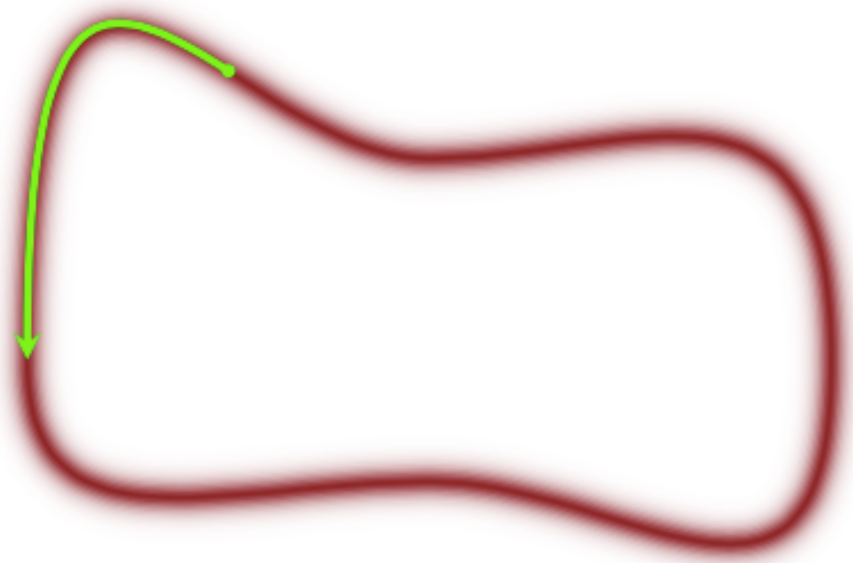
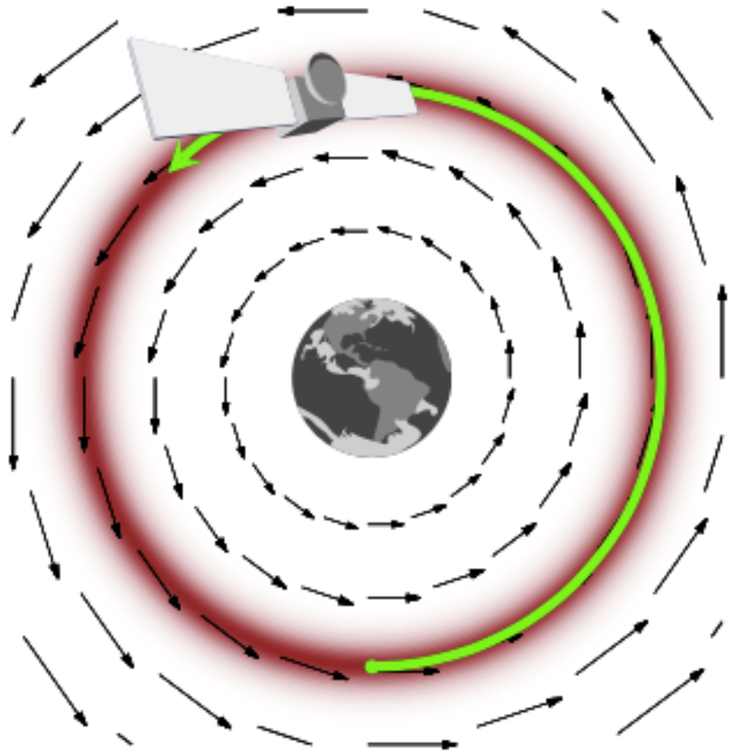
Lecture 17

HMC

The hierarchical gaussian

Recap of HMC ideas





Canonical distribution

$$p(p,q) = e^{-H(p,q)} = e^{-K(p,q)}e^{-V(q)} = p(p|q)p(q)$$

and thus: $H(p,q) = -log(p(p,q)) = -logp(p|q) - logp(q)$

$$\int dpp(p,q) = \int dpp(p|q)p(q) = p(q)\int p(p|q)dp = p(q)$$

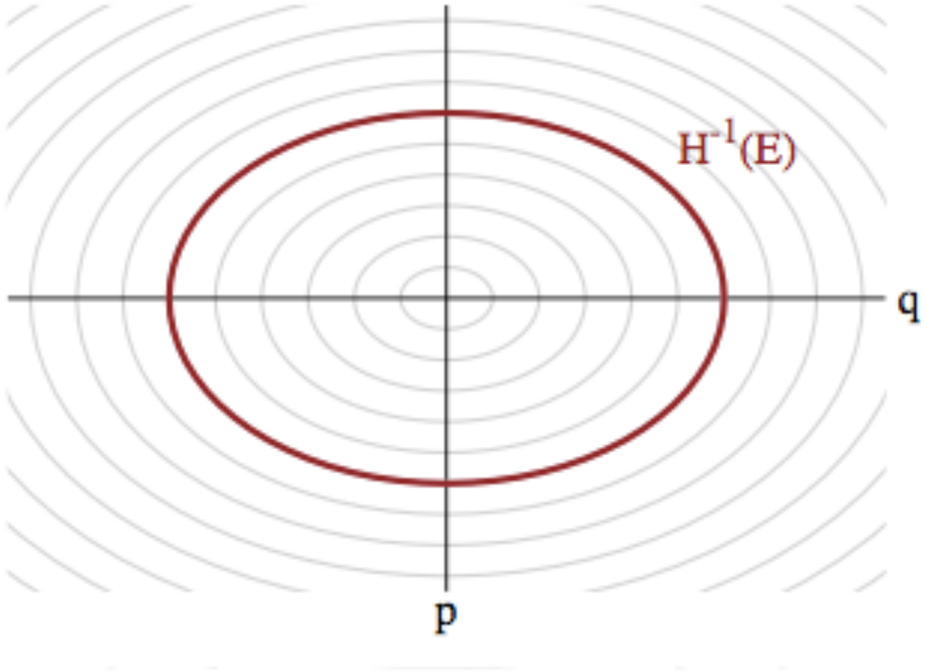
Phase Space level sets: Microcanonical Distribution

Typical Set decomposes into level sets of constant probability(energy)

The energy **Hamiltonian**

$$H(p,q) = \frac{p^2}{2m} + V(q) = E_i\,,$$

with E_i constants (constant energies) for each level-set foliate and where the **potential energy** $V(q) = -log(p(q))$ replaces the energy term we had earlier in simulated annealing.



Hamiltonian Mechanics

Physics equations of motion in the **Hamiltonian Formalism** set up the "glide" (over a level set).

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q}, \implies , \frac{dq}{dt} = \frac{\partial H}{\partial p}$$

Time independence: $\frac{\partial H}{\partial t} = 0 \implies \frac{dH}{dt} = 0$,

$H(t + \Delta t) = H(t) \, \forall t.$

Reversibility

T_s from $(q, p) \to (q', p')$ to a "later" time $t' = t + s$. Mapping is 1-1, inverse T_{-s}. This can be obtained by simply negating time:

$$\frac{dp}{d(-t)} = -\frac{\partial H}{\partial q}$$
$$\frac{dq}{d(-t)} = \frac{\partial H}{\partial p}$$

Superman transform

If we then transform $p \rightarrow -p$, we have the old equations back:

$$\frac{d(-p)}{d(-t)} = -\frac{\partial H}{\partial q}$$
$$\frac{dq}{d(-t)} = \frac{\partial H}{\partial(-p)}$$

To reverse T_s, flip the momentum, run Hamiltonian equations backwords in time until you get back to the original position and momentum in phase space at time t, then flip the momentum again so it is pointing in the right direction.

Volume in phase space is conserved

Jacobian:

$$det\left(\begin{bmatrix} 1+\delta\frac{\partial^2 H}{\partial q \partial p} & \delta\frac{\partial^2 H}{\partial p^2} \\ \delta\frac{\partial^2 H}{\partial q^2} & 1-\delta\frac{\partial^2 H}{\partial p \partial q} \end{bmatrix}\right) = 1 + O(\delta^2)$$

As a result of this, the momenta we augment our distribution with must be **dual** to our pdf's parameters, transforming in the opposite way so that phase space volumes are invariant.

Microcanonical distribution: states for given energy.

Time implicit H: flows constant energy, vol preserving, reversible.

