

**Theorem 1** (Monotonicity of LV-EBM ELBO over variational families). Fix a dataset  $\{x_i\}_{i=1}^N$  and a latent-variable energy-based model

$$p_\theta(x, z) = \frac{1}{Z(\theta)} \exp(-E_\theta(x, z)),$$

with  $Z(\theta) < \infty$  and such that, for each  $i$ , the conditional density  $p_\theta(z | x_i)$  exists and is strictly positive on its support.

Let  $\mathcal{Q}$  be the set of probability densities  $q(z)$  on the latent space with finite differential entropy, and let  $\tilde{\mathcal{Q}}$  be the analogous set of joint densities  $\tilde{q}(x, z)$  with finite differential entropy. For  $q \in \mathcal{Q}$  and  $\tilde{q} \in \tilde{\mathcal{Q}}$  define

$$A_i(q) := -\mathbb{E}_{q(z)}[E_\theta(x_i, z)] + H(q), \quad B(\tilde{q}) := -\mathbb{E}_{\tilde{q}(x, z)}[E_\theta(x, z)] + H(\tilde{q}),$$

and for any collections of admissible families  $S_{\text{pos}} = \{S_{\text{pos}}(x_i)\}_{i=1}^N$  with  $S_{\text{pos}}(x_i) \subseteq \mathcal{Q}$  and  $S_{\text{neg}} \subseteq \tilde{\mathcal{Q}}$  define

$$\text{ELBO}(\theta; S_{\text{pos}}, S_{\text{neg}}) := \frac{1}{N} \sum_{i=1}^N \sup_{q \in S_{\text{pos}}(x_i)} A_i(q) - \sup_{\tilde{q} \in S_{\text{neg}}} B(\tilde{q}).$$

Assume that, for all  $\theta$  and all admissible choices of  $S_{\text{pos}}, S_{\text{neg}}$ , the above suprema are finite. Let

$$S_{\text{pos}}^1 = \{S_{\text{pos}}^1(x_i)\}_{i=1}^N, \quad S_{\text{pos}}^2 = \{S_{\text{pos}}^2(x_i)\}_{i=1}^N$$

be two collections of positive-phase families with  $S_{\text{pos}}^1(x_i) \subseteq S_{\text{pos}}^2(x_i) \subseteq \mathcal{Q}$  for all  $i$ , and let  $S_{\text{neg}}^1 \subseteq S_{\text{neg}}^2 \subseteq \tilde{\mathcal{Q}}$  be two admissible negative-phase families. Then, for every  $\theta$ ,

$$\text{ELBO}(\theta; S_{\text{pos}}^1, S_{\text{neg}}^1) \leq \text{ELBO}(\theta; S_{\text{pos}}^2, S_{\text{neg}}^2) \leq \frac{1}{N} \sum_{i=1}^N \log p_\theta(x_i). \quad (1)$$

Moreover, the first inequality in (1) is strict for a given  $\theta$  whenever at least one of the following holds:

- (i) For some  $i$ , every maximizer of  $\sup_{q \in S_{\text{pos}}^2(x_i)} A_i(q)$  lies outside  $S_{\text{pos}}^1(x_i)$ .
- (ii) Every maximizer of  $\sup_{\tilde{q} \in S_{\text{neg}}^2} B(\tilde{q})$  lies outside  $S_{\text{neg}}^1$ .

*Proof.* By the Donsker–Varadhan variational formula applied to  $f_x(z) := -E_\theta(x, z)$  and  $f(x, z) := -E_\theta(x, z)$ , we have

$$\begin{aligned} \log p_\theta(x_i) &= \sup_{q \in \mathcal{Q}} A_i(q), \\ \log Z(\theta) &= \sup_{\tilde{q} \in \tilde{\mathcal{Q}}} B(\tilde{q}), \end{aligned}$$

with maximizers  $q^\star(\cdot) = p_\theta(\cdot | x_i)$  and  $\tilde{q}^\star = p_\theta(x, z)$ , respectively. Equivalently, using the identities

$$\mathbb{E}_{\tilde{q}}[E_\theta] - H(\tilde{q}) = \text{KL}(\tilde{q} \| p_\theta) - \log Z(\theta), \quad \mathbb{E}_q[E_\theta(x_i, \cdot)] - H(q) = \text{KL}(q \| p_\theta(\cdot | x_i)) - \log p_\theta(x_i),$$

we obtain

$$\begin{aligned} A_i(q) &= \log p_\theta(x_i) - \text{KL}(q \| p_\theta(\cdot | x_i)), \\ B(\tilde{q}) &= \log Z(\theta) - \text{KL}(\tilde{q} \| p_\theta). \end{aligned}$$

