta(\nabla_\phi w_\psi)/Z_\theta = \pi_\theta(w_\psi \nabla_\phi \log q_\phi)/Z_\theta = q_\phi(w_\psi^2 \nabla_\phi \log q_\phi)/Z_\theta^2 = q_\phi(w_\psi^2 \nabla_\phi \log q_\phi)\big|_{\psi' = \psi \circ h_\phi^{-1}})/Z_\theta^2 = \pi_\theta(2w_\psi \nabla_\phi \log q_\phi)\big|_{\psi' = \psi \circ h_\phi^{-1}})/Z_\theta,
\]

where the penultimate line follows from (6) with \( f_\phi = w_\psi^2 \). Replacing the numerator and denominator by the usual (self-normalised) importance-sampling approximations then yields the \text{AISLE} \( \phi \)-gradient estimator which coincides with the
reparametrised [IWAE] φ-gradient estimate from Tucker et al. (2019) given in (5) (up to the constant factor 2K). That is,
\[
\hat{\nabla}^{\text{AILSE}}_\phi(\theta, z^{1:K}) := \phi_\theta(z^{1:K}) (2w_\psi \nabla \phi z^{1:K}) / \tilde{Z}_\theta(\phi, z^{1:K})
\]
\[
= 2K \sum_{k=1}^K \left( \sum_{l=1}^K w_\psi(z_l) \right)^2 \nabla \phi \phi_\theta(z^1(z_k)) \ (14)
\]
for \( z^1, \ldots, z^K \sim q_\phi \). Note that if we normalise the gradients in the implementation, such as effectively done by popular optimisers such as ADAM (Kingma and Ba, 2015), the constant factor cancels out and both AISLE and IWAE become computationally equivalent. Finally, we note that without exploiting the identity from (6), the reparametrisation-gradient for minimising the above \( \chi^2 \)-divergence leads to a sampling-approximation which is proportional to the \( \phi \)-gradient proposed in Dieng et al. (2017) (see Subsection A.1 of the supplementary materials for details).

3.5 Extension to sequential Monte Carlo methods

Variational sequential Monte Carlo (SMC) approaches have recently been proposed in Maddison et al. (2017); Le et al. (2018a); Naesseth et al. (2018); Hirt and Dellaportas (2019). These are closely related to IWAEs. Indeed they optimise a multi-sample objective which may be viewed as a generalisation of the IWAE objective. For this reason, these methods struggle with the problem that resampling introduces latent variables into the objective which are discrete and which therefore cannot be reparametrised. This leaves certain high-variance terms in the gradient estimators which are typically simply ignored. However, this introduces a bias which is difficult to quantify and is detrimental to the optimisation of proposal kernels that take future observations into account (Lawson et al., 2018).

In contrast, AISLE extends more naturally to a SMC setting because it allows us to draw upon the numerous iterative schemes for optimising the proposal kernels used by SMC algorithms that have already been proposed in the literature (Cornebise et al., 2008; Gu et al., 2015; Guarniero et al., 2017; Heng et al., 2017). Furthermore, SMC-based generalisations of the \( \theta \)-gradient from (12) (as well as the corresponding Hessian) are also well understood (Poyiadjis et al., 2005; Del Moral et al., 2010) and often cheap to implement (Olsson and Westerborn, 2017).

4 Conclusion

We have introduced a simple, unified adaptive-importance-sampling framework termed adaptive importance sampling for learning (AISLE) and have proved that it admits various state-of-the-art variational methods as special cases, such as the importance weighted autoencoders (IWAEs) (Burda et al., 2016), the sticking the landing (STL) modification of IWAE (Roeder et al., 2017) and the reweighted wake-sleep (RWS) algorithm (Bornschein and Bengio, 2015).

