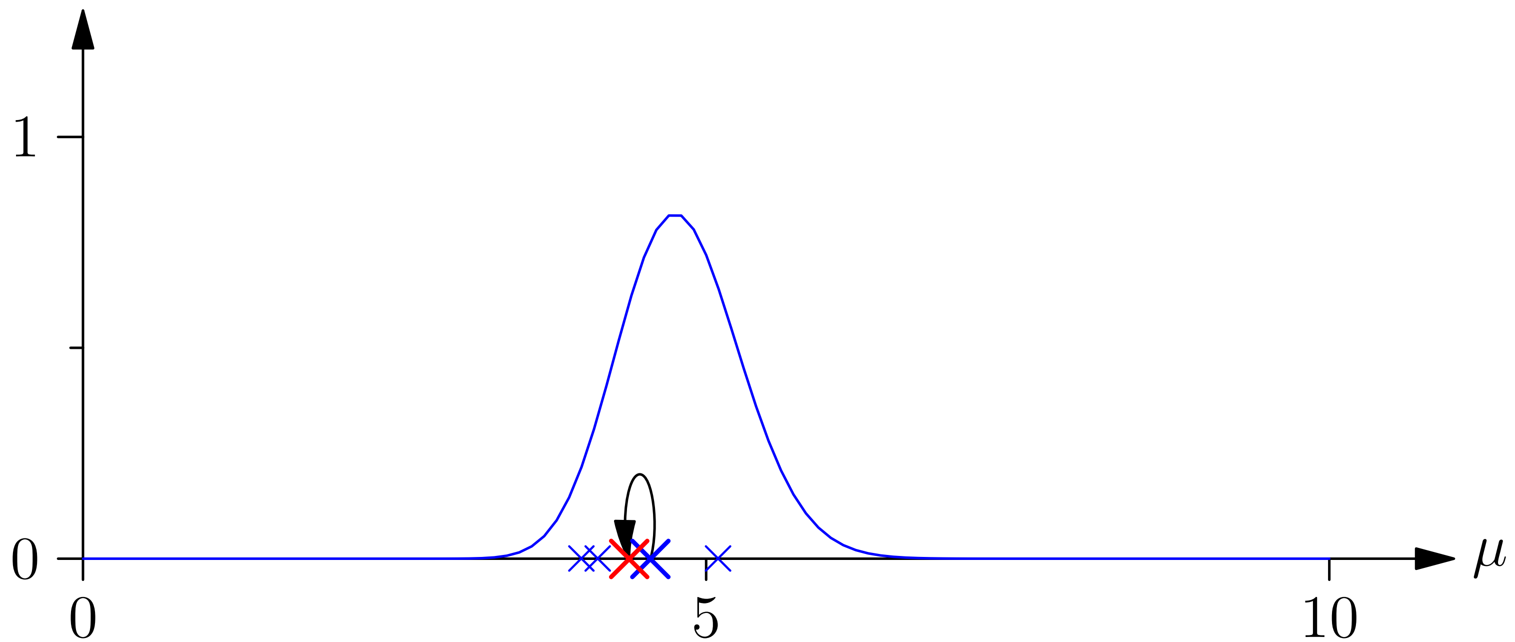
# Advanced Machine Learning

## *MCMC*

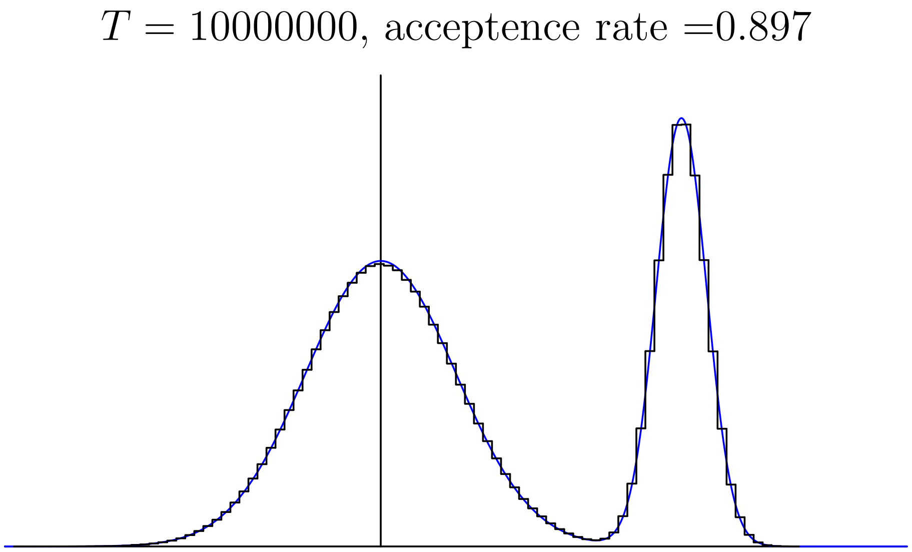
$$\mathcal{D} = \{4, 4, 6, 4, 2, 2, 5, 9, 5, 4, 3, 2, 5, 4, 4, 11, 6, 2, 3, 11\}$$




*Monte Carlo methods, MCMC, Variational Methods*

# Outline

1. **Sampling**
2. Random Number Generation
3. MCMC



# Bayesian Inference Gets Hard

- We saw that in some cases if we had a simple likelihood (normal, binomial, Poisson, multinomial) you can choose a conjugate prior (gamma-normal/Wishart, beta, gamma, Dirchlet) so that the posterior has the same form as the prior

- Very often we are working with more complex models where no conjugate prior exists

- The posterior is not described by a known distribution

- We have to work a lot harder—particularly with multivariate distributions

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$$\mathbb{P}(\boldsymbol{\theta}|\mathcal{D}) = \frac{\mathbb{P}(\mathcal{D}|\boldsymbol{\theta})\,\mathbb{P}(\boldsymbol{\theta})}{\mathbb{P}(\mathcal{D})} \qquad \text{or} \qquad f(\boldsymbol{\theta}|\mathcal{D}) = \frac{f(\mathcal{D}|\boldsymbol{\theta})\,f(\boldsymbol{\theta})}{f(\mathcal{D})}$$

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# Histograms, Samples and Means

- We could represent our posterior as a histogram, although for multivariate distributions (i.e. when we are modelling more than one variable) a histogram can be unwieldy

- A sample from the posterior distribution is often sufficient e.g. in our topic models (LDA) a typical set of topics is what we are after

- However, when samples vary a lot, often the most useful quantities are expectation, e.g.

$$\mathbb{E}[\boldsymbol{\Theta}] \qquad \mathbb{E}\left[\Theta_i^2\right] - \mathbb{E}[\Theta_i]^2$$

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- If we can draw independent **deviates** (aka **variates**), $\boldsymbol{\Theta}_i$, from our posterior distribution then we can obtain an estimate of our expectation

$$\mathbb{E}[g(\boldsymbol{\Theta})] \approx \frac{1}{n}\sum_{i=1}^{n} g(\boldsymbol{\Theta}_i)$$

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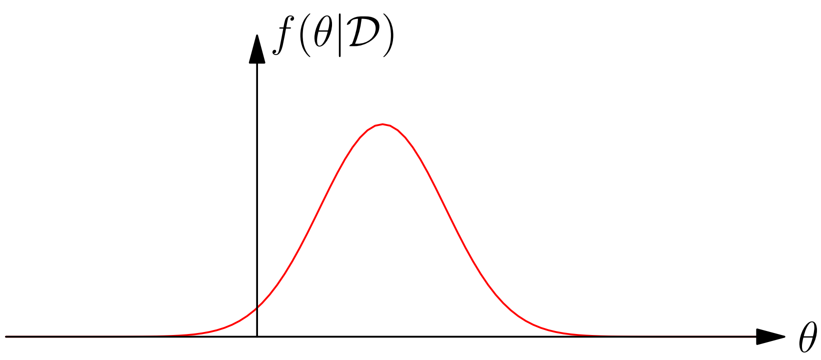


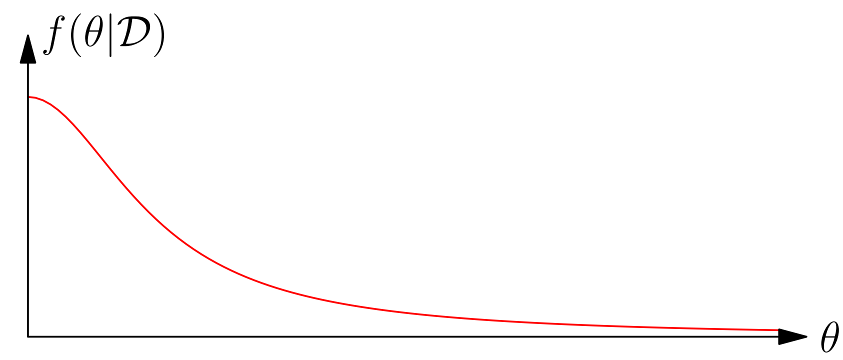

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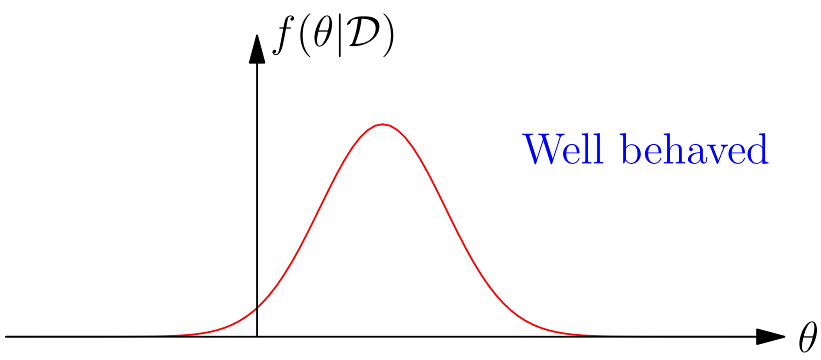


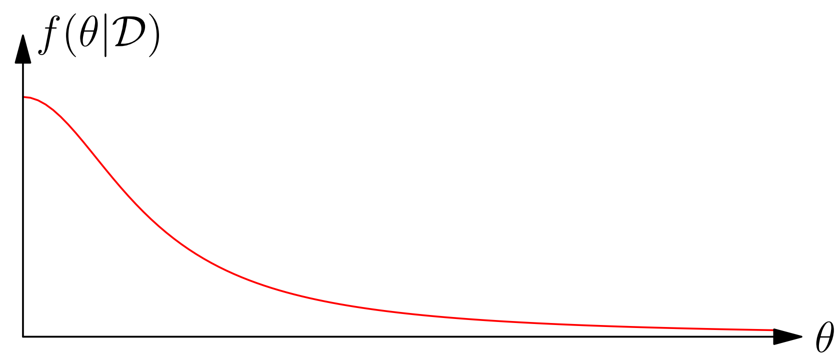

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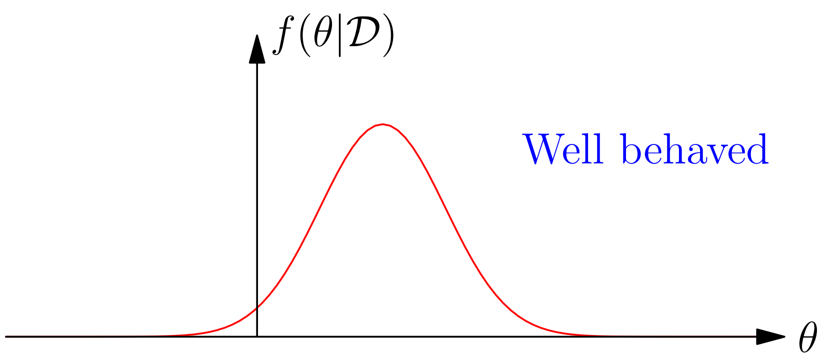


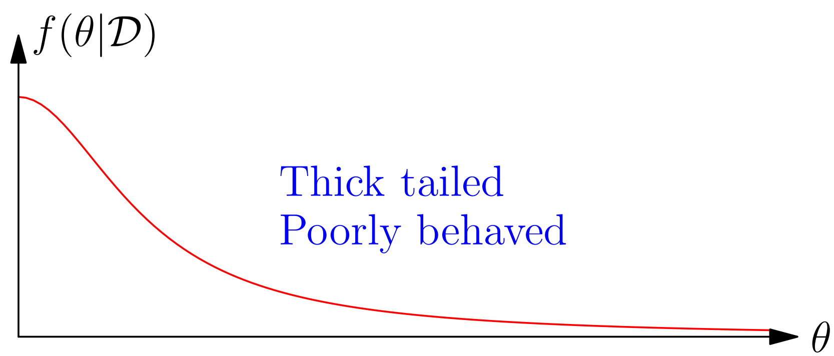

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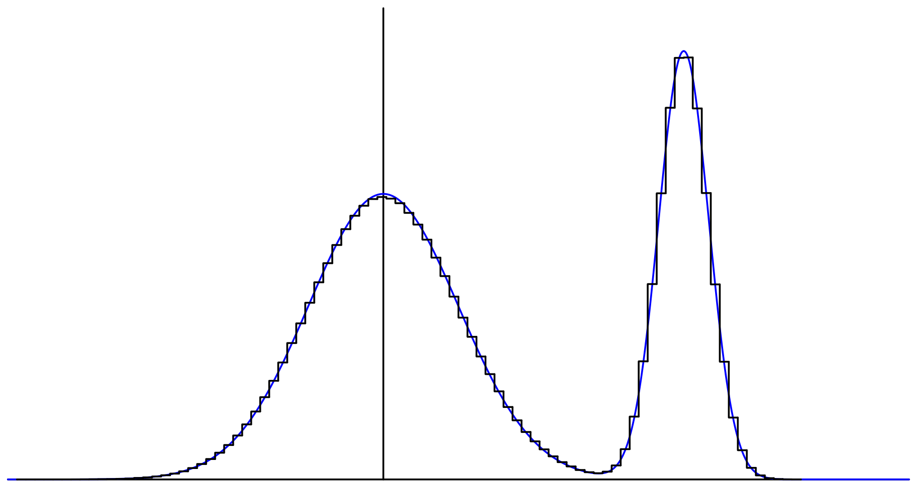

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- For some very simple distributions we can use the t**ransformation methods** to transform a uniform distribution

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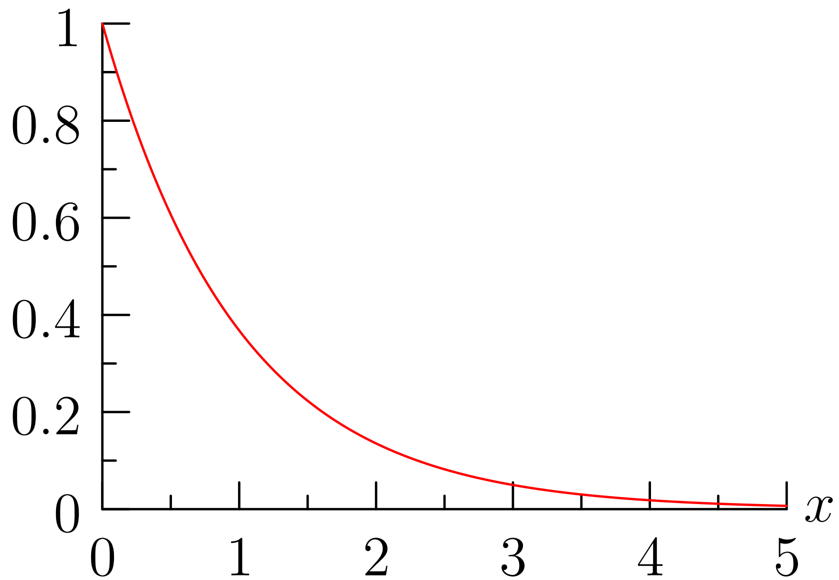


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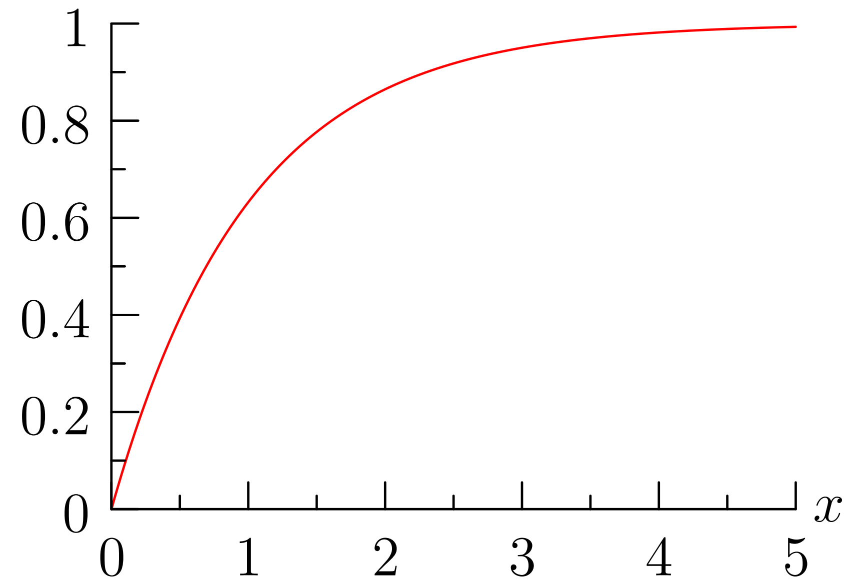

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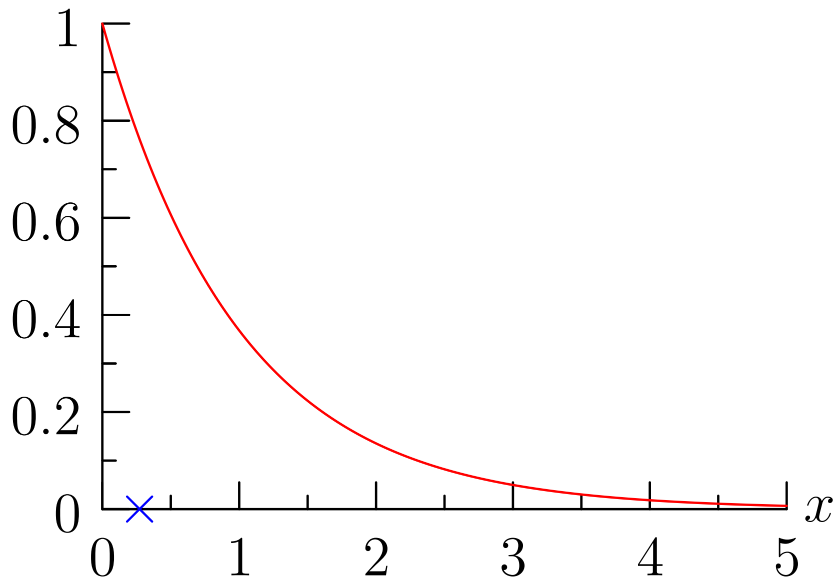


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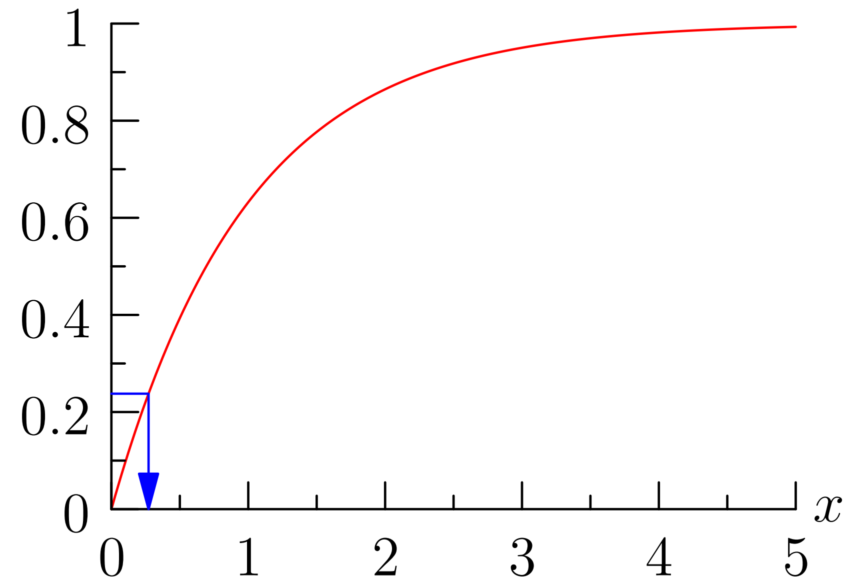

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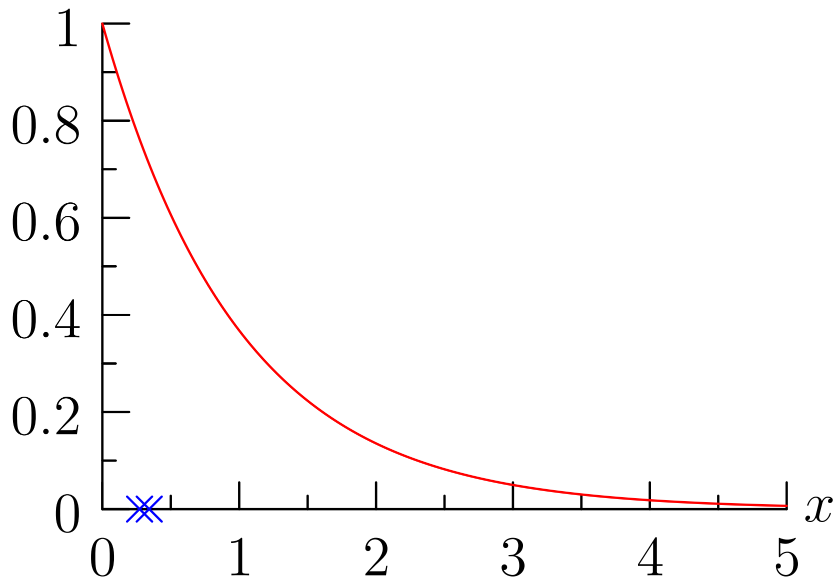


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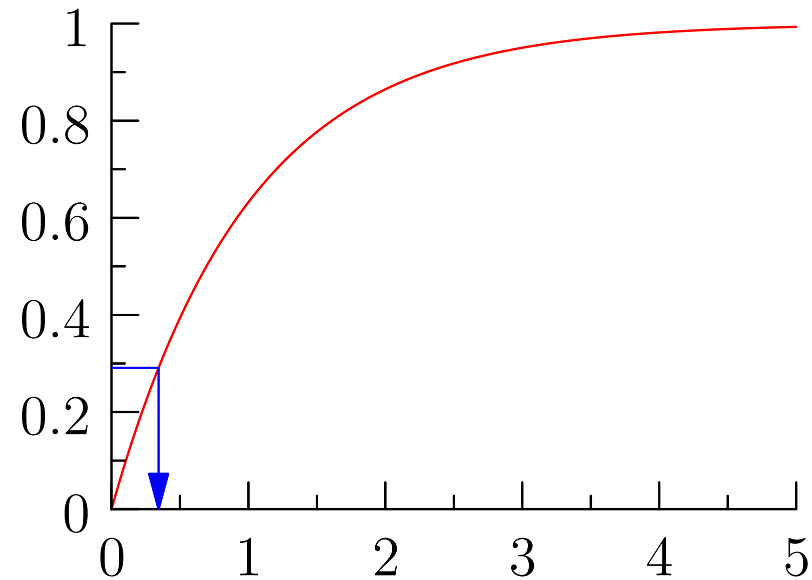

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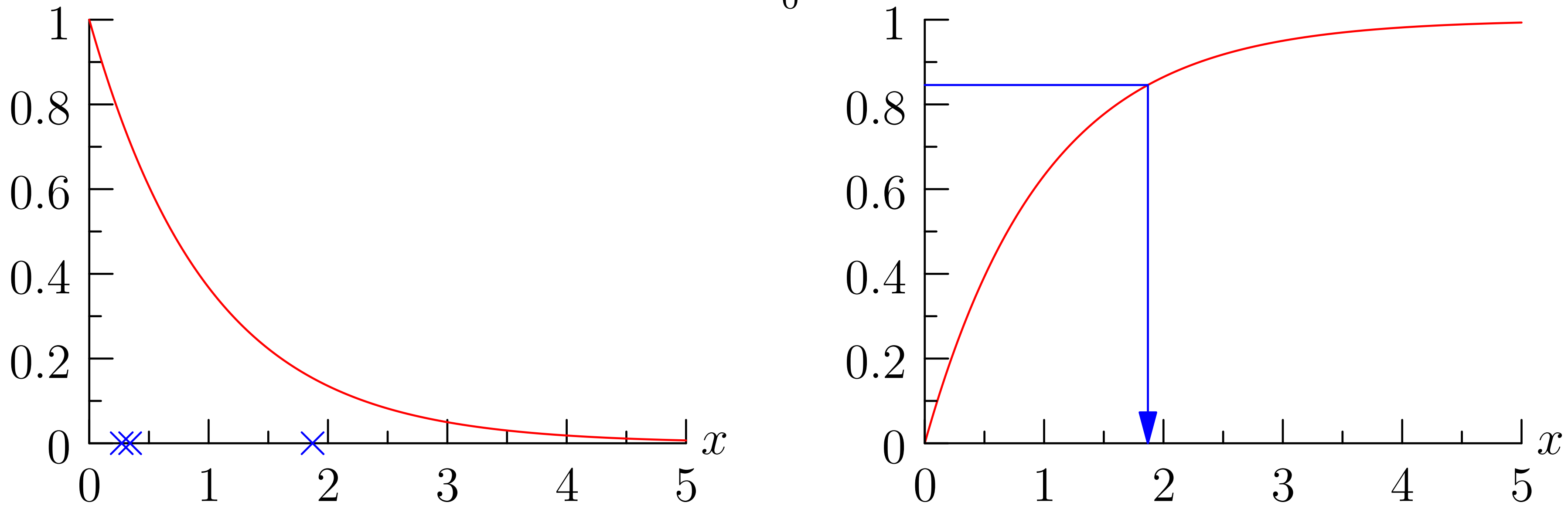

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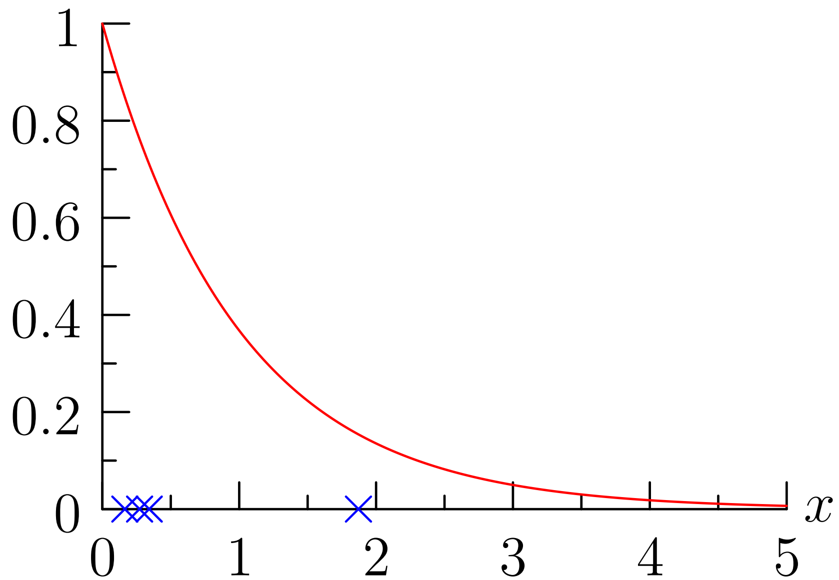

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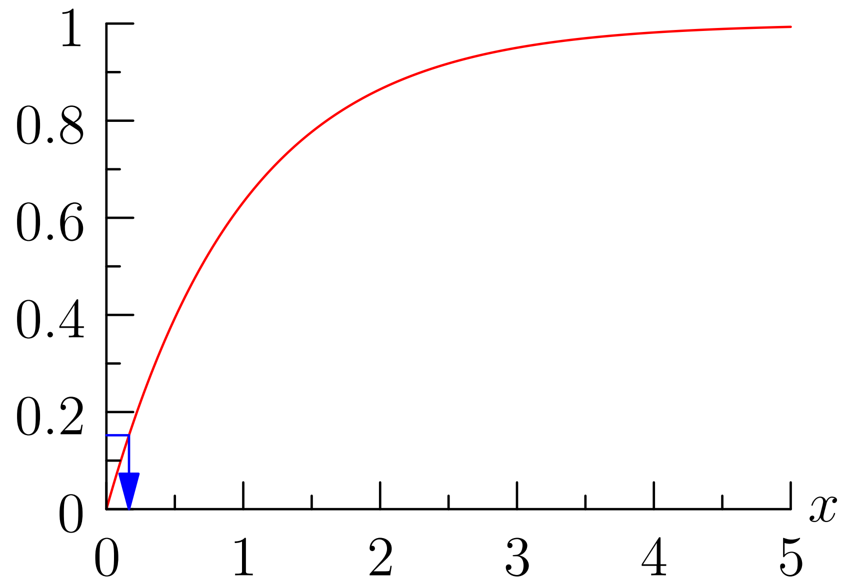

