

Markov Chain Monte Carlo and mixing rates

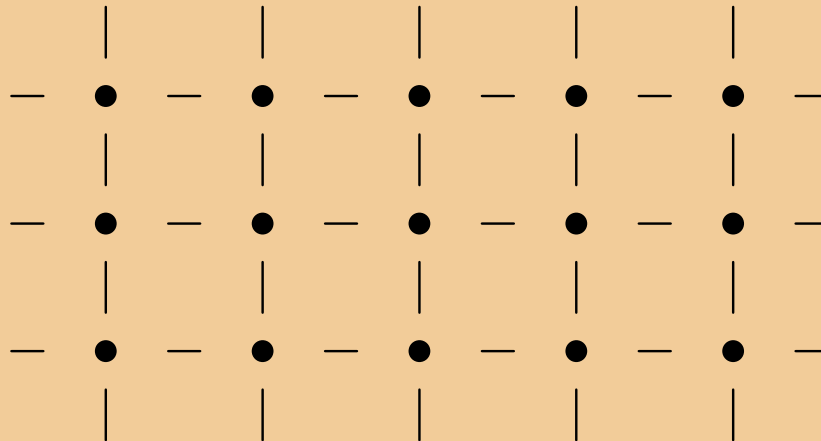
Yevgeniy Kovchegov

Department of Mathematics

Oregon State University

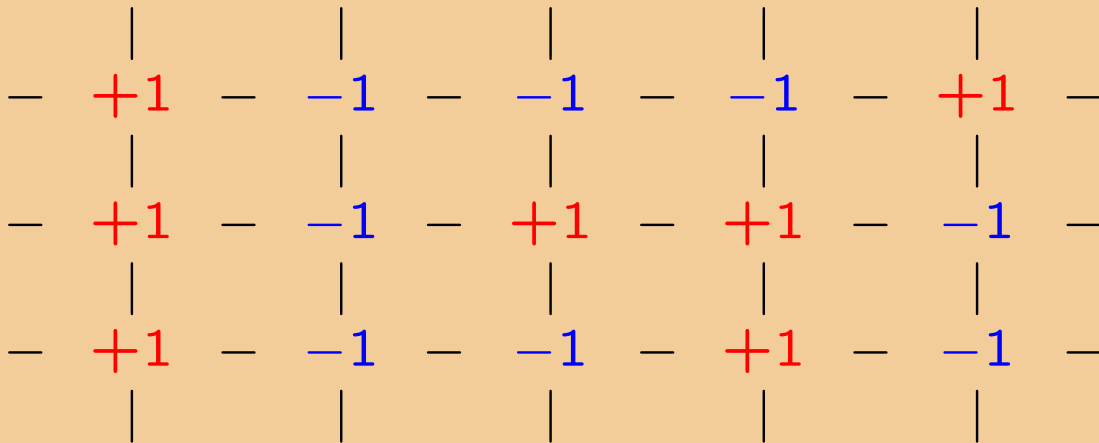
Ising Model. Every vertex v of $G = (V, E)$ is assigned a spin $\sigma(v) \in \{-1, +1\}$. The probability of a configuration $\sigma \in \{-1, +1\}^V$ is

$$\pi(\sigma) = \frac{e^{-\beta\mathcal{H}(\sigma)}}{Z(\beta)}, \quad \text{where } \beta = \frac{1}{T}$$



Ising Model. Every vertex v of $G = (V, E)$ is assigned a spin $\sigma(v) \in \{-1, +1\}$. The probability of a configuration $\sigma \in \{-1, +1\}^V$ is

$$\pi(\sigma) = \frac{e^{-\beta\mathcal{H}(\sigma)}}{Z(\beta)}, \quad \text{where } \beta = \frac{1}{T}$$



Ising Model. $\forall \sigma \in \{-1, +1\}^V$, the Hamiltonian

$$\mathcal{H}(\sigma) = -\frac{1}{2} \sum_{u,v: u \sim v} \sigma(u)\sigma(v) = - \sum_{\text{edges } e=[u,v]} \sigma(u)\sigma(v)$$

and probability of a configuration $\sigma \in \{-1, +1\}^V$ is

$$\pi(\sigma) = \frac{e^{-\beta \mathcal{H}(\sigma)}}{Z(\beta)}, \quad \text{where } \beta = \frac{1}{T}$$

$Z(\beta) = \sum_{\sigma \in \{-1, +1\}^V} e^{-\beta \mathcal{H}(\sigma)}$ - normalizing factor.

Ising Model: local Hamiltonian

$$\mathcal{H}(\sigma) = -\frac{1}{2} \sum_{u,v: u \sim v} \sigma(u)\sigma(v) = - \sum_{\text{edges } e=[u,v]} \sigma(u)\sigma(v)$$

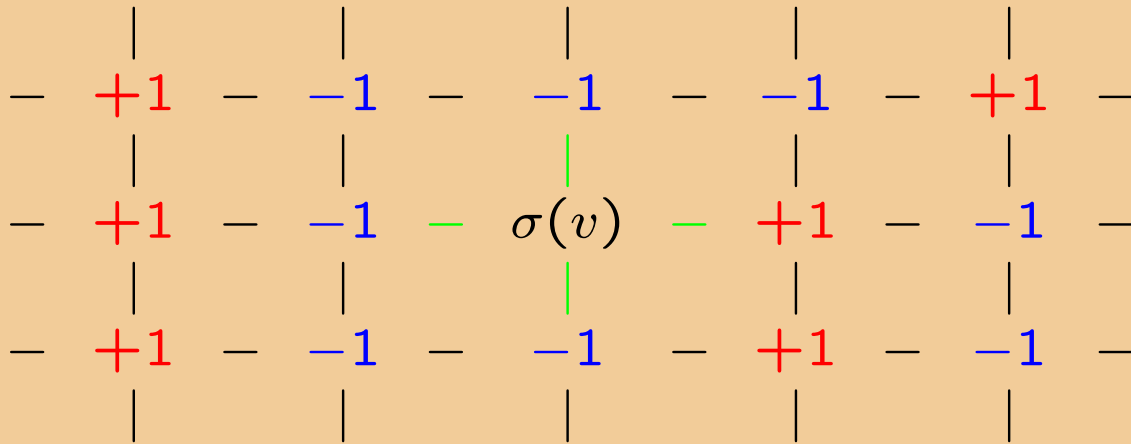
The local Hamiltonian

$$\mathcal{H}_{\text{local}}(\sigma, v) = - \sum_{u: u \sim v} \sigma(u)\sigma(v) .$$

Observe: conditional probability for $\sigma(v)$ is given by $\mathcal{H}_{\text{local}}(\sigma, v)$:

$$\mathcal{H}(\sigma) = \mathcal{H}_{\text{local}}(\sigma, v) - \sum_{e=[u_1, u_2]: u_1, u_2 \neq v} \sigma(u_1)\sigma(u_2)$$

