

No-U-Turn Sampler : Adaptively Setting Path Lengths in HMC

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CONTENTS

- 1 Hamiltonian Monte Carlo
- 2 Time-Reversibility
- 3 No-U-Turn Sampler
- 4 Tuning ϵ
- 5 Evaluation

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- $\theta(t)$: location at t
- $r(t)$: momentum at t
- $U(\theta)$: potential energy

$$U(\theta) = -\log(f(\theta))$$

- $K(r)$: kinetic energy

$$K(r) = \frac{r^T r}{2}$$

- $H(\theta, r) = U(\theta) + K(r)$

Leapfrog Method

- Hamilton's equation

$$\begin{aligned}\frac{dr}{dt} &= \frac{\partial H}{\partial p} = \frac{\partial U}{\partial p} \\ \frac{d\theta}{dt} &= \frac{\partial H}{\partial r} = \frac{\partial K}{\partial r}\end{aligned}$$

- Leapfrog integrator

$$r(t + \epsilon/2) = r(t) - (\epsilon/2) \frac{\partial U}{\partial \theta}(\theta(t))$$

$$\theta(t + \epsilon) = \theta(t) + \epsilon \frac{\partial K}{\partial r}(r(t + \epsilon/2))$$

$$r(t + \epsilon) = r(t + \epsilon/2) - (\epsilon/2) \frac{\partial U}{\partial \theta}(\theta(t + \epsilon))$$

Algorithm 1 Hamiltonian Monte Carlo

Given θ^0 , ϵ , L , \mathcal{L} , M :

for $m = 1$ to M **do**

 Sample $r^0 \sim \mathcal{N}(0, I)$.

 Set $\theta^m \leftarrow \theta^{m-1}$, $\tilde{\theta} \leftarrow \theta^{m-1}$, $\tilde{r} \leftarrow r^0$.

for $i = 1$ to L **do**

 Set $\tilde{\theta}, \tilde{r} \leftarrow \text{Leapfrog}(\tilde{\theta}, \tilde{r}, \epsilon)$.

end for

 With probability $\alpha = \min \left\{ 1, \frac{\exp\{\mathcal{L}(\tilde{\theta}) - \frac{1}{2}\tilde{r} \cdot \tilde{r}\}}{\exp\{\mathcal{L}(\theta^{m-1}) - \frac{1}{2}r^0 \cdot r^0\}} \right\}$, set $\theta^m \leftarrow \tilde{\theta}$, $r^m \leftarrow -\tilde{r}$.

end for

function Leapfrog(θ, r, ϵ)

 Set $\tilde{r} \leftarrow r + (\epsilon/2)\nabla_{\theta}\mathcal{L}(\theta)$.

 Set $\tilde{\theta} \leftarrow \theta + \epsilon\tilde{r}$.

 Set $\tilde{r} \leftarrow \tilde{r} + (\epsilon/2)\nabla_{\theta}\mathcal{L}(\tilde{\theta})$.

return $\tilde{\theta}, \tilde{r}$.

- L : number of steps
- ϵ : step size
- L is too small : random walk behavior
- L is too large : loop back and retrace their steps
- ϵ is too small : computational waste
- ϵ is too large : inaccurate

CONTENTS

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Time-Reversibility

- P : transition probability matrix

$$P_{ij} = P(X_{m+1} = j | X_m = i)$$

- Detailed balance equation

$$\pi_i P_{ij} = \pi_j P_{ji}$$

- Time reversible

$$P(X_{m+1} = j | X_m = i) = P(X_m = i | X_{m+1} = j)$$

CONTENTS

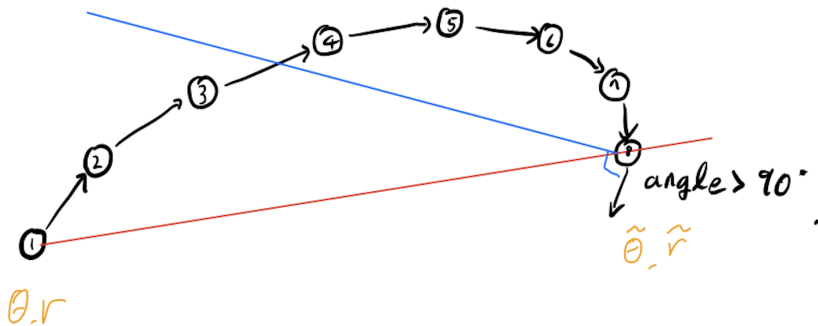
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- Running the simulation for more steps until no longer increase the distance between the proposal $\tilde{\theta}$ and the initial value of θ .

$$\frac{d}{dt} \frac{(\tilde{\theta} - \theta) \cdot (\tilde{\theta} - \theta)}{2} = (\tilde{\theta} - \theta) \cdot \frac{d}{dt}(\tilde{\theta} - \theta) = (\tilde{\theta} - \theta) \cdot \tilde{r}$$

- Simulating until $(\tilde{\theta} - \theta) \cdot \tilde{r} < 0$.