Our framework explicitly views these these techniques as seeking to minimise an \( f \)-divergence of the form \( D_f(\pi_\theta / q_\phi) \) instead of \( D_f(q_\phi / \pi_\theta) \), e.g. the “inclusive”
KL-divergence instead of the “exclusive” KL-divergence. Minimising the former is often viewed as less favourable because minimising the latter (a) uses φ-gradient approximations that do not rely on importance-weighting and thus scale better to higher dimensions, (b) induces a mode-seeking behaviour which is often desirable in high-dimensional or multi-modal scenarios. We are currently exploring the possibility of explicitly incorporating such a bias–variance trade-off into AISLE by replacing $\pi_\theta(z)$ by a regularised distribution, e.g. by a distribution proportional to $\pi_\theta(z)^\alpha q_\phi(z)^{1-\alpha}$ for $\alpha \in (0, 1]$ (and also replacing $\theta$ by $(\vartheta, \varphi)$).

We hope that this work highlights the potential for further improving variational techniques by drawing upon the vast body of research on (adaptive) importance sampling in the computational statistics literature; for instance, annealed importance sampling (Jarzynski, 1997a,b; Neal, 2001) has already been successfully combined with variational methods (Huang et al., 2018). Conversely, the methodological connections established in this work may also serve to emphasise the utility of the reparametrisation trick from Kingma and Welling (2014); Tucker et al. (2019) to computational statisticians.

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A Illustrations

A.1 Algorithms

In these supplementary materials, we illustrate the different $\phi$-gradient estimators (recall that all algorithms discussed in this work share the same $\theta$-gradient estimator). Specifically, we compare the following approximations.

- **AISLE-KL-NOREP.** The gradient for $\text{AISLE}$ based on the KL-divergence without any further reparametrisation, i.e. this coincides with the standard RWS-gradient from [9].

- **AISLE-KL.** The gradient for $\text{AISLE}$ based on the KL-divergence after reparametrisising and exploiting the identity from [6]; it is given by [13] which also shows that it coincides with the STL-gradient from [7].

- **AISLE-CHISQ-NOREP.** The gradient for $\text{AISLE}$ based on the $\chi^2$-divergence without any reparametrisation. This gradient was not explicitly stated above. It is based on the representation $-\nabla_\phi \chi^2(\pi_\theta \| q_\phi) = \pi_\theta(w_\phi \nabla_\phi \log q_\phi) / Z_\theta$ which
has the sampling-approximation
\[ \tilde{\pi}_\theta(\phi, z^{1:K}) (w_\psi \nabla_{\phi} \log q_\phi) / \tilde{Z}_\theta(\phi, z^{1:K}) = K \sum_{k=1}^{K} \left( \frac{w_\psi(z_k)}{\sum_{l=1}^{K} w_\psi(z_l)} \right)^2 \nabla_{\phi} \log q_\phi(z_k). \]

- **AISLE-CHISQ.** The gradient for **AISLE** based on the $\chi^2$-divergence after reparametrisation and exploiting the identity from [6]; it is given by [14] which also shows that it is proportional to the reparametrised **IWAE** gradient proposed in [Tucker et al. (2019)] which was stated in [5]. When normalising the gradients (as, e.g. implicitly done by optimisers such as **ADAM** [Kingma and Ba, 2015]), the proportionality constant cancels out so that both these gradient approximations lead to computationally the same algorithm.

- **IWAE-NOREP.** The gradient for **IWAE** without any reparametrisation. Its sampling approximation is given by the terms inside the expectation in [3].

- **IWAE.** The gradient for **IWAE** employing the reparametrisation trick from [Kingma and Welling (2014)]. Its sampling approximation is given in [4]. Recall that this is the gradient whose signal-to-noise ratio degenerates with $K$ as pointed out in [Rainforth et al. (2018)].

- **IWAE-TUCKER.** The reparametrisated **IWAE** gradient proposed in [Tucker et al. (2019)] which was stated in [5] and which, as mentioned above, is proportional to the gradient for **AISLE** based on the $\chi^2$-divergence after reparametrisation and exploiting the identity from [6].

- **RWS-TUCKER.** The gradient for **RWS** given in [10]. It was proposed in [Tucker et al. (2019)] who derived it by applying the identity from [6] to the default **RWS** gradient estimate.

