# LECTURE 4

# LOCAL INFERENCE ALGORITHMS

**Saifuddin Syed**

# TARGET DISTRIBUTIONS IN PHYSICS

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  - Gaussians correspond to quadradic potentials

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$$q' = q + \Delta q, \quad \Delta q = \epsilon p$$

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  - $M$ is referred to the **mass matrix**

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- Can fix this if we track position and momentum. Let $z = (q, p) \in \mathbb{R}^{2d}$ be the phase space.

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- Can express in terms of $z(t) = (q(t), p(t))$ and hamiltonian

$$\frac{\mathrm{d}z}{\mathrm{d}t} = J\nabla_z H(z), \qquad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

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$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} H(z(t)) &= \frac{\mathrm{d}}{\mathrm{d}t} U(q(t)) + \frac{\mathrm{d}}{\mathrm{d}t} K(p(t)) \\ &= \nabla U(q(t))^\top \dot{q}(t) + \nabla K(p(t))^\top \dot{p}(t) \\ &= \nabla U(q(t))^\top \nabla K(p(t)) \quad - \nabla K(q(t))^\top \nabla U(q(t)) \\ &= 0 \end{aligned}$$

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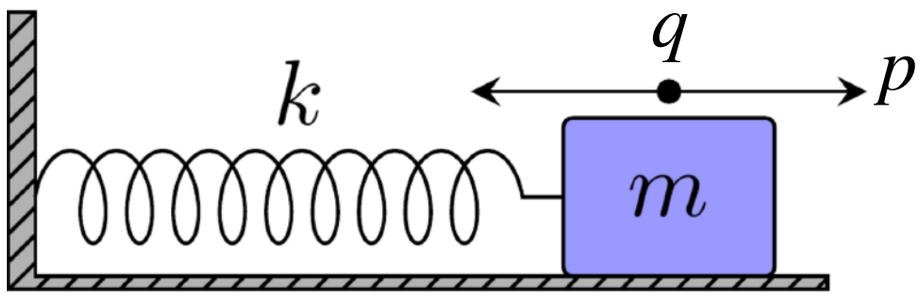
- Corresponds to the motion of mass spring system:

$$m\ddot{q}_t = -kq$$




$$\omega^2 = \frac{k}{m}$$

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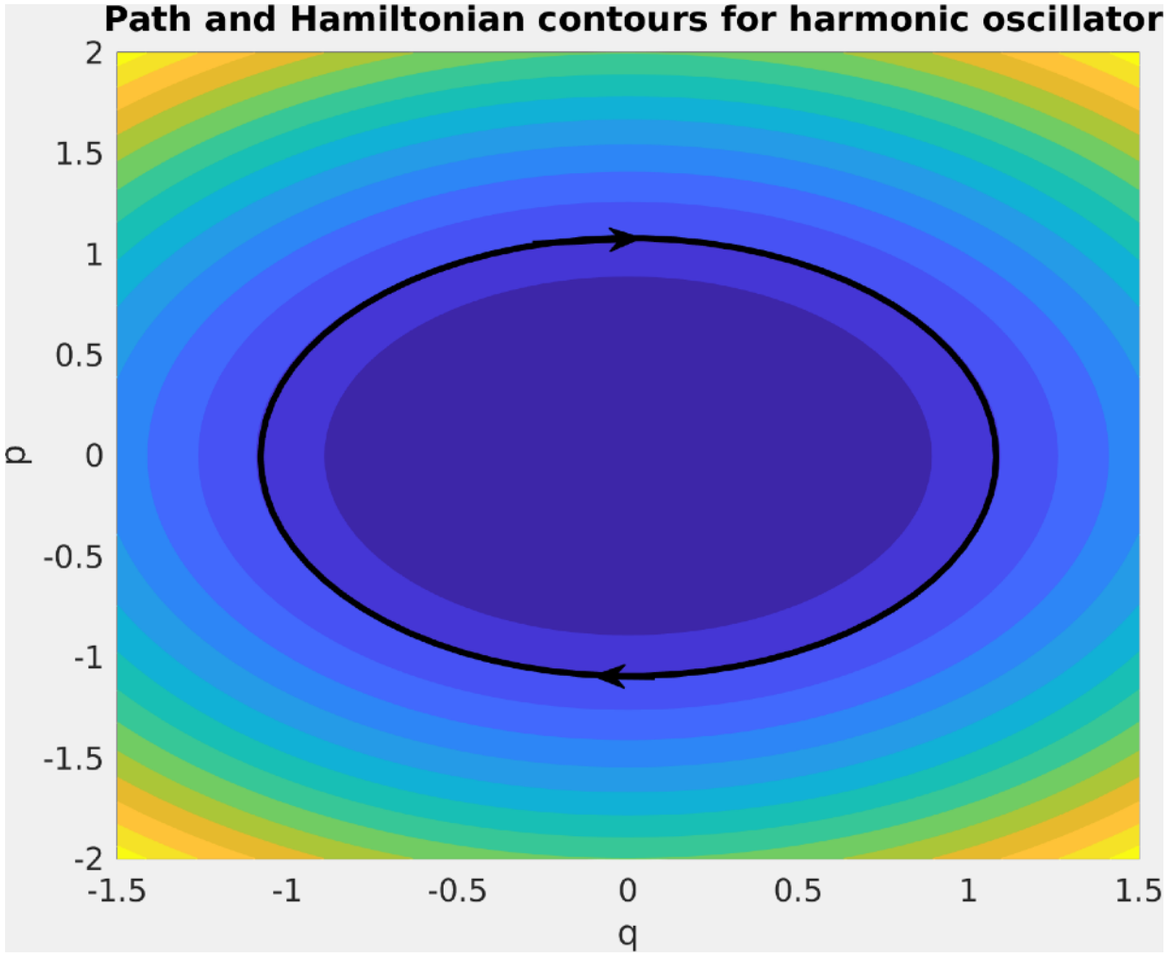
- Note that the hamiltonian is conserved:

$$H(q(t), p(t)) = \frac{1}{2}\omega^2 q(t)^2 + \frac{1}{2}p(t)^2 = \omega^2$$



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- **Proposition:** The time reversal solves Hamiltons equations and

$$z(t) = \Psi_t(z(0)), \quad \iff \quad z(0) = \Psi_t(N \circ z(t))$$

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  - Hence for all $t$ we have

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- Let $K_R(z, \mathrm{d}z')$ be the Markov kernel that resample the momentum according to the Gaussian distribution with covariance matrix $M$

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- The combination $K_R K_t$ defines an irriducible and ergodic Markov kernel!
  - Hamiltonian dynamics propogates withina level set
  - Momentum refresh propogates between level sets

# HAMILTONIAN MONTE CARLO

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- **Theorem:** Let $\pi(q) \propto \exp(-U(q))$ and Let $T \sim \nu_T$ with positive density on an interval $[0,\tau]$ for $\tau > 0$. Let $K(q, \mathrm{d}q)$ be the Markov kernel for the position variables corresponding to:

    1. Sampling a momentum $p \sim \mathcal{N}(0,I)$ and $T \sim \nu_T$
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- Then $K$ is strongly $\pi$-irreducible and $\pi$-reversible

