This is a Markov process since x_{n+1} only depends on x_n.

We generalize this:

$$x_{n+1} = \sum_{k=1}^{K} a_k x_{n+1-k} + z_n$$

uncorrelated noise:

$$\langle x_{n+1-k} z_n \rangle = 0$$

for $k = 1, 2, .., K$.

The coefficients a_k define a <u>Memory function.</u>

For a Markov process:

$$\underline{\underline{a_k = a\,\delta_{k,1}}}$$

Usually, we do not know

$$a_k, \; k = 1, 2, \ldots, K.$$

Rather, we typically know the <u>autocorrelation function</u> (from e.g. experiments.):

$$C_m = \langle x_n \, x_{n+m} \rangle, \; m = 0, 1, 2, \ldots$$

Assume $C_m = 0$ for $m > M$.

We now relate C_m and a_k:

$$x_{n+m} = \sum_{k=1}^{K} a_k \, x_{n+m-k} + z_{n+m-1}.$$

$$m = 1, 2, \ldots, M.$$

Multiply by x_n and then average:

$$\langle x_n \, x_{n+m} \rangle = C_m = \sum_{k=1}^{K} a_k \, C_{m-k}$$

In matrix notation:

$$\underline{\vec{c} = \overleftrightarrow{\mathcal{C}} \cdot \vec{a}}$$

Yule - Walker equation.

$$\vec{c} = \begin{pmatrix} c_1 \\ \vdots \\ c_M \end{pmatrix} \qquad \vec{a} = \begin{pmatrix} a_1 \\ \vdots \\ a_K \end{pmatrix}$$

$$\overleftrightarrow{\mathcal{C}} = \begin{pmatrix} c_0 & c_1 & \cdots & c_{K-1} \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ c_{M-1} & \cdots & \cdots & c_{M-K} \end{pmatrix}$$

Symmetry: $\mathcal{C}_{-m} = \mathcal{C}_m$

$\overleftrightarrow{\mathcal{C}}$ is a <u>Toeplitz matrix</u>.

It is easy to invert since it is Toeplitz.

For $K < M$, $c_m = \sum_{k=1}^{K} a_k c_{m-k}$

is overdetermined.

In this case, define

$$\epsilon_m = c_m - \sum_{k=1}^{K} c_{m-k} a_k$$

$$\delta^2 = \sum_{m=1}^{M} \epsilon_m^2$$

Minimize $\delta^2 = \underbrace{\overleftrightarrow{C}^T \cdot \overleftrightarrow{C} \cdot \vec{a} = \overleftrightarrow{C}^T \cdot \vec{c}}_{\text{Solve with respect to } \vec{a}.}$ $(*)$

Why? $\delta^2 = (\vec{c}^{\,T} - \vec{a}^{\,T} \cdot \overleftrightarrow{C}^T) \cdot (\vec{c} - \overleftrightarrow{C} \cdot \vec{a})$

$$\vec{\nabla}_{\vec{a}}\, \delta^2 = 0 \implies (*).$$

Hence, knowing $\vec{c} \implies \vec{a}$, a_k, $k = 1, \ldots, K$.

We now generate a stochastic sequence $\{x_n\}$ where the memory function is a_k.

$$\underline{\langle z_m^2 \rangle} = \langle (x_{m+1} - \sum_{k=1}^{K}{}' a_k \, x_{m+1-k})^2 \rangle$$

$$= \langle x_{m+1}^2 \rangle - 2 \sum_{k=1}^{K}{}' a_k \langle x_{m+1} \, x_{m+1-k} \rangle$$

$$+ \sum_{k=1}^{K}{}' \sum_{l=1}^{K}{}' a_k \, a_l \langle x_{m+1-k} \, x_{m+1-l} \rangle$$

$$= c_0 - 2 \sum_{k=1}^{K}{}' a_k \, c_{-k}$$

$$+ \sum_{k=1}^{K}{}' a_k \Big(\underbrace{\sum_{l=1}^{K}{}' a_l \, c_{k-l}}_{= c_k} \Big)$$

$$\underline{= c_0 - \sum_{k=1}^{K}{}' a_k c_k .} \qquad = \langle z^2 \rangle$$

Knowing $\langle z^2 \rangle$, we may generate realizations of x_n.