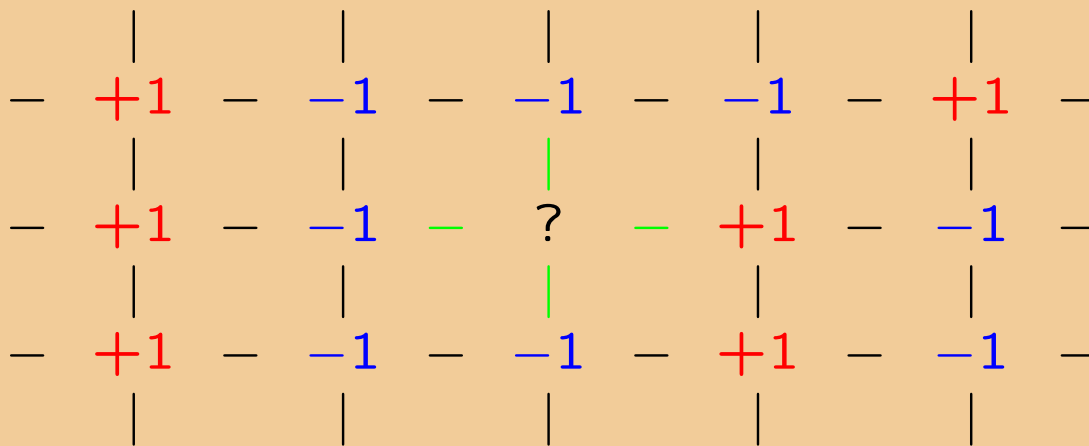
Ising Model via Glauber dynamics.



Observe: conditional probability for $\sigma(v)$ is given by $\mathcal{H}_{local}(\sigma, v)$:

$$\mathcal{H}(\sigma) = \mathcal{H}_{local}(\sigma, v) - \sum_{e=[u_1, u_2]: u_1, u_2 \neq v} \sigma(u_1)\sigma(u_2)$$

Ising Model via Glauber dynamics.



Randomly pick $v \in G$, erase the spin $\sigma(v)$.
Choose σ_+ or σ_- :

$$\begin{aligned} \text{Prob}(\sigma \rightarrow \sigma_+) &= \frac{e^{-\beta\mathcal{H}(\sigma_+)}}{e^{-\beta\mathcal{H}(\sigma_-)} + e^{-\beta\mathcal{H}(\sigma_+)}} \\ &= \frac{e^{-\beta\mathcal{H}_{local}(\sigma_+,v)}}{e^{-\beta\mathcal{H}_{local}(\sigma_-,v)} + e^{-\beta\mathcal{H}_{local}(\sigma_+,v)}} = \frac{e^{-2\beta}}{e^{-2\beta} + e^{2\beta}}. \end{aligned}$$

Glauber dynamics: Rapid mixing.

Glauber dynamics - a random walk on state space S (here $\{-1, +1\}^V$) s.t. needed π is stationary w.r.t. Glauber dynamics.

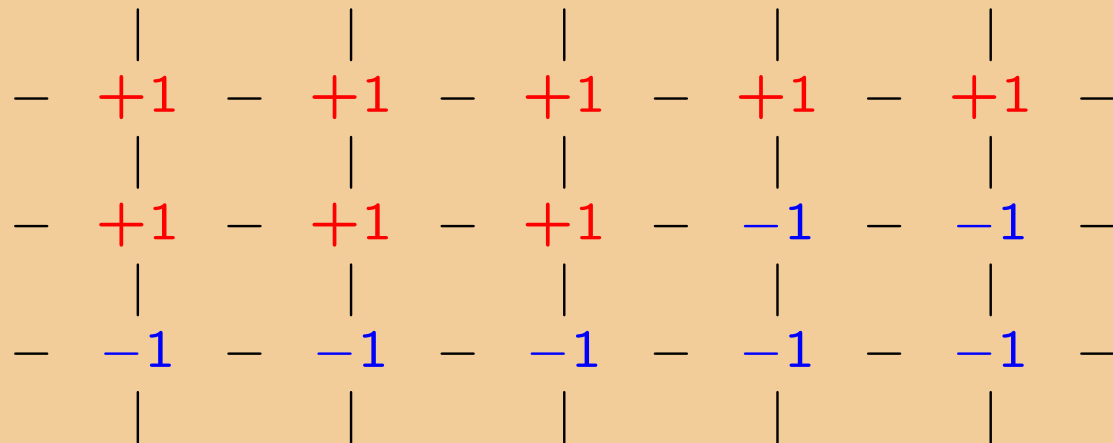
In high temperatures (i.e. $\beta = \frac{1}{T}$ small enough) it takes $O(n \log n)$ iterations to get “ ε -close” to π . Here $|V| = n$.

Need: $\max_{v \in V} \deg(v) \cdot \tanh(\beta) < 1$

Thus the Glauber dynamics is a fast way to generate π . It is an important example of **Gibbs sampling**.

Close enough distribution and mixing time.

What is “ ε -close” to π ? Start with σ_0 :



If $P_t(\sigma)$ is the probability distribution after t iterations, the total variation distance

$$\|P_t - \pi\|_{TV} = \frac{1}{2} \sum_{\sigma \in \{-1, +1\}^V} |P_t(\sigma) - \pi(\sigma)| \leq \varepsilon .$$

Who researched mixing times? D.Aldous,
P.Diaconis, J.A.Fill, M.Jerrum, A.Sinclair and
many more names.

Close enough distribution and mixing time.

Total variation distance:

$$\|\mu - \nu\|_{TV} := \frac{1}{2} \sum_{x \in S} |\mu(x) - \nu(x)| = \sup_{A \subset S} |\mu(A) - \nu(A)|$$

Mixing time:

$$t_{mix}(\varepsilon) := \inf \{t : \|P_t - \pi\|_{TV} \leq \varepsilon, \quad \text{all } \sigma_0\} .$$

In high temperature, $t_{mix}(\varepsilon) = O(n \log n)$.

Coupling Method.

S - sample space

$\{p(i, j)\}_{i, j \in S}$ - transition probabilities

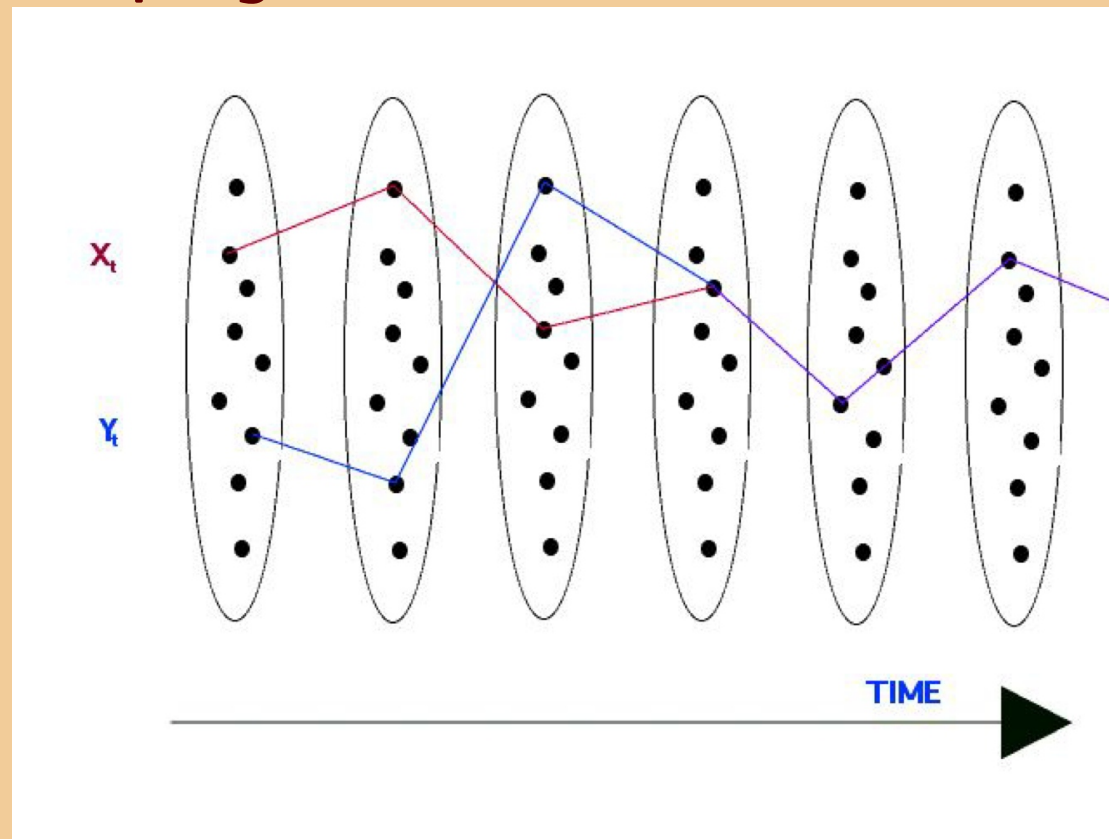
Construct process $\begin{pmatrix} X_t \\ Y_t \end{pmatrix}$ on $S \times S$ such that

