# On the speed of convergence of Markov chain Monte Carlo methods

# Outline

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- Myth busting
- More negative results
- Some hope
- Or proving that there's no hope...

# Markov chain Monte Carlo

"Almost all Markov chains can be modified to converge to a prescribed distribution"

Primer Markov chain with transition probabilities T(Y|X), aperiodic, irreducible and for all X and Y,

$$T(Y|X) \neq 0 \implies T(X|Y) \neq 0$$

Metropolis-Hastings algorithm:

Step 1. (proposal) Propose a $Y \sim T(\cdot|X_n)$

Step 2. (acceptance) Accept Y with probability

$$\min\left\{1, \frac{\pi(Y)T(X_n|Y)}{\pi(X)T(Y|X_n)}\right\}$$

# Mixing of Markov chains

"Mixing correlates with the second largest eigenvalue"

SLEM: Second largest eigenvalue modulus

$$\rho = \min\{\lambda_2, |\lambda_r|\}$$

Relaxation time

$$\tau_{rel} := \frac{1}{1-\lambda_2}$$

$$\tau_i(\varepsilon) := \min\left\{k_0 : \forall k > k_0, d_v(P^k\delta_i, \pi) \leq \varepsilon\right\}$$

Theorems (Aldous, 1982; Diaconis & Stroock,1991)

$$\tau_i(\varepsilon) \leq \frac{1}{1-\rho}\left(\ln\left(\frac{1}{\pi(i)}\right) + \ln\left(\frac{1}{\varepsilon}\right)\right)$$

$$\max_{i\in I} \tau_i(\varepsilon) \geq \frac{\rho}{2(1-\rho)} \ln(1/\varepsilon)$$

# Cheeger inequalities

“A Markov chain mixes slowly if and only if there is a bottleneck in it”

Ergodic flow:

$$F(S) := \sum_{i \in S, j \in i \setminus S} \pi(i) p_{ij}$$

Conductance:

$$\Phi := \min_{S \in I} \left\{ \frac{\sum_{i \in S, j \in i \setminus S} \pi(i) p_{ij}}{\pi(S)} \middle| 0 < \pi(S) \leq \frac{1}{2} \right\}$$

Cheeger inequality:

$$1 - 2\Phi \leq \lambda_2 \leq 1 - \frac{\Phi^2}{2}$$

# MCMC convergence

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$D_1$ $D_2$ $D_3$ $D_4$ $D_5$ $D_6$ $D_7$ ... $D_n$

# MCMC convergence

$$\begin{tikzcd}
D_1 \arrow[d] & D_2 \arrow[d] & D_3 \arrow[d] & D_4 \arrow[d] & D_5 \arrow[d] & D_6 \arrow[d] & D_7 \arrow[d] & \dots \arrow[d] & D_n \arrow[d] \\
M_1 & M_2 & M_3 & M_4 & M_5 & M_6 & M_7 & \dots & M_n
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## Fast convergence

$\exists\, k\ \forall\, D_n\ (|D_n| \leq n)$ the series of $1/(n^k(1-\lambda_{n,2}))$ built from the $\lambda_{n,2}$'s of the Markov chains $M_n$ defined by the algorithms converges to 0.

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## Slow convergence

$\exists D_n$ $(|D_n| \leq n)$ s.t. $\forall k$ the series of $1/(n^k(1-\lambda_{n,2}))$ built from the $\lambda_{n,2}$'s of the Markov chains $M_n$ defined by the algorithms does not converge to 0.

# Fast converging Markov chains

FPRAS:

(Fully Polynomial Randomized Approximation Scheme)

$$\text{given } x \in \Sigma^*, \varepsilon > 0, 0 < \delta < 1:$$
$$\Pr((1-\varepsilon) f(x) \le OUT \le (1+\varepsilon) f(x)) \ge 1-\delta$$

Algorithm polynomial in $|x|$, $1/\epsilon$ and $-\log(\delta)$

#P: Hard counting problem

# Fast converging Markov chains

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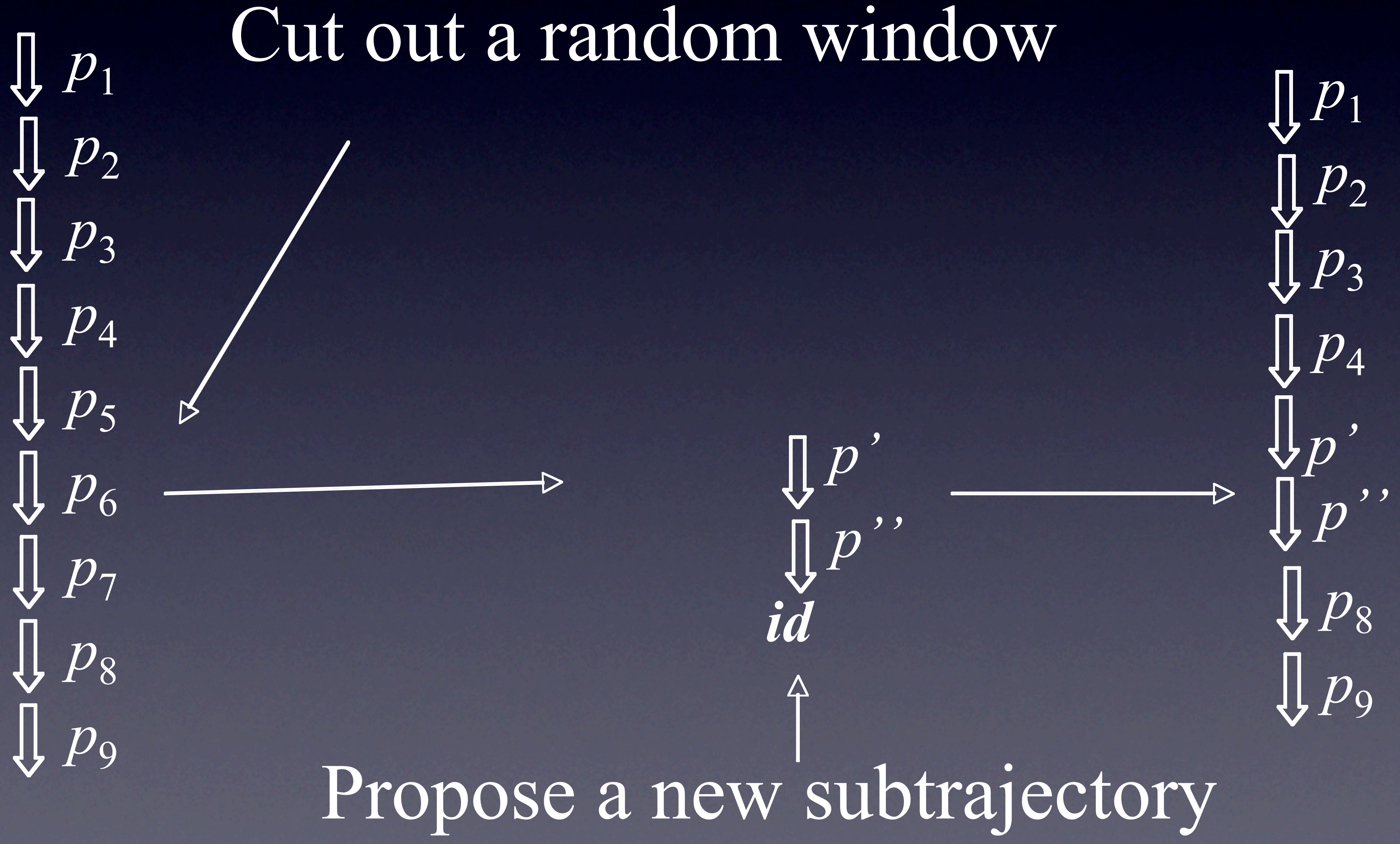
Algorithm polynomial in |x|, 1/ϵ and -log(δ)

#P: Hard counting problem

It is known that the intersection of #P and FPRAS is not empty. For example linear extension of partially ordered sets.