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- **Leapfrog scheme:**

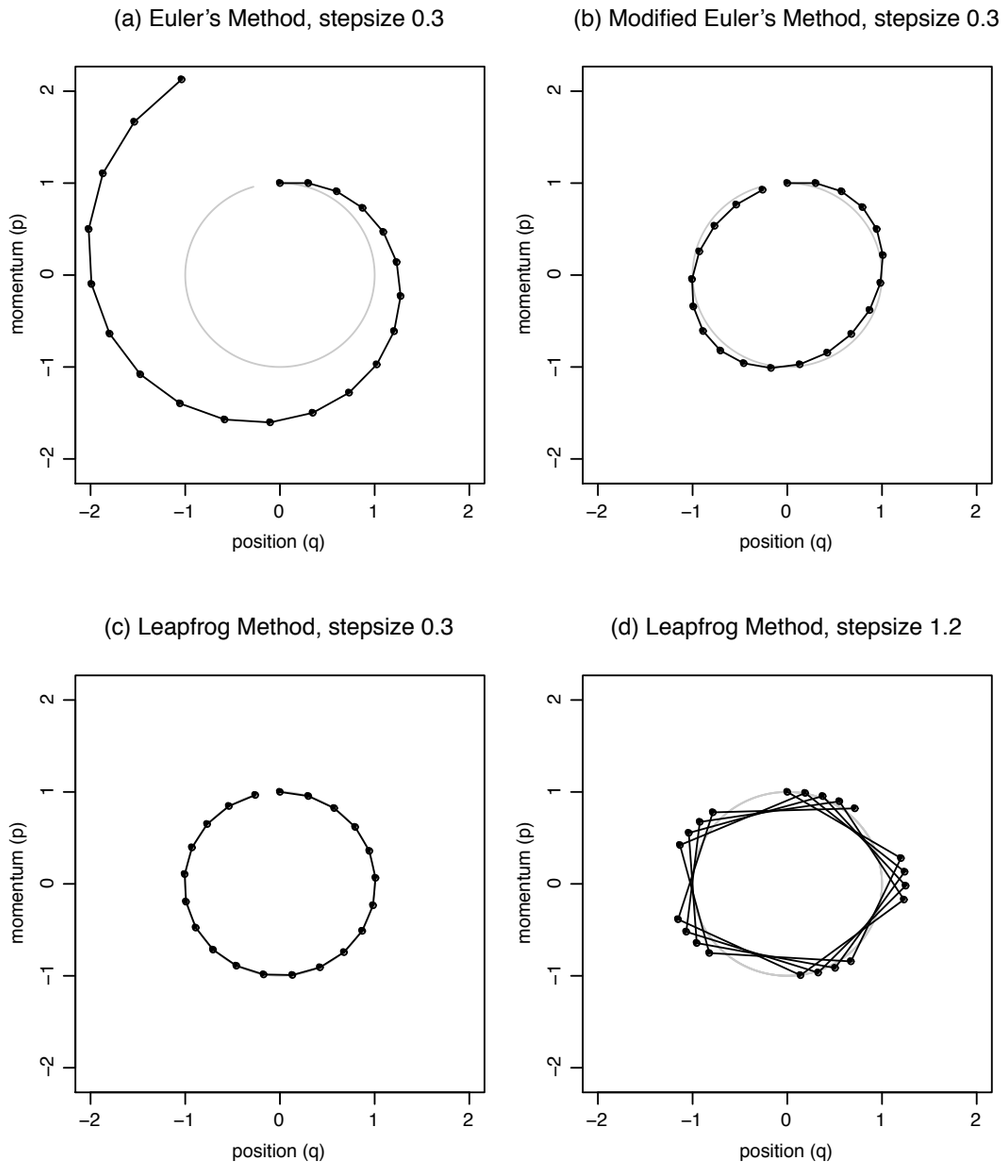
$$p(t+\epsilon/2) = p(t) - \frac{\epsilon}{2}\nabla U(q(t))$$
$$q(t+\epsilon) = q(t) + \epsilon M^{-1}p(t+\epsilon/2)$$
$$p(t+\epsilon) = p(t+\epsilon/2) - \frac{\epsilon}{2}\nabla U(q(t+\epsilon))$$

# DISCRETISATION



- Consider the simple harmonic oscillator $H(q,p) = \frac{1}{2}p^2 + \frac{1}{2}q^2$

- Approximation of Hamiltonian dynamics by 3 schemes. 20 steps in each case in black, the true trajectory in grey



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- Demo:

  https://www.saifsyed.com/sampling-demo/app.html?algorithm=HMC

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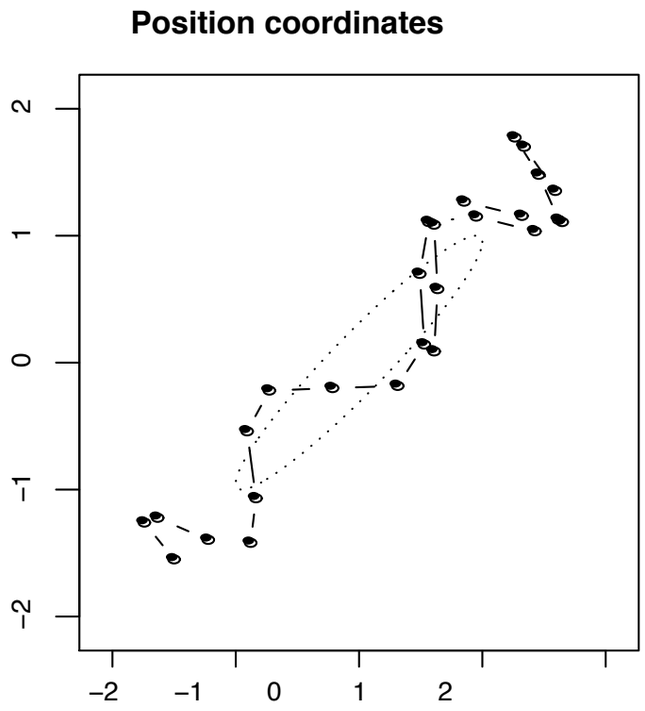
- HMC is a very good default sampler understanding the shape of a mode

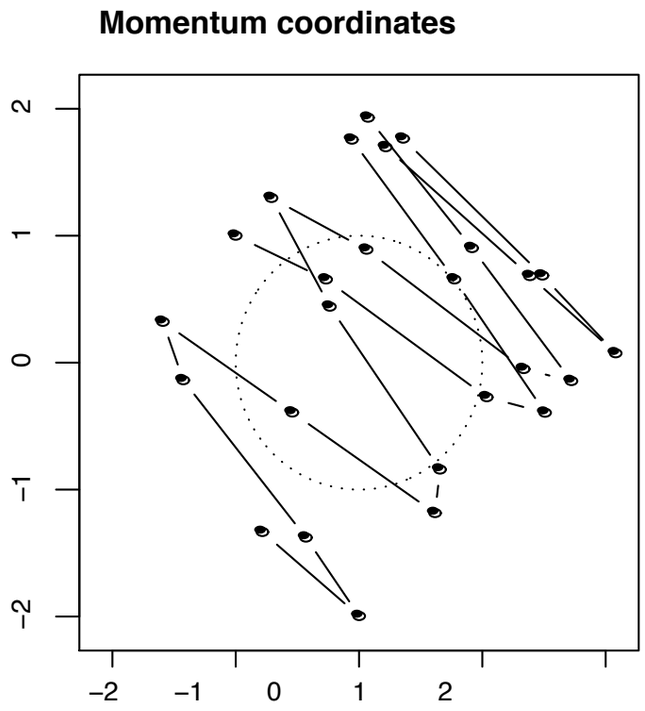
# EXAMPLE

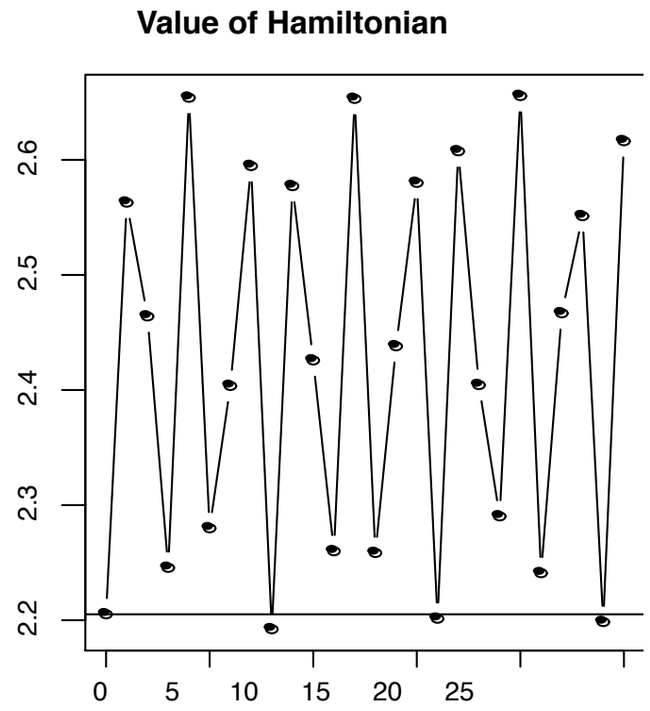


- Consider a 2D Gaussian distribution with covariance matrix $\Sigma = \begin{pmatrix} 1 & 0.98 \\ 0.98 & 1 \end{pmatrix}$

- We let $M = I$, and do $L = 25$ leapfrog steps per iteration using stepsize $\epsilon = 0.25$.