- **DIENG.** The gradient for **AISLE** based on the $\chi^2$-divergence employing the reparametrisation trick from [Kingma and Welling (2014)]. This gradient was not explicitly stated above. It is based on the representation
\[ -\nabla_{\phi} \chi^2(\pi_\theta \| q_\phi) = -\pi_\theta(\nabla_{\phi} \log w_\psi^2 \circ h_\phi \circ h_\phi^{-1}) / Z_\theta \] which leads to the following sampling-approximation which is proportional to the gradient proposed in [Dieng et al. (2017)]
\[ -\tilde{\pi}_\theta(\phi, z^{1:K}) (\nabla_{\phi} \log w_\psi^2 \circ h_\phi \circ h_\phi^{-1}) / \tilde{Z}_\theta(\phi, z^{1:K}) = -2K \sum_{k=1}^{K} \left( \frac{w_\psi(z_k)}{\sum_{l=1}^{K} w_\psi(z_l)} \right)^2 \nabla_{\phi} \log w_\psi \circ h_\phi(\circ h_\phi^{-1}(z_k)). \]

### A.2 Model

**Generative model.** We have $N \times D$-dimensional observations $x^{(1)}, \ldots, x^{(N)} \in \mathbb{R}^{D \times 1}$ and $N \times D$-dimensional latent variables $z^{(1)}, \ldots, z^{(N)} \in \mathbb{R}^{D \times 1}$. Hereafter, wherever
necessary, we add an additional subscript to make the dependence on the observations explicit. The joint law (the “generative model”), parametrised by \( \theta \), of the observations and latent variables then factorises as

\[
\prod_{n=1}^{N} p_{\theta}(z^{(n)} \mid x^{(n)}) = \prod_{n=1}^{N} \gamma_{\theta,x}(z^{(n)}).
\]

We model each latent variable–observation pair \((z, x)\) as

\[
p_{\theta}(z) := N(z; \mu, \Sigma), \\
p_{\theta}(x \mid z) := N(x; z; I_D),
\]

where \( \theta := \mu = \mu_{1:D} \in \mathbb{R}^{D \times 1} \), where \( \Sigma := (\sigma_{d,e})_{(d,e) \in \{1, \ldots, D\}^2} \in \mathbb{R}^{D \times D} \) is assumed to be known and where \( I_D \) denotes the \( D \times D \) identity matrix. For any \( \theta \),

\[
Z_{\theta,x} = p_{\theta}(x) = N(x; \mu, I_D + \Sigma), \\
\pi_{\theta,x}(z) = p_{\theta}(z \mid x) = N(z; \nu_{\theta,x}, \Gamma),
\]

with \( \Gamma := (\Sigma^{-1} + I_D)^{-1} \) and \( \nu_{\theta,x} := \Gamma(\Sigma^{-1}\mu + x) \). In particular, (15) implies that \( \theta^{ml} = \frac{1}{N} \sum_{n=1}^{N} x^{(n)} \).

**Proposal/variational approximation.** We take the proposal distributions as a fully-factored Gaussian:

\[
q_{\phi,x}(z) := N(z; Ax + b, C),
\]

where \( A = (a_{d,e})_{(d,e) \in \{1, \ldots, D\}^2} \in \mathbb{R}^{D \times D}, b = b_{1:D} \in \mathbb{R}^{D \times 1} \) and, for \( c_{1:D} := c \in \mathbb{R}^{D \times 1}, C := \text{diag}(e^{2c_1}, \ldots, e^{2c_D}) \). The parameters to optimise are thus

\[
\phi := (a_1^T, \ldots, a_D^T, b^T, c^T),
\]

where \( a_d := [a_{d,1}, a_{d,2}, \ldots, a_{d,D}]^T \in \mathbb{R}^{D \times 1} \) denotes the column vector formed by the elements in the \( d \)th row of \( A \). Furthermore, for the reparametrisation trick, we take \( q(\varepsilon) := N(\varepsilon; 0_D, I_D) \), where \( 0_D \in \mathbb{R}^{D \times 1} \) is a vector whose elements are all 0, so that

\[
h_{\phi,x}(\varepsilon) := Ax + b + C^{1/2}\varepsilon,
\]

which means that \( h_{\phi,x}^{-1}(z) = C^{-1/2}(z - Ax - b) \).