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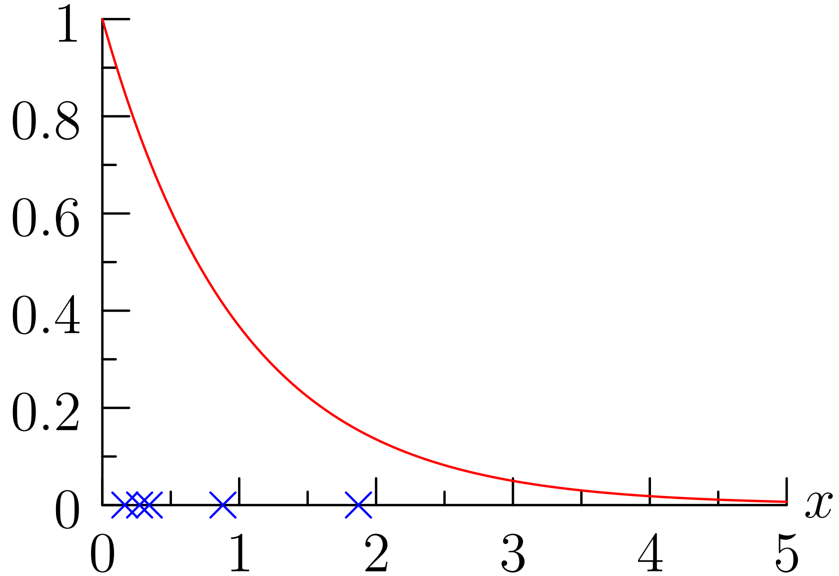


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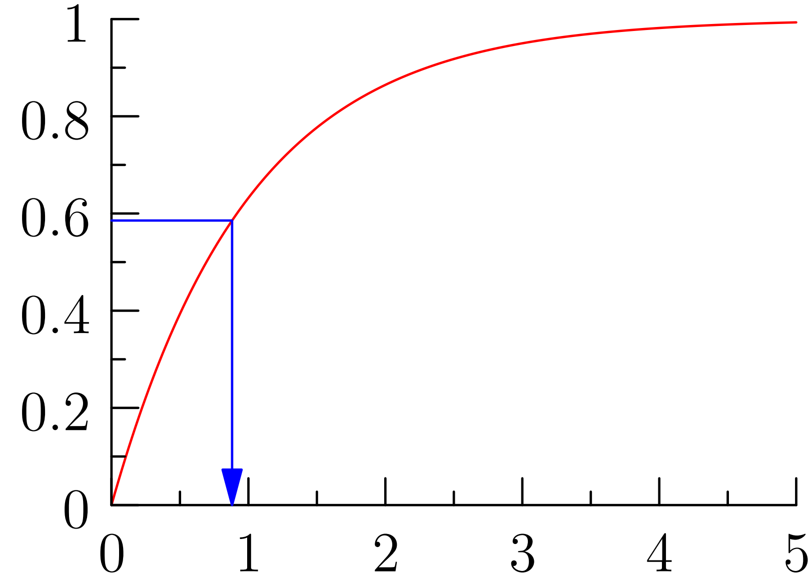

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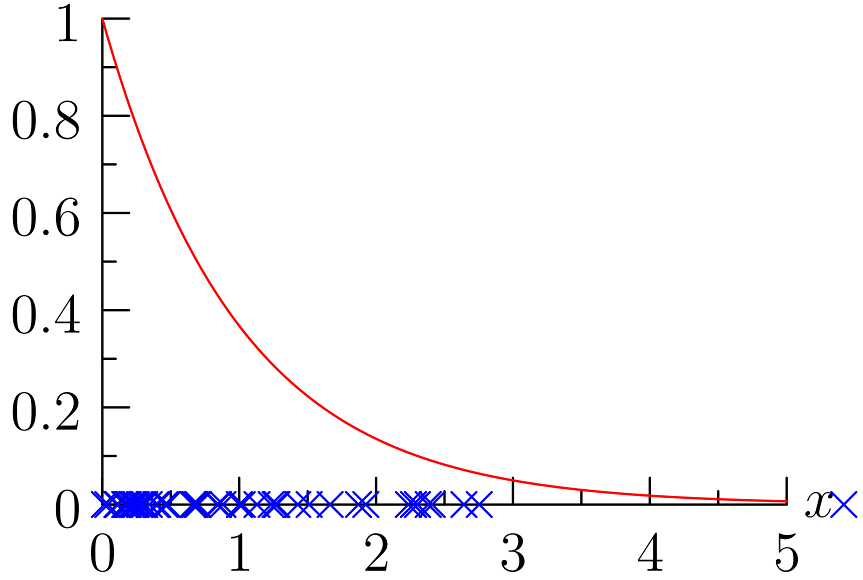


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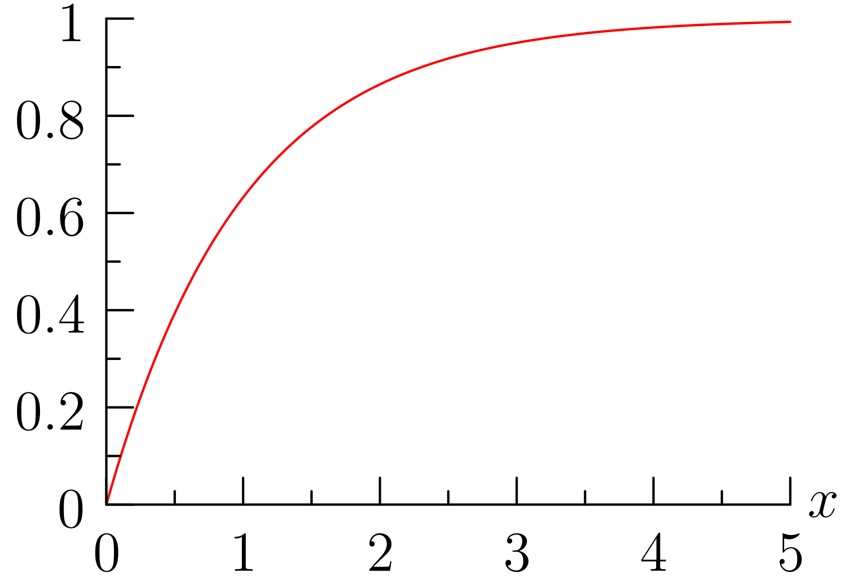

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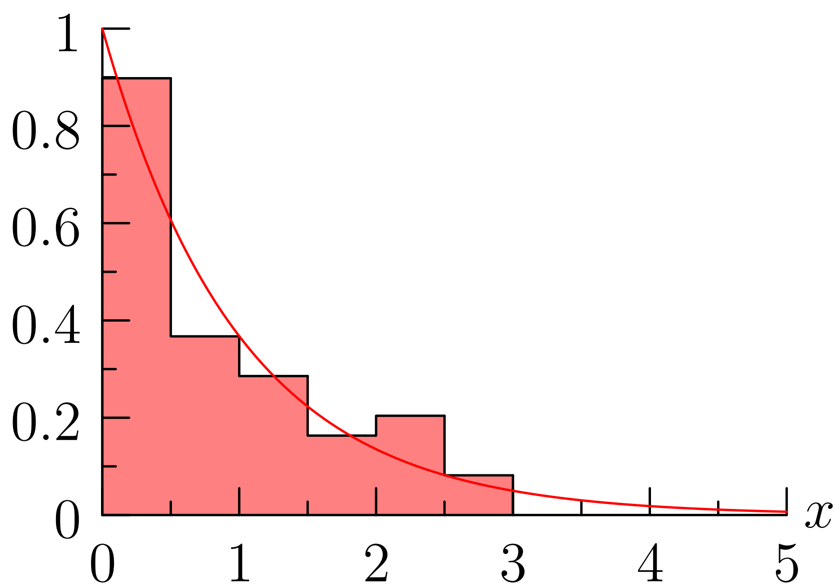


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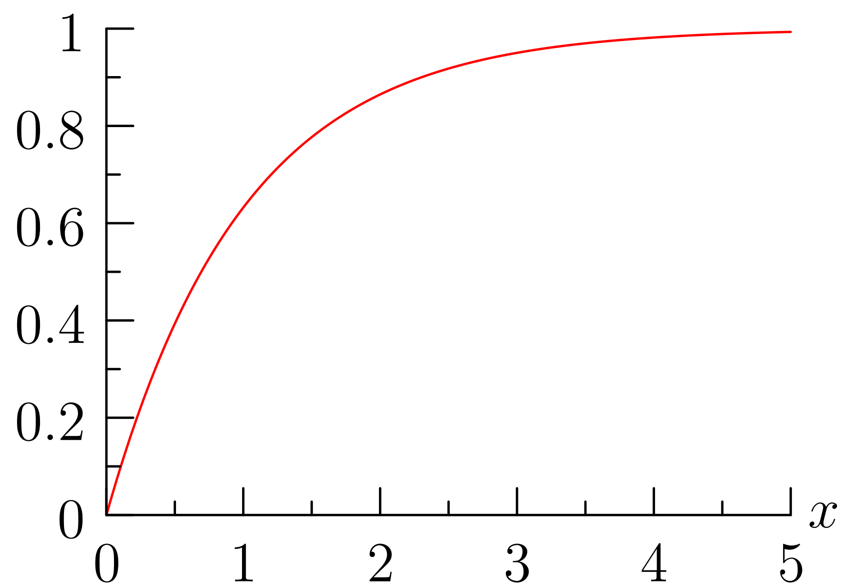

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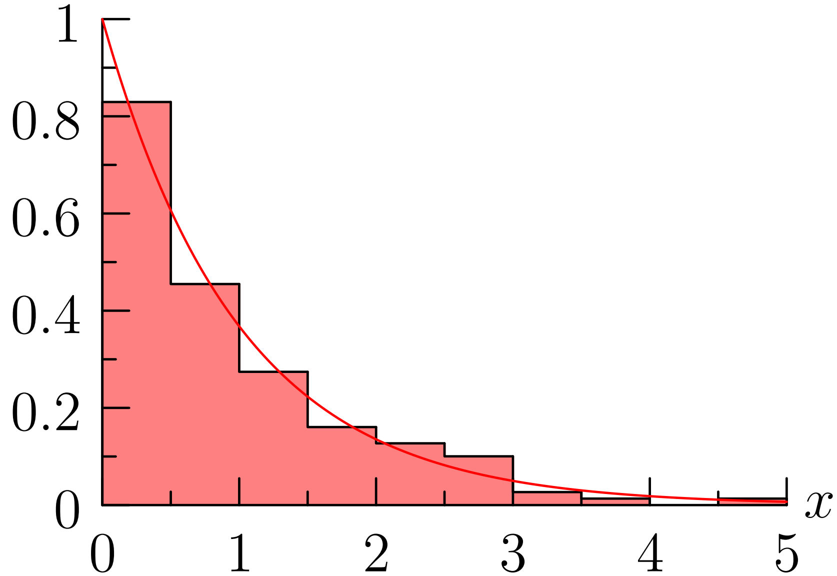


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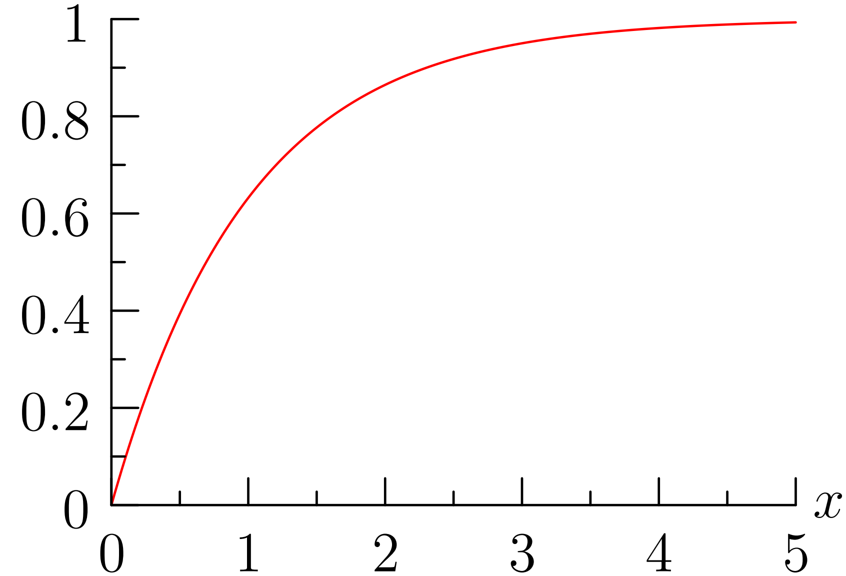

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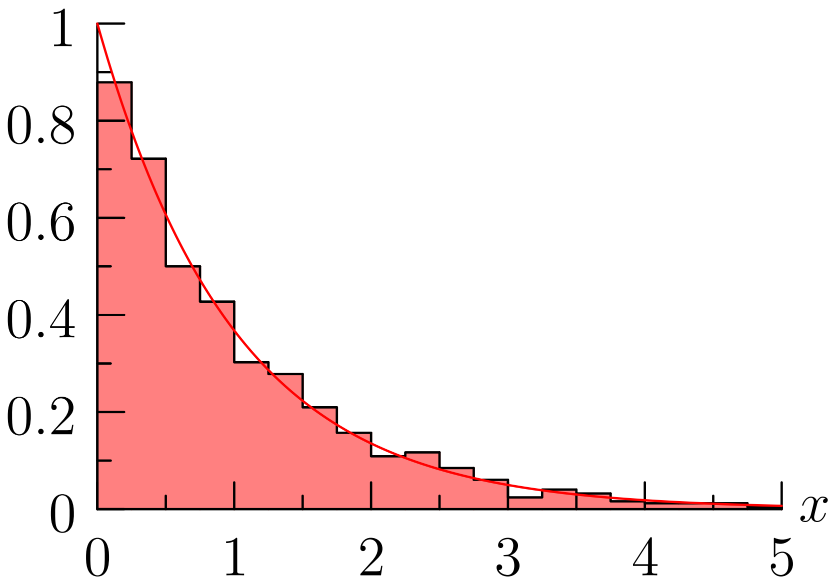


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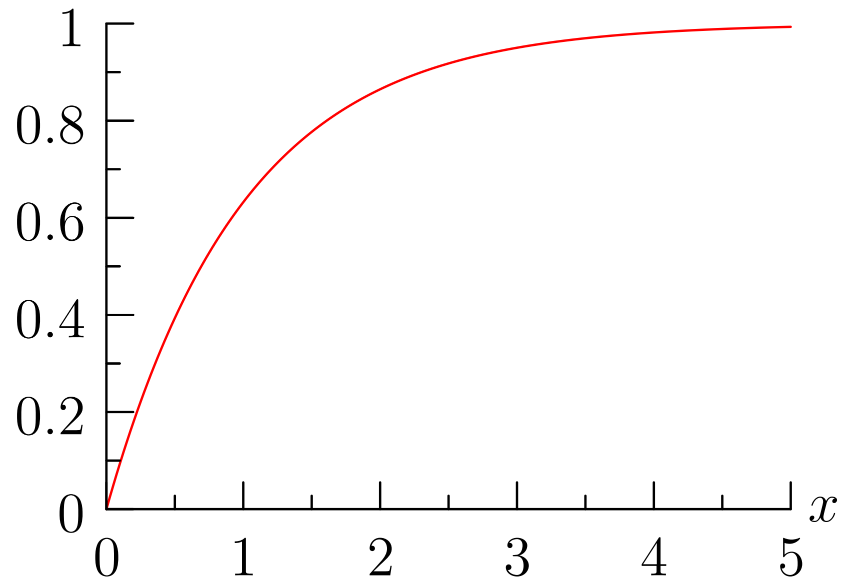

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- The transformation method only works when we can easily compute the inverse *cumulative distribution function* (CDF)
- A more general technique is the **rejection method** where we generate deviates from $g_Y(y)$ such that $c g_Y(x) \geq f_X(x)$
- To draw deviates from $f_X(x)$ we draw a deviate $Y \sim g_Y$ and then accept the deviate with probability $f_X(Y)/(c g_Y(Y))$
- The expected rejection rate is $c - 1$
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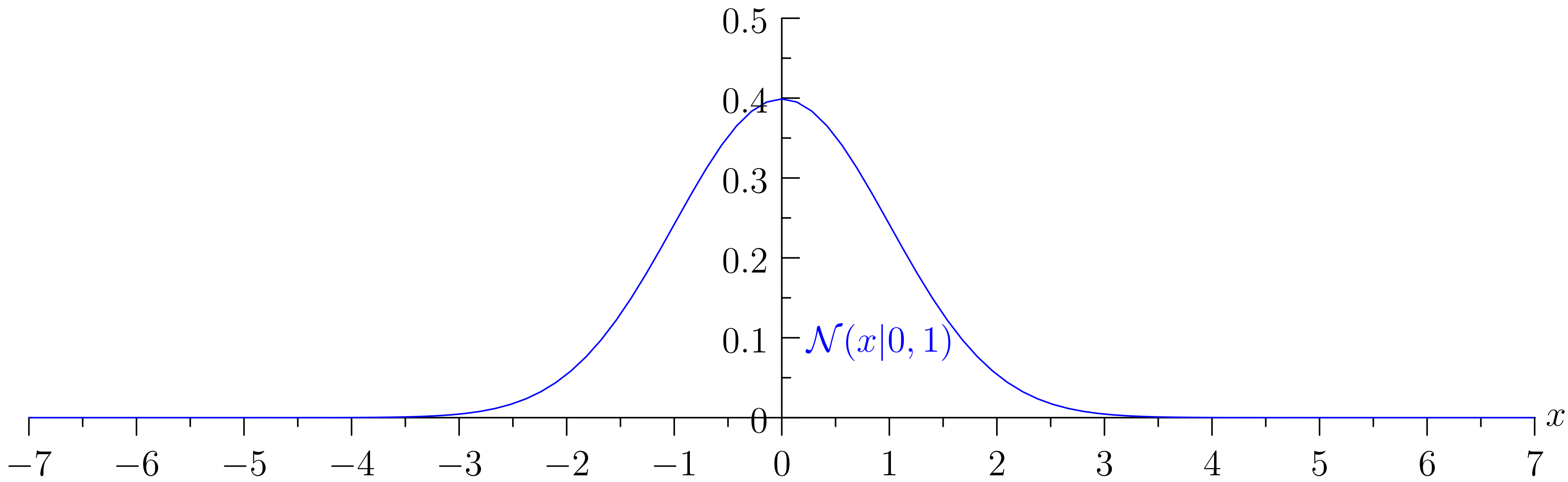

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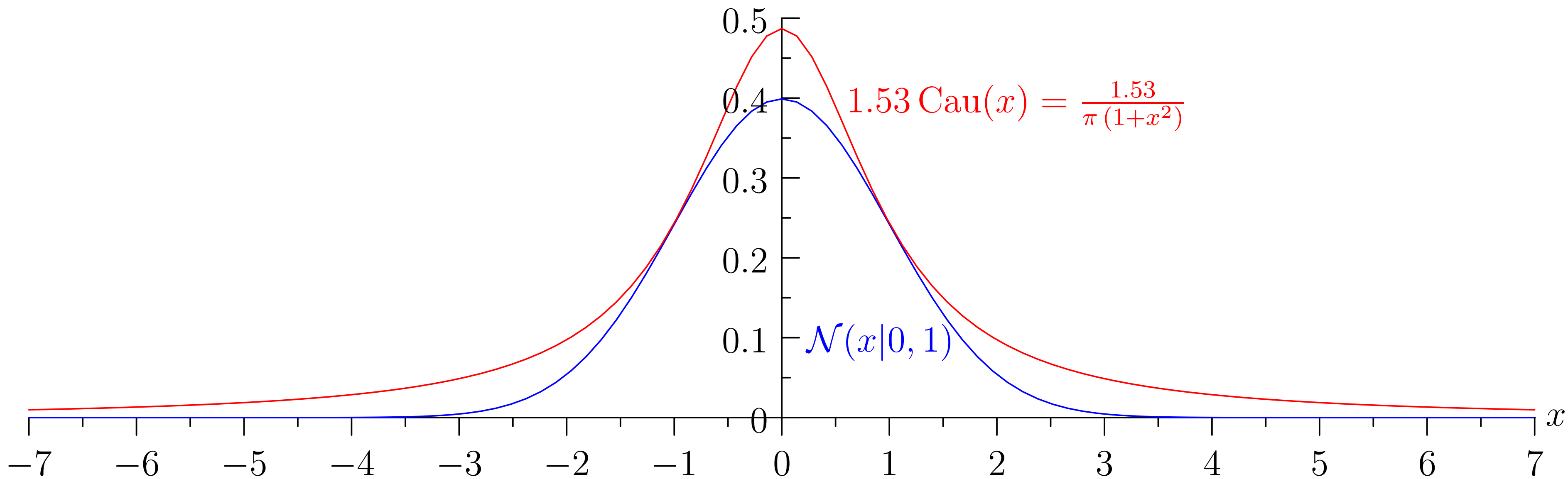

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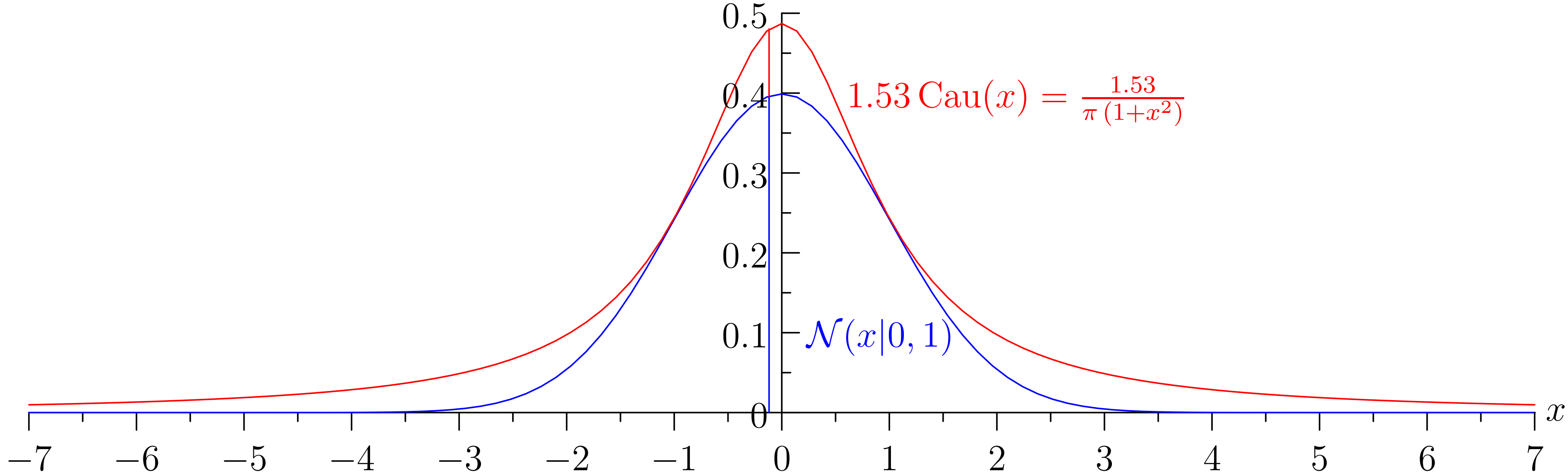

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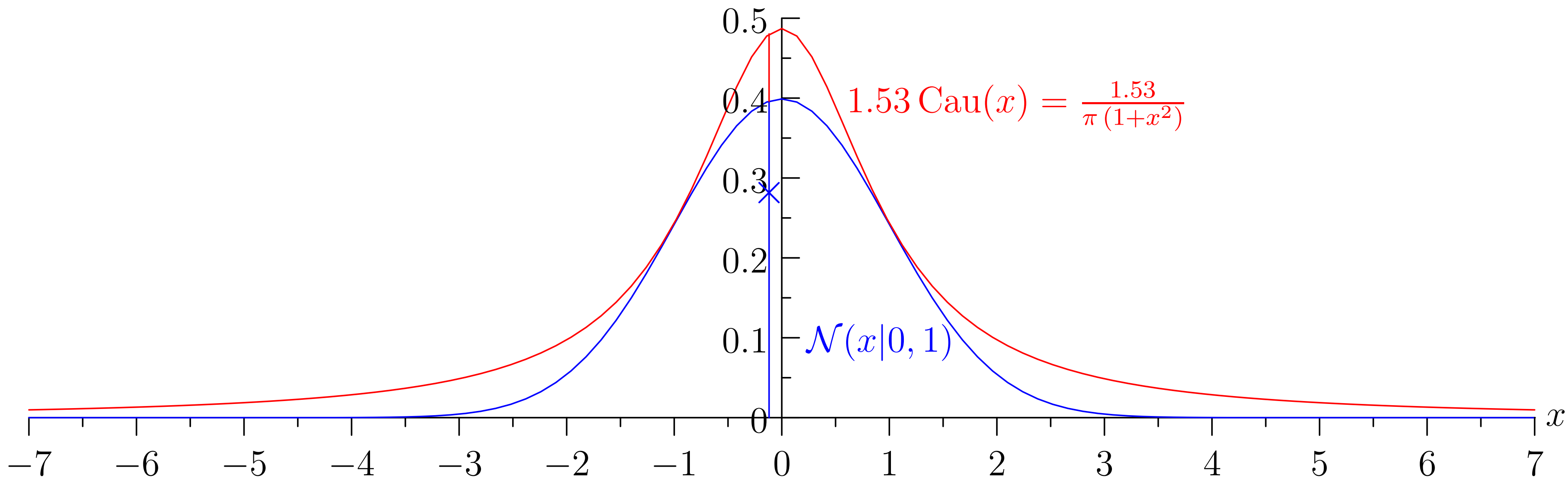

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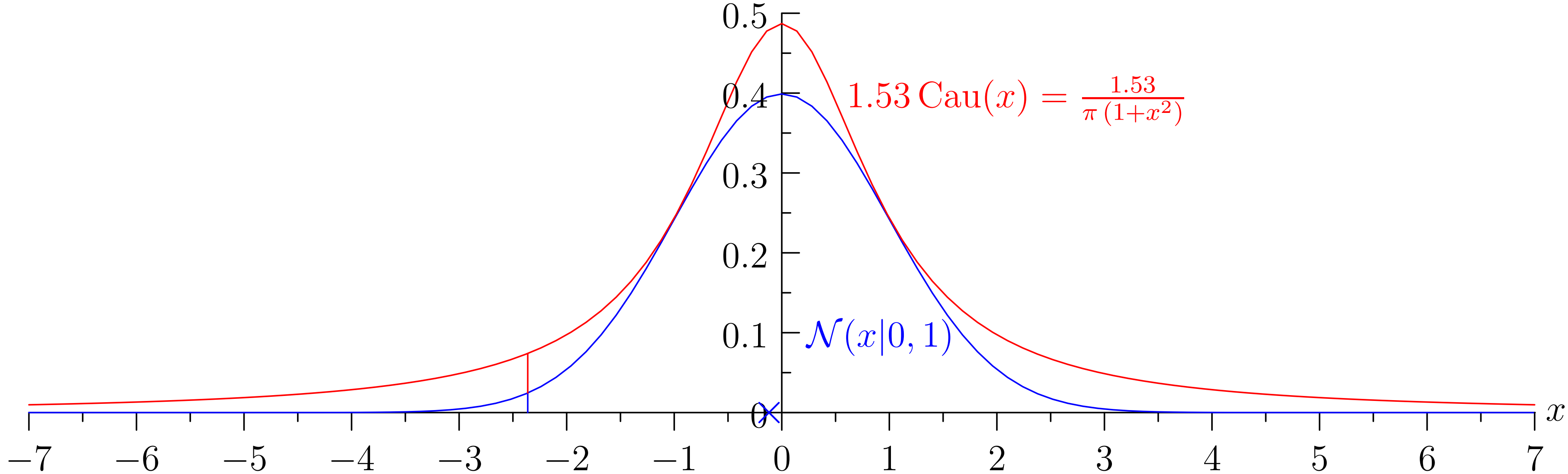

