Advanced Machine Learning

Bayesian Inference

Bayes, Conjugate Priors, Uninformative Priors

Outline

1. **Bayes' Rule**
2. Conjugate Priors
3. Uninformative Priors

Dealing with Uncertainty

- In machine learning we are attempting to make inference under uncertainty
- The natural language for discussing uncertainty is probability
- The natural framework for making inferences is Bayesian statistics
- However, this requires that we encode our prior knowledge of the problem and specify a likelihood
- In consequence, probabilistic methods tend to be bespoke, rather then general purpose black boxes

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Revision on Bayes

- Bayes' rule

$$\mathbb{P}(\mathcal{H}_i|\mathcal{D}) = \frac{\mathbb{P}(\mathcal{D}|\mathcal{H}_i)\,\mathbb{P}(\mathcal{H}_i)}{\mathbb{P}(\mathcal{D})}$$

  - ⋆ $\mathbb{P}(\mathcal{H}_i|\mathcal{D})$ is the **posterior** probability of a hypothesis $\mathcal{H}_i$ (i.e. the probability of $\mathcal{H}_i$ **after** we see the data)
  - ⋆ $\mathbb{P}(\mathcal{D}|\mathcal{H}_i)$ is the **likelihood** of the data given the hypothesis. Note, that we calculated this from the forward problem
  - ⋆ $\mathbb{P}(\mathcal{H}_i)$ is the **prior** probability (i.e. the probability of $\mathcal{H}_i$ **before** we see the data)
  - ⋆ $\mathbb{P}(\mathcal{D})$ is the **evidence**

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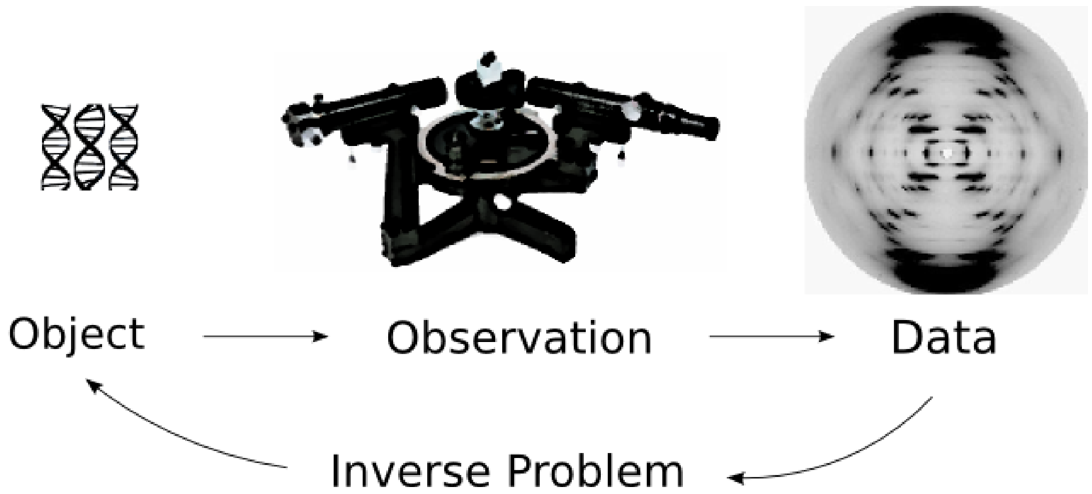
Solving Inverse Problems



- We want the posterior $\mathbb{P}(\mathcal{H}_i|\mathcal{D})$ (i.e. the probability of what happened given some evidence)
- The Bayesian formalism converts this into the forward problem

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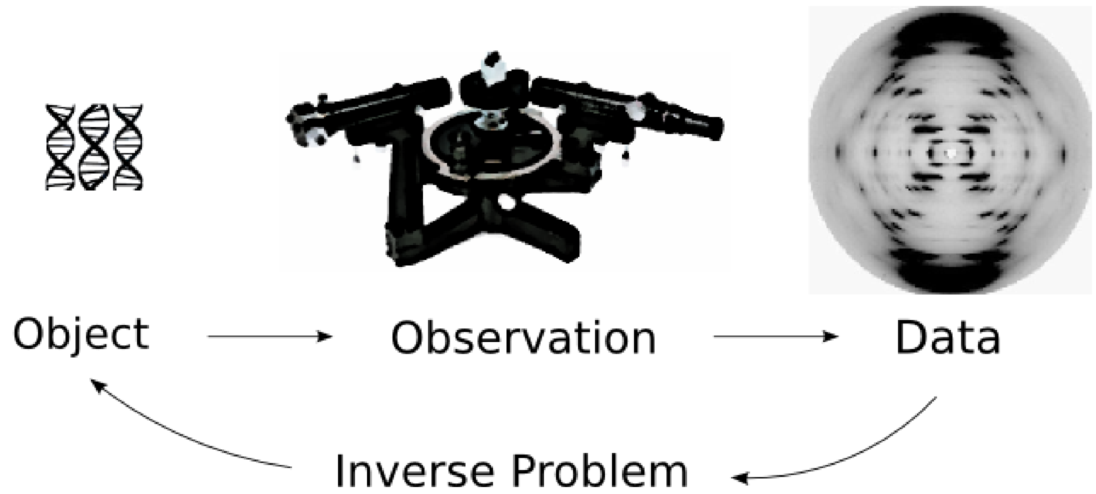

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- We calculate the likelihood $\mathbb{P}(\mathcal{D}|\mathcal{H}_i)$ (i.e. assuming the hypothesis, what is the chance of obtaining the data?)
- We consider the process of how the data is generated
- This uses the data we have (doesn't care about missing data)
- But we also need to know the prior $\mathbb{P}(\mathcal{H}_i)$
- Also, this can get difficult when we have many hypotheses

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Evidence

- The normalisation term

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  tells you how likely the data is (given the prior and likelihood function)

- It is called the **marginal likelihood**

- If we have two models M_1 and M_2 we can do **model selection** by choosing the model with the largest evidence $\mathbb{P}(\mathcal{D} \mid M_1)$ or $\mathbb{P}(\mathcal{D} \mid M_2)$

- This also allows us to select hyperparameters for a model

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Probability Density

- When we are working with continuous variables it is more natural to work with probability densities

$$f_X(x) = \lim_{\delta x \to 0} \frac{\mathbb{P}(x \le X < x + \delta x)}{\delta x}$$

- Note that densities are non-negative, but can be greater than 1 (they are not probabilities)

- However

$$\mathbb{P}(a \le X \le b) = \int_a^b f_X(x) \mathrm{d}x$$

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Densities and Bayes

- Bayes' rule also applies to densities

$$\mathbb{P}(x \le X < x + \delta x | Y) = \frac{\mathbb{P}(Y|x)\,\mathbb{P}(x \le X < x + \delta x)}{\mathbb{P}(Y)}$$

- Dividing by δx and taking the limit $\delta x \to 0$

$$f_{X|Y}(x|Y) = \frac{\mathbb{P}(Y|x)\, f_X(x)}{\mathbb{P}(Y)}$$

- Similarly if X is discrete and Y continuous

$$\mathbb{P}(X|y) = \frac{f_{Y|X}(y|X)\,\mathbb{P}(X)}{f_Y(y)}$$

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Practical Bayesian Inference

- Often consider learning parameters $\boldsymbol{\theta}$

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{p(\mathcal{D}|\boldsymbol{\theta})\,p(\boldsymbol{\theta})}{p(\mathcal{D})}$$

- This can be hard for large data sets as the posterior, $p(\boldsymbol{\theta}|\mathcal{D})$, is often a mess

- If we are lucky and have a simple likelihood then if we choose the right prior we end up with a posterior of the same form as the prior

- This occurs in some classic probabilistic inference problems, but as we will see soon it is also true for Gaussian Processes

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- Suppose we have a coin and we want to establish the probability of a head

- We want to learn this from a series of independent trials

- (Independent trials with two possible outcomes are known in probability theory as Bernoulli trials)

- Let X_i equal 1 if the i^{th} trial is a head and 0 otherwise

- If the probability of a head is p then the **likelihood** of a X_i is

$$\mathbb{P}(X_i|p) = p^{X_i}(1-p)^{1-X_i}$$

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$$\mathbb{P}(X_i|p) = p^{X_i}(1-p)^{1-X_i} = \begin{cases} p & \text{if } X_i = 1 \\ (1-p) & \text{if } X_i = 0 \end{cases}$$

Prior

- We may have a prior belief (e.g. we have made a few trials or we see the coin looks like a normal penny)

- We will suppose we can model our prior belief in terms of a **Beta distribution**

$$f(p) = \mathrm{Beta}(p|a,b) = \frac{p^{a-1}(1-p)^{b-1}}{B(a,b)}$$

- $B(a,b)$ is just a normalisation constant

$$B(a,b) = \int_0^1 p^{a-1}(1-p)^{b-1}\mathrm{d}p = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$$

- This is a useful function for modelling the distribution of a random variable in the range 0 to 1

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Uninformative Prior

- Suppose we have no idea about p what should we do?
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- This corresponds to a beta distribution with $a = b = 1$
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Independent Trials

- Using Bayes' rule

$$f(p|\mathcal{D}) = \frac{\mathbb{P}(\mathcal{D}|p)\, f(p)}{\mathbb{P}(\mathcal{D})}$$

- Assuming the trials are independent (a reasonably fair assumption for tossing coins) then the likelihood factorises

$$\begin{aligned}
\mathbb{P}(\mathcal{D}|p) &= \prod_{i=1}^{n} p^{X_i}(1-p)^{1-X_i} \\
&= p^{X_1}(1-p)^{1-X_1} p^{X_2}(1-p)^{1-X_2} \ldots p^{X_n}(1-p)^{1-X_n} \\
&= p^{\sum_i X_i}(1-p)^{\sum_i (1-X_i)} = p^s(1-p)^{n-s}
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$s = \sum_i X_i$ (number of successes/heads)

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- The denominator is a normalising factor

$$\mathbb{P}(\mathcal{D}) = \int_0^1 \mathbb{P}(\mathcal{D}|p)\, f(p)\mathrm{d}p = \int_0^1 \frac{p^{s+a_0-1}(1-p)^{n-s+b_0-1}}{B(a_0, b_0)} \mathrm{d}p$$
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- The posterior distribution is Beta distribution

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Incremental Updating

- For independent data we can update incrementally
  $\mathcal{D} = (X_1, X_2, \ldots, X_n)$

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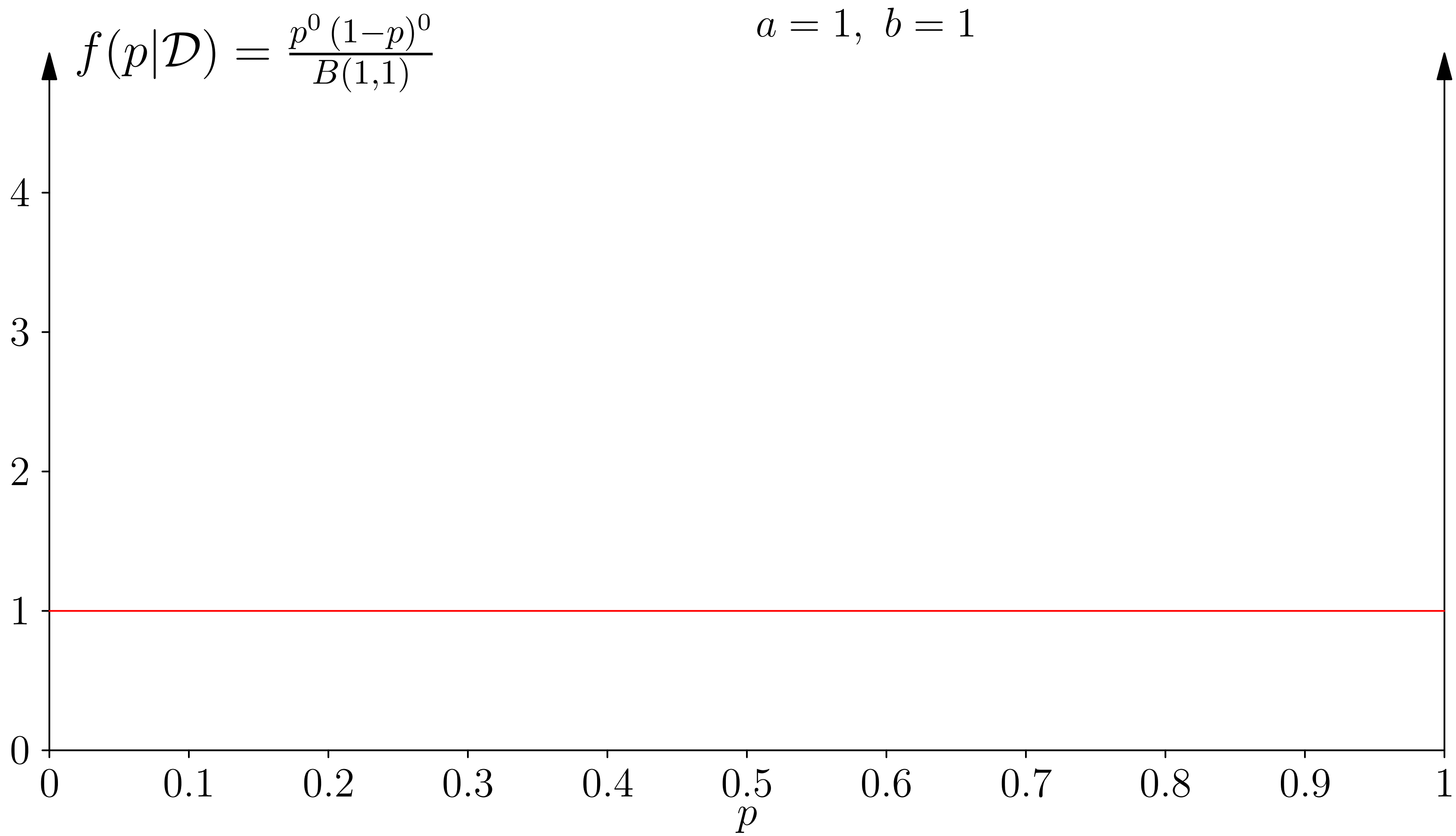
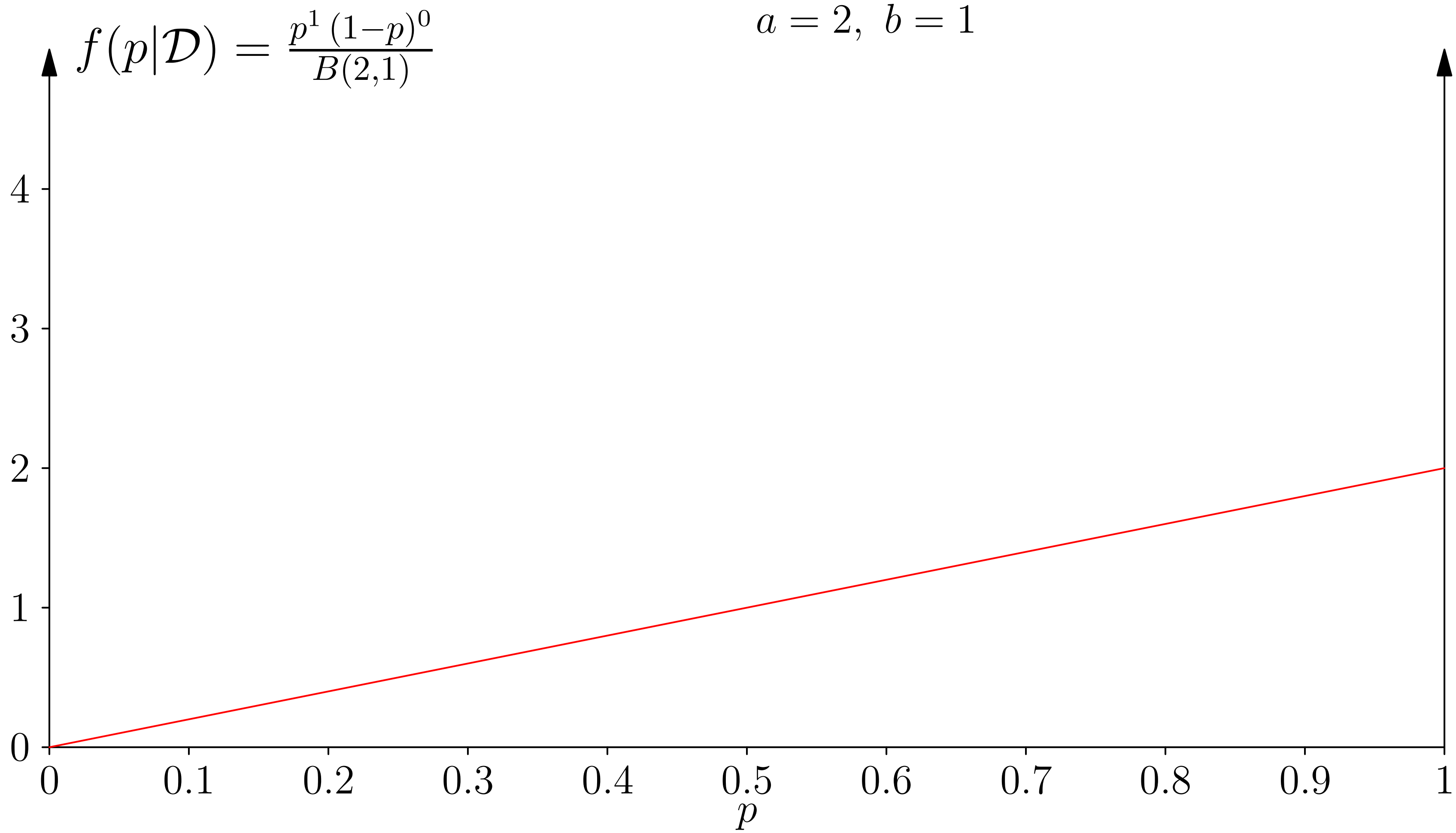
Example (p=0.7)



$f(p|\mathcal{D}) = \frac{p^0\,(1-p)^0}{B(1,1)}$
$a = 1,\ b = 1$
4
3
2
1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
p

Example (p=0.7)

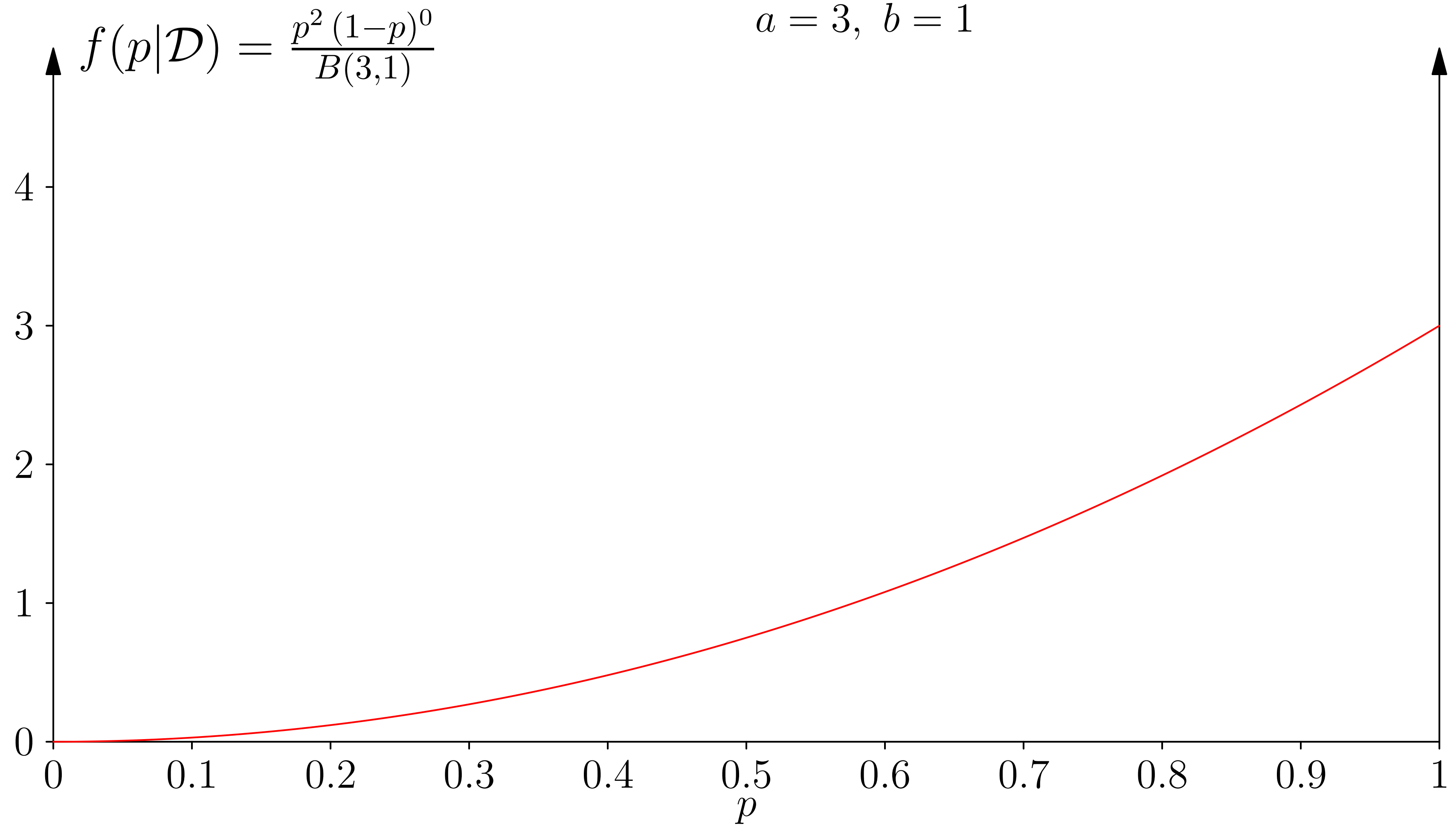
$\mathcal{D} = \{\mathrm{H},$



Example (p=0.7)

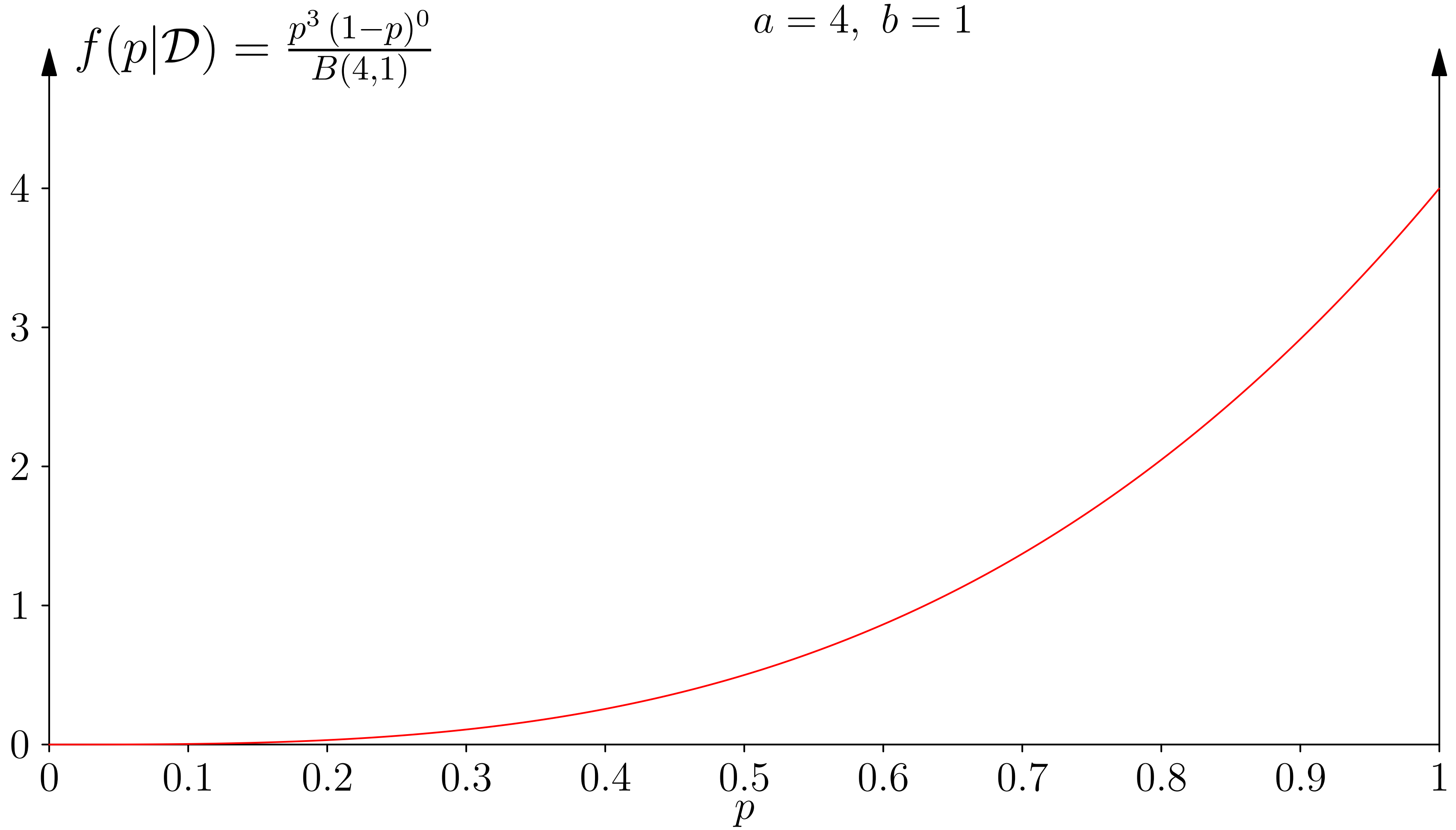
$\mathcal{D} = \{$H,H,

$a = 3, \; b = 1$



Example (p=0.7)