Note that the mean of the proposal in (17) coincides with the mean of the posterior in (16) if \( A = \Gamma \) and \( b = \Gamma \Sigma^{-1}\mu \).

This model is similar to the one used as a benchmark in Rainforth et al. (2018, Section 4) and also in Tucker et al. (2019, Section 6.1) who specified both the generative model and the variational approximation to be isotropic Gaussians. Specifically, their setting can be recovered by taking \( \Sigma := I_D \) and fixing \( c_d = \log(2/3)/2 \) so that \( C = \frac{3}{2}I_D \) throughout. Here, in order to investigate a slightly more realistic scenario, we also allow for the components of the latent vectors \( z \) to be *correlated/dependent* under the generative model. However, as the variational approximation remains restricted to being fully factored, it may fail to fully capture the uncertainty about the latent variables.
Gradient calculations. We end this subsection by stating the expressions needed to calculate the gradients in the Gaussian example presented above. Throughout, we use the denominator-layout notation for vector and matrix calculus and sometimes write $\varepsilon = \varepsilon_{1:D} = h_{\phi,x}^{-1}(z)$ to simplify the notation. Thus,

\begin{align*}
\nabla_{\theta} \log \gamma_{\theta,x}(z) &= \Sigma^{-1}(z - \mu) \in \mathbb{R}^{D \times 1}, \\
\nabla_{z} \log \gamma_{\theta,x}(z) &= \Sigma^{-1}(\mu - z) + x - z \in \mathbb{R}^{D \times 1}, \\
\nabla_{z} \log q_{\phi,x}(z) &= -C^{-1}(z - Ax - b) \\
&= -C^{-1/2}\varepsilon \in \mathbb{R}^{D \times 1}.
\end{align*}

(18)

Let $a_d := [a_{d,1}, a_{d,2}, \ldots, a_{d,D}]^T \in \mathbb{R}^{D \times 1}$ denote the column vector formed by the elements in the $d$th row of $A$. Then, letting $\odot$ denote elementwise multiplication,

\begin{align*}
\nabla_{a_d} \log q_{\phi,x}(z) &= C^{-1}(z_d - a_d^T x - b_d)x \\
&= C^{-1/2}\varepsilon_d x \in \mathbb{R}^{D \times 1}, \quad d \in \{1, \ldots, D\}, \\
\nabla_{b} \log q_{\phi,x}(z) &= C^{-1}(z - Ax - b) \\
&= C^{-1/2}\varepsilon \in \mathbb{R}^{D \times 1}, \\
\nabla_{c} \log q_{\phi,x}(z) &= C^{-1/2}(z - Ax - b) \odot C^{-1/2}(z - Ax - b) - 1_D \\
&= \varepsilon \odot \varepsilon - 1_D \in \mathbb{R}^{D \times 1},
\end{align*}

Furthermore, write $h_{\phi,x} = [h_{\phi,x,1}, \ldots, h_{\phi,x,D}]^T$, i.e.

\[ h_{\phi,x,d}(\varepsilon) = z_d = a_d^T x + b_d + \exp(c_d)\varepsilon_d, \]

and let $e^{(d)} = [0, \ldots, 0, 1, 0, \ldots, 0]^T \in \mathbb{R}^{D \times 1}$ be the vector whose entries are all 0 except for the $d$th entry which is 1. Then, for $d \in \{1, \ldots, D\}$,

\begin{align*}
\nabla_{a_d} h_{\phi,x,d}(\varepsilon) &= 1\{d = d'\} x \in \mathbb{R}^{D \times 1}, \quad d' \in \{1, \ldots, D\}, \\
\nabla_{b} h_{\phi,x,d}(\varepsilon) &= e^{(d)} \in \mathbb{R}^{D \times 1}, \quad (20) \\
\nabla_{c} h_{\phi,x,d}(\varepsilon) &= \exp(c_d)\varepsilon_d e^{(d)} \in \mathbb{R}^{D \times 1}. \quad (21)
\end{align*}