# EXAMPLE

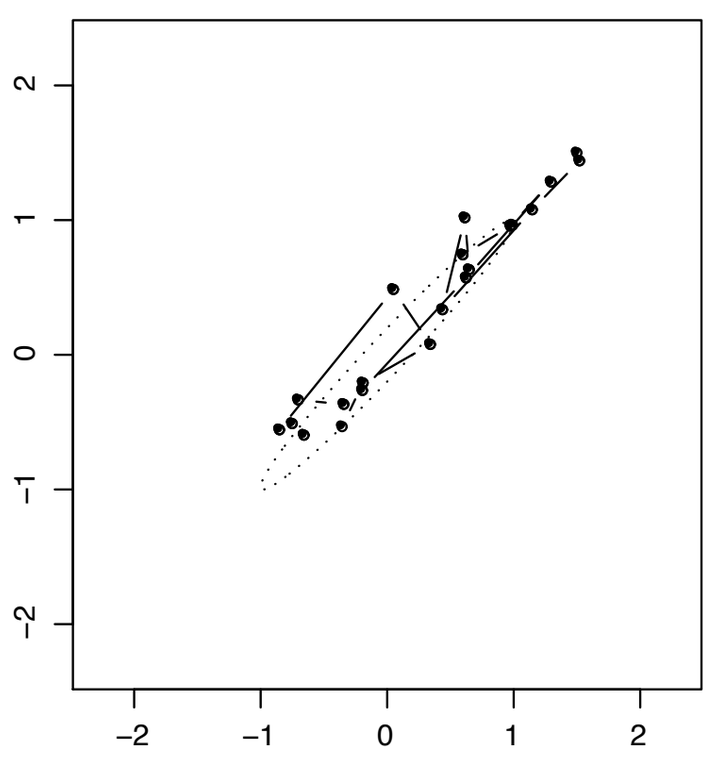


- Consider a 2D Gaussian distribution with covariance matrix $\Sigma = \begin{pmatrix} 1 & 0.98 \\ 0.98 & 1 \end{pmatrix}$

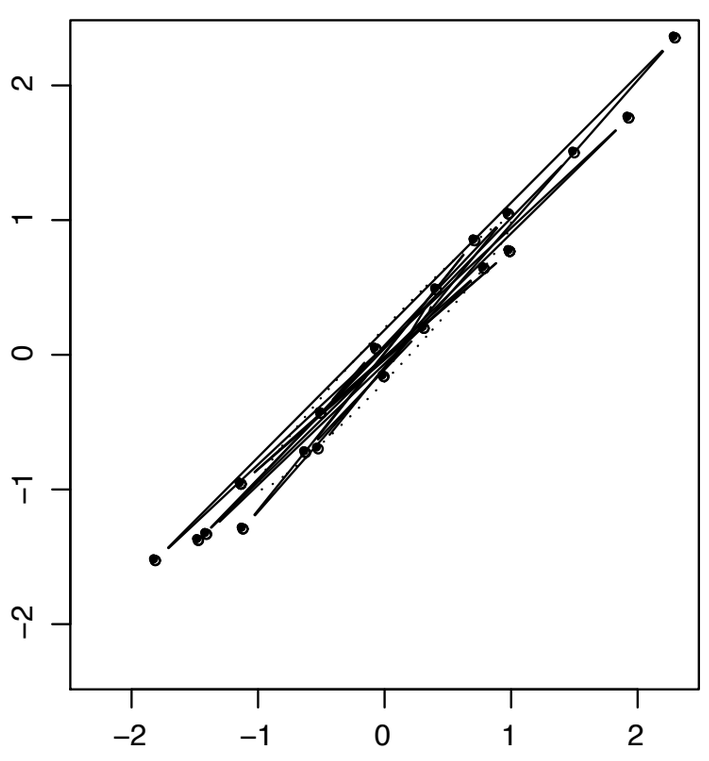
- We let $M = I$, and do $L = 25$ leapfrog steps per iteration using stepsize $\epsilon = 0.25$.

- Twenty iterations of the random walk Metropolis method (20 updates per iteration). HMC is making much larger moves and mixes faster than random walk Metropolis.

**Random–walk Metropolis**



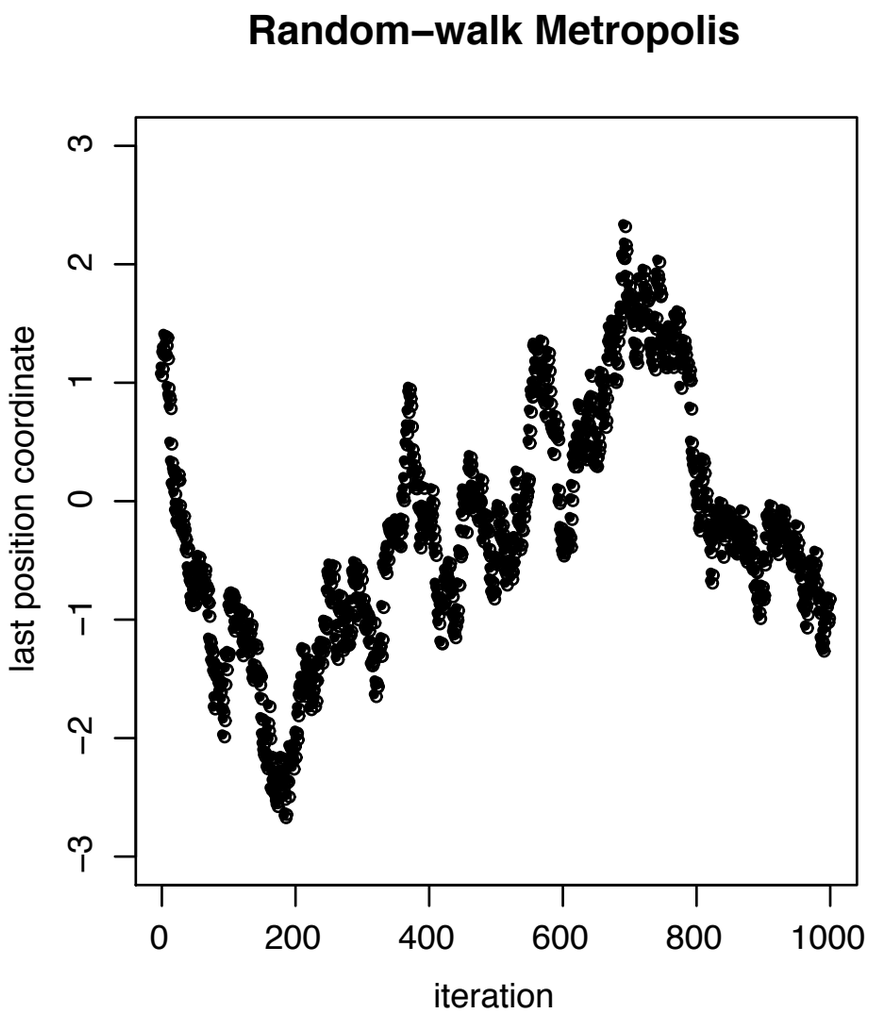

**Hamiltonian Monte Carlo**

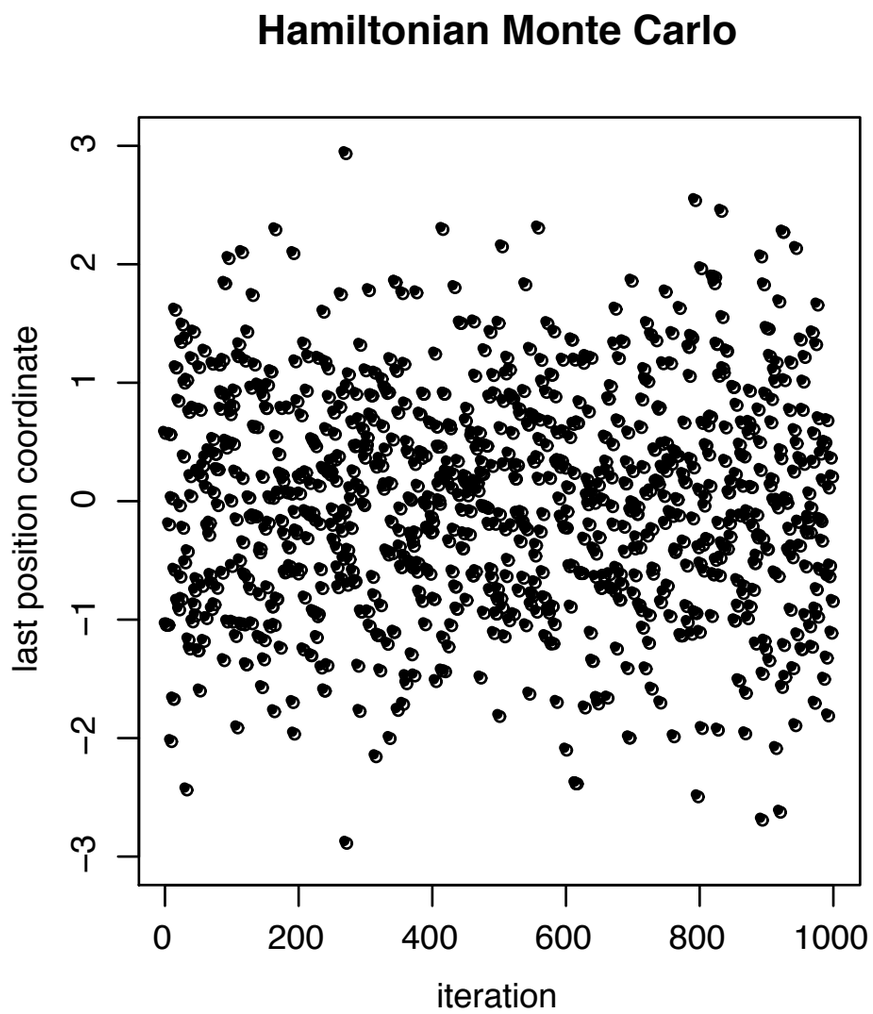


# EXAMPLE



- 100 dimensional multivariate Gaussian distribution with independent components of standard deviations $0.01,\ldots,1.00$, with $\epsilon = 0.1$ and $L = 150$ leapfrog steps. The figure shows the last component.