Therefore, for any  $S_{\text{pos}}, S_{\text{neg}}$ ,

$$\begin{aligned} \sup_{q \in S_{\text{pos}}(x_i)} A_i(q) &= \log p_\theta(x_i) - \inf_{q \in S_{\text{pos}}(x_i)} \text{KL}(q \| p_\theta(\cdot | x_i)), \\ \sup_{\tilde{q} \in S_{\text{neg}}} B(\tilde{q}) &= \log Z(\theta) - \inf_{\tilde{q} \in S_{\text{neg}}} \text{KL}(\tilde{q} \| p_\theta), \end{aligned}$$

and hence

$$\text{ELBO}(\theta; S_{\text{pos}}, S_{\text{neg}}) = \frac{1}{N} \sum_{i=1}^N \log p_\theta(x_i) - \log Z(\theta) - \frac{1}{N} \sum_{i=1}^N \inf_{q \in S_{\text{pos}}(x_i)} \text{KL}(q \| p_\theta(\cdot | x_i)) + \inf_{\tilde{q} \in S_{\text{neg}}} \text{KL}(\tilde{q} \| p_\theta).$$

Now take two nested pairs  $(S_{\text{pos}}^1, S_{\text{neg}}^1)$  and  $(S_{\text{pos}}^2, S_{\text{neg}}^2)$  as in the statement. For each  $i$ ,

$$\inf_{q \in S_{\text{pos}}^2(x_i)} \text{KL}(q \| p_\theta(\cdot | x_i)) \leq \inf_{q \in S_{\text{pos}}^1(x_i)} \text{KL}(q \| p_\theta(\cdot | x_i)),$$

and likewise

$$\inf_{\tilde{q} \in S_{\text{neg}}^2} \text{KL}(\tilde{q} \| p_\theta) \leq \inf_{\tilde{q} \in S_{\text{neg}}^1} \text{KL}(\tilde{q} \| p_\theta),$$

since infima over supersets cannot be larger. Substituting these inequalities into the expression for  $\text{ELBO}(\theta; \cdot, \cdot)$  yields

$$\text{ELBO}(\theta; S_{\text{pos}}^1, S_{\text{neg}}^1) \leq \text{ELBO}(\theta; S_{\text{pos}}^2, S_{\text{neg}}^2)$$

for all  $\theta$ , with strict inequality whenever at least one of the two infima is strictly smaller over  $S_{\text{pos}}^2, S_{\text{neg}}^2$  than over  $S_{\text{pos}}^1, S_{\text{neg}}^1$ ; this is exactly conditions (i)–(ii).

Finally, taking  $S_{\text{pos}}^2(x_i) = \mathcal{Q}$  and  $S_{\text{neg}}^2 = \tilde{\mathcal{Q}}$ , we recover  $\sup_{q \in \mathcal{Q}} A_i(q) = \log p_\theta(x_i)$  and  $\sup_{\tilde{q} \in \tilde{\mathcal{Q}}} B(\tilde{q}) = \log Z(\theta)$ , so

$$\text{ELBO}(\theta; \mathcal{Q}, \tilde{\mathcal{Q}}) = \frac{1}{N} \sum_{i=1}^N \log p_\theta(x_i),$$

which gives the upper bound in (1).  $\square$

**Corollary 1** (LV–EBM gradient-flow families dominate parametric VI). In the setting of Theorem 1, fix  $\theta$  and let  $S_{\text{pos}}^{\text{VI}}(x_i) \subseteq \mathcal{Q}$  and  $S_{\text{neg}}^{\text{VI}} \subseteq \tilde{\mathcal{Q}}$  be any finite-dimensional “variational inference” families (e.g. diagonal Gaussian conditionals and a parametric joint). Define the corresponding VI objective by

$$\text{ELBO}_{\text{VI}}(\theta) := \text{ELBO}(\theta; S_{\text{pos}}^{\text{VI}}, S_{\text{neg}}^{\text{VI}}).$$