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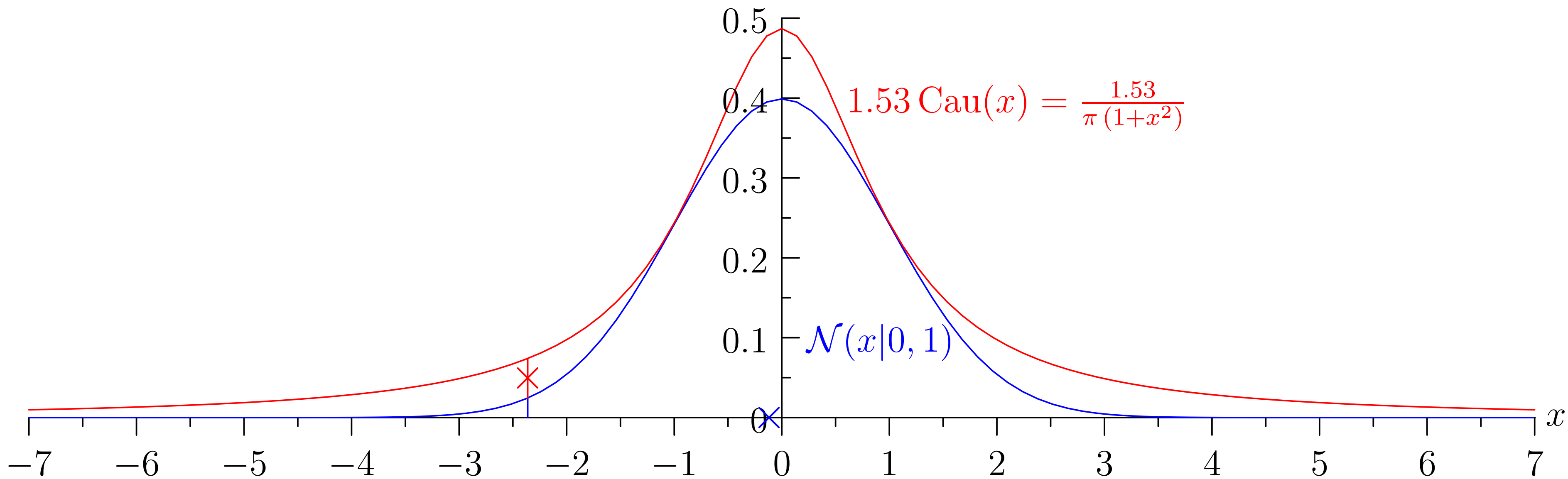

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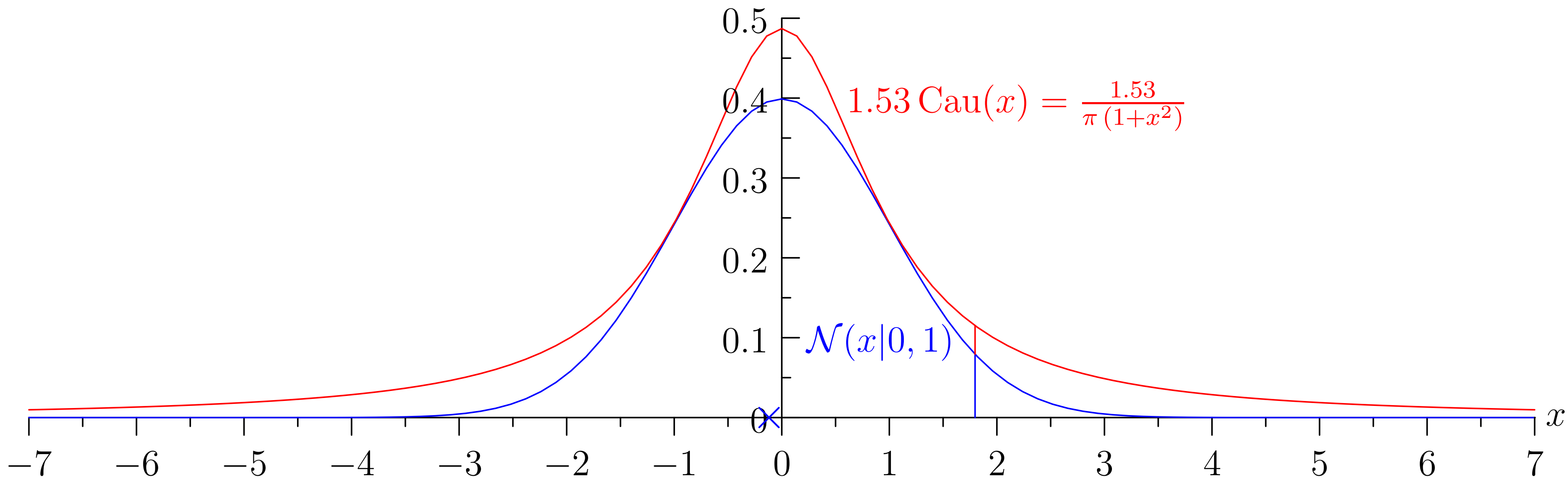

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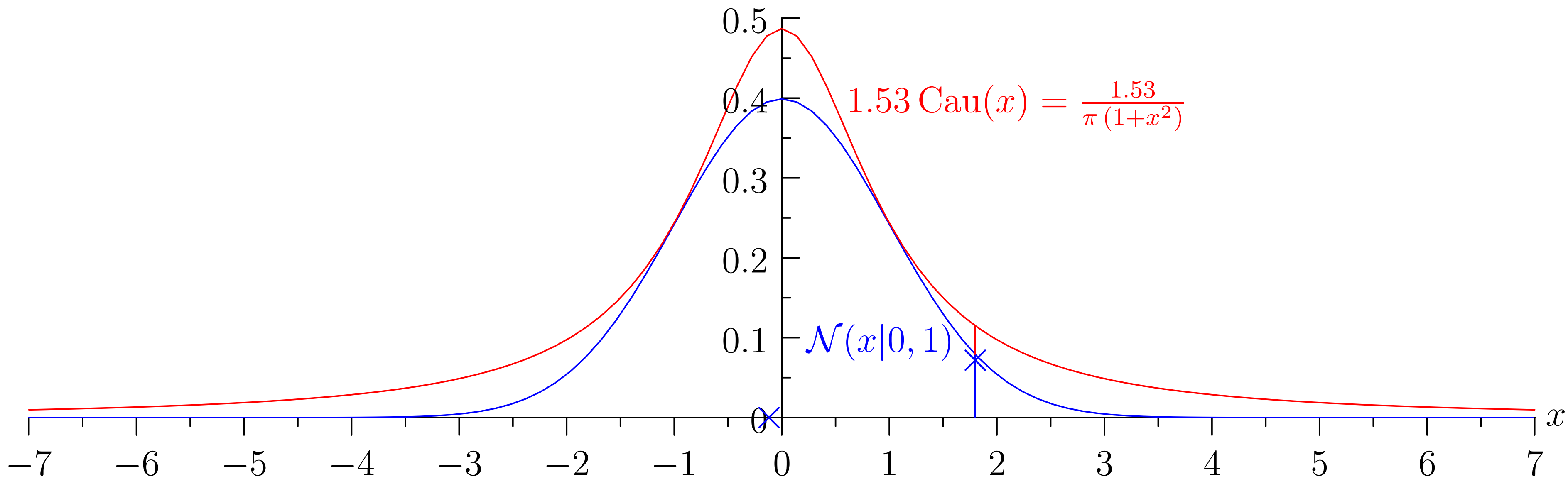

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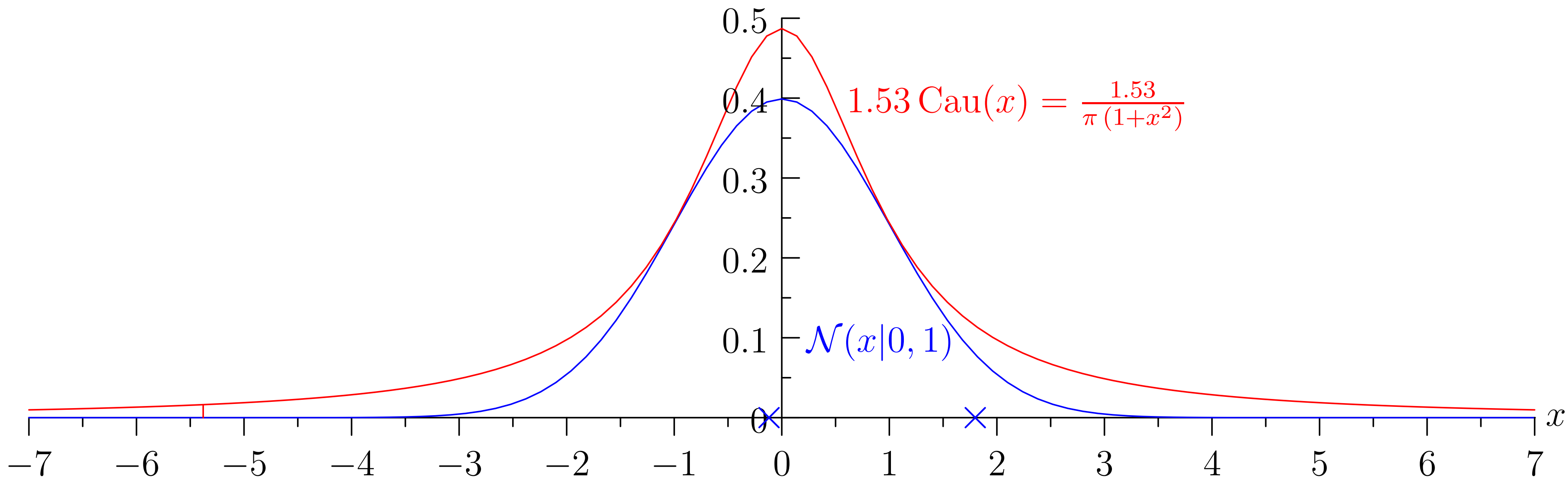

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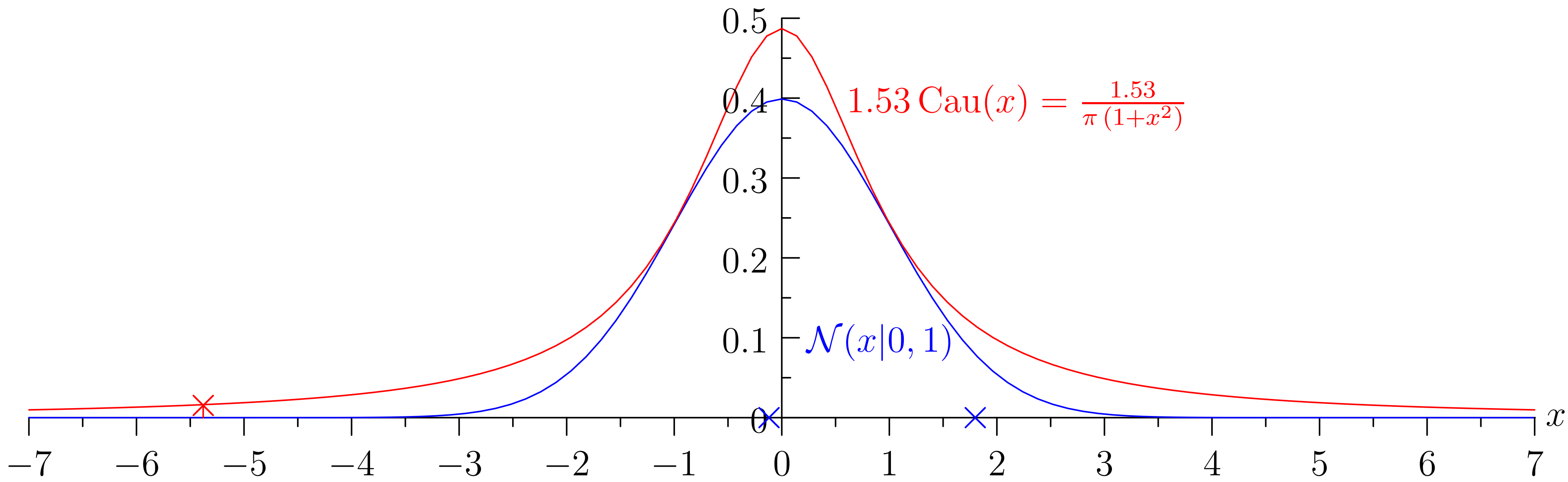

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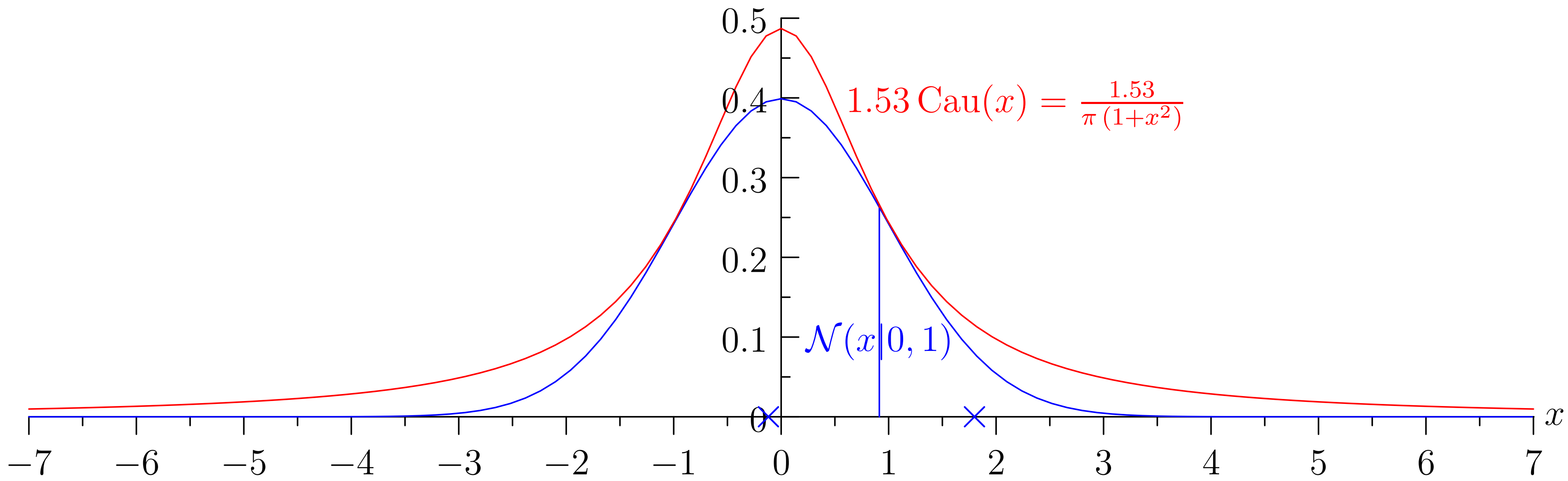

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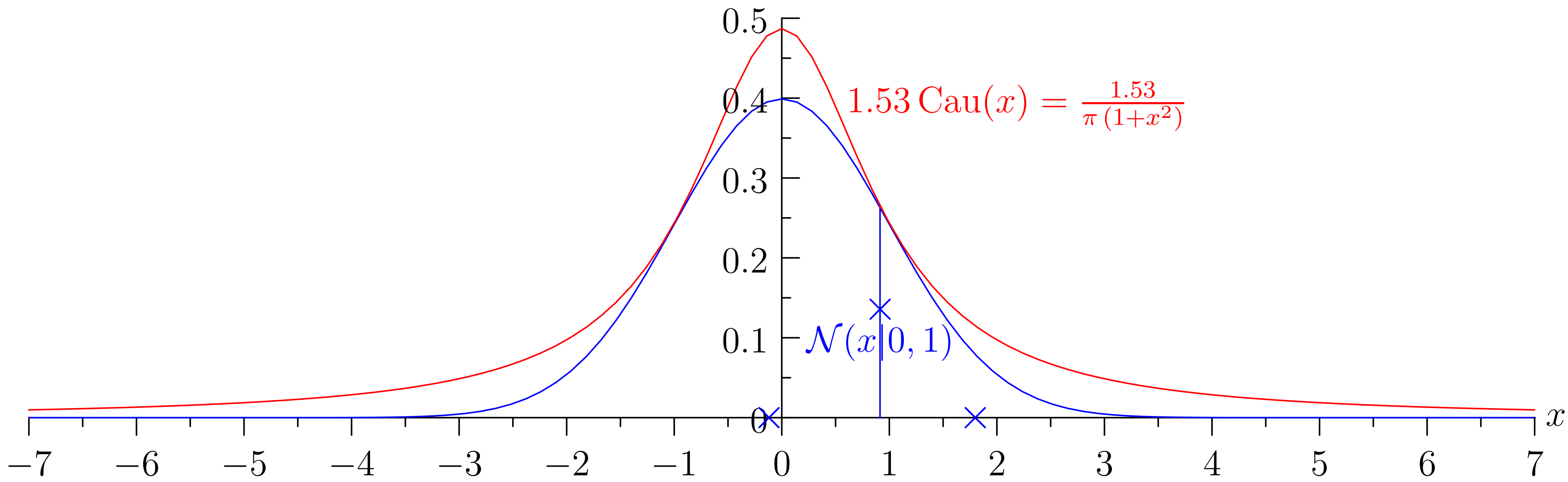

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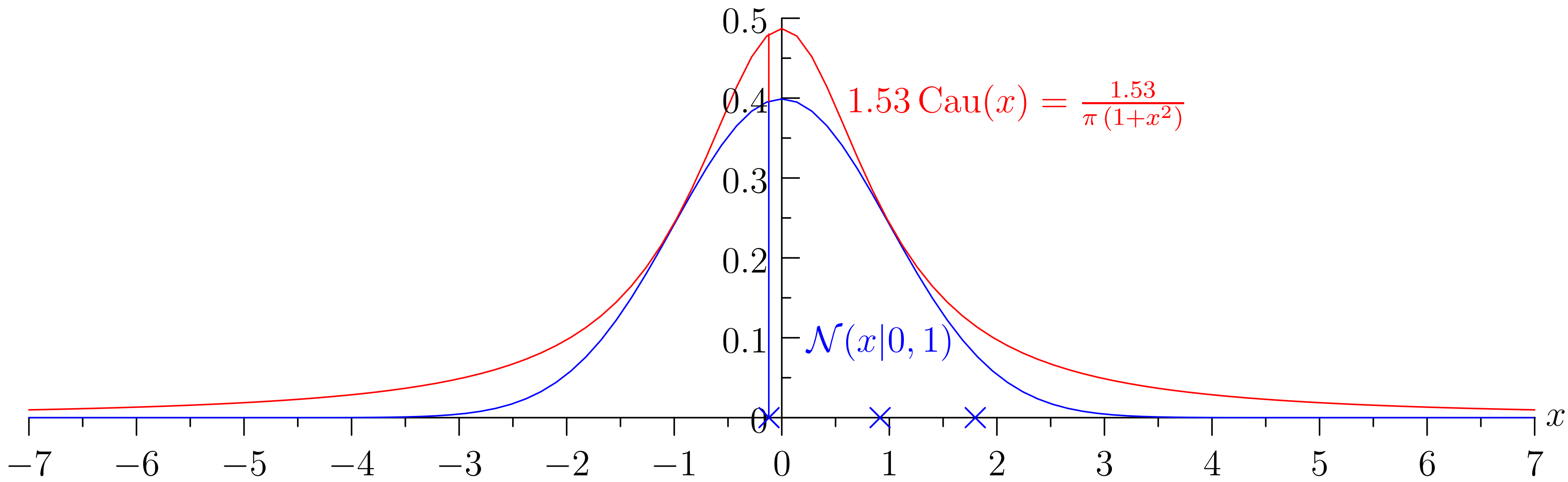

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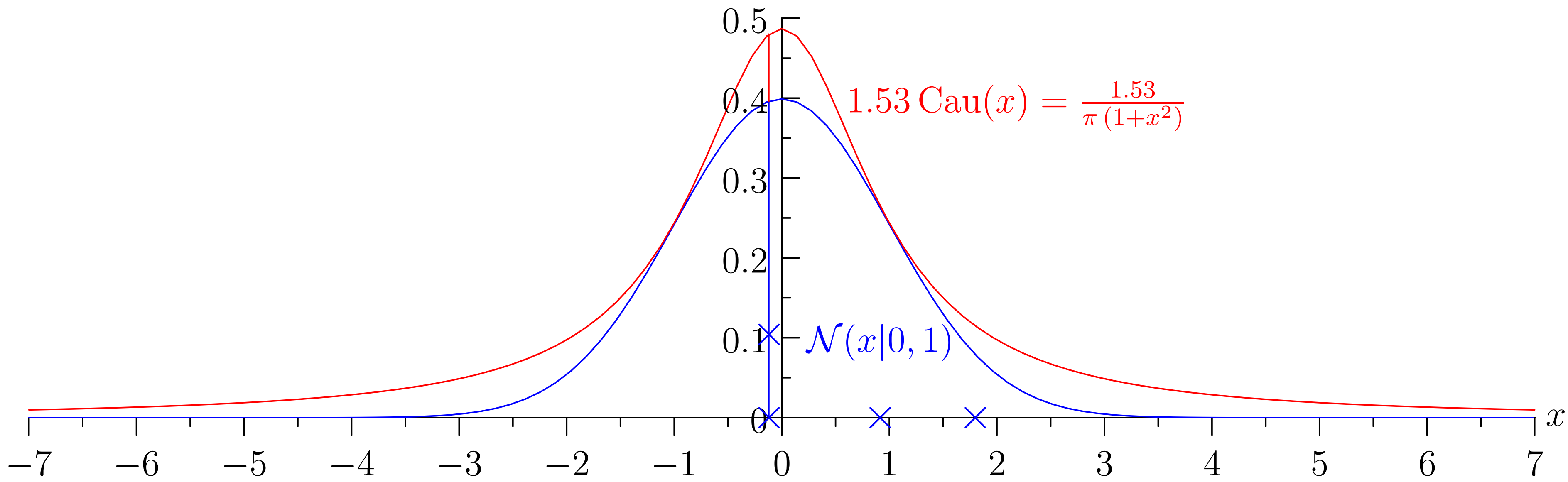

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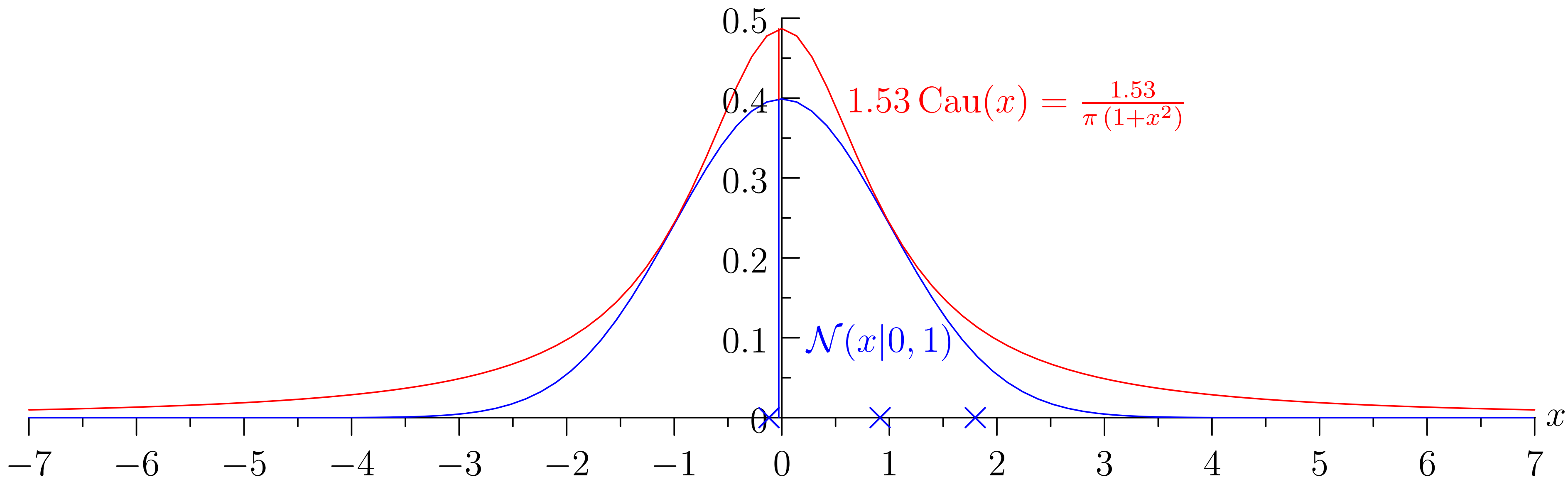

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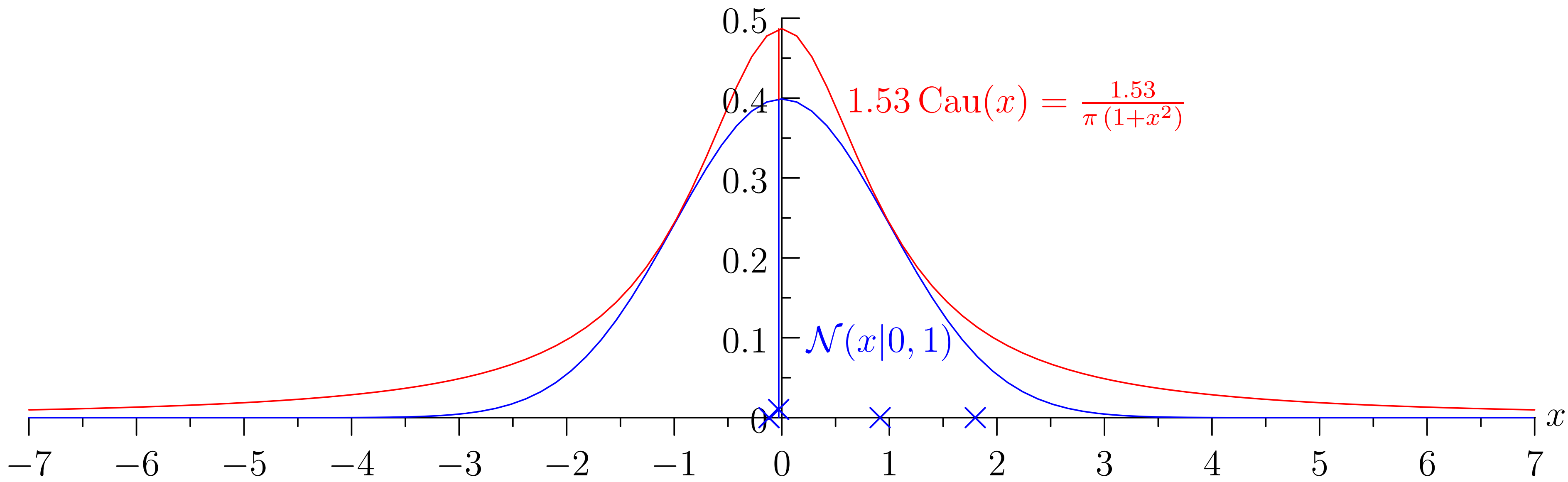

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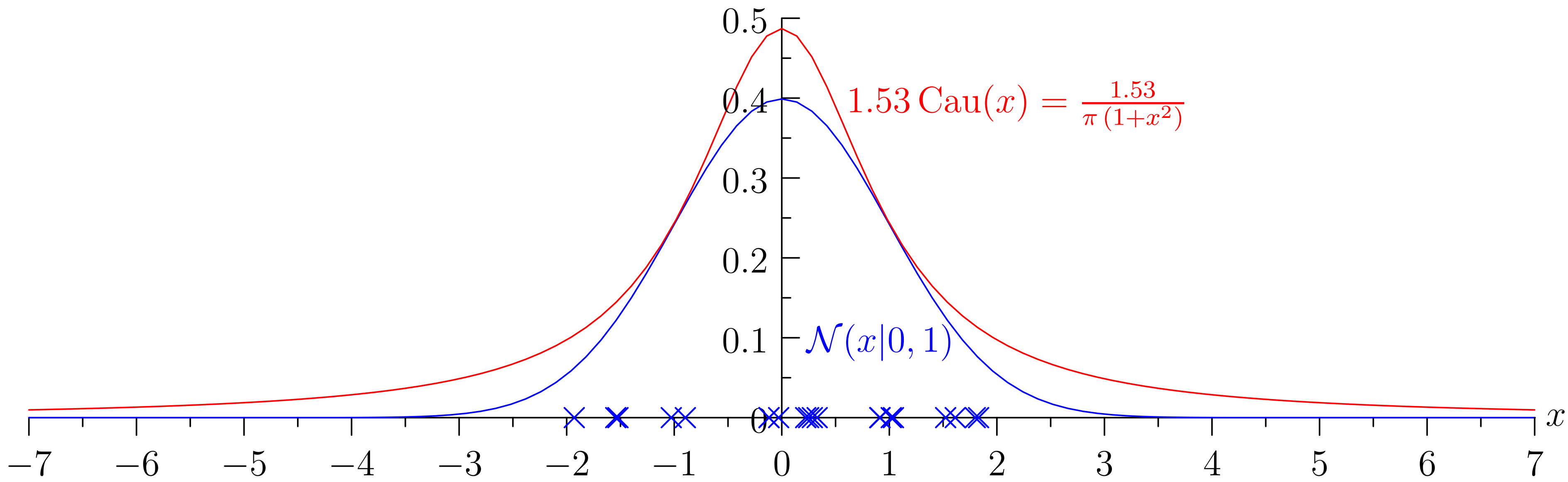