# ParIS: Partial Importance Sampling



Cut out a random window

$\Downarrow p_1$
$\Downarrow p_2$
$\Downarrow p_3$
$\Downarrow p_4$
$\Downarrow p_5$
$\Downarrow p_6$
$\Downarrow p_7$
$\Downarrow p_8$
$\Downarrow p_9$

$\Downarrow p'$
$\Downarrow p''$
$\boldsymbol{id}$

$\Downarrow p_1$
$\Downarrow p_2$
$\Downarrow p_3$
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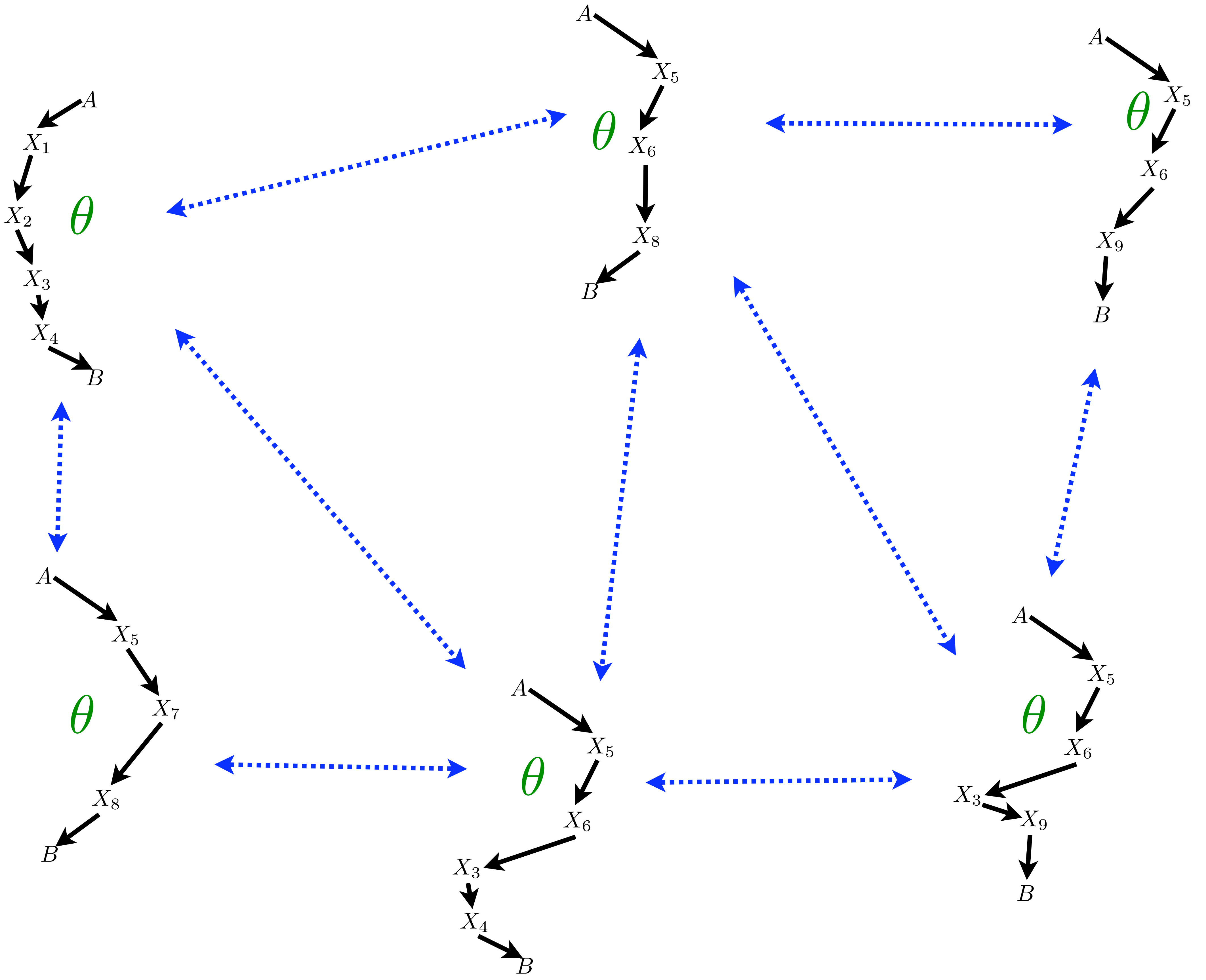
$\Downarrow p''$
$\Downarrow p_8$
$\Downarrow p_9$

Propose a new subtrajectory

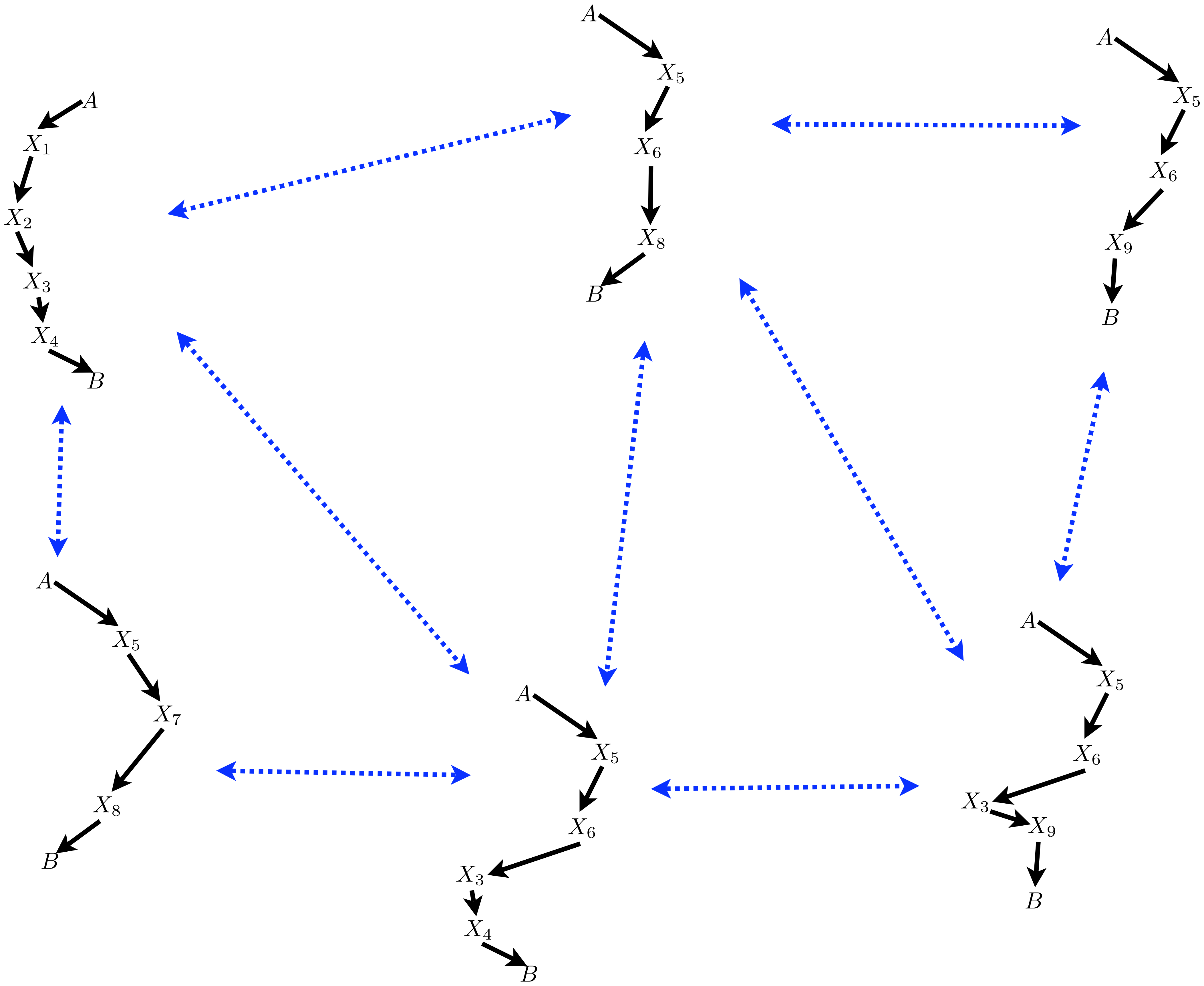
# Random walk on random walks



# Examples for RWoRWs

- Genome rearrangement paths
- Ancestral states in the infinite site recombination model
- Sequence alignment
- etc.