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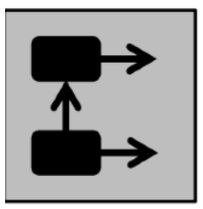
- **Example:** an ODE parameter inference problem from Leonhardt et al (2014)

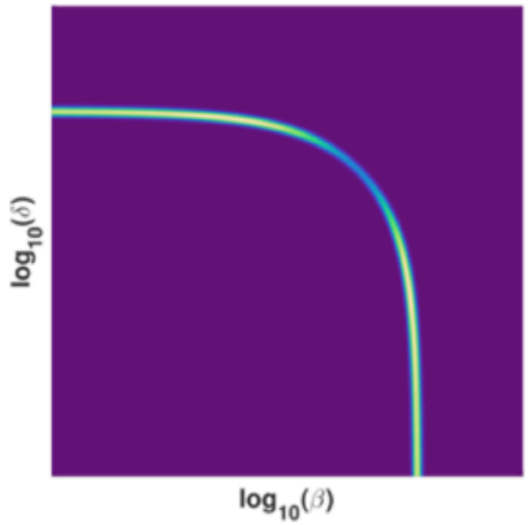


## (M1) mRNA Transfection

- Equally weighted modes; Parameters $\delta$ and $\beta$ exchangable
- Analytical solution available
- Only one of two states observable: $y_1(t) = G(t)$
- $\forall\, t < t_0 : m(t) = G(t) = 0$
- Two data sets: Experimental (a) and Artificial (b)

$$\dot{G} = k_{TL} m - \beta G, \qquad G(t_0) = 0$$

$$\dot{m} = -\delta m, \qquad m(t_0) = m_0$$



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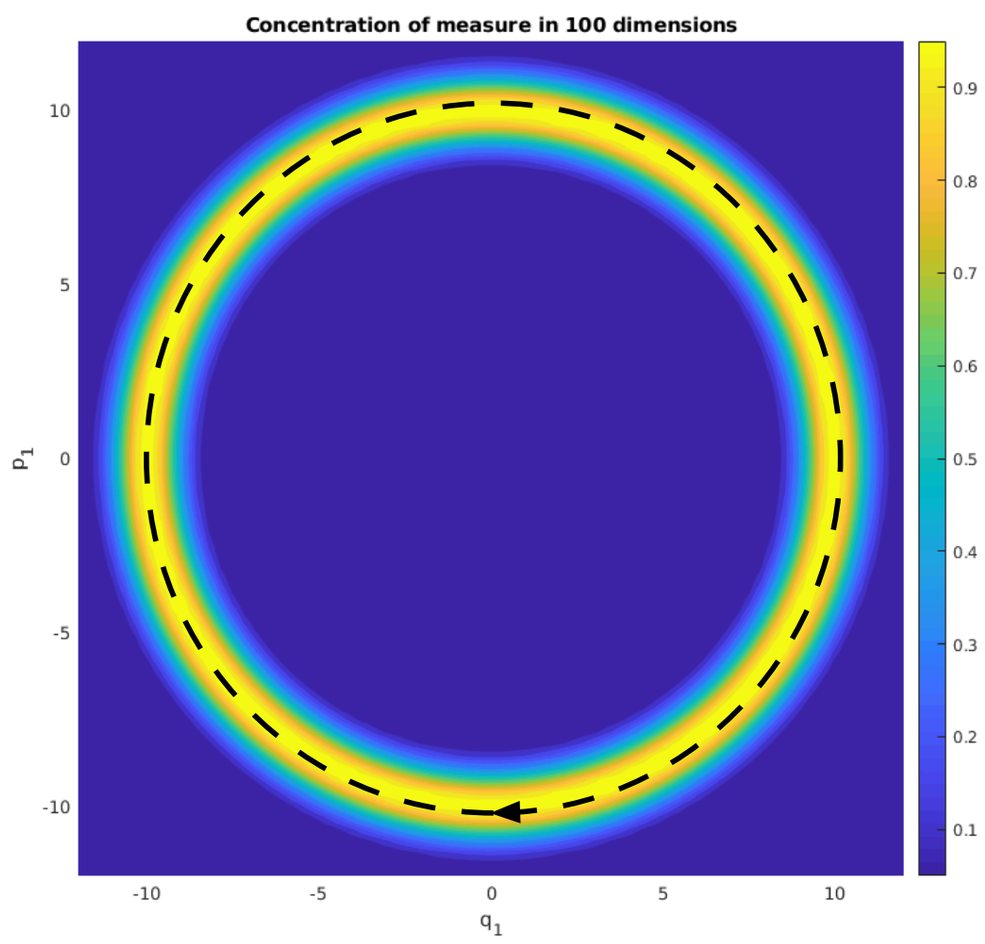

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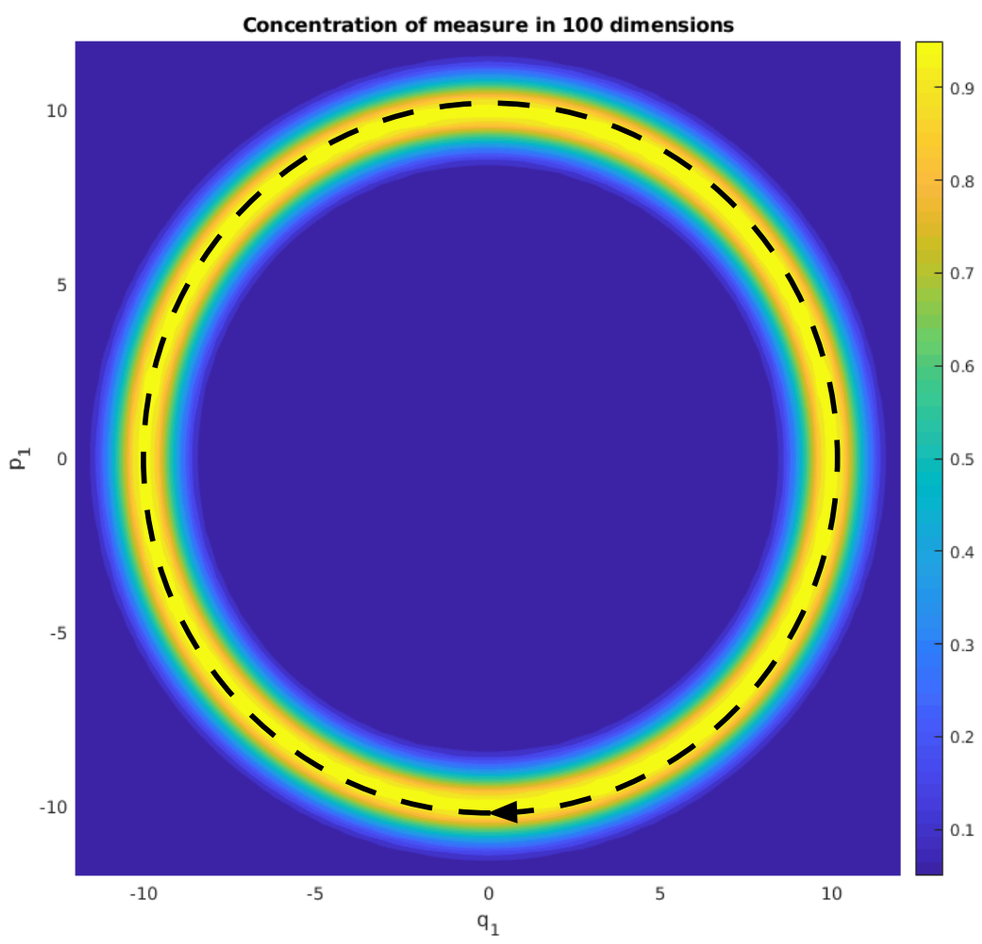

