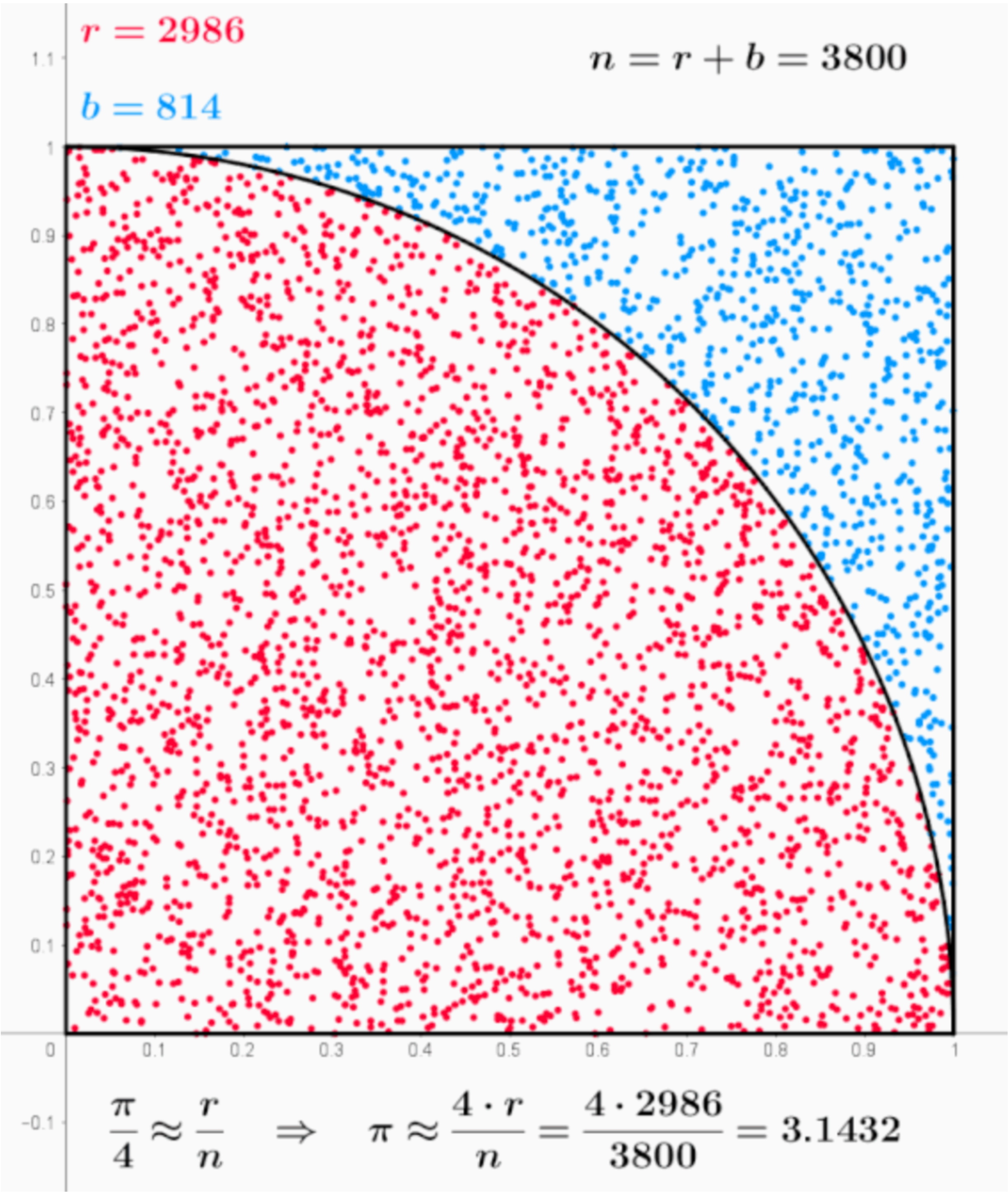
Markov Chain Monte Carlo Methods

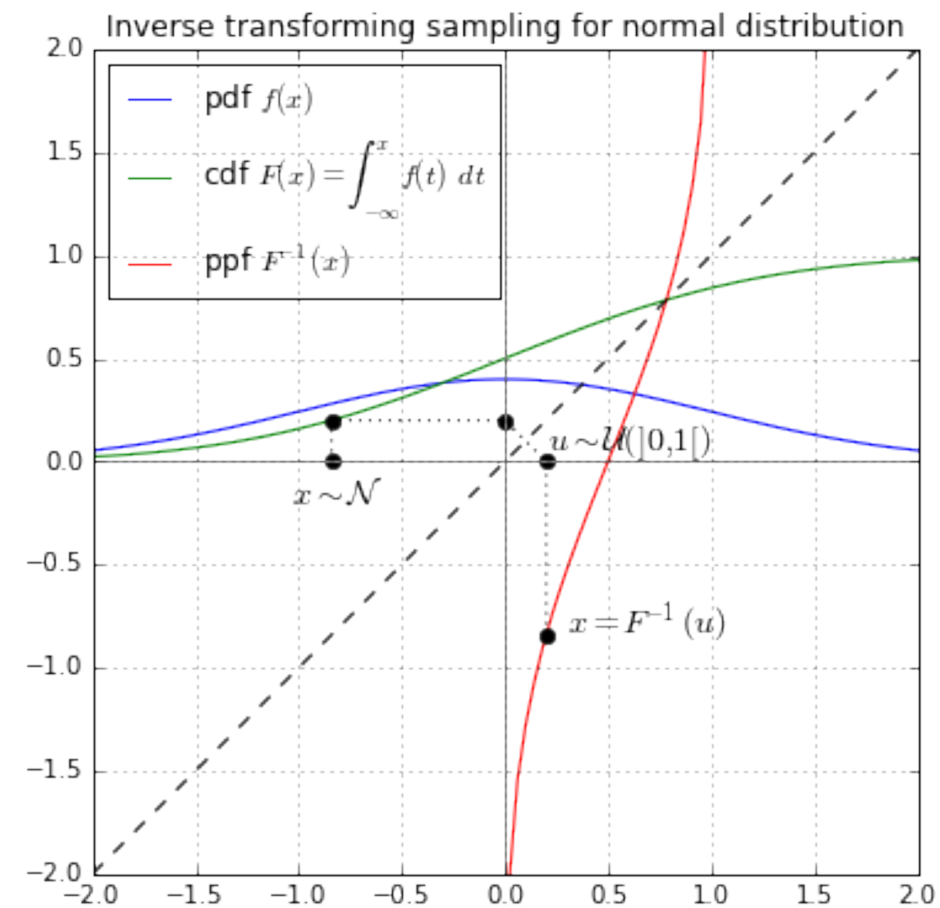
Monte Carlo Methods



Inverse transform sampling

$$
\begin{aligned}
& \Pr(X \le x) \\
= {} & \Pr(F_X^{-1}(U) \le x) \\
= {} & \Pr(U \le F_X(x)) \\
= {} & F_X(x)
\end{aligned}
$$