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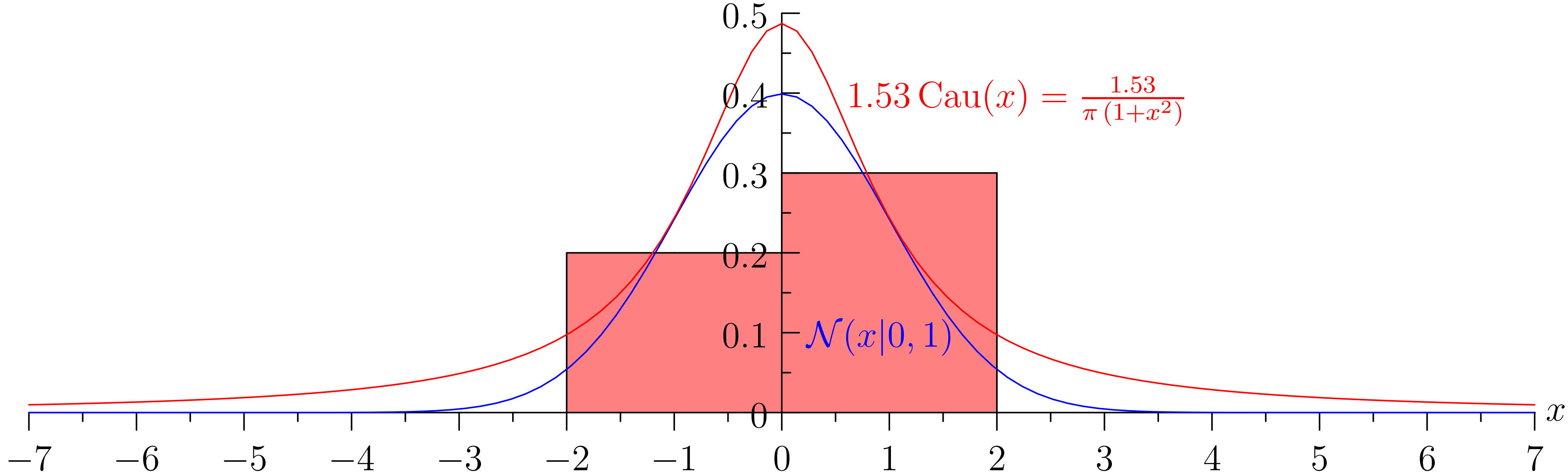

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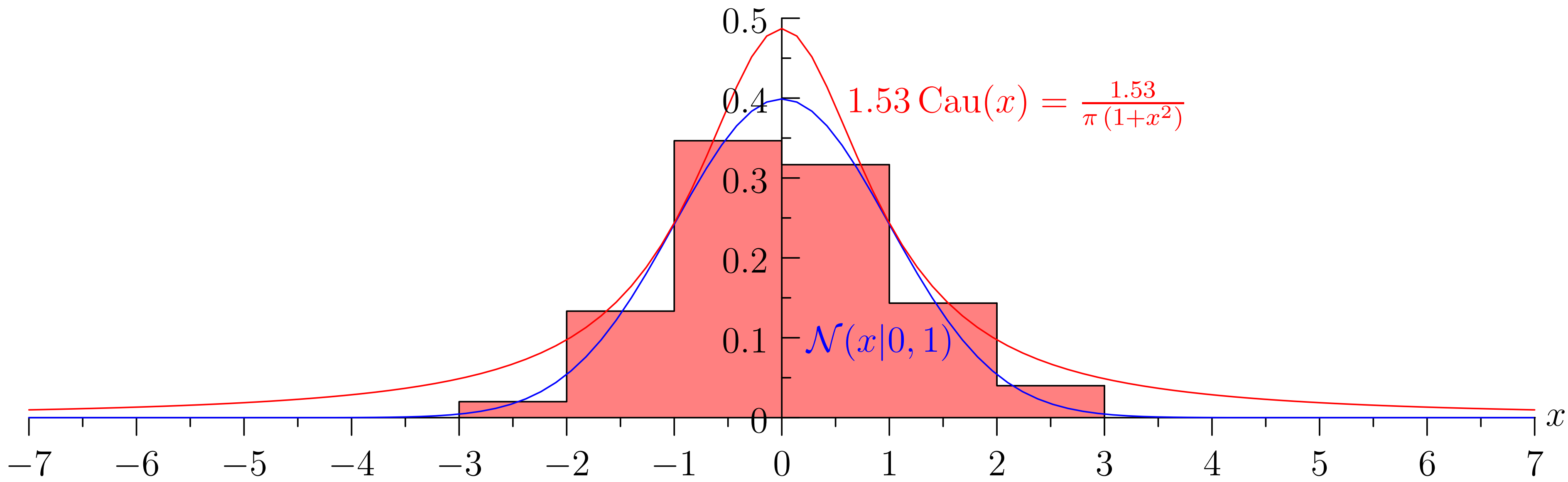

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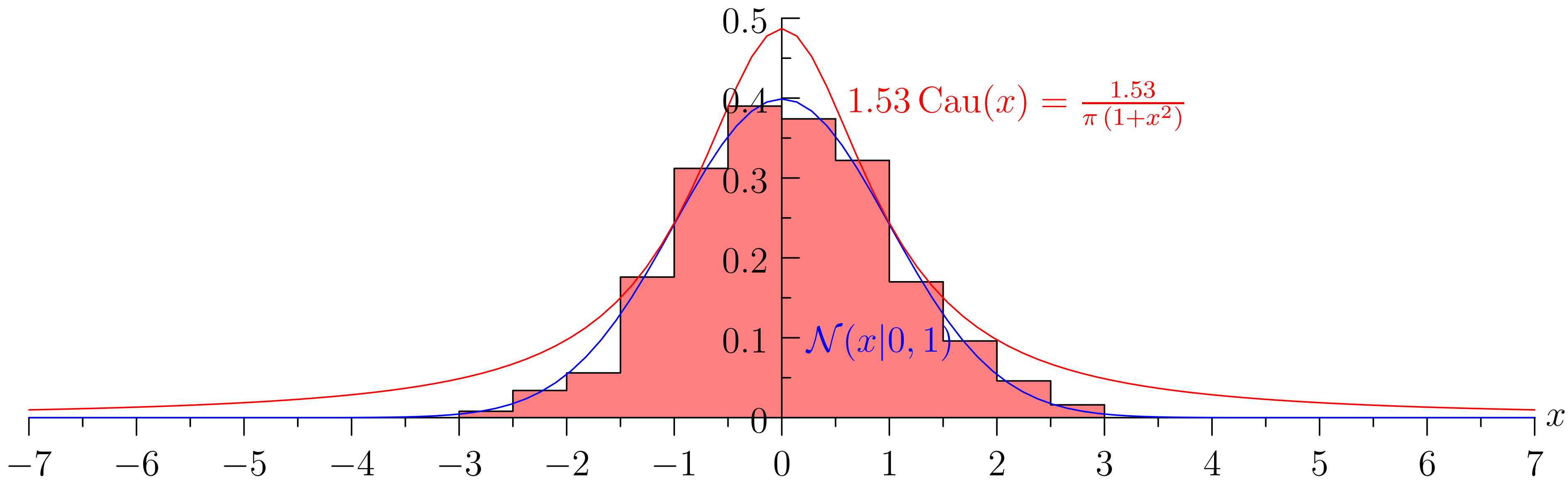

# Problems with Rejection

- The rejection method is very general and often the method of choice (although for normal deviates there is a clever transformation method which is faster)

- However, for complicated probability distributions it can be difficult to find a good proposal distribution $g_Y(y)$

- This is particular true for multivariate distributions

- If the proposal distribution is poor $c$ might be very high and the number of rejections is stupidly high

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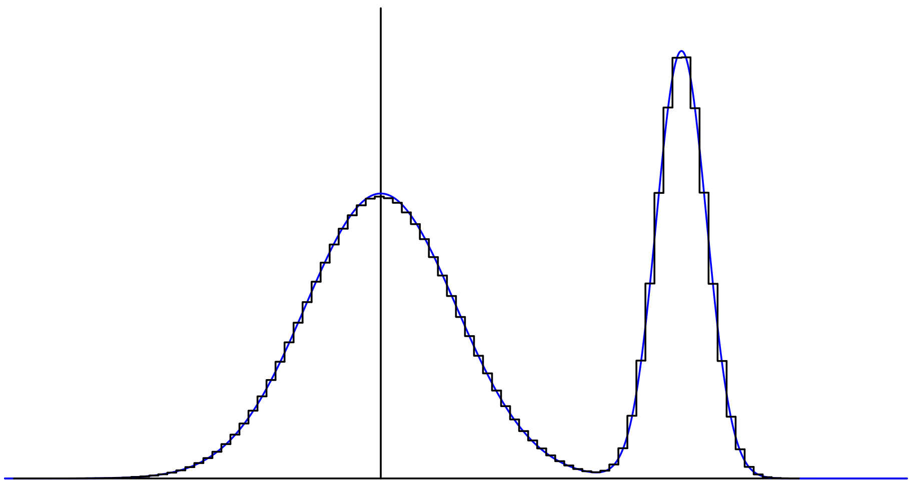
# Outline

1. Sampling
2. Random Number Generation
3. **MCMC**



# Detailed Balance

- Suppose we have a set of states $\mathcal{S}$ and want to draw sample from a probability distribution $\boldsymbol{\pi} = (\pi_i | i \in \mathcal{S})$
- We invent a dynamical system with a transition probability $M_{ij}$ from state $j$ to state $i$ such that

$$M_{ij}\pi_j = M_{ji}\pi_i$$

- This is known as **detailed balance**
- Summing both sides over $j$

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# Convergence of MCMC

- Suppose we start from a state $\boldsymbol{x}(0) = \sum_i c_i \boldsymbol{v}^{(i)}$ where the $\boldsymbol{v}^{(i)}$'s are an eigenvectors of the transition matrix $\mathbf{M}$ with eigenvalues $\lambda_i$

- It I apply $\mathbf{M}$ many times then

$$\boldsymbol{x}(t) = \mathbf{M}^t \boldsymbol{x}(0)$$

- And $\lim_{t \to \infty} \boldsymbol{x}(t) = \boldsymbol{v}^*$ where $\boldsymbol{v}^*$ is the eigenvector with the maximum eigenvalue

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# Metropolis Algorithm

- A very easy way to achieve detailed balance is starting from state $j$ choose a "neighbouring" state, $i$ with equal probability
- We accept the move if either
  - ⋆ $\pi_i > \pi_j$ or
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# Continuous Variables

- If we are working with continuous variables $\boldsymbol{\theta}$ then the equation for detailed balance for the transition probability $W(\boldsymbol{\theta} \to \boldsymbol{\theta}')$ is

$$W(\boldsymbol{\theta} \to \boldsymbol{\theta}')\pi(\boldsymbol{\theta}) = W(\boldsymbol{\theta}' \to \boldsymbol{\theta})\pi(\boldsymbol{\theta}')$$

- where $\pi(\boldsymbol{\theta})$ is the probability distribution we wish to sample from
- The update rule is to choose a nearby value $\boldsymbol{\theta}'$, compute $r = \pi(\boldsymbol{\theta}')/\pi(\boldsymbol{\theta})$ and accept the update with probability $\min(1,r)$
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- Because we are free to choose where we move (and choose close by neighbours) $\pi(\boldsymbol{\theta}') \approx \pi(\boldsymbol{\theta})$ so that moves are not too infrequent

- Also very importantly the updates depend only on the ratio $\pi(\boldsymbol{\theta}')/\pi(\boldsymbol{\theta})$

- We only need to know our probabilities up to a multiplicative scaling factor

- For sampling from the posterior we only need to know the likelihood and prior $\mathbb{P}(\mathcal{D}|\boldsymbol{\theta})\,\mathbb{P}(\boldsymbol{\theta})$

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- We don't even know how long we have to wait
- Even when we have reached this *equilibration time* each sample is correlated with the previous sample
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- It can take a long time until our states occur with the probability $\pi$ (i.e. we have forgotten our initial state)
- We don't even know how long we have to wait
- Even when we have reached this *equilibration time* each sample is correlated with the previous sample
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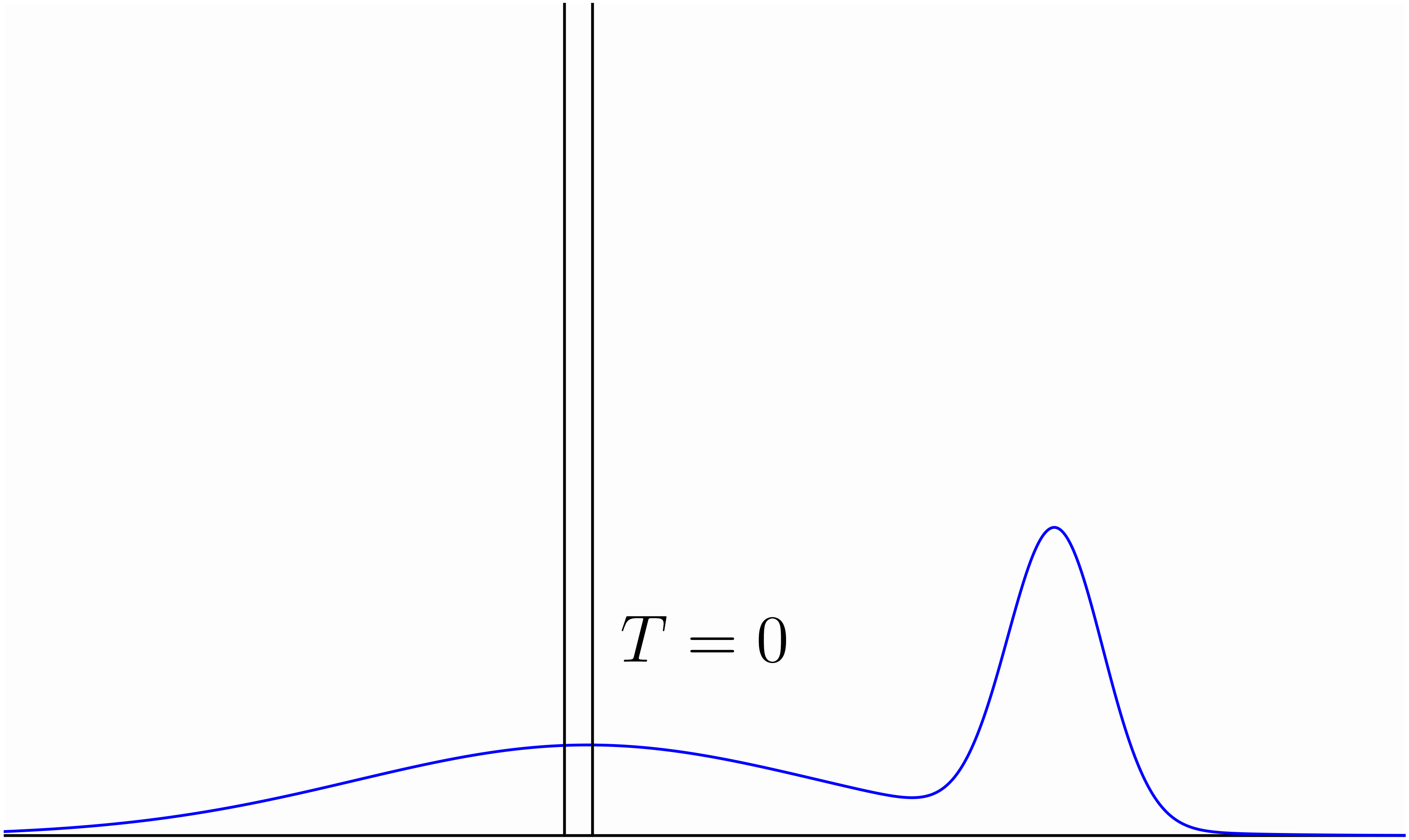

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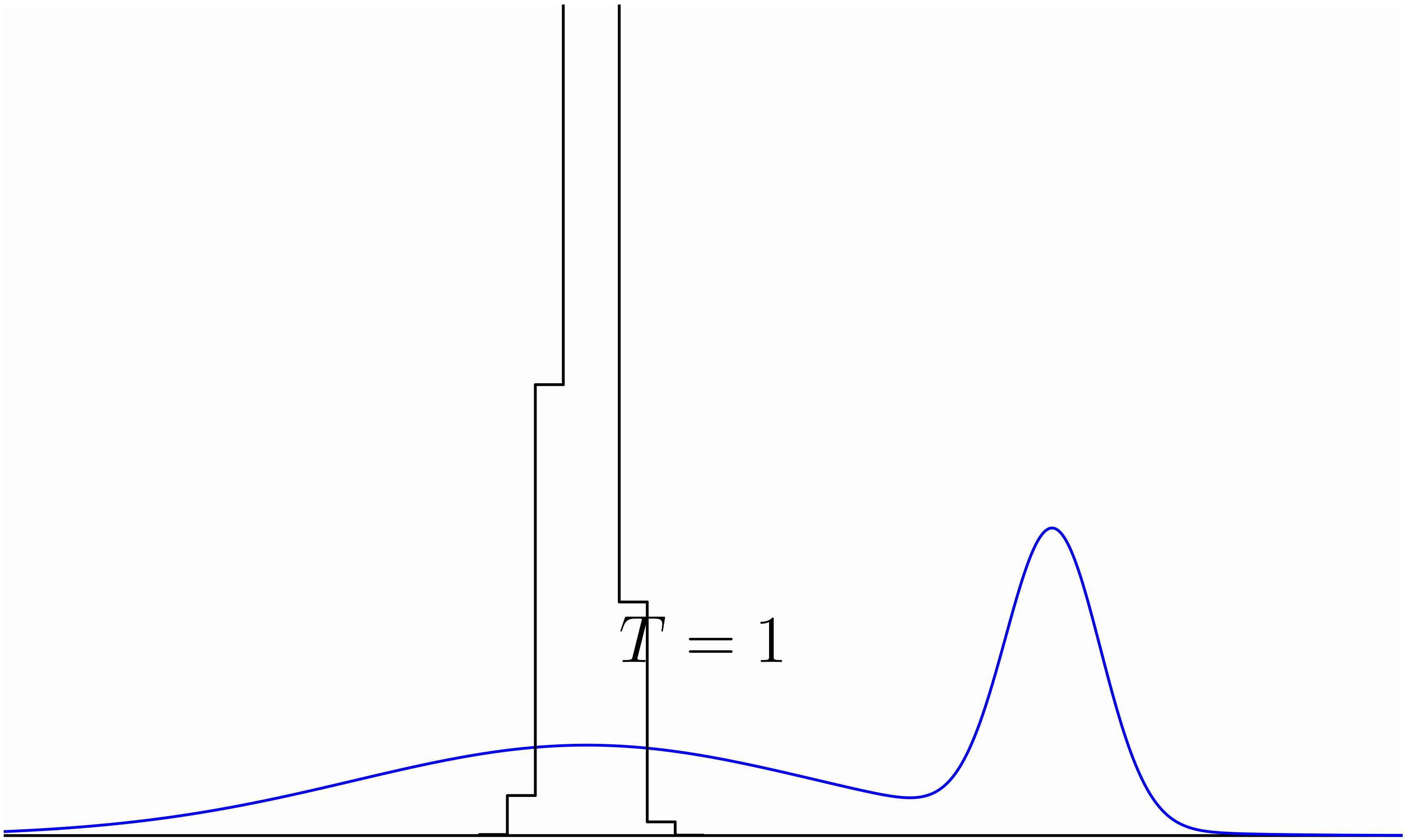

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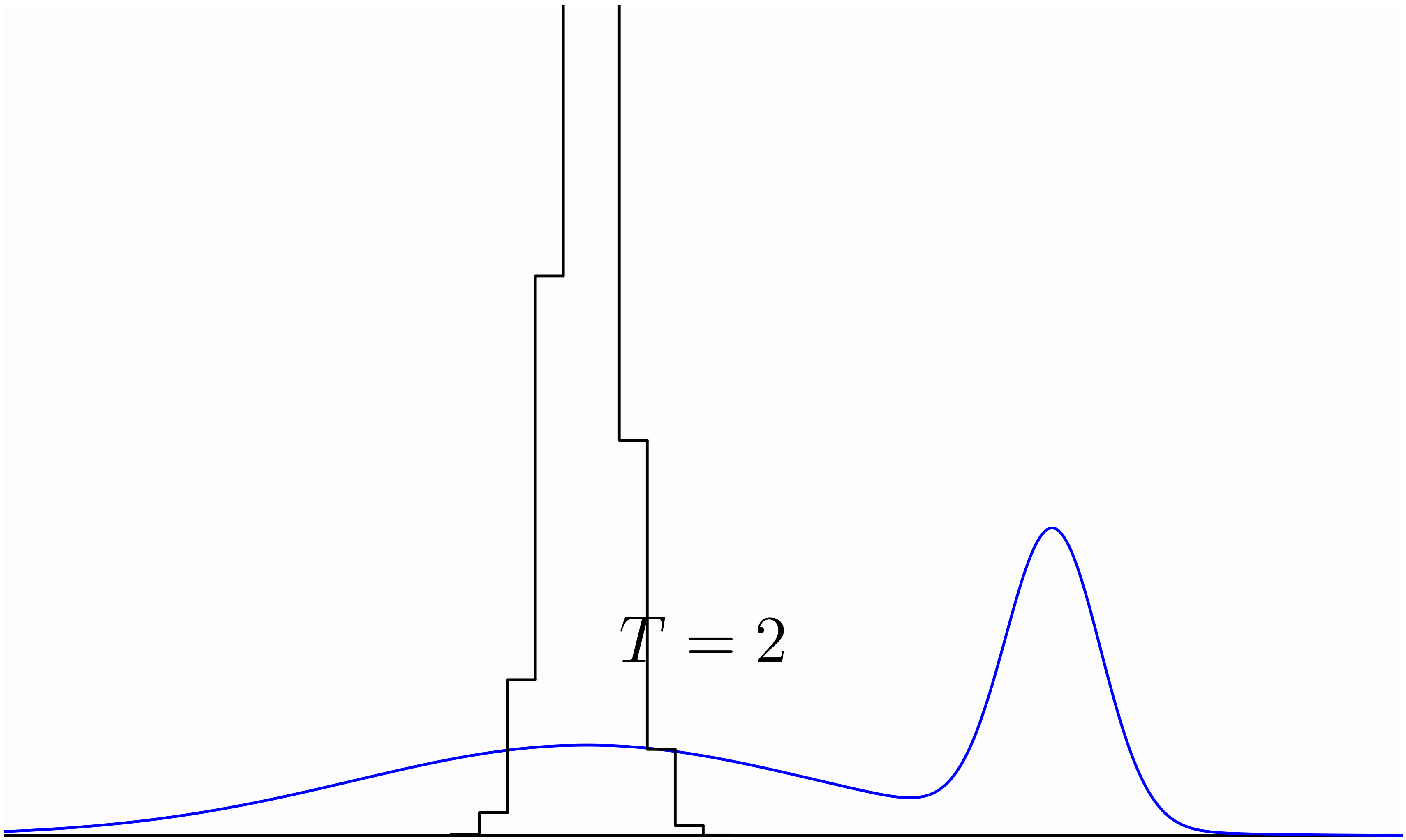

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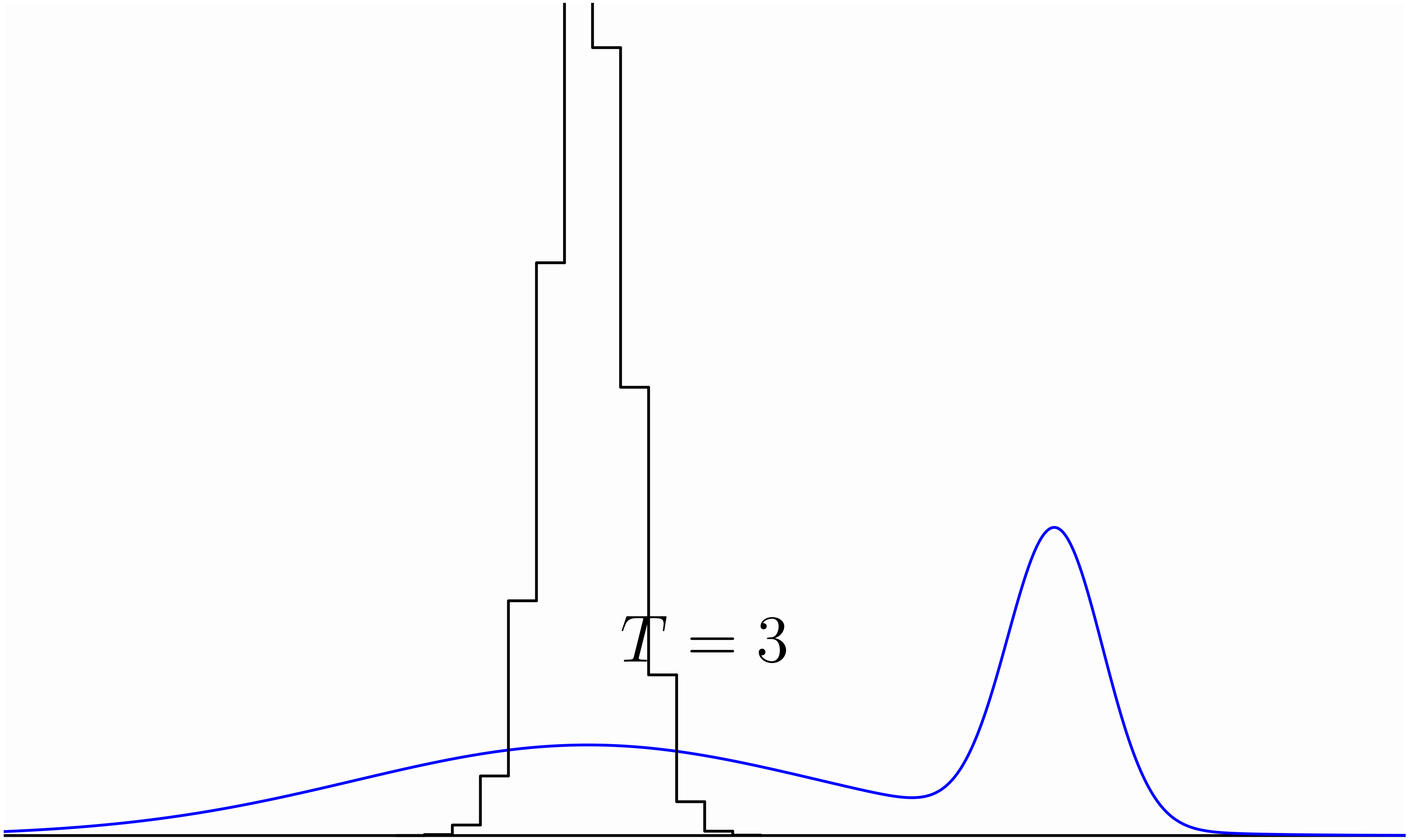