(21)

Again writing $\varepsilon = h_{\phi,x}^{-1}(z)$ implies that

\begin{align*}
\nabla_{\phi} \log \circ w_{\psi,x} \circ h_{\phi,x}|_{\psi=\psi}(\varepsilon) &= [\nabla_{\phi} h_{\phi,x,1}, \ldots, \nabla_{\phi} h_{\phi,x,D}] (\varepsilon) \nabla_{z} \log w_{\psi,x}(z),
\end{align*}

so that, letting $[\nabla_{z} \log w_{\psi,x}(z)]_d$ denote the $d$th element of the vector $\nabla_{z} \log w_{\psi,x}(z)$,

\begin{align*}
\nabla_{a_d} \log \circ w_{\psi,x} \circ h_{\phi,x}|_{\psi=\psi}(\varepsilon) &= [\nabla_{z} \log w_{\psi,x}(z)]_d x, \\
\nabla_{b} \log \circ w_{\psi,x} \circ h_{\phi,x}|_{\psi=\psi}(\varepsilon) &= \nabla_{z} \log w_{\psi,x}(z), \\
\nabla_{c} \log \circ w_{\psi,x} \circ h_{\phi,x}|_{\psi=\psi}(\varepsilon) &= \varepsilon \odot C^{1/2} \nabla_{z} \log w_{\psi,x}(z).
\end{align*}

From this, since

\begin{align*}
\nabla_{\phi} \log \circ w_{\psi,x} \circ h_{\phi,x}|_{\psi=\psi}(\varepsilon) &= \nabla_{\phi} \log \circ w_{\psi,x} \circ h_{\phi,x}|_{\psi=\psi}(\varepsilon) - \nabla_{\phi} \log q_{\phi,x}(z),
\end{align*}

we have that

\begin{align*}
\nabla_{a_d} \log \circ w_{\psi,x} \circ h_{\phi,x}(\varepsilon) &= ([\nabla_{z} \log w_{\psi,x}(z)]_d - C^{-1/2}\varepsilon_d) x, \\
\nabla_{b} \log \circ w_{\psi,x} \circ h_{\phi,x}(\varepsilon) &= \nabla_{z} \log w_{\psi,x}(z) - C^{-1/2}\varepsilon, \\
\nabla_{c} \log \circ w_{\psi,x} \circ h_{\phi,x}(\varepsilon) &= \varepsilon \odot C^{1/2} \nabla_{z} \log w_{\psi,x}(z) - \varepsilon \odot \varepsilon + 1_D.
\end{align*}

(19)
A.3 Analytical illustration

In this subsection, we analytically illustrate the impact of the reparametrisation trick combined with the identity from [Tucker et al., 2019] which was given in (6). Recall that this approach yields $\phi$-gradients that are expressible as integrals of path-derivative functions $\nabla \phi \log w_{\psi,x} \circ h_{\phi,x} |_{\psi' = \psi}$. Thus, if there exists a value $\phi$ such that $q_{\phi,x} = \pi_{\theta,x}$ then $w_{\psi,x} \propto \pi_{\theta,x} / q_{\phi,x} \equiv 1$ is constant so that we obtain zero-variance $\phi$-gradients (see, e.g., Roeder et al., 2017, for a discussion on this).

For simplicity, assume that $\Sigma = I_D$ and recall that we then have $q_{\phi,s,x} = \pi_{\theta,x}$ if the values $(A,b,C)$ implied by $\phi^*$ are $(A^*,b^*,C^*) = (\frac{1}{2}I_D, \frac{1}{2}\mu, \frac{1}{2}I_D)$. By (18) and (19), and with the usual convention $\varepsilon = h_{\phi,x}^{-1}(z)$, we then have

$$\nabla_z \log w_{\psi,x}(z) = (x + \mu) - 2z + C^{-1}(z - Ax - b) = 2[(A^*x + b^*) - (Ax + b) + C^{-1/2}(C^* - C)\varepsilon]. \quad (23)$$