X_t is a $\{p(i, j)\}$ -Markov chain

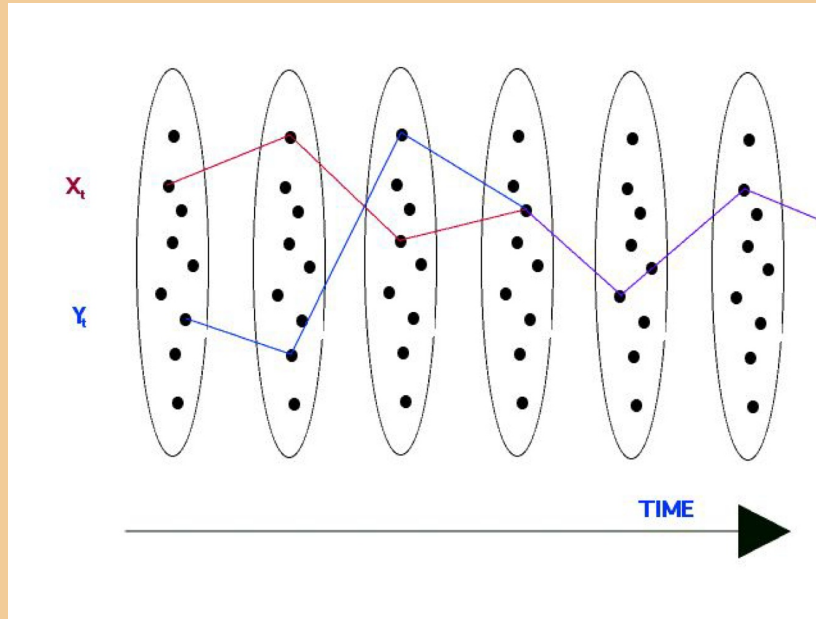
Y_t is a $\{p(i, j)\}$ -Markov chain

Once $X_t = Y_t$, let $X_{t+1} = Y_{t+1}$, $X_{t+2} = Y_{t+2}, \dots$

Coupling Method.



Coupling Method.



Coupling time: $T_{coupling} = \min\{t : X_t = Y_t\}$

Successful coupling: $\text{Prob}(T_{coupling} < \infty) = 1$

Mixing times via coupling.

Let $T_{i,j}$ be coupling time for $\begin{pmatrix} X_t \\ Y_t \end{pmatrix}$ given $X_0 = i$ and $Y_0 = j$. Then

$$\|P_{X_t} - P_{Y_t}\|_{TV} \leq P[T_{i,j} > t] \leq \frac{E[T_{i,j}]}{t}$$

Now, if we let $Y_0 \sim \pi$, then for any $X_0 \in S$,

$$\|P_{X_t} - \pi\|_{TV} = \|P_{X_t} - P_{Y_t}\|_{TV} \leq \frac{\max_{i,j \in S} E[T_{i,j}]}{t} \leq \varepsilon$$

whenever $t \geq \frac{\max_{i,j \in S} E[T_{i,j}]}{\varepsilon}$.

Mixing times via coupling.

$$\|P_{X_t} - \pi\|_{TV} \leq \varepsilon \text{ whenever } t \geq \frac{\max_{i,j \in S} E[T_{i,j}]}{\varepsilon}.$$

Thus

$$t_{mix}(\varepsilon) = \inf \left\{ t : \|P_{X_t} - \pi\|_{TV} \leq \varepsilon \right\} \leq \frac{\max_{i,j \in S} E[T_{i,j}]}{\varepsilon}.$$

So,

$$O(t_{mix}) \leq O(T_{coupling}) .$$

Thus constructing a coupled process that minimizes $E[T_{coupling}]$ gives an effective upper bound on mixing time.

Coupon collector.



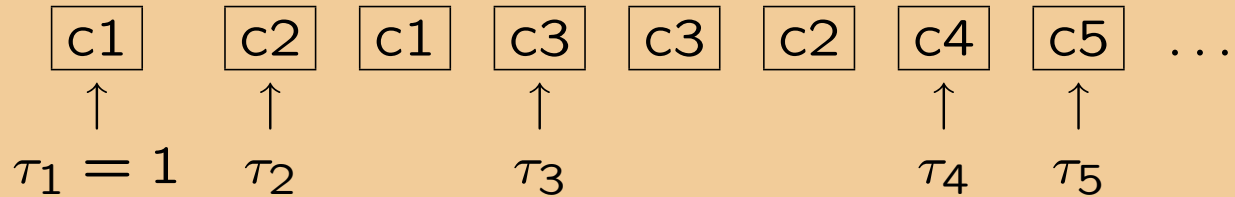
n types of coupons: $\boxed{1}, \boxed{2}, \dots, \boxed{n}$

Collecting coupons: coupon / unit of time,
each coupon type is equally likely.

Goal: To collect a coupon of each type.

Question: How much time will it take?

Coupon collector.



Here $\tau_1 = 1$, $E[\tau_2 - \tau_1] = \frac{n}{n-1}$,
 $E[\tau_3 - \tau_2] = \frac{n}{n-2}, \dots, E[\tau_n - \tau_{n-1}] = n$.

Hence

$$E[\tau_n] = n \left(1 + \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{n} \right) = n \log n + O(n)$$

Coupon collector and random card-to-random location shuffling.

Shuffling a deck of n different cards:

1 2 3 4 5 6 7 8

Coupon collector and random card-to-random location shuffling.

Shuffling a deck of n different cards:

1 2 3 4 5 6 7 8

Pick a card at random:

1 2 3 4 5 6 7 8

Coupon collector and random card-to-random location shuffling.

Shuffling a deck of n different cards:

1 2 3 4 5 6 7 8

Pick a card at random:

1 2 3 4 5 6 7 8

Pool it out, and place it anywhere in the deck:

1 2 5 3 4 6 7 8

Iterate. **Question:** $t_{mix}(\varepsilon) = ?$

Random card-to-random location:

Cover time: T_{cover} - each card was selected at least once.

