# Understanding MCMC

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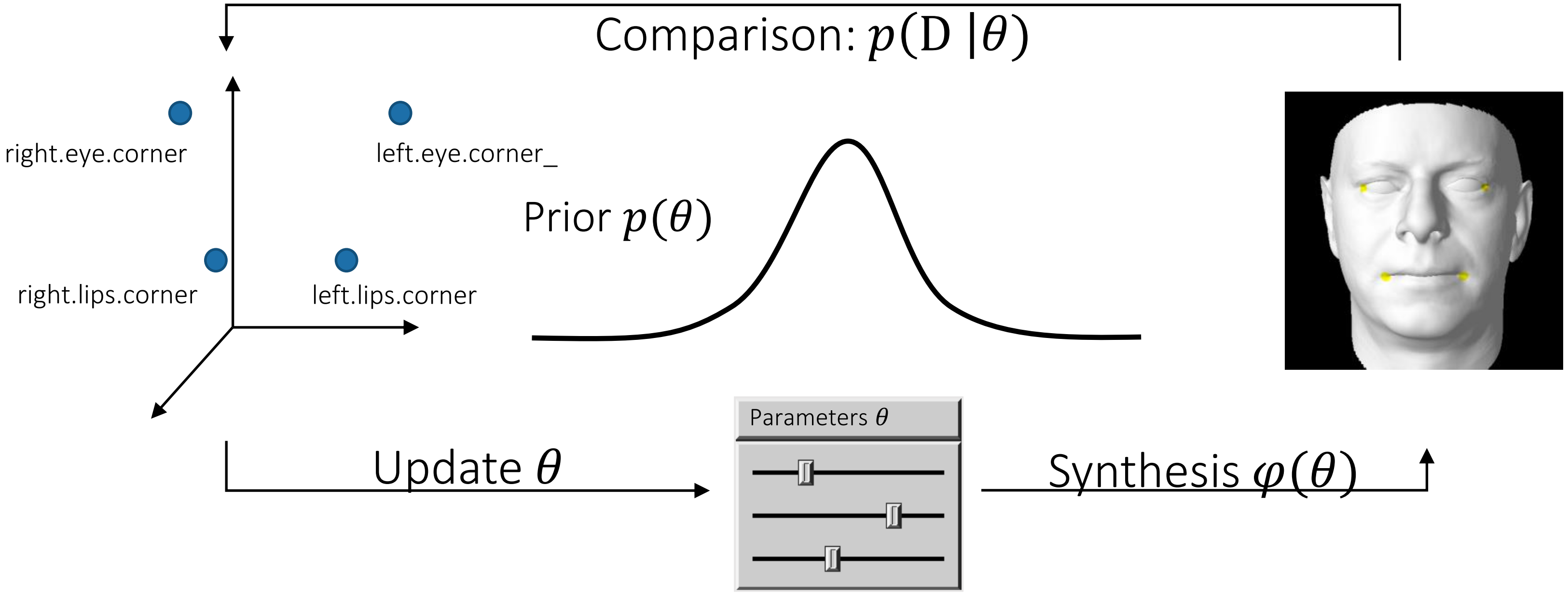
Slides based on presentation by Sandro Schönborn

# Reminder: Analysis by synthesis



Comparison: $p(\mathrm{D}\ |\theta)$

right.eye.corner

left.eye.corner_

right.lips.corner

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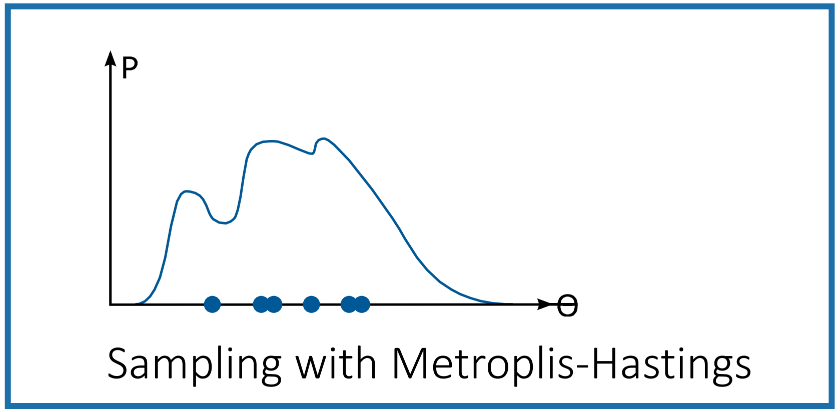
Prior $p(\theta)$