Note that the only source of randomness in this expression is the multivariate normal random variable $\varepsilon$. Thus, by (20) and (21), for any values of $A$ and $b$ and any $K \geq 1$, the variance of the $A$- and $b$-gradient approximations from AISLE-KL (a.k.a. STL) and AISLE-CHISQ/IWAE-TUCKER goes to zero as $C \to C^* = \frac{1}{2}I_D$. In other words, in this model, these algorithms have (near) zero-variance gradients for the parameters governing the proposal mean as soon as the variance-parameters fall within a neighbourhood of their optimal values. Furthermore, (22) combined with (23) shows that for any $K \geq 1$, the variance of the $C$-gradient also goes to zero as $(A,b,C) \to (A^*,b^*,C^*)$. A more thorough analysis of the benefits of reparametrisation-trick gradients in Gaussian settings is carried out in Xu et al. (2019).

A.4 Empirical illustration

Setup. We end this section by empirically comparing the algorithms from Subsection A.1. We run each of these algorithms for a varying number of particles, $K \in \{1, 10, 100\}$, and varying model dimensions, $D \in \{2, 5, 10\}$. Each of these configurations is repeated independently 250 times. Each time using a new synthetic data set consisting of $N = 25$ observations sampled from the generative model after generating a new “true” prior mean vector as $\mu \sim N(0_D, I_D)$. Since all the algorithms share the same $\theta$-gradient, we focus only on the optimisation of $\phi$ and thus simply fix $\theta := \theta_{\text{ml}}$ throughout. To initialise the gradient-ascent algorithm, we draw each component of the initial values $\phi_0$ of $\phi \overset{\text{IID}}{\sim} \mathcal{N}(0, I_D)$ according to a standard normal distribution. We use both plain stochastic gradient-ascent (with the gradients normalised to have unit $L_1$-norm) and the ADAM optimiser (Kingma and Ba, 2015) with default parameter values. The total number of iterations is $10,000$; in each case, the learning-rate parameters at the $i$th step are $i^{-1/2}$. We show results for the four following settings.

- **Figure 1** The generative model is specified via $\Sigma = I_D$. In this case, there exists a value $\phi^*$ of $\phi$ such that $q_{\phi,x}(z) = \pi_{\theta,x}(z)$. Plain stochastic gradient-ascent is used.
• **Figure 2.** Same as Figure 1 except that we use ADAM instead of plain gradient-ascent.

• **Figure 3.** The generative model is specified via $\Sigma = (0.95^{d-|d+1|})_{(d,e) \in \{1,\ldots,D\}^2}$. Note that in this case, the fully-factored variational approximation cannot fully mimic the dependence structure of the latent variables under the generative model. That is, in this case, $q_{\phi,x}(z) \neq \pi_{\theta,x}(z)$ for any values of $\phi$.

• **Figure 4.** Same as Figure 3 except that we use ADAM instead of plain gradient-ascent.

We note that the algorithms DIENG and, less surprisingly IWAE-NOREP, did not yield useful results in the tested configurations (which are therefore omitted from Figures 1–4). We also ran the algorithms in each of the above-mentioned scenarios with fixed values of $c_d$, e.g. as in Rainforth et al. (2018); Tucker et al. (2019). However, we omit the results as this did not significantly change the relative performance of the different algorithms. For the same reason, we omit the graphs related to the optimisation of the parameters governing $A$ and $C$.

**Summary of results.** Below, we outline what we believe to be the main takeaways from these simulation results for this particular model. However, further theoretical analysis is required to determine whether these hold in more general scenarios.