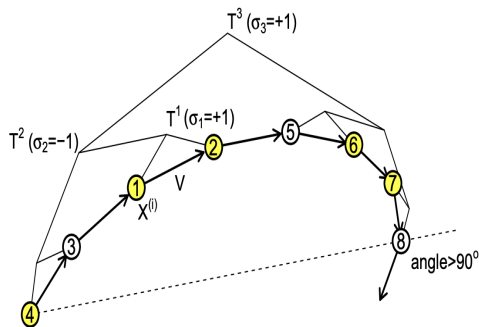
Main Idea



Problem

- This algorithm does not guarantee time reversibility.
- NUTS overcomes this issue by running the Hamiltonian simulation both forward and backward in time.
- Introduce a slice variable u for simplifying the NUTS.

Simple algorithm



- Choosing a random direction $\sigma_i \sim U(-1, 1)$
- Taking 2^j leapfrog steps of size $\sigma_j \epsilon$
- θ^-, r^- and θ^+, r^+ : the state of leftmost and rightmost leaves.
- Simulating until $(\theta^+ - \theta^-) \cdot r^- < 0$ or $(\theta^+ - \theta^-) \cdot r^+ < 0$

Slice sampling

- $\theta \sim \pi(\theta)$
 - $V = \{(\theta, u) : 0 < u < \pi(\theta)\}$
 - Sampling (θ, u) uniformly over the region V .
- Step 1 : $p(u|\theta) \propto \mathbb{I}[0 < u < \pi(\theta)]$
- Step 2 : $p(\theta|u) \propto \mathbb{I}[u < \pi(\theta)]$
- Slice sampling can suppress random walks.

- \mathcal{B} : all position-momentum states
- \mathcal{C} : candidate position-momentum states
- C.1 : All elements of \mathcal{C} must be chosen in a way that preserves volume.
- C.2 : $P((\theta, r) \in \mathcal{C} | \theta, r, u, \epsilon) = 1$
- C.3 : $P(u \leq \exp\{-U(\theta') - \frac{r'^T r'}{2}\} | (\theta', r') \in \mathcal{C}) = 1$
- C.4 : If $(\theta, r) \in \mathcal{C}$ and $(\theta', r') \in \mathcal{C}$ then for any \mathcal{C} ,
 $P(\mathcal{B}, \mathcal{C} | \theta, r, u, \epsilon) = P(\mathcal{B}, \mathcal{C} | \theta', r', u, \epsilon)$

- Step
 1. sample $r \sim N(0, I)$
 2. sample $u \sim U([0, \exp(-U(\theta) - r \cdot r/2)])$
 3. sample \mathcal{B}, \mathcal{C} from $P(\mathcal{B}, \mathcal{C} | \theta(t), r, u, \epsilon)$
 4. sample $\theta(t+1), r \sim T(\theta_t, r, \mathcal{C})$
- T : transition kernel
- $u \leq \exp\{-U(\theta') - r' \cdot r'/2\}$ then $(\theta', r') \in \mathcal{C}$
- Stop doubling if the tree includes a leaf node whose state θ, r satisfies $\log(f(\theta)) - r \cdot r/2 - \log(u) < -\Delta_{max}$

Algorithm 2 Naive No-U-Turn Sampler

Given θ^0 , ϵ , \mathcal{L} , M :

for $m = 1$ to M **do**

Resample $r^0 \sim \mathcal{N}(0, I)$.