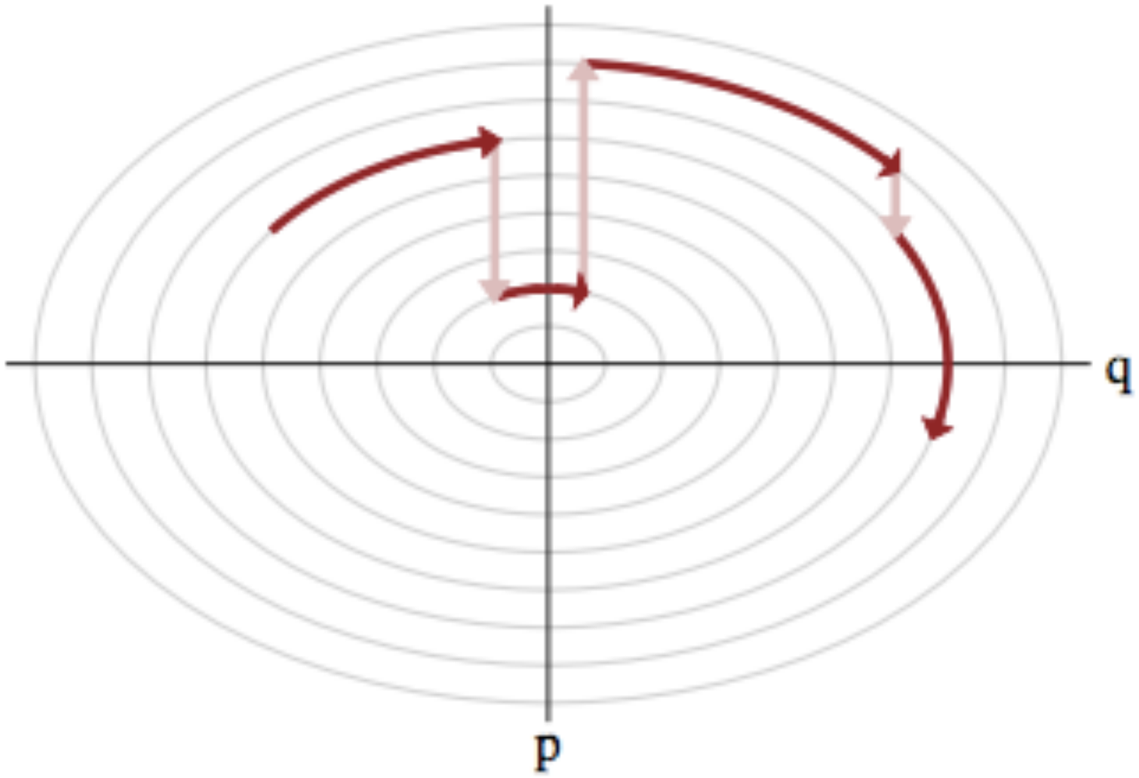
The canonical distribution can be written as a product of this microcanonical distribution and a **marginal energy distribution**:

$$p(q,p) = p(\theta_E|E)p(E)$$

where θ_E indexes the position on the level set.

Marginal Energy Distrib: probability of level set in the typical set.

Momentum resampling



Draw p from a distribution that is determined by the distribution of momentum, i.e. $p \sim N(0, \sqrt{M})$ for example, and attempt to explore the level sets.

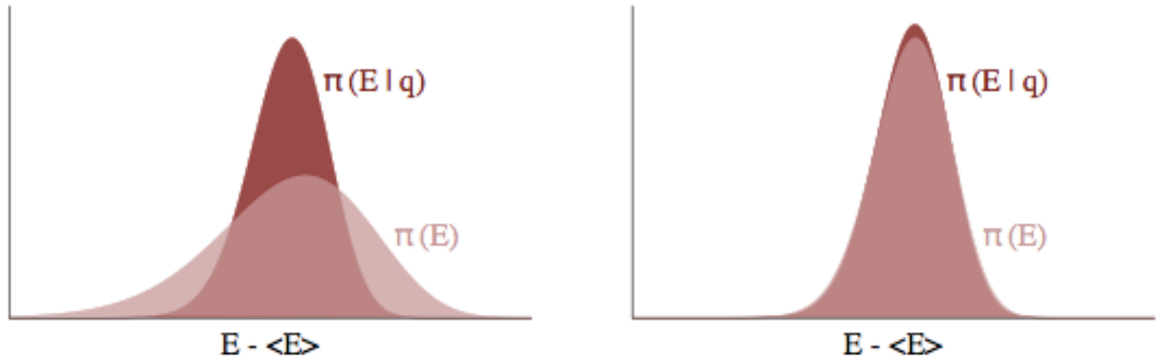
Firing the thruster moves us between level sets!

Resampling Efficiency

Let $p(E|q)$ as the transition distribution of energies induced by a momentum resampling using $p(p|q) = -log\, K(p, q)$ at a given position q.

If $p(E|q)$ narrow compared to the marginal energy distribution $p(E)$: random walk amongst level sets proceeds slowly.

If $p(E|q)$ matches $p(E)$: independent samples generated from the marginal energy distribution very efficiently.



Tuning: choice of Kinetic energy

- Ideal kinetic energy: microcanonical exploration easy and uniform, marginal exploration matched by the transition distrib.
- In practice we often use $K(p) = \frac{1}{2} p' M^{-1} p = \sum_i p_i^2 / 2m_i$
- Set M^{-1} to the covariance of the target distribution: maximally de-correlate the target. Do in warmup (tune) phase.
- can see this by $p \to p/\sqrt{M}$, Then $q \to q\sqrt{M}$

See this for Gaussian:

$$H = \frac{1}{2} p' M^{-1} p + \frac{1}{2} q' \Sigma^{-1} q$$

On transformation

$$H = \frac{1}{2}(p'p + q'q) \text{ if } M^{-1} = \Sigma$$

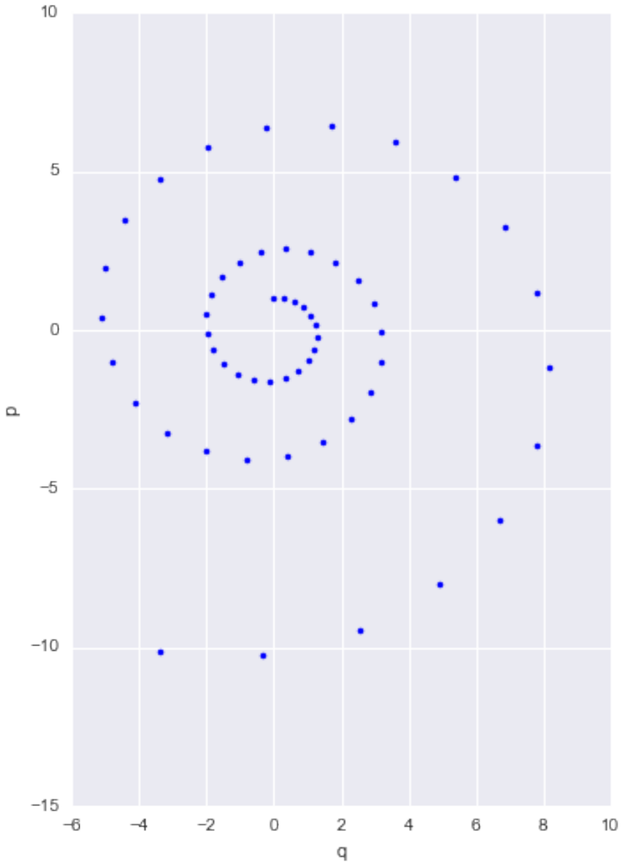
Thus de-correlate target.

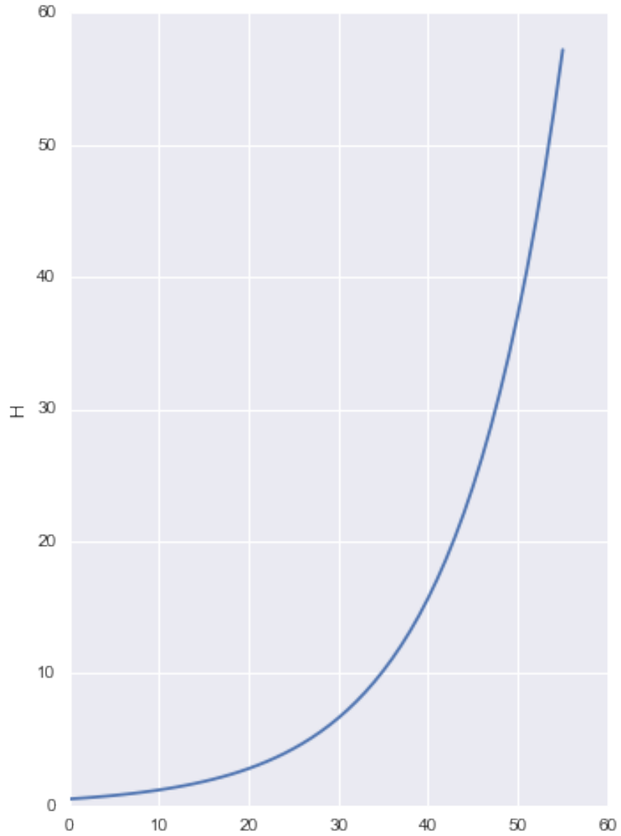
Generalize to arbitrary distributions.

