# Gibbs flow transport for Bayesian inference

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# Problem specification

- **Target** distribution on $\mathbb{R}^d$

$$\pi(dx) = \frac{\gamma(x)\,dx}{Z}$$

where $\gamma : \mathbb{R}^d \to \mathbb{R}_+$ can be evaluated pointwise and

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- **Problem 1**: Obtain consistent estimator of $\pi(\varphi) := \int_{\mathbb{R}^d} \varphi(x)\,\pi(dx)$

- **Problem 2**: Obtain unbiased and consistent estimator of $Z$

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- MCMC can fail in practice, for e.g. when $\pi$ is highly multi-modal

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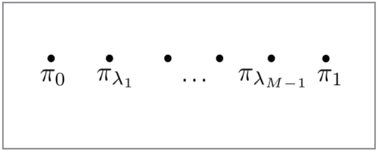

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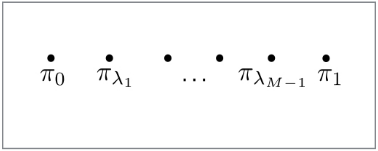


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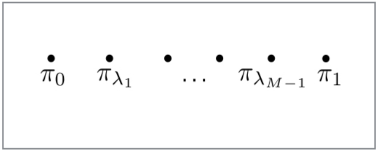


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  - **Annealed importance sampling** constructs $w : (\mathbb{R}^d)^{M+1} \to \mathbb{R}_+$ so that

$$\pi(\varphi) = \frac{\mathbb{E}\left[\varphi(X_M)w(X_{0:M})\right]}{\mathbb{E}\left[w(X_{0:M})\right]}, \quad Z = \mathbb{E}\left[w(X_{0:M})\right]$$

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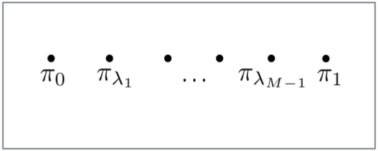


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  - AIS (Neal, 2001) and SMC samplers (Del Moral et al., 2006) are considered state-of-the-art in statistics and machine learning

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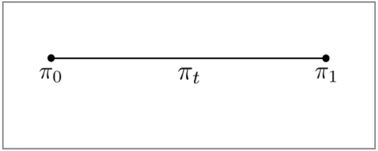

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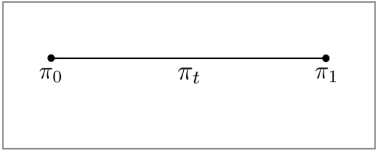

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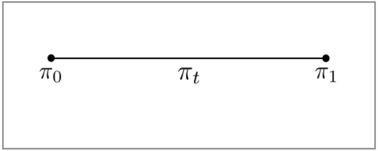


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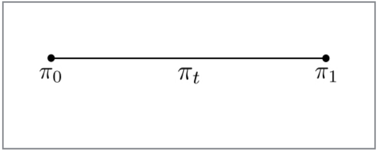


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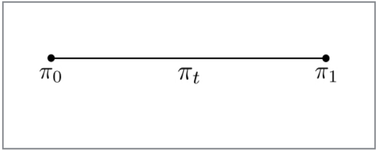


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- To what extent is this state-of-the-art in molecular dynamics?

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- Zero lag also achieved by running **deterministic dynamics**

$$dX_t = f(t, X_t)dt, \quad X_0 \sim \pi_0$$

# Time evolution of distributions

- Time evolution of $\pi_t$ is given by

$$\partial_t \pi_t(x) = \lambda'(t) \left(\log L(x) - I_t\right) \pi_t(x),$$

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- Integrating recovers **path sampling** (Gelman and Meng, 1998) or **thermodynamic integration** (Kirkwood, 1935) identity

$$\log\left(\frac{Z(1)}{Z(0)}\right) = \int_0^1 \lambda'(t) I_t \, dt.$$

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satisfying Liouville PDE

$$-\nabla \cdot (\tilde{\pi}_t f) = \partial_t \tilde{\pi}_t, \quad \tilde{\pi}_0 = \pi_0$$