Resample $u \sim \text{Uniform}([0, \exp\{\mathcal{L}(\theta^{m-1} - \frac{1}{2}r^0 \cdot r^0)\}])$

Initialize $\theta^- = \theta^{m-1}$, $\theta^+ = \theta^{m-1}$, $r^- = r^0$, $r^+ = r^0$, $j = 0$, $\mathcal{C} = \{(\theta^{m-1}, r^0)\}$, $s = 1$.

while $s = 1$ **do**

Choose a direction $v_j \sim \text{Uniform}(\{-1, 1\})$.

if $v_j = -1$ **then**

$\theta^-, r^-, -, -, \mathcal{C}', s' \leftarrow \text{BuildTree}(\theta^-, r^-, u, v_j, j, \epsilon)$.

else

$-, -, \theta^+, r^+, \mathcal{C}', s' \leftarrow \text{BuildTree}(\theta^+, r^+, u, v_j, j, \epsilon)$.

end if

if $s' = 1$ **then**

$\mathcal{C} \leftarrow \mathcal{C} \cup \mathcal{C}'$.

end if

$s \leftarrow s' \mathbb{I}[(\theta^+ - \theta^-) \cdot r^- \geq 0] \mathbb{I}[(\theta^+ - \theta^-) \cdot r^+ \geq 0]$.

$j \leftarrow j + 1$.

end while

Sample θ^m, r uniformly at random from \mathcal{C} .

end for

Algorithm

function BuildTree($\theta, r, u, v, j, \epsilon$)

if $j = 0$ **then**

Base case—take one leapfrog step in the direction v .

$\theta', r' \leftarrow \text{Leapfrog}(\theta, r, v\epsilon).$

$C' \leftarrow \begin{cases} \{(\theta', r')\} & \text{if } u \leq \exp\{\mathcal{L}(\theta') - \frac{1}{2}r' \cdot r'\} \\ \emptyset & \text{else} \end{cases}$

$s' \leftarrow \mathbb{I}[\mathcal{L}(\theta') - \frac{1}{2}r' \cdot r' > \log u - \Delta_{\max}].$

return $\theta', r', \theta', r', C', s'.$

else

Recursion—build the left and right subtrees.

$\theta^-, r^-, \theta^+, r^+, C', s' \leftarrow \text{BuildTree}(\theta, r, u, v, j - 1, \epsilon).$

if $v = -1$ **then**

$\theta^-, r^-, -, -, C'', s'' \leftarrow \text{BuildTree}(\theta^-, r^-, u, v, j - 1, \epsilon).$

else

$-, -, \theta^+, r^+, C'', s'' \leftarrow \text{BuildTree}(\theta^+, r^+, u, v, j - 1, \epsilon).$

end if

$s' \leftarrow s' s'' \mathbb{I}[(\theta^+ - \theta^-) \cdot r^- \geq 0] \mathbb{I}[(\theta^+ - \theta^-) \cdot r^+ \geq 0].$

$C' \leftarrow C' \cup C''.$

return $\theta^-, r^-, \theta^+, r^+, C', s'.$

end if

- Naive NUTS algorithm requires that we store 2^j position and momentum vectors.
- Naive NUTS cannot guarantee large jumps.