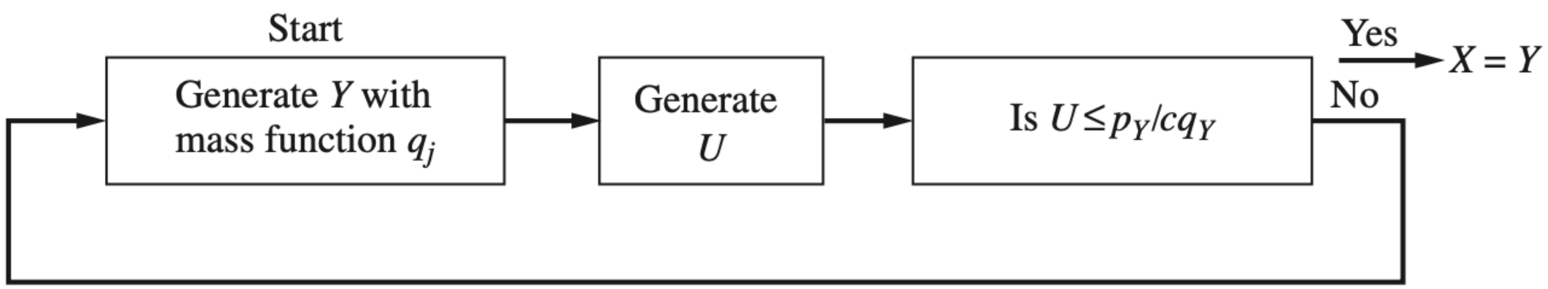
$$\implies X \sim F_X^{-1}(U)$$

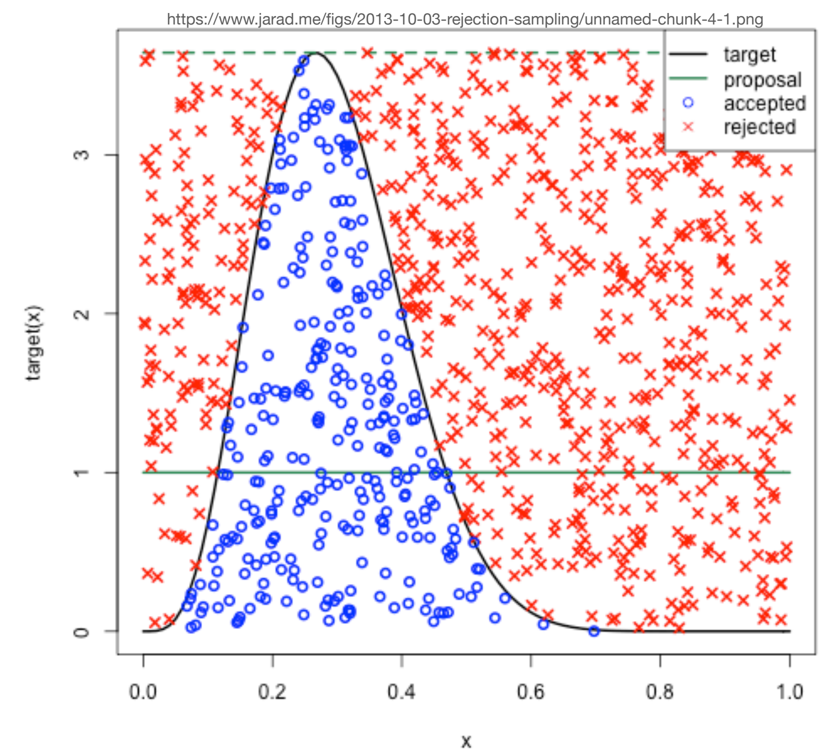


https://upload.wikimedia.org/wikipedia/commons/6/68/

u	$F^{-1}(u)$
.5	0
.975	1.95996
.995	2.5758
.999999	4.75342
$1\text{-}2^{-52}$	8.12589