Tuning: integration time

- find the point at which the orbital expectations converge to the spatial expectations..a sort of ergodicity
- L, number of iterations for which we run the Hamiltonian dynamics, and ϵ which is the (small) length of time each iteration is run.
- generally static not good, under-samples tails (high-energy micro-canonicals). Estimate dynamically: NUTS (pymc3 and Stan)

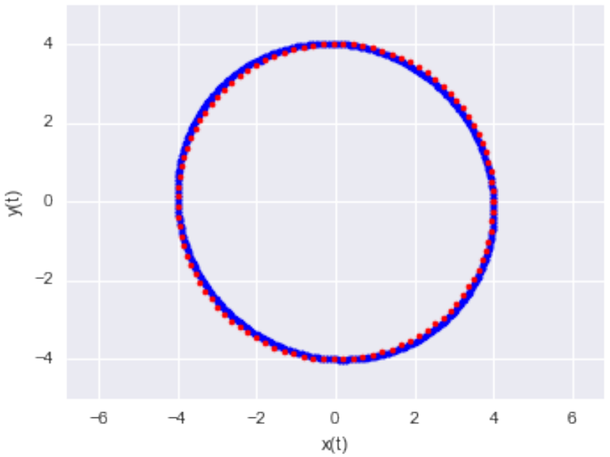
Discretization: Non symplectic integration

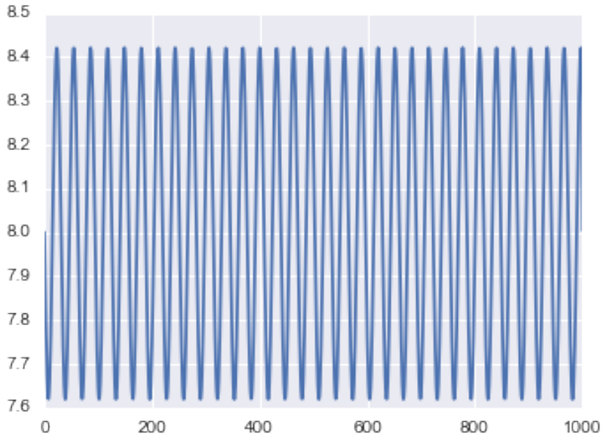




- $p_i(t+\epsilon) = p_i(t) - \epsilon \frac{\partial U}{\partial q_i}|_{q(t)}$
- $q_i(t+\epsilon) = q_i(t) + \epsilon \frac{p_i(t)}{m_i}$
- off-diagonal terms of size ϵ makes volume not preserved
- leads to drift over time

Sympletic Leapfrog



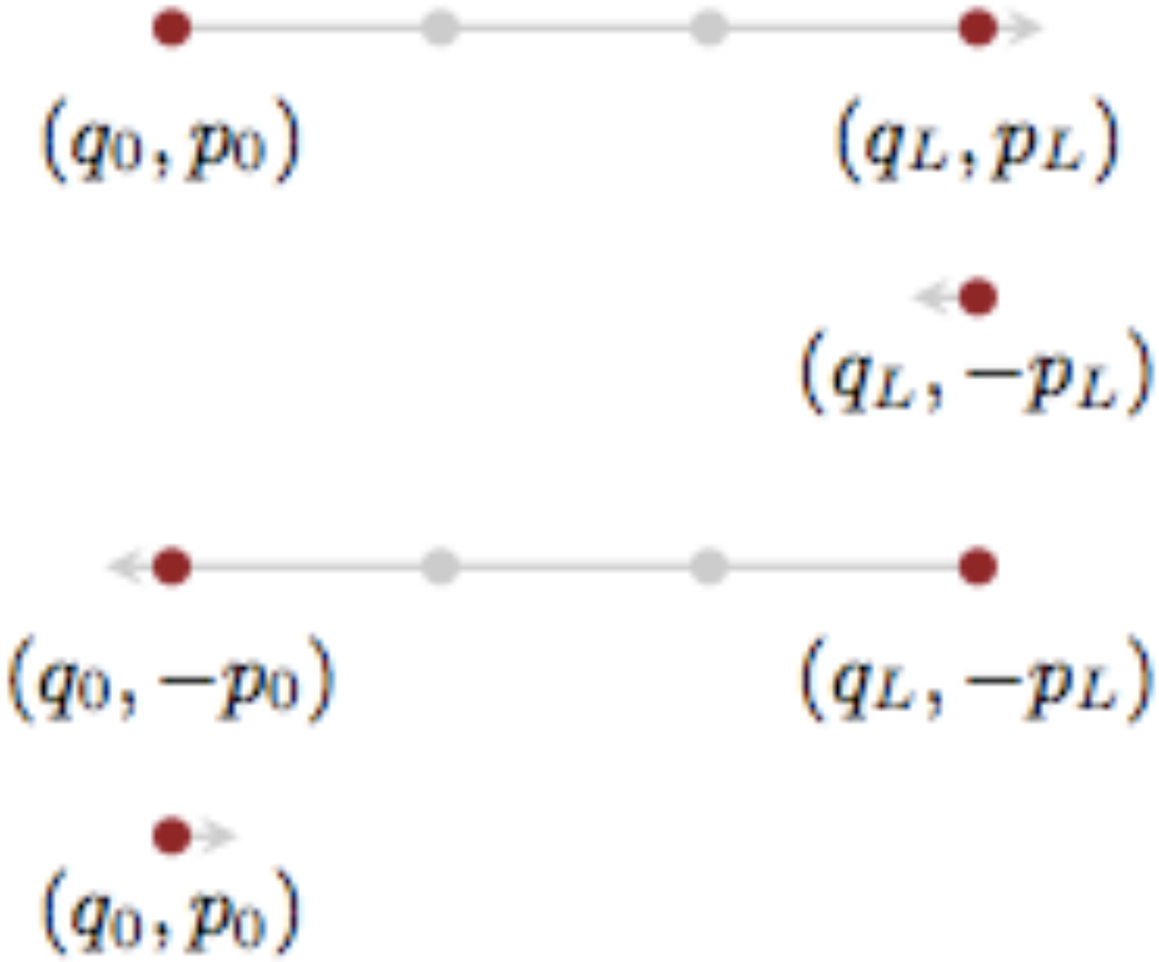


- Only *shear* transforms allowed, will preserve volume.
- $p_i(t+\frac{\epsilon}{2}) = p_i(t) - \frac{\epsilon}{2}\frac{\partial V}{\partial q_i}|_{q(t)}$
- $q_i(t+\epsilon) = q_i(t) + \epsilon\frac{p_i(t+\frac{\epsilon}{2})}{m_i}$
- $p_i(t+\epsilon) = p_i(t+\frac{\epsilon}{2}) - \frac{\epsilon}{2}\frac{\partial V}{\partial q_i}|_{q(t+\epsilon)}$
- still error exists, oscillatory, so reversibility not achieved

Acceptance probability

- might choose $Q(q', p'|q, p) = \delta(q' - q_L)\delta(p' - p_L)$.
- but small symplectic errors means this is only forward in time
- tack on sign change $(q, p) \rightarrow (q_L, -p_L)$. Superman to the rescue!
- proposal now: $Q(q', p'|q, p) = \delta(q' - q_L)\delta(p' + p_L)$.
- Acceptance: $A = \mathbf{min}[1, \frac{p(q_L, -p_L)\delta(q_L - q_L)\delta(-p_L + p_L)}{p(q, p)\delta(q - q)\delta(p - p)}]$

- thus:
  $A = \min[1, \exp(-U(q_L) + U(q) - K(p_L) + K(p)]$
- critical thing with HMC is that our **time evolution is on a level set**. So our A always closer to 1, and we have a very efficient sampler. Optimal acceptance can be shown: 65% roughly.
- In general we'll want to sum over all such points in the orbit
- momentum reversal could be left out if not within a more complex sampling scheme