Parameters $\theta$

Update $\theta$

Synthesis $\varphi(\theta)$



Sampling with Metroplis-Hastings

# Reminder: The Metropolis-Hastings Algorithm

**Requirements**:

- Proposal distribution $Q(\boldsymbol{x}'|\boldsymbol{x})$ – *must generate samples*
- Target distribution $P(\boldsymbol{x})$ – *with point-wise evaluation*

Tuning "knob" – influences convergence

Target distribution
In our case: $p(\theta|Data)$

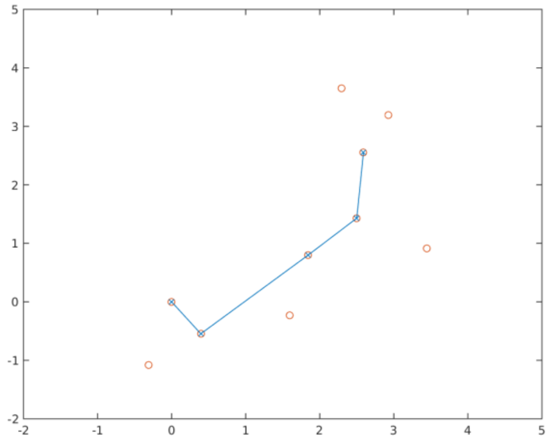
**Result**:

- Stream of samples approximately from $P(\boldsymbol{x})$

- Initialize with sample $\boldsymbol{x}$
- Generate next sample, with current sample $\boldsymbol{x}$
  1. Draw a sample $\boldsymbol{x}'$ from $Q(\boldsymbol{x}'|\boldsymbol{x})$ ("proposal")
  2. With *probability* $\alpha = \min\left\{\frac{P(x')}{P(x)}\frac{Q(x|x')}{Q(x'|x)}, 1\right\}$ accept $\boldsymbol{x}'$ as new state $\boldsymbol{x}$
  3. Emit current state $\boldsymbol{x}$ as sample

# Reminder: The Metropolis-Hastings Algorithm

- Target: $P(\boldsymbol{x})$
- Proposal: $Q(\boldsymbol{x}'|\boldsymbol{x}) = \mathcal{N}(\boldsymbol{x}'\,|\,\boldsymbol{x}, \sigma^2 I_2)$
- Initial State $x_0$