# Big islands


$A$
$X_1$
$X_2$
$X_3$
$X_4$
$B$
$A$
$X_5$
$X_6$
$X_8$
$B$
$A$
$X_5$
$X_6$
$X_9$
$B$
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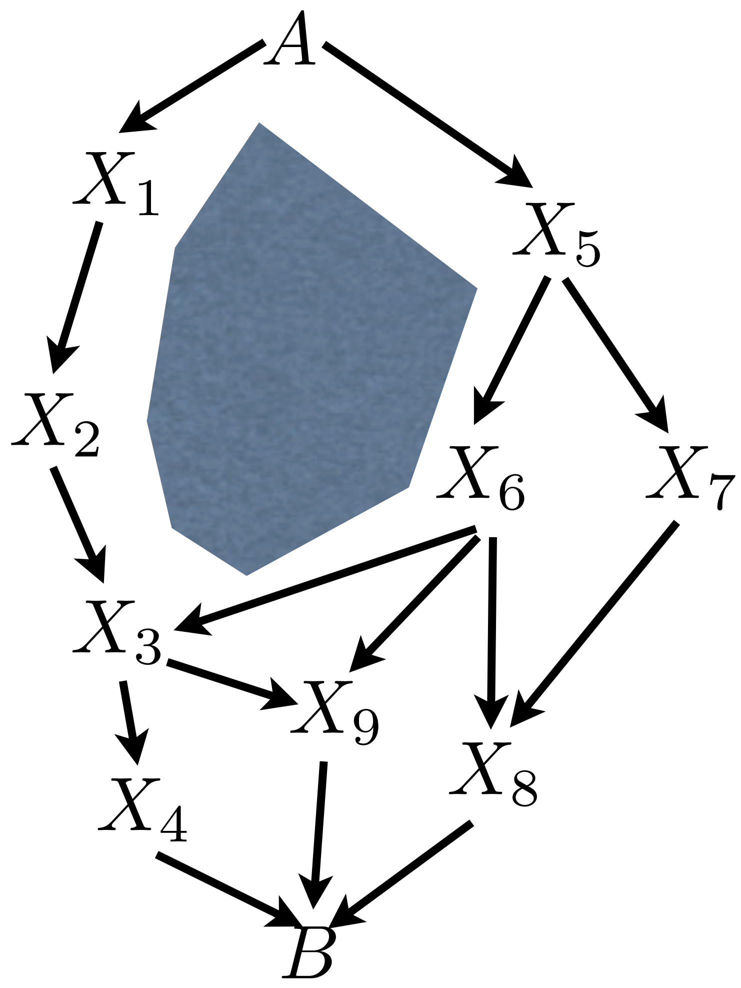
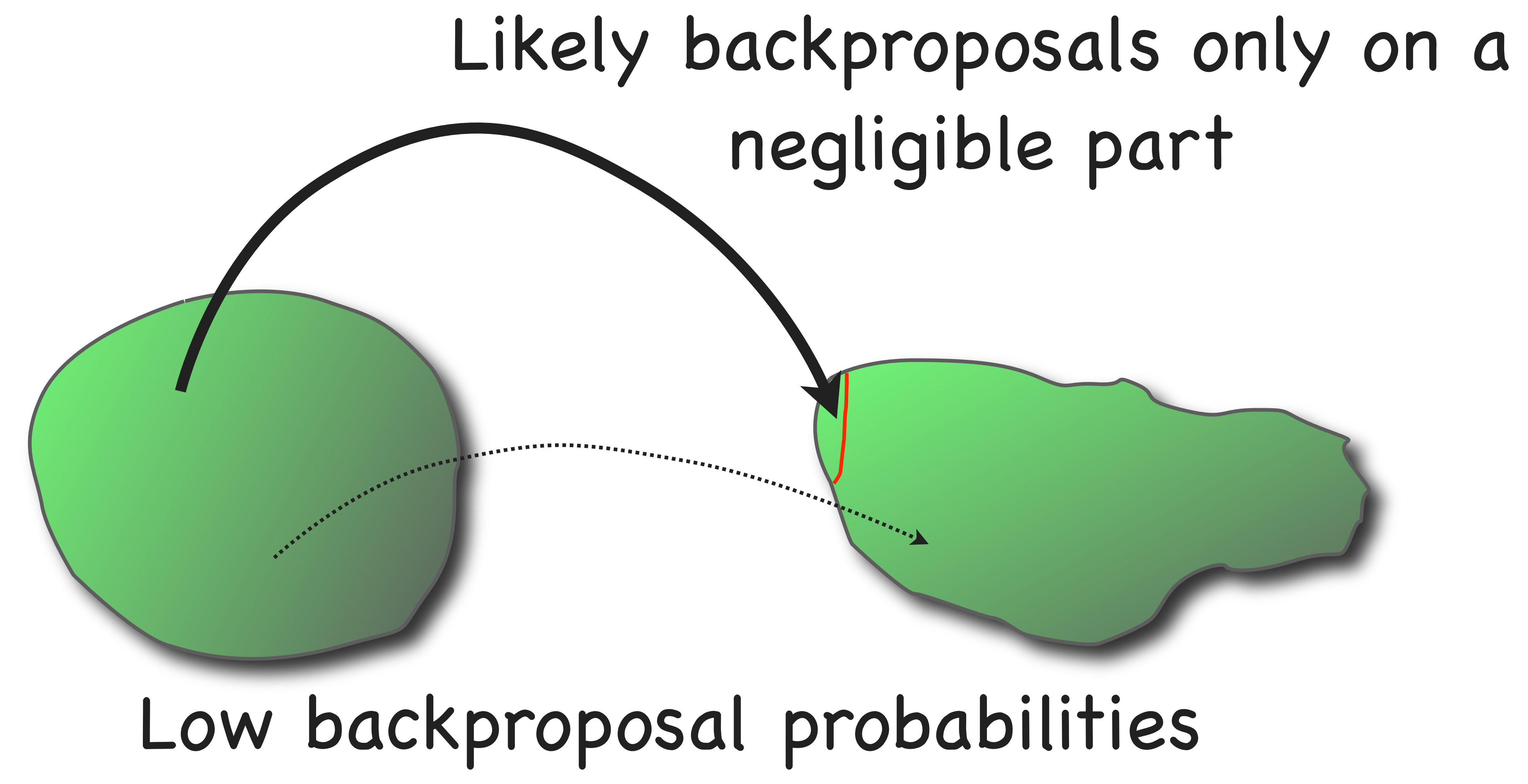