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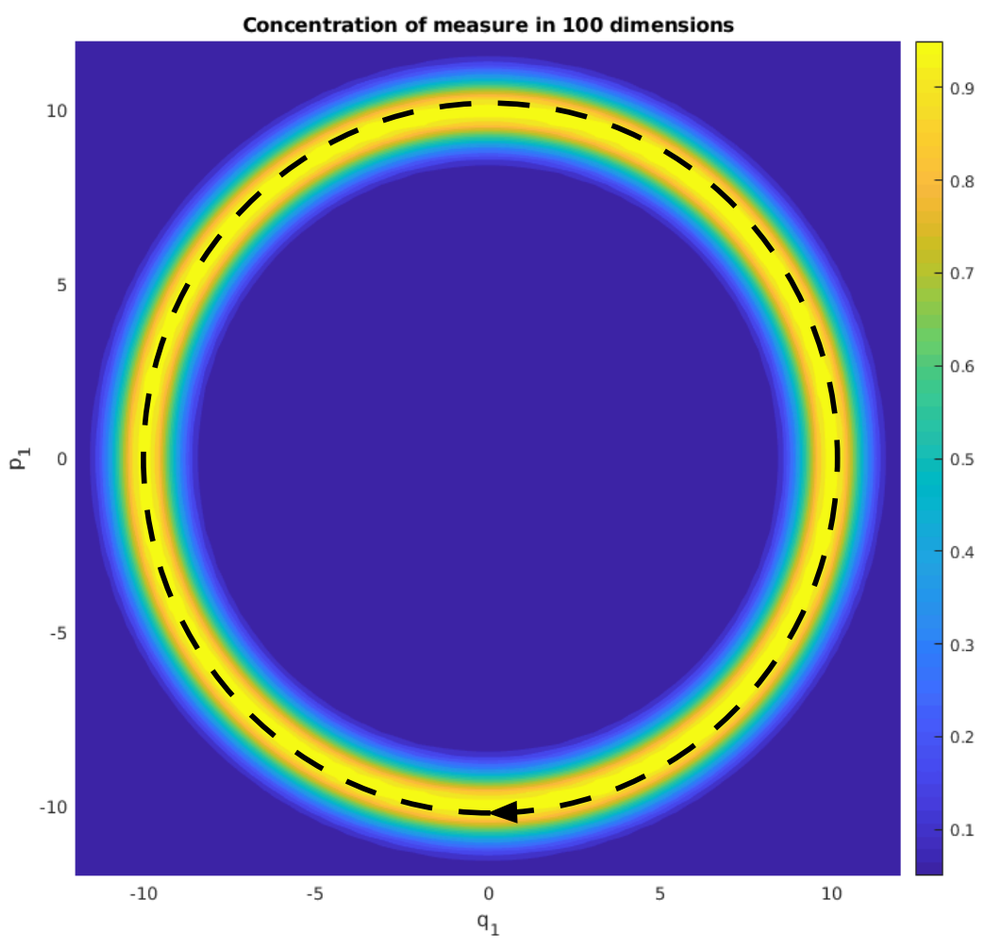

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$$q' = q_L$$

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- When $L = 1$ an HMC is equivalent to corresponds to iteration of MALA with $M = \Sigma^{-1}$

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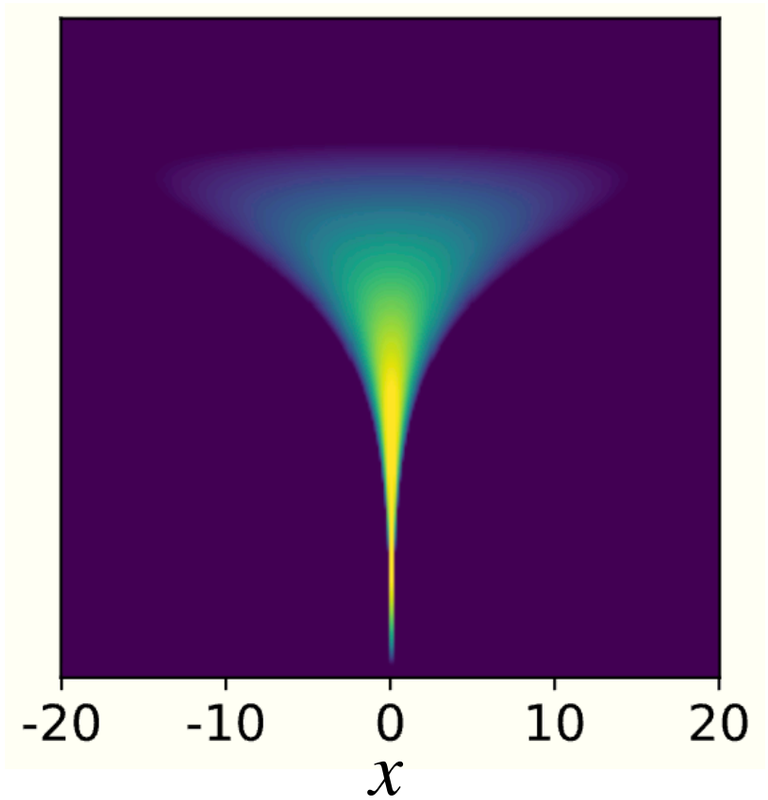

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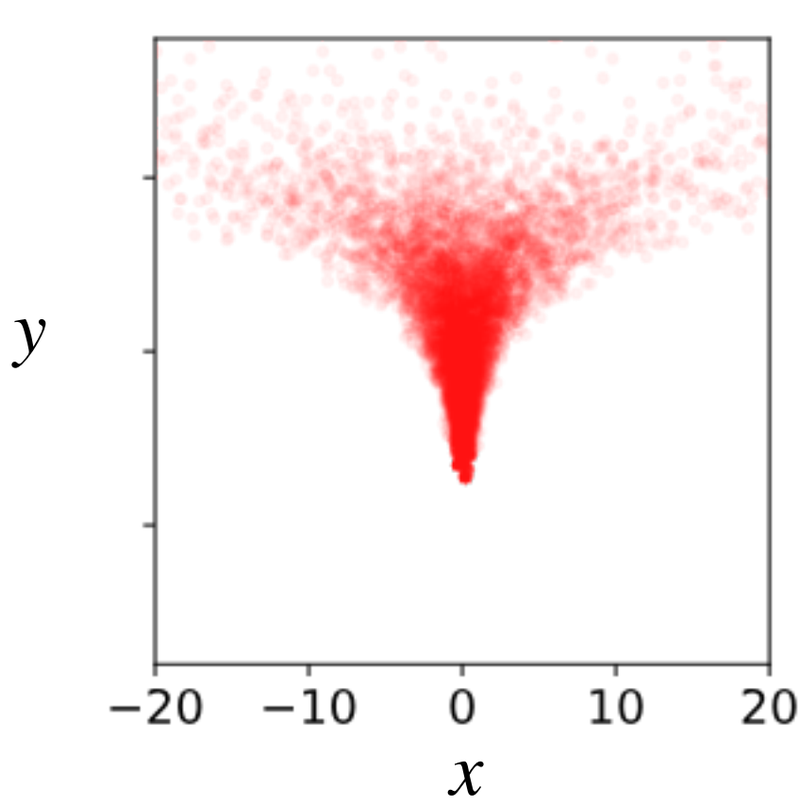