# Defining the flow transport problem

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- Define **flow transport problem** as solving Liouville $(L)$ for $f$ that satisfies [A1] & [A2]

# Ill-posedness and regularization

- **Under-determined**: consider $\pi_t = \mathcal{N}((0,0), I_2)$ for $t \in [0,1]$,

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- Analytical solution available when distributions are (mixtures of) Gaussians (Reich, 2012)

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$$|\pi_t f|(t,x) = \left| \int_{-\infty}^{x} \partial_t \pi_t(u)\,du \right| \to 0 \text{ as } |x| \to \infty$$

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- **Optimality**: $f = \nabla \varphi$ holds trivially

# Flow transport problem on $\mathbb{R}$

- Re-write solution as

$$f(t,x) = \frac{\lambda'(t) I_t \left\{F_t(x) - I_t^x / I_t\right\}}{\pi_t(x)}$$

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- **Sign** is given by difference between $F_t(x)$ and $I_t^x / I_t \in [0,1]$

# Flow transport problem on $\mathbb{R}^d, d \geq 1$

- Multivariate solution for $d = 3$

$$(\pi_t f_1)(t, x_{1:3}) = -\int_{-\infty}^{x_1} \partial_t \pi_t(u_1, x_2, x_3)\, du_1 + g_1(t, x_1) \int_{-\infty}^{\infty} \partial_t \pi_t(u_1, x_2, x_3)\, du_1$$

$$(\pi_t f_2)(t, x_{1:3}) = -g_1'(t, x_1) \int_{-\infty}^{\infty} \int_{-\infty}^{x_2} \partial_t \pi_t(u_1, u_2, x_3)\, du_{1:2} + g_1'(t, x_1) g_2(t, x_2) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \partial_t \pi_t(u_1, u_2, x_3)\, du_{1:2}$$

$$(\pi_t f_3)(t, x_{1:3}) = -g_1'(t, x_1) g_2'(t, x_2) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{x_3} \partial_t \pi_t(u_1, u_2, u_3)\, du_{1:3}$$

where $g_1, g_2 \in C^2([0,1] \times \mathbb{R}, [0,1])$

# Flow transport problem on $\mathbb{R}^d, d \geq 1$

- Checking **Liouville**

$$
\begin{aligned}
\partial_{x_1}(\pi_t f_1)(t, x_{1:3}) = &- \partial_t \pi_t(x_1, x_2, x_3) \\
&+ g_1'(t, x_1) \int_{-\infty}^{\infty} \partial_t \pi_t(u_1, x_2, x_3)\, du_1 \\
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- Taking divergence gives telescopic sum

$$-\nabla \cdot (\pi_t f)(t, x_{1:3}) = -\sum_{i=1}^{3} \partial_{x_i}(\pi_t f_i)(t, x_{1:3}) = \partial_t \pi_t(x_{1:3})$$

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A1 For $f$ to be **locally Lipschitz**, assume

$$\pi_0, L \in C^1(\mathbb{R}^d, \mathbb{R}_+) \Longrightarrow f \in C^1([0,1] \times \mathbb{R}^d, \mathbb{R}^d)$$

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$$|\pi_t f|(t,x)| \to 0 \text{ as } |x| \to \infty$$

if $\{g_i\}$ are **non-decreasing** functions with **tail behaviour**

$$g_i(t, x_i) \to 0 \quad \text{as } x_i \to -\infty,$$
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- Choosing $g_i(t,x_i) = F_t(x_i)$ as **marginal CDF** of $\pi_t$ allows $f$ to decouple if distributions are independent

# Approximate Gibbs flow transport

- Solution involved integrals of **increasing dimension** as it tracks **increasing conditional** distributions

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$$-\nabla_{x_i} \cdot \left\{ \pi_t(x_i|x_{-i}) \tilde{f}_i(t,x) \right\} = \partial_t \pi_t(x_i|x_{-i}),$$

each defined on $(0,1) \times \mathbb{R}^{d_i}$

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- Otherwise, analogous to Metropolis-within-Gibbs, **split into one dimensional components** and apply above