# ParIS mixes slowly on minimal reversal sorting paths

Miklós, Mélykúti, Swenson, manuscript submitted



Likely backproposals only on a negligible part

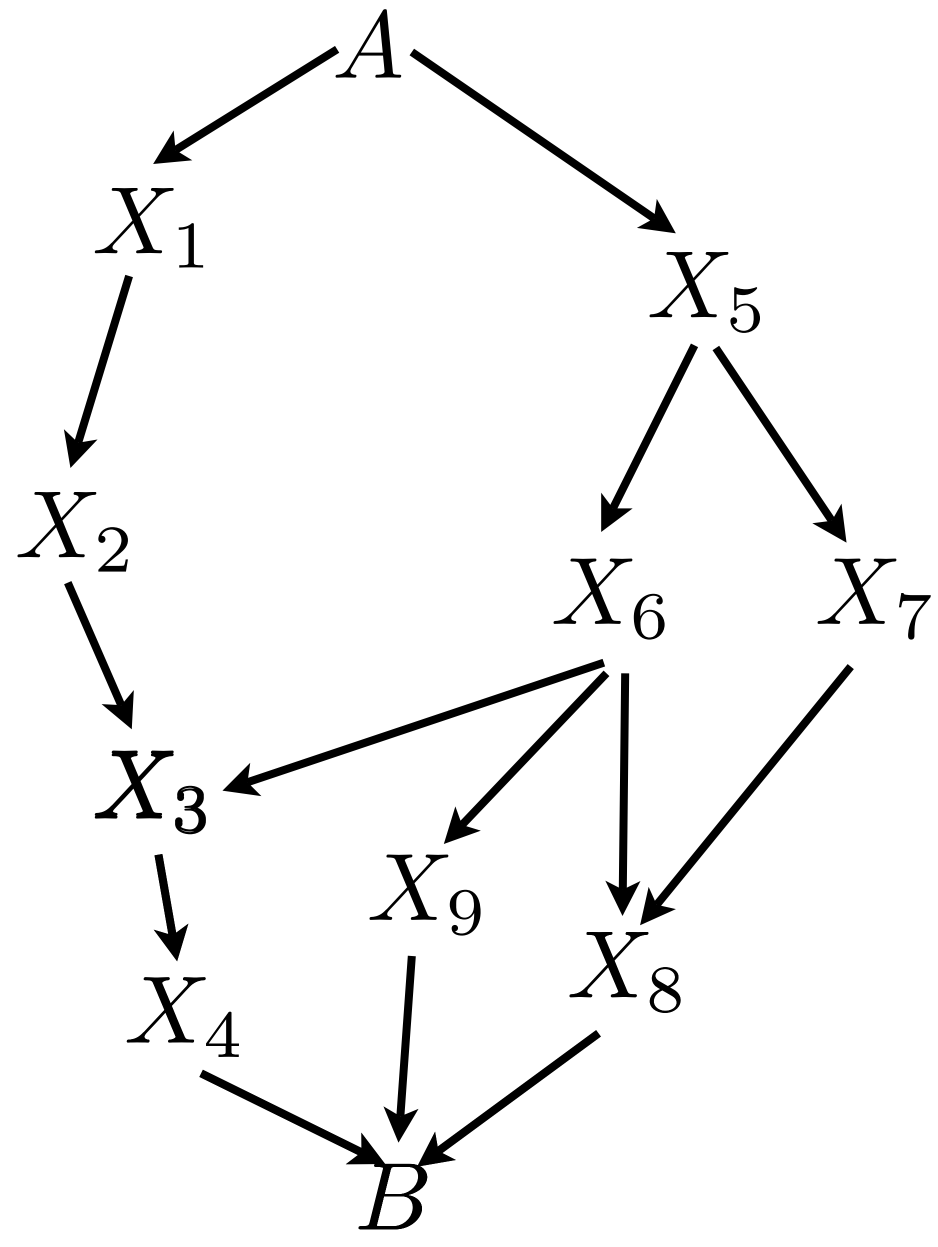
Low backproposal probabilities


Pascal = N
Crack
MOMENT OF IMPACT
NOT TO SCALE
LAWYER FRAME FOR CORRECT MASS DIST.
56" SHOULDER
SANDBAG ON EVERY RUNG
YTH STERS

# Myth I.

# It is worth jumping big

# Random walks as decision trees



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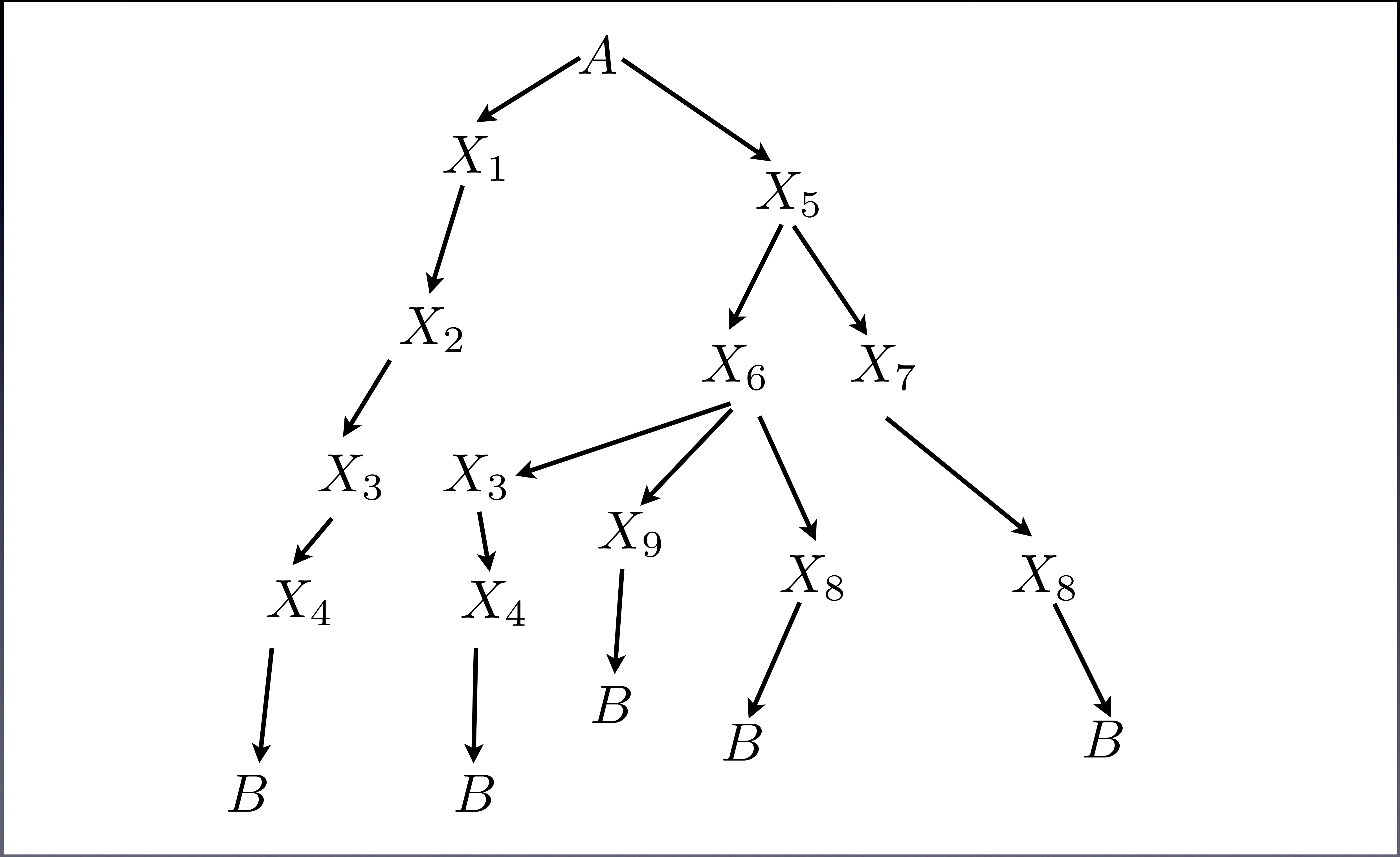