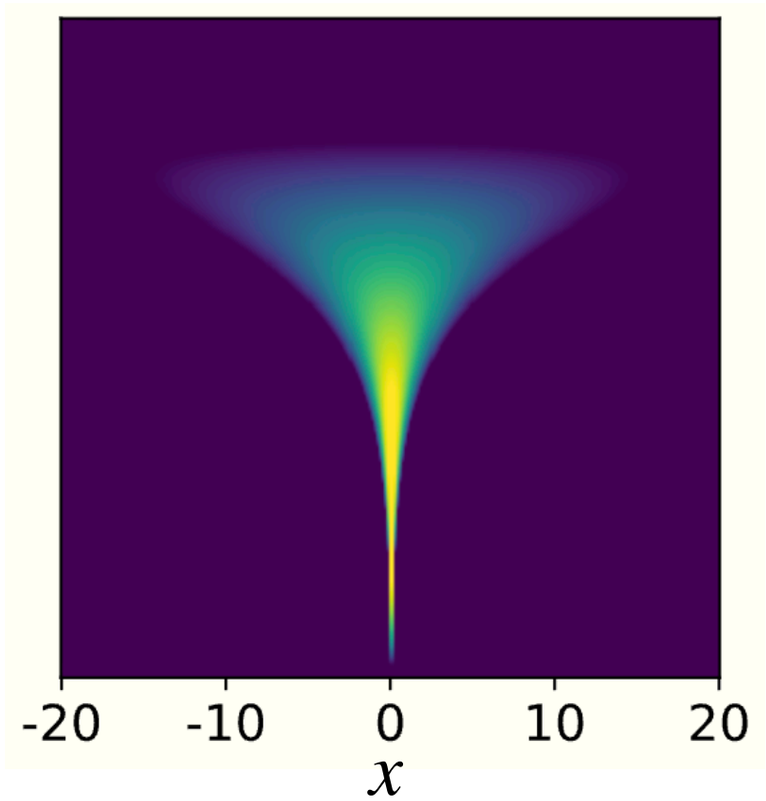

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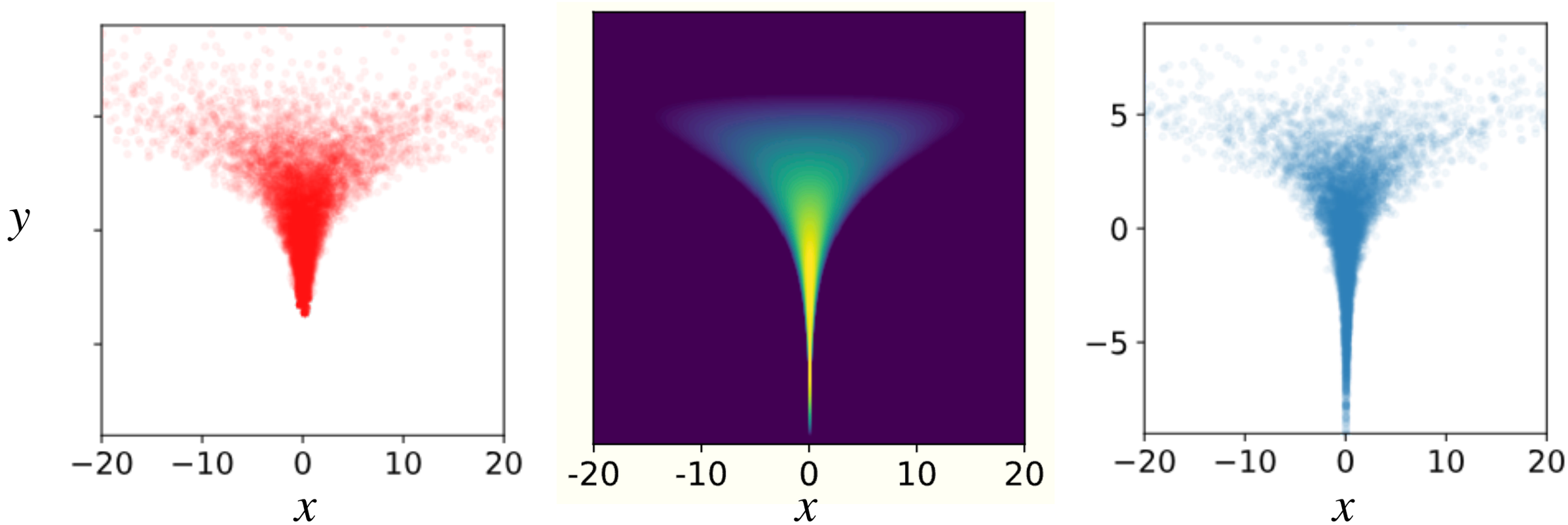

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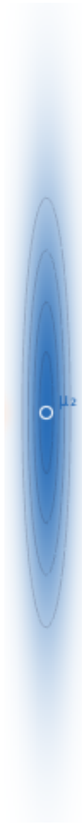

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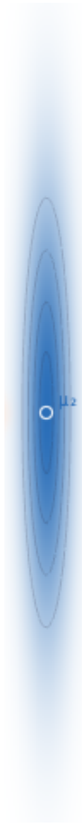

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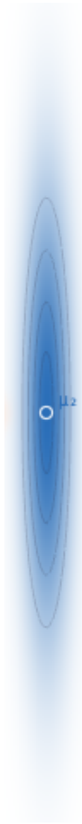

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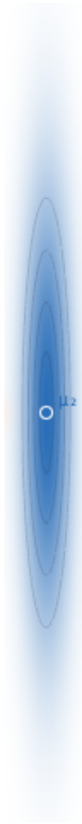

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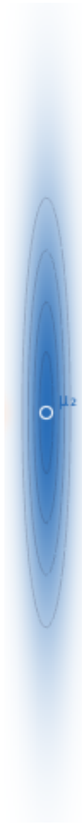

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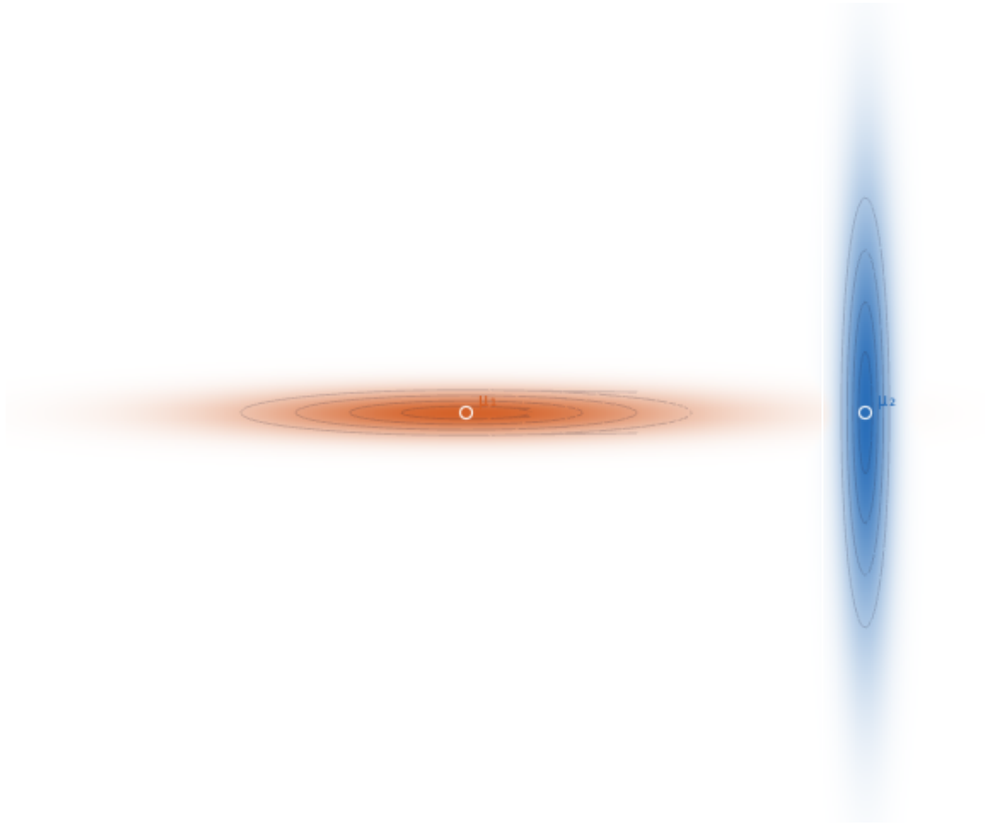

# TUNING MASS/COVARIANCE



- The mass/covariance matrix $M = \Sigma^{-1}$ is a locally should match the covariance structure of mode
  - Move faster (low mass) in directions where mode stretches
  - Move slow (high mass) in direction where mode contracts
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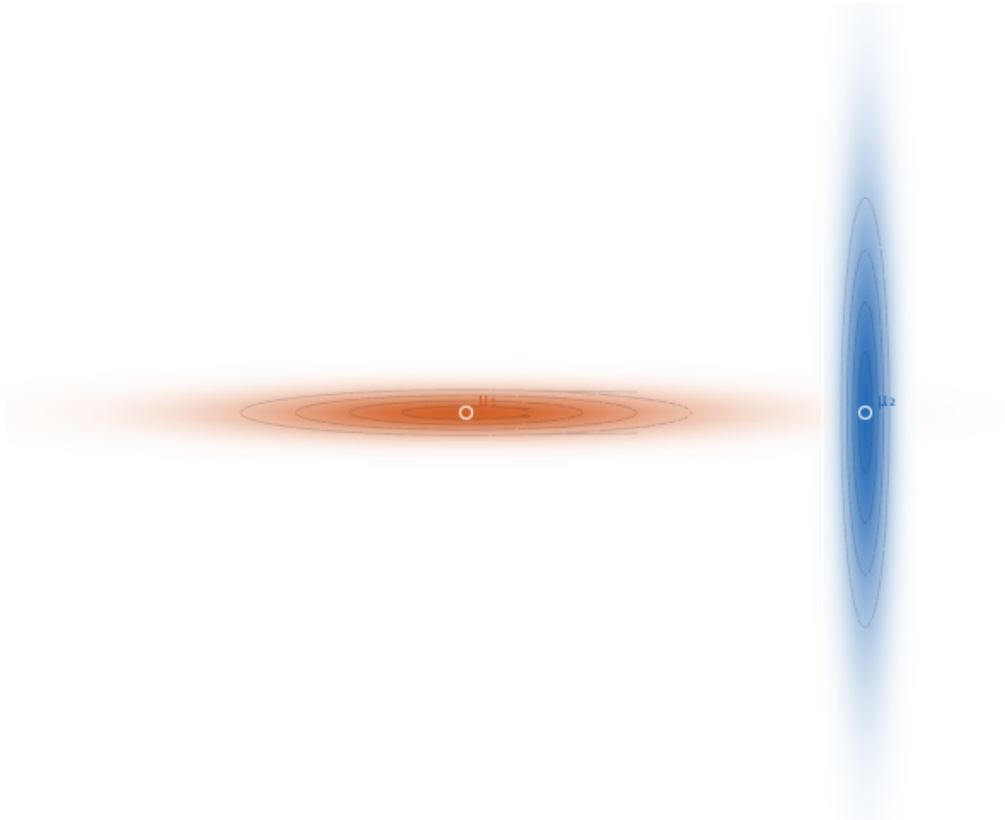
  - The best matrix in one mode can be the worst matrix in another…