# Error control

- Define **local error**

$$\begin{aligned}\varepsilon_t(x) &= \left|\partial_t \pi_t(x) + \nabla \cdot (\pi_t(x)\tilde{f}(t,x))\right| \\ &= \left|\partial_t \pi_t(x) - \sum_{i=1}^{p} \partial_t \pi_t(x_i|x_{-i})\pi_t(x_{-i})\right|\end{aligned}$$

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- If Gibbs flow induces $\{\tilde{\pi}_t\}_{t\in[0,1]}$ with $\tilde{\pi}_0 = \pi_0$

$$\|\tilde{\pi}_t - \pi_t\|_{L^2}^2 \leq t\int_0^t \|\varepsilon_u\|_{L^2}^2\, du \cdot \exp\left(1 + \int_0^t \|\nabla \cdot \tilde{f}\,(u,\cdot)\,\|_\infty\, du\right)$$

# Numerical integration of Gibbs flow

- Previously, we considered the **forward Euler scheme**

$$Y_m = Y_{m-1} + \Delta t\, \tilde{f}(t_{m-1}, Y_{m-1}) = \Phi_m(Y_{m-1})$$

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- In contrast, this scheme mimicking a **systematic Gibbs scan**

$$Y_m[i] = Y_{m-1}[i] + \Delta t\, \tilde{f}(t_{m-1}, Y_m[1:i-1], Y_{m-1}[i:p])$$
$$Y_m = \Phi_{m,d} \circ \cdots \circ \Phi_{m,1}(Y_{m-1})$$

is also **order one**, and costs $O(d)$

# Mixture modelling example

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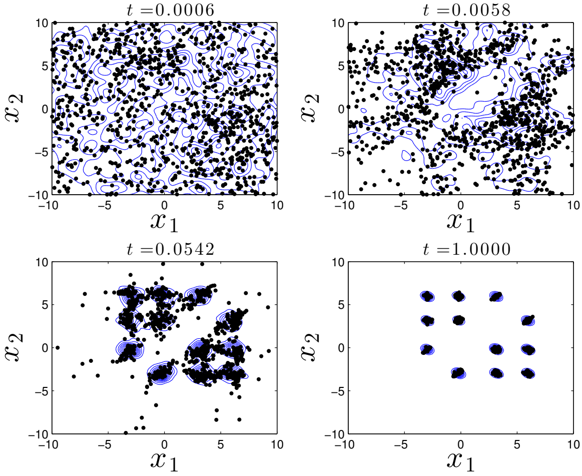
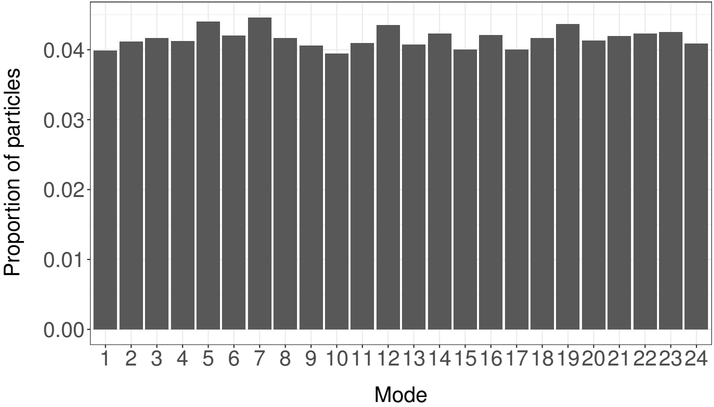
- Gibbs flow approximation



