A connection between Tempering and Entropic Mirror Descent

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Sampling

- **Aim 1:** sample from a probability distribution π on $\mathbb{R}^d$ and approximate expectations w.r.t. $\pi(x) = \eta(x)/\mathcal{Z}$ whose normalising constant might be unknown

$$\int f(x)\pi(x)\mathrm{d}x$$

- **Motivation:** compute posterior expectations in Bayesian inference
- **Aim 2:** estimate the unknown normalising constant $\mathcal{Z}$
- **Motivation:** model selection/parameter inference

Sampling as optimisation over distributions

$$\min_{\mu \in \mathcal{P}(\mathbb{R}^d)} \mathrm{KL}(\mu|\pi)$$

where $\mathrm{KL}(\mu|\pi) = \int_{\mathbb{R}^d} \log(\mu/\pi)\mathrm{d}\mu$ denotes the Kullback–Leibler divergence.

- Variational Inference (Blei et al., 2017)
- Algorithms based on the Langevin diffusion (Jordan et al., 1998)
- Stein Variational Gradient Descent (SVGD; Liu (2017))
- Algorithms based on tempering (this work and Domingo-Enrich and Pooladian (2023))

Why tempering?

1. can tackle multimodal targets
2. normalising constant estimated for free
3. used as alternatives to poorly mixing MCMC algorithms

Gradient Descent

Gradient descent in **Euclidean space** amounts to solving

$$\dot{x}_t = -\nabla \mathcal{F}(x_t)$$

Gradient descent in the **space of distributions** amounts to solving

$$\partial_t \mu_t = \mathrm{div}\left(\mu_t \nabla \mathrm{KL}(\mu_t|\pi)\right)$$

Algorithms based on the Langevin diffusion (ULA, MALA, HMC, etc.), SVGD and continuous time tempering all implement gradient for the KL in different geometries.

Gradient Descent

Langevin diffusion $dX_t = \nabla \log \pi(X_t)dt + \sqrt{2}dB_t$

Geometry: Wasserstein-2

Gradient: $\nabla_{W_2} \mathrm{KL}(\mu_t|\pi) = \nabla \log \left(\frac{\mu_t}{\pi}\right)$

Stein Variational Gradient Descent

$dX_t^i = 1/N \sum_{j=1}^N \left[k(X_t^i, X_t^j) \nabla \log \pi(X_t^j) - \nabla_1 k(X_t^j, X_t^i) \right]$

Geometry: Stein

Gradient: $\nabla_{\mathrm{Stein}} \mathrm{KL}(\mu_t|\pi) = \int k(x, \cdot) \nabla \log \left(\frac{\mu_t}{\pi}(x)\right) d\mu_t(x)$

Tempering $\mu_t \propto \mu_0^{e^{-t}} \pi^{1-e^{-t}}$

Geometry: Fisher-Rao

Gradient: $\nabla_{\mathrm{FR}} \mathrm{KL}(\mu_t|\pi)$

Mirror Descent

Let $\mathcal{F} : \mathcal{P}(\mathbb{R}^d) \to \mathbb{R}^+$ be a functional on $\mathcal{P}(\mathbb{R}^d)$. **Mirror Descent** proceeds iteratively solving (Aubin-Frankowski et al., 2022)

$$\mu_{n+1} = \operatorname*{argmin}_{\mu \in \mathcal{P}(\mathbb{R}^d)} \left\{ \mathcal{F}(\mu_n) + \langle \nabla \mathcal{F}(\mu_n), \mu - \mu_n \rangle \; + (\gamma_{n+1})^{-1} B_\phi(\mu|\mu_n) \right\}. \quad (1)$$

- $(\gamma_n)_{n \geq 0}$ is a sequence of step-sizes
- $B_\phi(\nu|\mu) = \phi(\nu) - \phi(\mu) - \langle \nabla \phi(\mu), \nu - \mu \rangle$ for some positive and convex ϕ is the **Bregman divergence**
- $\langle \nabla \mathcal{F}(\nu), \xi \rangle = \lim_{\epsilon \to 0} \frac{1}{\epsilon}(\mathcal{F}(\nu + \epsilon \xi) - \mathcal{F}(\nu))$ is the **first variation** of $\mathcal{F}$

Entropic Mirror Descent (MD)

Using the first order conditions of (1) we obtain the dual iteration

$$\nabla\phi(\mu_{n+1}) - \nabla\phi(\mu_n) = -\gamma_{n+1}\nabla\mathcal{F}(\mu_n).$$

In the case $B_\phi(\nu|\mu) = \mathrm{KL}(\nu|\mu)$ we have the following multiplicative update named **entropic mirror descent**:

$$\mu_{n+1} \propto \mu_n e^{-\gamma_{n+1}\nabla\mathcal{F}(\mu_n)}.$$

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If $\mathcal{F}(\mu) = \mathrm{KL}(\mu|\pi)$, $\nabla\mathcal{F}(\mu) = \log(\frac{\mu}{\pi})$ and we obtain entropic mirror descent on the KL:

$$\mu_{n+1} \propto \mu_n^{(1-\gamma_{n+1})}\pi^{\gamma_{n+1}}.$$

Tempering/Annealing

In the Monte Carlo literature, it is common to consider the following **tempering (or annealing)** sequence

$$\mu_{n+1} \propto \mu_0^{1-\lambda_{n+1}} \pi^{\lambda_{n+1}},$$

where $0 = \lambda_0 < \lambda_1 < \cdots < \lambda_T = 1$.