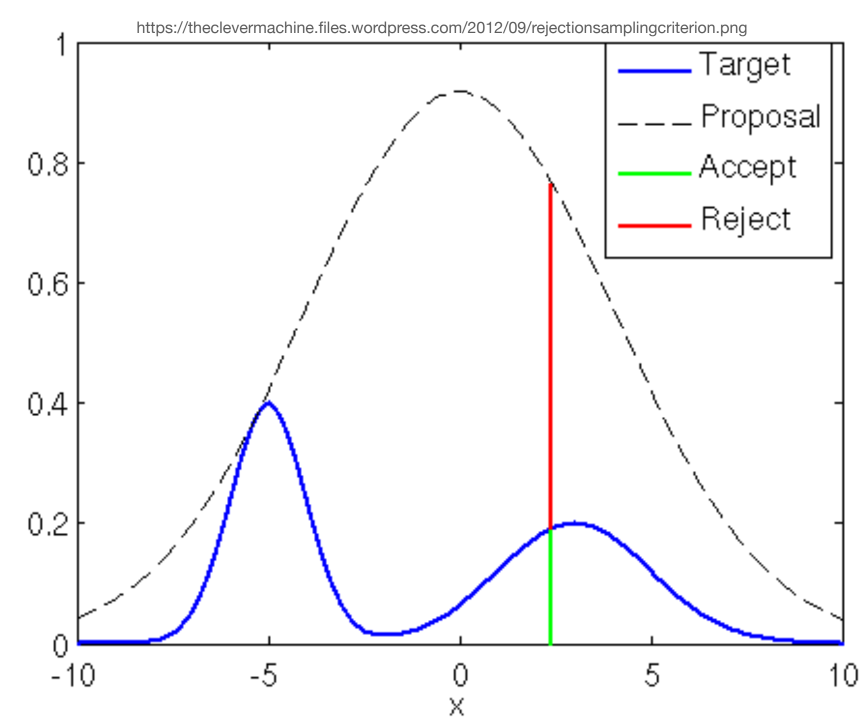
Rejection sampling





If $u \leq \dfrac{p(y)}{cq(y)}$, *accept*

If $u > \dfrac{p(y)}{cq(y)}$, *reject*



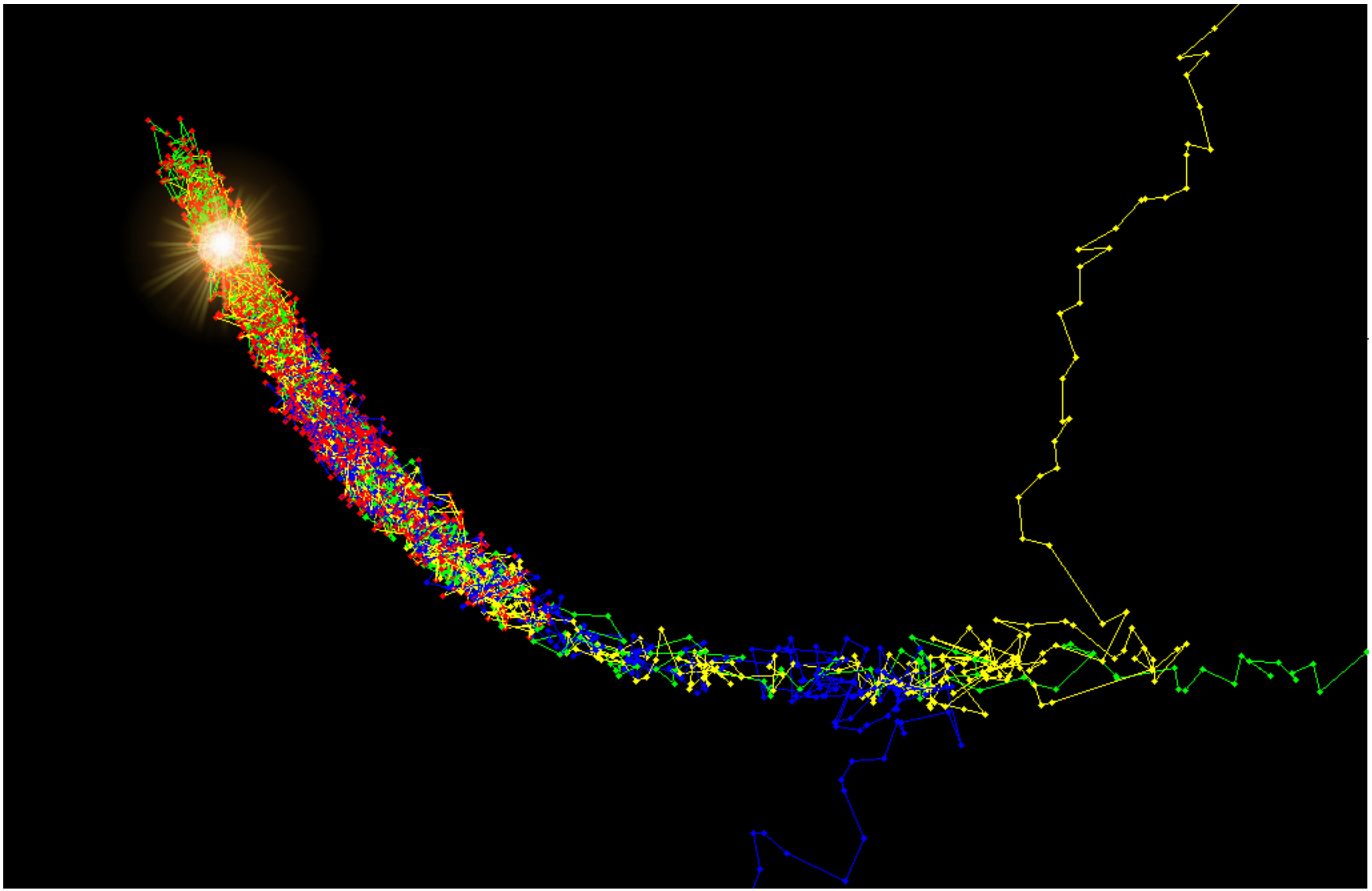
Rejection sampling: proof

$$
\begin{aligned}
P\{Y = j, \text{it is accepted}\} &= P\{Y = j\}P\{\text{accept}|Y = j\} \\
&= q_j \frac{p_j}{cq_j} \\
&= \frac{p_j}{c}
\end{aligned}
$$

$$
P\{\text{accepted}\} = \sum_j \frac{p_j}{c} = \frac{1}{c}
$$

$$
\begin{aligned}
P\{X = j\} &= \sum_n P\{j \text{ accepted on iteration } n\} \\
&= \sum_n (1 - 1/c)^{n-1} \frac{p_j}{c} \\
&= p_j \quad \square
\end{aligned}
$$