2 5 3 1 6 8 7 4

Coupon collector $\Rightarrow E[T_{cover}] = n \log n + O(n)$

Cover time as well as coupling time (both strong stationary time) provides an effective upper and lower bound on mixing time.

Here $E[t_{mix}(\varepsilon)] = n \log n + O(n)$

Shuffling by random transpositions.

Pick two cards at random:

1 2 3 4 5 6 7 8

Transpose them:

1 2 3 4 7 6 5 8

Iterate:

3 2 1 4 7 6 5 8

3 2 6 4 7 1 5 8

... etc.

Shuffling by random transpositions.

3 2 6 4 7 1 5 8

Here coupon collector gives only a lower bound of $\frac{1}{2}n \log n$.

Goal: get $O(n \log(n))$ upper bound with coupling method - hidden coupon collector.

Obtaining $O(n \log(n))$ via super-fast coupling. (Joint work with R.Burton)

Diaconis and Shahshahani (early 80's):

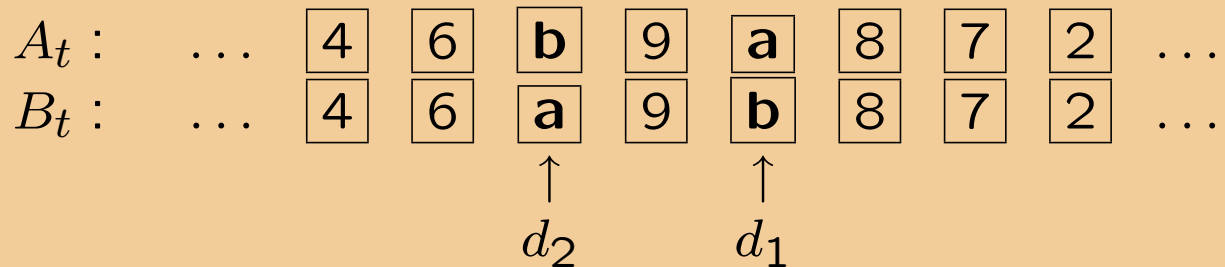
The mixing time for shuffling a deck of n cards by random transpositions is of order $O(n \log(n))$ with cut-off asymptotics at $\frac{1}{2}n \log(n)$.

Method used: **representation theory.**

We answer an **open problem** (Y. Peres):
Provide a coupling proof of $O(n \log(n))$ mixing rate.

A coupling. (Aldous and Fill) $\ll \boxed{\mathbf{a}}, i \gg$:
 moves card $\boxed{\mathbf{a}}$ to location i in both processes, A_t and B_t .

Even in case of **two discrepancies** ($d = 2$)
 at d_1 and d_2 :

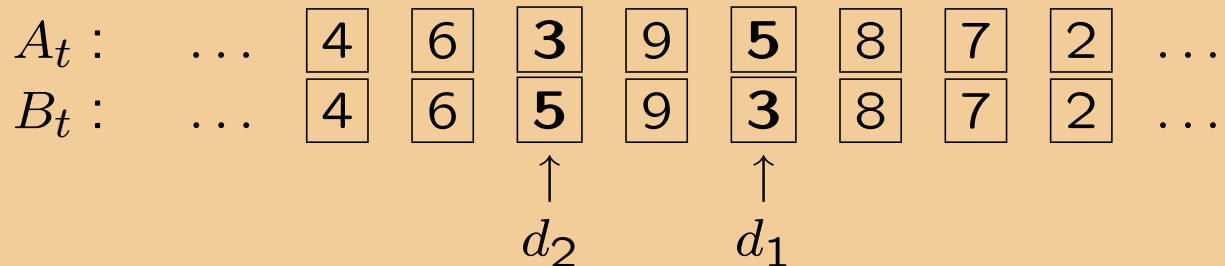


Label-to-location coupling:

$$E[T_{coupling}] = \frac{n^2}{4} \quad \text{– too large.}$$

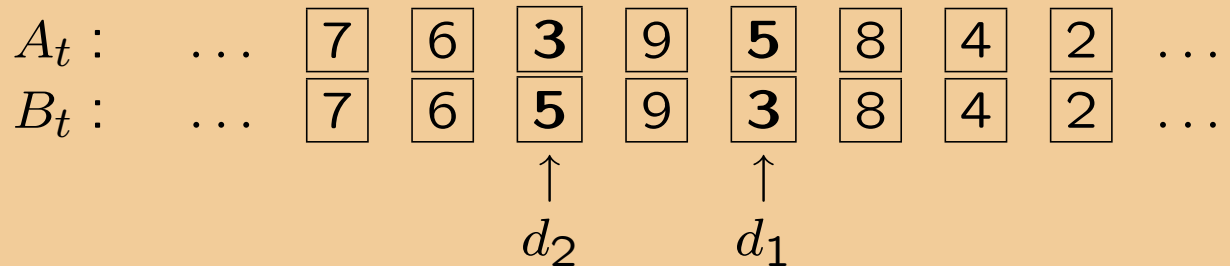
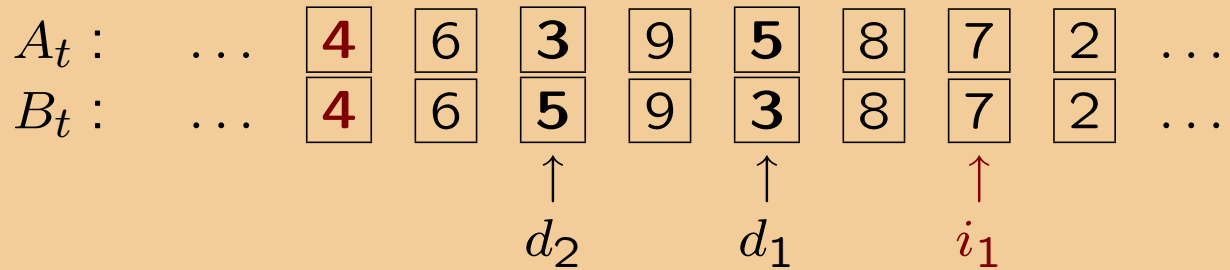
A coupling. (Aldous and Fill) $\ll \boxed{\mathbf{a}}, i \gg$:
 moves card $\boxed{\mathbf{a}}$ to location i in both processes, A_t and B_t .

Case of **two discrepancies** ($d = 2$):