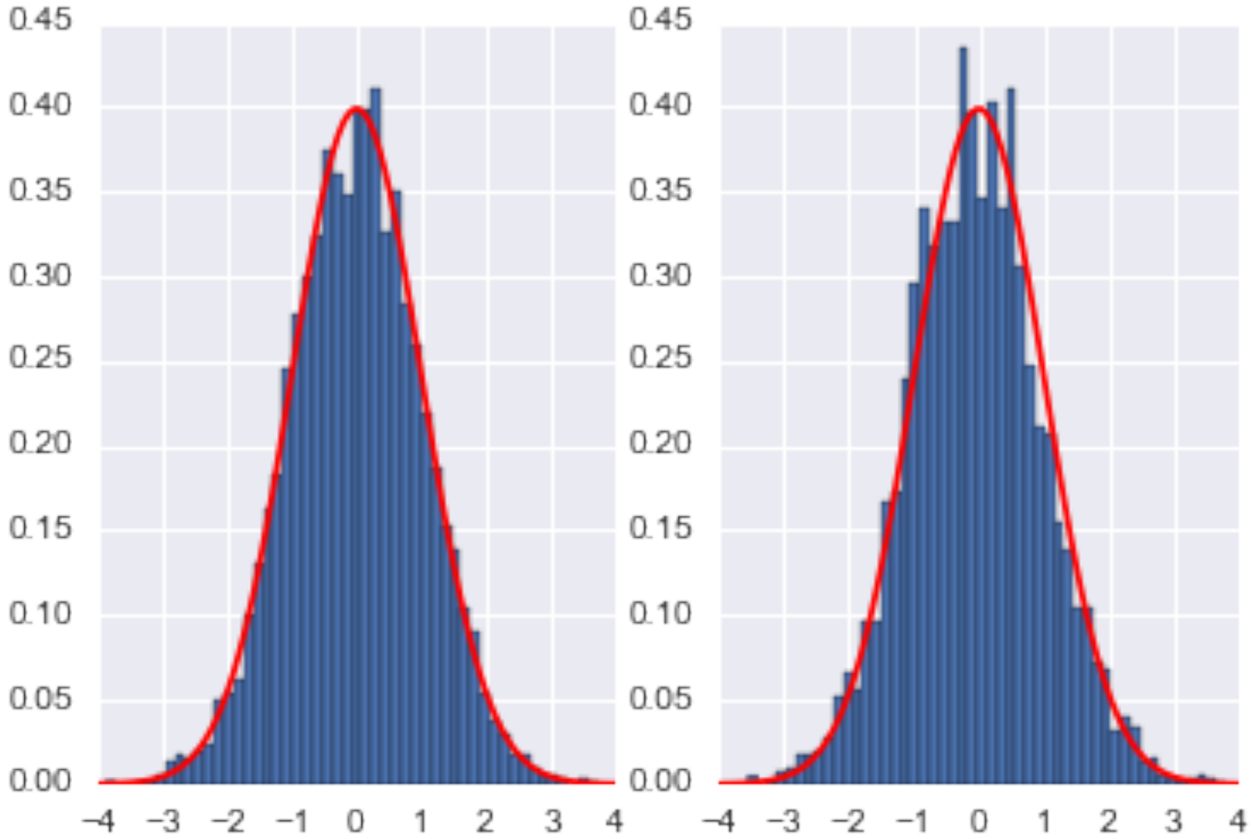
HMC Algorithm

- for i=1:N_samples
  - 1. Draw $p \sim N(0, M)$
  - 2. Set $q_c = q^{(i)}$ where the subscript c stands for current
  - 3. $p_c = p$
  - 4. Update momentum before going into LeapFrog stage: $p^* = p_c - \frac{\epsilon * \nabla U(q_c)}{2}$
  - 5. LeapFrog to get new proposals. For j=1:L (first/third steps together)
    - $q^* = q^* + \epsilon p$
    - if not the last step, $p = p - \epsilon \nabla U(q)$
  - 6. Complete leapfrog: $p = p - \frac{\epsilon \nabla U(q)}{2}$

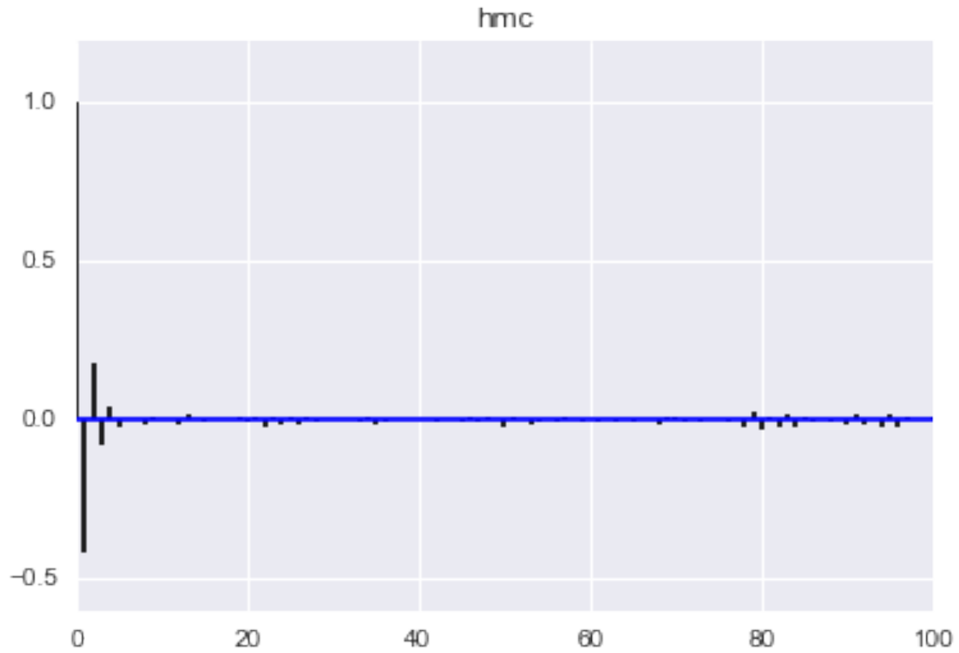
HMC (contd)

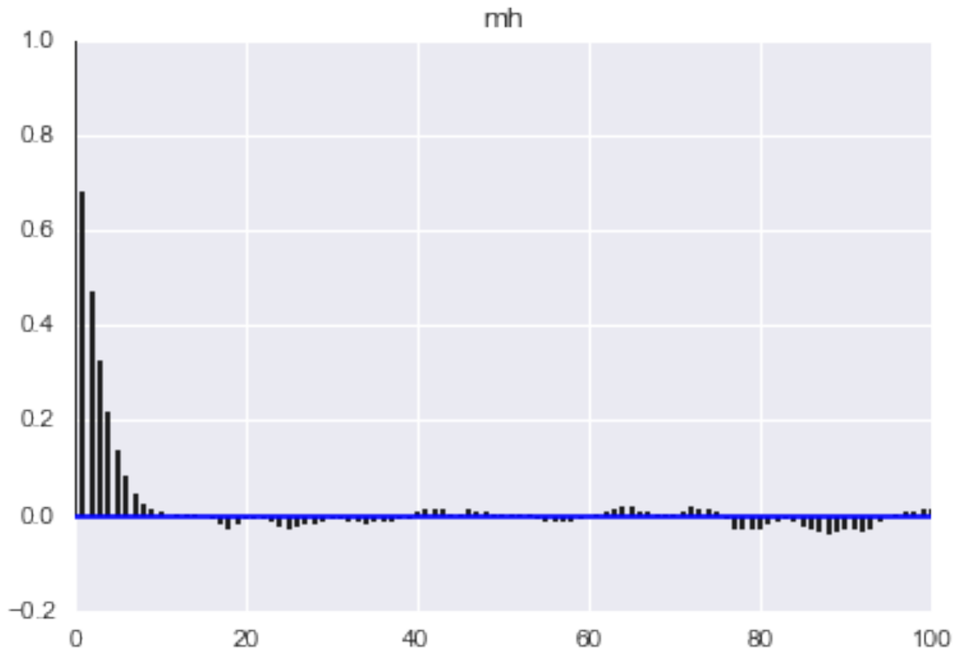
- for i=1:N_samples
  - 7. $p^* = -p$
  - 8. $V_c = V(q_c), \;\; K_c = \frac{p_c^\top M^{-1} p_c}{2}$
  - 9. $V^* = V(q^*), \;\; K^* = \frac{p^{\top *} M^{-1} p^*}{2}$
  - 10. $r \sim \mathbf{Unif}(0,1)$
  - 11. if $r < e^{(U_c - U^* + K_c - K^*)}$
    - accept $q_i = q^*$
    - otherwise reject

```python
def HMC(U,K,dUdq,N,q_0, p_0, epsilon=0.01, L=100):
    current_q = q_0
    current_p = p_0
    H = np.zeros(N)
    qall = np.zeros(N)
    accept=0
    for j in range(N):
        q = current_q
        p = current_p
        #draw a new p
        p = np.random.normal(0,1)
        current_p=p
        # leap frog
        # Make a half step for momentum at the beginning
        p = p - epsilon*dUdq(q)/2.0
        # alternate full steps for position and momentum
        for i in range(L):
            q = q + epsilon*p
            if (i != L-1):
                p = p - epsilon*dUdq(q)
        #make a half step at the end
        p = p - epsilon*dUdq(q)/2.
        # negate the momentum
        p= -p;
        current_U = U(current_q)
        current_K = K(current_p)
        proposed_U = U(q)
        proposed_K = K(p)
        A=np.exp( current_U-proposed_U+current_K-proposed_K)
        # accept/reject
        if np.random.rand() < A:
            current_q = q
            qall[j]=q
            accept+=1
        else:
            qall[j] = current_q
        H[j] = U(current_q)+K(current_p)
    print("accept=",accept/np.double(N))
    return H, qall
```