$\mathcal{D} = \{\mathrm{H,H,H,}$



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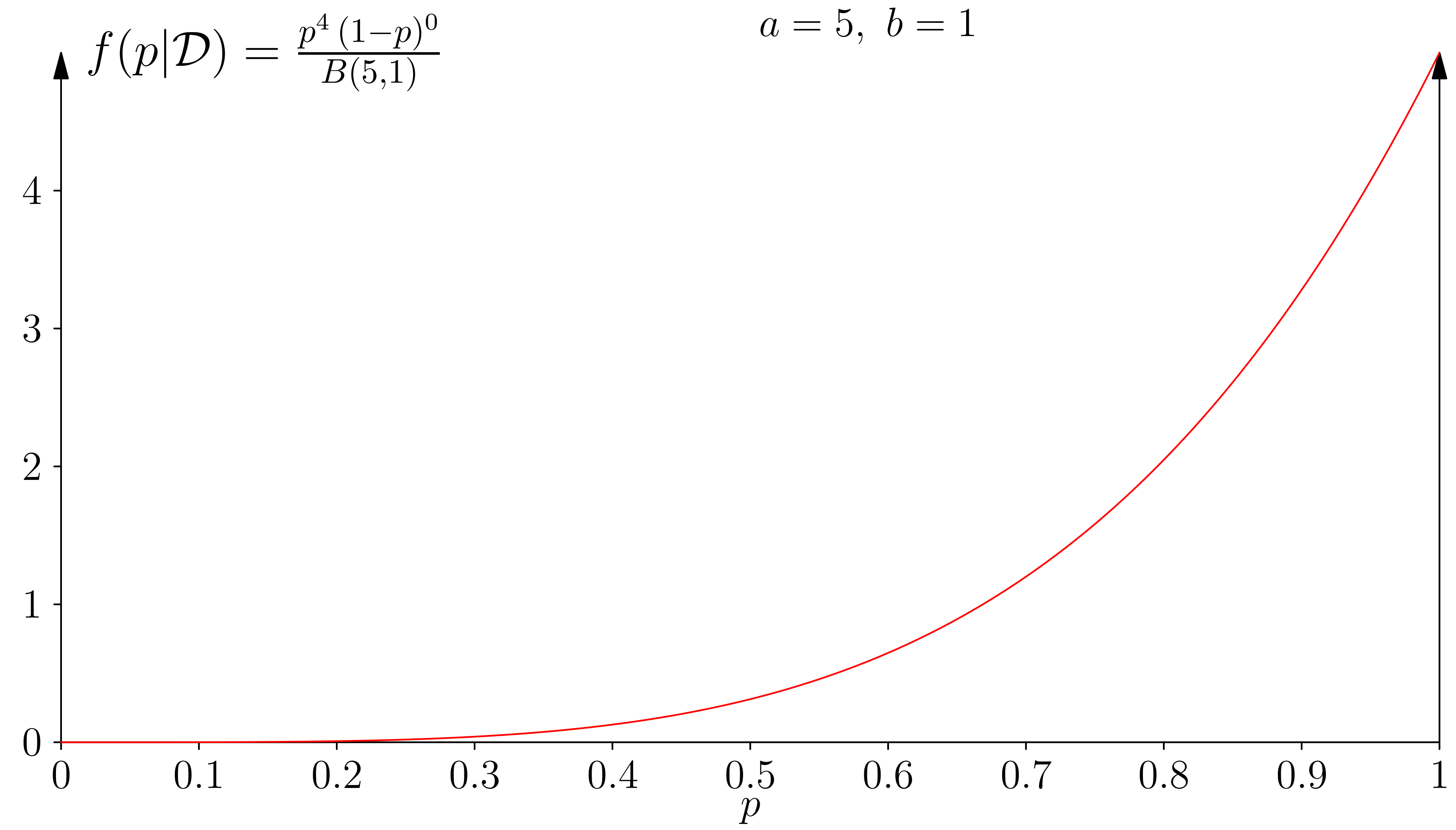

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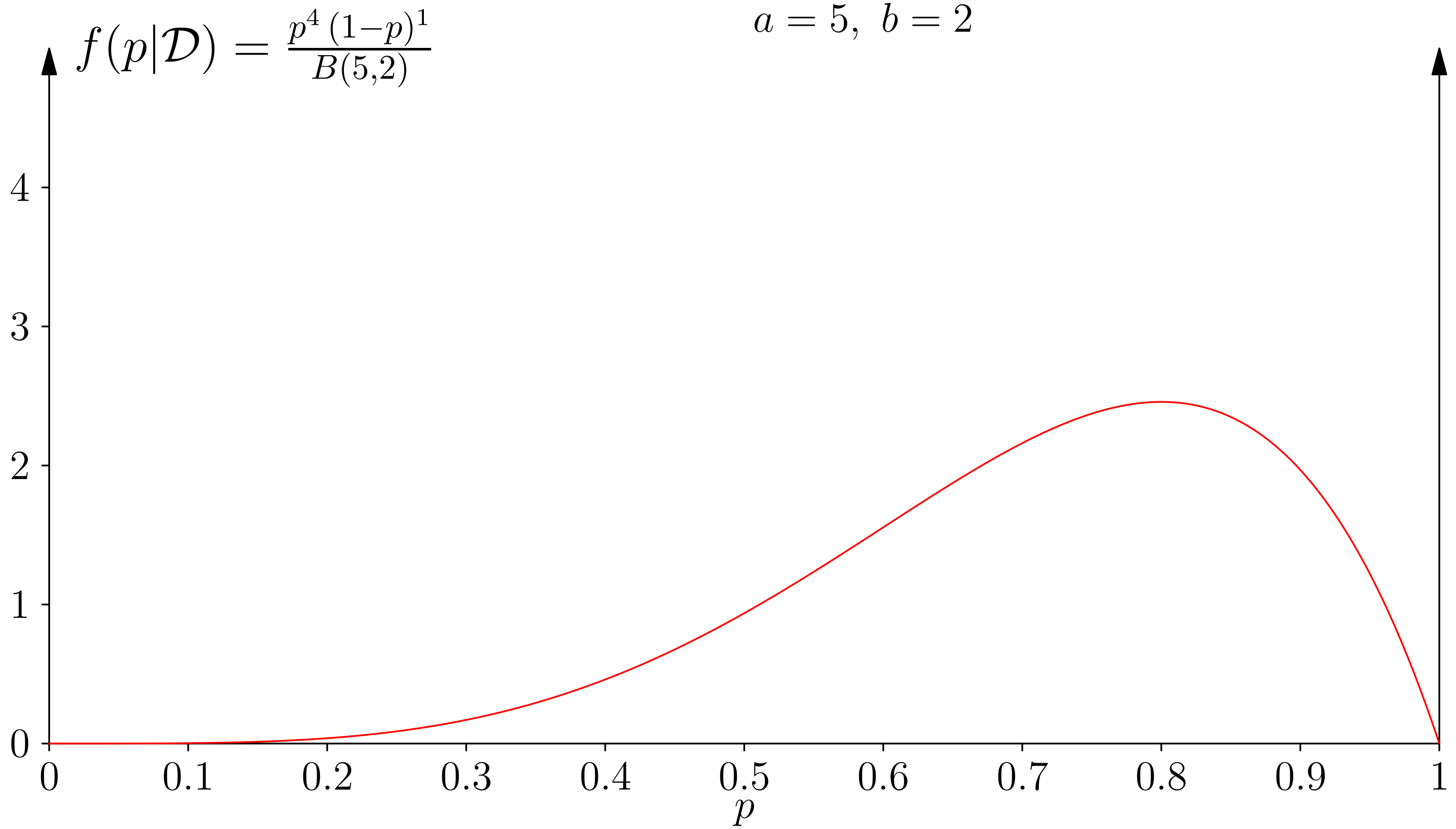

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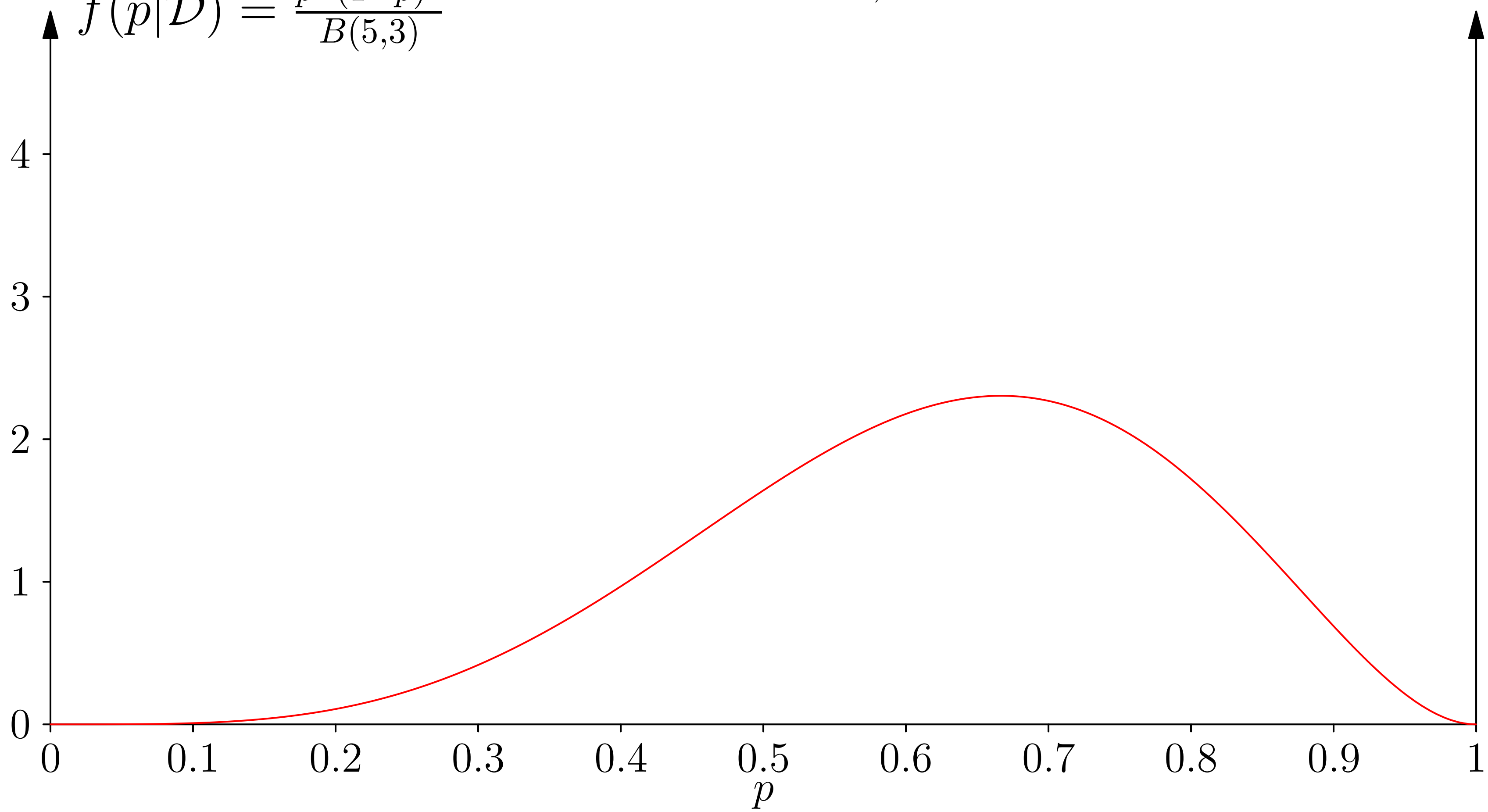
$f(p|\mathcal{D}) = \frac{p^4\,(1-p)^2}{B(5,3)}$

$a = 5,\ b = 3$



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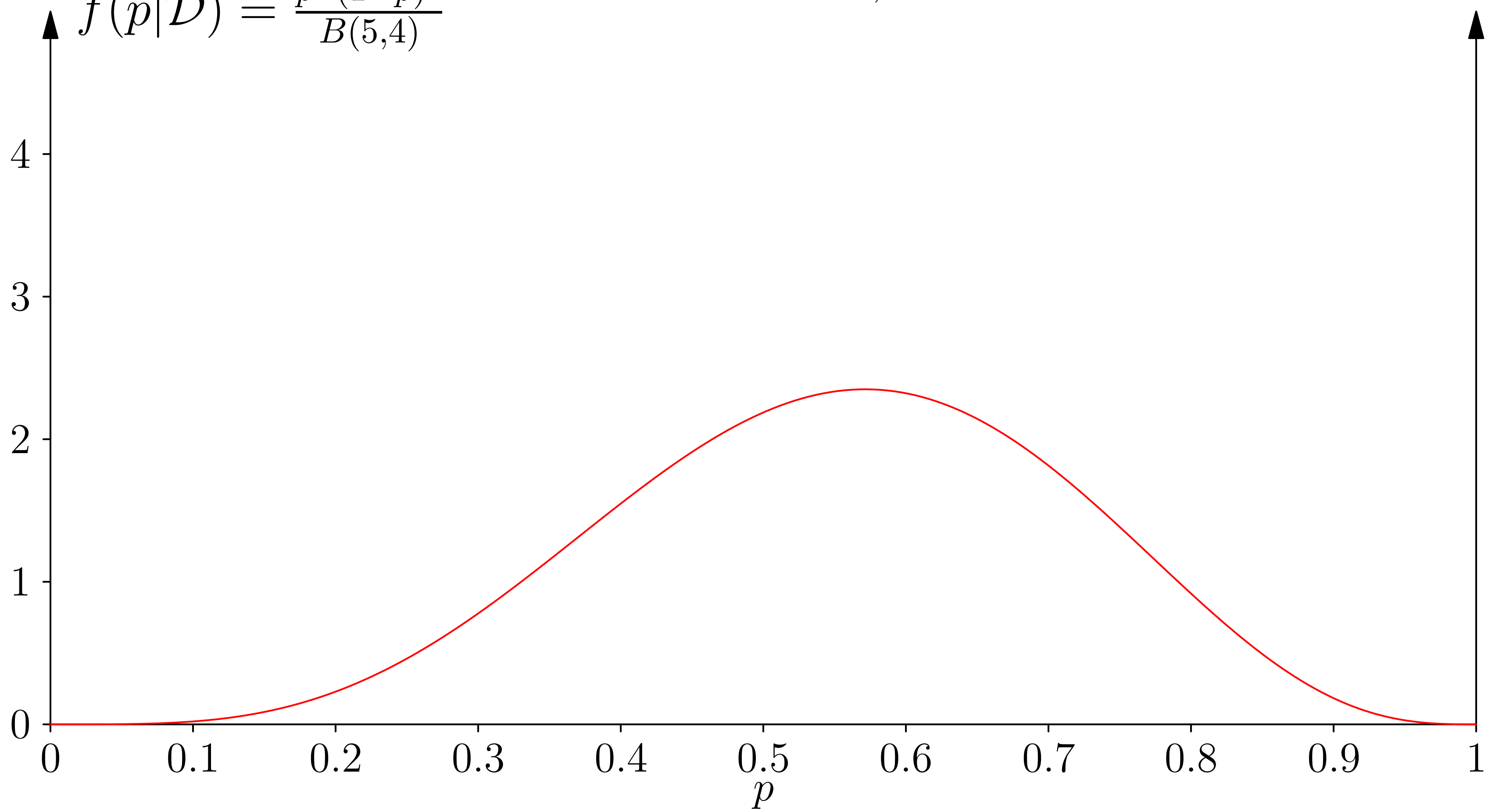

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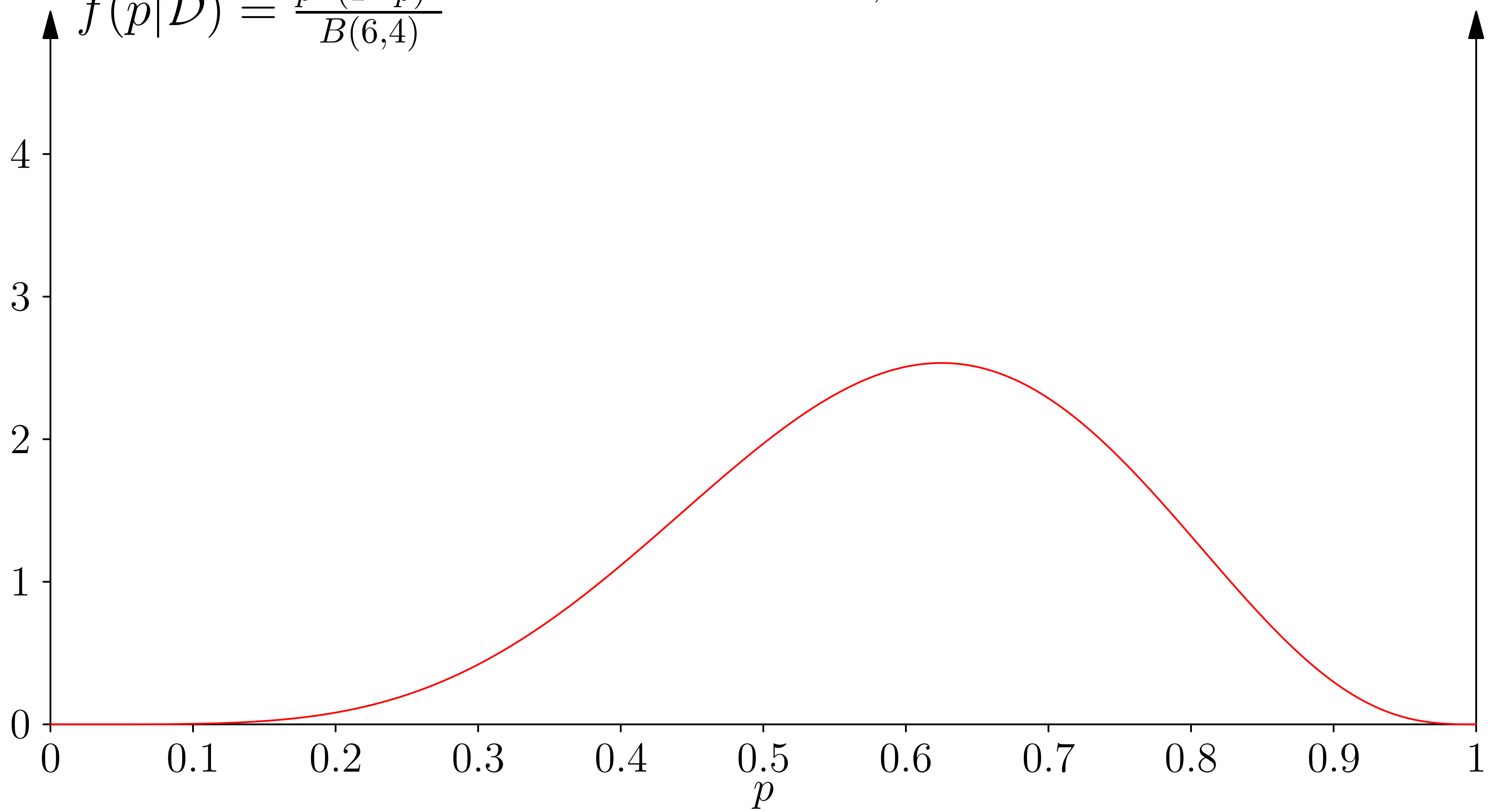

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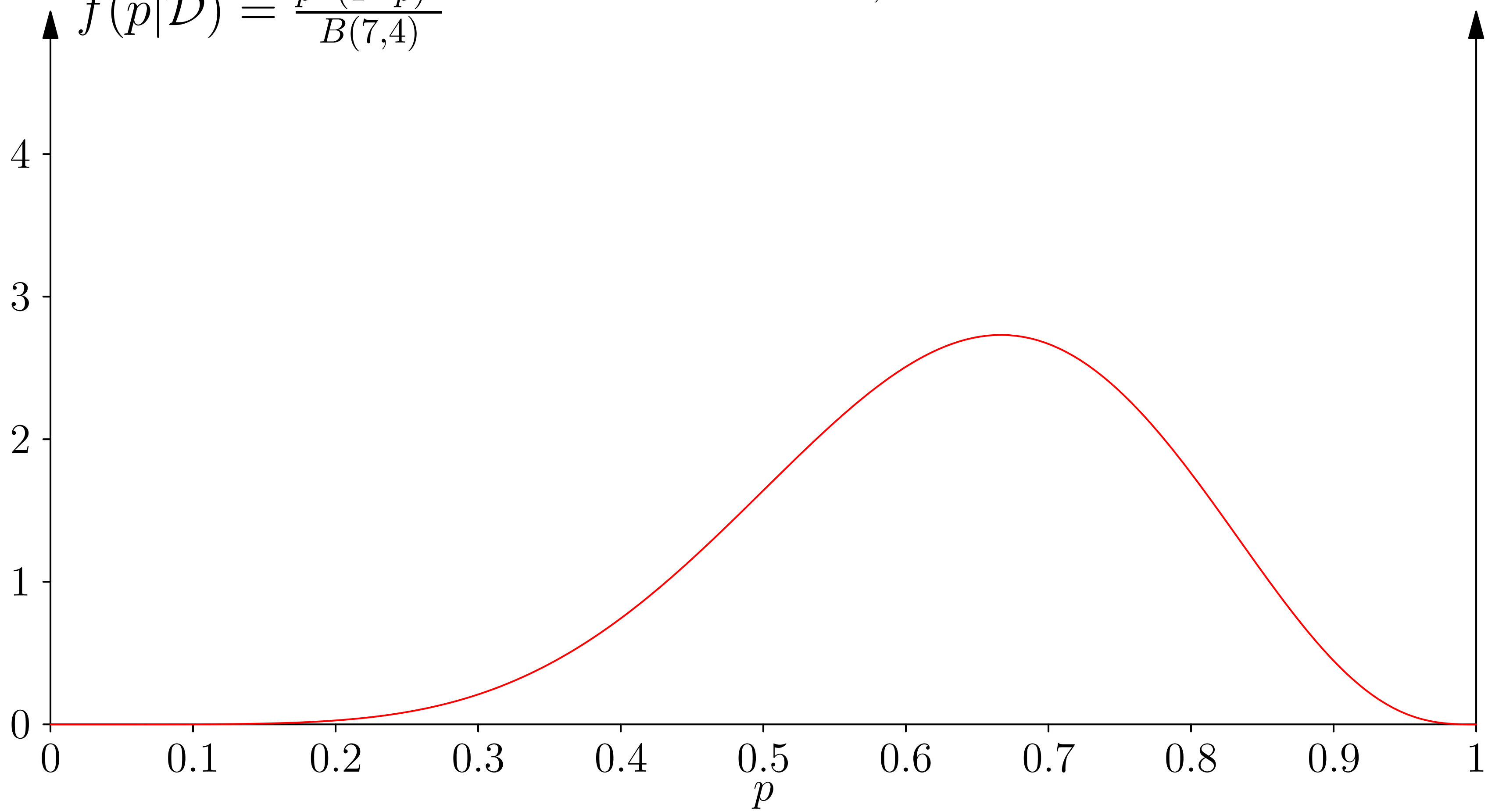