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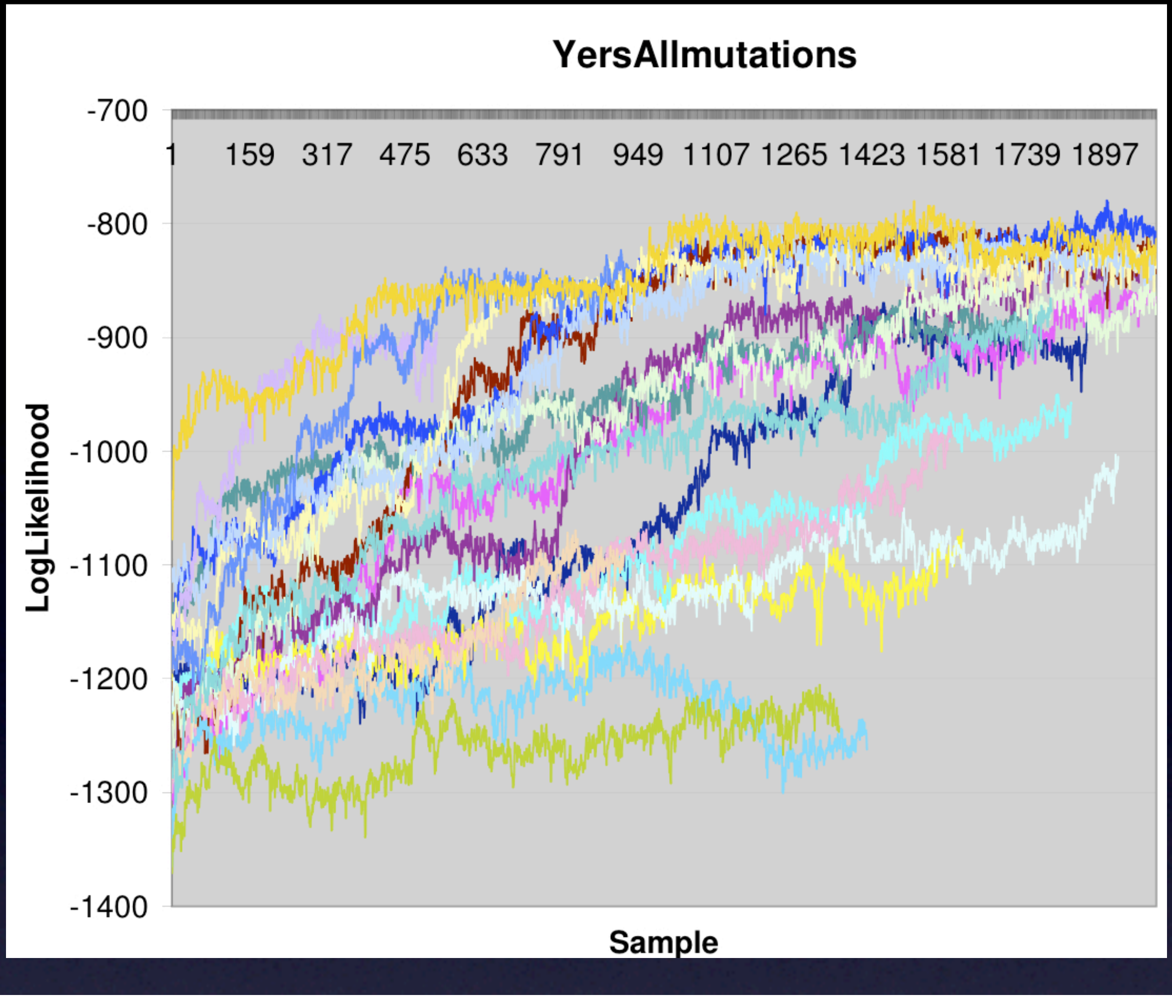
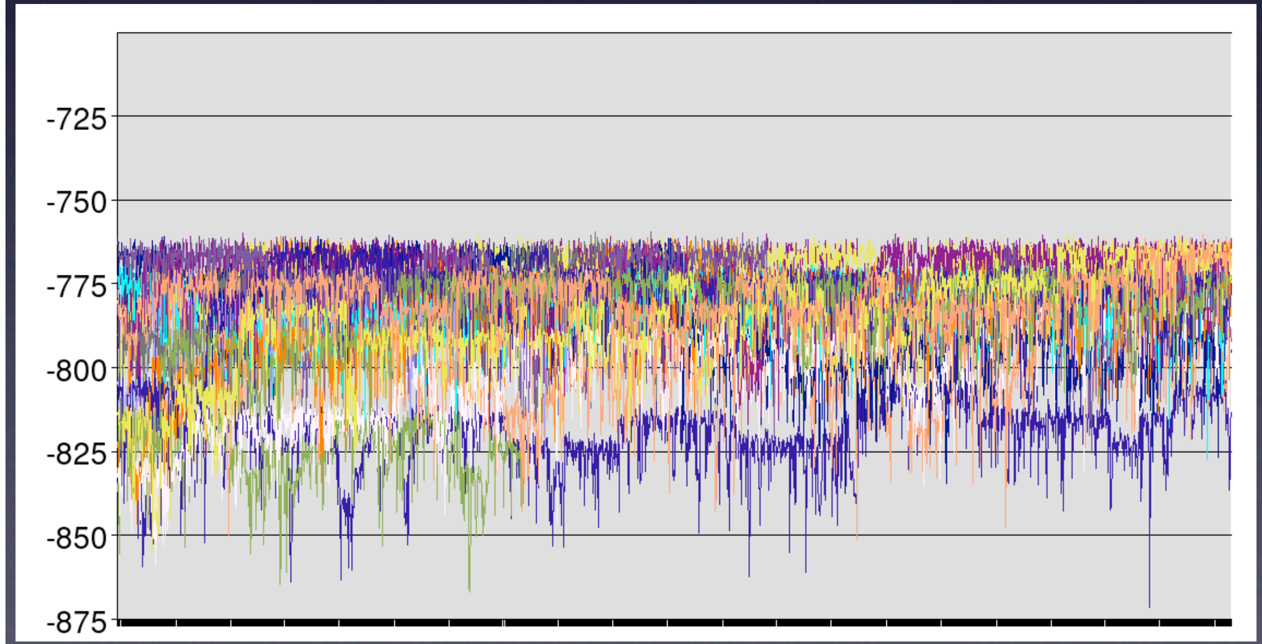
We cannot jump big in discrete, high dimensional distributions.

# Myth II.

# Small acceptance rate is caused by bad proposals





Pre-burnin without proposal ratio!

# Myth II.
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The ‘curse of small backproposal probabilities’.

# ParIS: indeed speeded up computation?

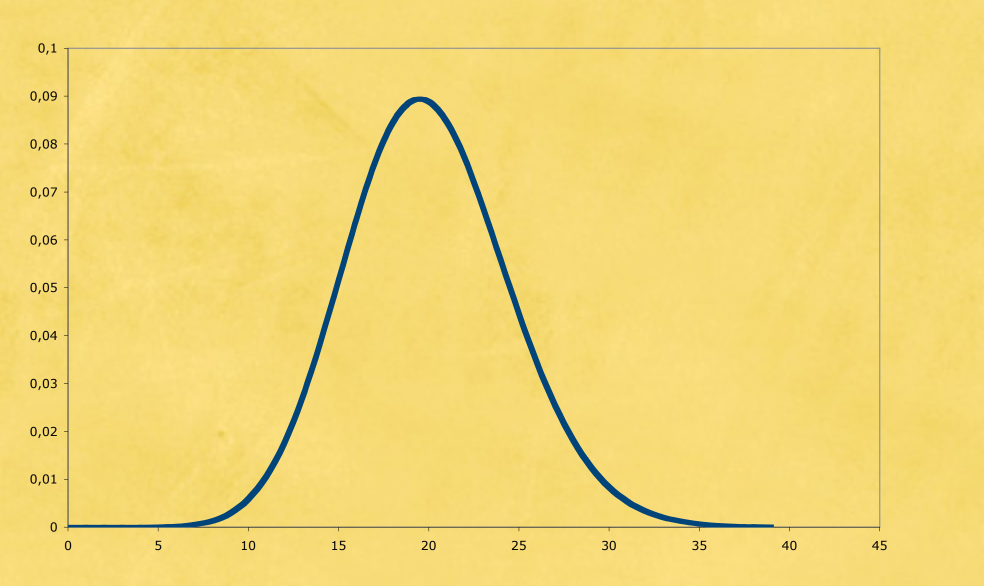
It is enough to calculate proposal probabilities for a 'window' (Green, 1995; Lunter, Miklos, etc, 2005)