Autocorrelation: HMC vs MH

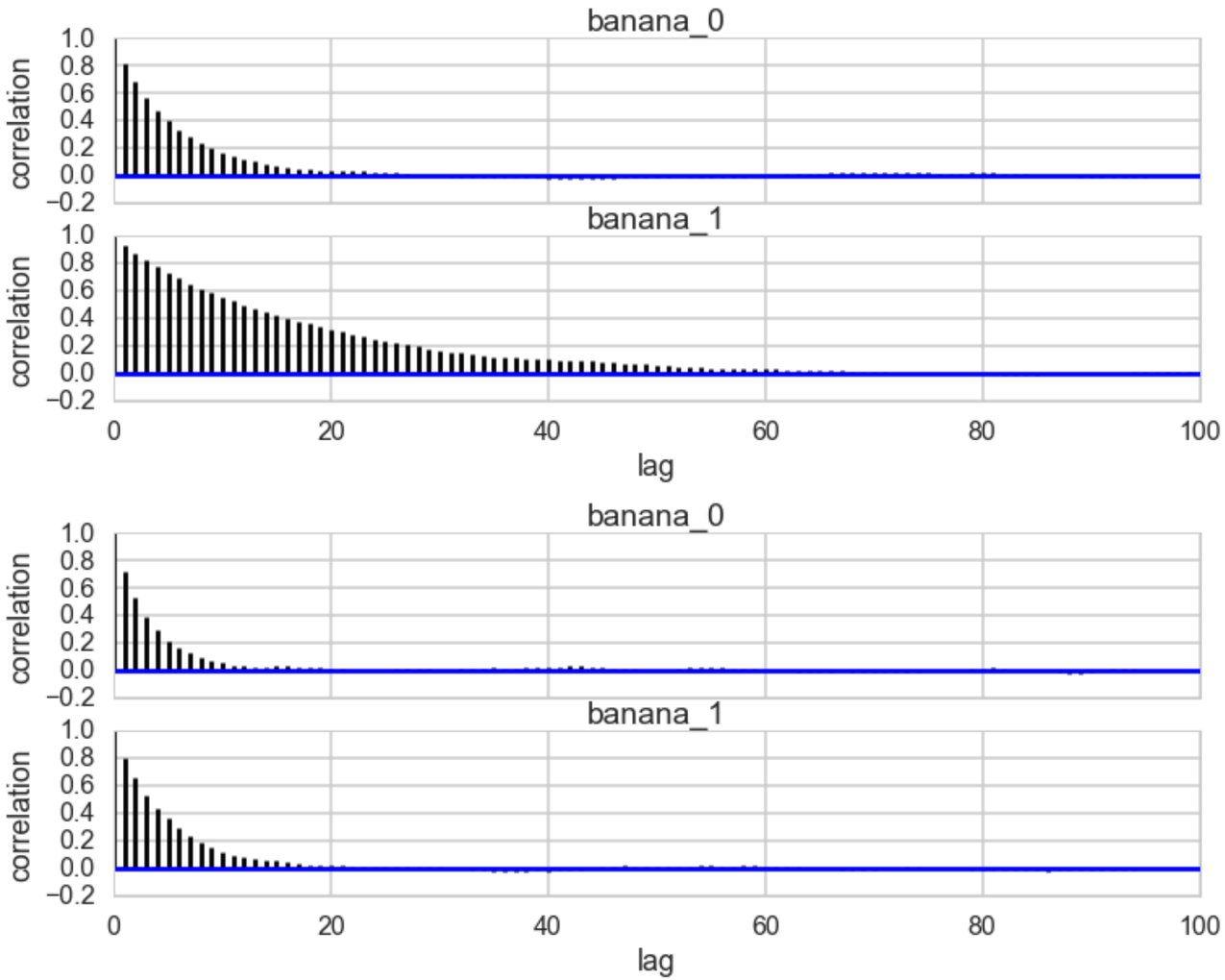





```
H, qall= HMC(U=U,K=K,dUdq=dUdq,N=10000,q_0=0, p_0=-4, epsilon=0.01, L=200)

samples_mh = MH_simple(p=P, n=10000, sig=4.0, x0=0)
```

HMC/NUTS in pymc3

```
def clike2(value):
    x = value[0]
    y = value[1]
    val = -100 * (T.sqrt(y**2+x**2)-1)**2 + (x-1)**3 - y -5
    return (val)

with pm.Model() as model:
    banana = pm.DensityDist("banana", clike2, shape=2, testval=[1,1])

with model:
    start = pm.find_MAP()
    stepper=pm.Metropolis()
    trace=pm.sample(100000, step=stepper, start=start)
pm.autocorrplot(trace[20000::5])

with model:
    start_nuts = pm.find_MAP()
    stepper_nuts=pm.NUTS()
    trace_nuts=pm.sample(100000, step=stepper_nuts)
pm.autocorrplot(trace_nuts[:16000])
```



Tumors in pymc3 with NUTS

```
with Model() as tumor_model:
    # Uniform priors on the mean and variance of the Beta distributions
    mu = Uniform("mu",0.00001,1.)
    nu = Uniform("nu",0.00001,1.)
    # Calculate hyperparameters alpha and beta as a function of mu and nu
    alpha = pm.Deterministic('alpha', mu/(nu*nu))
    beta = pm.Deterministic('beta', (1.-mu)/(nu*nu))
    # Priors for each theta
    thetas = Beta('theta', alpha, beta, shape=N)
    # Data likelihood
    obs_deaths = Binomial('obs_deaths', n=tumorn, p=thetas, observed=tumory)

with tumor_model:
    # Use ADVI for initialization
    mu, sds, elbo = pm.variational.advi(n=100000)
    step = pm.NUTS(scaling=tumor_model.dict_to_array(sds)**2,
                   is_cov=True)
    tumor_trace = pm.sample(5000, step, start=mu)
```

Normal-Normal Hierarchical Model

J independent experiments, experiment j estimating the parameter θ_j from n_j independent normally distributed data points, y_{ij}, each with known error variance σ^2; that is,

$$y_{ij}|\theta_j \sim N(\theta_j, \sigma^2),\ i = 1, \ldots, n_j; j = 1, \ldots, J.$$

Gelman 8-schools problem: estimated coaching effects $\bar{y}_j$ to improve SAT scores for school j, with sampling variances, σ_j^2.

Sample mean of each group j

$\bar{y}_j = \frac{1}{n_j}\sum_{i=1}^{n_j} y_{ij}$ with sampling variance

$\sigma_j^2 = \sigma^2/n_j.$

Likelihood for θ_j using suff-stats, $\bar{y}_j$:

$$\bar{y}_j|\theta_j \sim N(\theta_j, \sigma_j^2).$$

Notation flexible in allowing a separate variance σ_j^2 for the mean of each group j.

Appropriate when the variances differ for reasons other than number of data pts.

School	Estimated treatment effect, y_j	Standard error of effect estimate, σ_j
A	28	15
B	8	10
C	−3	16
D	7	11
E	−1	9
F	1	11
G	18	10
H	12	18

Installation

```
pip install theano==0.9
pip install pymc3==3.1rc2
```

```
pm.__version__
'3.1.rc2'
```