Markov Chain Monte Carlo Methods



https://en.wikipedia.org/wiki/File:3dRosenbrock.png

Hastings algorithm

Target distribution: $P(x) = cf(x)$

Choose $x_0, g(x \mid y)$

$$x' \sim g(x' \mid x_t)$$

$$\alpha = f(x')/f(x_t)$$

If $u \leq \alpha$, *accept*

If $u > \alpha$, *reject*

Hastings algorithm: derivation

$$P(x'|x)P(x) = P(x|x')P(x')$$

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

$$P(x'|x) = g(x'|x)A(x',x)$$

$$\implies \frac{A(x',x)}{A(x,x')} = \frac{P(x')}{P(x)}\frac{g(x|x')}{g(x'|x)}$$

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

Bayesian Inference with Hastings algorithm

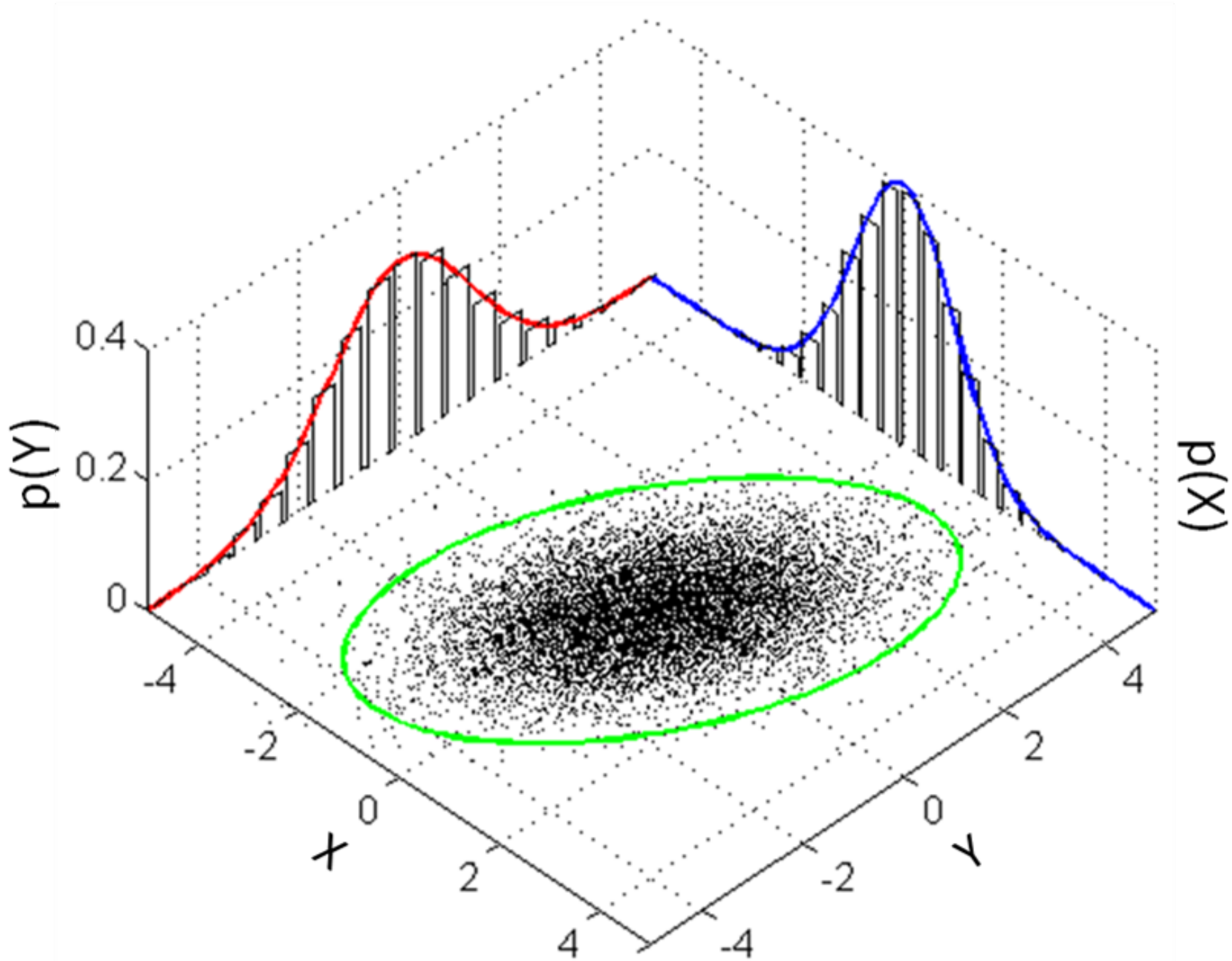
$$A(x', x) = \min\left(1, \frac{P(x')}{P(x)} \frac{g(x \mid x')}{g(x' \mid x)}\right)$$

$$P(H \mid E) = \frac{P(E \mid H) P(H)}{P(E)}$$

$$\implies A(x', x) = \min\left(1, \frac{P(x' \mid E)}{P(x \mid E)} \frac{g(x \mid x')}{g(x' \mid x)}\right)$$

$$\implies A(x', x) = \min\left(1, \frac{P(E \mid x') P(x')}{P(E \mid x) P(x)} \frac{g(x \mid x')}{g(x' \mid x)}\right)$$

Gibbs sampling



Hamiltonian Monte Carlo

https://arogozhnikov.github.io/images/ml_demonstrations/hmc_explained.png