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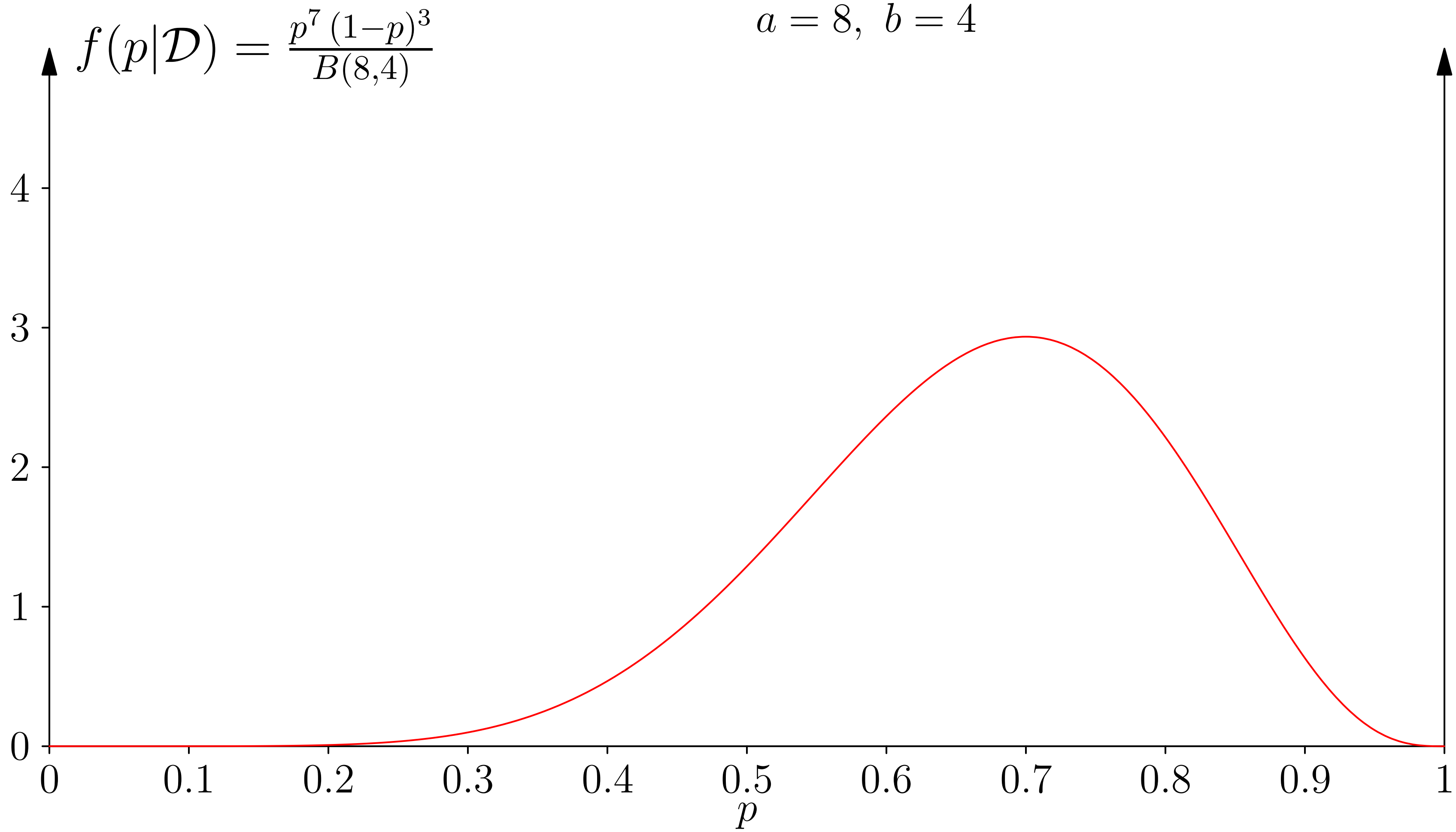

Example (p=0.7)

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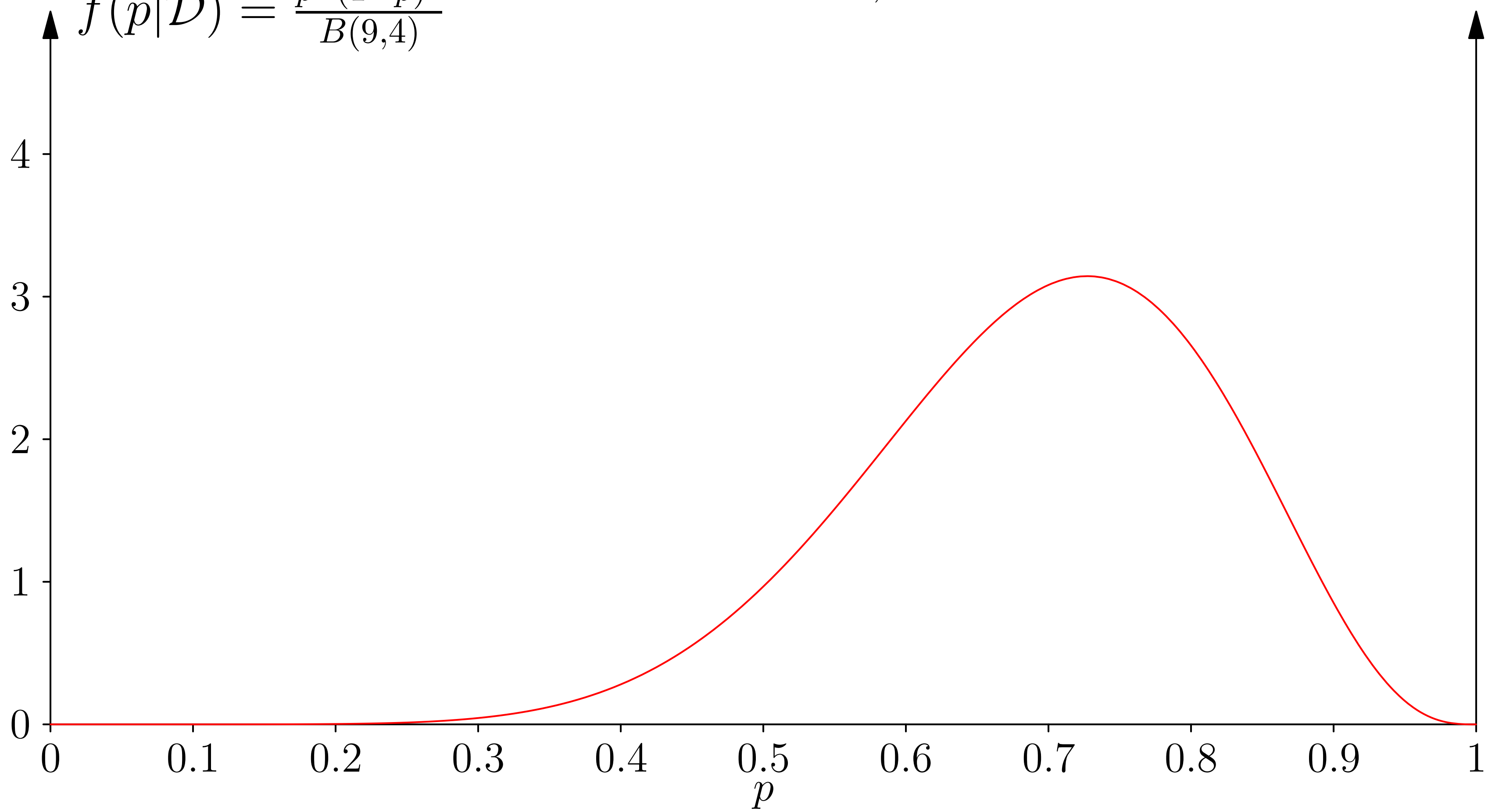
$a = 9,\ b = 4$



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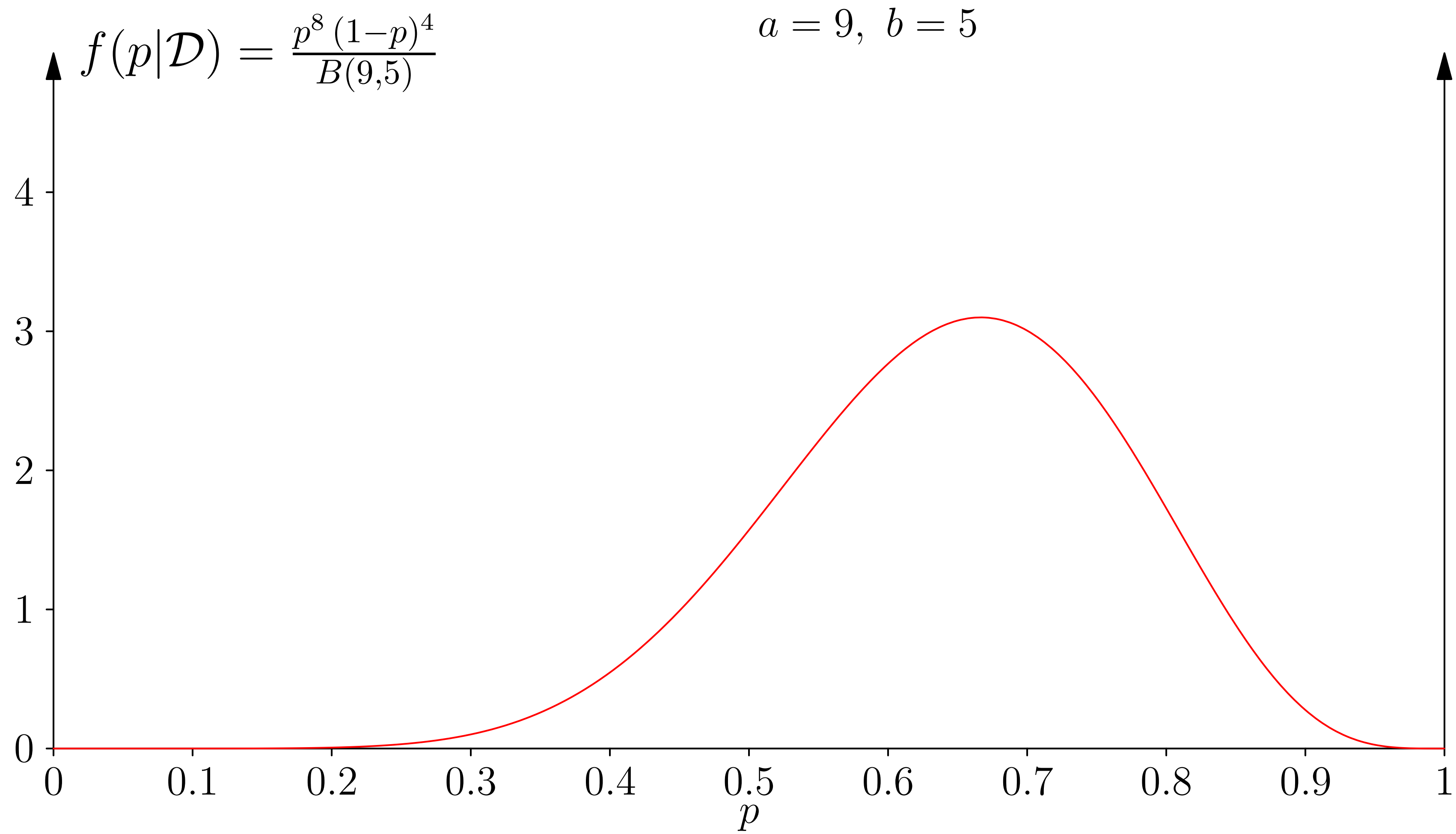

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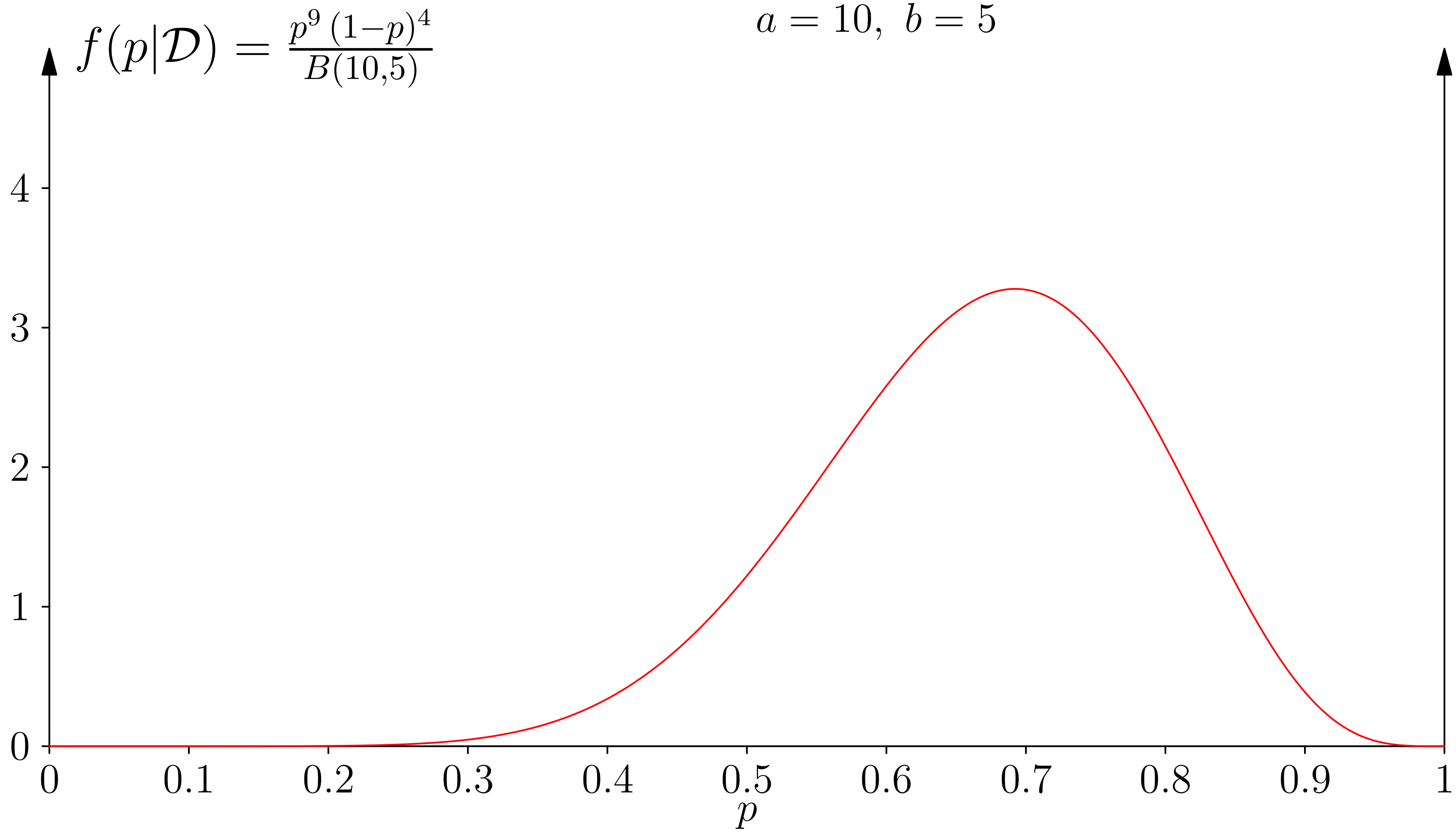

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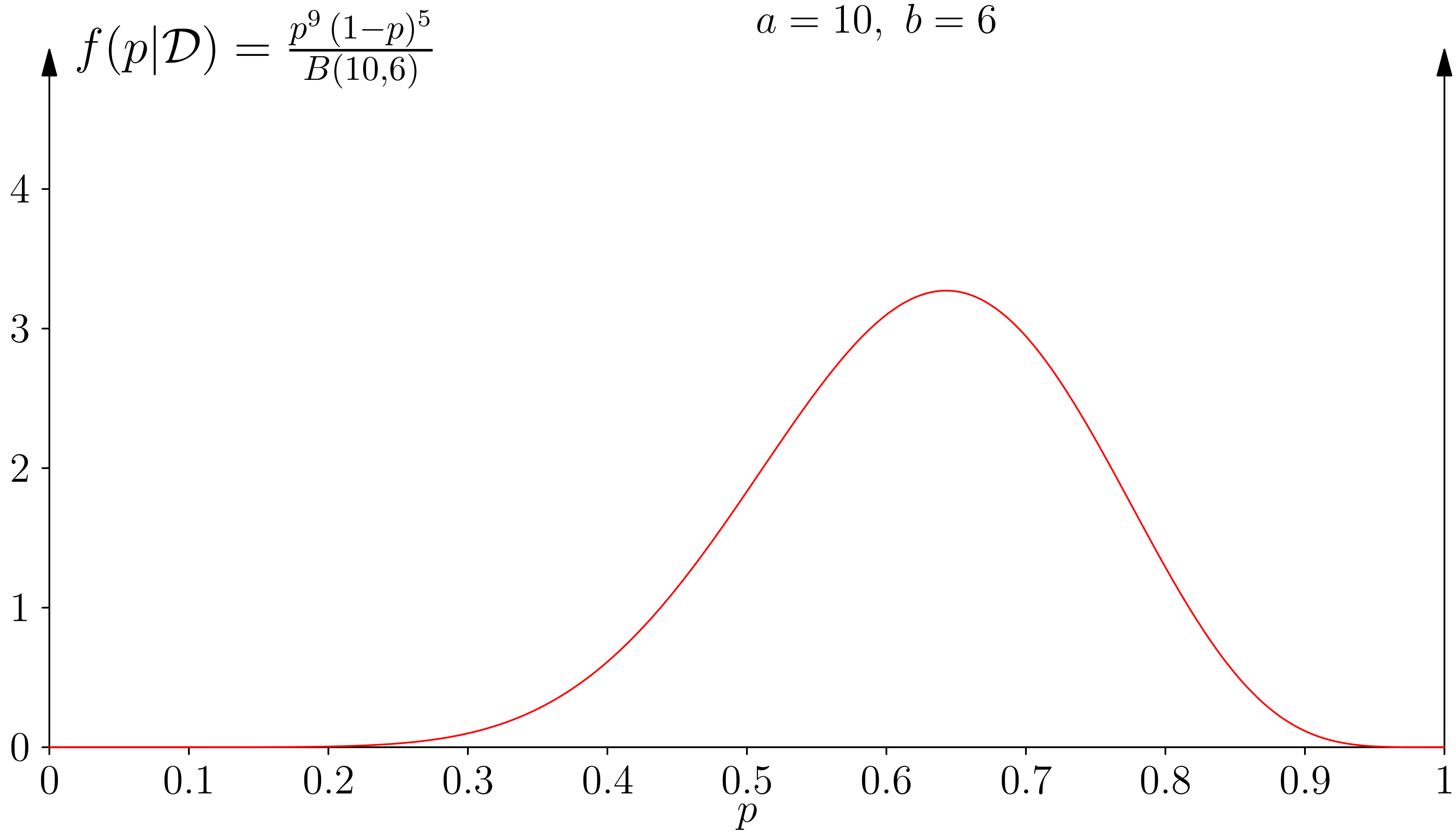

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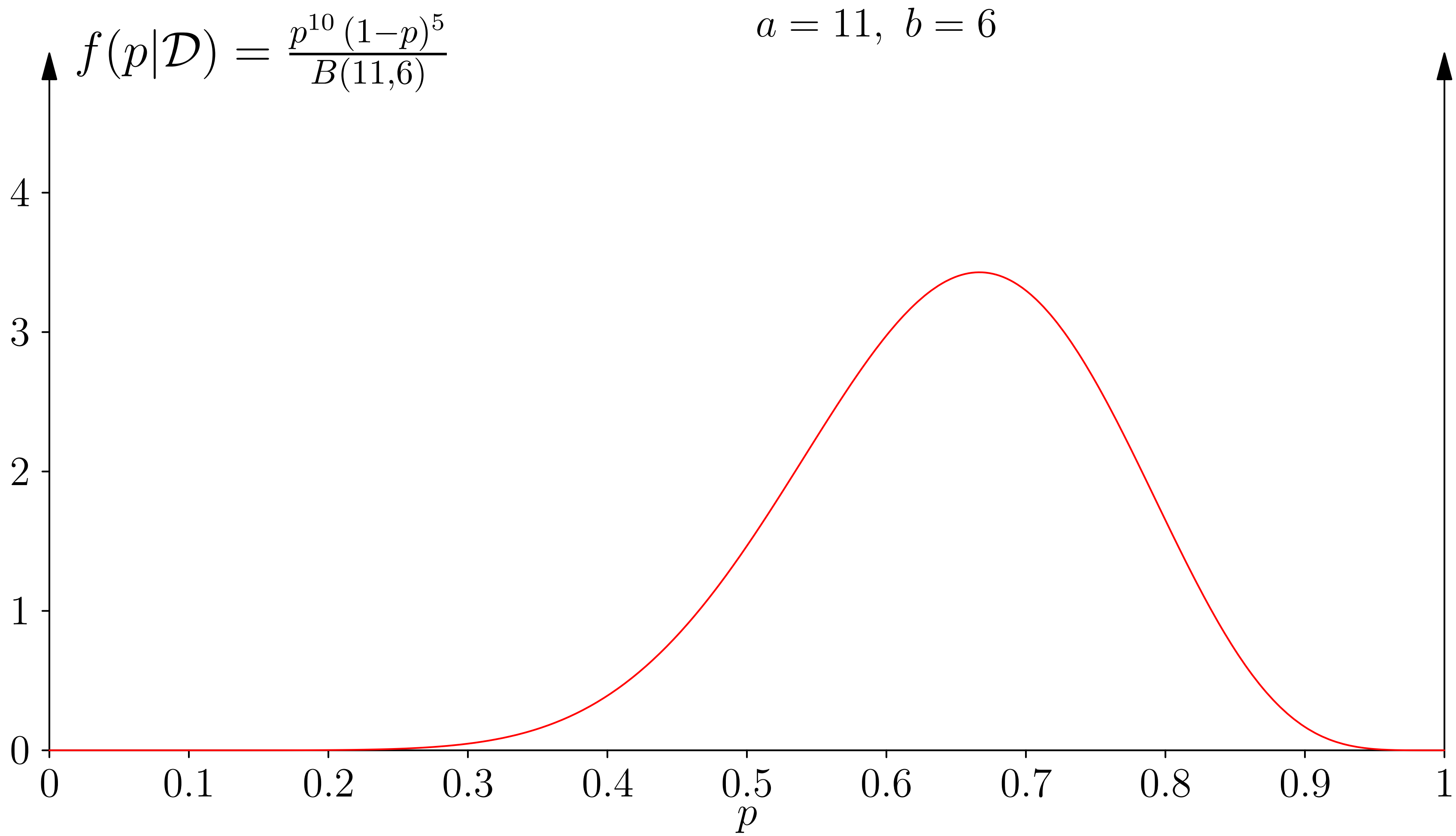