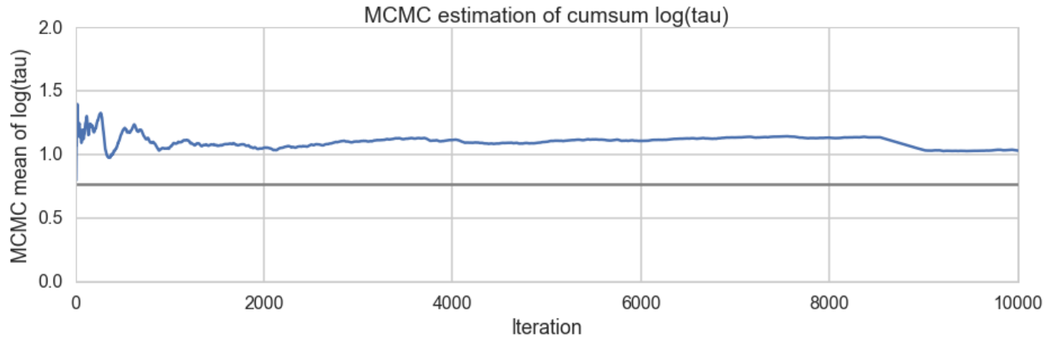
Centered Hierarchical Model

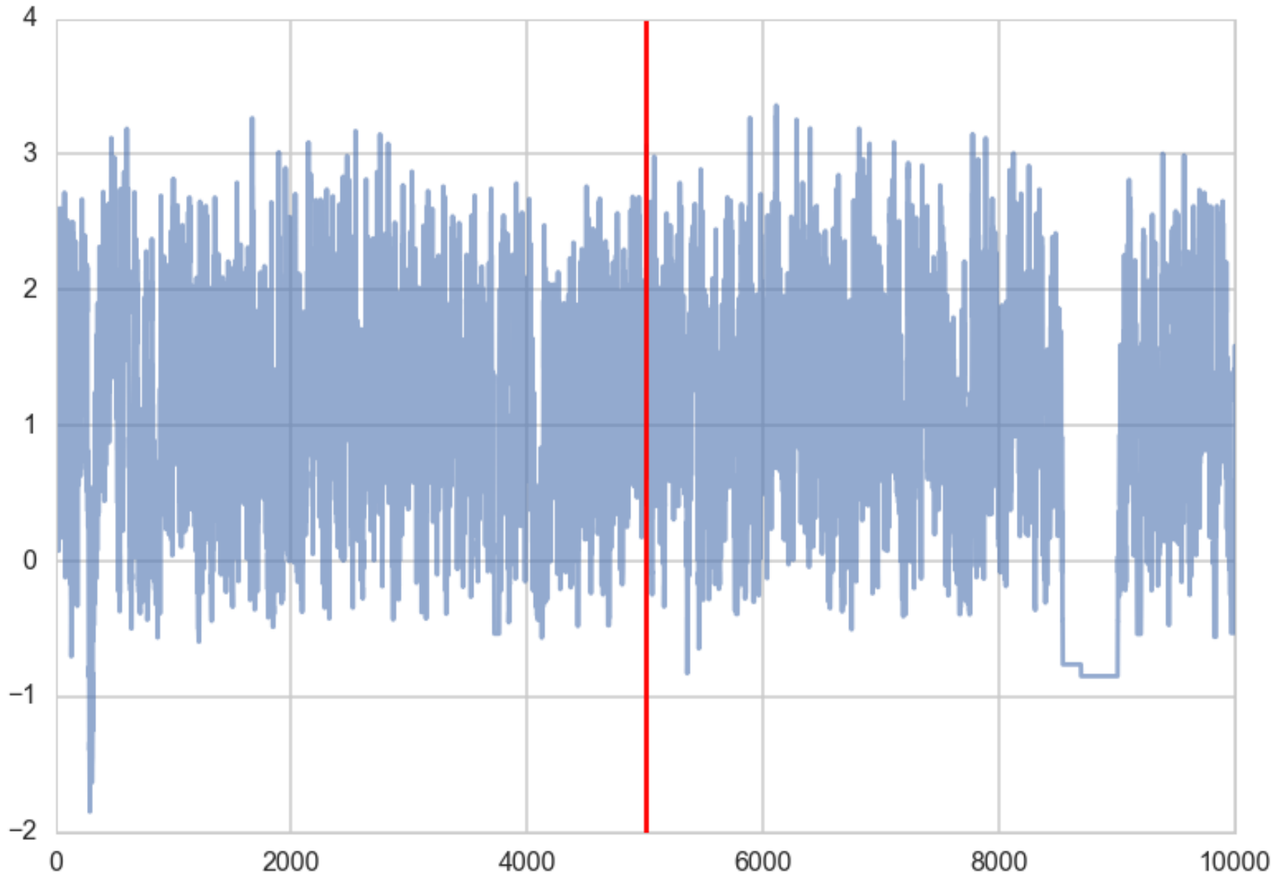
$$\mu \sim \mathcal{N}(0, 5)$$
$$\tau \sim \text{Half-Cauchy}(0, 5)$$
$$\theta_j \sim \mathcal{N}(\mu, \tau)$$
$$\bar{y}_j \sim \mathcal{N}(\theta_j, \sigma_j)$$

```
with pm.Model() as schools1:

    mu = pm.Normal('mu', 0, sd=5)
    tau = pm.HalfCauchy('tau', beta=5)
    theta = pm.Normal('theta', mu=mu, sd=tau, shape=J)
    obs = pm.Normal('obs', mu=theta, sd=sigma, observed=y)

with schools1:
    trace1 = pm.sample(5000, init=None, njobs=2, tune=500)
```

Small n_{eff}:

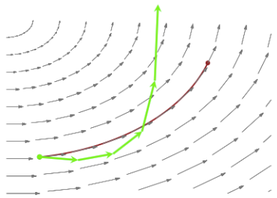
```
{'mu': 101.0,
  'tau': 273.0,
  'tau_log_': 77.0,
  'theta': array([ 169.,  199.,  236.,  193.,  211.,  231.,  139.,  204.])})
```



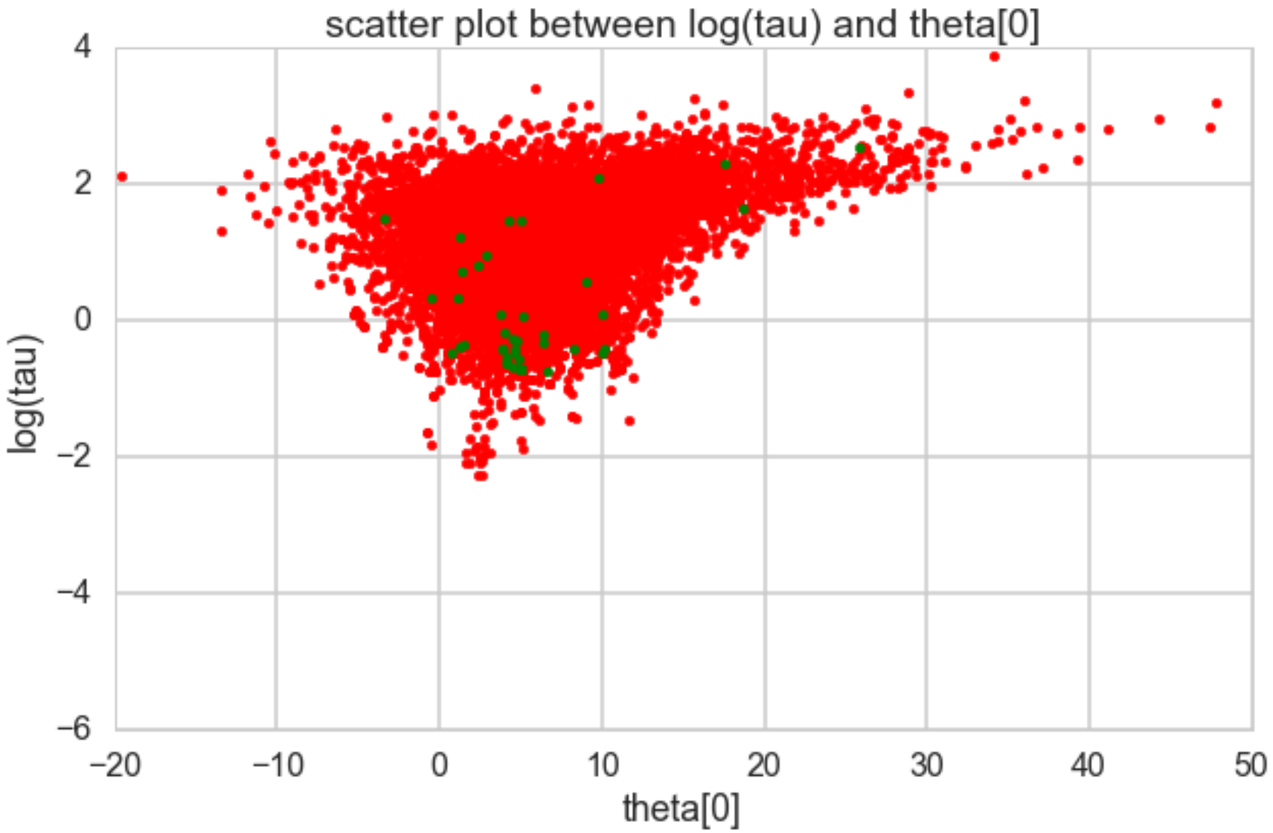


- stickys are actually trying to drive down value of trace
- we are in a region of high curvature

High Curvature Issues



- symplectic integration diverges: good diagnostic
- sampler needs to have real small steps to not diverge, but then becomes sticky
- regions of high curvature often have high energy differences, causing trouble for microcanonical jump transitions.



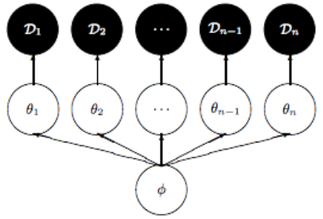
Diagnosed thus:

```
divergent = trace1['diverging']
print('Number of Divergent %d' % divergent.nonzero()[0].size)
divperc = divergent.nonzero()[0].size/len(trace1)
print('Percentage of Divergent %.5f' % divperc)
```

