# Algorithm for Sampling Maximal Couplings of Markov Chains

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#### Defining a Maximal Coupling

Given two Markov Chains  $X_t, Y_t$  with initial distributions  $\mu, \nu$  and shared transition function P, a coupling introduces some kind of dependence between  $X_t, Y_t$ 







Here  $X_t$  and  $Y_t$  are independent; the path of  $X_t$  does not affect the path of  $Y_t$ .



 $X_t$  and  $Y_t$  are **maximally coupled**; the dependence maximizes the rate at which they reach the same state.

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#### **Constructing a Maximal Coupling**

Let T be the first time the paths of  $X_t, Y_t$  meet (the coupling time)

**Theorem 1.** If  $X_t, Y_t$  are maximally coupled, we can recursively compute:

$$\begin{split} m_t(x) &= \mathbb{P}[X_T = Y_T = x, T = t] \\ \alpha_{\mu,t}(x) &= \mathbb{P}[X_t = x, T > t] \\ C_{\mu,t}(x) &= \mathbb{P}[T = t | X_t = x, T \ge t] \end{split} \qquad \begin{array}{l} \alpha_{\nu,t}(y) &= \mathbb{P}[Y_t = y, T > t] \\ C_{\nu,t}(y) &= \mathbb{P}[T = t | Y_t = x, T \ge t] \end{array}$$

Probability that maximally coupled X takes on path  $\bar{x} = (x_0, \ldots, x_t)$  and T = t:

$$\mathbb{P}(X_{[0,t]} = \bar{x}, T = t) = \mu(x_0)C_{\mu,t}(x_t)\prod_{s=0}^{t-1} (1 - C_{\mu,s}(x_s))P(x_s, x_{s+1})$$

#### **Time Reversal**

Note the substitutions:

$$q_t(y, x) := \frac{\alpha_{\nu, t-1}(x) P(x, y) (1 - C_{\nu, t}(y))}{\alpha_t(y)}$$
$$Q_t(y, x) := \frac{\alpha_{\nu, t-1}(x) P(x, y) C_{\nu, t}(y)}{m_t(y)}$$

This reverses the time in our original path decomposition formula:

$$\mathbb{P}(Y_{[0,t]} = \bar{y} \mid T = t, X_t = Y_t = y_t) = Q_t(y_t, y_{t-1}) \prod_{n=1}^{t-1} q_n(y_n, y_{n-1}) = Q_t(y_t, y_t, y_{t-1}) = Q_t(y_t, y_t, y_{t-1$$

### Algorithm

We first sample the X path, and then iterate backward to sample the Y path:

```
Sample a Maximal Coupling
procedure SAMPLE(P, \mu, \nu)
   t = 0
   X_0 \sim \mu
   while Uniform[0, 1] < C_{\mu,t}(X_t) do
      X_{t+1} \sim P(X_t, \cdot)
     t = t + 1
   end while
   Y_t = X_t
   Y_{t-1} \sim Q_t(Y_t, \,\cdot\,)
  t = t - 1
   while t > 0 do
     Y_{t-1} \sim q_t(Y_t, \,\cdot\,)
    t = t - 1
   end while
```





## Simulating a Maximal Coupling



#### Maximally Coupled Walks on a $50 \times 50$ Grid

Theoretical TV vs. Empirical TV of Maximally Coupled Walks on a  $50 \times 50$  Grid



#### References

#### References

- [1] Levin, David A., Peres, Yuval and Wilmer, Elizabeth L. Markov chains and mixing times. : American Mathematical Society, 2006.
- [2] Pitman, J.W. On coupling of Markov chains. Z. Wahrscheinlichkeitstheorie verw Gebiete 35, 315–322 (1976).