⇒ Introduce other transition kernel

New transition kernel

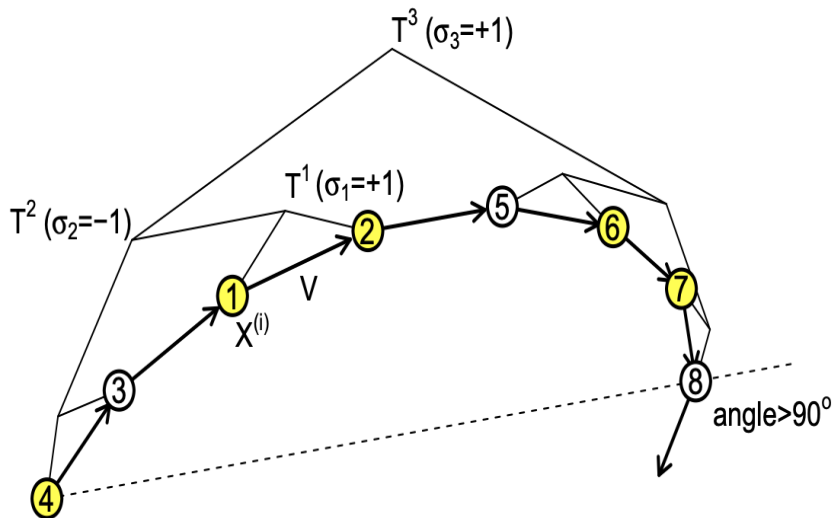
Consider the transition kernel

$$T(w'|w, \mathcal{C}) = \begin{cases} \frac{\mathbb{I}[w' \in \mathcal{C}^{\text{new}}]}{|\mathcal{C}^{\text{new}}|} & \text{if } |\mathcal{C}^{\text{new}}| > |\mathcal{C}^{\text{old}}|, \\ \frac{|\mathcal{C}^{\text{new}}|}{|\mathcal{C}^{\text{old}}|} \frac{\mathbb{I}[w' \in \mathcal{C}^{\text{new}}]}{|\mathcal{C}^{\text{new}}|} + \left(1 - \frac{|\mathcal{C}^{\text{new}}|}{|\mathcal{C}^{\text{old}}|}\right) \mathbb{I}[w' = w] & \text{if } |\mathcal{C}^{\text{new}}| \leq |\mathcal{C}^{\text{old}}| \end{cases}$$

- $\mathcal{C} = \mathcal{C}^{\text{old}} \cup \mathcal{C}^{\text{new}}, w \in \mathcal{C}^{\text{old}}$
- T propose a move from \mathcal{C}^{old} to a random state in \mathcal{C}^{new} and accept the move with probability $\frac{|\mathcal{C}^{\text{new}}|}{|\mathcal{C}^{\text{old}}|}$
- It satisfies detailed balance with respect to the uniform distribution on \mathcal{C} , that is,

$$p(w|\mathcal{C})T(w'|w, \mathcal{C}) = p(w'|\mathcal{C})T(w|w', \mathcal{C})$$

New transition kernel



Algorithm 3 Efficient No-U-Turn Sampler

Given θ^0 , ϵ , \mathcal{L} , M :

for $m = 1$ to M **do**

Resample $r^0 \sim \mathcal{N}(0, I)$.

Resample $u \sim \text{Uniform}([0, \exp\{\mathcal{L}(\theta^{m-1} - \frac{1}{2}r^0 \cdot r^0)\}])$

Initialize $\theta^- = \theta^{m-1}$, $\theta^+ = \theta^{m-1}$, $r^- = r^0$, $r^+ = r^0$, $j = 0$, $\theta^m = \theta^{m-1}$, $n = 1$, $s = 1$.

while $s = 1$ **do**

Choose a direction $v_j \sim \text{Uniform}(\{-1, 1\})$.

if $v_j = -1$ **then**

$\theta^-, r^-, -, -, \theta', n', s' \leftarrow \text{BuildTree}(\theta^-, r^-, u, v_j, j, \epsilon)$.

else

$-, -, \theta^+, r^+, \theta', n', s' \leftarrow \text{BuildTree}(\theta^+, r^+, u, v_j, j, \epsilon)$.

end if

if $s' = 1$ **then**

With probability $\min\{1, \frac{n'}{n}\}$, set $\theta^m \leftarrow \theta'$.

end if

$n \leftarrow n + n'$.

$s \leftarrow s' \mathbb{I}[(\theta^+ - \theta^-) \cdot r^- \geq 0] \mathbb{I}[(\theta^+ - \theta^-) \cdot r^+ \geq 0]$.

$j \leftarrow j + 1$.

end while

end for

Algorithm

```
function BuildTree( $\theta, r, u, v, j, \epsilon$ )
if  $j = 0$  then
    Base case—take one leapfrog step in the direction  $v$ .
     $\theta', r' \leftarrow \text{Leapfrog}(\theta, r, v\epsilon)$ .
     $n' \leftarrow \mathbb{I}[u \leq \exp\{\mathcal{L}(\theta') - \frac{1}{2}r' \cdot r'\}]$ .
     $s' \leftarrow \mathbb{I}[\mathcal{L}(\theta') - \frac{1}{2}r' \cdot r' > \log u - \Delta_{\max}]$ 
    return  $\theta', r', \theta', r', \theta', n', s'$ .
else
    Recursion—implicitly build the left and right subtrees.
     $\theta^-, r^-, \theta^+, r^+, \theta', n', s' \leftarrow \text{BuildTree}(\theta, r, u, v, j - 1, \epsilon)$ .
    if  $s' = 1$  then
        if  $v = -1$  then
             $\theta^-, r^-, -, -, \theta'', n'', s'' \leftarrow \text{BuildTree}(\theta^-, r^-, u, v, j - 1, \epsilon)$ .
        else
             $-, -, \theta^+, r^+, \theta'', n'', s'' \leftarrow \text{BuildTree}(\theta^+, r^+, u, v, j - 1, \epsilon)$ .
        end if
        With probability  $\frac{n''}{n' + n''}$ , set  $\theta' \leftarrow \theta''$ .
         $s' \leftarrow s'' \mathbb{I}[(\theta^+ - \theta^-) \cdot r^- \geq 0] \mathbb{I}[(\theta^+ - \theta^-) \cdot r^+ \geq 0]$ 
         $n' \leftarrow n' + n''$ 
    end if
    return  $\theta^-, r^-, \theta^+, r^+, \theta', n', s'$ .
end if
```


