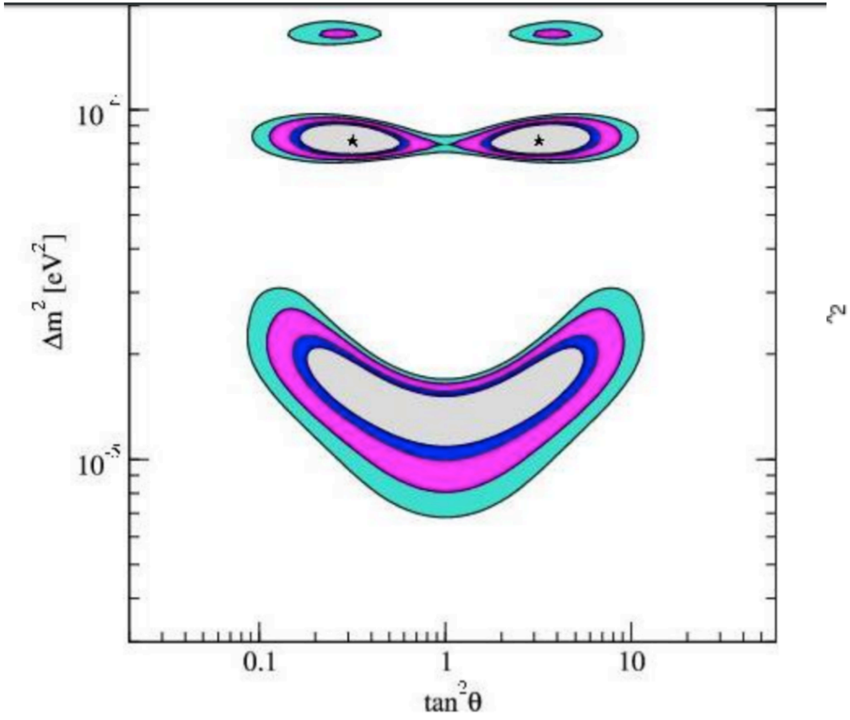
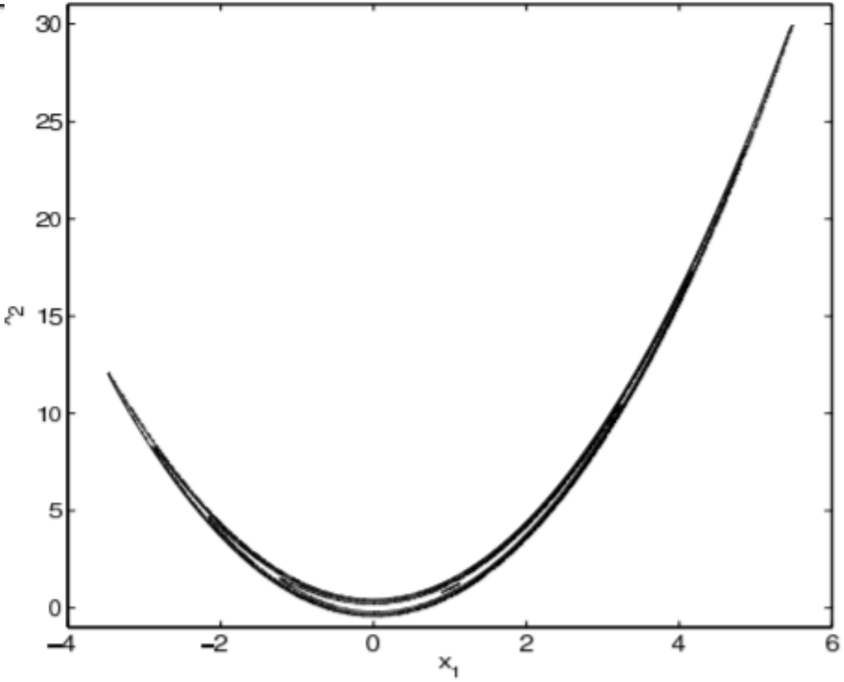
Ensemble Samplers with Affine Invariance

Jonathan Goodman & Jonathan Weare
(2010)

E. S. Martiny and A. K. Ravn
Niels Bohr Institute

The Problem





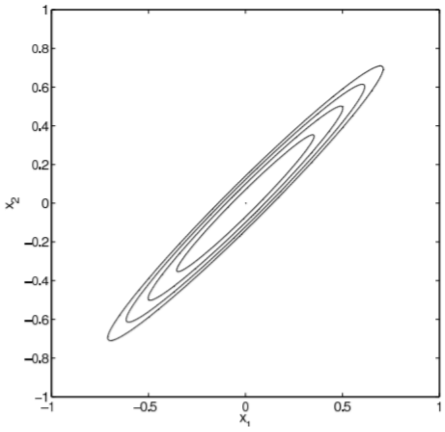
Affine invariance

- An affine transformation is a transformation on the form *Ax + b* that preserves points, parallel lines and parallel planes.
- A move is affine invariant iff the same affine transformation performed before the move algorithm or after the move algorithm produces the same result.