- Parallel Tempering (Geyer, 1991)
- Annealed Importance Sampling (Neal, 2001)
- Sequential Monte Carlo samplers (Del Moral et al., 2006)
- Termodynamic Integration (Gelman and Meng, 1998)

Connection between Tempering and MD

MD

$$\mu_{n+1} \propto \mu_n^{(1-\gamma_{n+1})} \pi^{\gamma_{n+1}}$$

Tempering

$$\mu_{n+1} \propto \mu_0^{1-\lambda_{n+1}} \pi^{\lambda_{n+1}}$$

are equivalent if

$$\lambda_n = 1 - \prod_{k=1}^{n} (1 - \gamma_k)$$

and can both be written in exponential family form

$$\mu_{n+1}(x) \equiv \mu_{\lambda_{n+1}}(x) \propto \mu_0 \exp\{\lambda_{n+1} s(x)\}$$

where $s(x) := \log \pi(x)/\mu_0(x)$.

Convergence Rates

The connection between MD and tempering allows us to obtain explicit rates of convergence for the tempering iterates:

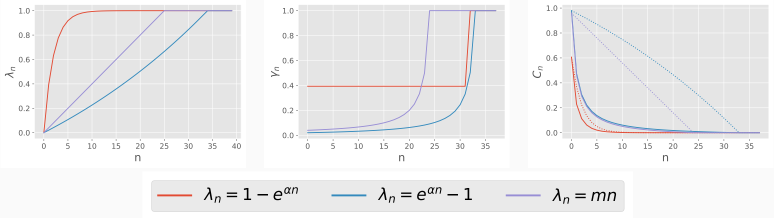
$$\mathrm{KL}(\mu_n|\pi) \leq (\gamma_1)^{-1} \prod_{k=1}^{n}(1-\gamma_k)\,\mathrm{KL}(\pi|\mu_0) = (\lambda_1)^{-1}(1-\lambda_n)\,\mathrm{KL}(\pi|\mu_0)$$

Adaptive choice of tempering

$$\int \mu_\lambda f(\mu_{\lambda'}/\mu_\lambda) = \frac{f''(1)\mathrm{I}(\lambda)}{2} \times (\lambda' - \lambda)^2 + \mathcal{O}\left((\lambda' - \lambda)^3\right),$$

where $\mathrm{I}(\lambda) = \mathrm{Var}_{\mu_\lambda}[s(X)]$ is the Fisher information. The above suggests the following recipe to choose successive λ_n values:

$$\lambda_n - \lambda_{n-1} = c\mathrm{I}(\lambda_{n-1})^{-1/2} \tag{2}$$



Algorithms

$$\mu_{n+1} \propto q_n \exp(-\gamma_n g_n)$$

where g_n is an approximation of the gradient of the KL objective $\log(\mu_n/\pi)$; and q_n is an approximation of μ_n.

We focus on algorithms which use:

- importance weights corresponding to $\exp(-\gamma_n g_n)$
- mixtures corresponding to q_n

Particle Mirror Descent (PMD)

In PMD (Dai et al., 2016), the mirror descent iterate at time n is approximated by a kernel density estimator $q_n^{\mathrm{PMD}}(x) := \sum_{i=1}^{N} V_n^i K_{h_n}(x - X_n^i)$

- $\{X_n^i, V_n^i\}_{i=1}^N$ weighted particle set with

$$V_n(x) = \left(\frac{\pi(x)}{q_{n-1}^{\mathrm{PMD}}(x)} \right)^{\gamma_n}.$$

- K_{h_n} a smoothing kernel with bandwidth h_n
- at each iteration a new N-particle set is resampled from q_n^{PMD}

Safe and Regularized Adaptive Importance Sampling (SRAIS)

In SRAIS (Korba and Portier, 2022), the mirror descent iterate at time n is approximated by a kernel density estimator $q_n^{\mathrm{SRAIS}}(x) = \sum_{i=1}^n U_i K_{h_i}(x - X_i)$

- $\{X_n^i, U_n^i\}_{i=1}^N$ weighted particle set with

$$U_n(x) = \left(\frac{\pi(x)}{q_{n-1}^{\mathrm{SRAIS}}(x)} \right)^{\gamma_n} .$$

- K_{h_i} a smoothing kernel with bandwidth h_i
- at each iteration a new particle is added sampling from q_n^{SRAIS}

Sequential Monte Carlo (SMC) samplers

In SMC (Del Moral et al., 2006), the mirror descent iterate at time n is approximated by $q_n^{\mathrm{SMC}}(x) = \sum_{i=1}^N W_n^i \delta_{X_n^i}(x)$

- $\{X_n^i, W_n^i\}_{i=1}^N$ weighted particle set with

$$W_n(x) = \left(\frac{\pi(x)}{\mu_0(x)}\right)^{\lambda_n - \lambda_{n-1}} = \left(\frac{\pi(x)}{\mu_{n-1}(x)}\right)^{\gamma_n}.$$

- at each iteration a new N-particle set is resampled using W_n^i and a μ_n-invariant Markov kernel

Which algorithm is better?