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- 5 Evaluation

- HMC : Optimal value of ϵ for a given simulation length ϵL is the one that produces an average Metropolis acceptance probability of approximately 0.65.

$$H_t^{HMC} = \min\left\{1, \frac{p(\theta^t, r^t)}{p(\theta^{t-1}, r^{t,0})}\right\}; \quad h^{HMC}(\epsilon) = \mathbb{E}[H_t^{HMC}|\epsilon]$$

- NUTS : Since there is no single accept/reject step, we must define an alternative statistic to Metropolis acceptance probability.

$$H_t^{NUTS} = \frac{1}{|\mathcal{B}_t^{final}|} \sum_{\theta, r \in \mathcal{B}_t^{final}} \min\left\{1, \frac{p(\theta, r)}{p(\theta^{t-1}, r^{t,0})}\right\};$$

$$h^{NUTS}(\epsilon) = \mathbb{E}[H_t^{NUTS}|\epsilon]$$

Dual Averaging

- Assuming that we want to find a setting of a parameter $x \in \mathbb{R}$ such that $h(x) = \mathbb{E}_t[H_t|x] = 0$, we can apply the updates

$$x_{t+1} \leftarrow \mu - \frac{\sqrt{t}}{\gamma} \frac{1}{t + t_0} \sum_{i=1}^t H_i; \quad \bar{x}_{t+1} \leftarrow \eta_t x_{t+1} + (1 - \eta_t) \bar{x}_t$$

- $\eta_t = t^{-\kappa}$, $\kappa \in (0.5, 1]$
- Assuming that h is nondecreasing as a function of x

$\implies \bar{x}_t$ is guaranteed to converge to a value such that $h(\bar{x}_t)$ converges to 0.

Algorithm(HMC with Dual Averaging)

Algorithm 5 Hamiltonian Monte Carlo with Dual Averaging

Given $\theta^0, \delta, \lambda, \mathcal{L}, M, M^{\text{adapt}}$.

Set $\epsilon_0 = \text{FindReasonableEpsilon}(\theta), \mu = \log(10\epsilon_0), \bar{\epsilon}_0 = 1, \bar{H}_0 = 0, \gamma = 0.05, t_0 = 10, \kappa = 0.75$.

for $m = 1$ to M **do**

 Resample $r^0 \sim \mathcal{N}(0, I)$.

 Set $\theta^m \leftarrow \theta^{m-1}, \tilde{\theta} \leftarrow \theta^{m-1}, \tilde{r} \leftarrow r^0, L_m = \max\{1, \text{Round}(\lambda/\epsilon_{m-1})\}$.

for $i = 1$ to L_m **do**

 Set $\tilde{\theta}, \tilde{r} \leftarrow \text{Leapfrog}(\tilde{\theta}, \tilde{r}, \epsilon_{m-1})$.

end for

 With probability $\alpha = \min\left\{1, \frac{\exp\{\mathcal{L}(\tilde{\theta}) - \frac{1}{2}\tilde{r} \cdot \tilde{r}\}}{\exp\{\mathcal{L}(\theta^{m-1}) - \frac{1}{2}r^0 \cdot r^0\}}\right\}$, set $\theta^m \leftarrow \tilde{\theta}, r^m \leftarrow -\tilde{r}$.

if $m \leq M^{\text{adapt}}$ **then**

 Set $\bar{H}_m = \left(1 - \frac{1}{m+t_0}\right) \bar{H}_{m-1} + \frac{1}{m+t_0}(\delta - \alpha)$.