1. The performance of the reparametrisation gradients (AISLE-KL, AISLE-CHISQ, IWAE, IWAE-TUCKER) did not appear to improve with an increase in the number of particles, $K \geq 1$. Indeed, the performance appeared to become worse with increasing $K$. While Rainforth et al. (2018) offer an explanation of this behaviour in the case of IWAE (see Subsection 2.2), this explanation does not extend to AISLE-KL, AISLE-CHISQ, IWAE-TUCKER as these can not be viewed as self-normalised importance-sampling approximation of an integral that is equal to zero. We conjecture that in this model, the direction of the gradient $\nabla_{\phi}[\log w_{\psi,x} \circ h_{\phi,x}]_{\psi'=\psi} \circ h_{\psi,x}^{-1}(z)$ yield slower convergence for values of $z$ for which the weight $w_{\psi,x}(z)$ is large and as the number of particles is increased, it becomes more likely to propose particles in such a region (whose cumulative self-normalised weights are then also close to one). To counteract this issue, it may be beneficial to regularise the weights in each of these estimators, e.g. to replace $w_{\psi,x}(z^k)/\sum_{l=1}^K w_{\psi,x}(z^l)$ by $w_{\psi,x}^\alpha(z^k)/\sum_{l=1}^K w_{\psi,x}^\alpha(z^l)$, for some $\alpha \in (0,1)$.

2. The performance of the gradients AISLE-KL and AISLE-CHISQ (which are not based on any reparametrisation) benefited drastically from moderate (relative to the dimension of the latent variables) increases in the number of particles.

3. The KL-divergence based AISLE algorithms performed somewhat better than their $\chi^2$-divergence based AISLE counterparts, i.e. AISLE-KL-NOREP outperformed AISLE-CHISQ-NOREP while AISLE-KL outperformed AISLE-CHISQ (the latter being computationally equivalent to IWAE-TUCKER). We
Figure 1. Average $L_1$-error of the estimates of the constants $b = b_{1,D}$ in the mean of the Gaussian variational/proposal distribution. The average is taken over the $D$ components of $b$ and the figure displays the median error at each iteration over 250 independent runs of each algorithm, each using a different data set consisting of 25 observations sampled from the model. Here, the covariance matrix $\Sigma = I_D$ is diagonal. The results are obtained using stochastic gradient-ascent. Note the logarithmic scaling on the second axis.

Figure 2. The same setting as in Figure 1 except that ADAM is used instead of plain stochastic gradient-ascent.
Figure 3. The same setting as in Figure 1 except that here, the covariance matrix \( \Sigma = (0.95^{d-e+1})_{(d,e) \in \{1, \ldots, D\}^2} \) is not a diagonal matrix. Again, note the logarithmic scaling on the second axis.

Figure 4. The same setting as in Figure 3 except that ADAM is used instead of plain stochastic gradient-ascent.
conjecture that this is due to the fact that the χ²-divergence based variants square the (self-normalised) importance weights which increases the variance of the φ-gradients.

4. RWS-TUCKER given in (10) performed well for a moderate to large number of particles $K > 1$ in settings in which the variance of the importance weights, $\text{var}_{z \sim q_{\phi,x}}[w_{\psi,x}(z)]$ is small (or at least if it becomes small as $\phi$ is optimised), e.g. in the scenario from Figures 1-2. However, this requires that $q_{\phi,x}$ can be made very close to $\pi_{\theta,x}$ for an appropriate choice of $\phi$ which is typically only possible in low-dimensional settings and if the variational family is sufficiently expressive. Otherwise, e.g. in dimension $D = 10$ in the scenario from Figures 3-4, the performance of RWS-TUCKER was worse than that of any AISLE variants and also worse than the standard WAE reparametrisation-trick gradient. We conjecture that this is because the variance of the weights is so large that typically one of the self-normalised weights $w_{\psi,x}(z^k) / \sum_{l=1}^{K} w_{\psi,x}(z^l)$ is numerically equal to 1 while all the others are numerically equal to 0. Note that whenever this happens, the resulting gradient reduces to a vector of 0s. Again, regularising the weights, e.g. by replacing $w_{\psi,x}(z^k) / \sum_{l=1}^{K} w_{\psi,x}(z^l)$ by $w_{\psi,x}^{\alpha}(z^k) / \sum_{l=1}^{K} w_{\psi,x}^{\alpha}(z^l)$, for some $\alpha \in (0, 1)$, could be beneficial in this case.