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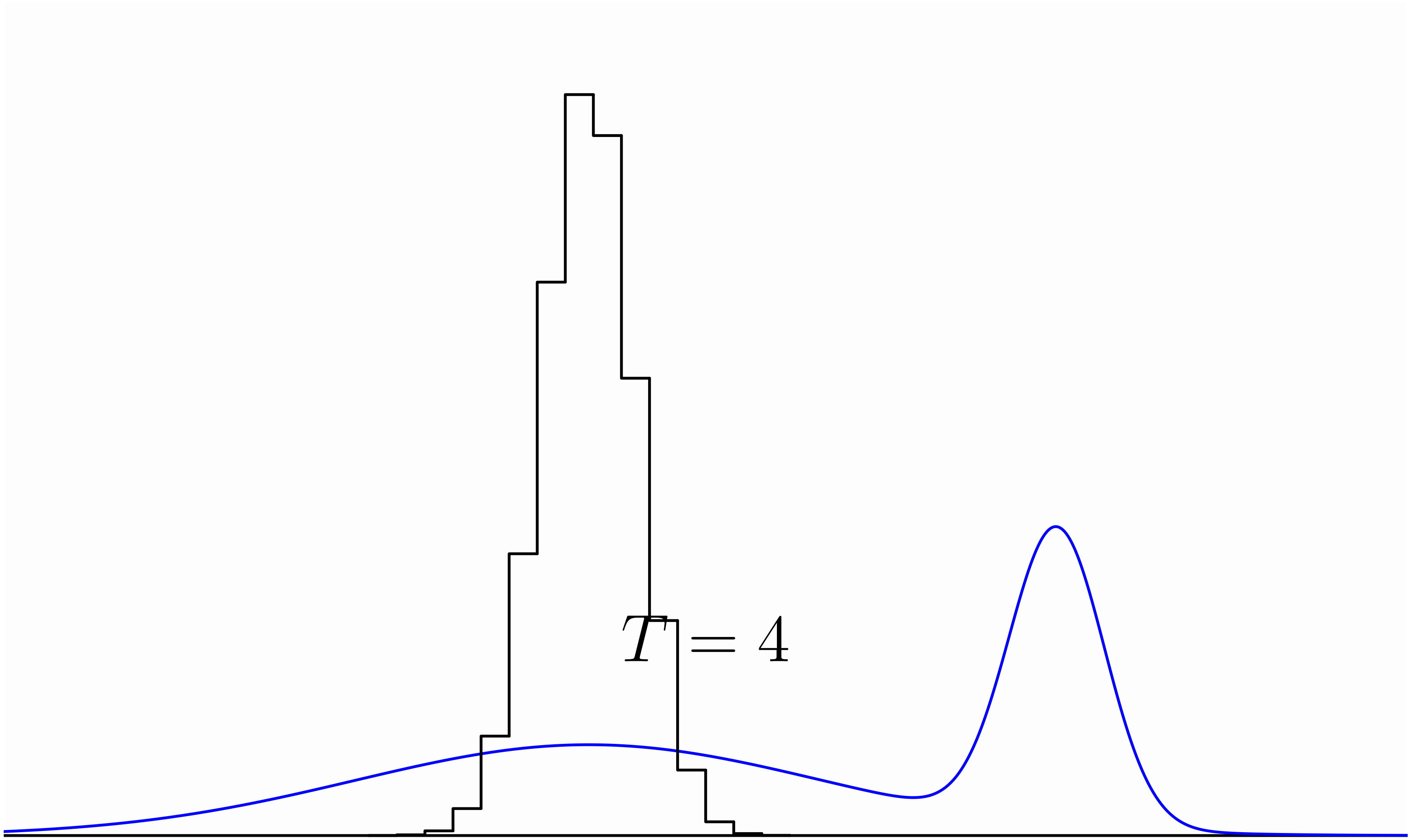

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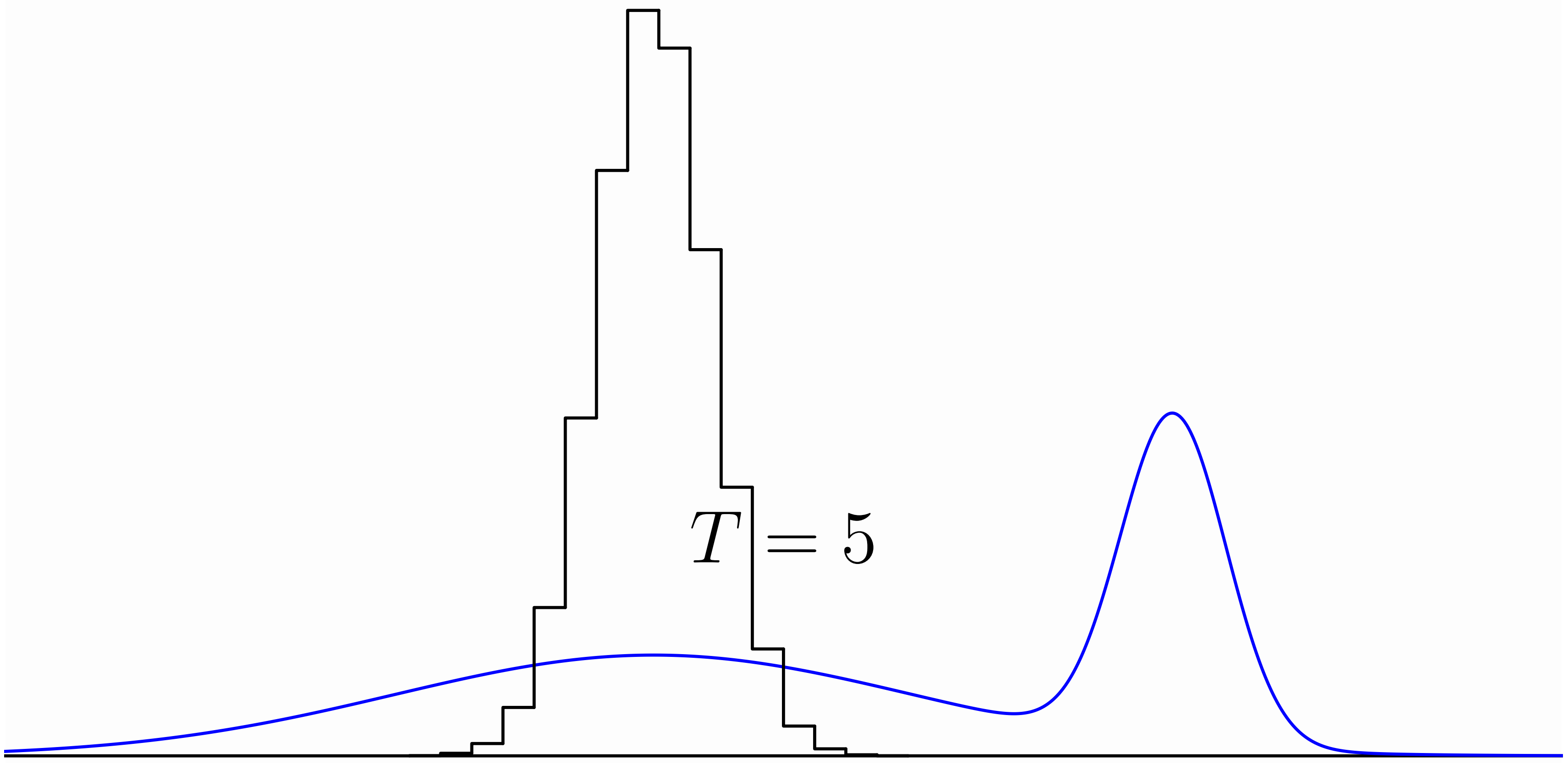

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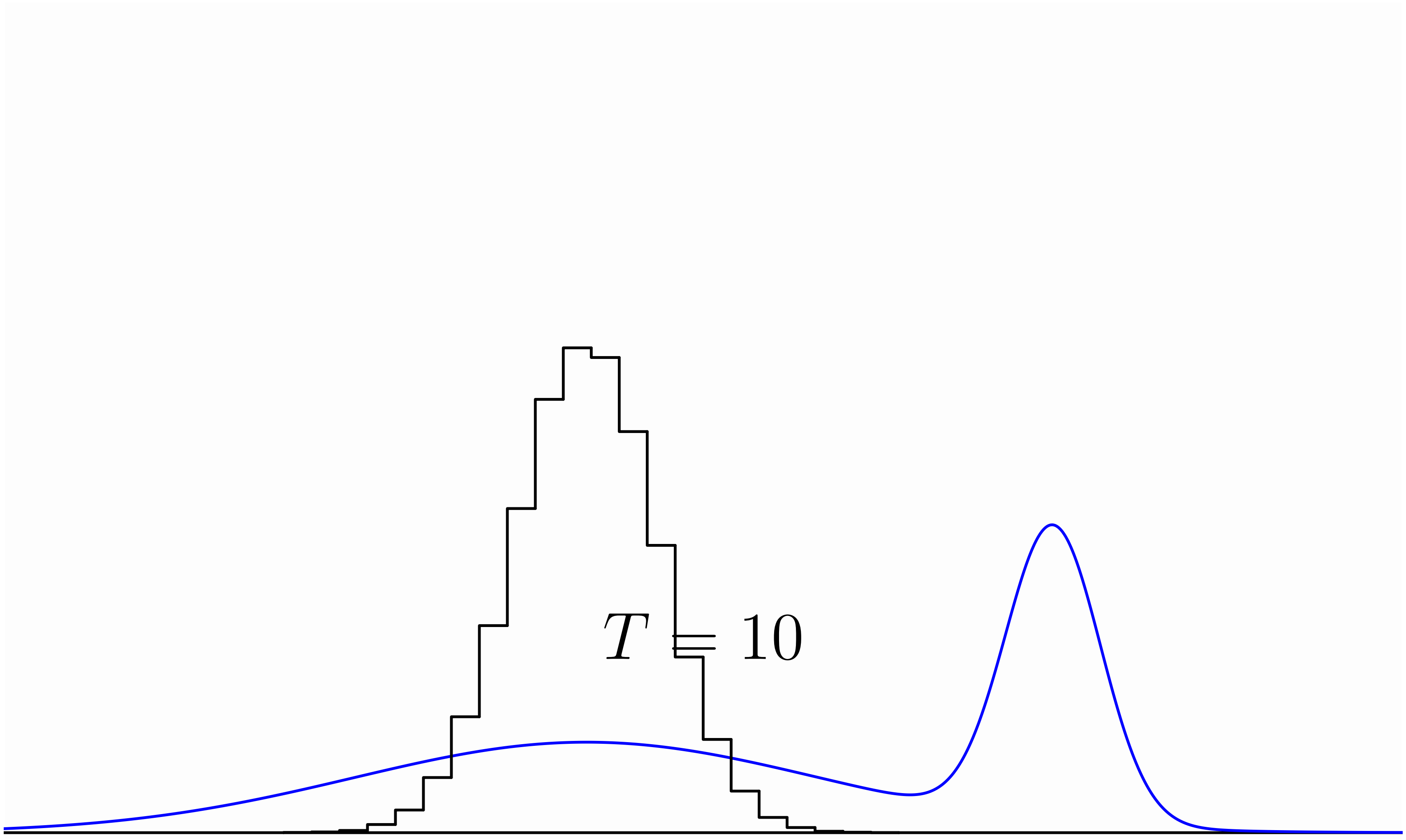

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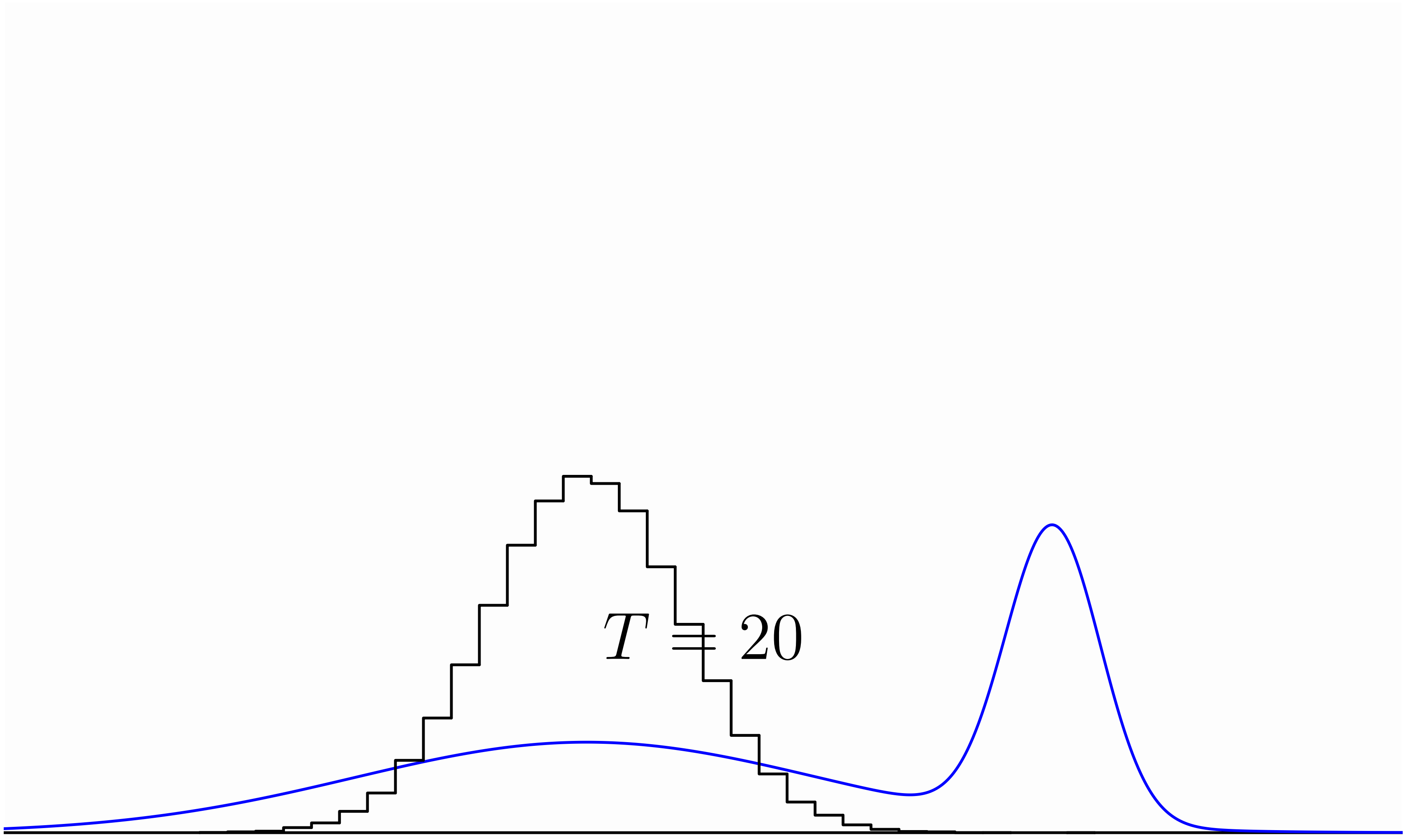

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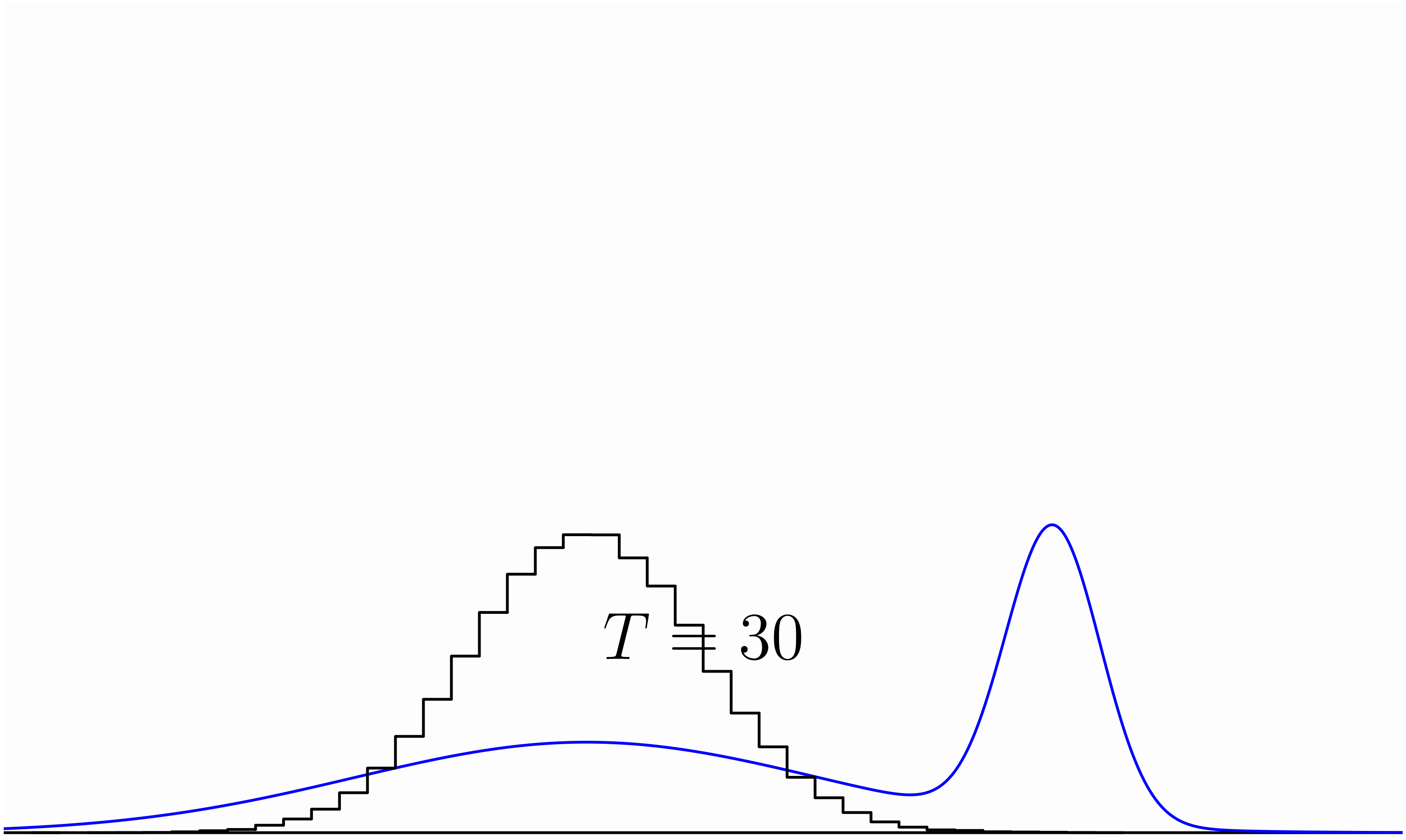

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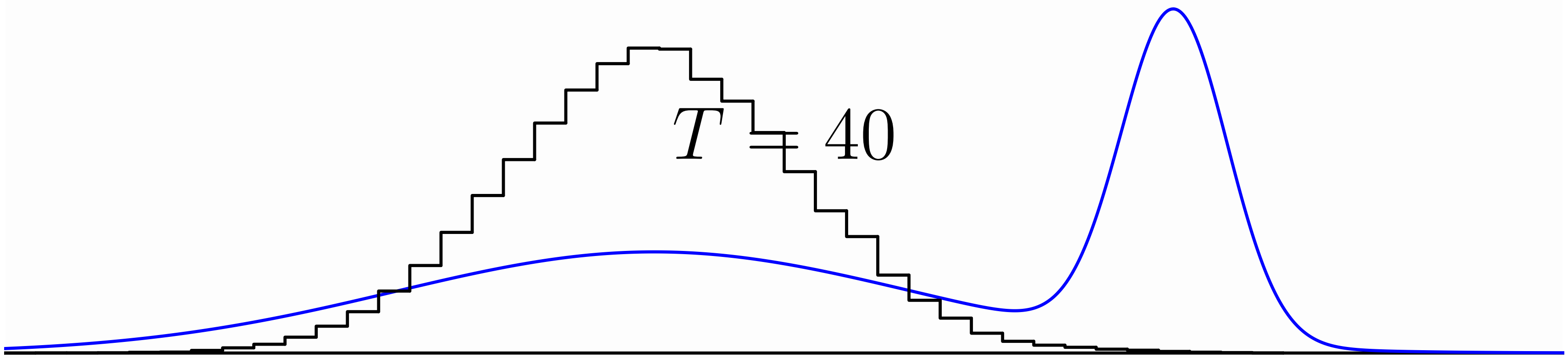

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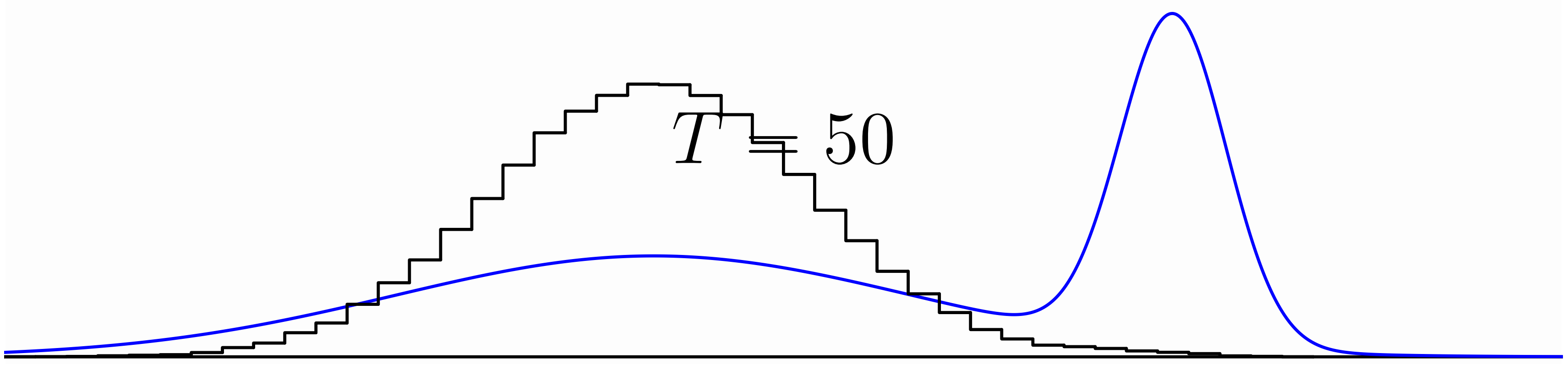

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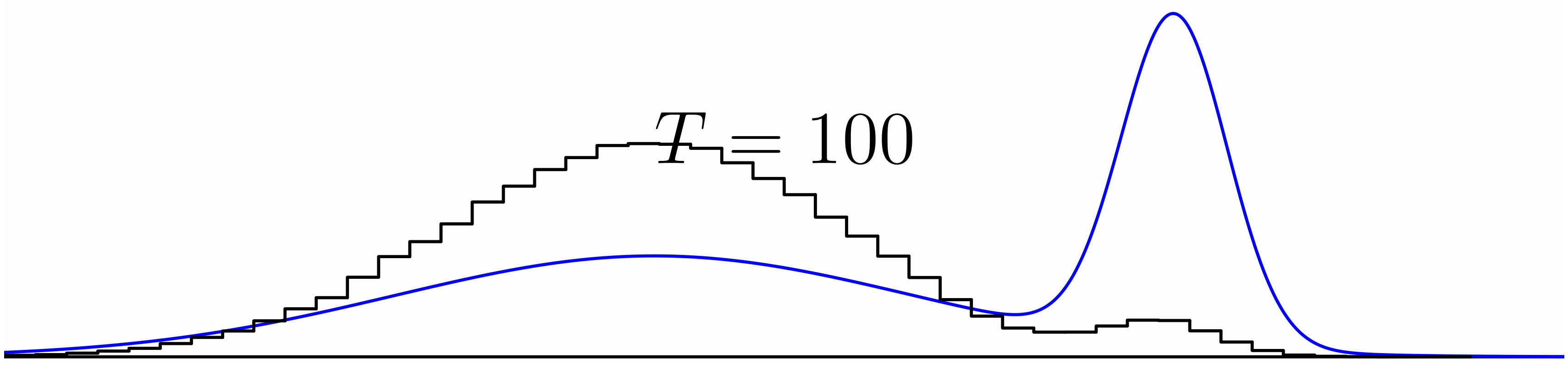

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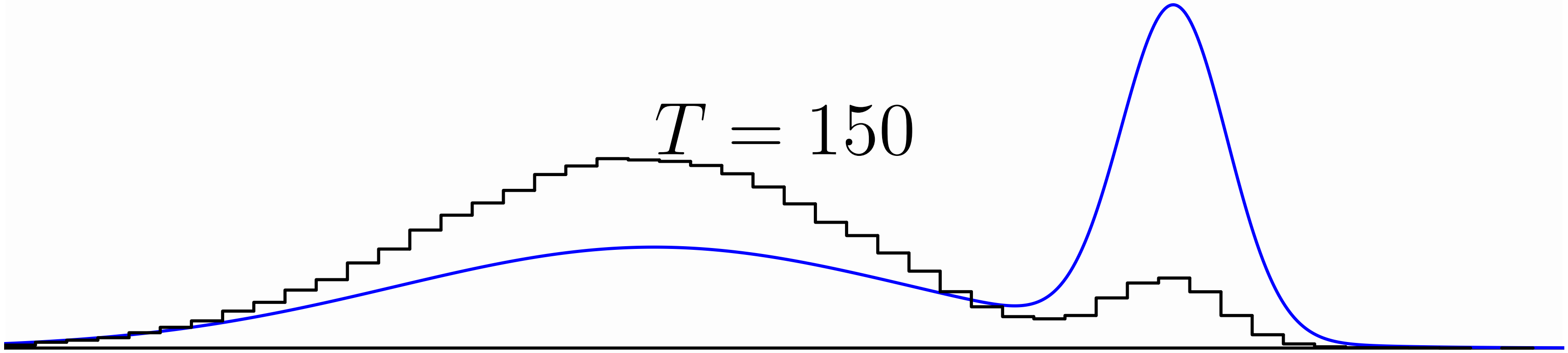

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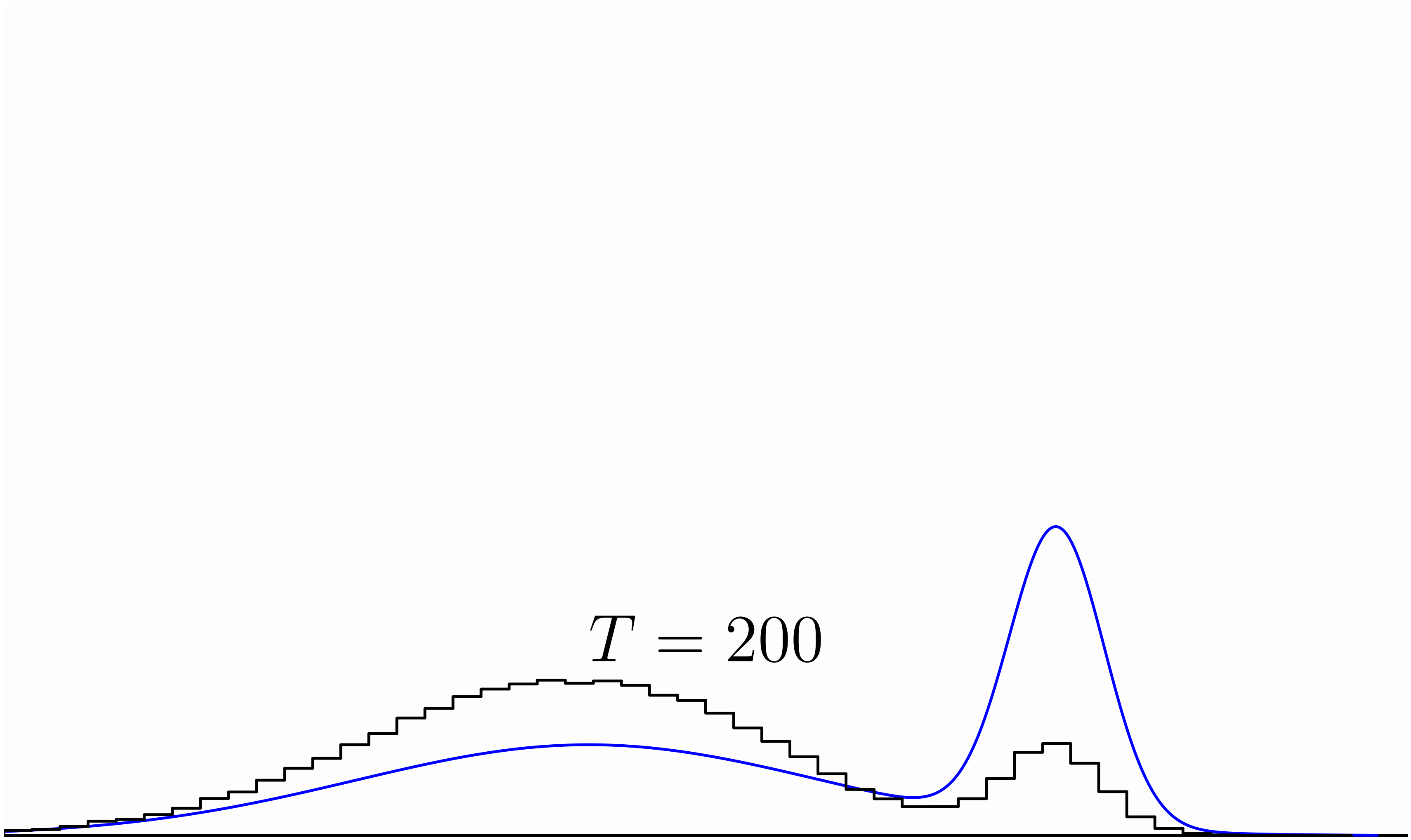