 Set $\log \epsilon_m = \mu - \frac{\sqrt{m}}{\gamma} \bar{H}_m, \log \bar{\epsilon}_m = m^{-\kappa} \log \epsilon_m + (1 - m^{-\kappa}) \log \bar{\epsilon}_{m-1}$.

else

 Set $\epsilon_m = \bar{\epsilon}_{M^{\text{adapt}}}$.

end if

end for

Algorithm(NUTS with Dual Averaging)

Algorithm 6 No-U-Turn Sampler with Dual Averaging

Given θ^0 , δ , \mathcal{L} , M , M^{adapt} :

Set $\epsilon_0 = \text{FindReasonableEpsilon}(\theta)$, $\mu = \log(10\epsilon_0)$, $\bar{\epsilon}_0 = 1$, $\bar{H}_0 = 0$, $\gamma = 0.05$, $t_0 = 10$, $\kappa = 0.75$.

for $m = 1$ to M **do**

 Sample $r^0 \sim \mathcal{N}(0, I)$.

 Resample $u \sim \text{Uniform}([0, \exp\{\mathcal{L}(\theta^{m-1} - \frac{1}{2}r^0 \cdot r^0)\}])$

 Initialize $\theta^- = \theta^{m-1}$, $\theta^+ = \theta^{m-1}$, $r^- = r^0$, $r^+ = r^0$, $j = 0$, $\theta^m = \theta^{m-1}$, $n = 1$, $s = 1$.

while $s = 1$ **do**

 Choose a direction $v_j \sim \text{Uniform}(\{-1, 1\})$.

if $v_j = -1$ **then**

$\theta^-, r^-, -, -, \theta', n', s', \alpha, n_\alpha \leftarrow \text{BuildTree}(\theta^-, r^-, u, v_j, j, \epsilon_{m-1}\theta^{m-1}, r^0)$.

else

$-, -, \theta^+, r^+, \theta', n', s', \alpha, n_\alpha \leftarrow \text{BuildTree}(\theta^+, r^+, u, v_j, j, \epsilon_{m-1}\theta^{m-1}, r^0)$.

end if

if $s' = 1$ **then**

 With probability $\min\{1, \frac{n'}{n}\}$, set $\theta^m \leftarrow \theta'$.

end if

$n \leftarrow n + n'$.

$s \leftarrow s' \mathbb{I}[(\theta^+ - \theta^-) \cdot r^- \geq 0] \mathbb{I}[(\theta^+ - \theta^-) \cdot r^+ \geq 0]$.

$j \leftarrow j + 1$.

end while

if $m \leq M^{\text{adapt}}$ **then**

 Set $\bar{H}_m = \left(1 - \frac{1}{m+t_0}\right) \bar{H}_{m-1} + \frac{1}{m+t_0} (\delta - \frac{\alpha}{n_\alpha})$.

 Set $\log \epsilon_m = \mu - \frac{\sqrt{m}}{\gamma} \bar{H}_m$, $\log \bar{\epsilon}_m = m^{-\kappa} \log \epsilon_m + (1 - m^{-\kappa}) \log \bar{\epsilon}_{m-1}$.

else

 Set $\epsilon_m = \bar{\epsilon}_{M^{\text{adapt}}}$.