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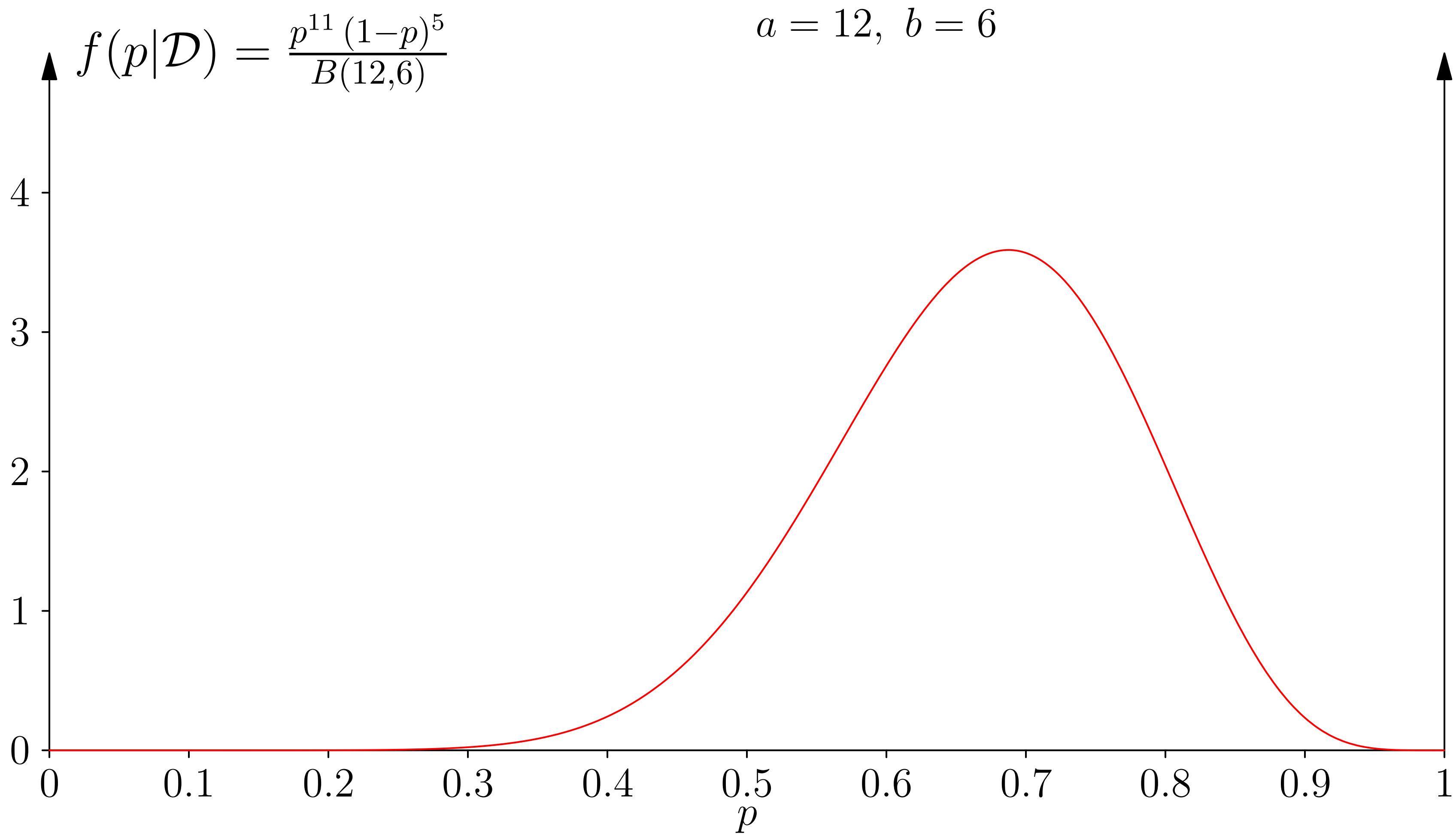

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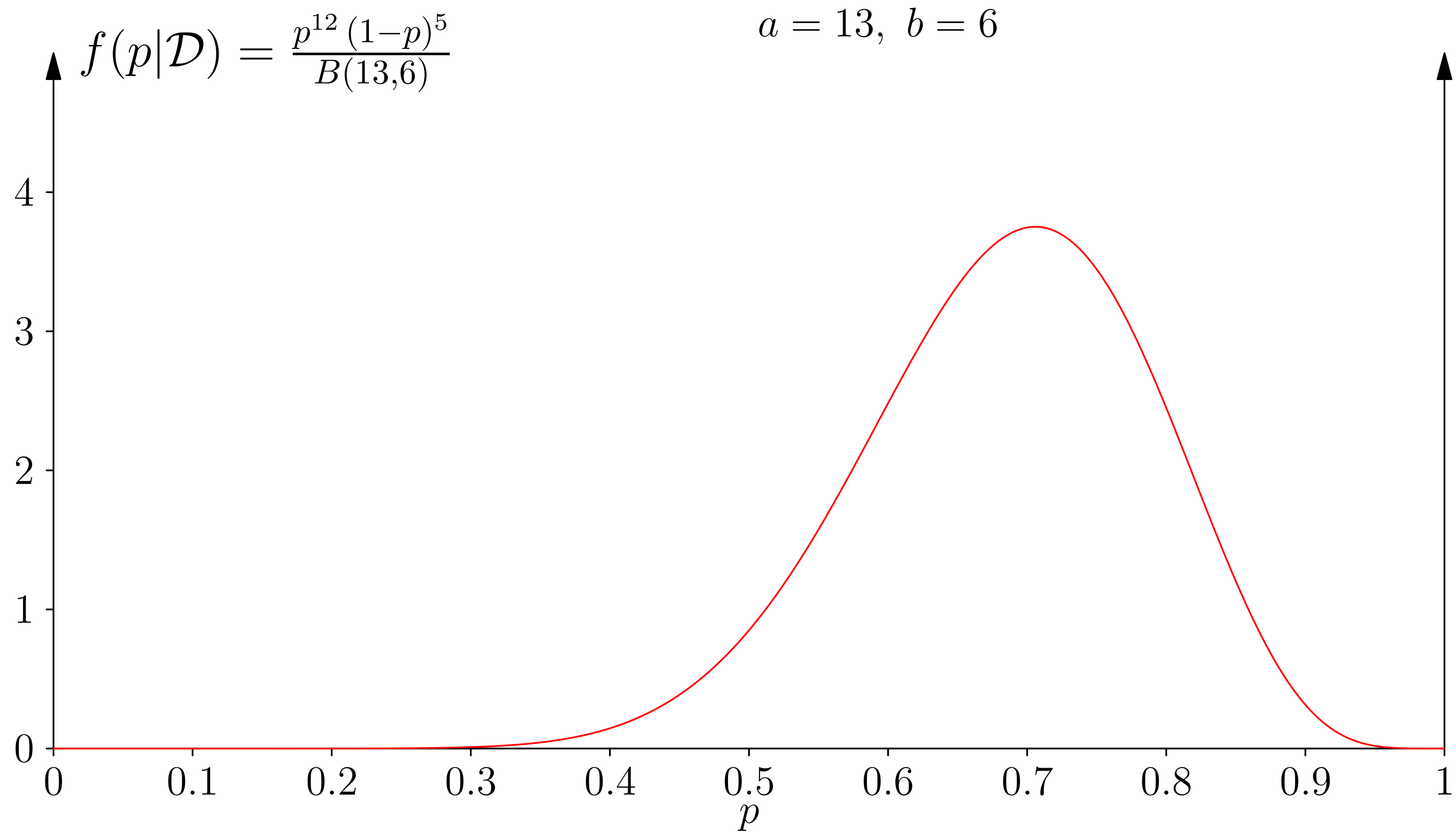

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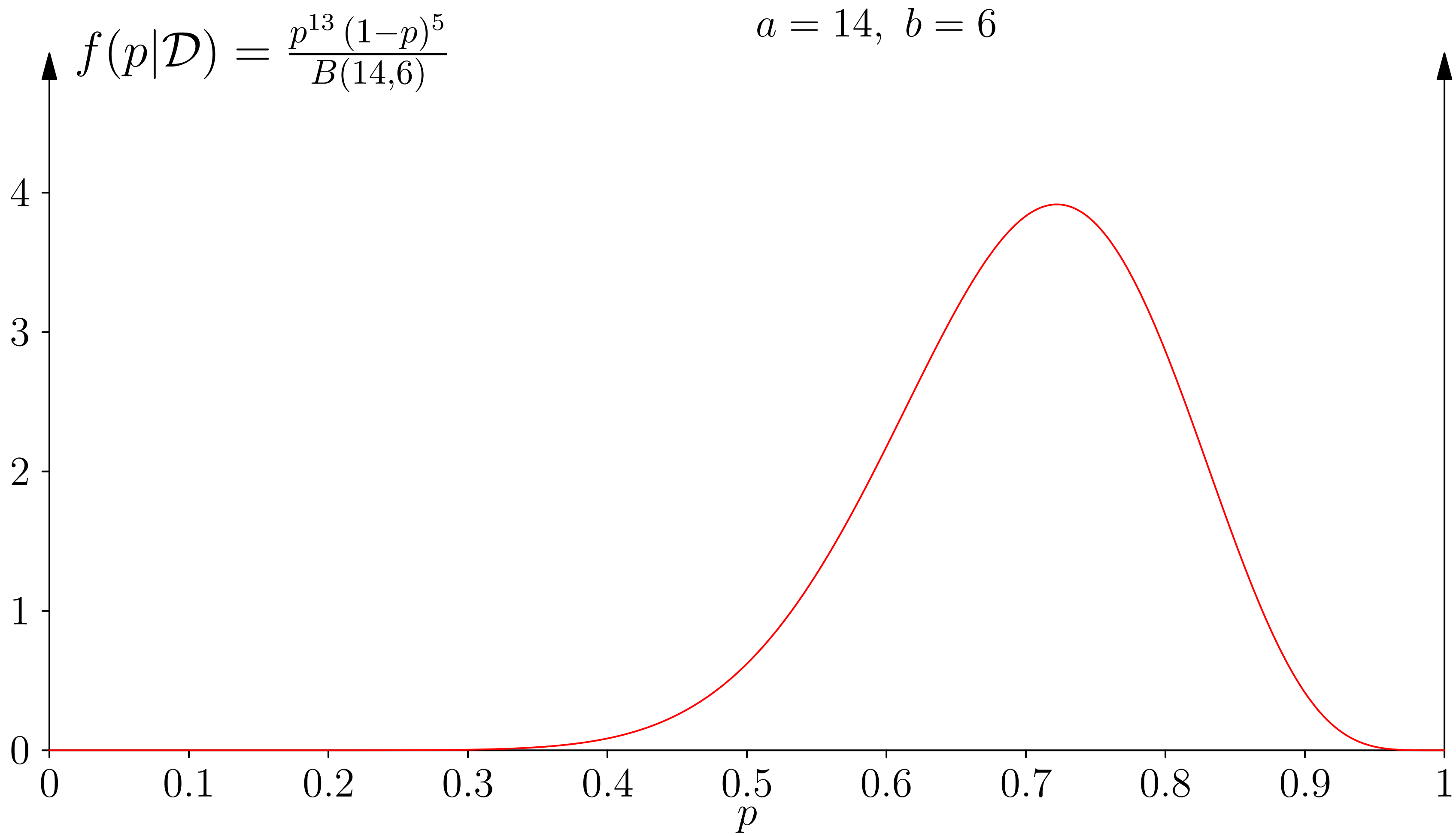
$\mathcal{D} = \{$H,H,H,H,T,T,T,H,H,H,H,T,H,T,H,H,H,H,



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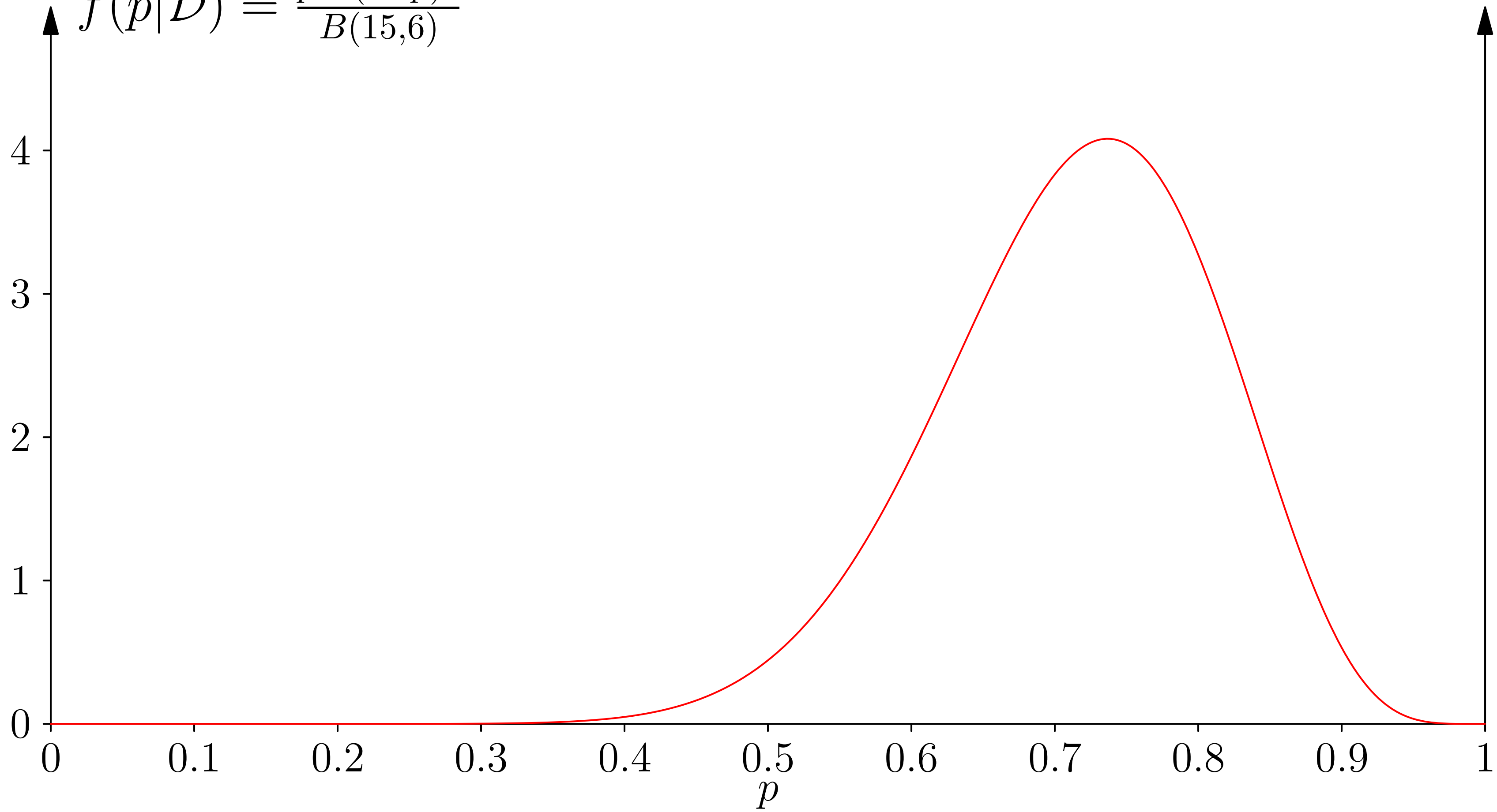
$f(p|\mathcal{D}) = \frac{p^{14}\,(1-p)^5}{B(15,6)}$

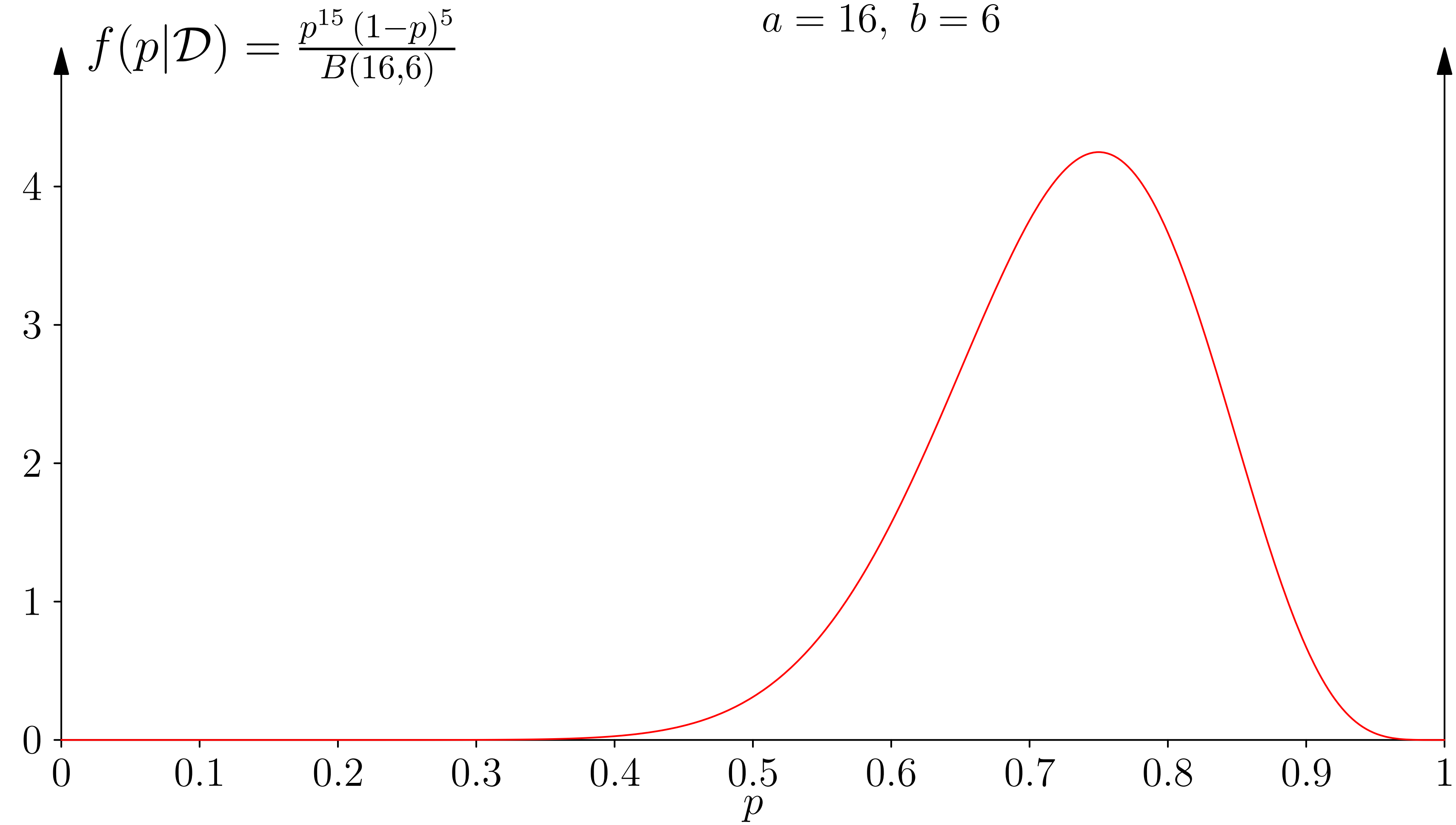
$a = 15,\ b = 6$



Example (p=0.7)

$\mathcal{D} = \{$H,H,H,H,T,T,T,H,H,H,H,T,H,T,H,H,H,H,H,H,

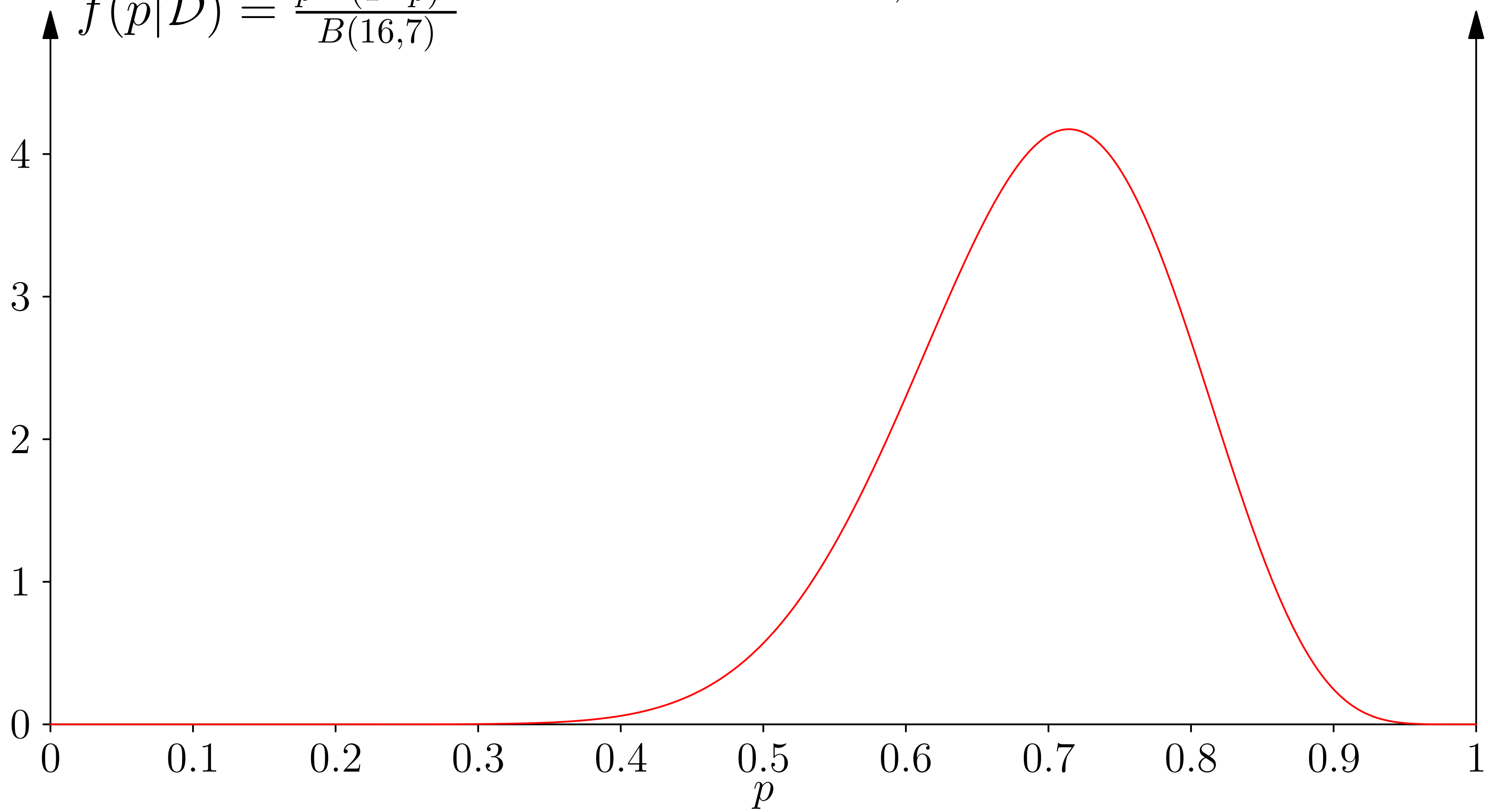
$a = 16, \; b = 6$



Example (p=0.7)

$\mathcal{D} = \{\text{H,H,H,H,T,T,T,H,H,H,H,T,H,T,H,H,H,H,H,H,T,}$

$f(p|\mathcal{D}) = \frac{p^{15}\,(1-p)^{6}}{B(16,7)}$ $\qquad a = 16,\ b = 7$



Example (p=0.7)

