MCMC

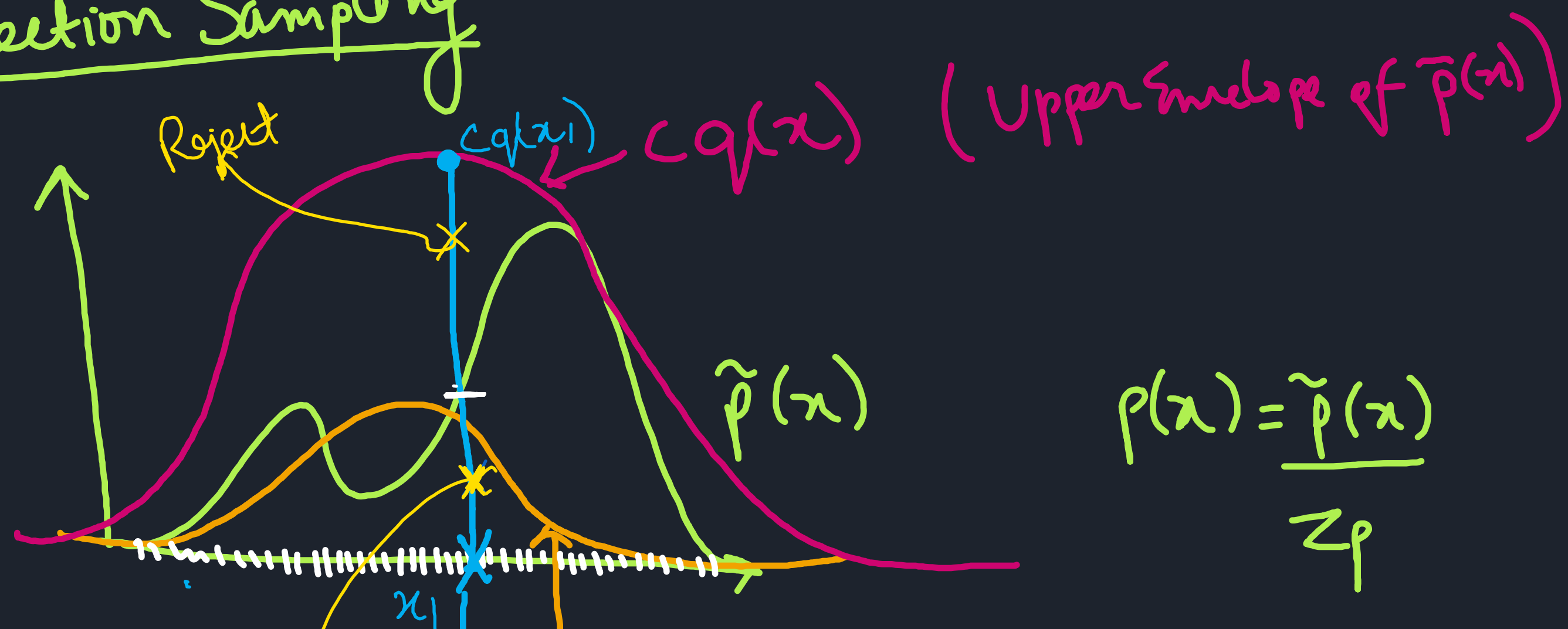# Sampling

$$P(\Theta | D) = \frac{P(D | \Theta) \cdot P(\Theta)}{P(D)}$$

Post. predictive $= P(y^* | x^*, D) = \int P(y^* | x^*, \Theta) \cdot P(\Theta | D) \, d\Theta \approx \frac{1}{N} \sum_{i=1}^{N} P(y^* | x^*, \Theta_i) \quad ; \quad \Theta_i \underset{i.i.d}{\sim} P(\Theta | D)$

(Monte Carlo)

Rejection Sampling

$(cq(x_1))$

$Cq(x)$ (Upper Envelope of $\bar{p}(x)$)