end if

end for

Algorithm(NUTS with Dual Averaging)

```
function BuildTree( $\theta, r, u, v, j, \epsilon, \theta^0, r^0$ )  
if  $j = 0$  then  
    Base case—take one leapfrog step in the direction  $v$ .  
     $\theta', r' \leftarrow \text{Leapfrog}(\theta, r, v\epsilon)$ .  
     $n' \leftarrow \mathbb{I}[u \leq \exp\{\mathcal{L}(\theta') - \frac{1}{2}r' \cdot r'\}]$ .  
     $s' \leftarrow \mathbb{I}[u < \exp\{\Delta_{\max} + \mathcal{L}(\theta') - \frac{1}{2}r' \cdot r'\}]$ .  
    return  $\theta', r', \theta', r', \theta', n', s', \min\{1, \exp\{\mathcal{L}(\theta') - \frac{1}{2}r' \cdot r' - \mathcal{L}(\theta^0) + \frac{1}{2}r^0 \cdot r^0\}\}, 1$ .  
else  
    Recursion—implicitly build the left and right subtrees.  
     $\theta^-, r^-, \theta^+, r^+, \theta', n', s', \alpha', n'_\alpha \leftarrow \text{BuildTree}(\theta, r, u, v, j-1, \epsilon, \theta^0, r^0)$ .  
    if  $s' = 1$  then  
        if  $v = -1$  then  
             $\theta^-, r^-, -, -, \theta'', n'', s'', \alpha'', n''_\alpha \leftarrow \text{BuildTree}(\theta^-, r^-, u, v, j-1, \epsilon, \theta^0, r^0)$ .  
        else  
             $-, -, \theta^+, r^+, \theta'', n'', s'', \alpha'', n''_\alpha \leftarrow \text{BuildTree}(\theta^+, r^+, u, v, j-1, \epsilon, \theta^0, r^0)$ .  
        end if  
        With probability  $\frac{n''}{n' + n''}$ , set  $\theta' \leftarrow \theta''$ .  
        Set  $\alpha' \leftarrow \alpha' + \alpha''$ ,  $n'_\alpha \leftarrow n'_\alpha + n''_\alpha$ .  