$$x_{n+1} = \sum_{k=1}^{K'} a_k \, x_{n+1-k} + z_n .$$

Wiener-Lévy random walk

$$\dot{x}(t) = -\beta x(t) + \eta(t)$$

Set $\beta = 0$

$\langle \eta(t) \rangle = 0$

$\langle \eta(t') \eta(t'') \rangle = A \delta(t' - t'')$

$$t \to \underbrace{t_n = t_0 + \Delta t \, n}_{\text{discrete time.}}$$

$$x_{n+1} = x_n + z_n$$

$\beta \neq 0$:

$$x_n e^{-\beta \Delta t} + z_n$$

$$z_n = \int_0^{\Delta t} \eta(t_n + t') \, dt'$$

Gaussian random variable with $\langle z \rangle = 0$,

$\langle z^2 \rangle = \frac{A}{2\beta}(1 - e^{-\beta \Delta t}) = A\Delta t + O(\beta)$ $\longleftarrow$ $\langle z^2 \rangle = A \Delta t$

Then we have

$$\langle x_n^2 \rangle = n A \Delta t$$

– no longer stationary!

Markov chains

x may only take on N discrete values (but $N \to \infty$).

Transition probabilities:

$$p_{\alpha\beta} = \mathrm{Prob}\{x_n = x_\beta \mid x_{n-1} = x_\alpha\}$$

States α and β.

$N \times N$ matrix: $\overleftrightarrow{P} = \{p_{\alpha\beta}\}$

Individual probabilities:

$$\vec{p} = \{p_\alpha\}.$$

Reversible Markov chains

$$\boxed{p_\alpha P_{\alpha\beta} = p_\beta P_{\beta\alpha}}$$

This property is called <u>detailed balance</u>.

$\overleftrightarrow{P}$ contains N^2 elements $P_{\alpha\beta}$.

$p_\alpha P_{\alpha\beta} = p_\beta P_{\beta\alpha}$ constitute $\frac{N(N-1)}{2}$ equations.

There are not equations enough to determine $\overleftrightarrow{P}$ given $\vec{p}$.

For a given $\vec{p} = \{p_\alpha\}$ there are many $\overleftrightarrow{P}$ that fulfill <u>detailed balance</u>.

One possible choice:

Asymmetric rule

(= Metropolis)

Given a state α.

We define a set of neighboring states $\{\beta\}$.

The number of neighboring states is z.

We now pick one of the neighboring states β.

The probability for this is

$$\boxed{\pi_{\alpha\beta} = \frac{1}{z}}$$

- All neighboring states are equaly liable for being picked.

The neighborhood must be constructed in such a way that

$$\boxed{\pi_{\alpha\beta} = \pi_{\beta\alpha}.}$$

We now <u>define</u>:

$$\boxed{\begin{aligned} p_{\alpha\beta} &= \pi_{\alpha\beta} \quad \text{if} \quad p_\beta \geq p_\alpha \\ p_{\alpha\beta} &= \pi_{\alpha\beta} \frac{p_\beta}{p_\alpha} \quad \text{if} \quad p_\beta < p_\alpha. \end{aligned}}$$

This choice of transition probabilities fulfills detailed balance:

Assume $\quad p_\beta > p_\alpha$:

$$p_\alpha \, p_{\alpha\beta} = p_\alpha \, \pi_{\alpha\beta}$$

$$p_\beta \, p_{\beta\alpha} = p_\beta \, \pi_{\beta\alpha} \frac{p_\alpha}{p_\beta} = p_\alpha \, \pi_{\beta\alpha}$$

$$= p_\alpha \, \pi_{\alpha\beta}.$$

Another choice: <u>Symmetric rule</u>

(= Glauber)

$$\boxed{p_{\alpha\beta} = \pi_{\alpha\beta} \frac{p_\beta}{p_\alpha + p_\beta}}$$

Detailed balance is fulfilled:

$$p_\alpha \, p_{\alpha\beta} = \pi_{\alpha\beta} \frac{p_\alpha p_\beta}{p_\alpha + p_\beta}$$

$$p_\beta P_{\beta\alpha} = \pi_{\beta\alpha} \frac{p_\beta p_\alpha}{p_\beta + p_\alpha}$$

$$= \pi_{\alpha\beta} \frac{p_\alpha p_\beta}{p_\alpha + p_\beta}.$$

The Monte Carlo Method.

The theorem that lays the foundation for the Monte Carlo method:

> If a stationary Markov chain characterized by $\vec{p} = \{p_\alpha\}$ and $\overleftrightarrow{P} = \{P_{\alpha\beta}\}$ is reversible, then every state α will be visited in a sufficiently long chain with relative frequency proportional to p_α.