Reject

$\tilde{p}(x)$

Accept

x_1

Proposal $q(x)$

$C = 20$

$q \sim N(5, 100)$

$x_1 = 6.2$

$x_1 \sim q$

$U_1 \sim UNIF(0, Cq(x_1))$

$$p(x) = \frac{\tilde{p}(x)}{Z_p}$$

$$Z_p = \int \tilde{p}(x) dx$$

Rejection Sampling

```
For i in [0,...N_TRIES]:

    x_i ~ q
    u_i ~ UNIF(0, cq(x_i))
    if u_i > p̃(x_i): REJECT
    else: accept
```

```
For I in [0,...N]:
    x_i ~ q
    Accept x_i with prob:  p̃(x_i) / cq(x_i)
```

$$P(Accept) = \frac{Z_{\tilde{p}}}{C}$$

$$P(Sample | Accept) = \frac{P(Accept | Sample)\, P(Sample),}{P(Accept)}$$

$$= \frac{\frac{\tilde{p}(x)}{C\,q(x)}\; q(x)}{P(Accept)}$$

$$= \frac{\frac{\tilde{p}(x)}{C}}{\frac{Z_{\tilde{p}}}{C}}$$

$$= p(x)$$

$$P(Accept) = \int \frac{\tilde{p}(x)}{C}\, dx$$

$$= \frac{Z_{\tilde{p}}}{C}$$

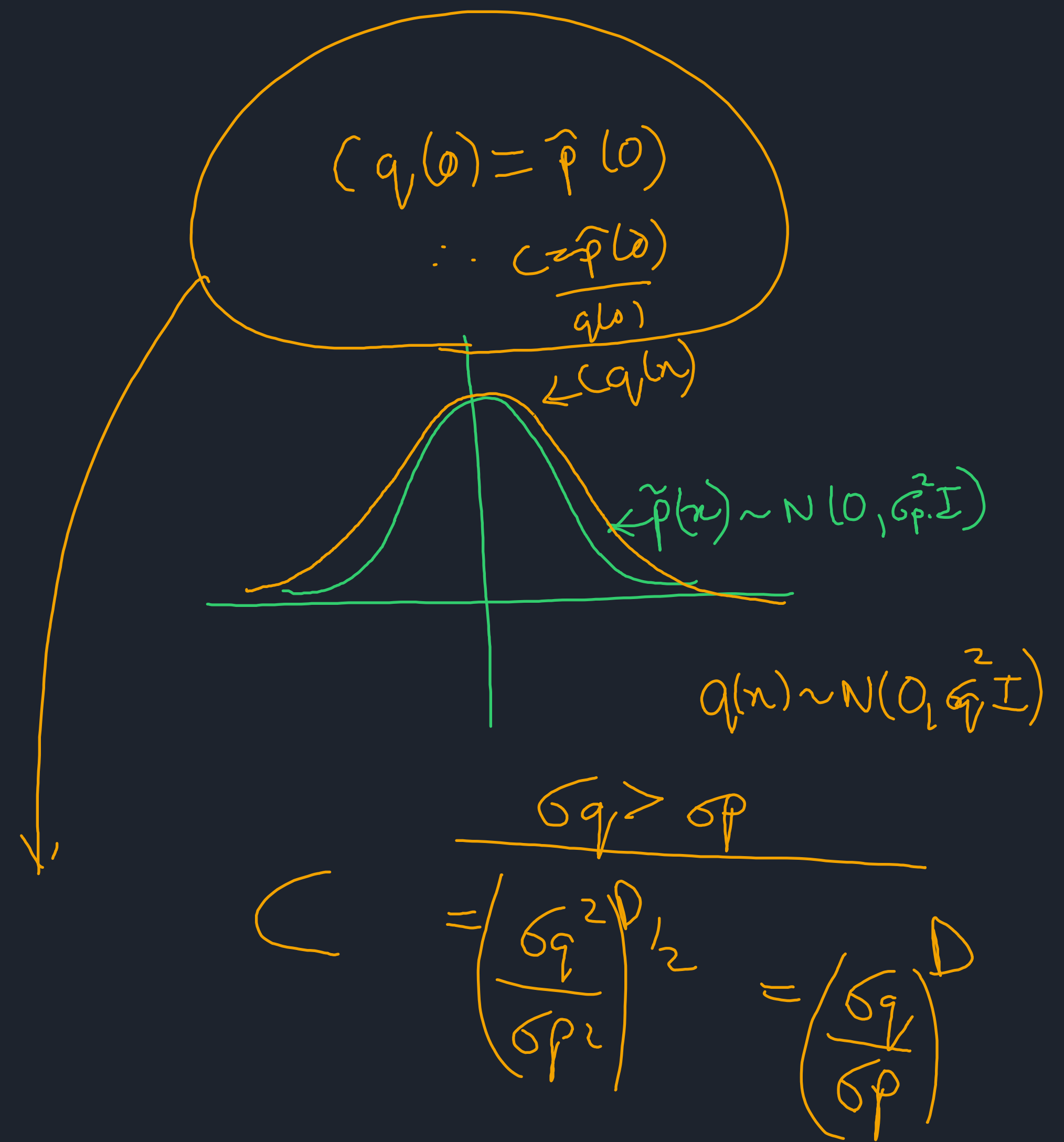$$P(\theta | D) = \frac{P(D | \theta) \cdot P(\theta)}{P(D)} = \frac{\tilde{p}(\theta)}{Z_p}$$
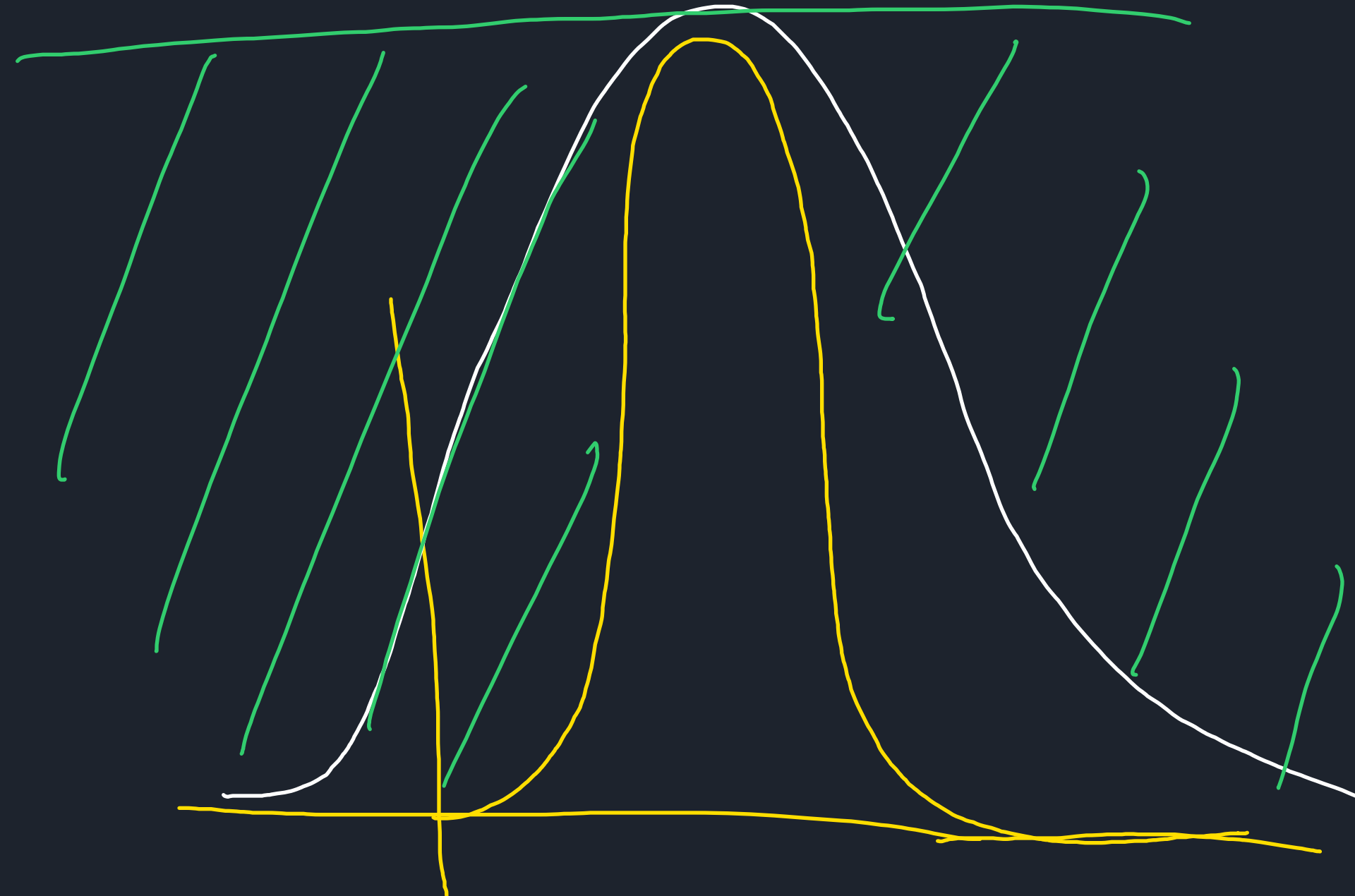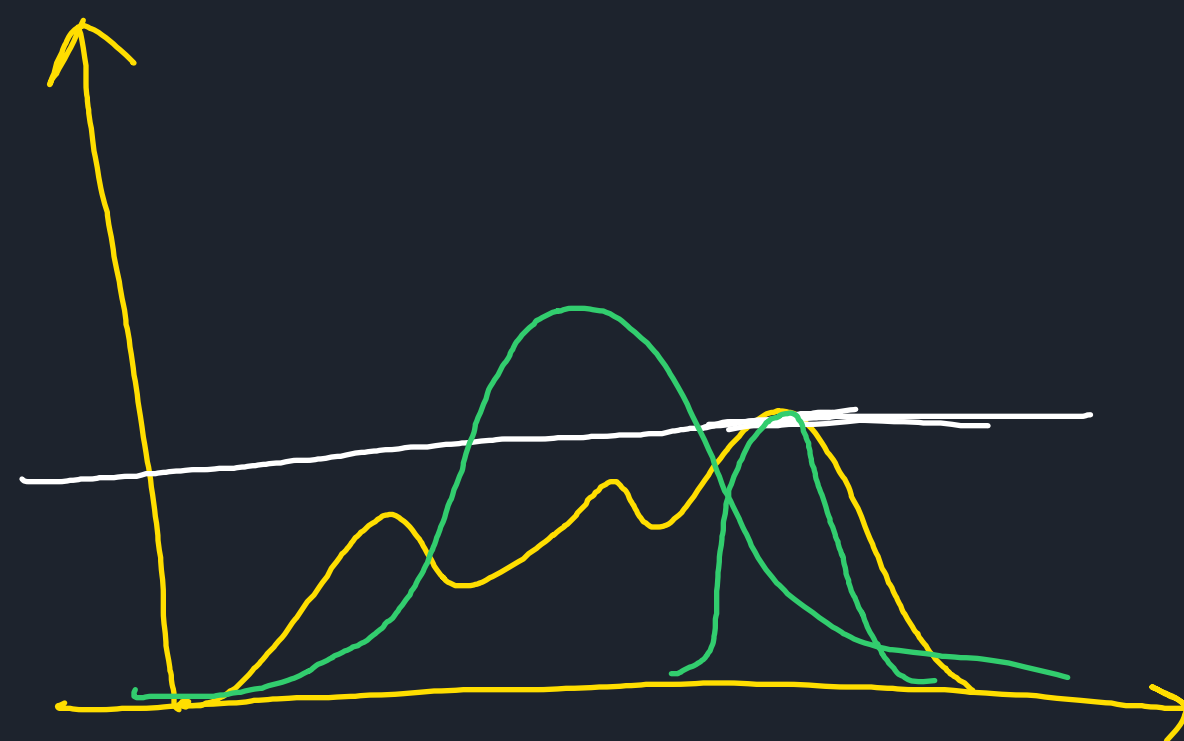
Limitations of Rejection Sampling