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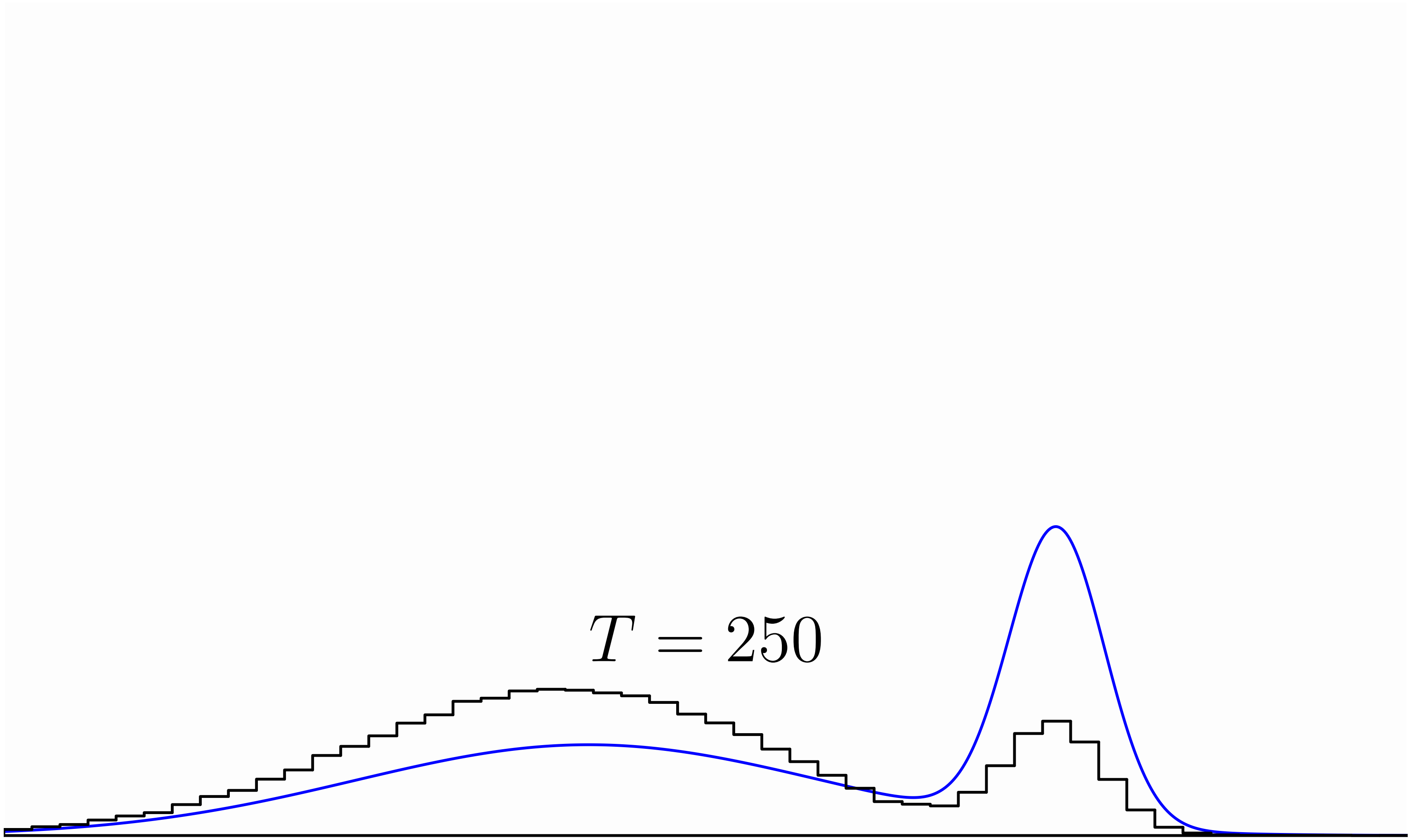

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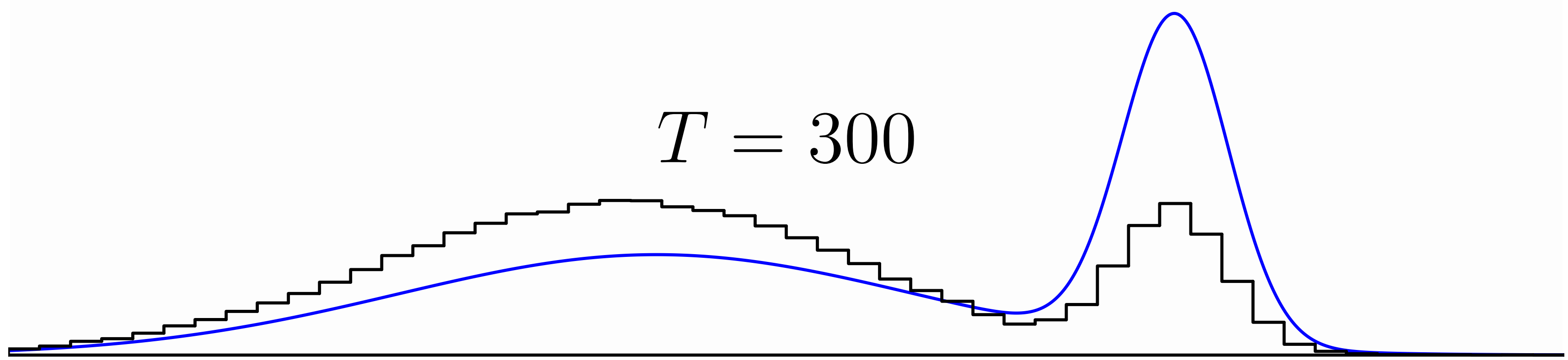

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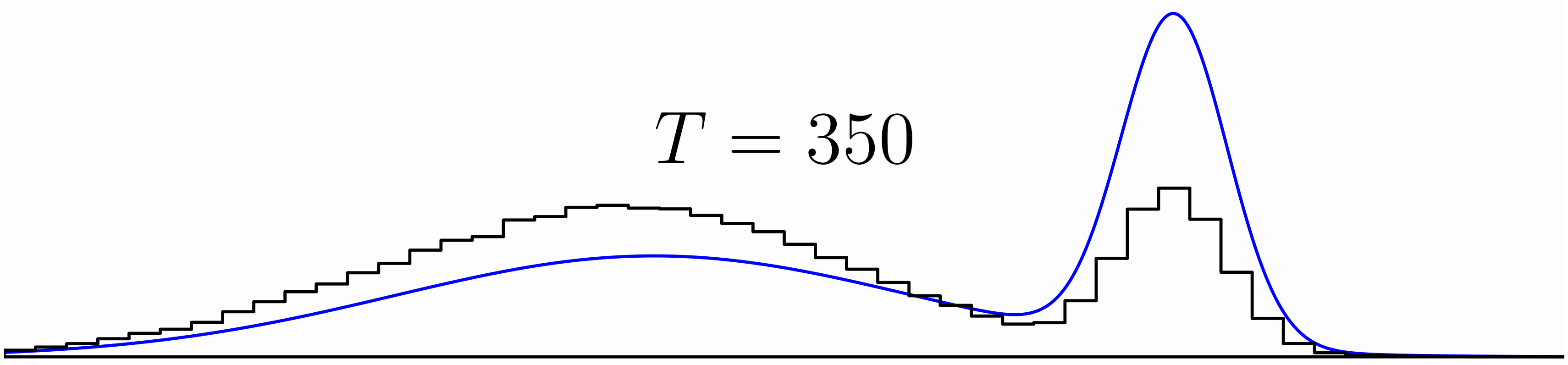

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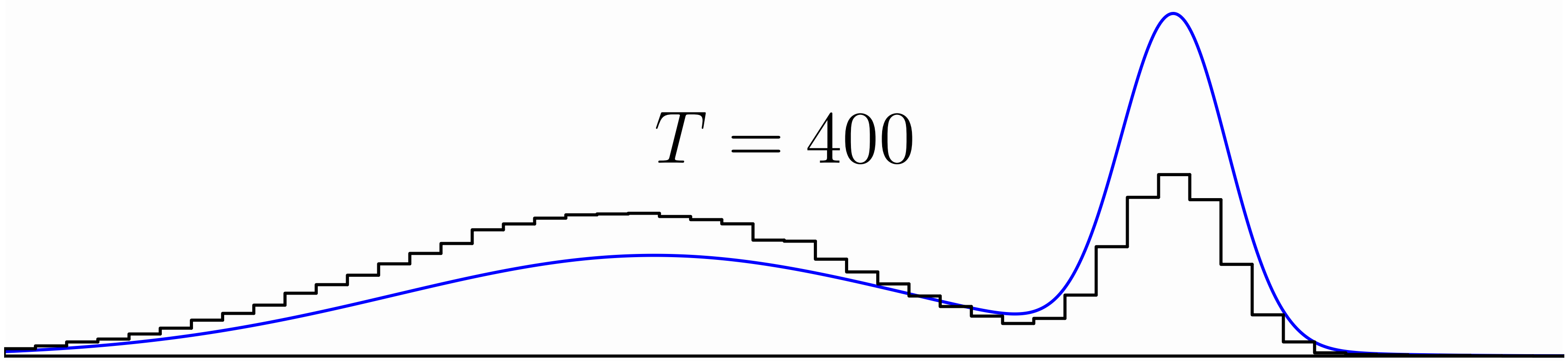

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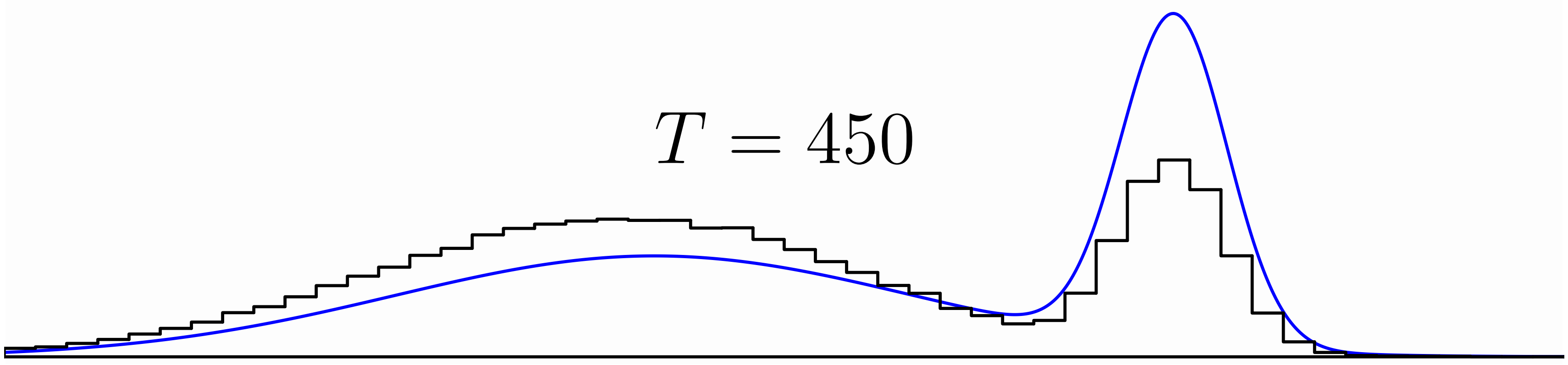

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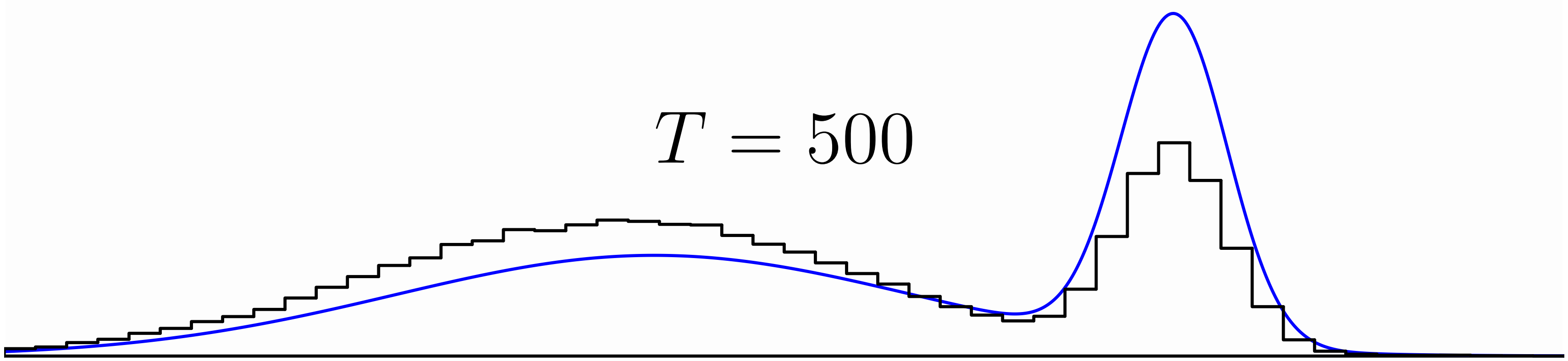

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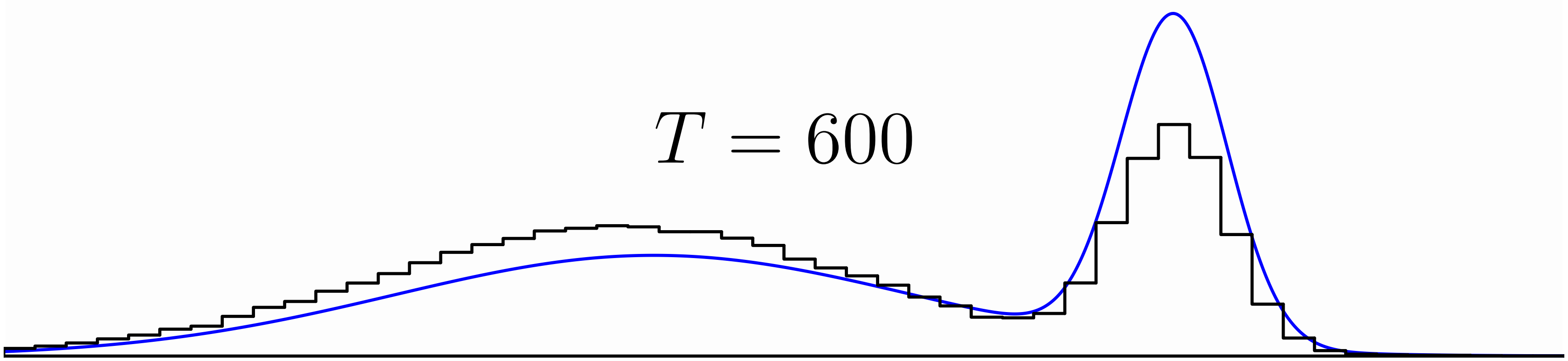

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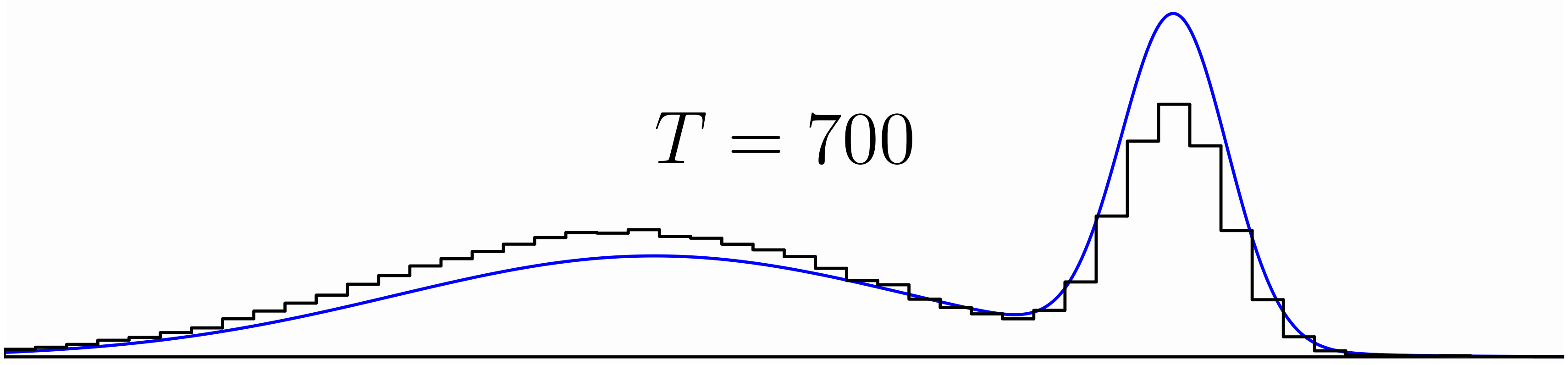

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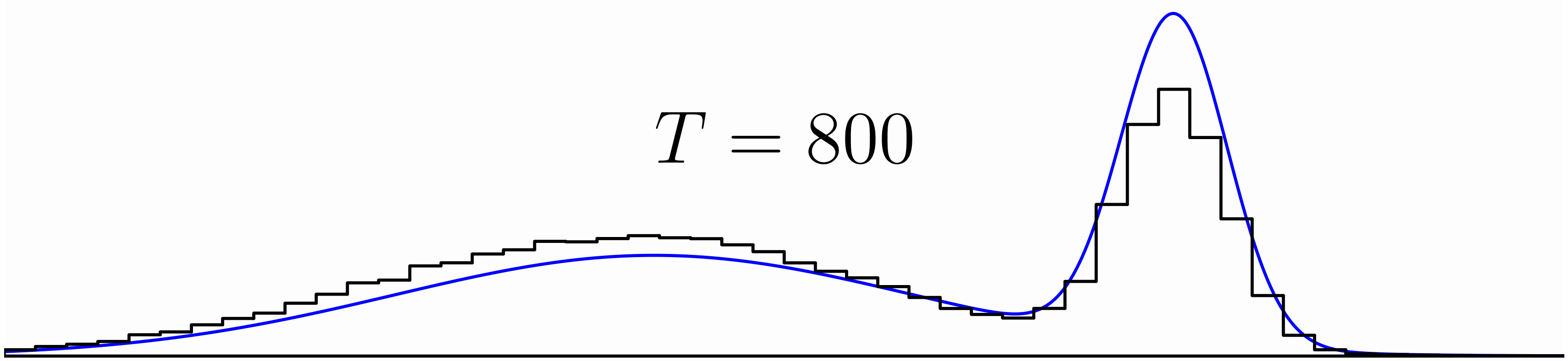

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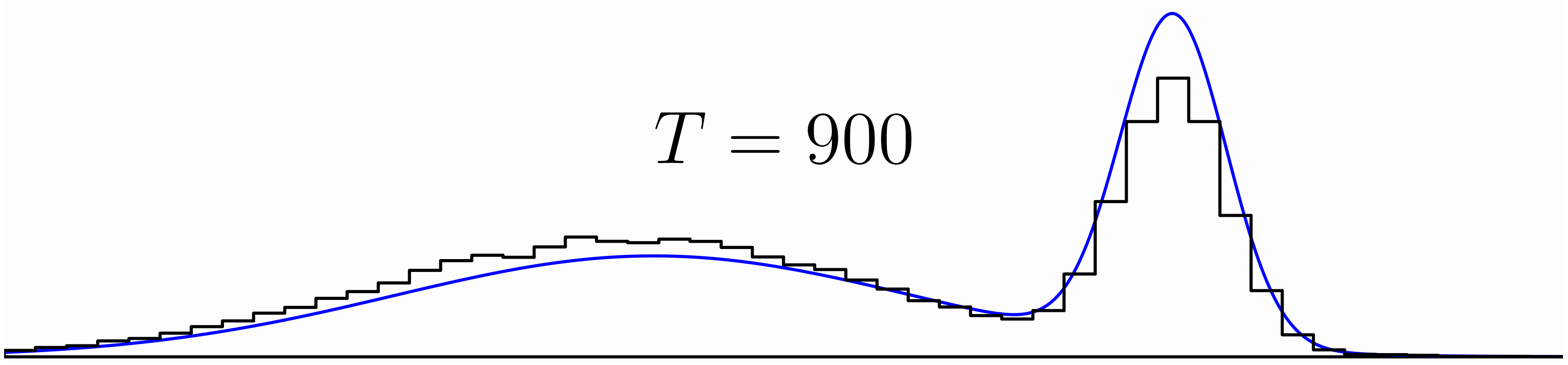

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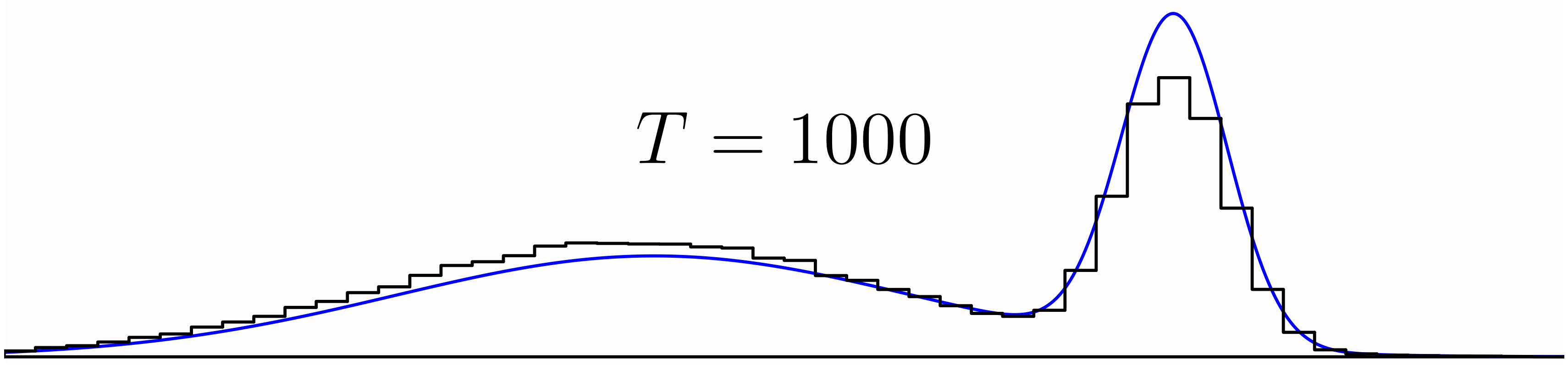

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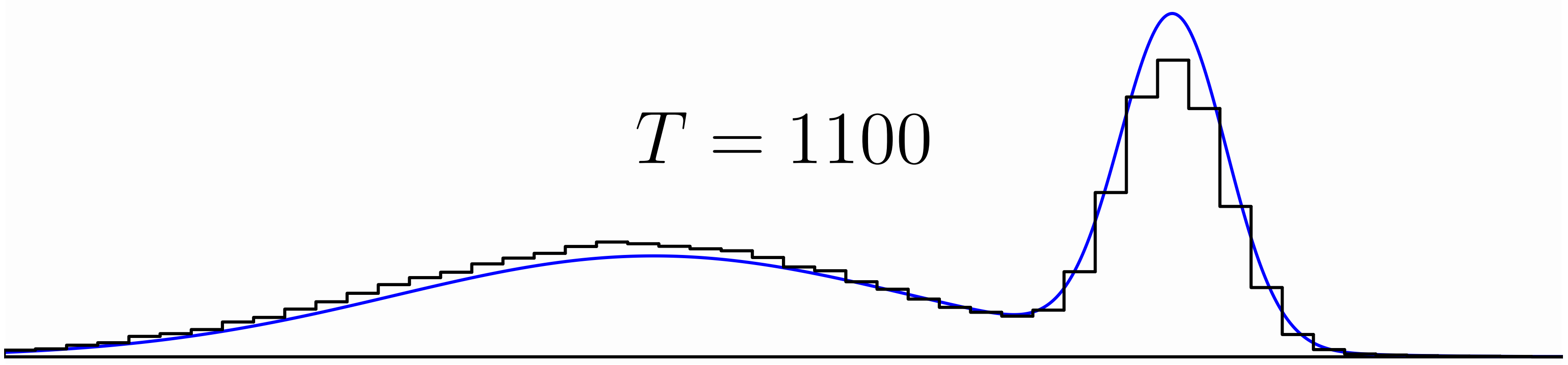

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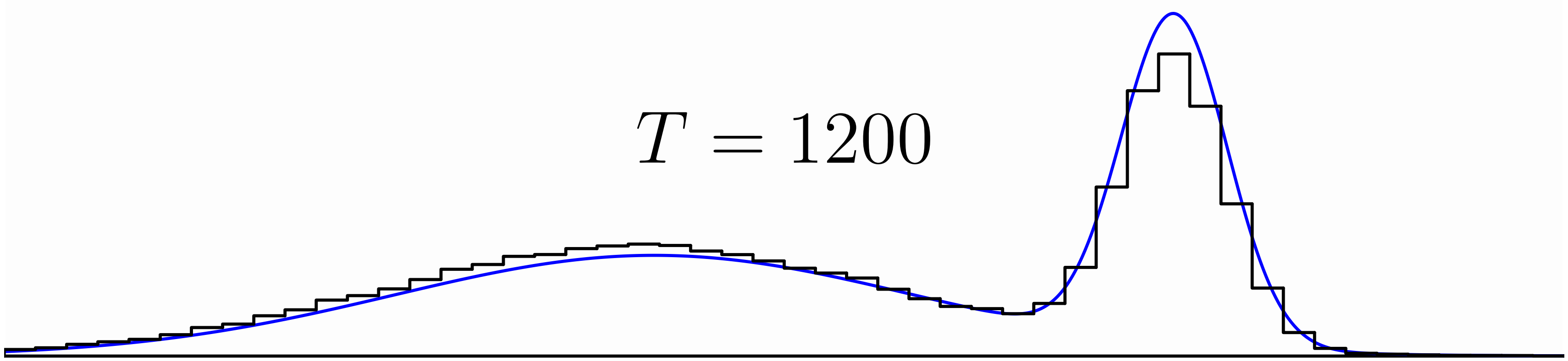

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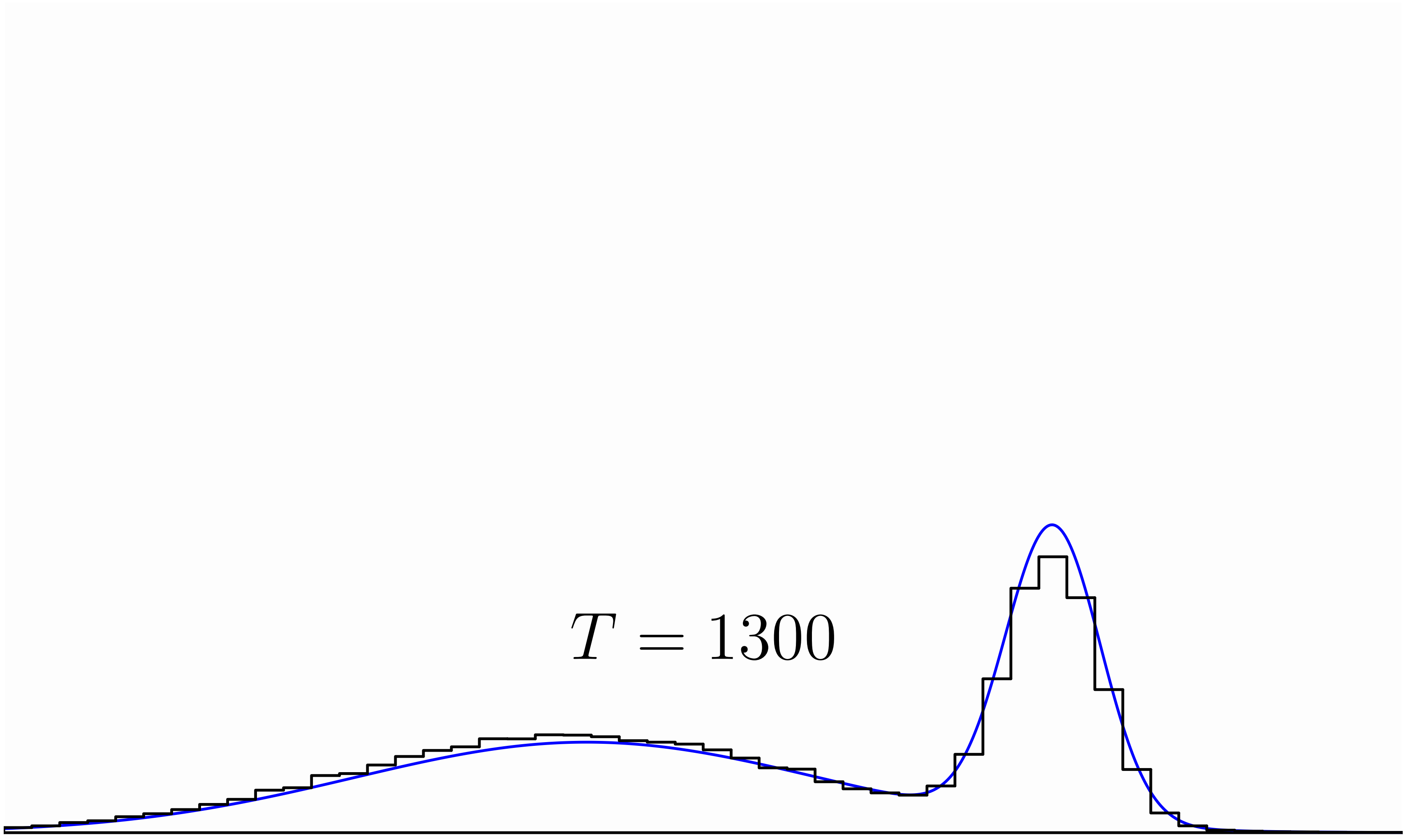