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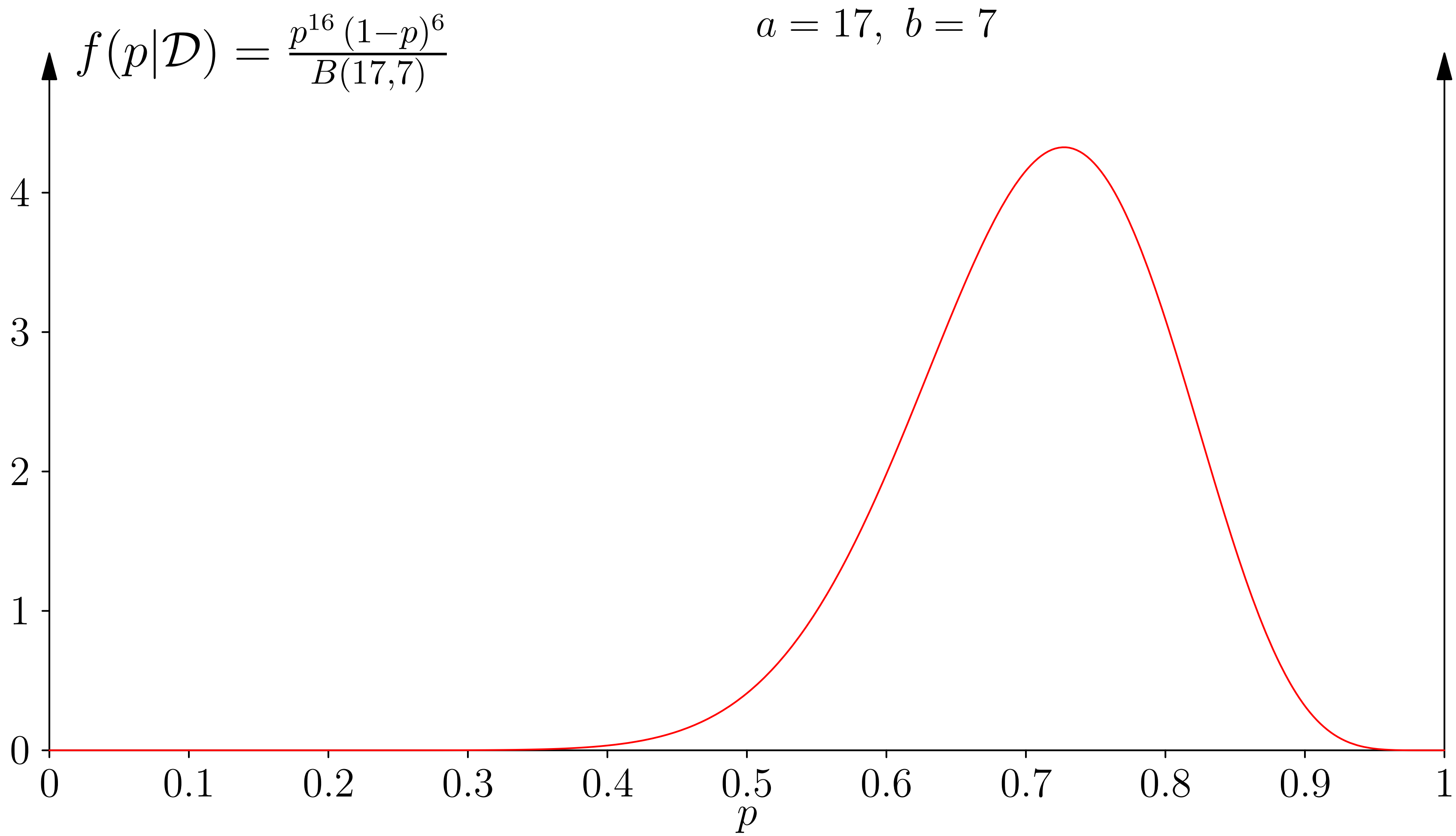
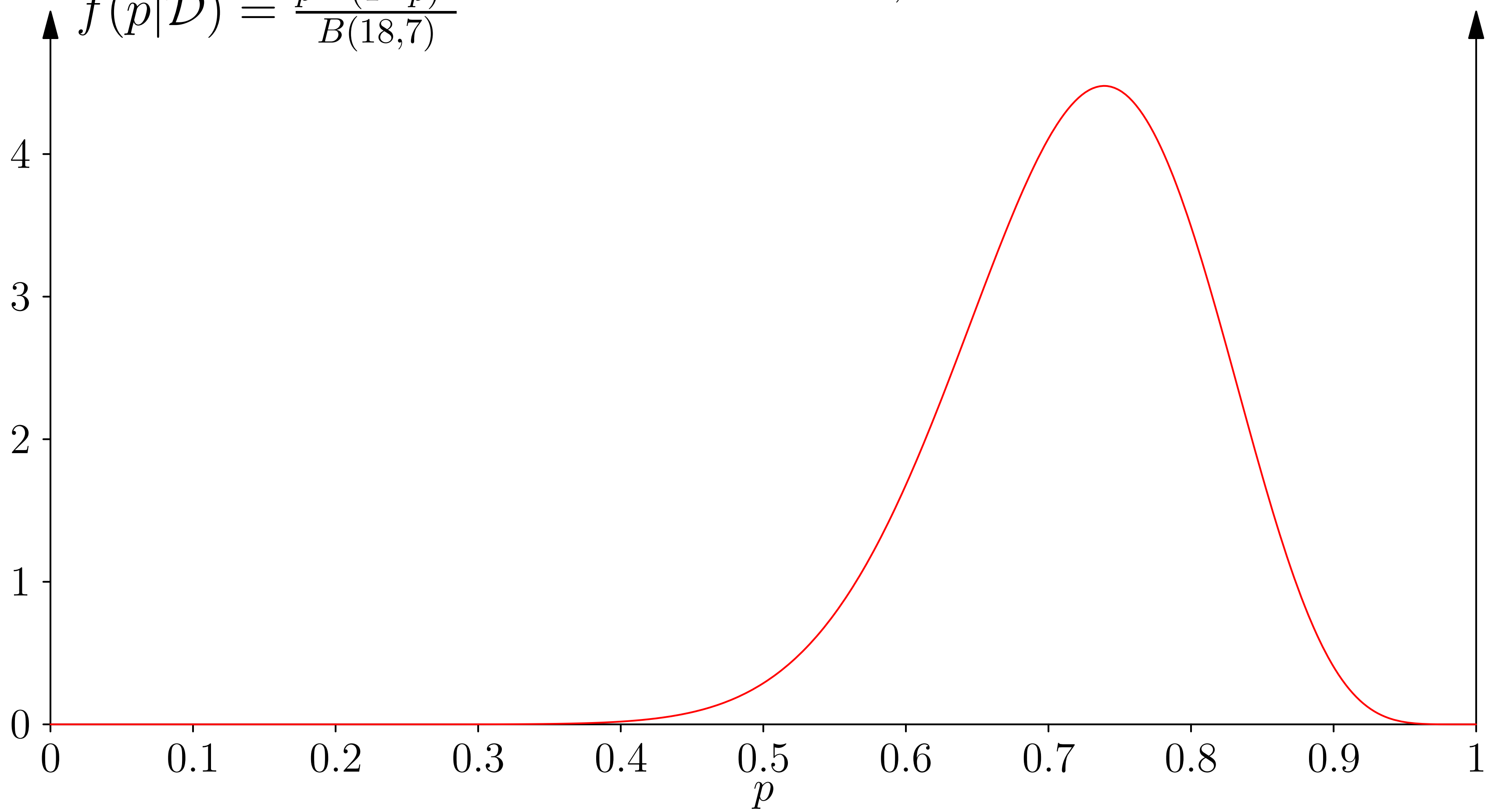


Example (p=0.7)

$\mathcal{D} = \{$H,H,H,H,T,T,T,H,H,H,H,T,H,T,H,H,H,H,H,H,T,H,H,

$a = 18,\ b = 7$

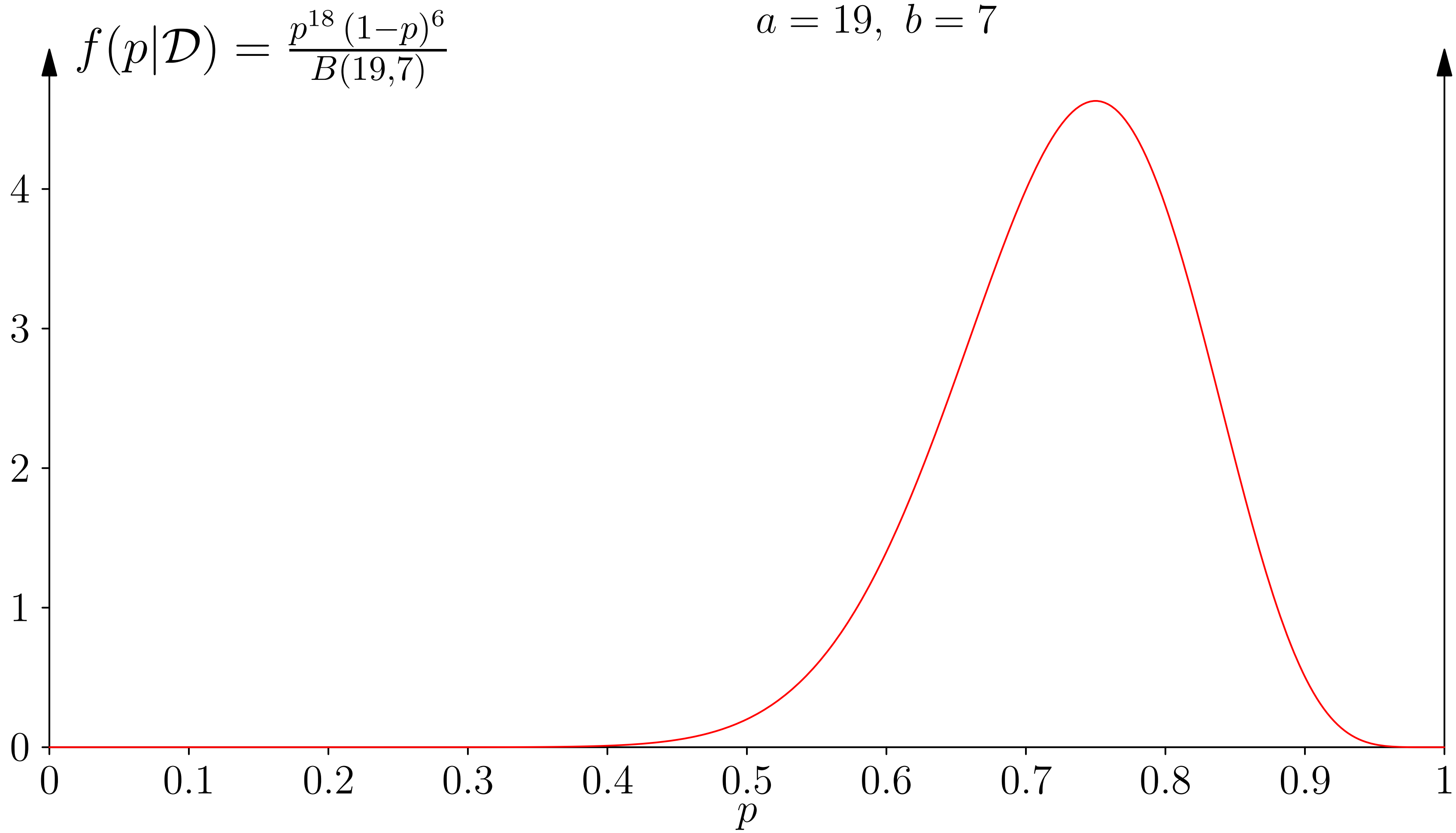
$f(p|\mathcal{D}) = \frac{p^{17}\,(1-p)^{6}}{B(18,7)}$



Example (p=0.7)

$\mathcal{D} = \{$H,H,H,H,T,T,T,H,H,H,H,T,H,T,H,H,H,H,H,H,T,H,H,H,

$a = 19,\ b = 7$



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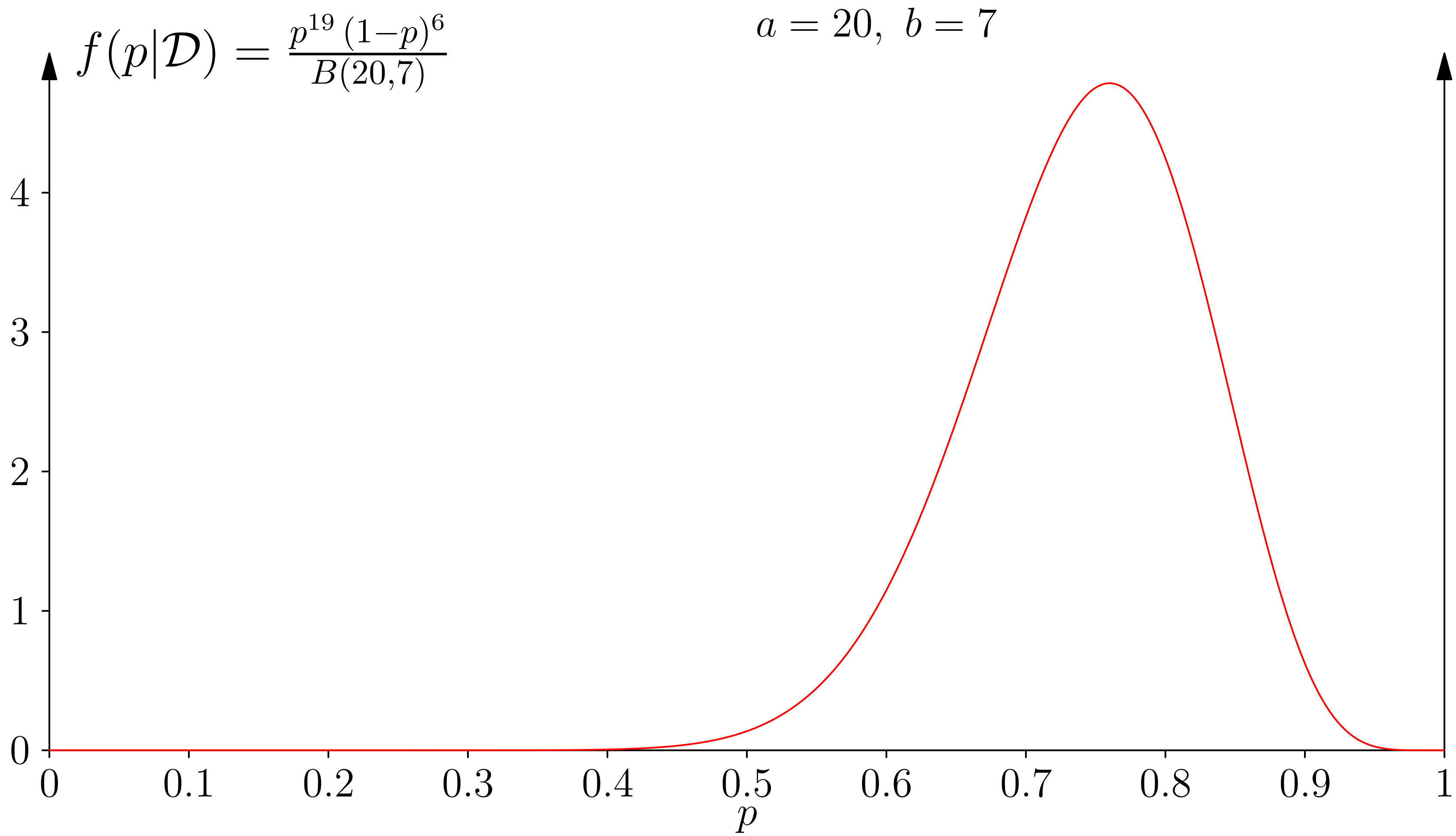

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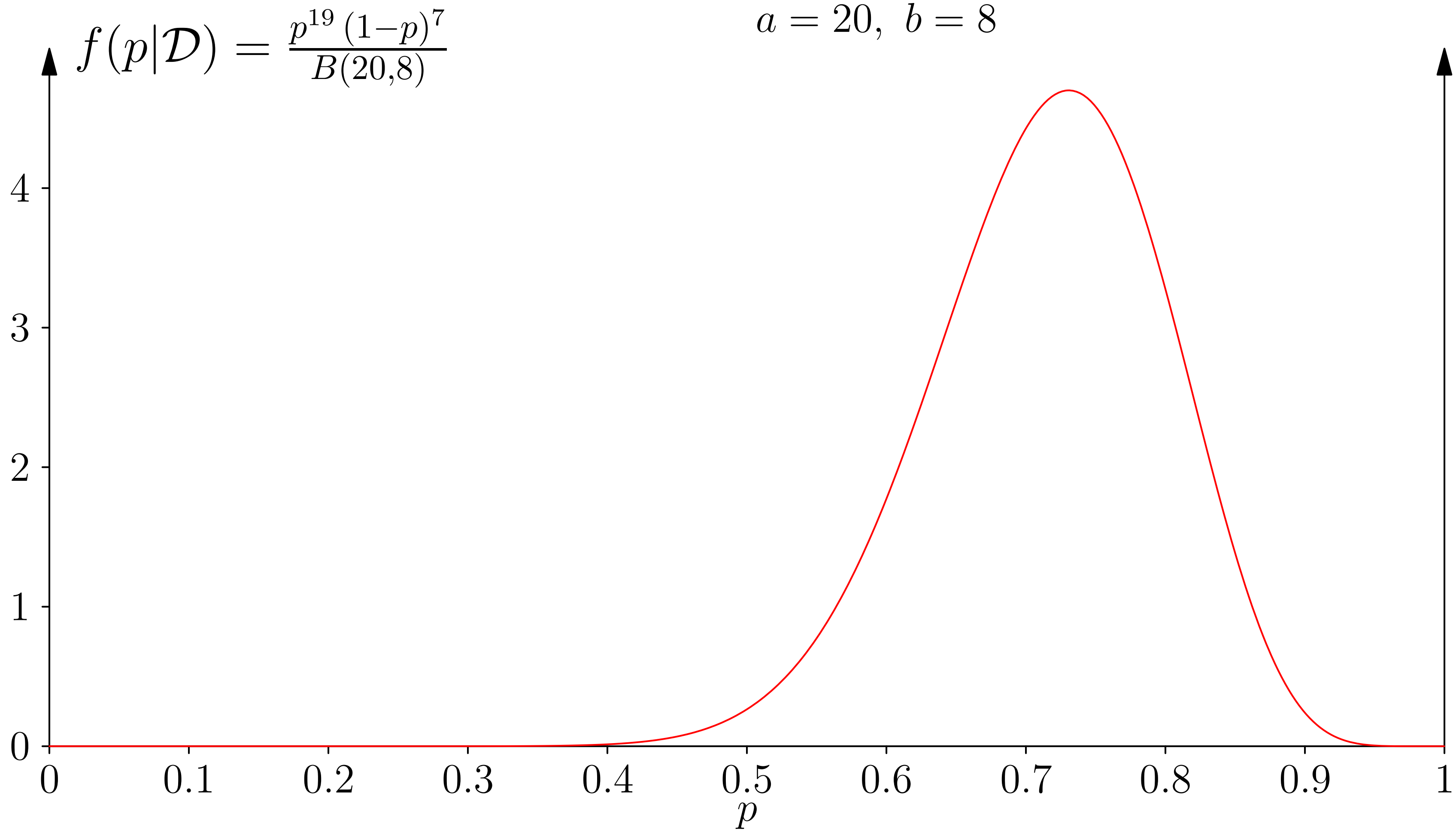
$\mathcal{D} = \{$H,H,H,H,T,T,T,H,H,H,H,T,H,T,H,H,H,H,H,H,T,H,H,H,H,T,

$a = 20,\ b = 8$



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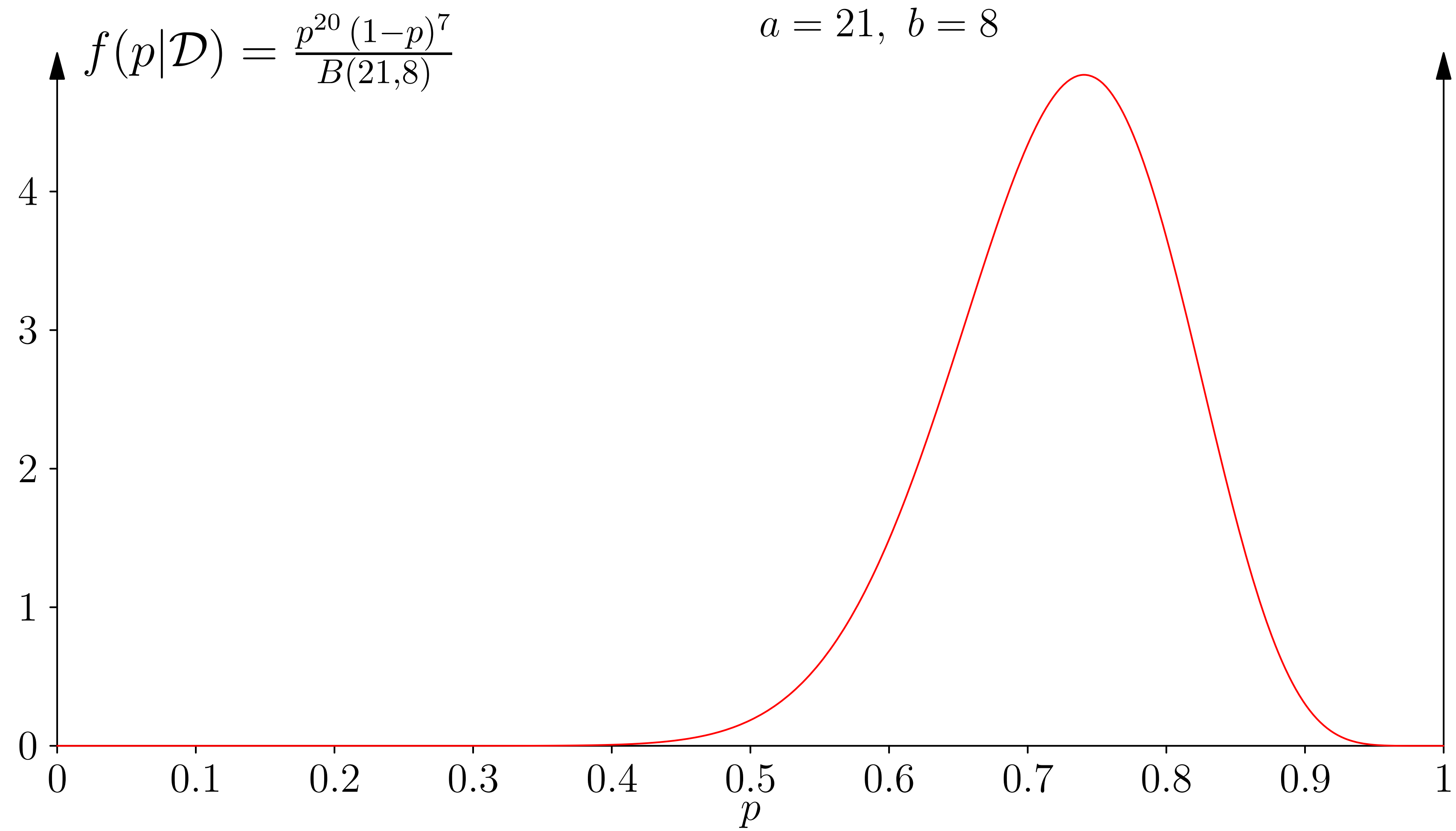