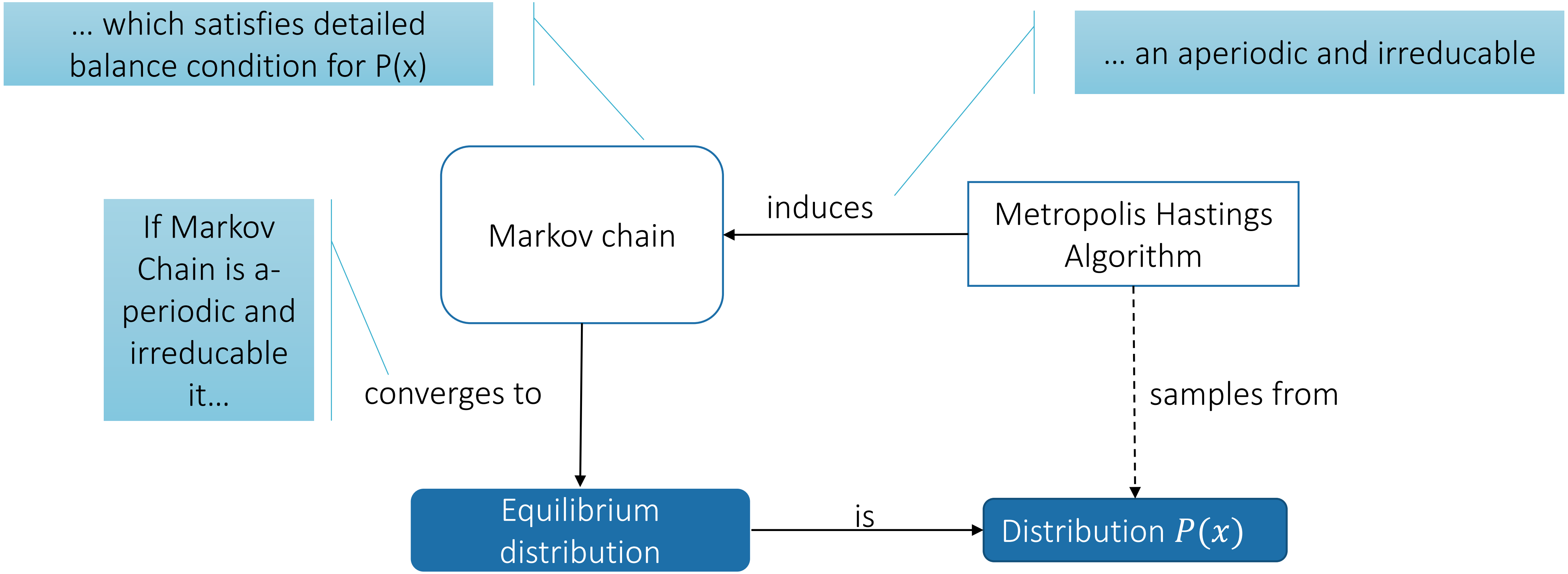


The sampled state at step $i$ is a random variable $X_i \sim P_i(x)$

- Initially close to our starting point $x_0$
- “forgets” starting point after some time

Convergence: Distribution of $X_i$ becomes $P(x)$ if $i \rightarrow \infty$

# The big picture



… which satisfies detailed balance condition for P(x)

… an aperiodic and irreducable

If Markov Chain is a-periodic and irreducable it…

# Understanding Markov Chains

# Markov Chain

State space

- Sequence of random variables $\{X_i\}_{i=1}^{N}$, $X_i \in S$ with Markov Property

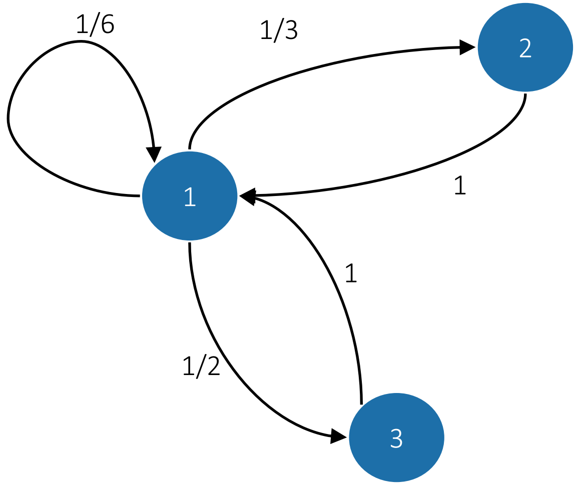
$$P(X_i|X_1, X_2, \dots, X_{i-1}) = P(X_i|X_{i-1})$$

Transition probability

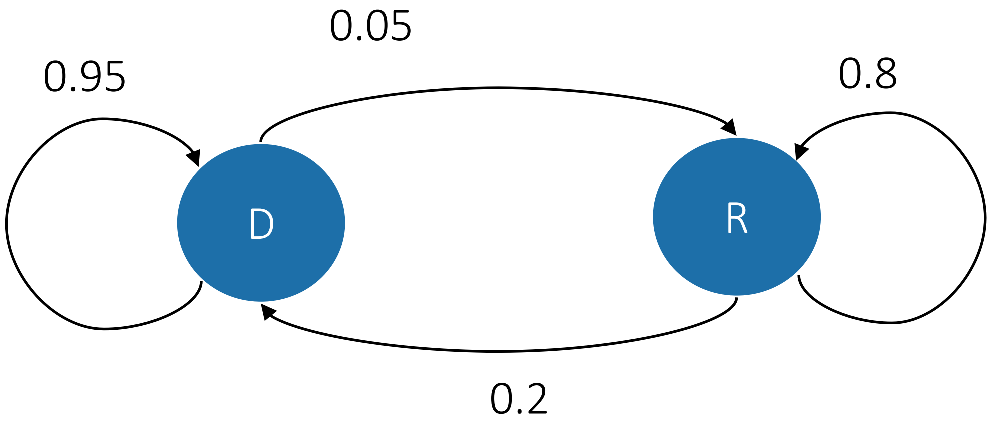
- Simplifications: (for our analysis)
  - Discrete state space: $S = \{1, 2, \dots, K\}$
  - Homogeneous Chain: $P(X_i = l|X_{i-1} = m) = T_{lm}$