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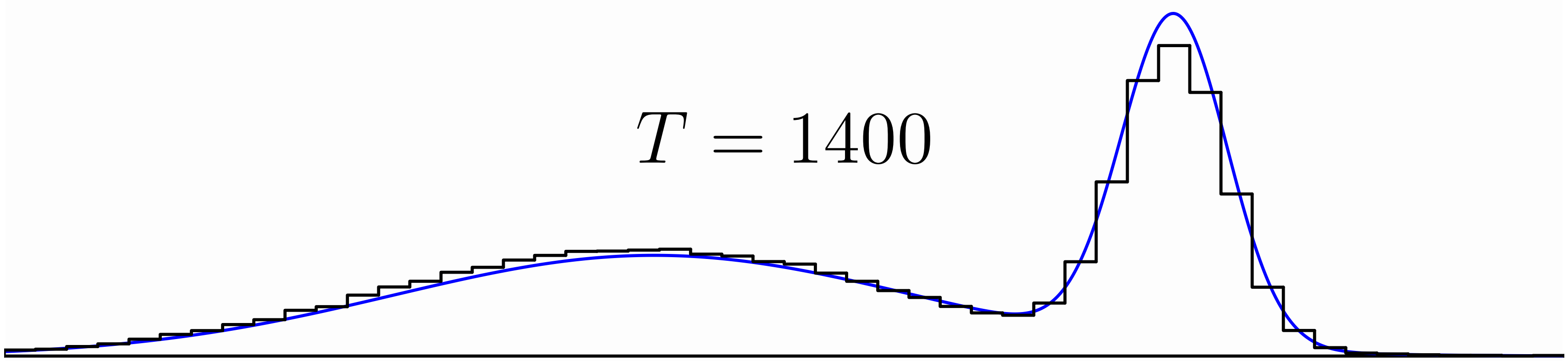

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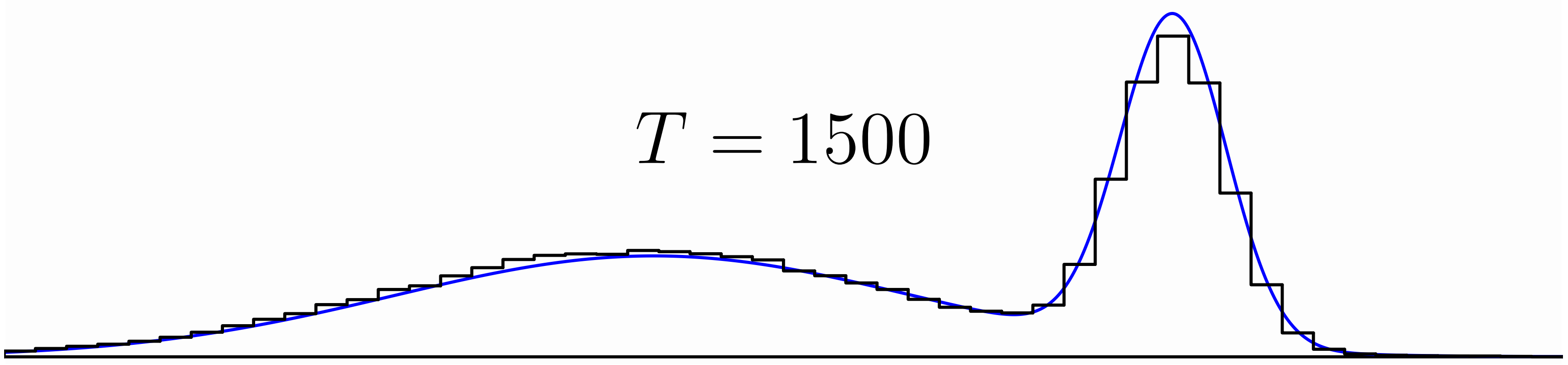

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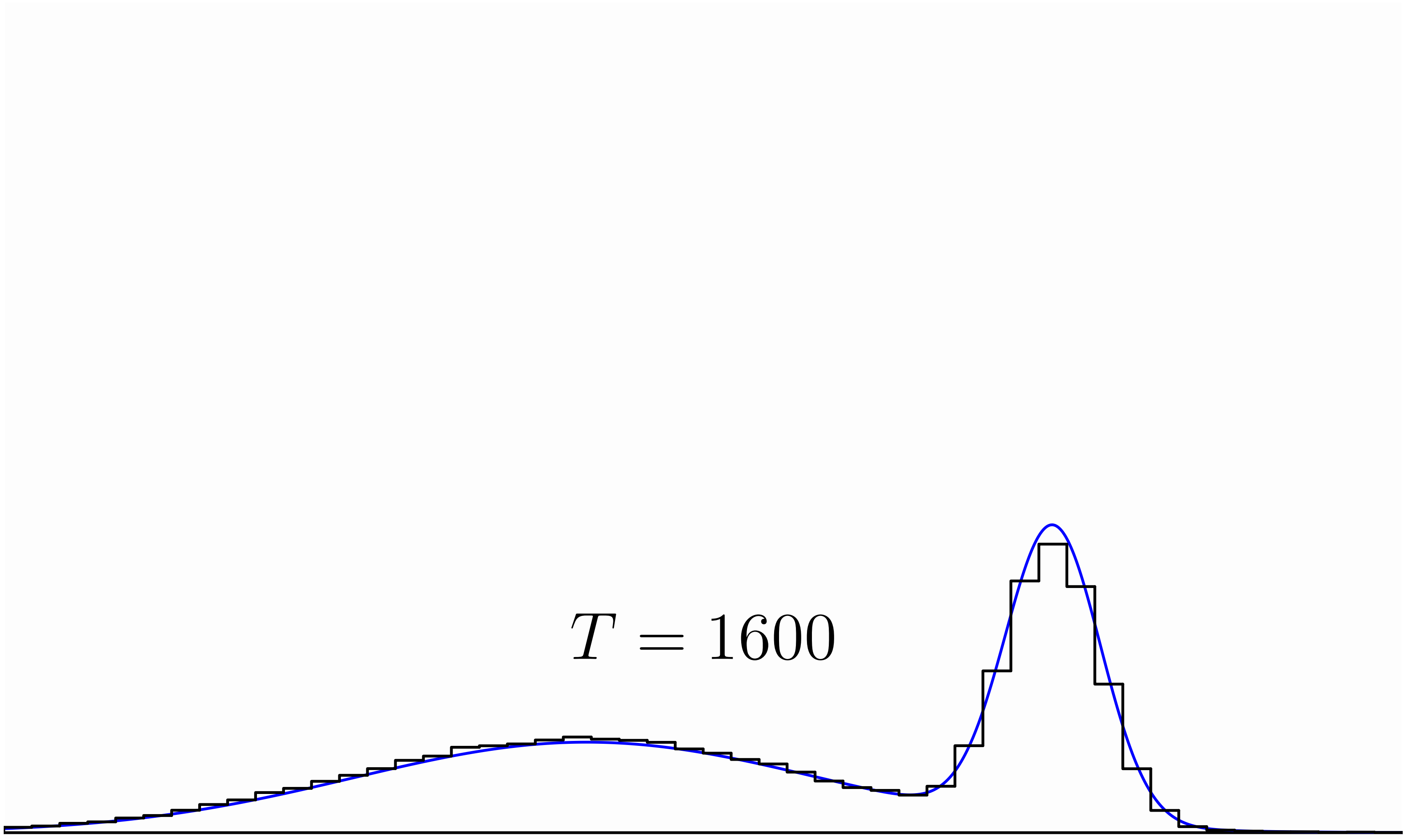

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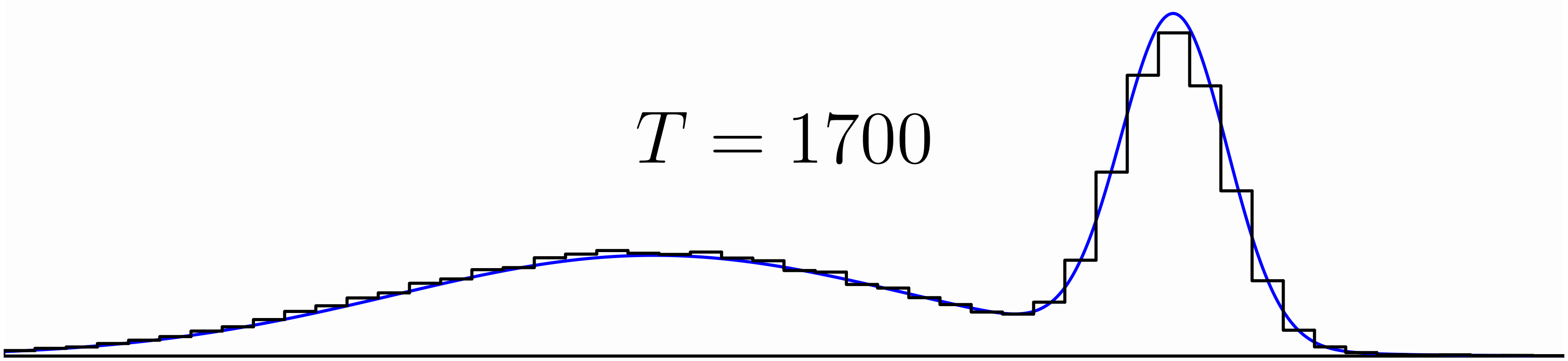

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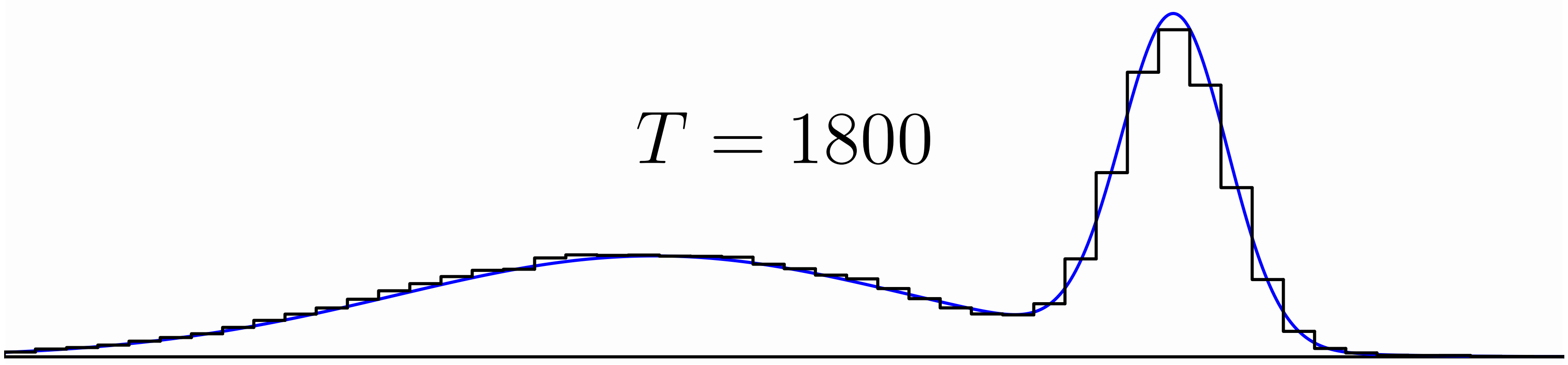

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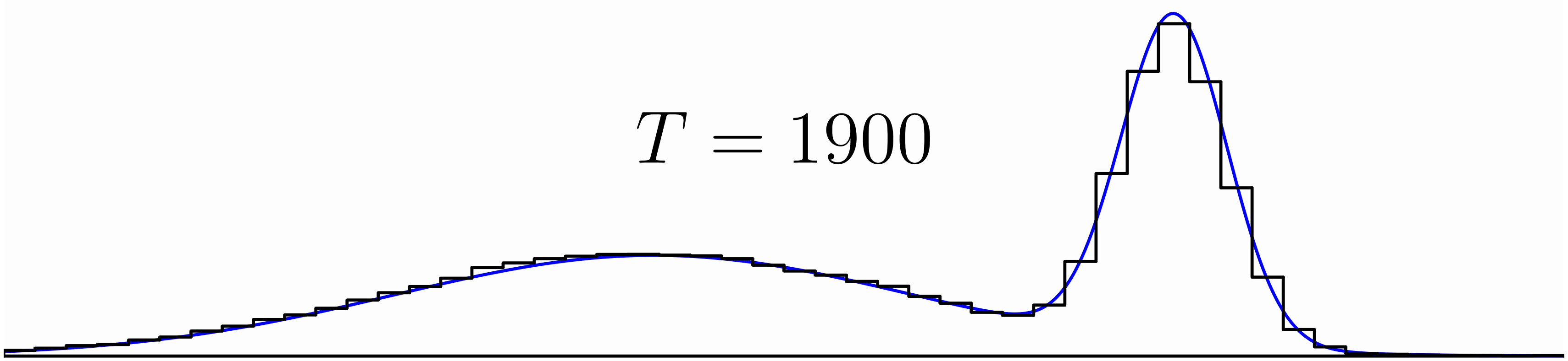

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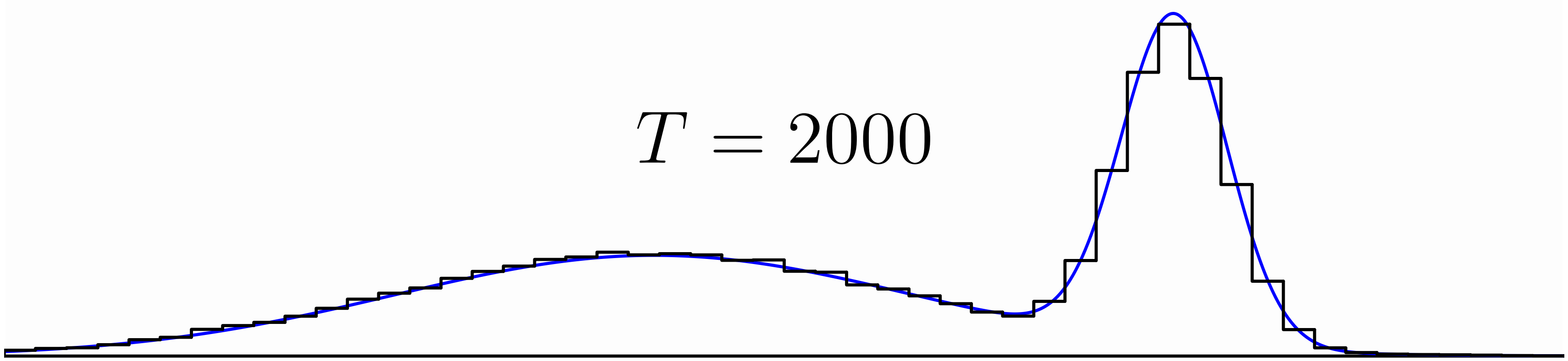

# Proposals and Metropolis-Hastings

- We have some freedom in choosing a new proposal $\boldsymbol{\theta}'$ from our current position $\boldsymbol{\theta}$—a good choice can increase the acceptance rate making the MCMC more efficient

- We define the proposal distribution $p(\boldsymbol{\theta}'|\boldsymbol{\theta})$

- For the standard Metropolis algorithm to work we require $p(\boldsymbol{\theta}'|\boldsymbol{\theta}) = p(\boldsymbol{\theta}|\boldsymbol{\theta}')$

- In some cases (e.g when $\theta_i \geq 0$) this can be hard to achieve

- We can modify our update rule to accept a move with probability

$$\min\left(1, \frac{p(\boldsymbol{\theta}|\boldsymbol{\theta}')\, f(\mathcal{D}|\boldsymbol{\theta}')\, f(\boldsymbol{\theta}')}{p(\boldsymbol{\theta}'|\boldsymbol{\theta})\, f(\mathcal{D}|\boldsymbol{\theta})\, f(\boldsymbol{\theta})}\right)$$

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# Traffic Rate

- Consider monitoring the flow of traffic where we have data

$$\mathcal{D} = (N_1, N_2, \ldots, N_n)$$

  where $N_i$ is the number of car that past on day $i$

- We assume $N_i \sim \mathrm{Poi}(\mu)$ and want to infer $\mu$
- The Poisson distribution has a beta conjugate prior
- We don't have any prior knowledge on $\mu$ so we use a non-informative prior $\mathrm{Gam}(\mu|0,0) = 1/\mu$
- Note that we can solve this problem exactly—however, lets compare with MCMC

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# Proposal Distribution

- If we can choose our proposal distribution $p(\mu'|\mu)$ to be close to the posterior distribution then our acceptance rate would be close to 1

- We choose $p(\mu'|\mu) = \mathrm{Gam}(\mu'|\mu,\mu^2)$ which has $\mathbb{E}[\mu'] = \mu$ and variance 1

- We update with probability $\min(1,r)$ where

$$
\begin{aligned}
r &= \frac{\mathrm{Gam}(\mu|\mu'^2,\mu')\frac{1}{\mu'}\prod_{i=1}^n \mathrm{Poi}(N_i|\mu')}{\mathrm{Gam}(\mu'|\mu^2,\mu)\frac{1}{\mu}\prod_{i=1}^n \mathrm{Poi}(N_i|\mu)} \\
&= \frac{\mu\,\mathrm{Gam}(\mu|\mu'^2,\mu')}{\mu'\,\mathrm{Gam}(\mu'|\mu^2,\mu)} \mathrm{e}^{-n(\mu'-\mu)+\sum\limits_{i=1}^n N_i \log\left(\frac{\mu'}{\mu}\right)}
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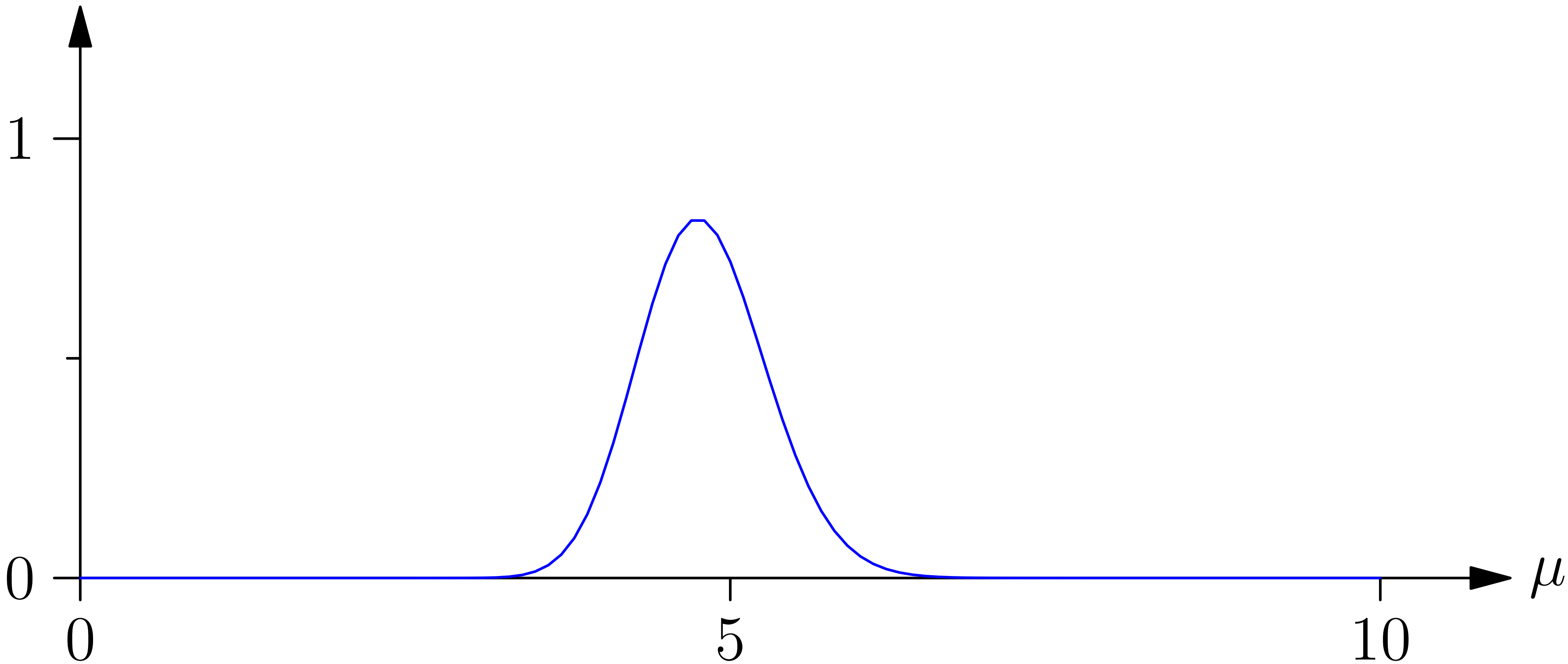
# MCMC in Practice

$$\mathcal{D} = \{4, 4, 6, 4, 2, 2, 5, 9, 5, 4, 3, 2, 5, 4, 4, 11, 6, 2, 3, 11\}$$



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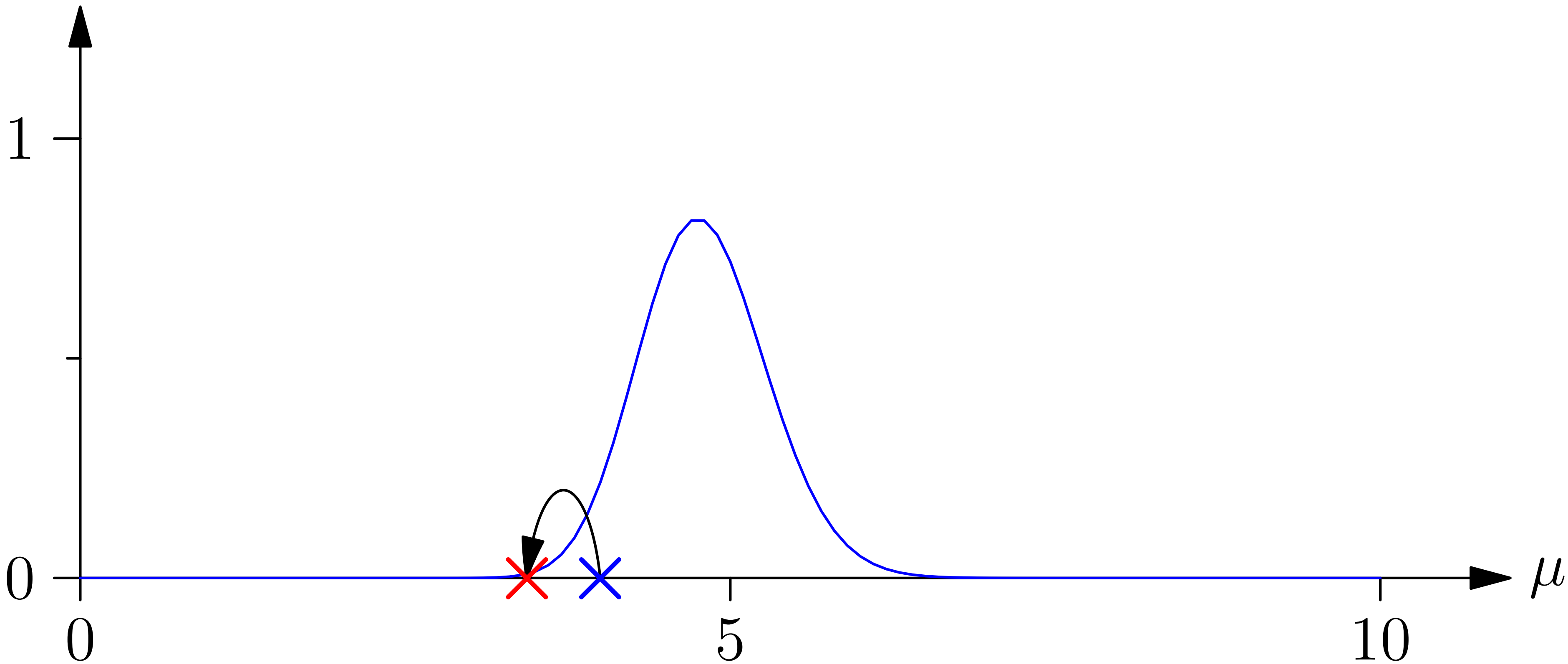

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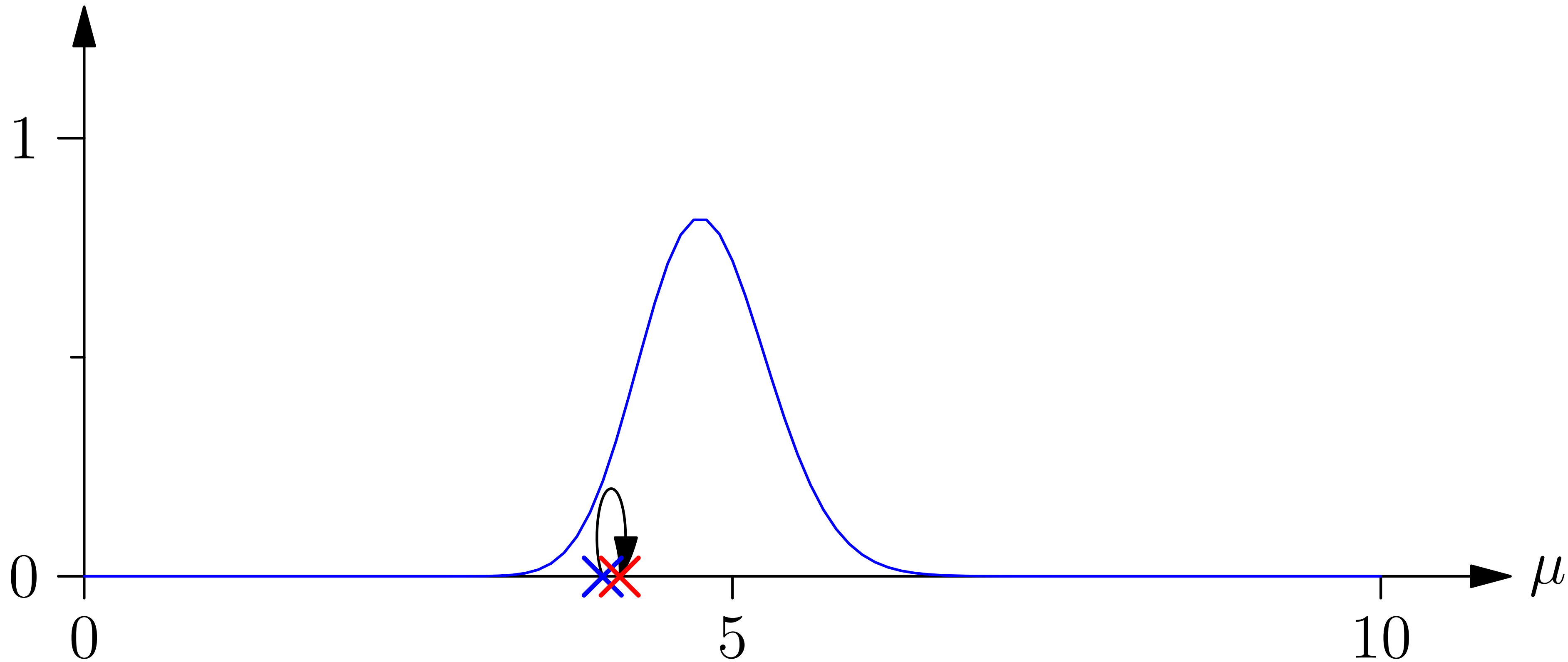