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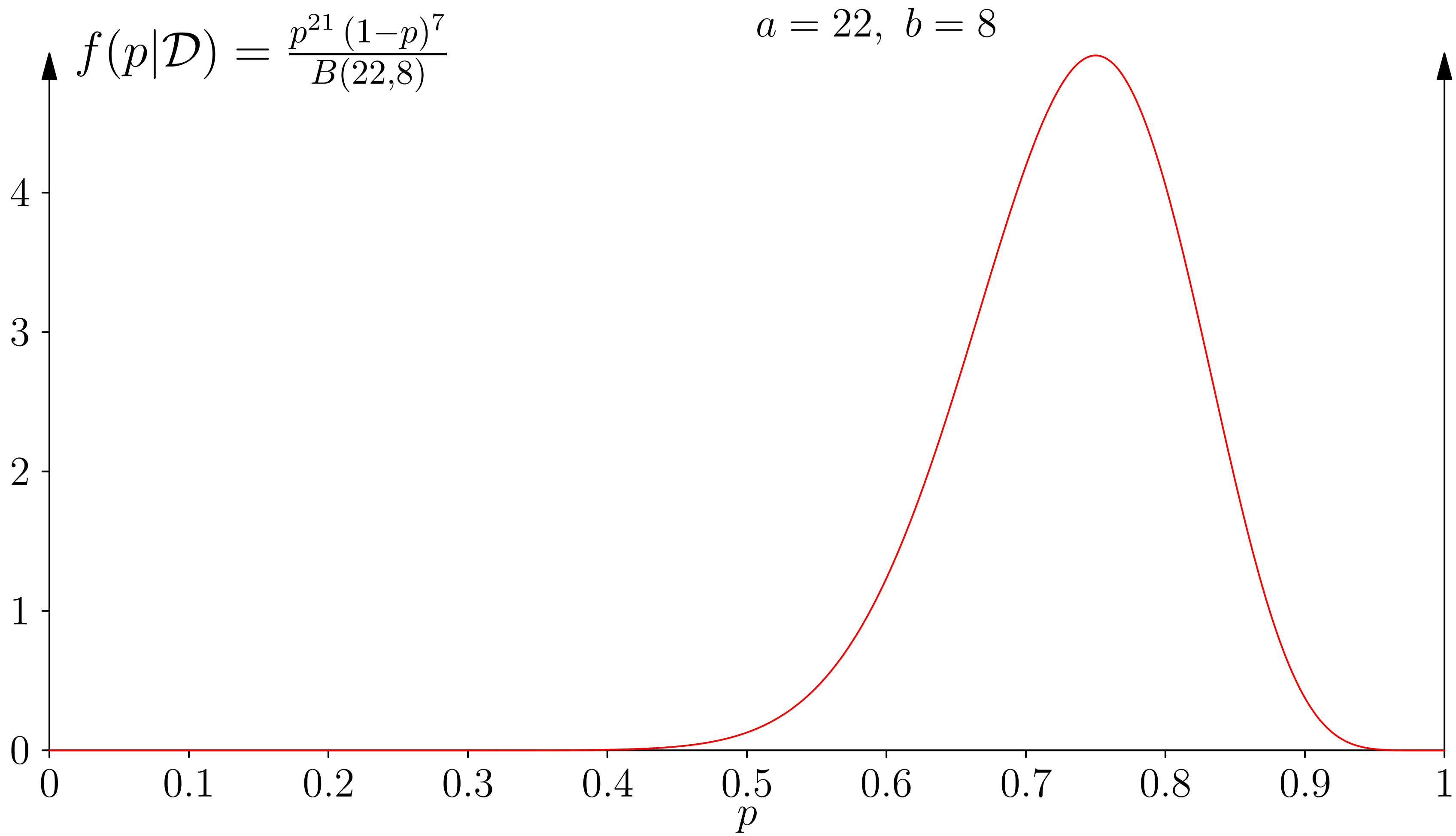

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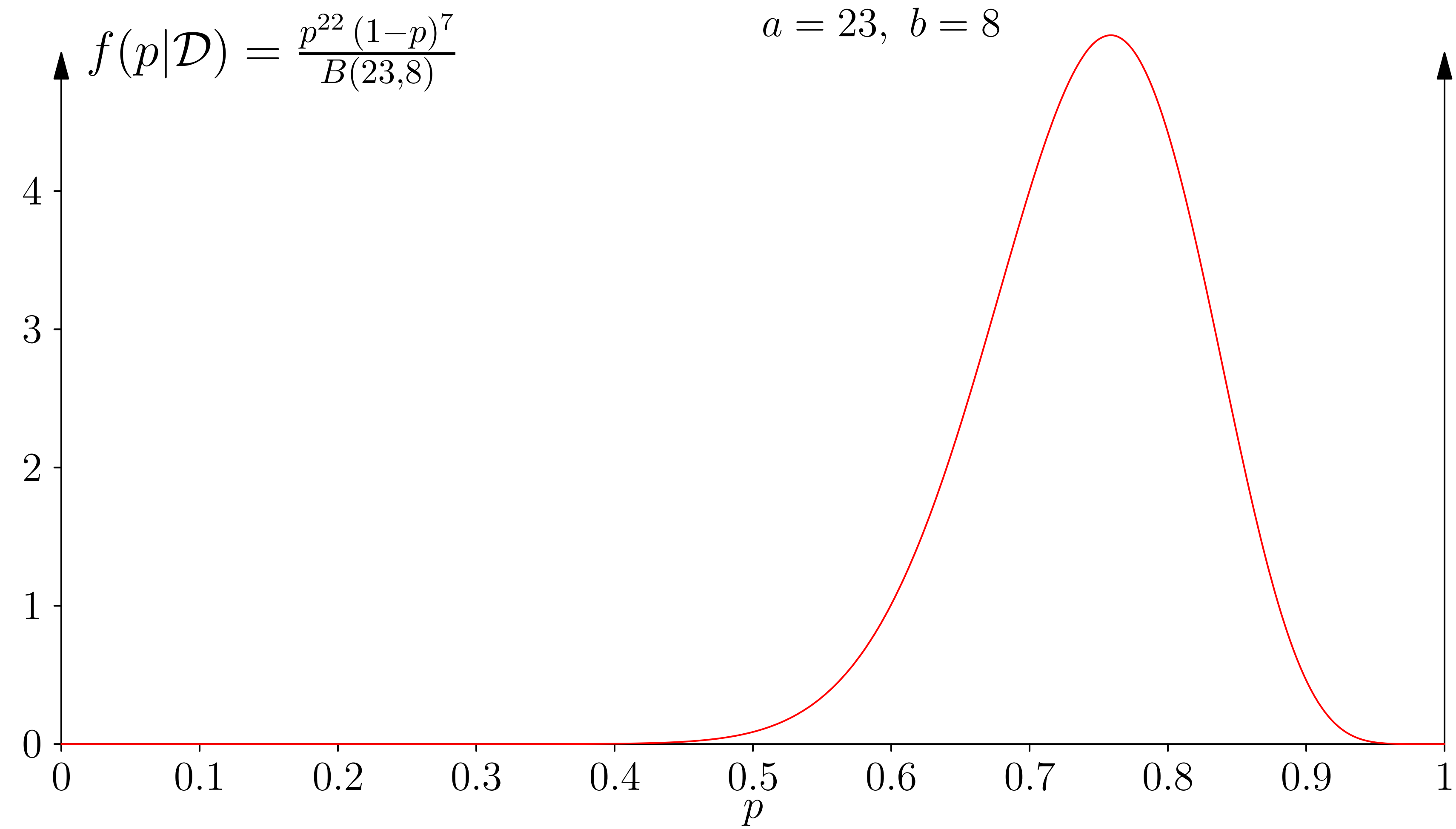

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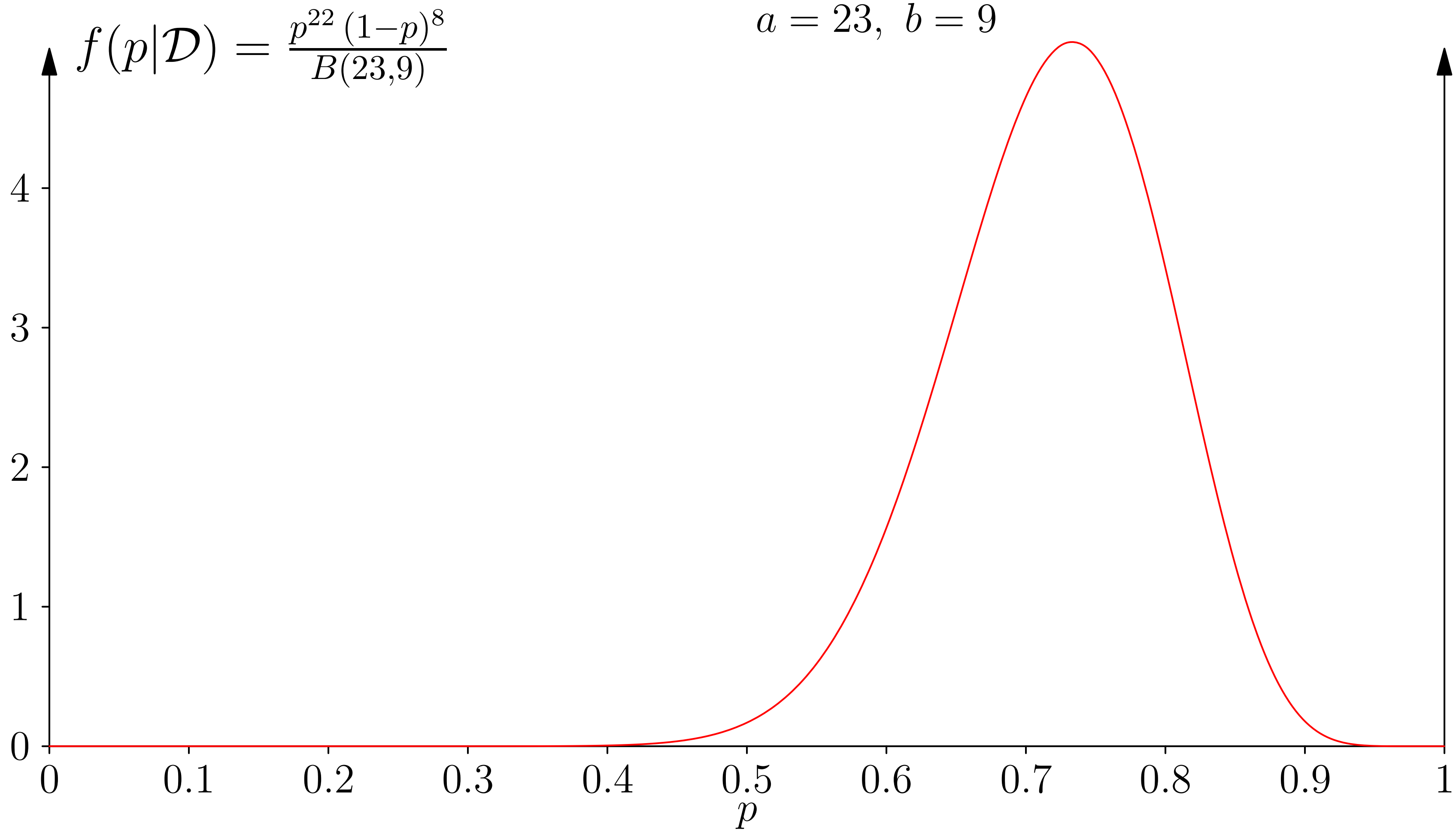

Estimating Prediction Errors

- A full Bayesian treatment gives a prediction of its own error
- Assuming $f(p|\mathcal{D}) = \mathrm{Beta}(p|a,b)$
- The expected value of p is given by $a/(a+b) = 23/32 = 0.719$
- The standard deviation is

$$\sqrt{\frac{ab}{(a+b)^2(a+b+1)}} = 0.078$$

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Poisson Likelihoods

- Let's look at a second example of conjugate priors
- Suppose we want to find the rate of traffic along a road between 1:00pm and 2:00pm
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$$\mathbb{P}(N) = \mathrm{Pois}(N|\mu) = \frac{\mu^N}{N!}\mathrm{e}^{-\mu}$$

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Using Bayes

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$$p(\mu) = \Gamma(\mu|a_0,b_0) = \frac{b_0^{a_0}\mu^{a_0-1}\mathrm{e}^{-b_0\mu}}{\Gamma(a)}$$

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Posterior

- The posterior after seeing the first piece of data is

$$
\begin{aligned}
p(\mu|N_1) &\propto \mathbb{P}(N_1|\mu)\, p(\mu) \\
&\propto \frac{\mu^{N_1}}{N_1!} \mathrm{e}^{-\mu} \mu^{a_0-1} \mathrm{e}^{-b_0 \mu} \\
&\propto \mu^{N_1+a_0-1} \mathrm{e}^{-(b_0+1)\mu}
\end{aligned}
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- The posterior is also a Gamma distribution $\Gamma(\mu|a_1,b_1)$ with $a_1 = a_0 + N_1$, $b_1 = b_0 + 1$

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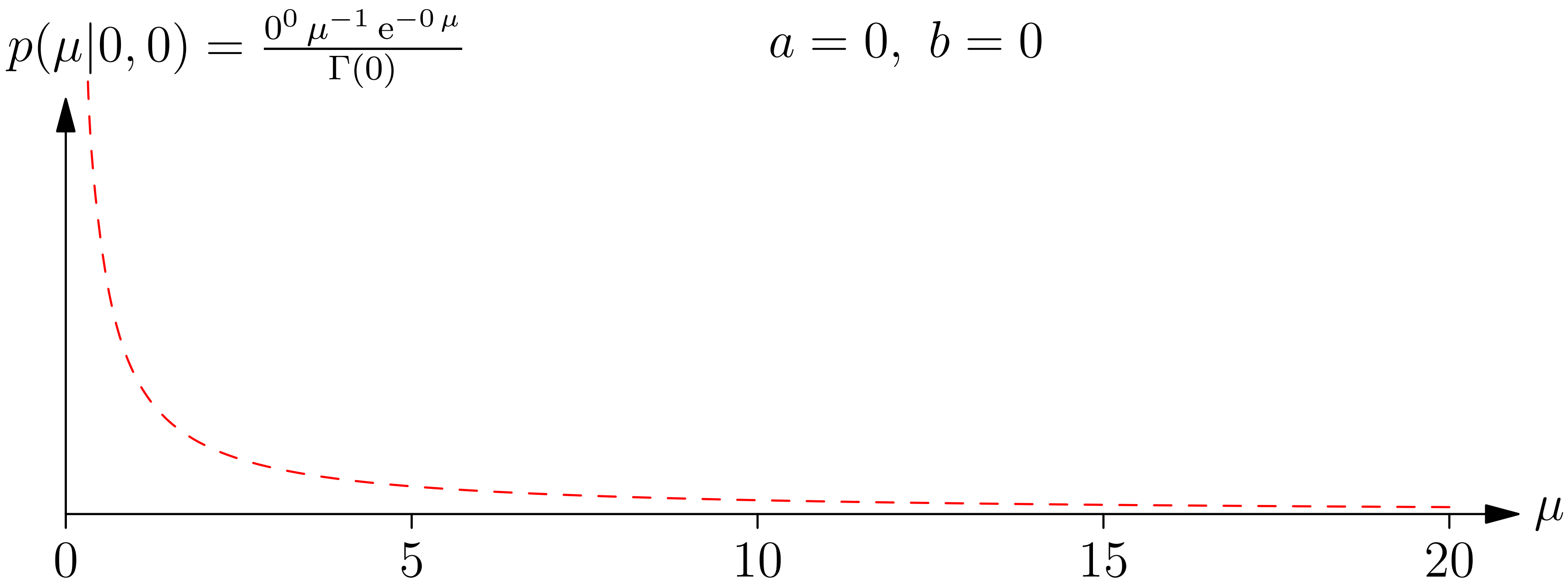
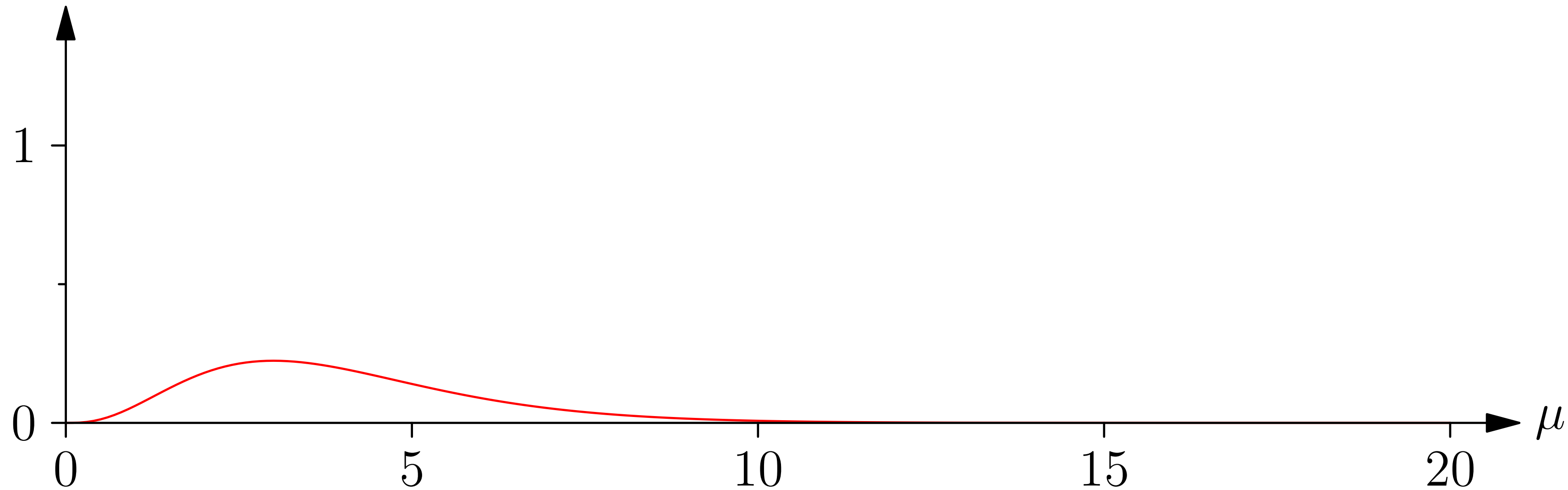
Example ($\mu = 5$)



Example ($\mu = 5$)

$\mathcal{D} = \{4\}$

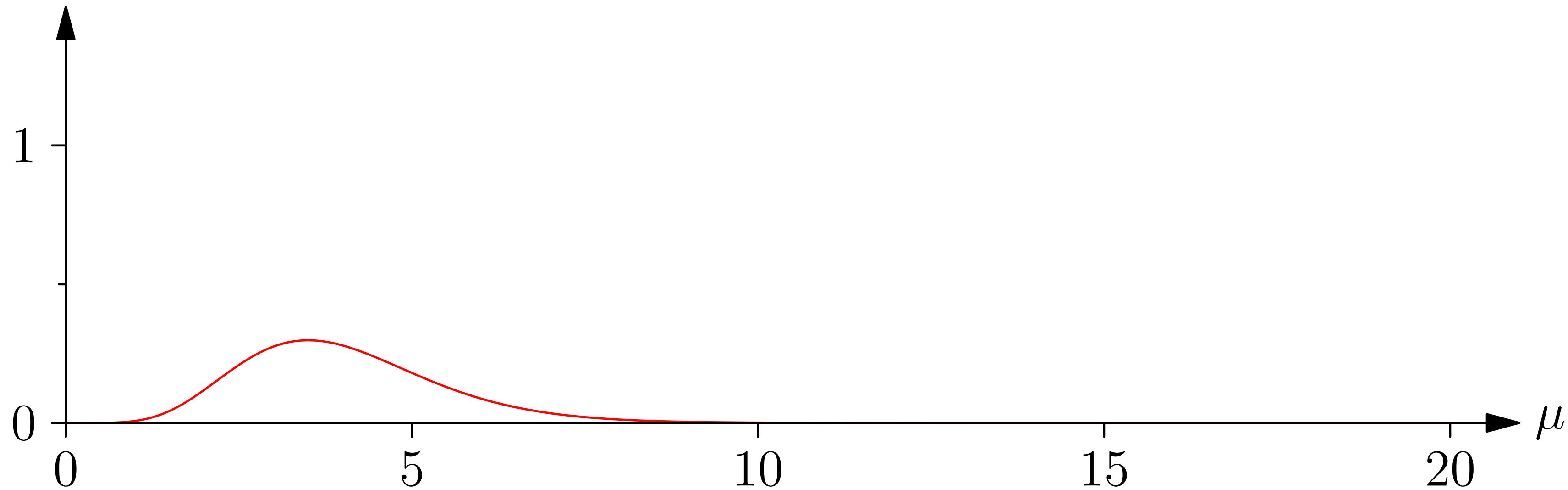
$p(\mu|4,1) = \frac{1^4\,\mu^3\,\mathrm{e}^{-1\,\mu}}{\Gamma(4)}$ $\qquad a = 4,\ b = 1$



Example ($\mu = 5$)

$$\mathcal{D} = \{4, 4\}$$

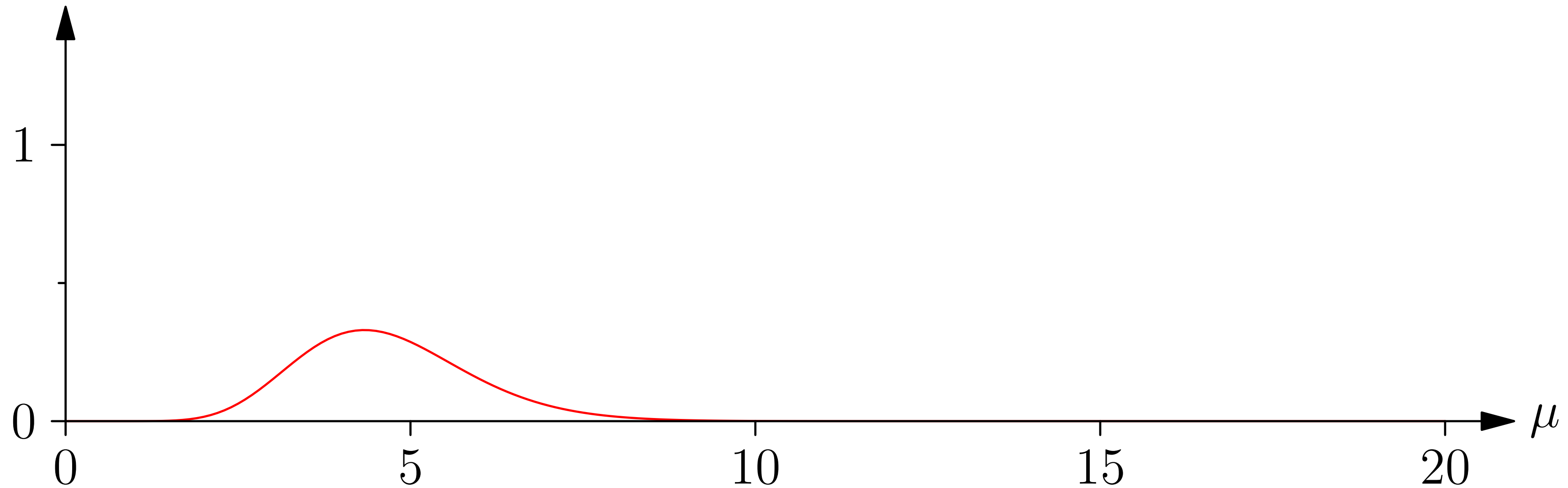
$$p(\mu|8,2) = \frac{2^8\,\mu^7\,\mathrm{e}^{-2\,\mu}}{\Gamma(8)} \qquad a = 8,\; b = 2$$