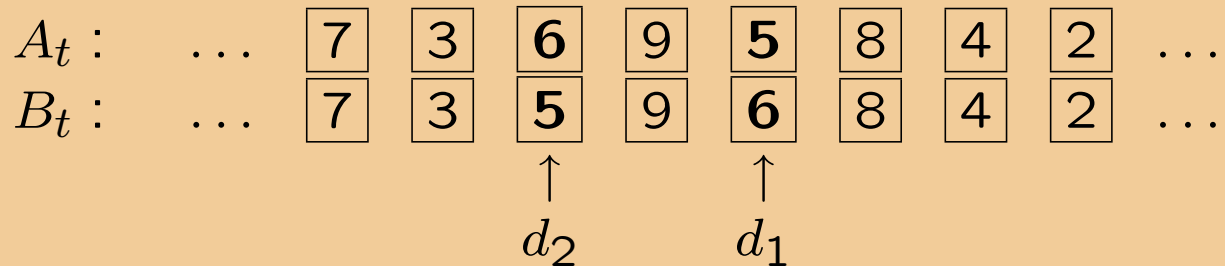
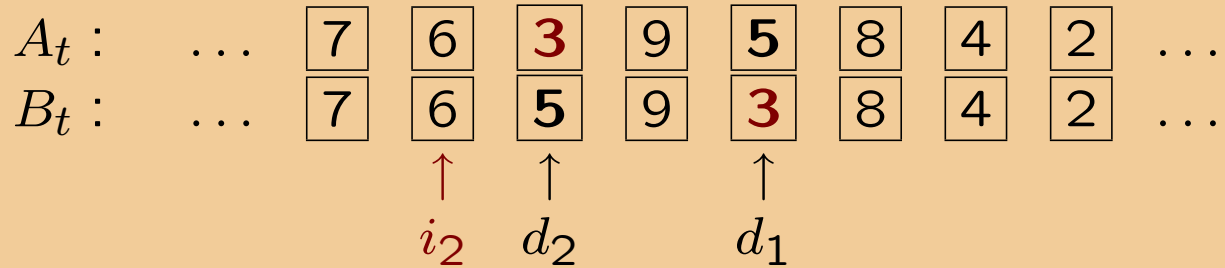
A coupling. (Aldous and Fill) $\ll \boxed{\mathbf{a}}, i \gg$:
 moves card $\boxed{\mathbf{a}}$ to location i in both processes, A_t and B_t .

Case of **two discrepancies** ($d = 2$):



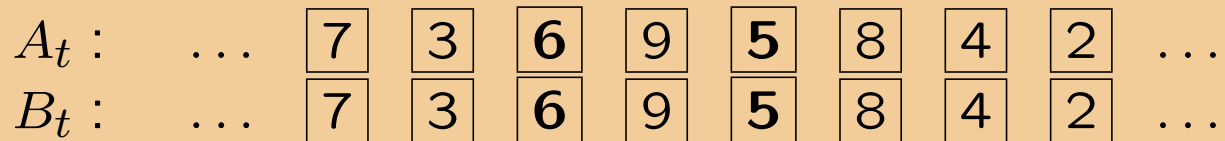
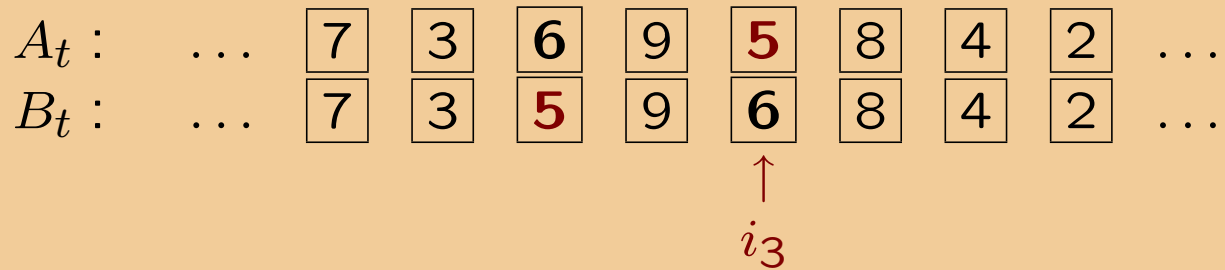
A coupling. (Aldous and Fill) $\ll \boxed{\mathbf{a}}, i \gg$:
 moves card $\boxed{\mathbf{a}}$ to location i in both processes, A_t and B_t .

Case of **two discrepancies** ($d = 2$):



A coupling. (Aldous and Fill) $\ll \boxed{\mathbf{a}}, i \gg$:
 moves card $\boxed{\mathbf{a}}$ to location i in both processes, A_t and B_t .

Case of **two discrepancies** ($d = 2$):



Label-to-location coupling: $E[T_{coupling}] = \frac{n^2}{4}$

A coupling. (Aldous and Fill) $\ll \boxed{\mathbf{a}}, i \gg$: moves card $\boxed{\mathbf{a}}$ to location i in both processes, A_t and B_t .

Mixing: order $O(n^2)$ instead of $O(n \log n)$;

$$E[T_{coupling}] \approx \sum_{d=2}^n \frac{n^2}{d^2} \approx \left(\frac{\pi^2}{6} - 1 \right) n^2$$

Problem: slows down significantly when the number of discrepancies is small enough.

Obtaining $O(n \log(n))$ via super-fast coupling. (Joint work with R.Burton)

Tunneling into the future approach.

Coupling time:

$$E[T_{coupling}] \leq \left[\frac{1}{2\varepsilon} + \frac{\kappa}{(1-\kappa)(\kappa-\varepsilon)} \right] \cdot n \log n$$

for any $0 < \varepsilon < \kappa < 1$.

Two discrepancies ($d = 2$) at d_1 and d_2 :

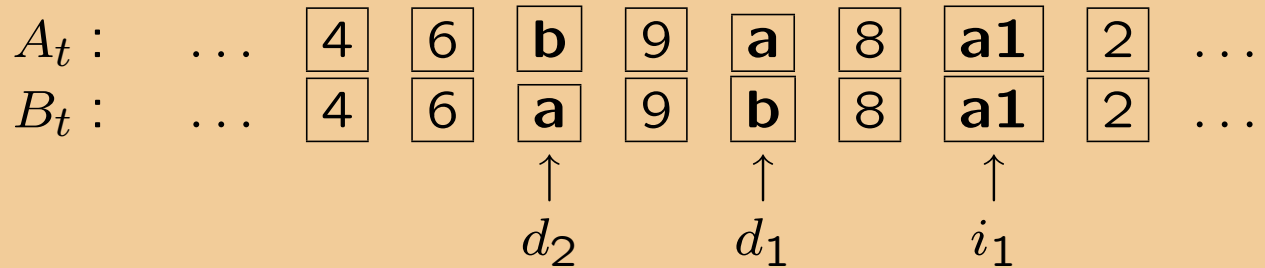
A_t :	...	4	6	b	9	a	8	a1	2	...
B_t :	...	4	6	a	9	b	8	a1	2	...
				↑		↑		↑		
				d_2		d_1		i_1		

Label-to-location coupling:

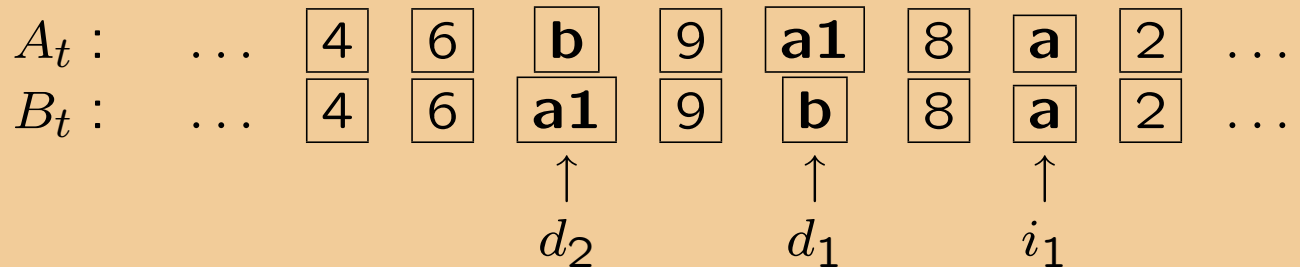
$$E[T_{coupling}] = \frac{n^2}{4} \quad - \text{ too large.}$$