# Mixture modelling example

- Proportion of particles in each of the 24 modes



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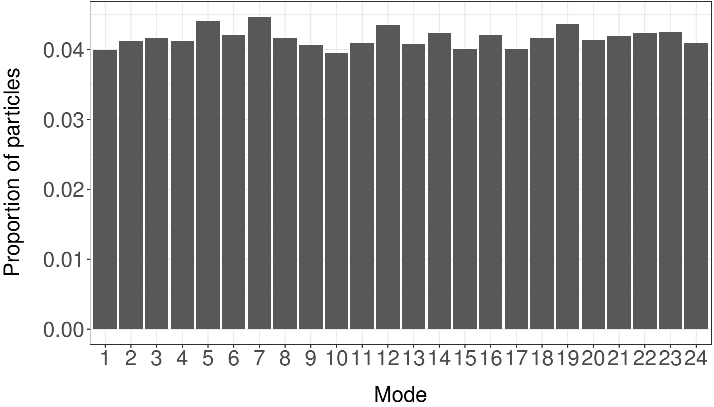
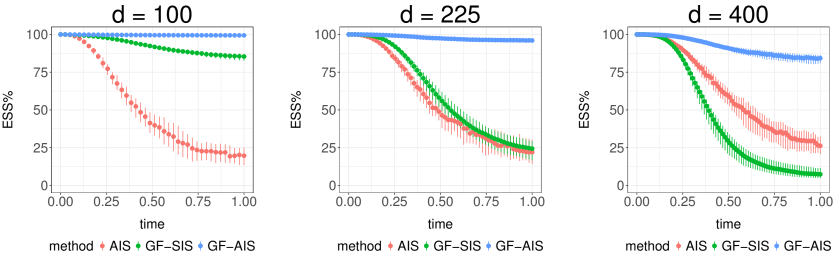



- Pearson's Chi-squared test for uniformity gives p-value of 0.85

# Cox point process model

- Effective sample size % in dimension $d$



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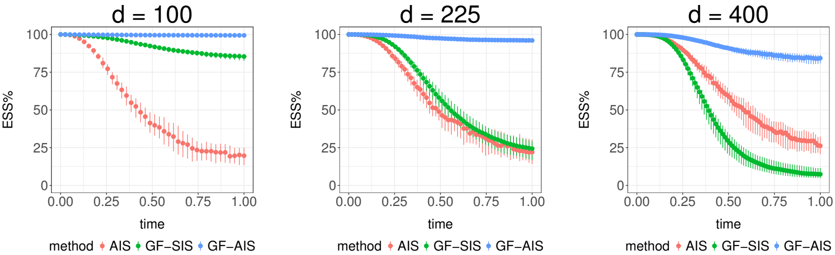

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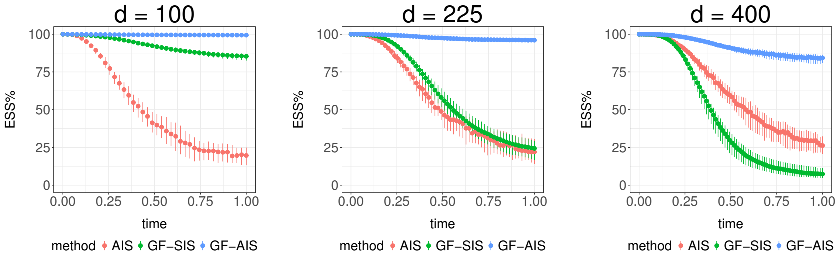

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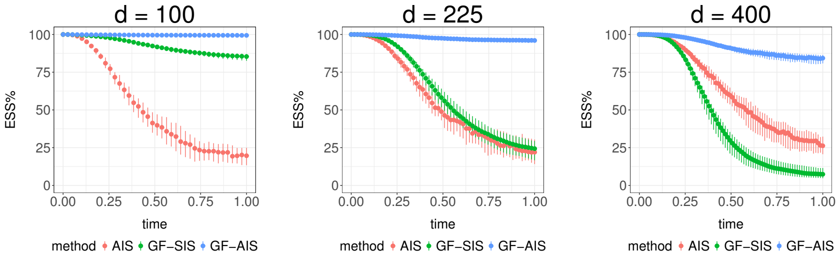

# End


- Heng, J., Doucet, A., & Pokern, Y. (2015). Gibbs Flow for Approximate Transport with Applications to Bayesian Computation. arXiv preprint arXiv:1509.08787.


- Updated article and `R` package coming soon!