Example ($\mu = 5$)

$$\mathcal{D} = \{4, 4, 6\}$$

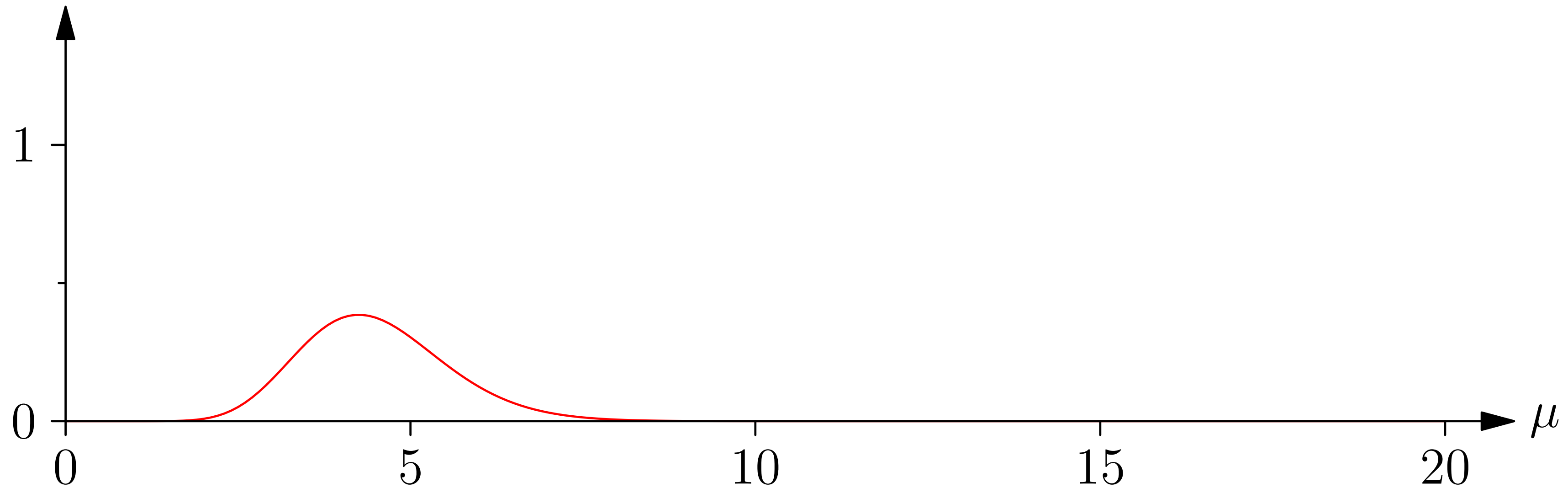
$$p(\mu|14,3) = \frac{3^{14}\,\mu^{13}\,\mathrm{e}^{-3\,\mu}}{\Gamma(14)} \qquad a = 14,\ b = 3$$



Example ($\mu = 5$)

$\mathcal{D} = \{4, 4, 6, 4\}$

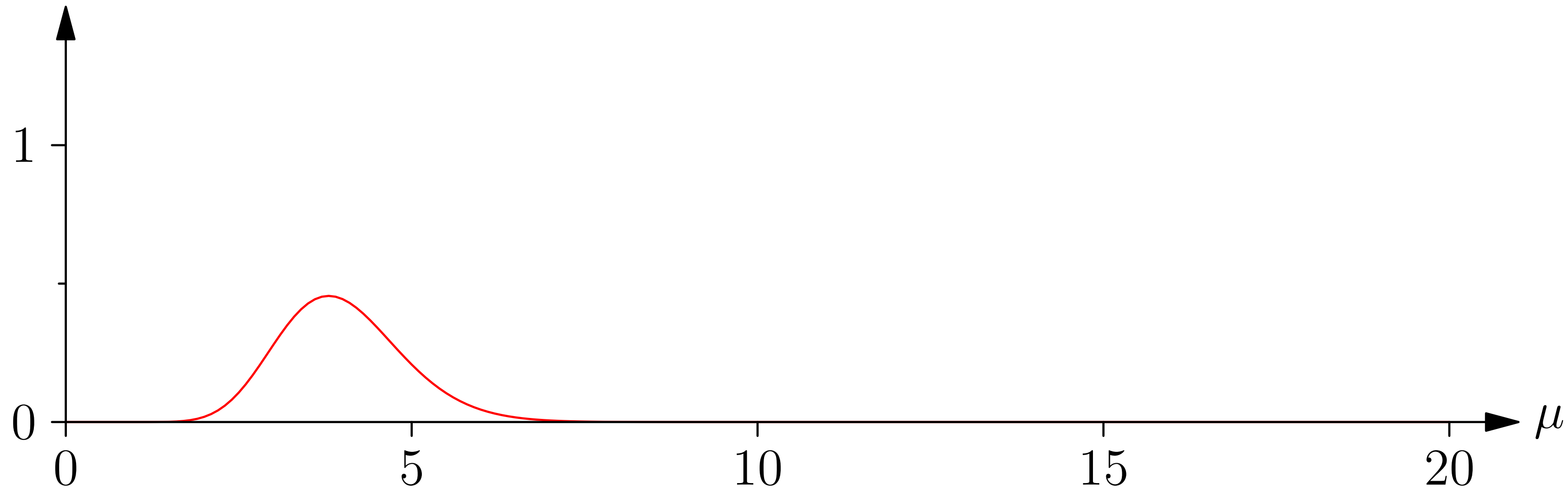
$p(\mu|18,4) = \frac{4^{18}\,\mu^{17}\,\mathrm{e}^{-4\,\mu}}{\Gamma(18)}$ $\qquad a = 18,\ b = 4$



Example ($\mu = 5$)

$$\mathcal{D} = \{4, 4, 6, 4, 2\}$$

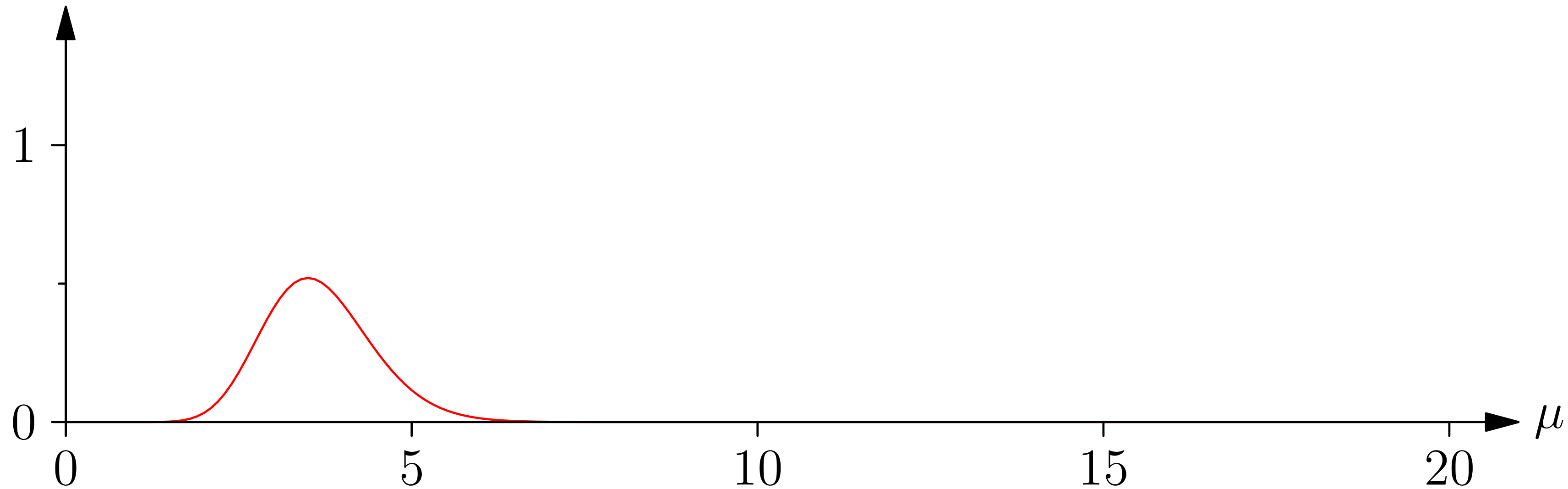
$$p(\mu|20, 5) = \frac{5^{20}\,\mu^{19}\,\mathrm{e}^{-5\,\mu}}{\Gamma(20)} \qquad a = 20,\; b = 5$$



Example ($\mu = 5$)

$$\mathcal{D} = \{4, 4, 6, 4, 2, 2\}$$

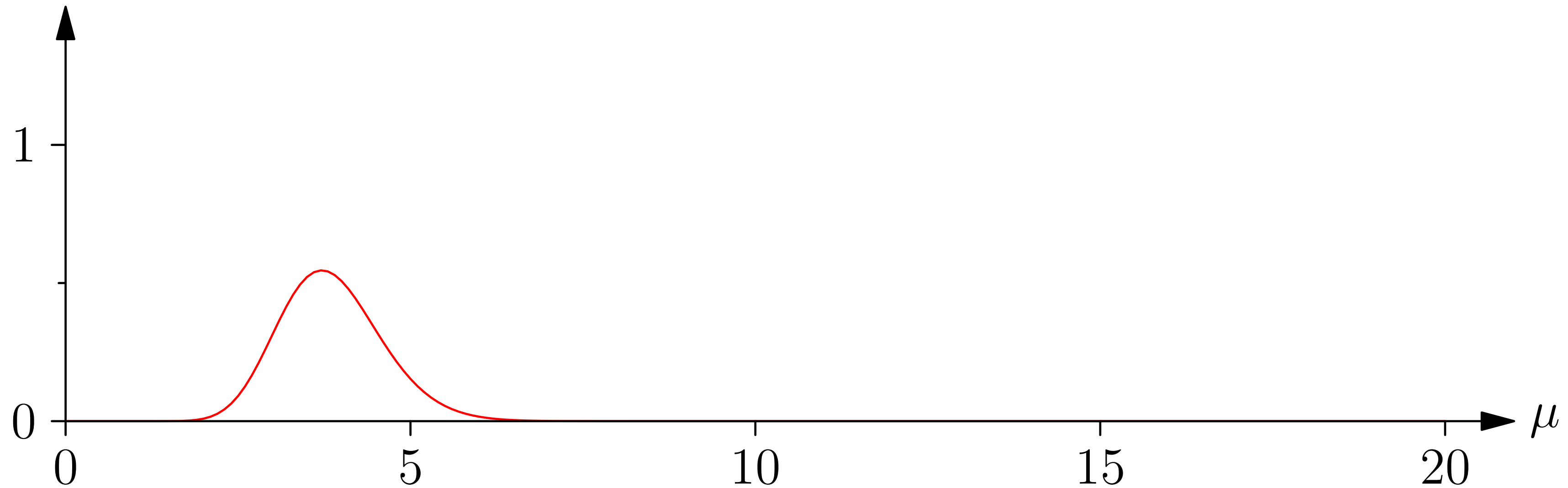
$$p(\mu|22,6) = \frac{6^{22}\,\mu^{21}\,\mathrm{e}^{-6\,\mu}}{\Gamma(22)} \qquad a = 22,\ b = 6$$



Example ($\mu = 5$)

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

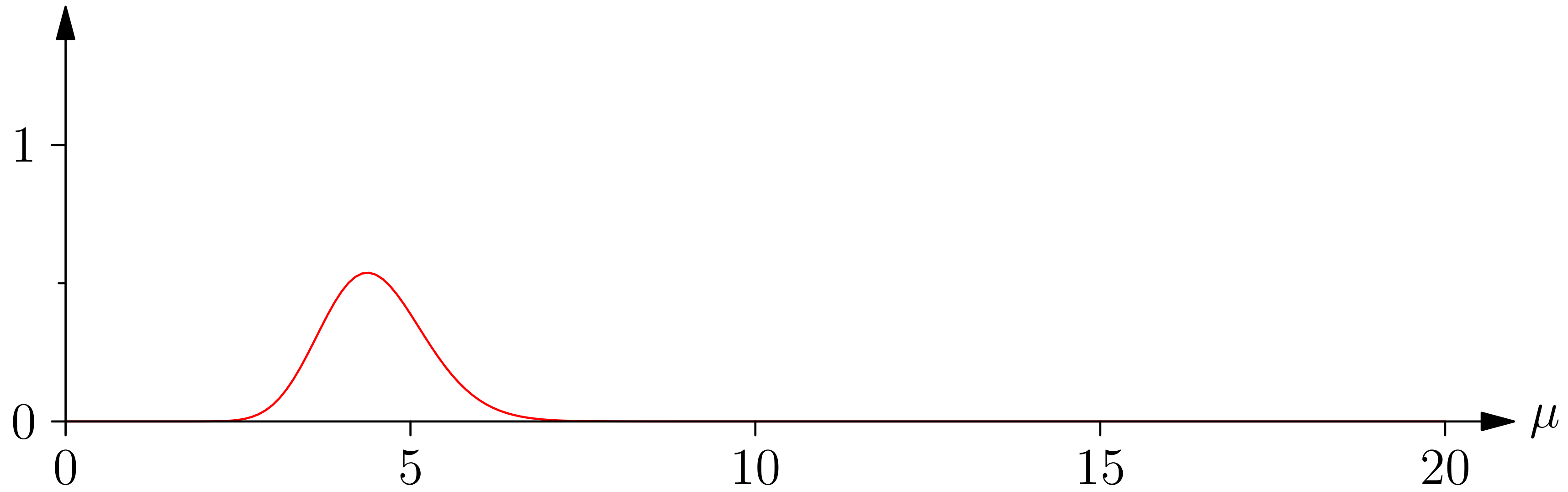
$$p(\mu|27, 7) = \frac{7^{27}\, \mu^{26}\, \mathrm{e}^{-7\,\mu}}{\Gamma(27)} \qquad a = 27,\ b = 7$$



Example ($\mu = 5$)

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

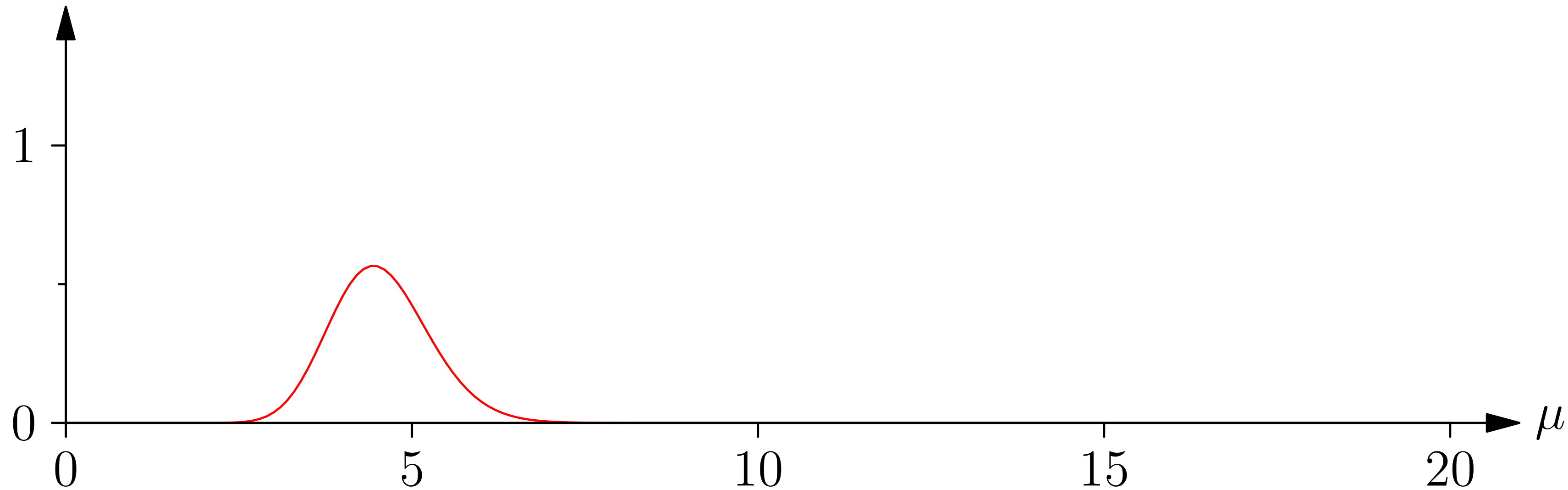
$$p(\mu|36, 8) = \frac{8^{36}\,\mu^{35}\,\mathrm{e}^{-8\,\mu}}{\Gamma(36)} \qquad a = 36,\ b = 8$$



Example ($\mu = 5$)

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

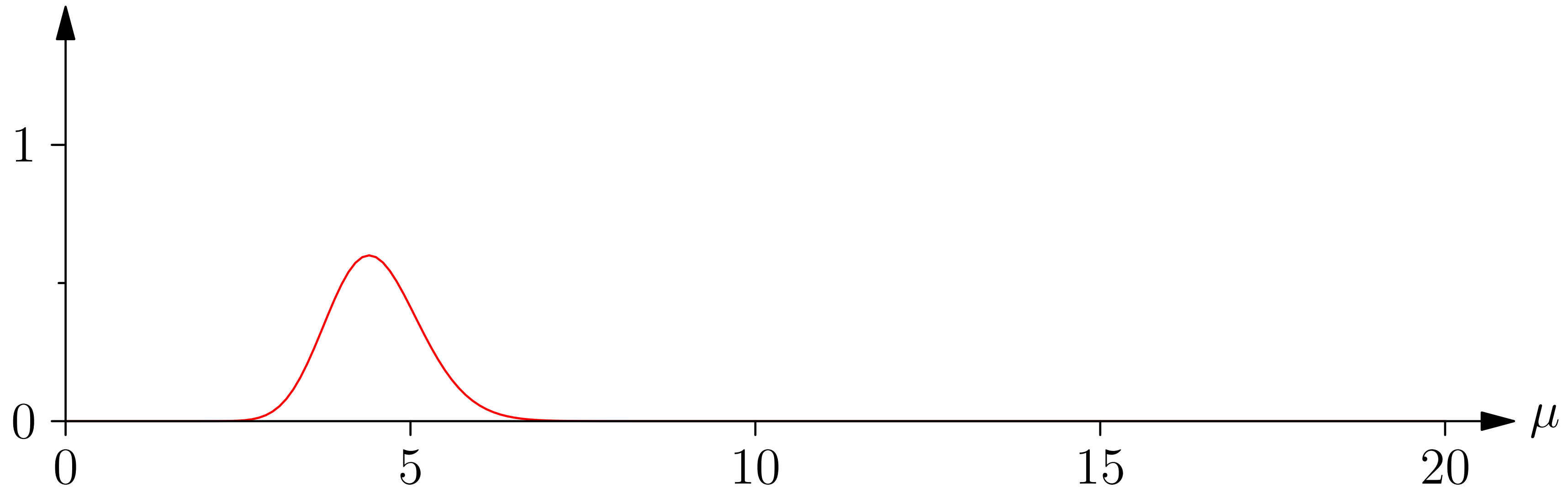
$$p(\mu|41, 9) = \frac{9^{41}\,\mu^{40}\,\mathrm{e}^{-9\,\mu}}{\Gamma(41)} \qquad a = 41,\ b = 9$$



Example ($\mu = 5$)

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

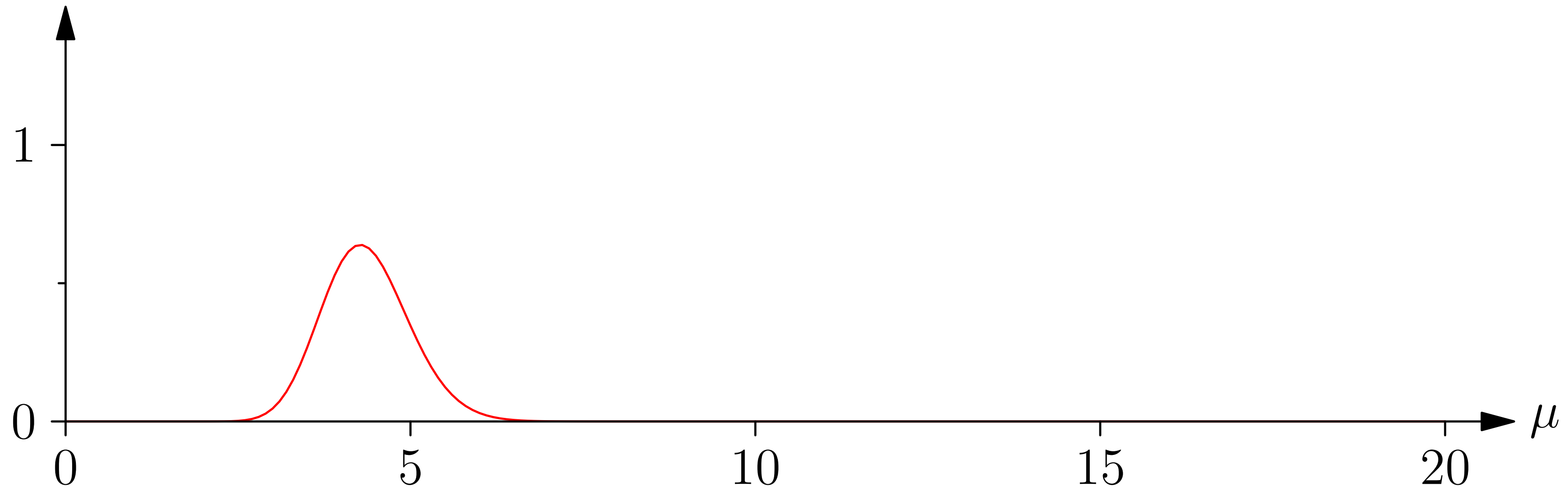
$$p(\mu|45, 10) = \frac{10^{45}\,\mu^{44}\,\mathrm{e}^{-10\,\mu}}{\Gamma(45)} \qquad a = 45,\ b = 10$$



Example ($\mu = 5$)

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

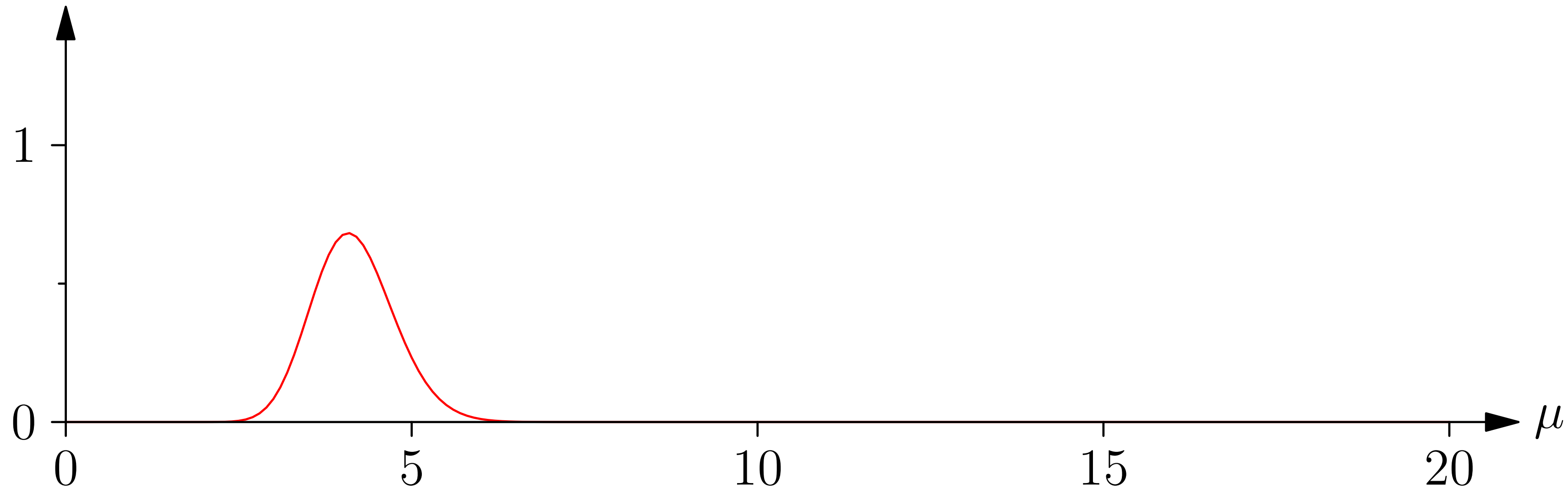
$$p(\mu|48, 11) = \frac{11^{48}\,\mu^{47}\,\mathrm{e}^{-11\,\mu}}{\Gamma(48)} \qquad a = 48,\ b = 11$$



Example ($\mu = 5$)