Jump $\ll \boxed{\mathbf{a}}, i_1 \gg$ of $\boxed{\mathbf{a}}$ to random location i_1 at exponential time t_1 :

From

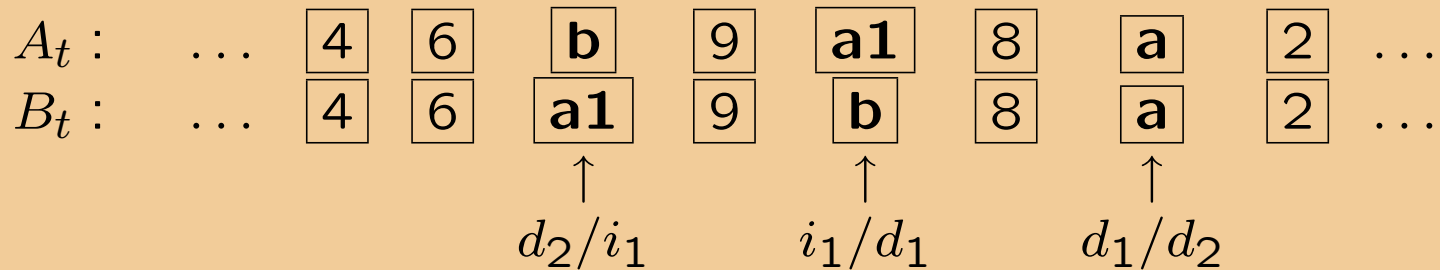


to



Different way of saying the same:

Start with

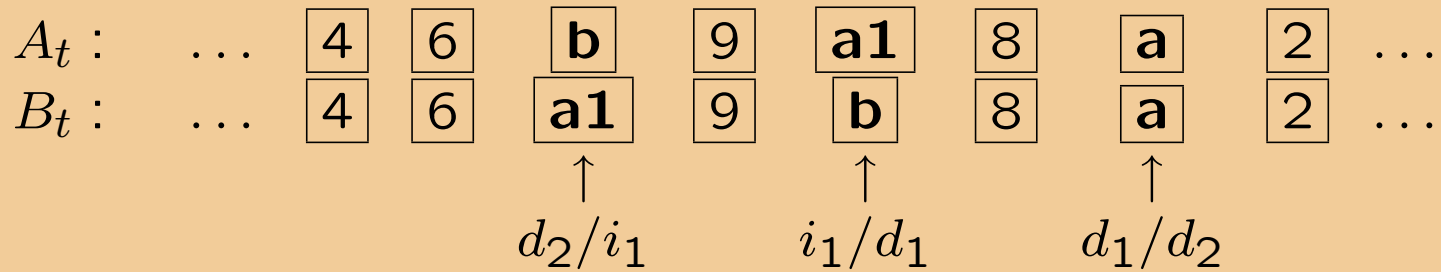


where at time t_1 the locations relabel according to

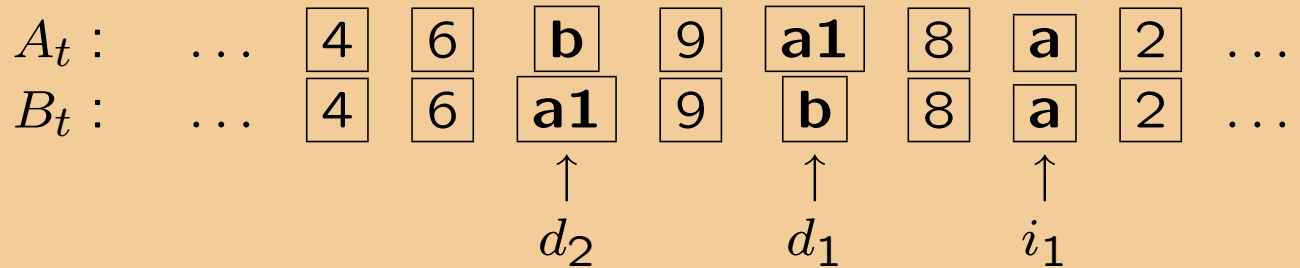
$d_1/d_2 \longrightarrow i_1$
$i_1/d_1 \longrightarrow d_1$
$d_2/i_1 \longrightarrow d_2$

Jump $\ll \boxed{\mathbf{a}}, i_1 \gg$ at time $t_1 \sim \text{exponential} \left(\frac{1}{n} \right)$.

From



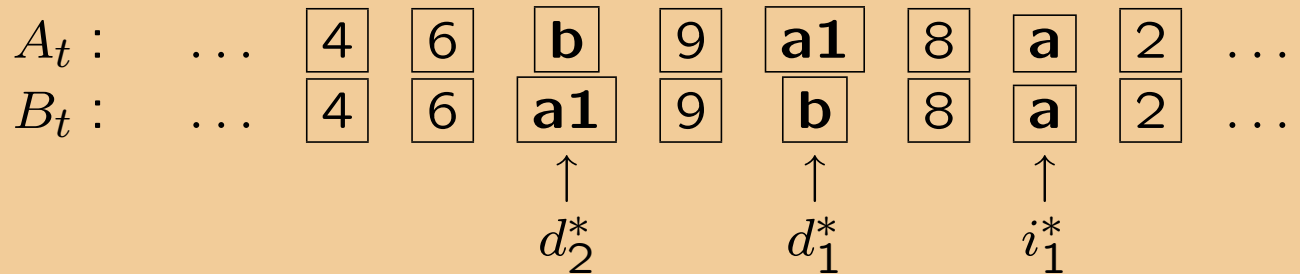
to



The following **association map** will determine jumps of **a1**.

A_t :	...	4	6	b	9	a1	8	a	2	...
B_t :	...	4	6	a1	9	b	8	a	2	...

Card **a1** will jump to position i_2 on the assoc. map at time t_2 , even if $t_2 < t_1$.



Now $i_2 \neq i_1^*$ and

$$t_2 \sim \text{exponential} \left((1 - 1/n) \cdot \frac{1}{n} \right)$$

$\ll \boxed{\mathbf{a1}}, i_1^* \gg = \ll \boxed{\mathbf{a1}}, \boxed{\mathbf{a}} \gg$ is label-to-label,
we can skip.

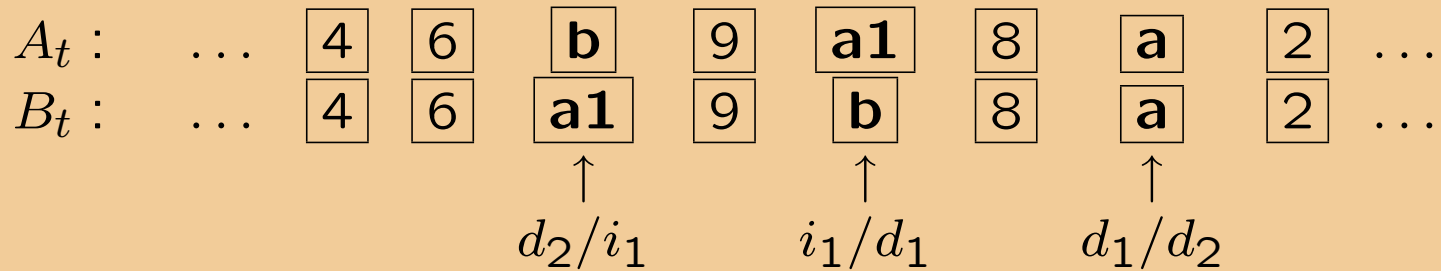
If $i_1 = d_1$ or d_2 , discrepancies cancel at t_1 ;

if $i_2^* = d_1^*$ or d_2^* , discrepancies cancel on the assoc. map at t_2 .