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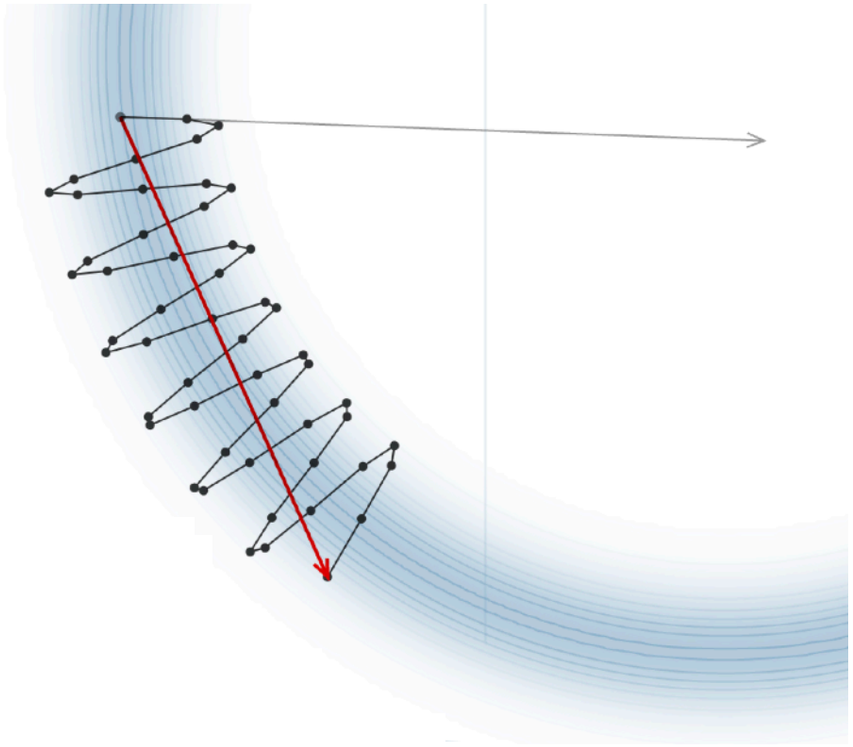

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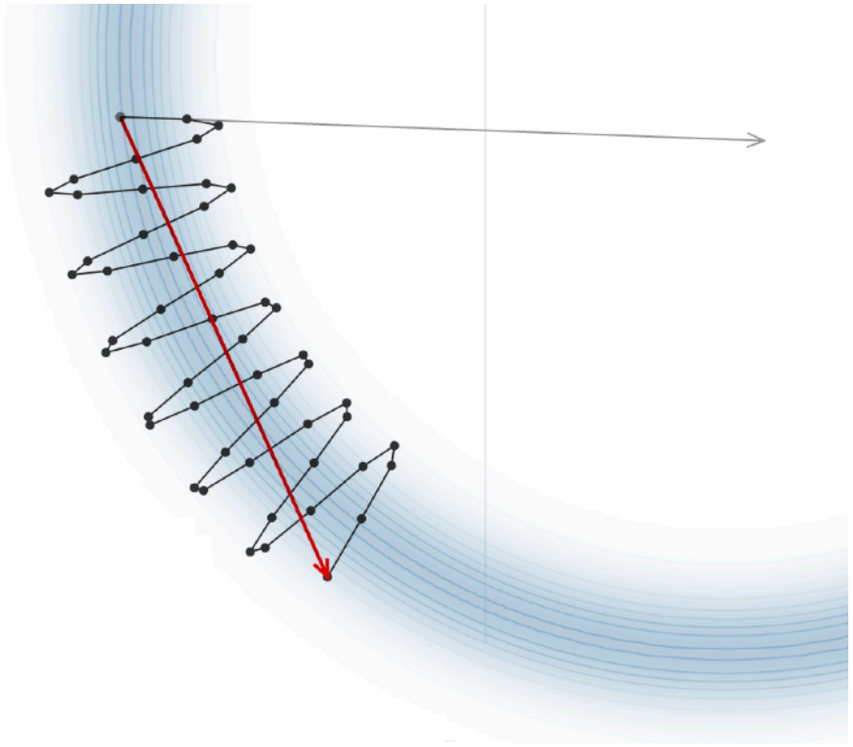
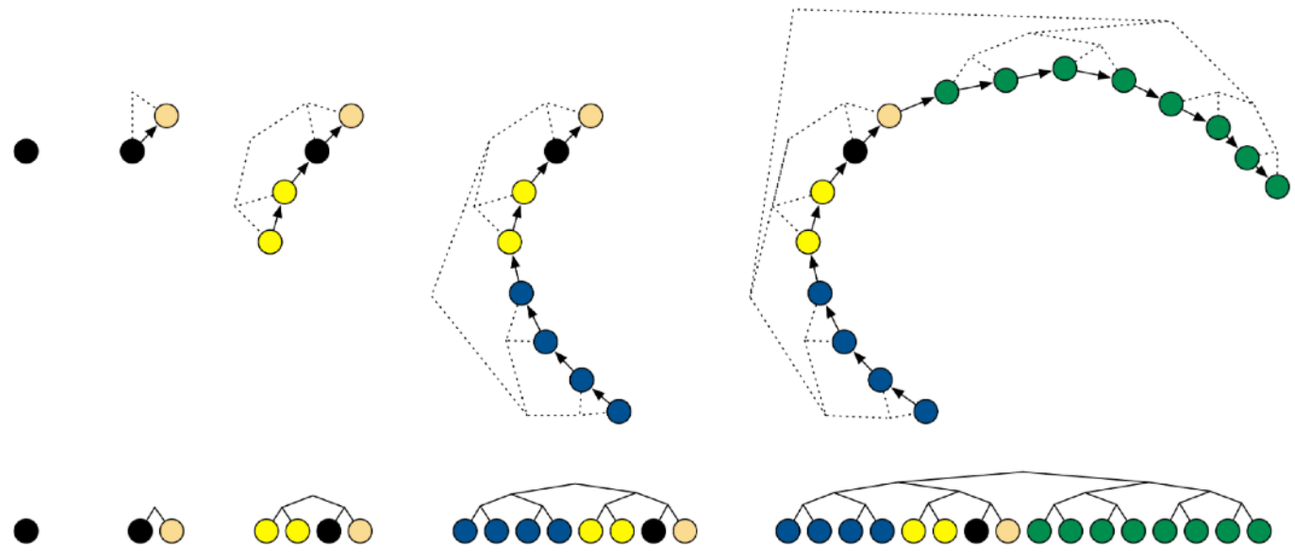
- No U-Turn Samplers (NUTS) (Hoffman et al, 2011) avoid this issue by choosing a clever proposal
  - Admits random run-time for each iteration





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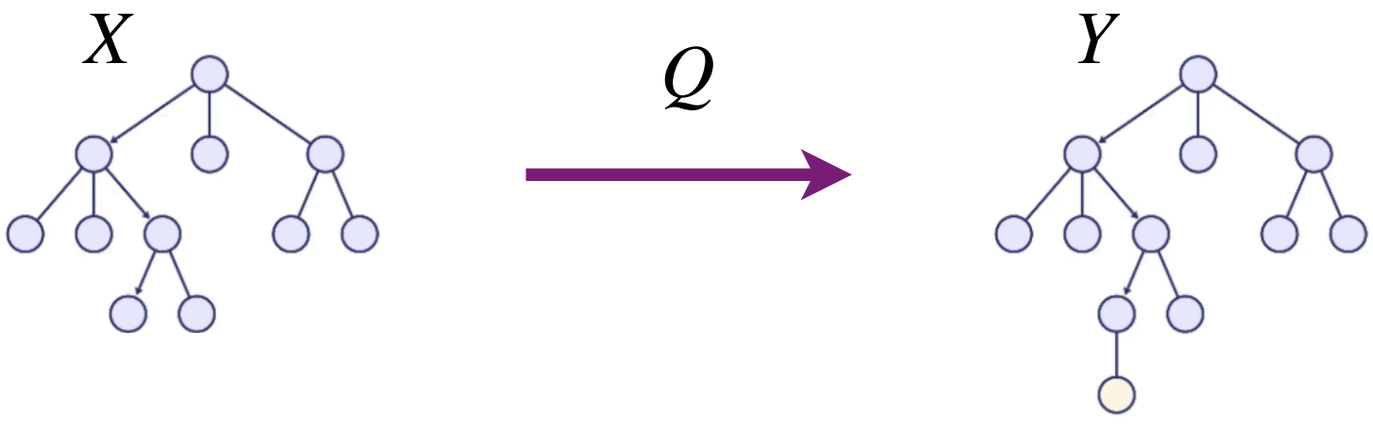