Automatically true if we use computers (e.g. 32 bit floats)

- Can be simulated, for any given initial distribution $X_1$



# Example: Markov Chain



- Simple weather model: *dry* (D) or *rainy* (R) hour
  - Condition in next hour? $X_{t+1}$
  - State space $S = \{D, R\}$
  - Stochastic: $P(X_{t+1}|X_t)$
  - Depends only on *current* condition $X_t$
- Draw samples from chain:
  - Initial: $X_0 = D$
  - Evolution: $P(X_{t+1}|X_t)$
- Long-term Behavior
  - Does it converge? *Average* probability of rain?
  - Dynamics? How *quickly* will it converge?

$DDDDDDDDRRRRRRRRRRRDDDDDDDDDDD$
$DDDDDDDDDDDDDDDDDDDDDDDDDDDDDD$
$DDDDDDDDDRDD...$

# Discrete Homogeneous Markov Chain

Formally linear algebra:

- Distribution (vector):

$$P(X_i):\ \boldsymbol{p_i} = \begin{bmatrix} P(X_i = 1) \\ \vdots \\ P(X_i = K) \end{bmatrix}$$

- Transition probability (transition matrix):

$$P(X_i|X_{i-1}):\ T = \begin{bmatrix} P(1 \leftarrow 1) & \cdots & P(1 \leftarrow K) \\ \vdots & \ddots & \vdots \\ P(K \leftarrow 1) & \cdots & P(K \leftarrow K) \end{bmatrix}$$

$$T_{lm} = P(l \leftarrow m) = P(X_i = l|X_{i-1} = m)$$

# Evolution of the Initial Distribution

- Evolution of $P(X_1) \rightarrow P(X_2)$:

$$P(X_2 = l) = \sum_{m \in S} P(l \leftarrow m) P(X_1 = m)$$

$$\boldsymbol{p}_2 = T\boldsymbol{p}_1$$

- Evolution of $n$ steps:

$$\boldsymbol{p}_{n+1} = T^n \boldsymbol{p}_1$$

- Is there a *stable* distribution $\boldsymbol{p}^*$? (steady-state)

$$\boldsymbol{p}^* = T\boldsymbol{p}^*$$

A stable distribution is an *eigenvector* of $T$ with eigenvalue $\lambda = 1$

# Steady-State Distribution: $\boldsymbol{p}^*$

- It exists:
  - $T$ subject to normalization constraint: *left* eigenvector to eigenvalue 1

$$\sum_l T_{lm} = 1 \quad \Leftrightarrow \quad [1 \quad \dots \quad 1]T = [1 \quad \dots \quad 1]$$

  - T has eigenvalue $\lambda = 1$ (left-/right eigenvalues are the same)
  - Steady-state distribution as corresponding right eigenvector

$$T\boldsymbol{p}^* = \boldsymbol{p}^*$$

- Does *any* arbitrary initial distribution *evolve* to $\boldsymbol{p}^*$?
  - Convergence?
  - Uniqueness?

# Equilibrium Distribution: $\boldsymbol{p}^*$

- Additional requirement for $T$: $(\mathrm{T}^{\mathrm{n}})_{lm} > 0 \ \text{ for all } n > N_0$

  The chain is called *irreducible* and *aperiodic* (implies *ergodic*)

    - All states are connected using at most $N_0$ steps
    - Return intervals to a certain state are irregular

- *Perron-Frobenius* theorem for positive matrices:
  - PF1: $\lambda_1 = 1$ is a simple eigenvalue with 1d eigenspace (*uniqueness*)
  - PF2: $\lambda_1 = 1$ is dominant, all $|\lambda_i| < 1, \ \ i \neq 1$ (*convergence*)