$$\pi(X)T(Y \mid X) =$$

$$\pi(X)\sum_i P(Y, w_i \mid X)\min\left(1, \frac{\pi(Y)P(X, w_i \mid Y)}{\pi(X)P(Y, w_i \mid X)}\right) =$$

$$\sum_i \min\big(\pi(X)P(Y, w_i \mid X), \pi(Y)P(X, w_i \mid Y)\big)$$

# But does it help?



Proposing alignment window lengths from Poisson distribution

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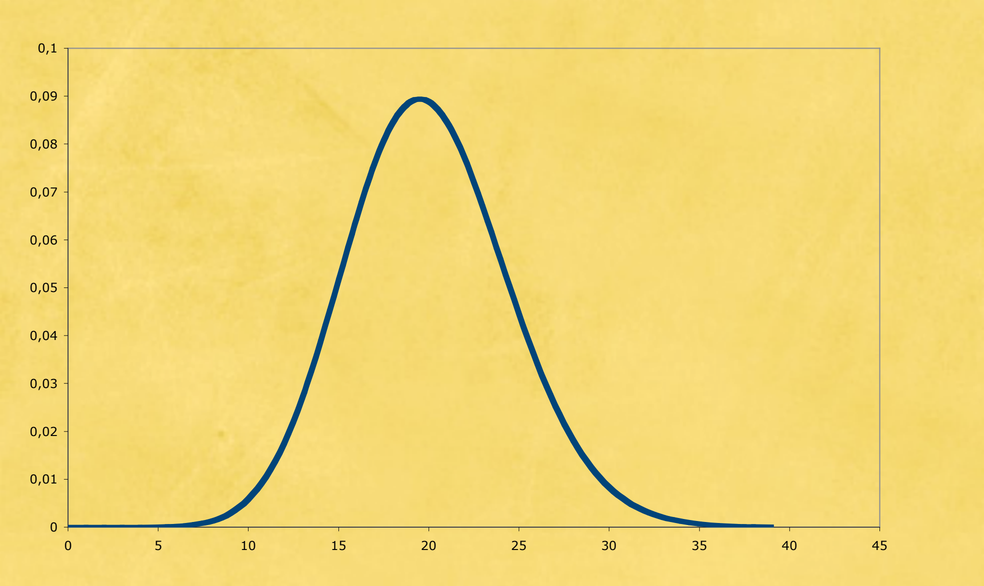

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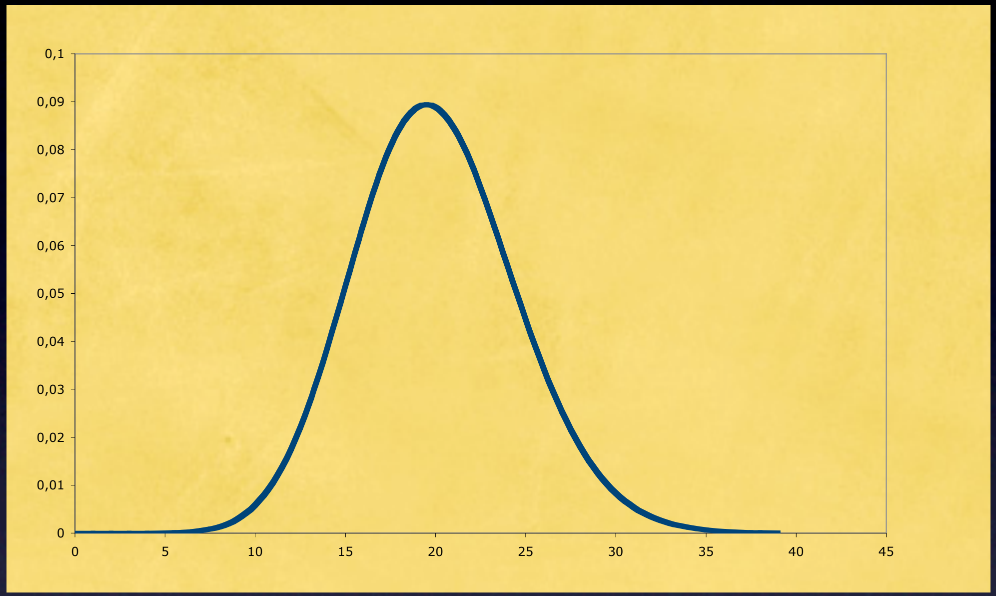

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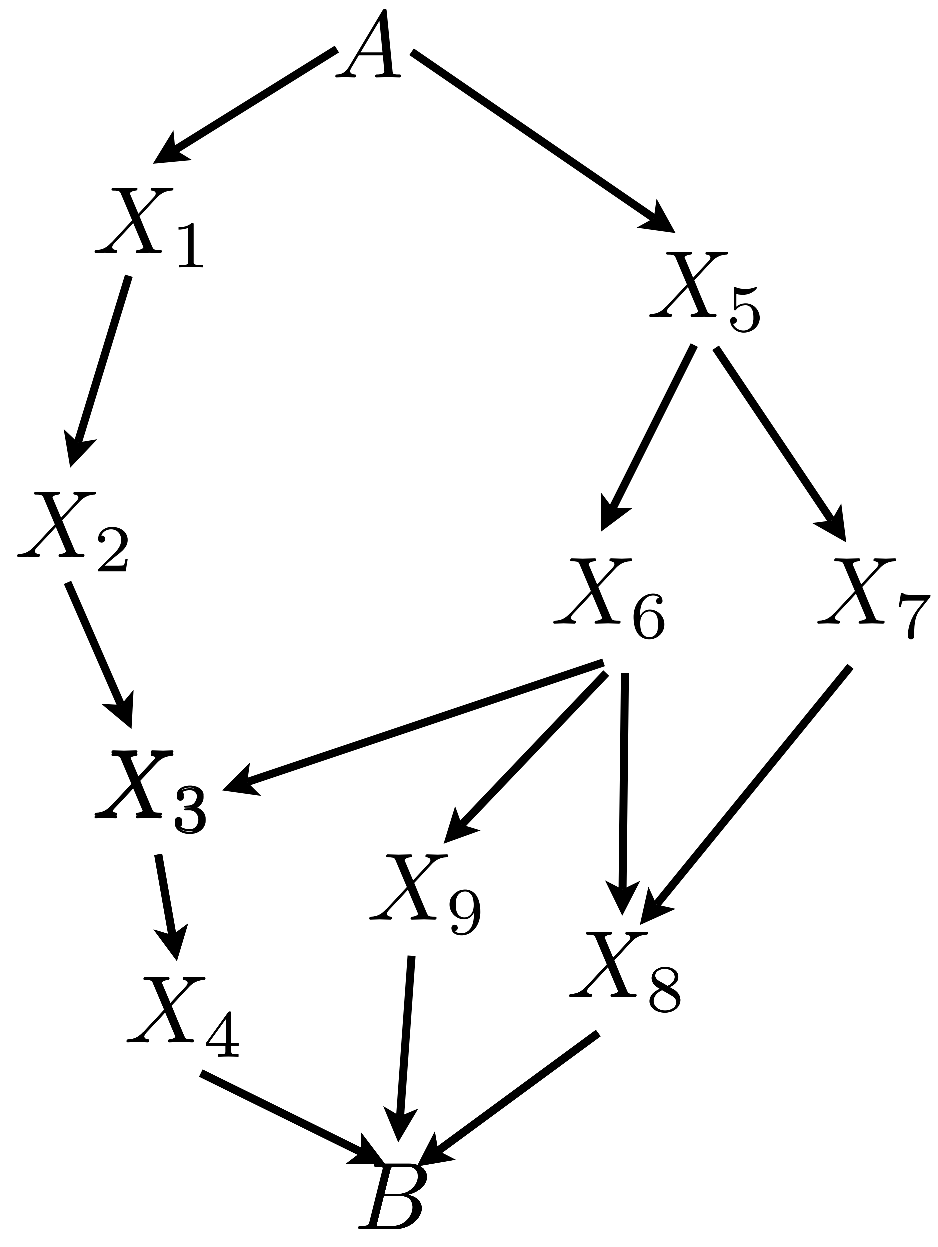
A mixture distribution helps