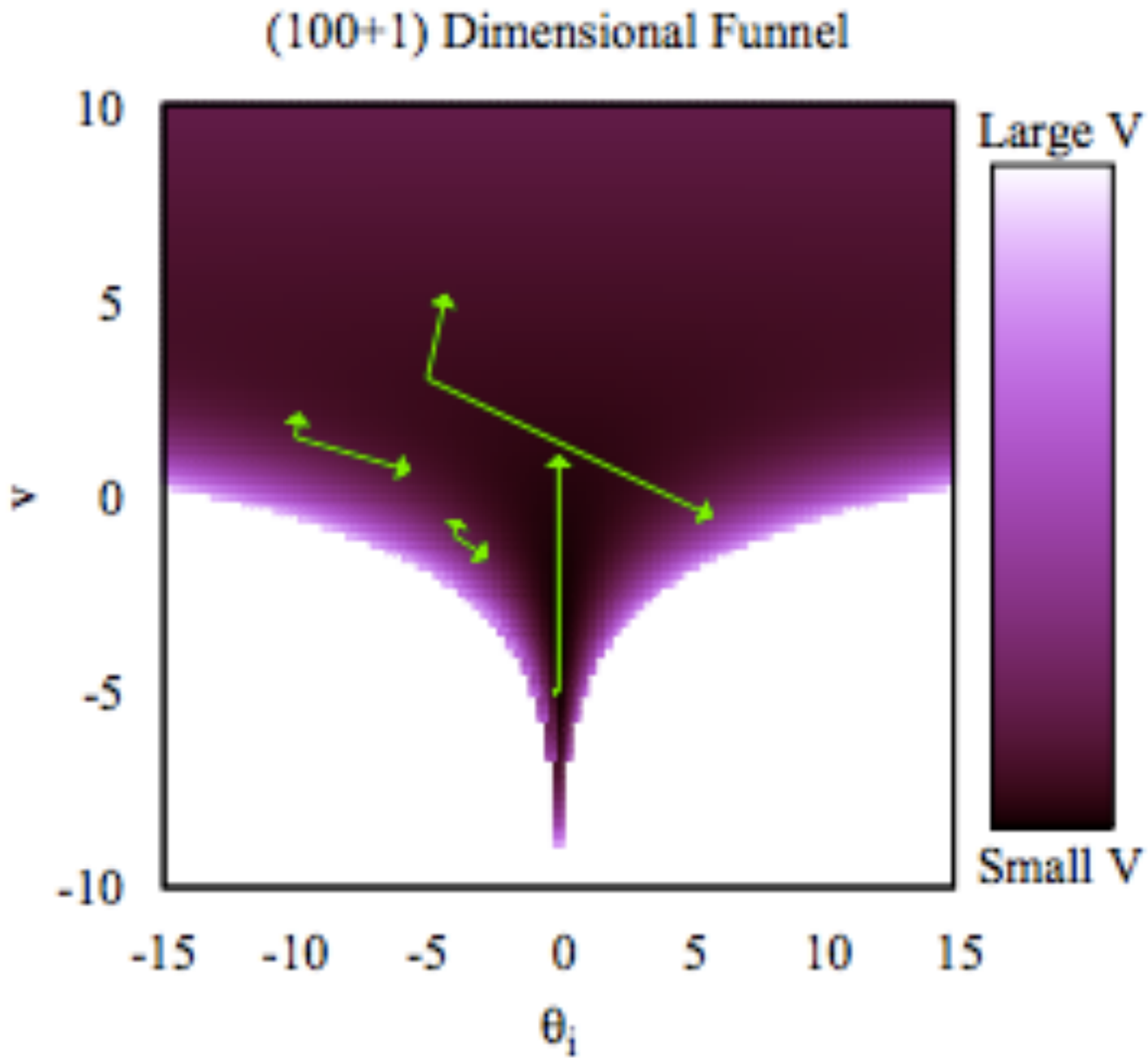
```
Number of Divergent 74
Percentage of Divergent 0.01480
```

- Not characterizing neck well
- No confidence in postrior in this region

Hierarchical Models have high curvature

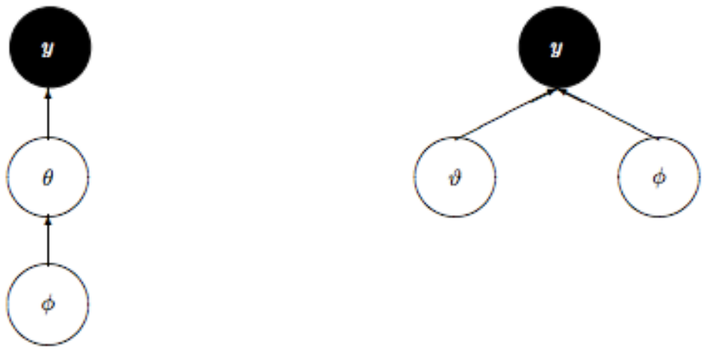


- characteristic funnel, also there in MH and gibbs
- reflects high correlation between levels in tree
- divergences occur in neck



Non-centered model

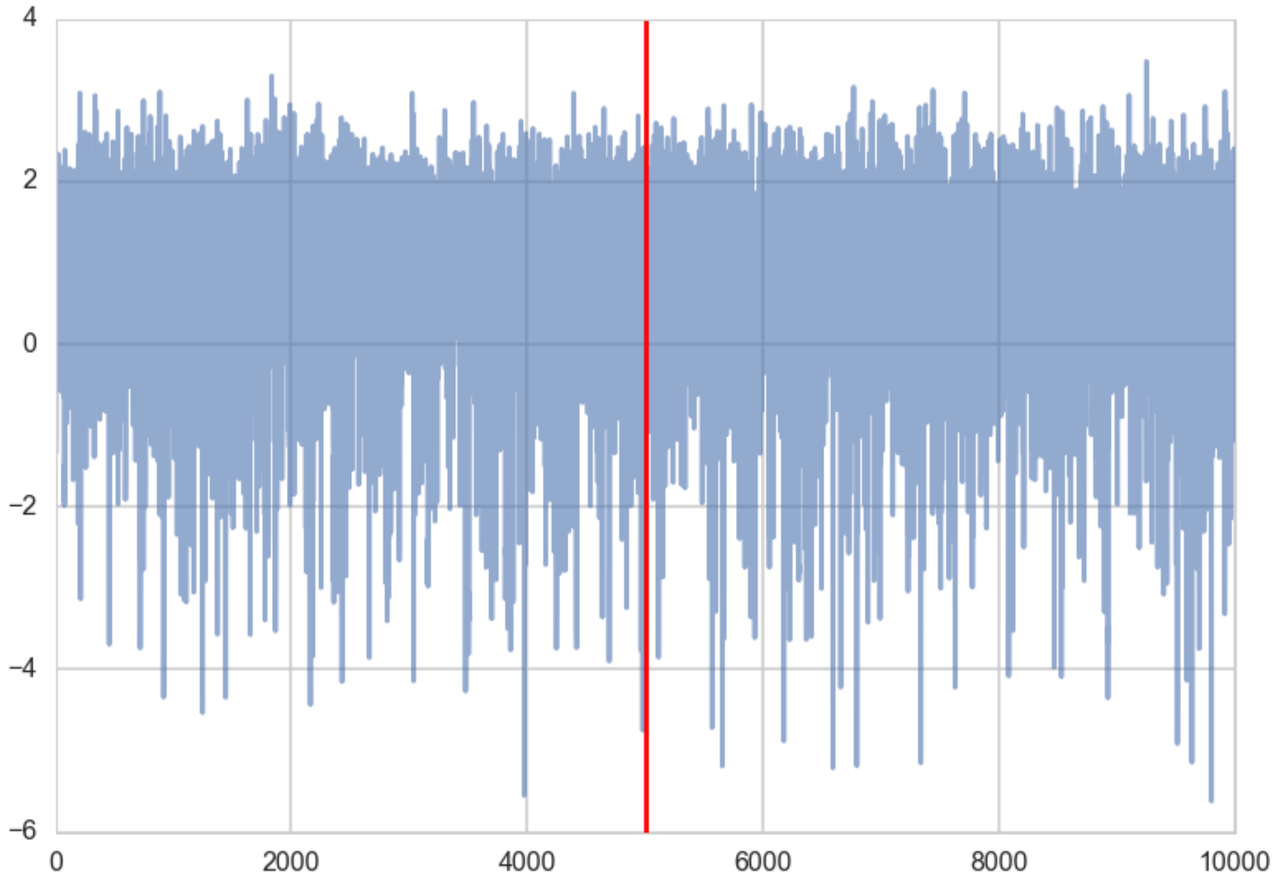
- could change kinetic energy (riemannian HMC) to make mass matrix dependent upon position
- simpler: reparametrize to reduce levels in hierarchy

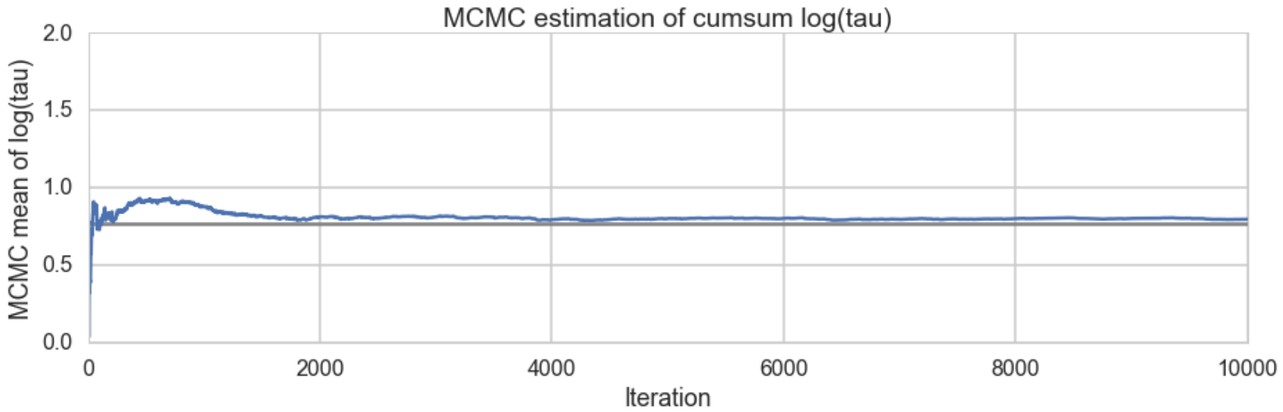


$$\mu \sim \mathcal{N}(0, 5)$$
$$\tau \sim \text{Half-Cauchy}(0, 5)$$
$$\nu_j \sim \mathcal{N}(0, 1)$$
$$\theta_j = \mu + \tau\nu_j$$
$$\bar{y}_j \sim \mathcal{N}(\theta_j, \sigma_j)$$