- $\boldsymbol{p}^*$ is a stable attractor, called *equilibrium distribution*

$$T\boldsymbol{p}^* = \boldsymbol{p}^*$$

# Convergence

- Time evolution of arbitrary distribution $\boldsymbol{p}_0$

$$\boldsymbol{p}_n = T^n \boldsymbol{p}_0$$

- Expand $\boldsymbol{p}_0$ in Eigen basis of $T$

$$T\boldsymbol{p}_0 = \mathrm{T}\sum_i^K c_i e_i = \sum_i^K c_i \mathrm{T} e_i = \sum_i^K c_i \lambda_i \boldsymbol{e}_i$$

$$T^n \boldsymbol{p}_0 = \sum_i^K c_i \lambda_i^n \boldsymbol{e}_i = c_1 \boldsymbol{e}_1 + \lambda_2^n c_2 \boldsymbol{e}_2 + \lambda_3^n c_3 \boldsymbol{e}_3 + \cdots$$

Eigenbasis:

$$T\boldsymbol{e}_i = \lambda_i \boldsymbol{e}_i, |\lambda_i| < \lambda_1 = 1, |\lambda_k| \geq |\lambda_{k+1}|$$

$$\boldsymbol{p}_0 = \sum_i^K c_i \boldsymbol{e}_i$$

# Convergence (II)

$$T^n \boldsymbol{p}_0 = \sum_{i}^{K} c_i \lambda_i^n \boldsymbol{e}_i = c_1 \boldsymbol{e_1} + \lambda_2^n c_2 \boldsymbol{e}_2 + \lambda_3^n c_3 \boldsymbol{e}_3 + \cdots$$

$$(n \gg 1) \qquad \approx \boldsymbol{p}^* + \lambda_2^n c_2 \boldsymbol{e}_2$$

$c_1 \boldsymbol{e_1} = \boldsymbol{p}^*$

Normalizations:
$\|\boldsymbol{e}_1\| = 1$
$\sum_i p_i^* = 1$

- We have *convergence*:

$$T^n \boldsymbol{p}_0 \xrightarrow{n \to \infty} \boldsymbol{p}^*$$

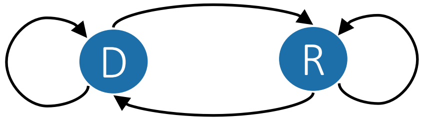
- *Rate* of convergence:

$$\|\boldsymbol{p}_n - \boldsymbol{p}^*\| \approx \|\lambda_2^n c_2 \boldsymbol{e}_2\| = |\lambda_2|^n |c_2|$$

# Example: Weather Dynamics

Rain forecast for stable versus mixed weather:

stable $W_s = \begin{bmatrix} 0.95 & 0.2 \\ 0.05 & 0.8 \end{bmatrix}$



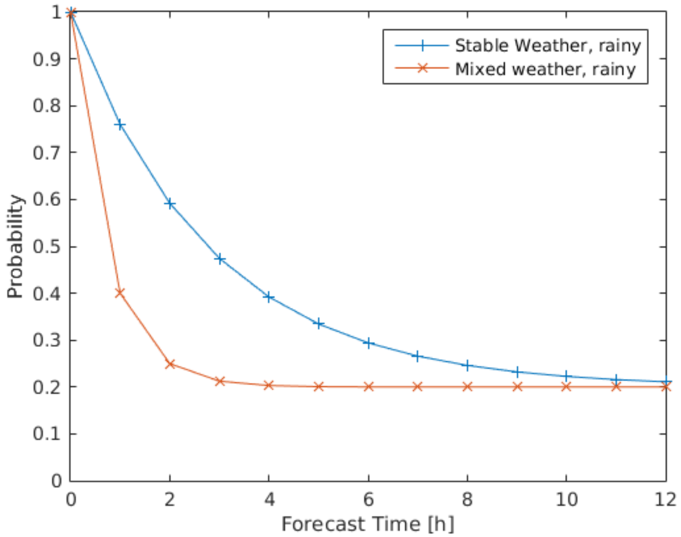
mixed $W_m = \begin{bmatrix} 0.85 & 0.6 \\ 0.15 & 0.4 \end{bmatrix}$

$\boldsymbol{p}^* = \begin{bmatrix} 0.8 \\ 0.2 \end{bmatrix}$ ← Long-term average probability of rain: **20%** → $\boldsymbol{p}^* = \begin{bmatrix} 0.8 \\ 0.2 \end{bmatrix}$

Eigenvalues: 1, **0.75**

Rainy now, next hours?