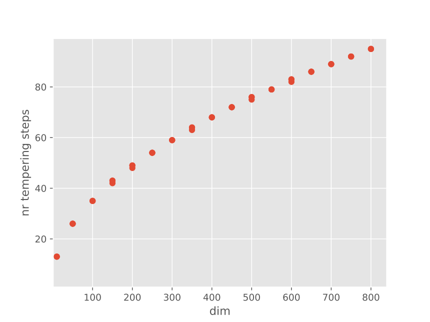
- **computational cost:** SMC is cheaper than PMD (no weight approximation)
- **approximation error:** SMC targets π exactly, PMD and SRAIS target a smoothed version of π
- PMD allows for minibatching while simple SMC does not (but a different version does)
- the convergence properties of SMC are very well studied

Adaptive strategies

The SMC literature offers an easy way to tune the stepsize/tempering sequence adaptively: aim for iterates which keep constant

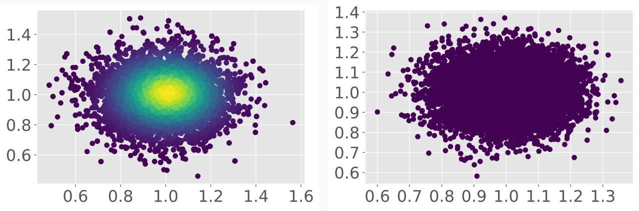
$$\mathrm{ESS}_n(\lambda) := 1/\sum_{i=1}^{N}(W_n^i)^2.$$

1. easy and inexpensive to approximate with particle cloud
2. can be linked to χ^2 divergence
3. guarantees $T = \mathcal{O}(\sqrt{d})$



Example

Approximations of $\pi = \mathcal{N}(1_d, 0.1^2 Id)$ from $\mu_0 = \mathcal{N}(0_d, Id)$.



Left: Adaptive SMC, Right: Fixed γ SMC.

Conclusions

- the connection between mirror descent (MD) and tempering justifies tempering from an optimisation point of view and provides the MD literature with a new class of algorithms (which is very well-studied!)
- opens the door to extensions of tempering through the use of other divergences
- clarifies when and in which case each algorithm should be used

Conclusions

- the connection between mirror descent (MD) and tempering justifies tempering from an optimisation point of view and provides the MD literature with a new class of algorithms (which is very well-studied!)
- opens the door to extensions of tempering through the use of other divergences
- clarifies when and in which case each algorithm should be used

Thank you!

References

Pierre-Cyril Aubin-Frankowski, Anna Korba, and Flavien Léger. Mirror descent with relative smoothness in measure spaces, with application to Sinkhorn and EM. *Advances in Neural Information Processing Systems*, 35:17263–17275, 2022.

David M Blei, Alp Kucukelbir, and Jon D McAuliffe. Variational inference: A review for statisticians. *Journal of the American Statistical Association*, 112(518):859–877, 2017.

Bo Dai, Niao He, Hanjun Dai, and Le Song. Provable Bayesian inference via particle mirror descent. In *Artificial Intelligence and Statistics*, pages 985–994. PMLR, 2016.

Pierre Del Moral, Arnaud Doucet, and Ajay Jasra. Sequential Monte Carlo samplers. *Journal of the Royal Statistical Society Series B: Statistical Methodology*, 68(3):411–436, 2006.

Carles Domingo-Enrich and Aram-Alexandre Pooladian. An Explicit Expansion of the Kullback-Leibler Divergence along its Fisher-Rao Gradient Flow. *arXiv preprint arXiv:2302.12229*, 2023.

Andrew Gelman and Xiao-Li Meng. Simulating normalizing constants: From importance sampling to bridge sampling to path sampling. *Statistical Science*, pages 163–185, 1998.

Charles J Geyer. Markov chain Monte Carlo maximum likelihood. In E. M. Keramides, editor, *Computing Science and Statistics: Proceedings of the 23rd Symposium on the Interface*, pages 156–163, 1991.

Richard Jordan, David Kinderlehrer, and Felix Otto. The variational formulation of the Fokker–Planck equation. *SIAM Journal on Mathematical Analysis*, 29(1):1–17, 1998.

Anna Korba and François Portier. Adaptive importance sampling meets mirror descent: a bias-variance tradeoff. In *International Conference on Artificial Intelligence and Statistics*, pages 11503–11527. PMLR, 2022.

Qiang Liu. Stein variational gradient descent as gradient flow. In I. Guyon, U. Von Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 30. Curran Associates, Inc., 2017. URL `https://proceedings.neurips.cc/paper_files/paper/2017/file/17ed8abedc255908be746d245e50263a-Paper.pdf`.

Radford M Neal. Annealed importance sampling. *Statistics and Computing*, 11:125–139, 2001.