$$\pi(x) \propto \exp\left(\frac{-(x_1 - x_2)^2}{2\epsilon} - \frac{(x_1 + x_2)^2}{2}\right)$$

$$y_1 = \frac{x_1 - x_2}{\sqrt{\epsilon}}, \qquad y_2 = x_1 + x_2,$$

$$\pi_A(y) \propto e^{-(y_1^2 + y_2^2)/2}.$$

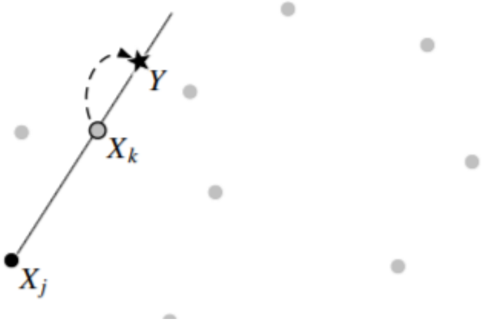


$$X(t+1) = R(X(t), \xi(t), \pi)$$

$$R(Ax + b, \xi(t), \pi_{A,b}) = AR(x(t), \xi(t), \pi) + b$$

Stretch move

- The stretch move uses another walker in the ensamble to make the proposal for the next move.
- All possible proposals lie on the line that contains both walkers positions in parameter space.

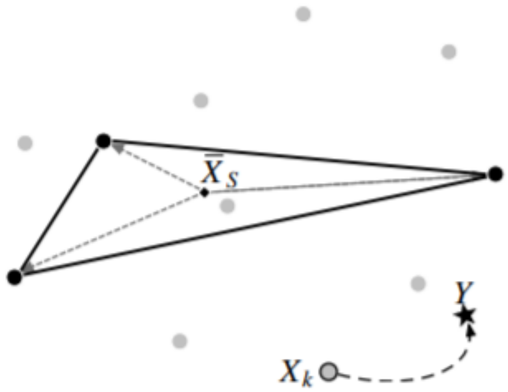


$$X_k(t) \rightarrow Y = X_j + Z(X_k(t) - X_j)$$

$$g(z) \propto \begin{cases} \frac{1}{\sqrt{z}} & \text{if } z \in \left[\frac{1}{a}, a\right], \\ 0 & \text{otherwise.} \end{cases}$$

Walk move

- The walk move uses at least two other walkers in the ensemble (sub-ensemble) to make a proposal for a new move.
- The proposal adds a stochastic variable with same covariance as the sub-ensemble to the current position of the walker.

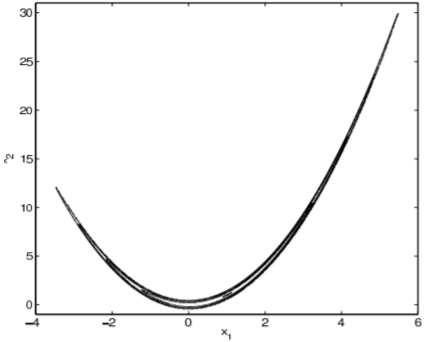


$$X_k(t) \to X_k(t) + W.$$

$$W = \sum_{X_j \in S} Z_j (X_j - \bar{X}_S)$$

Performance

Rosenbrock distribution test



method↓ ensemble size →	$f(x_1, x_2) = x_1$ 1	10	100	∞	$f(x_1, x_2) = x_2$ 1	10	100	∞
Metropolis	163	–	–	–	322	–	–	–
stretch moves	–	19.4	8.06	8.71	–	67.0	18.4	23.5
walk moves, $\|S\| = 3$	–	46.4	19.8	18.6	–	68.0	44.2	47.1

Sampling from invariant distribution of the stochastic Allen-Cahn equation.

method	time
Metropolis	80
stretch moves	5.2
walk moves, $\|S\| = 3$	1.4

Ending remarks

- These algorithms works the best when the walker ensemble is large.
- The `emcee` python package utilizes a stretch move algorithm optimized for parallelization to compute MCMCs.
- In the next big release of `emcee` (v3.0) they are going to implement the walk move along with other ensemble samplers, as well as single-particle Metropolis.