*RRRRDDDDDDDDDDDD*
*DDDDDDDDDDDDDD...*



Eigenvalues: 1, **0.25**

Rainy now, next hours?

*RDDDDDDDDDDDDDDDD*
*RDDDRDDDDDDDDD...*

# Markov Chain: First Results

- *Aperiodic* and *irreducible* chains are *ergodic*:
  (every state reachable after $> N$ steps, irregular return time)
  - Convergence towards a unique *equilibrium distribution* $\boldsymbol{p}^*$
- Equilibrium distribution $\boldsymbol{p}^*$
  - Eigenvector of $T$ with eigenvalue $\lambda = 1$:

$$T\boldsymbol{p}^* = \boldsymbol{p}^*$$

  - Rate of convergence:

Exponential decay with second largest eigenvalue $\propto |\lambda_2|^n$

*Only useful if we can design chain with desired equilibrium distribution!*

# Detailed Balance

- Special property of some Markov chains

  Distribution $p$ satisfies *detailed balance* if the total flow of probability between every pair of states is equal, (we have a local equilibrium):

$$p(l \leftarrow m)p(m) = p(m \leftarrow l)p(l)$$

- Detailed balance implies: $p$ is the equilibrium distribution

$$(T\boldsymbol{p})_l = \sum_m T_{lm} p_m = \sum_m T_{ml} p_l = p_l$$

- Most MCMC methods construct chains which satisfies detailed balance.

# The Metropolis-Hastings Algorithm

MCMC to draw samples from an arbitrary distribution

# Idea of Metropolis Hastings algorithm

- Design a Markov Chain, which satisfies the detailed balance condition

$$T_{MH}(x' \leftarrow x)P(x) = T_{MH}(x \leftarrow x')P(x')$$

- *Ergodicity ensures that chain converges to this distribution*

# Attempt 1: A simple algorithm

- Initialize with sample $\boldsymbol{x}$
- Generate next sample, with current sample $\boldsymbol{x}$
  1. Draw a sample $\boldsymbol{x}'$ from $Q(\boldsymbol{x}'|\boldsymbol{x})$ (“proposal”)
  2. Emit current state $\boldsymbol{x}$ as sample

- It’s a Markov chain
- Need to choose Q for every P to satisfy detailed balance

$$Q(x' \leftarrow x)P(x) = Q(x \leftarrow x')P(x')$$

# Attempt 2: More general solution

- Initialize with sample $\boldsymbol{x}$
- Generate next sample, with current sample $\boldsymbol{x}$
  1. Draw a sample $\boldsymbol{x}'$ from $Q(\boldsymbol{x}'|\boldsymbol{x})$ ("proposal")
  2. With *probability* $\alpha(\mathrm{x}, \mathrm{x}')$ emit $\boldsymbol{x}'$ as new sample
  3. With *probability* $1 - \alpha(\mathrm{x}, \mathrm{x}')$ emit $x$ as new sample

- It's a Markov chain
- Decouples Q from P through acceptance rule a
  - How to choose a?

# What is the acceptance function a?

$$T_{MH}(x' \leftarrow x)P(x) = T_{MH}(x \leftarrow x')P(x')$$
$$a(x'|x)Q(x'|x)P(x) = a(x|x')Q(x|x')P(x')$$

*Case A: x' = x*

- Detailed balance trivially satisfied for every a(x',x)

*Case B:* $x' \neq x$

- We have the following requirement

$$\frac{a(x'|x)}{a(x|x')} = \frac{Q(x|x')P(x')}{Q(x'|x)P(x)}$$

# What is the acceptance function a?

*Requirement: Choose* $a(x'|x)$ *such that*

$$\frac{a(x'|x)}{a(x|x')} = \frac{Q(x|x')P(x')}{Q(x'|x)P(x)}$$

- $a(x|x')$ is probability distribution $a(x|x') \leq 1$ and $a(x|x') \geq 0$
- Easy to check that:

$$a(x'|x) = \min\left(1, \frac{Q(x|x')P(x')}{Q(x'|x)P(x)}\right)$$

satisfies this property.