Factor dependency of θ on $\phi = \mu, \tau$ into a deterministic transformation between the layers, leaving the actively sampled variables uncorrelated.

```
with pm.Model() as schools2:
    mu = pm.Normal('mu', mu=0, sd=5)
    tau = pm.HalfCauchy('tau', beta=5)
    nu = pm.Normal('nu', mu=0, sd=1, shape=J)
    theta = pm.Deterministic('theta', mu + tau * nu)
    obs = pm.Normal('obs', mu=theta, sd=sigma, observed=y)
    trace2 = pm.sample(5000, init=None, njobs=2, tune=500)
```





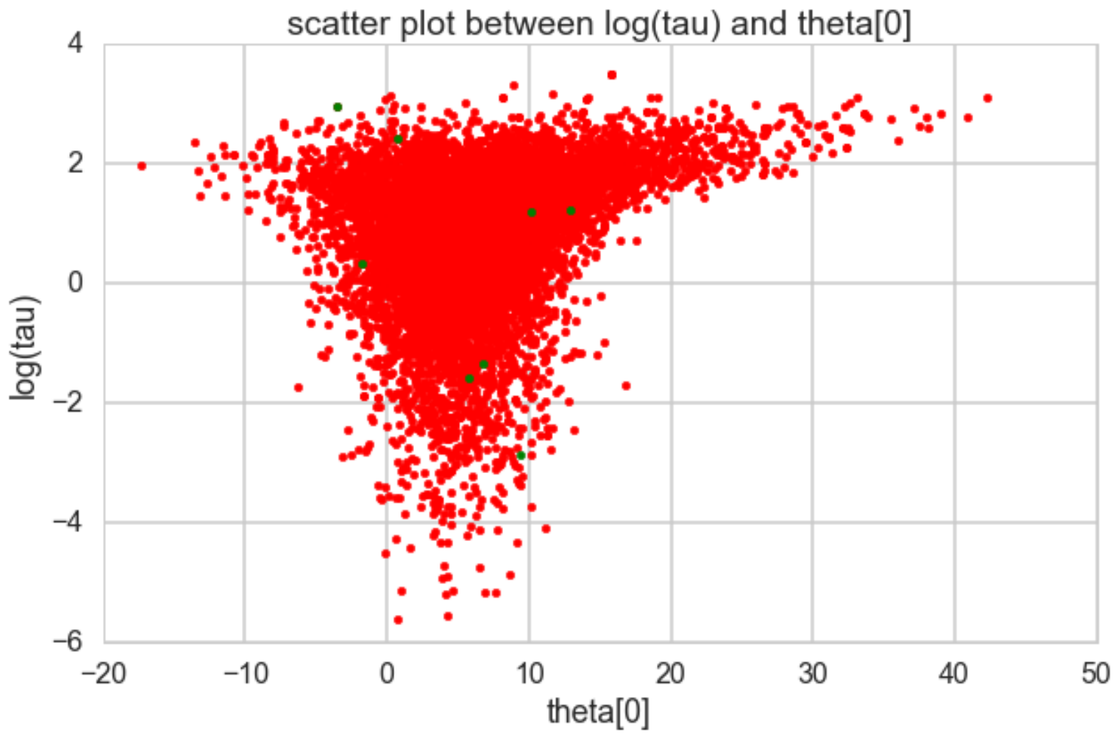
n_{eff}:

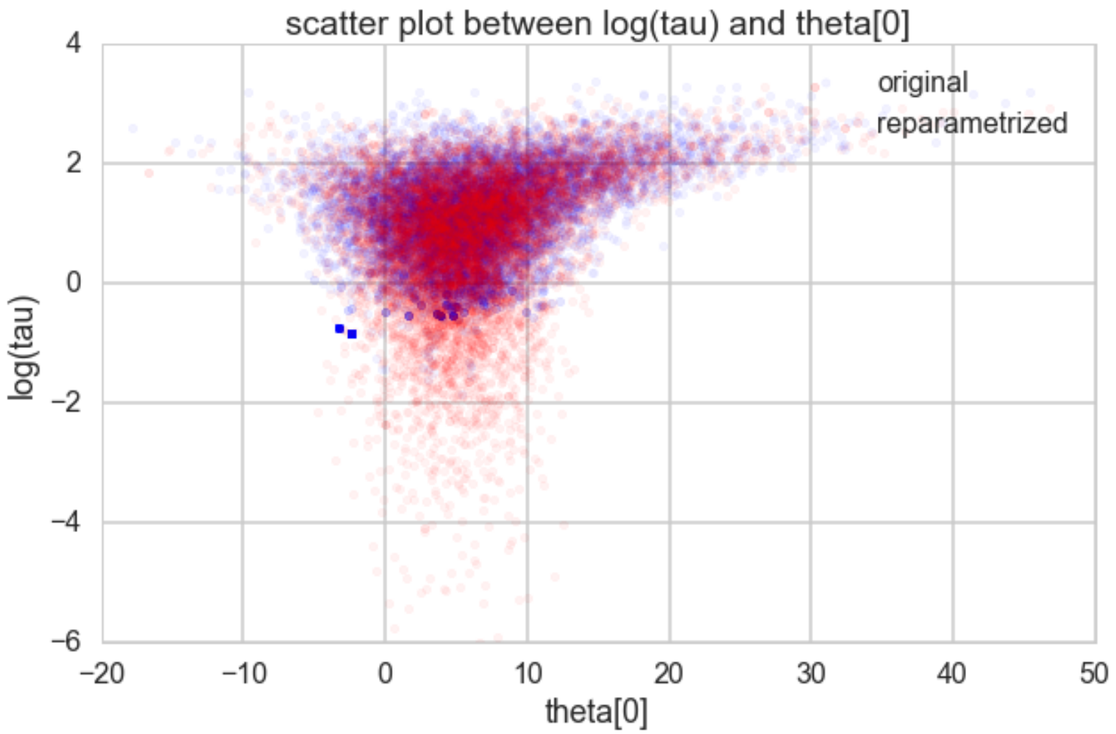
```
{'mu': 10000.0,
  'nu': array([ 10000.,  10000.,  10000.,  10000.,  10000.,  10000.,  10000.,
         10000.]),
  'tau': 6880.0,
  'tau_log_': 5193.0,
  'theta': array([  9624.,  10000.,  10000.,  10000.,  10000.,  10000.,  10000.,
          9829.])}
```

```
divergent = trace2['diverging']
print('Number of Divergent %d' % divergent.nonzero()[0].size)
divperc = divergent.nonzero()[0].size/len(trace2)
print('Percentage of Divergent %.5f' % divperc)
```

```
Number of Divergent 8
Percentage of Divergent 0.00160
```

Divergences and true length of funnel





Speed of light experiment

- Simon Newcomb, 1882, times required for light to travel 7442 metres, recorded as deviations from 24,800 nanoseconds

```
light_speed = np.array([28, 26, 33, 24, 34, -44, 27, 16, 40, -2, 29, 22, 24, 21, 25,
                        30, 23, 29, 31, 19, 24, 20, 36, 32, 36, 28, 25, 21, 28, 29,
                        37, 25, 28, 26, 30, 32, 36, 26, 30, 22, 36, 23, 27, 27, 28,
                        27, 31, 27, 26, 33, 26, 32, 32, 24, 39, 28, 24, 25, 32, 25,
                        29, 27, 28, 29, 16, 23])
```

Use Normal model with weakly informative priors to model

```
with pm.Model() as light_model:
    mu = pm.Uniform('mu', lower=-1000,
                    upper=1000.0)
    sigma = pm.Uniform('sigma', lower=0.1, upper=1000.0)
    obsv = pm.Normal('obsv', mu=mu, sd=sigma, observed=light_speed)
```

```
with light_model:
    trace = pm.sample(10000)
```

```
Average ELBO = -408.66:  19%|██         | 37486/200000 [00:03<00:14, 11046.99it/s]16, 11779.39it/s]
100%|██████████| 10000/10000 [00:07<00:00, 1384.39it/s]
```