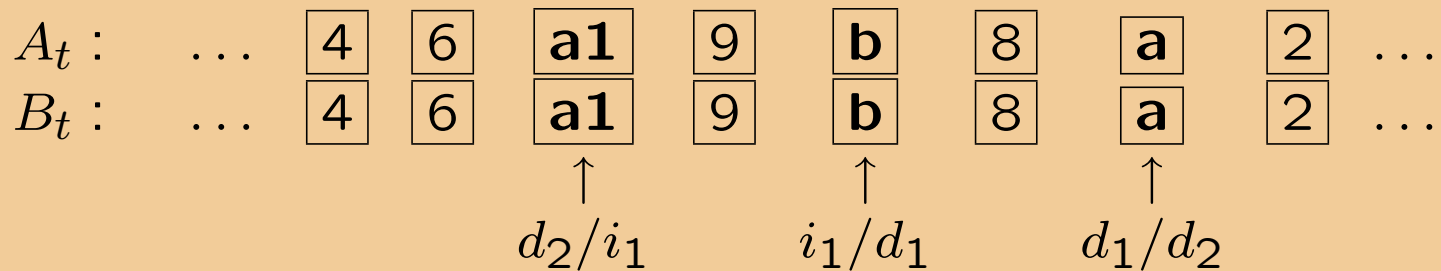
If $t_1 < t_2$, assoc. map \rightarrow real picture at t_1 , we create one more assoc. map.

Case $t_2 < t_1$, and $i_2^* = d_2^*$. **On association map:**

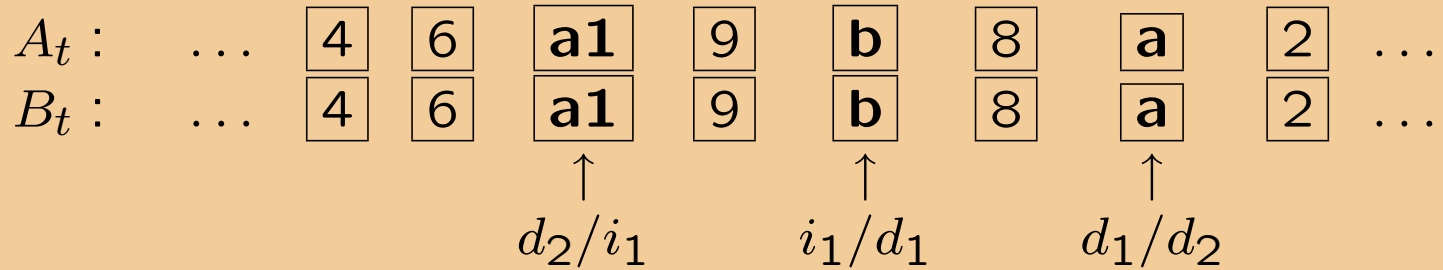
Start with



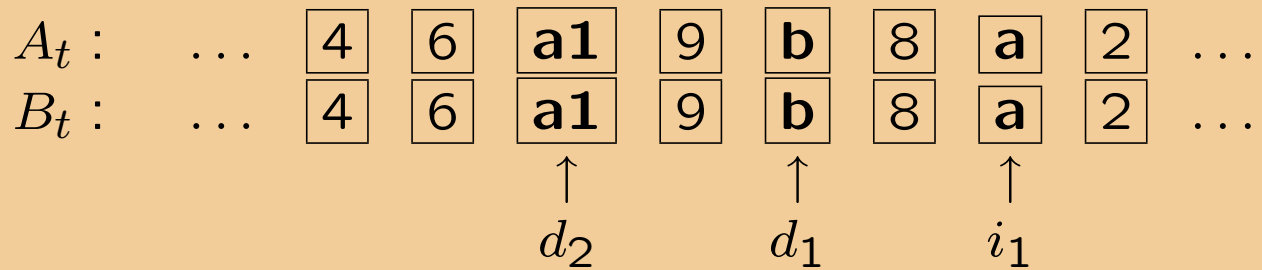
At time t_2 :



At time t_2 :

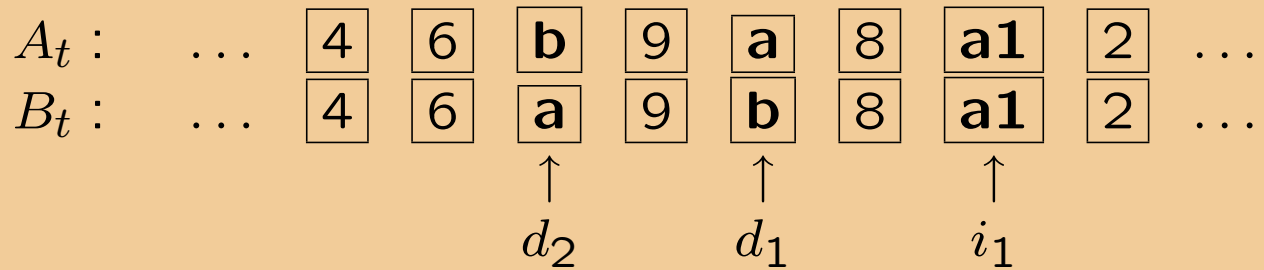


At time t_1 :