1) $P(\text{accept}) \not\propto \dfrac{1}{C}$; very wasteful

2) Hard to choose 'q'

3) high dimensions. ; $P(\text{Acceptance})$ very low
$$= \left(\dfrac{\sigma_p}{\sigma_q}\right)^D$$

$$(q(0) = \hat{p}(0))$$

$$\therefore \left(\dfrac{C \cdot \hat{p}(0)}{q(0)}\right)$$

$\leftarrow (C \, q(x))$

$\leftarrow \tilde{p}(x) \sim N(0, \sigma_p^2 \cdot I)$

$$q(x) \sim N(0, \sigma_q^2 I)$$

$$C = \dfrac{\sigma_q > \sigma_p}{\left(\dfrac{\sigma_q^2 D}{\sigma_p^2}\right)^{\frac{1}{2}}} = \left(\dfrac{\sigma_q}{\sigma_p}\right)^D$$

$$\text{MVN : PDF} \propto \frac{1}{\left| (2\pi\Sigma) \right|^{1/2}}$$

$$\Sigma = \sigma_q^2 I = \begin{bmatrix} \sigma_q^2 & & & \\ & \sigma_q^2 & & \\ & & \ddots & \\ & & & \sigma_q^2 \end{bmatrix}_{D \times D}$$

$$= \left(\sigma_q^2 \right)^{\frac{D}{2}}$$

$$PDF = \frac{1}{|2\pi\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\right)$$