# What is the acceptance function a?

*Case 1:*

$$\frac{Q(x'|x)P(x)}{Q(x|x')P(x')}>1$$

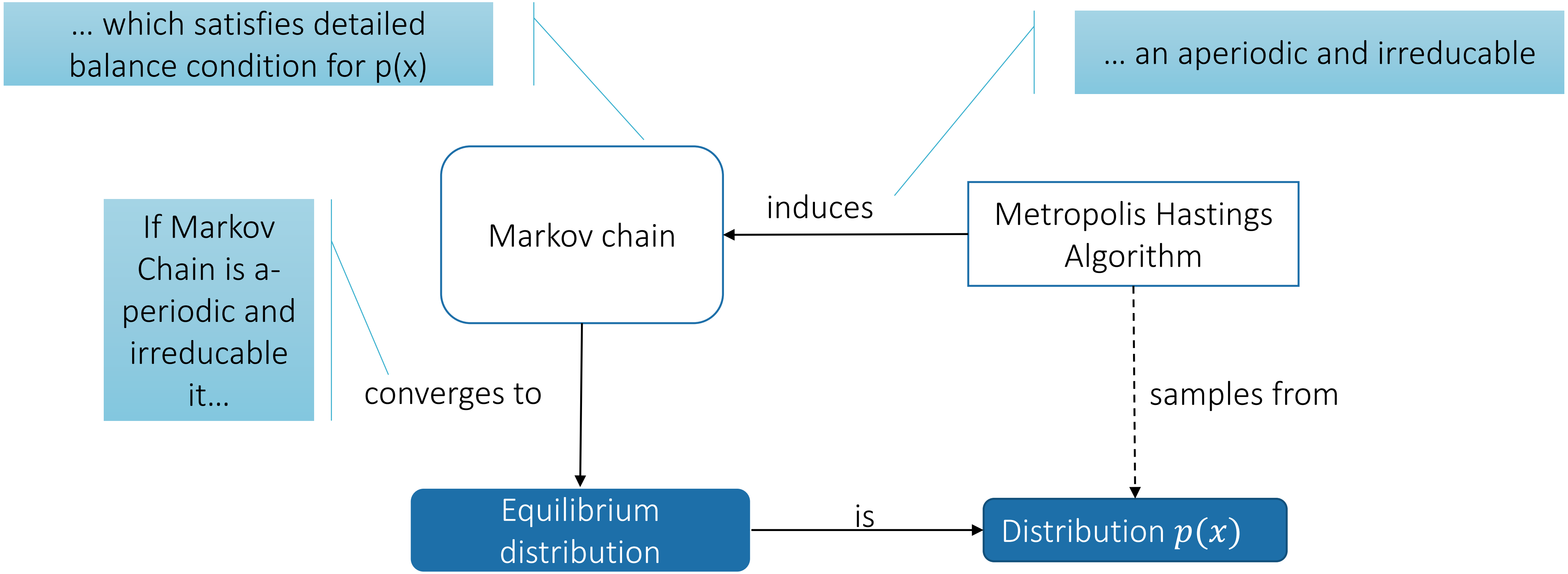
$$\frac{a(x'|x)}{a(x|x')}=\frac{\min\left(1,\frac{Q(x|x')P(x')}{Q(x'|x)P(x)}\right)}{\min\left(1,\frac{Q(x'|x)P(x)}{Q(x|x')P(x')}\right)}=\frac{\frac{Q(x|x')P(x')}{Q(x'|x)P(x)}}{1}=\frac{Q(x|x')P(x')}{Q(x'|x)P(x)}$$

*Case 2:*

$$\frac{Q(x|x')P(x')}{Q(x'|x)P(x)}>1$$

$$\frac{a(x'|x)}{a(x|x')}=\frac{\min\left(1,\frac{Q(x|x')P(x')}{Q(x'|x)P(x)}\right)}{\min\left(1,\frac{Q(x'|x)P(x)}{Q(x|x')P(x')}\right)}=\frac{1}{\frac{Q(x'|x)P(x)}{Q(x|x')P(x')}}=\frac{Q(x|x')P(x')}{Q(x'|x)P(x)}$$

# The big picture



… which satisfies detailed balance condition for p(x)

… an aperiodic and irreducable

If Markov Chain is a-periodic and irreducable it…

Markov chain

induces

Metropolis Hastings Algorithm

converges to

samples from

Equilibrium distribution

is

Distribution $p(x)$