         $s' \leftarrow s'' \mathbb{I}[(\theta^+ - \theta^-) \cdot r^- \geq 0] \mathbb{I}[(\theta^+ - \theta^-) \cdot r^+ \geq 0]$   
         $n' \leftarrow n' + n''$   
    end if  
    return  $\theta^-, r^-, \theta^+, r^+, \theta', n', s', \alpha', n'_\alpha$ .  
end if
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CONTENTS

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- 2 Time-Reversibility
- 3 No-U-Turn Sampler
- 4 Tuning ϵ
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- 250-dim MVN

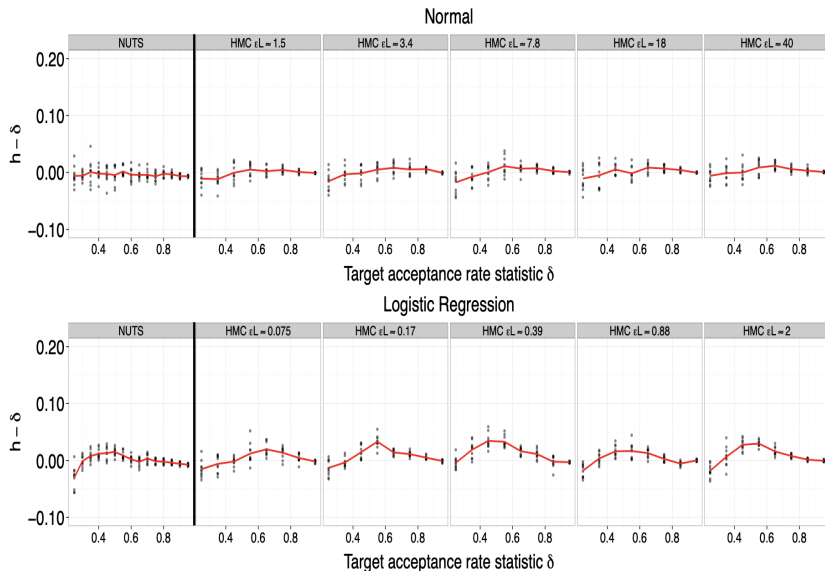
$$p(\theta) \propto \exp\left\{-\frac{1}{2}\theta^T A\theta\right\}$$

- Bayesian logistic regression
 - α : intercept term
 - β : vector of 24 regression coefficients

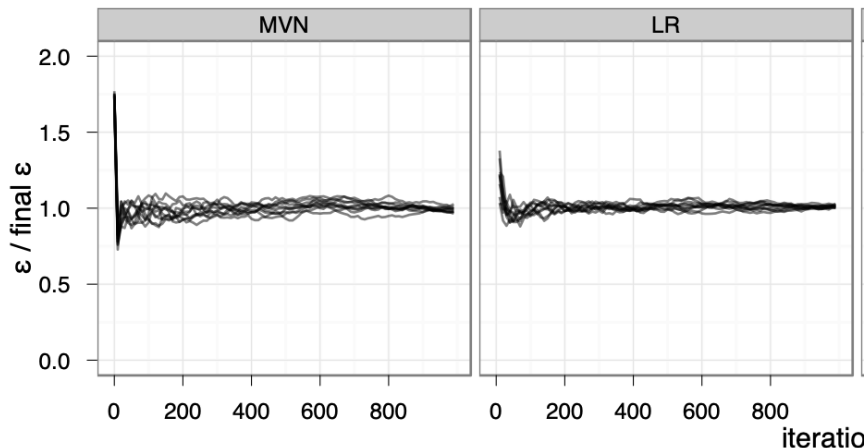
$$p(\alpha, \beta | x, y) \propto p(y | x, \alpha, \beta) p(\alpha) p(\beta)$$

$$\propto \exp\left\{-\sum_i \log(1 + \exp\{-y_i(\alpha + x_i \cdot \beta)\}) - \frac{\alpha^2}{2\sigma^2} - \frac{\beta \cdot \beta}{2\sigma^2}\right\}$$

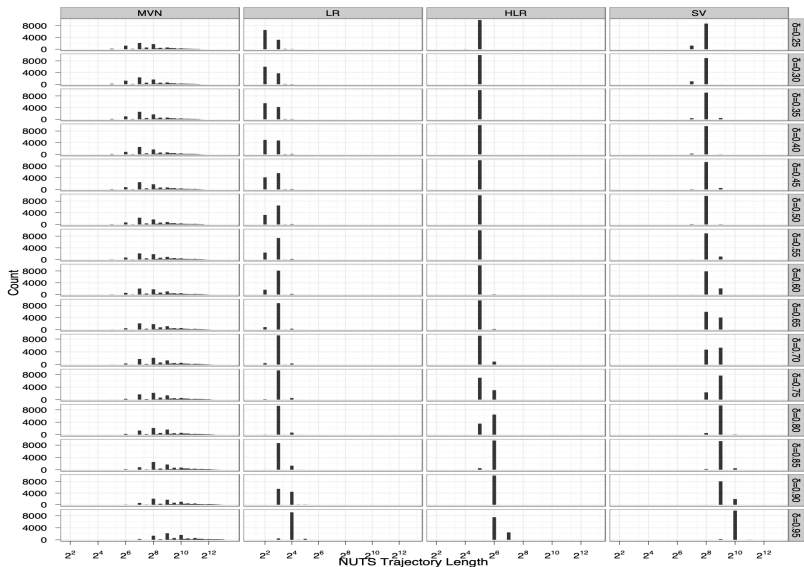
Convergence of Dual Averaging



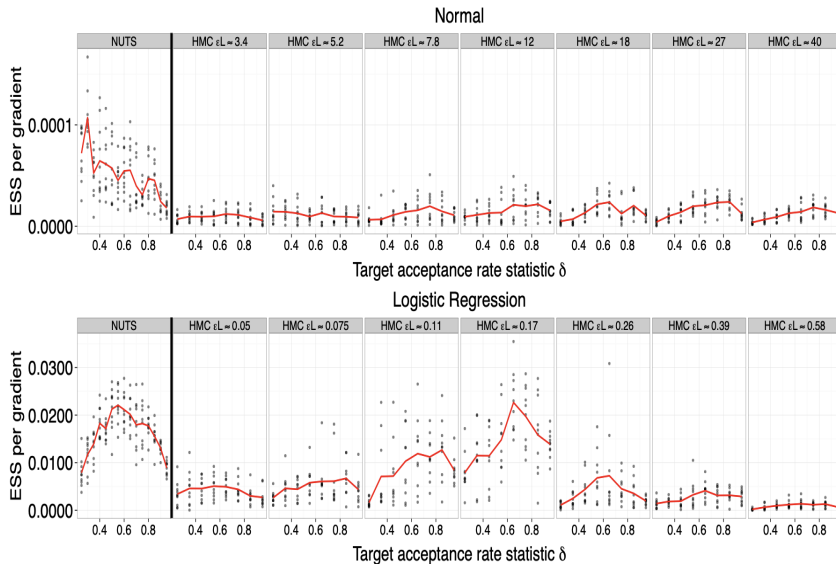
Convergence of Dual Averaging



NUTS Trajectory Lengths

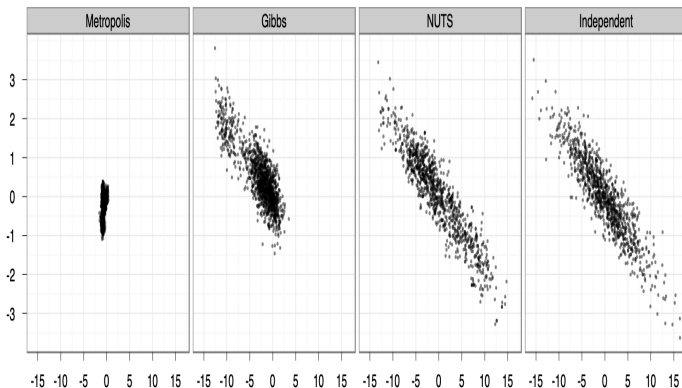


Efficiency of HMC and NUTS



Qualitative Comparison of NUTS,HMC and Gibbs

- Sampling on the 250-dim MVN.(projected onto the first two dimensions)
- 1,000,000 iteration (Gradient)





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