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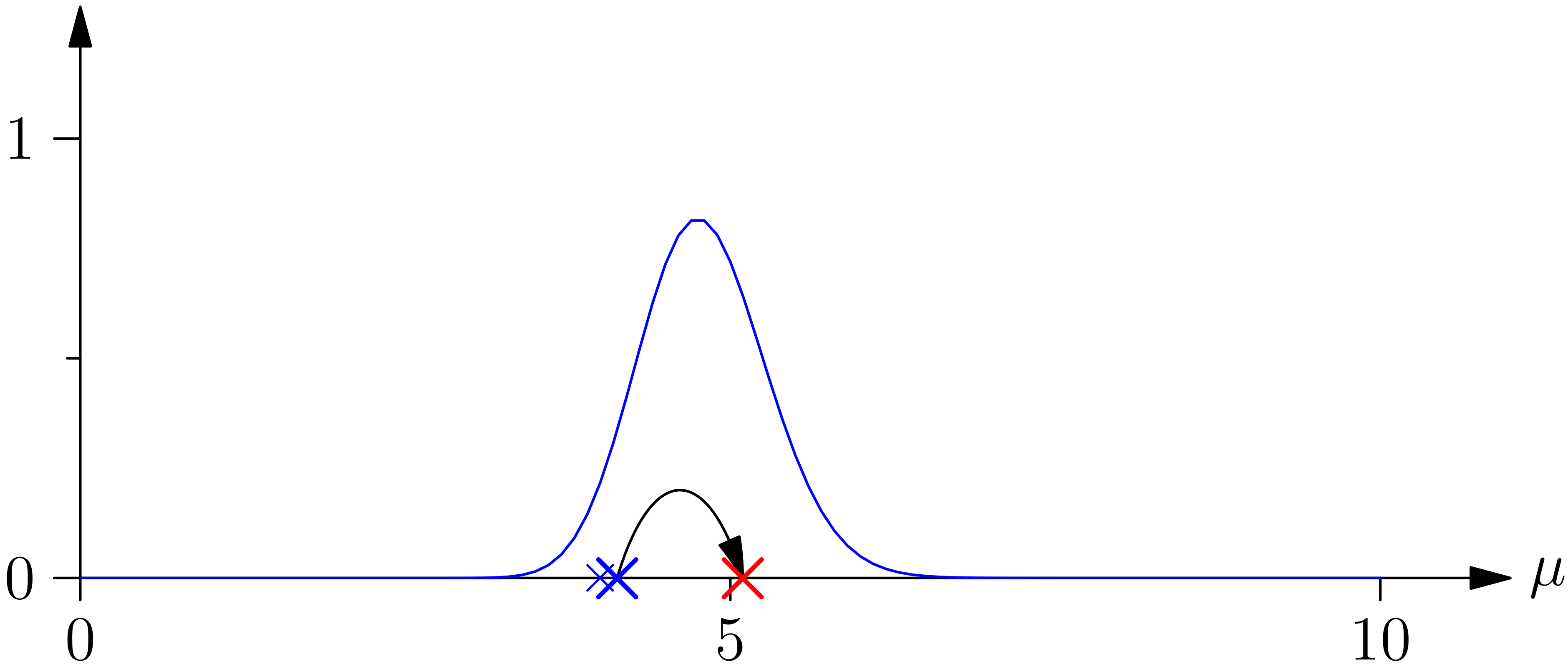

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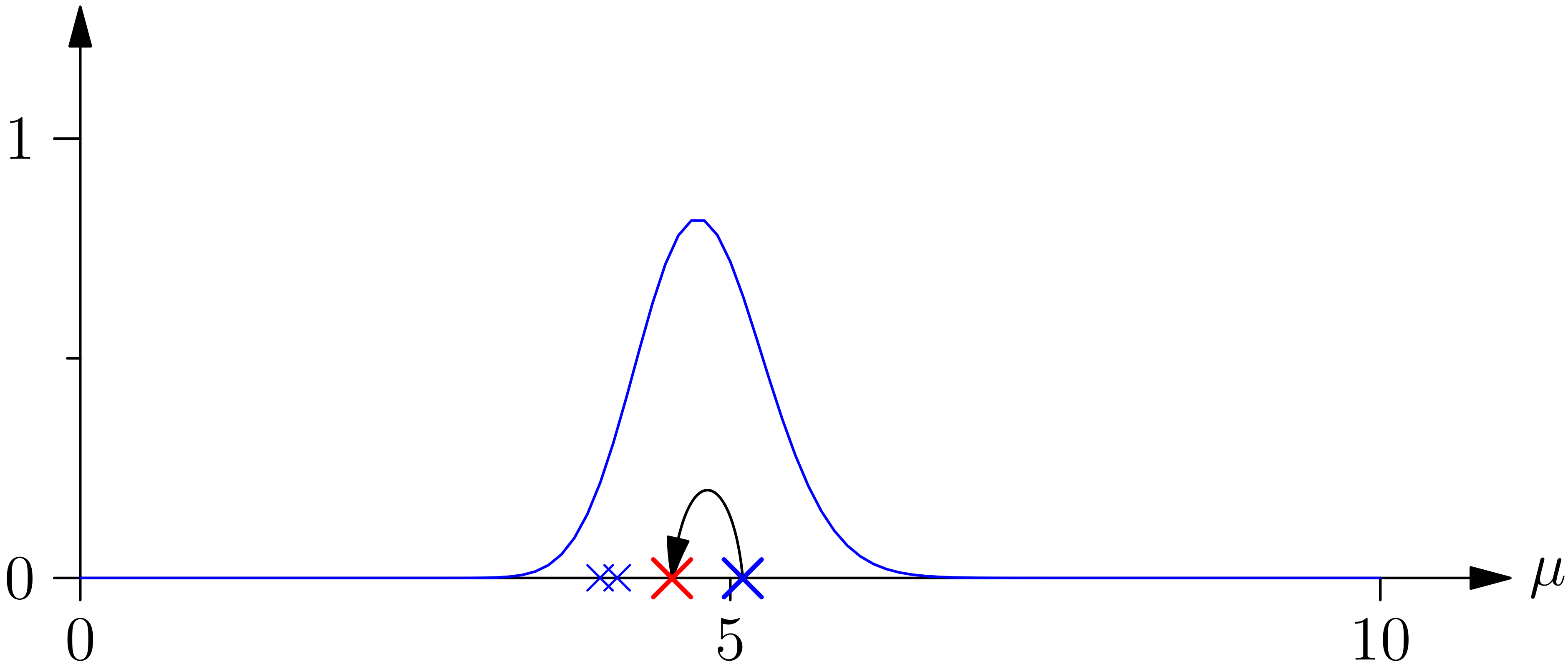

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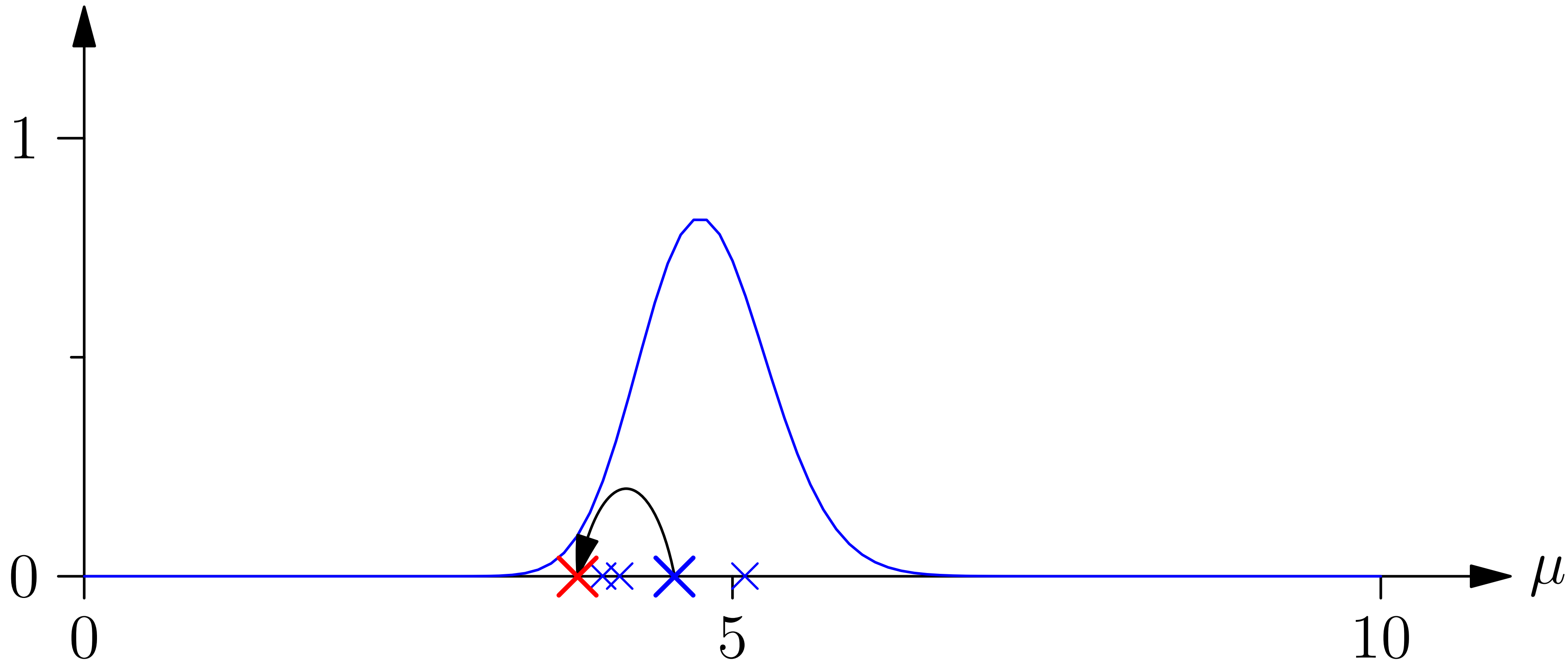

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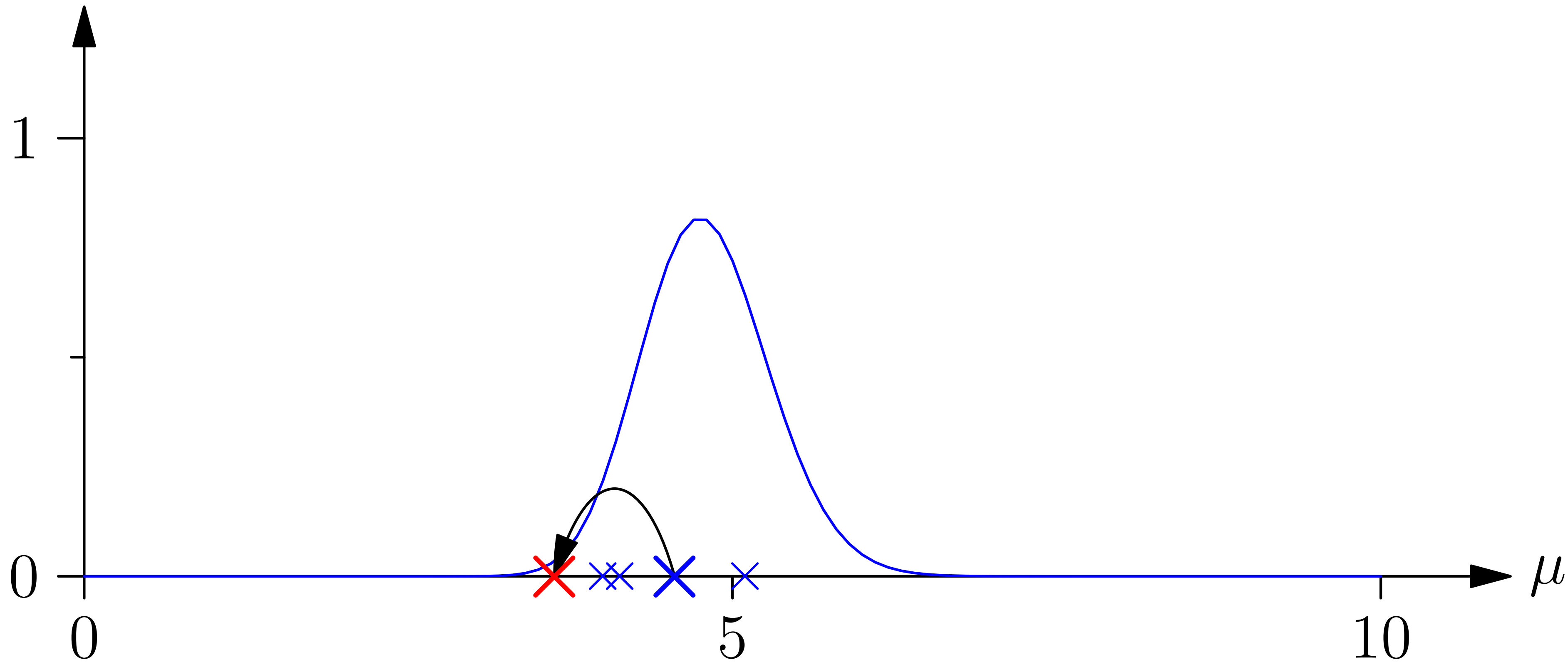

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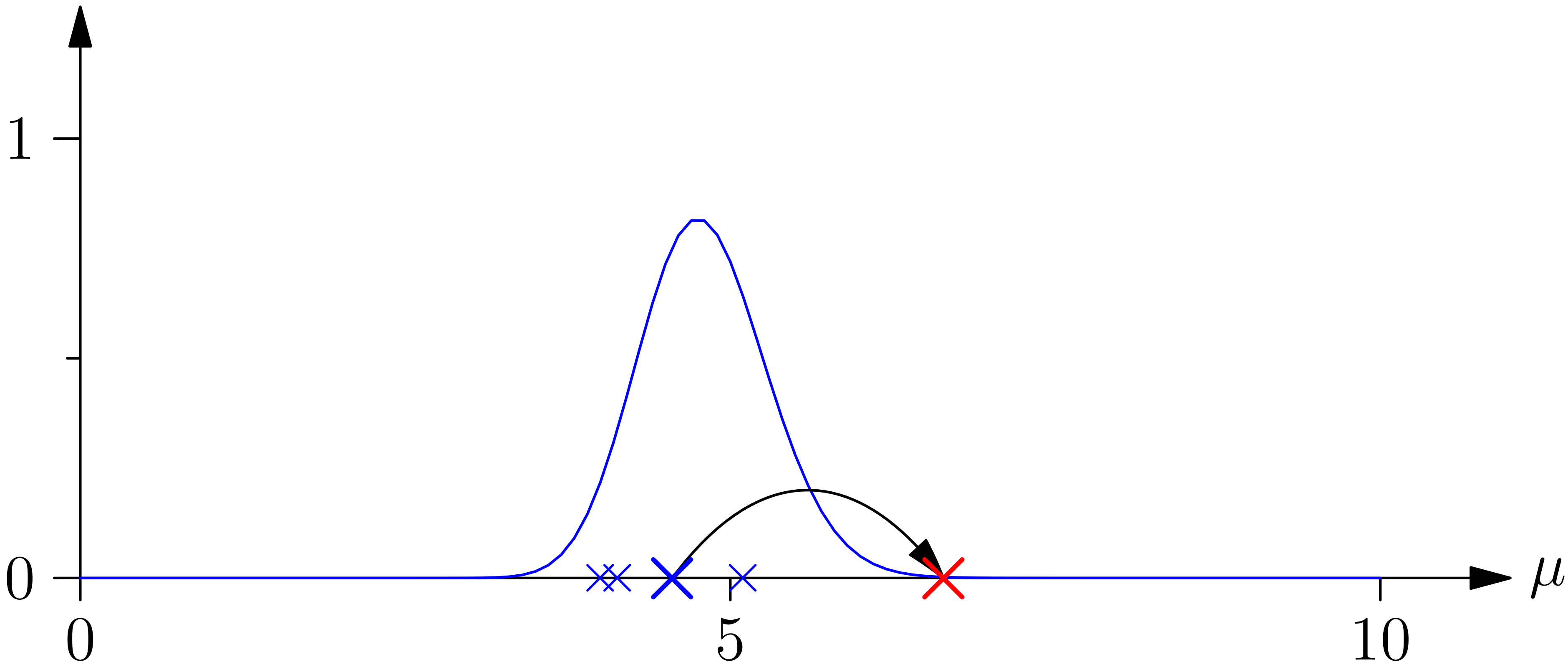

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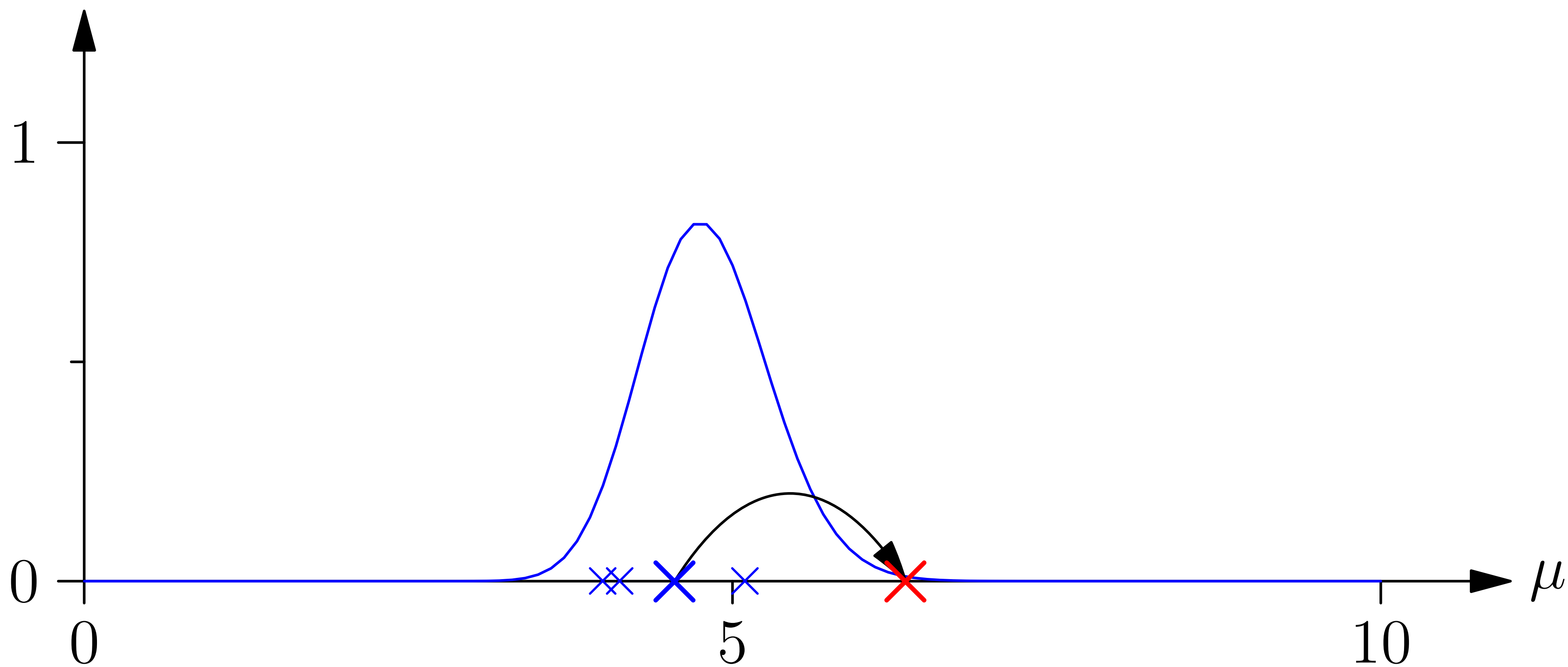

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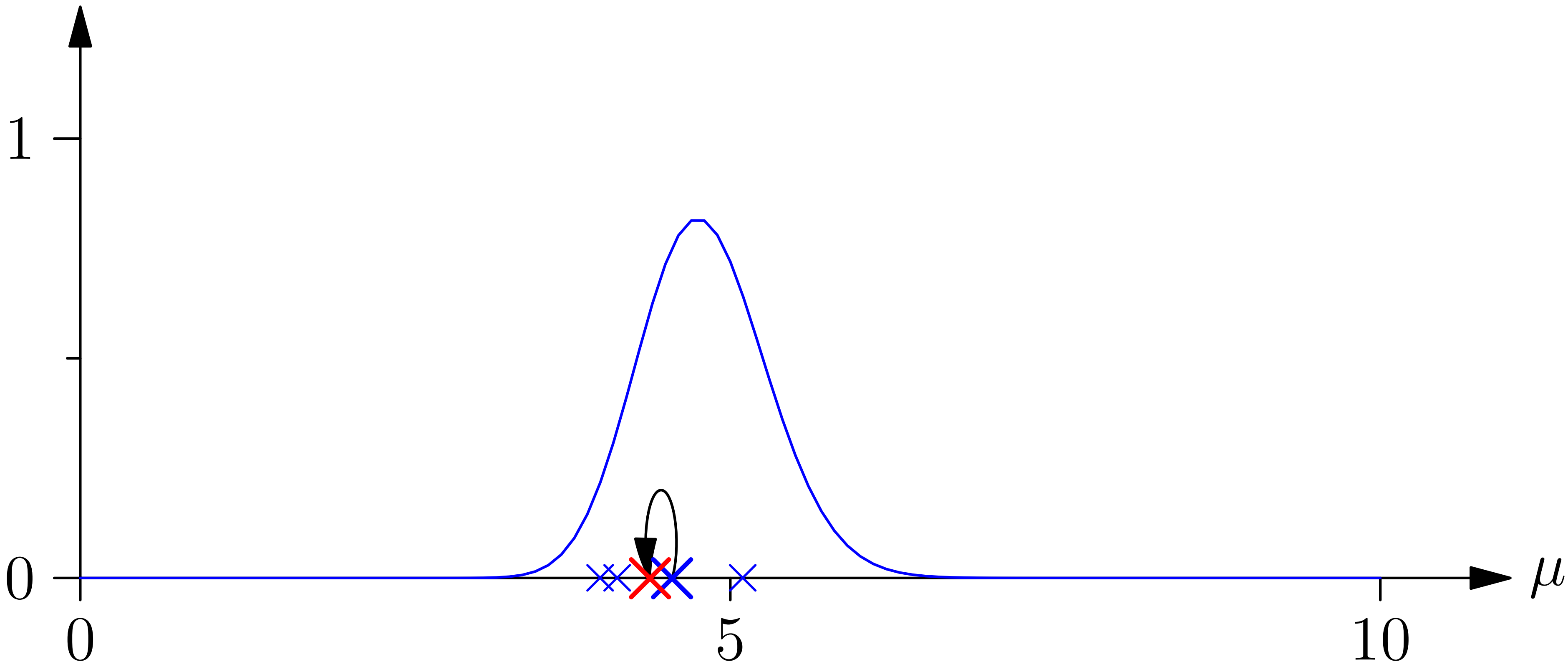

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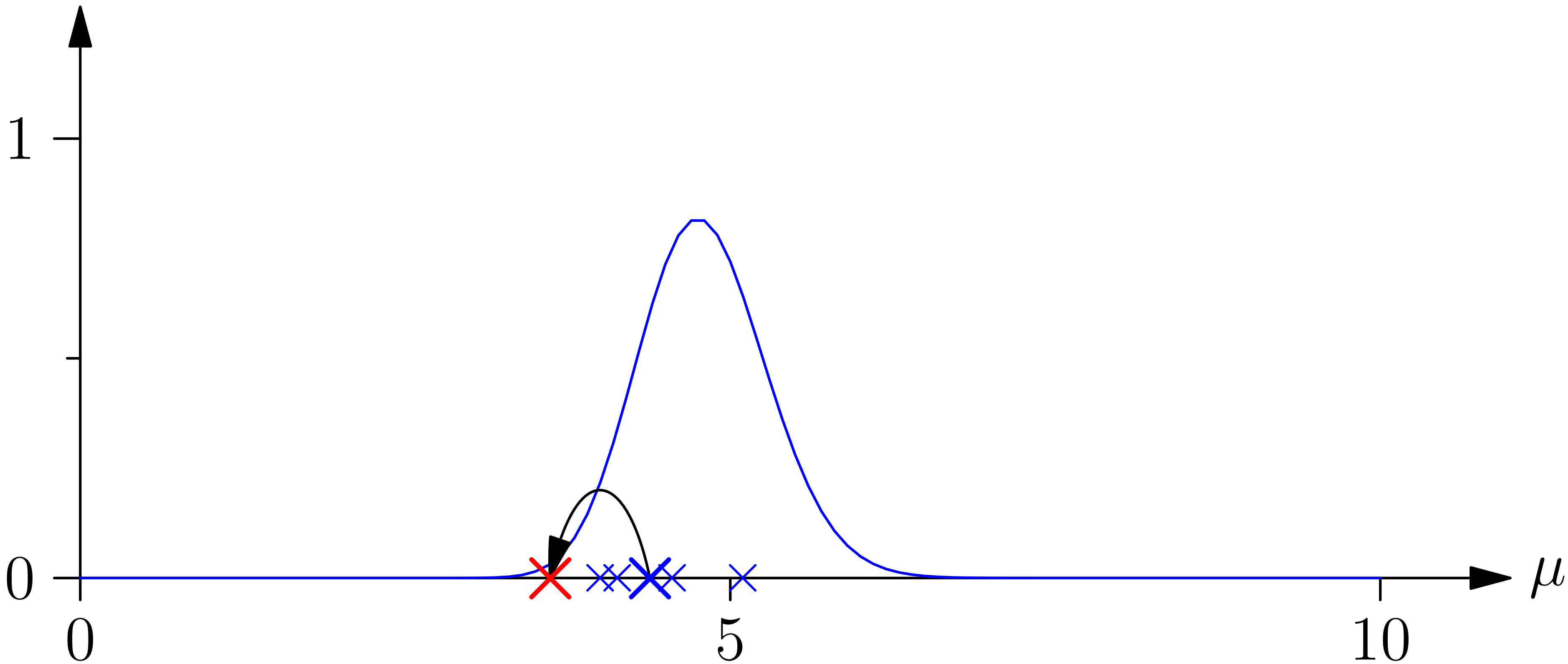

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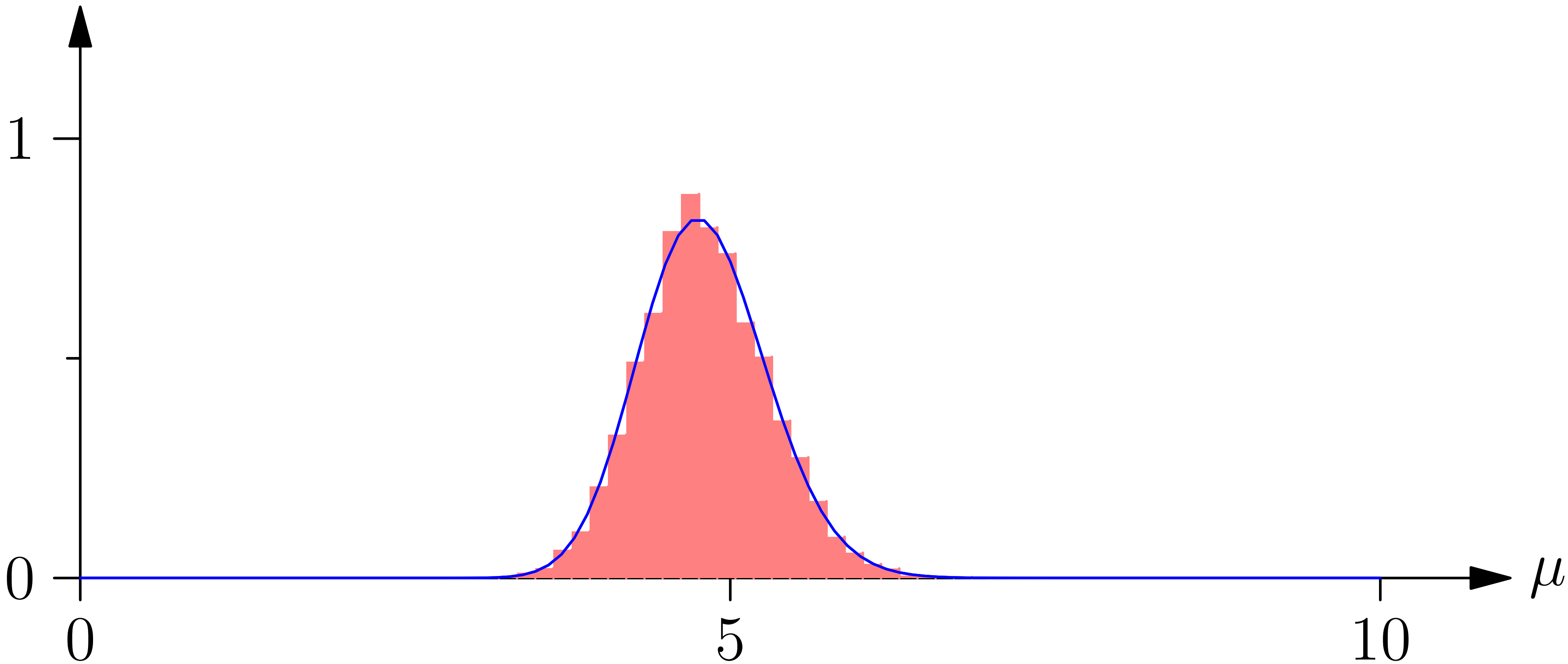

# MCMC Details

- To compute correct histograms you need to count samples where no move is made multiple times
- On modern computers its quite quick to compute millions of samples
- The code is not very difficult to write (although care is need to get everything correct)
- This can be used on complicated problems such as topic models (LDA) with thousands of parameters
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# The MCMC Industry

- MCMC provides a means to accurately sample from very complex models
- There have been many advanced techniques developed to improve MCMC performance
- E.g. hybrid MCMC simulates a dynamics to find good proposals with similar probability far from the starting point
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# Conclusions

- As soon as we use complex models we are no longer able to compute the posterior in closed form
- Monte Carlo techniques and particularly MCMC are a very general method for computing samples from the posterior
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