Let  $(\mathcal{T}_t^x)_{t \geq 0}$  and  $(\tilde{\mathcal{T}}_t)_{t \geq 0}$  denote the Markov semigroups associated with the conditional and joint Langevin dynamics used in LV–EBMs, assumed to be well-defined and Feller under the regularity assumptions on  $E_\theta$  in the main text. For any fixed time horizon  $t \geq 0$ , define the (infinite-dimensional) gradient-flow families

$$S_{\text{pos}}^{\text{flow}}(x_i) := \{\mathcal{T}_t^{x_i}(q_0) : q_0 \in \mathcal{Q}\} \subseteq \mathcal{Q}, \quad S_{\text{neg}}^{\text{flow}} := \{\tilde{\mathcal{T}}_t(\tilde{q}_0) : \tilde{q}_0 \in \tilde{\mathcal{Q}}\} \subseteq \tilde{\mathcal{Q}}.$$

Assume that every VI density can be realized as an admissible initial distribution for the semigroups, and that we include  $t = 0$  in the definition of the flow families (so that  $\mathcal{T}_0^x$  and  $\tilde{\mathcal{T}}_0$  are the identity maps on  $\mathcal{Q}$  and  $\tilde{\mathcal{Q}}$ ). Then

$$S_{\text{pos}}^{\text{VI}}(x_i) \subseteq S_{\text{pos}}^{\text{flow}}(x_i), \quad S_{\text{neg}}^{\text{VI}} \subseteq S_{\text{neg}}^{\text{flow}},$$

and, for all  $\theta$ ,

$$\text{ELBO}_{\text{VI}}(\theta) \leq \text{ELBO}(\theta; S_{\text{pos}}^{\text{flow}}, S_{\text{neg}}^{\text{flow}}) \leq \frac{1}{N} \sum_{i=1}^N \log p_\theta(x_i). \quad (2)$$

Moreover, the first inequality in (2) is strict whenever, for the given  $\theta$ , at least one of the VI families  $S_{\text{pos}}^{\text{VI}}(x_i)$  or  $S_{\text{neg}}^{\text{VI}}$  is misspecified in the sense that its best-approximation KL divergence to the true posterior  $p_\theta(z | x_i)$  or joint  $p_\theta(x, z)$  is strictly positive.

*Proof.* By definition of the semigroups,  $\mathcal{T}_0^x$  and  $\tilde{\mathcal{T}}_0$  act as the identity on  $\mathcal{Q}$  and  $\tilde{\mathcal{Q}}$ , so any VI density  $q_\phi(z | x_i)$  or  $q_\psi(x, z)$  can be written as  $\mathcal{T}_0^{x_i}(q_0)$  or  $\tilde{\mathcal{T}}_0(\tilde{q}_0)$  with  $q_0 = q_\phi$  and  $\tilde{q}_0 = q_\psi$ . Hence  $S_{\text{pos}}^{\text{VI}}(x_i) \subseteq S_{\text{pos}}^{\text{flow}}(x_i)$  and  $S_{\text{neg}}^{\text{VI}} \subseteq S_{\text{neg}}^{\text{flow}}$ . Applying Theorem 1 with  $(S_{\text{pos}}^1, S_{\text{neg}}^1) = (S_{\text{pos}}^{\text{VI}}, S_{\text{neg}}^{\text{VI}})$  and  $(S_{\text{pos}}^2, S_{\text{neg}}^2) = (S_{\text{pos}}^{\text{flow}}, S_{\text{neg}}^{\text{flow}})$  gives the inequalities in (2). Strictness follows from the strict part of Theorem 1 whenever at least one of the VI families cannot realize the exact posterior or joint.  $\square$