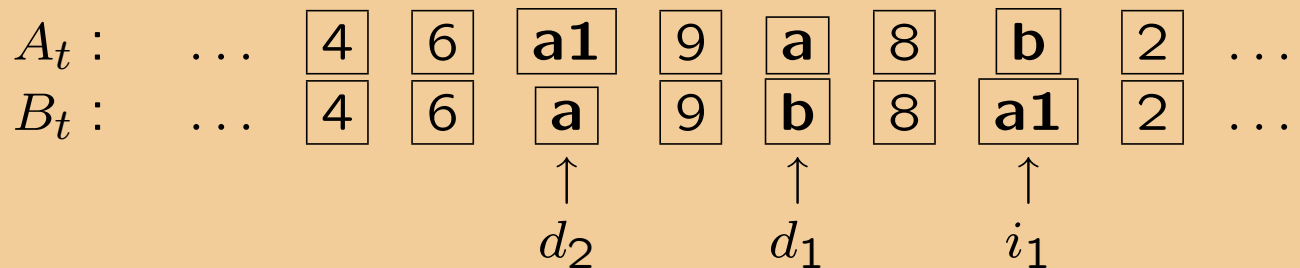


Case $t_2 < t_1$, and $i_2^* = d_2^*$. **Same evolution, original association:**

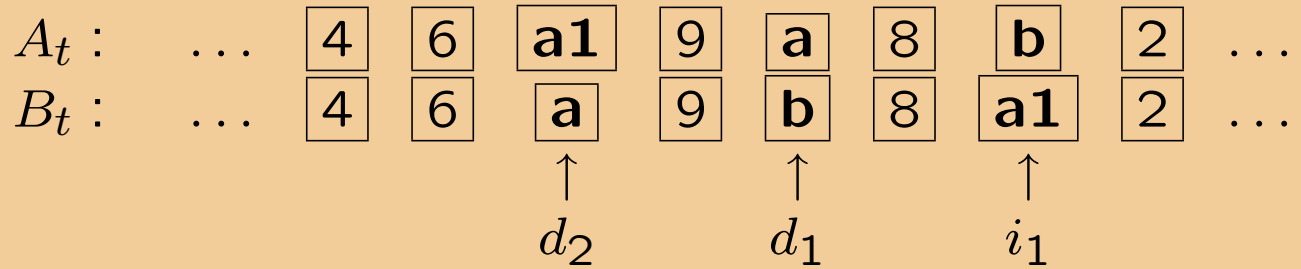
Start with



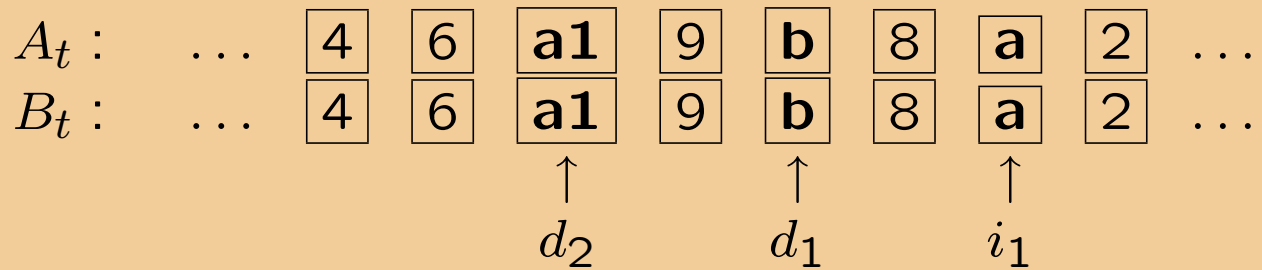
At time t_2 :



At time t_2 :



At time t_1 :

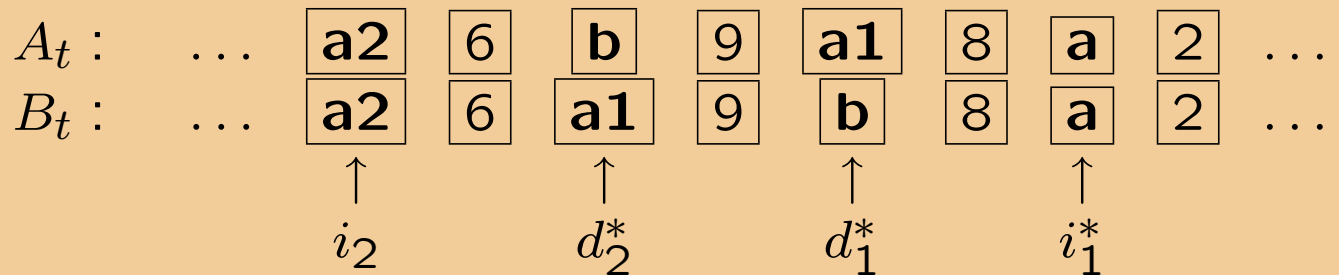


Here

$$E[T_{coupling}] \approx \frac{n^2}{8}$$

Chain of association maps:

$\ll \boxed{\mathbf{a1}}, i_2 \gg$ occurs at t_2

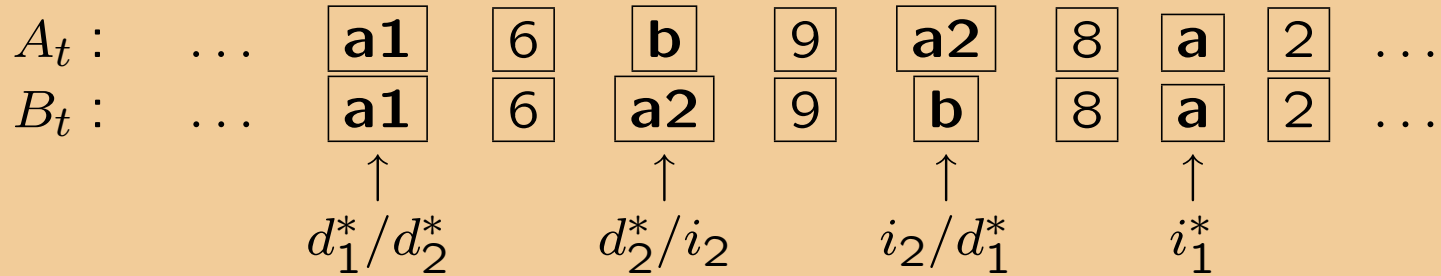


d_1^* is i_1/d_1 before t_1 , and d_1 after t_1 ;

d_2^* is d_2/i_1 before t_1 , and d_2 after t_1 ;

i_1^* is d_1/d_2 before t_1 , and i_1 after t_1 .

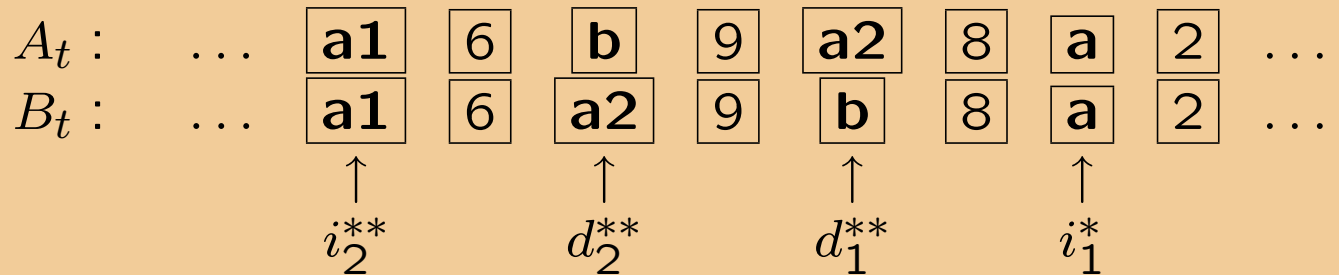
New association map:



where at t_2 ,

d_1^*/d_2^*	\longrightarrow	i_2
i_2/d_1^*	\longrightarrow	d_1^*
d_2^*/i_2	\longrightarrow	d_2^*

a2 will do label-to-location jump w.r.t. the following assoc. map



d_1^{**} is i_2/d_1^* before t_2 , and d_1^* after t_2 ;

d_2^{**} is d_2^*/i_2 before t_2 , and d_2^* after t_2 ;

i_2^{**} is d_1^*/d_2^* before t_2 , and i_2 after t_2 .

$\ll \mathbf{a2}, i_3 \gg$ occurs at $t_3 \sim \text{exponential} \left((1 - 2/n) \cdot \frac{1}{n} \right)$

And so on, creating a **chain** of $k = \lfloor \varepsilon n \rfloor$ association maps.

In case of $d = 2$ discrepancies, the avg. time of discrepancy cancelation on one of assoc. maps is

$$E[T_2] = \frac{n^2}{4(k+1)} = \frac{n}{4\varepsilon}.$$

General d :

$$E[T_d] = \frac{n^2}{2(k+1)d} \approx \frac{n}{2\epsilon d}.$$

Coupling time (all discrepancies):

$$E[T_{coupling}] \leq \left[\frac{1}{2\epsilon} + \frac{\kappa}{(1-\kappa)(\kappa-\epsilon)} \right] \cdot n \log n$$

for any $0 < \epsilon < \kappa < 1$.