# Random walks as decision trees



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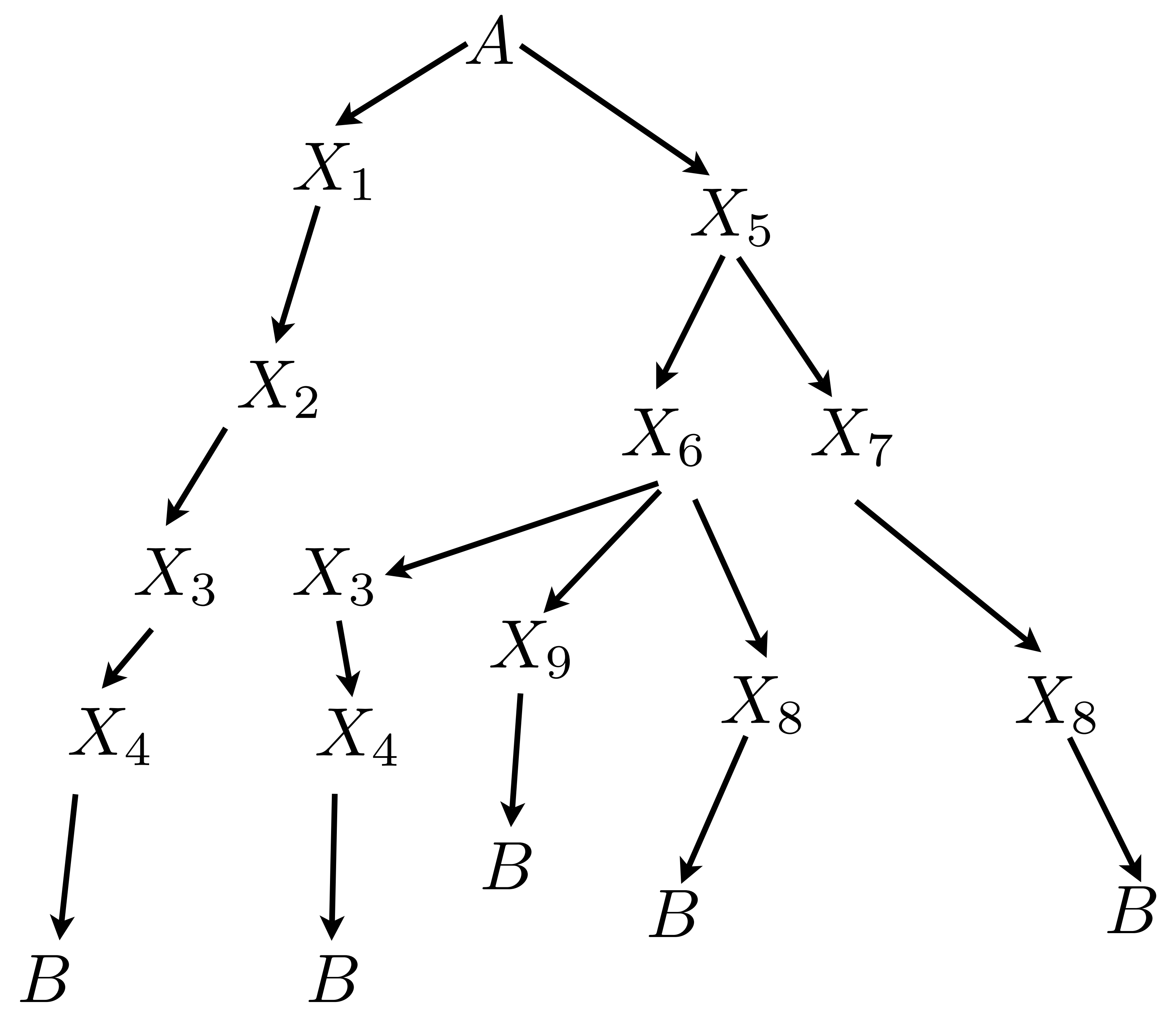
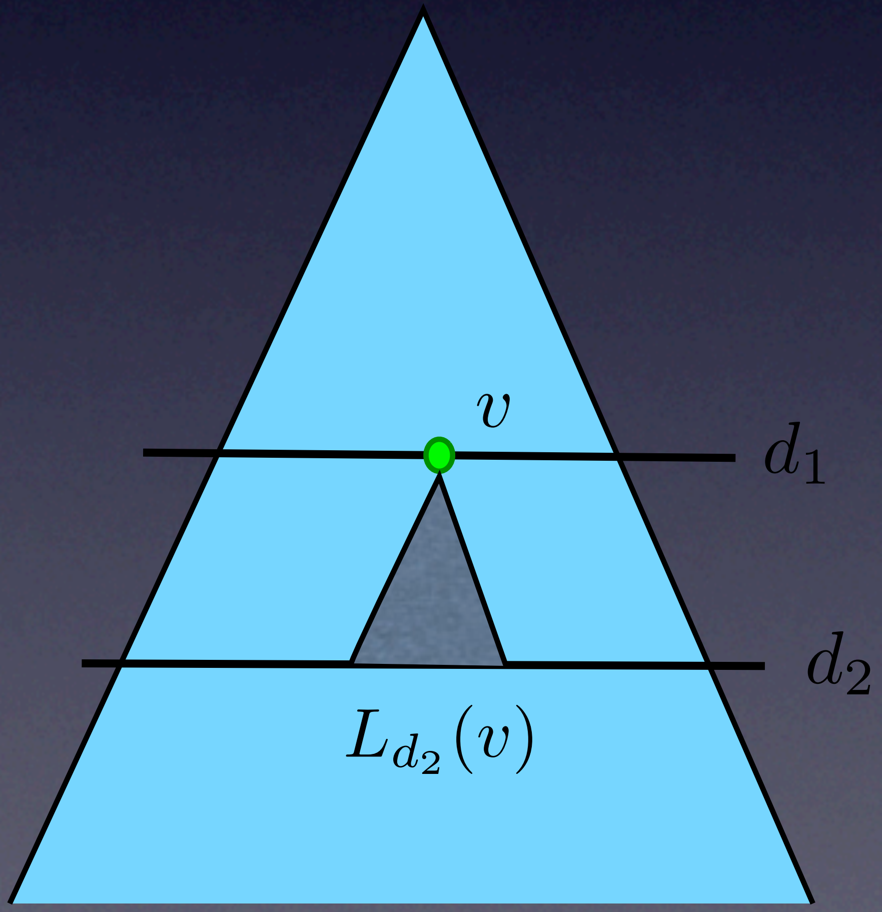