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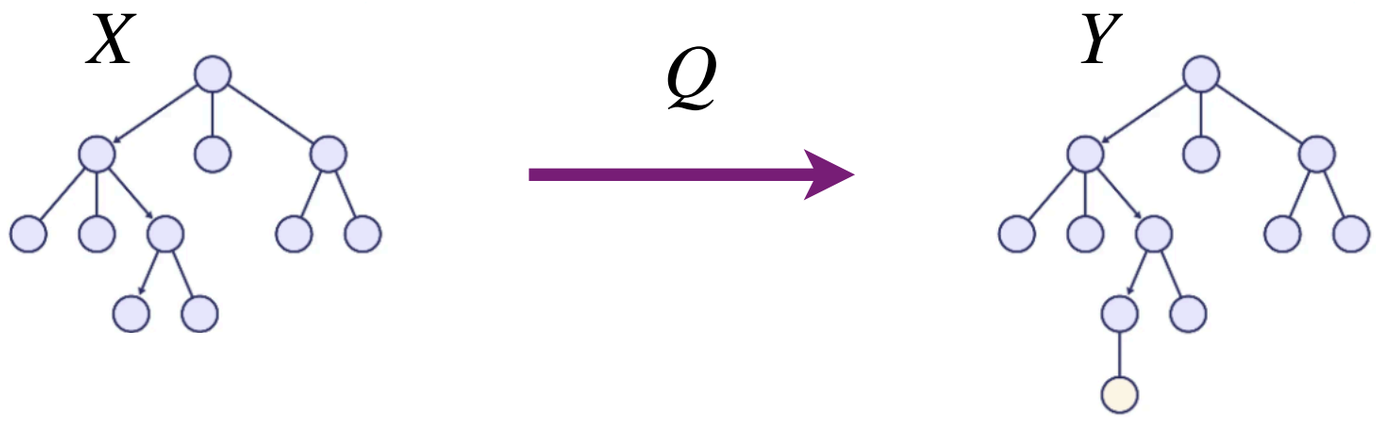


- Often appeals to the dynamics driven by a differential equation such as Langevin or Hamiltionian

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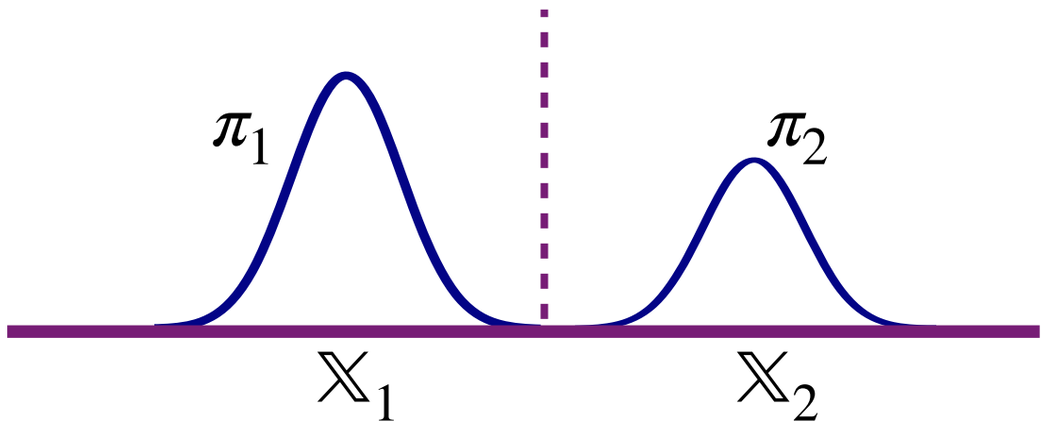

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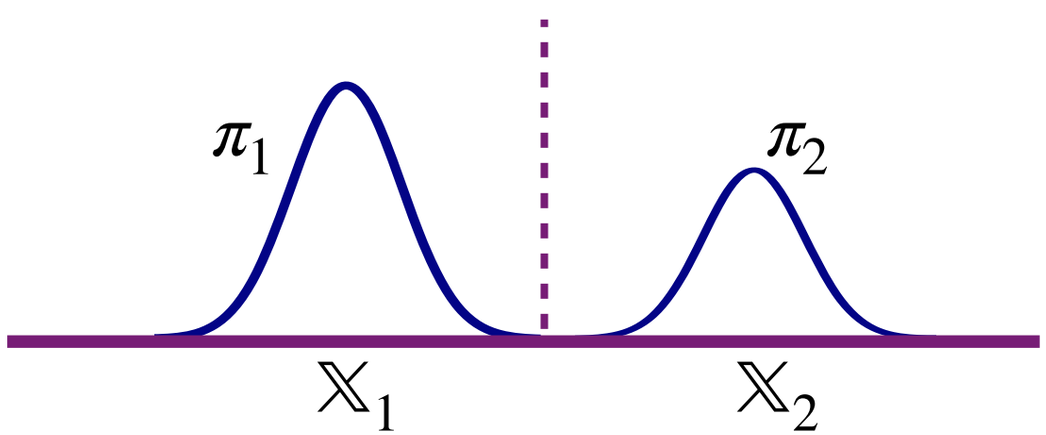

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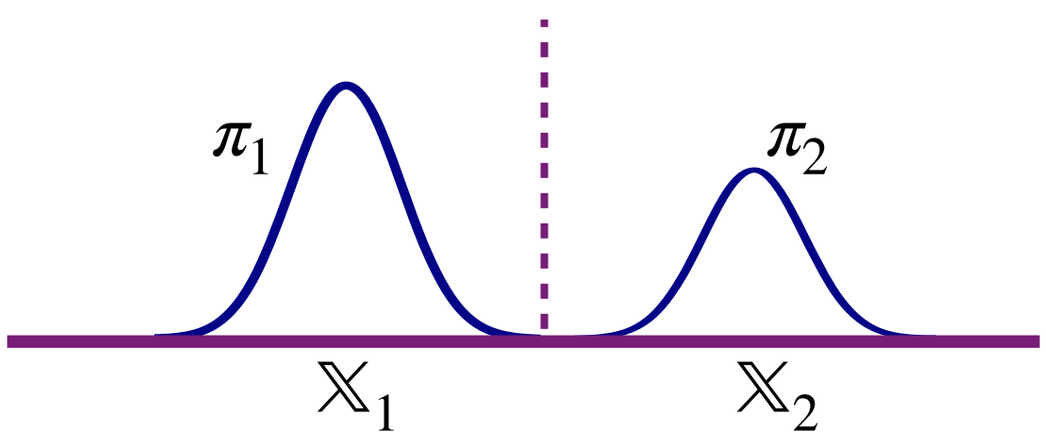

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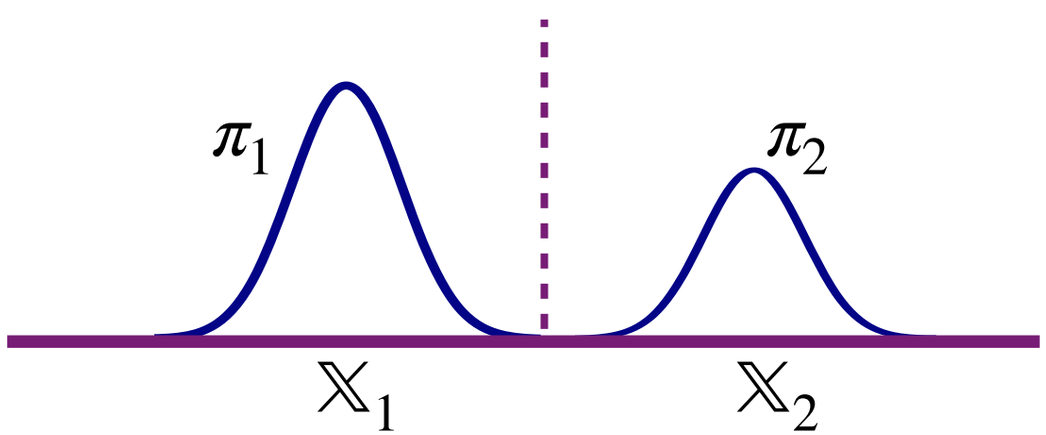
- Random initialisations don't help since attracted to the close modes not big big modes



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