MODE

$x_1 \sim q$ $x_3 \sim q$ $x_2 \sim q$

x_t
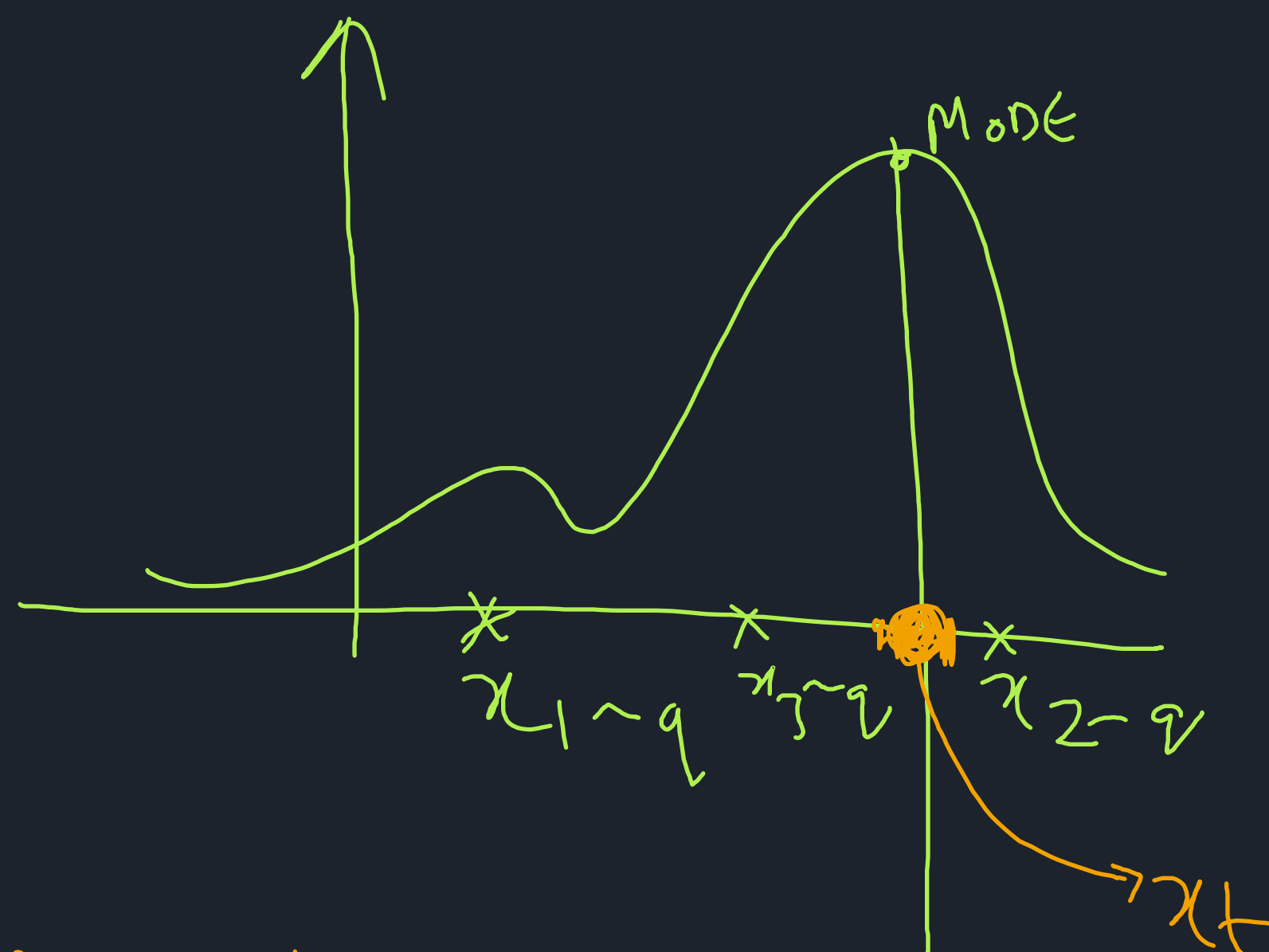
leverage when you are near mode

$x_{t+1} = x_t \pm 0.2$

$x_{t+1} \sim N(x_t, \sigma = 1)$

Stationary distribution

$$\pi_t(j) = P(\text{Being in state } j \text{ at time } t)$$

$$\pi_0 = \begin{bmatrix} 0.8 \\ 0.2 \end{bmatrix}$$

$$\pi_1(S) = 0.8 \times 0.8 + 0.2 \times 0.1 = 0.66$$

$$\pi_1(R) = 0.34$$

$$\pi_1 = \begin{bmatrix} 0.66 \\ .34 \end{bmatrix}$$

$$\pi_2(S) = \pi_1(S) * P(S \to S) \\ + \pi_1(R) * P(R \to S) \\ = 0.562$$

Diagram labels:
- Start → S: 0.8
- Start → R: 0.2
- S → R: 0.2
- R → S: 0.1
- S self-loop: 0.8
- R self-loop: 0.9

$$\pi_0 = \begin{bmatrix} 0.8 & 0.2 \end{bmatrix}_{1 \times 2}$$

← Start in S

Start in R

$$A = \begin{matrix} S \\ R \end{matrix} \begin{bmatrix} 0.8 & 0.2 \\ 0.1 & 0.9 \end{bmatrix}_{2 \times 2}$$

S R

Next close S

go from $R \to S$

$$\pi_1 = \pi_0 A$$

$$\pi_{t+1} = \pi_t A$$