# Hiddenness of decision trees

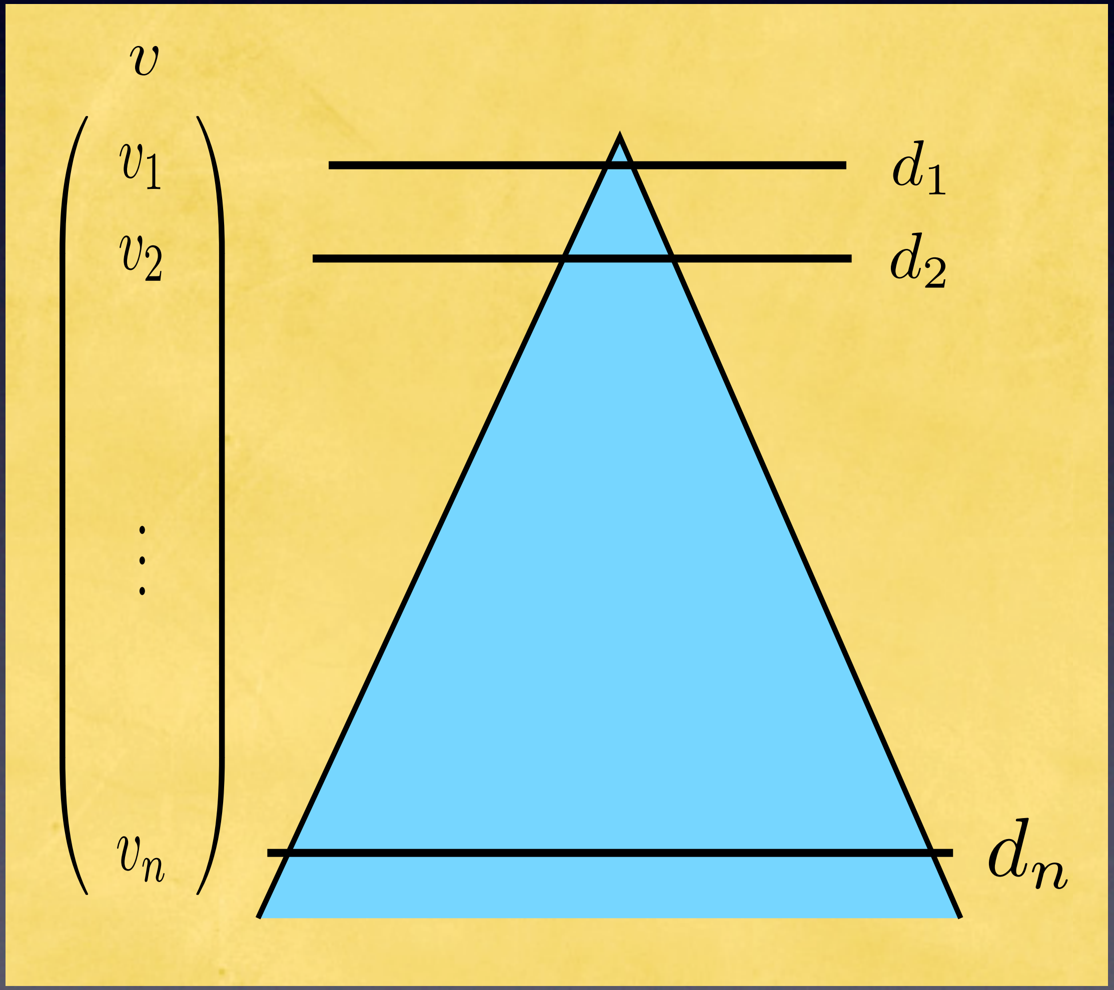


$$|L_{d_2}(v)| \leq k \times \frac{|d_2|}{|d_1|}$$

# MCMCMCMC

Model Changing Metropolis Coupled

Markov Chain Monte Carlo



PT-like MSIS

- No need to know the normalizing constant
- Parallelization is possible
- Too many chains?

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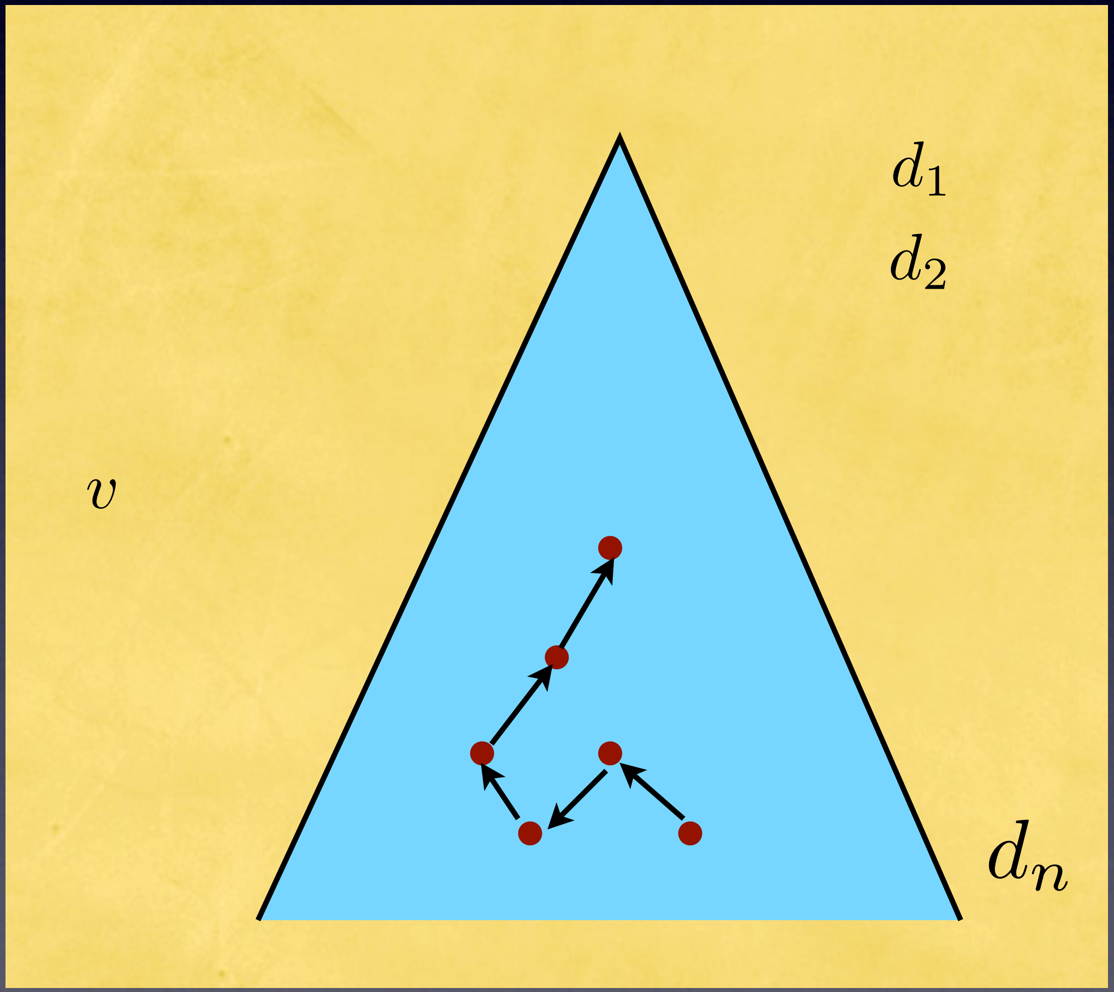

ST-like MSIS

- Unknown normalizing constant!
- Parallelization is not possible
- Single chain

# Convergence property of MCMCMCMC

For ST-like MSIS

$$\Omega(k) = \tau_{rel} = O(an^2k)$$

For PT-like MSIS

$$\Omega(k) = \tau_{rel} = O(an^{6+\log_2(k)})$$

Where k is the hiddenness rate, ‘a’ is the smallest transition probability, and n is the depth of the tree

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Hiddenness rate might grow exponentially with the length of the signed permutations!

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Fortunately, we can add more transition kernels, like swapping commuting mutations.

Mixing speed is unknown at the moment...

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When will an FPRAS be a BPP?

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If the decision problem is NP-complete, then it is unlikely that an FPRAS algorithm exists, unless BPP $\neq$ P or P=NP

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$$d_V(\delta_i^T P^n, \pi^T) \leq c(P, \pi)\rho^n$$

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$$d_V(\delta_i^T P^n, \pi^T) \leq c(P, \pi)\rho^n$$

$$c(P, \pi) = \min\left\{ \frac{1}{\rho}\left(\frac{p_{ii}}{\pi_i}\right)^{\frac{1}{2}}, \frac{1}{2}\left(\frac{1-\pi_i}{\pi_i}\right)^{\frac{1}{2}} \right\}$$

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How is this complexity class related to FPRAS?

# Conclusions

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I hope I spread non-knowledge significantly today!

# Thank you!