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

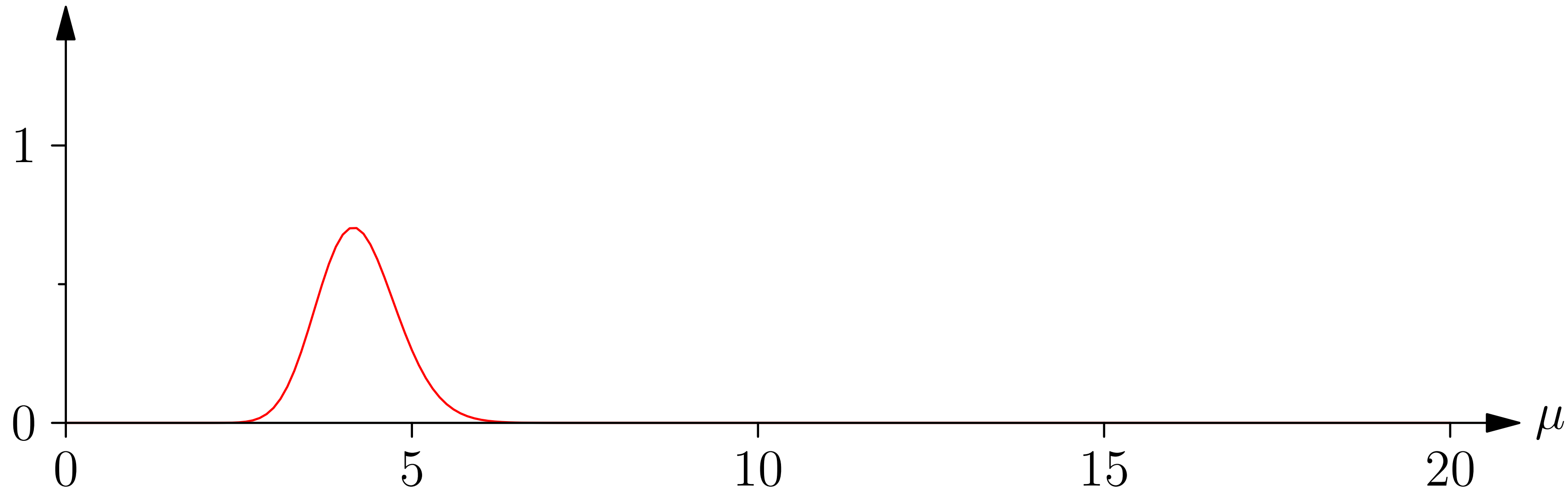
$$p(\mu|50, 12) = \frac{12^{50}\,\mu^{49}\,\mathrm{e}^{-12\,\mu}}{\Gamma(50)} \qquad a = 50,\ b = 12$$



Example ($\mu = 5$)

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

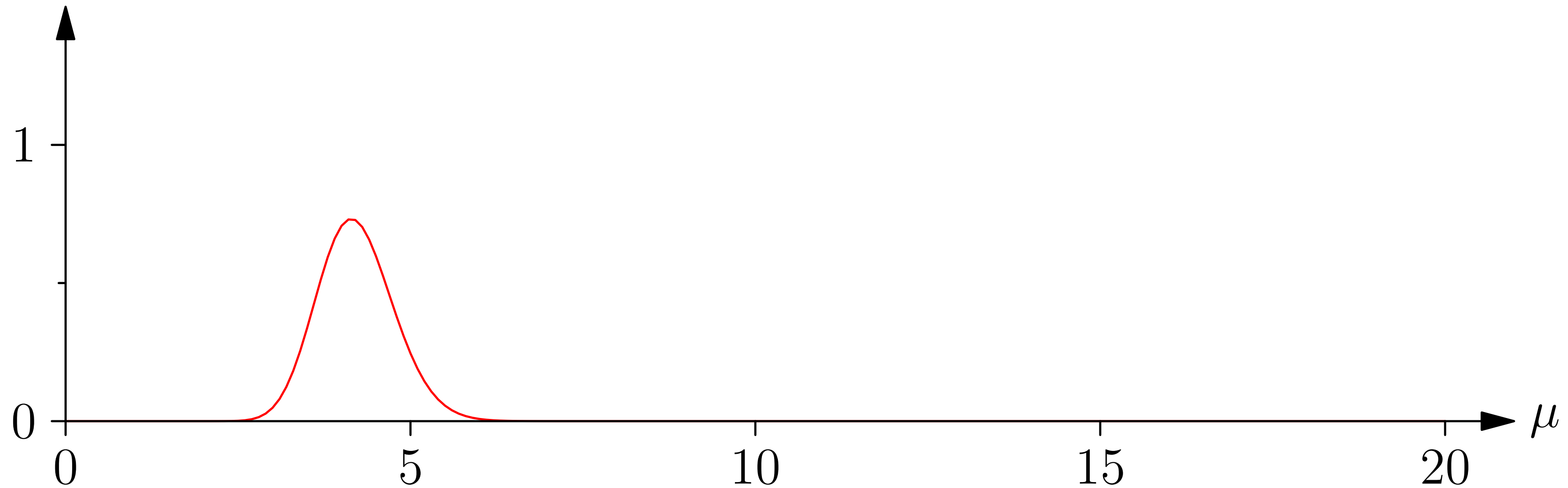
$$p(\mu|55, 13) = \frac{13^{55}\,\mu^{54}\,\mathrm{e}^{-13\,\mu}}{\Gamma(55)} \qquad a = 55,\ b = 13$$



Example ($\mu = 5$)

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

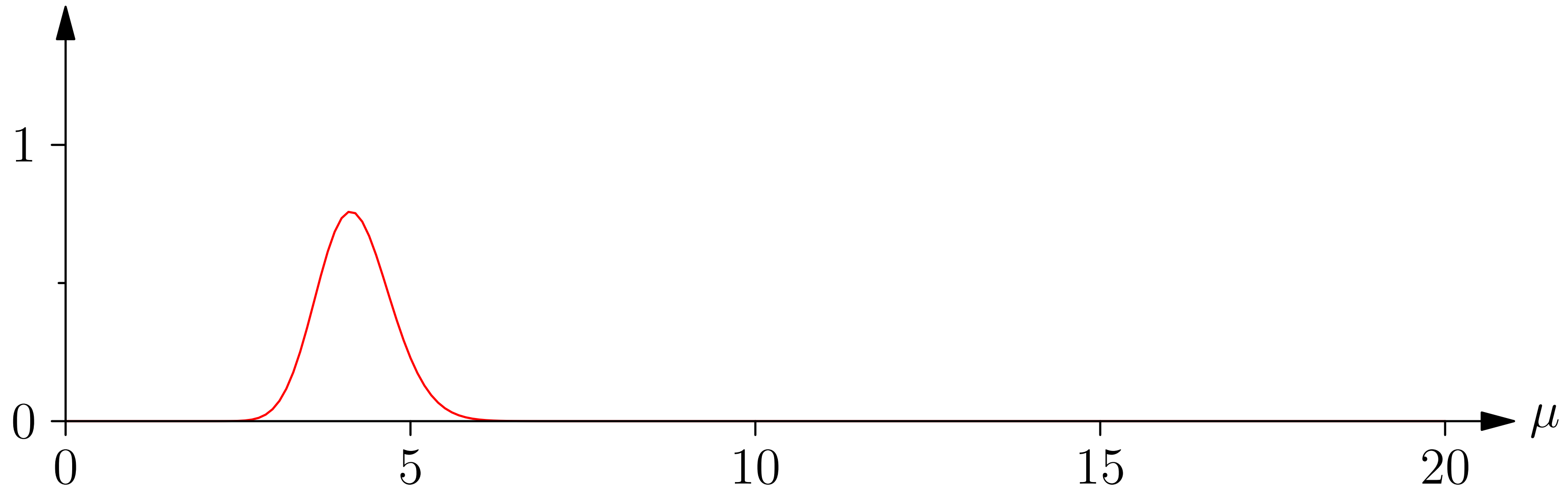
$$p(\mu|59, 14) = \frac{14^{59}\,\mu^{58}\,\mathrm{e}^{-14\,\mu}}{\Gamma(59)} \qquad a = 59,\ b = 14$$



Example ($\mu = 5$)

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

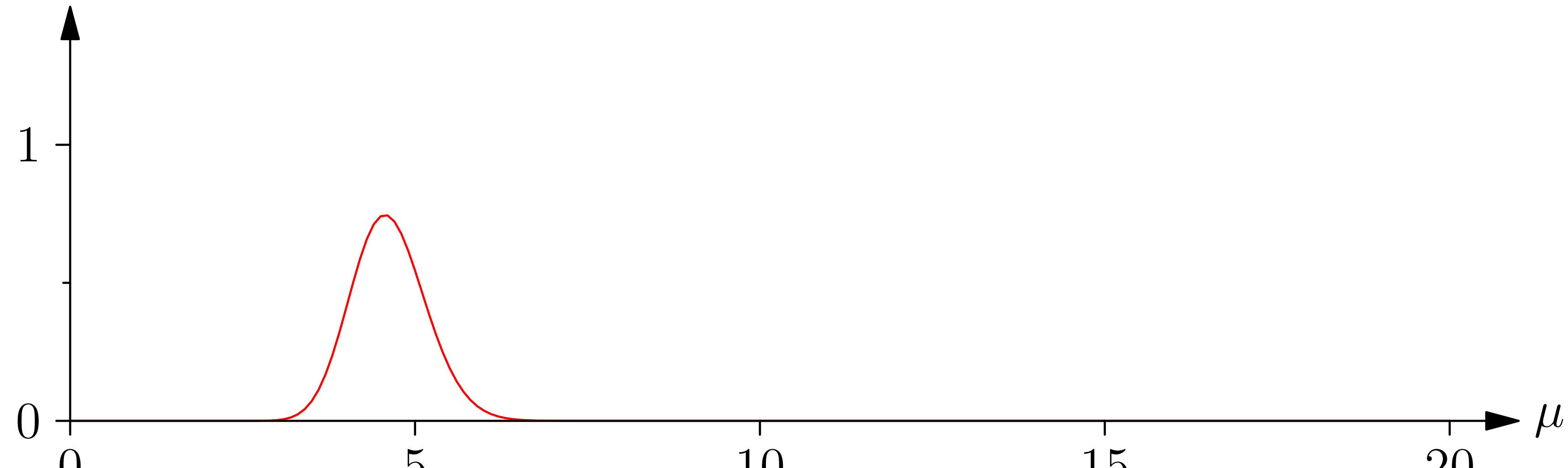
$$p(\mu|63, 15) = \frac{15^{63}\,\mu^{62}\,\mathrm{e}^{-15\,\mu}}{\Gamma(63)} \qquad a = 63,\; b = 15$$



Example ($\mu = 5$)

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

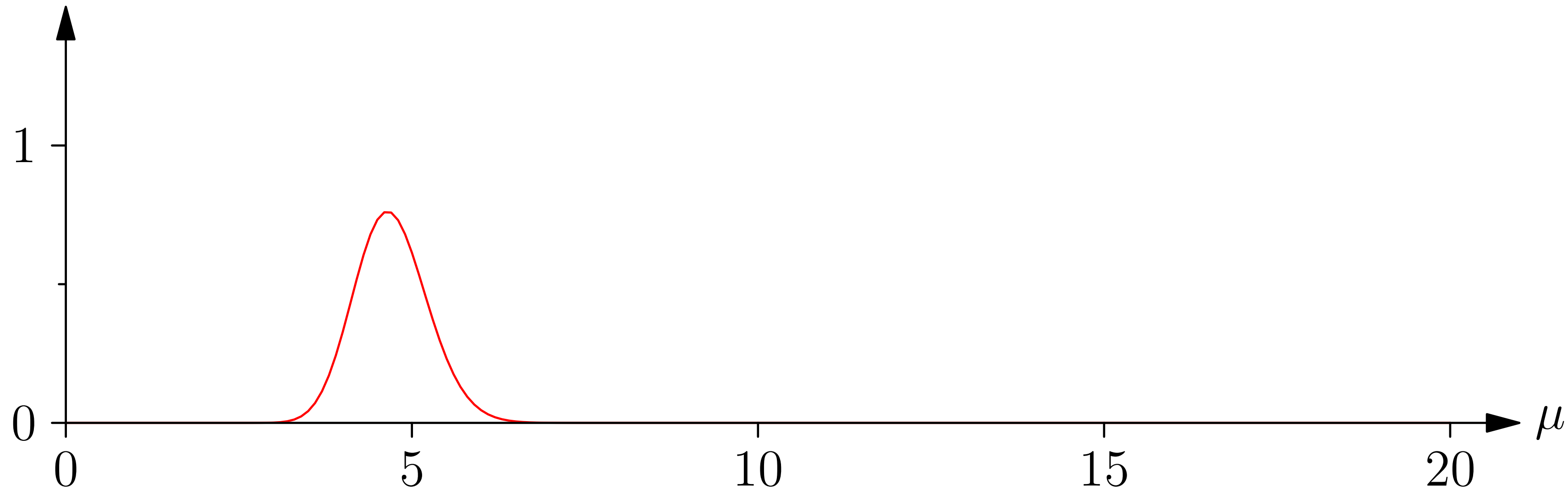
$$p(\mu|74, 16) = \frac{16^{74}\,\mu^{73}\,\mathrm{e}^{-16\,\mu}}{\Gamma(74)} \qquad a = 74,\ b = 16$$



Example ($\mu = 5$)

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

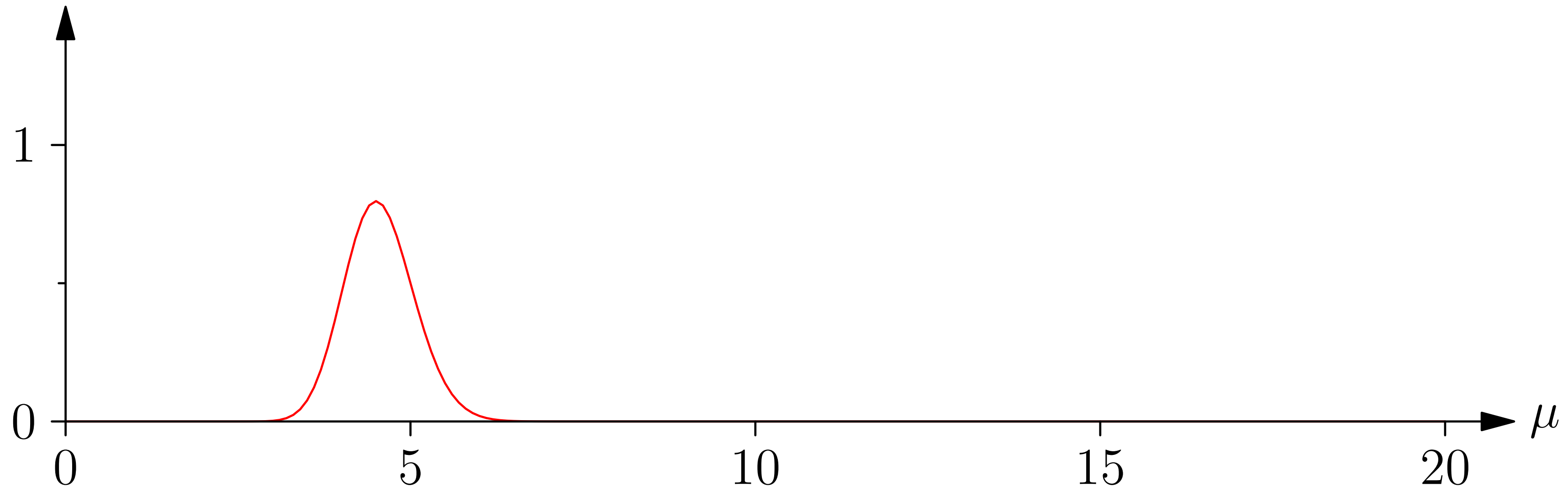
$$p(\mu|80, 17) = \frac{17^{80}\,\mu^{79}\,\mathrm{e}^{-17\,\mu}}{\Gamma(80)} \qquad a = 80,\ b = 17$$



Example ($\mu = 5$)

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

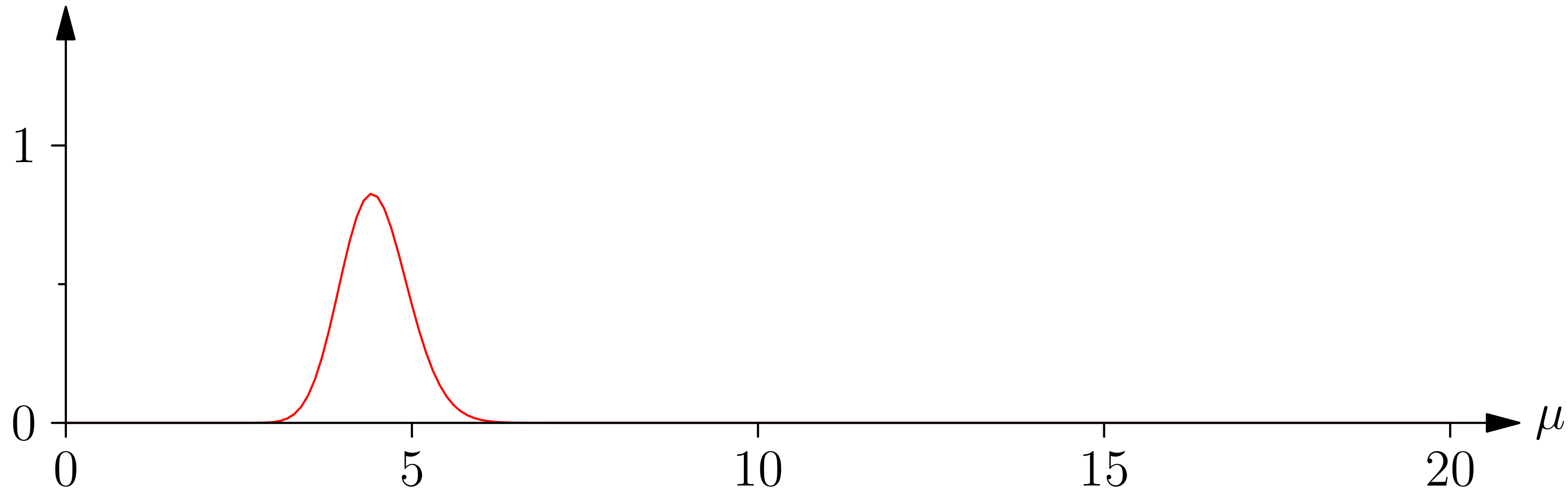
$$p(\mu|82, 18) = \frac{18^{82}\,\mu^{81}\,\mathrm{e}^{-18\,\mu}}{\Gamma(82)} \qquad a = 82,\ b = 18$$



Example ($\mu = 5$)

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

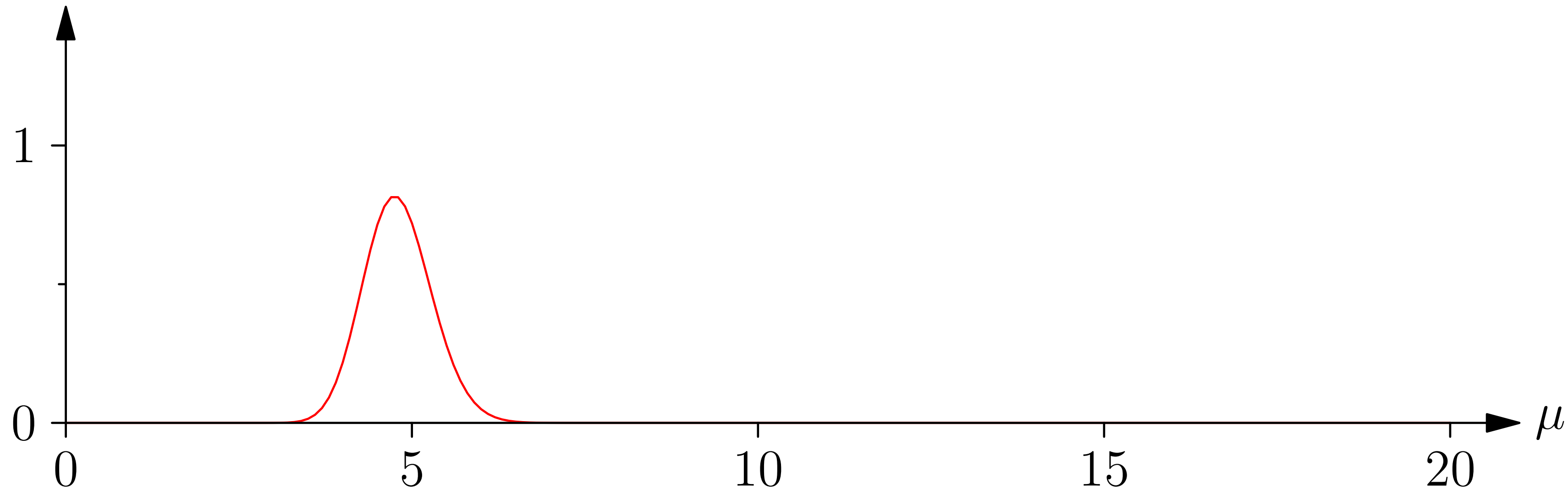
$$p(\mu|85, 19) = \frac{19^{85}\,\mu^{84}\,\mathrm{e}^{-19\,\mu}}{\Gamma(85)} \qquad a = 85,\ b = 19$$



Example ($\mu = 5$)

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

$$p(\mu|96, 20) = \frac{20^{96}\,\mu^{95}\,\mathrm{e}^{-20\,\mu}}{\Gamma(96)} \qquad a = 96,\ b = 20$$



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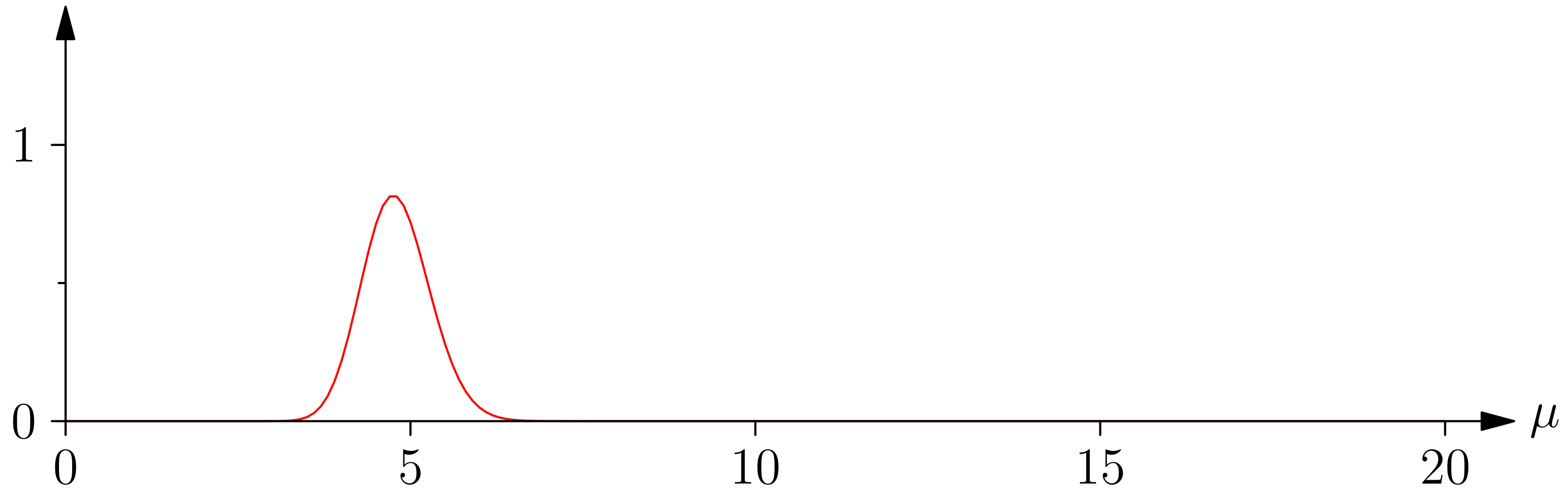

$$\mathbb{E}[\mu] = \frac{a}{b} = \frac{96}{20} = 4.8 \qquad \sqrt{\mathbb{V}\mathrm{ar}(\mu)} = \sqrt{\frac{a}{b^2}} = 0.49$$

Outline

1. Bayes' Rule
2. Conjugate Priors
3. **Uninformative Priors**

Uninformative Priors

- What if we have no prior knowledge, what should we do?
- OK usually we know whether we should make a measurement using a micrometer, ruler or car mileage, but we might still know almost nothing
- This led to Bayesian statistics being labelled as *subjective*
- However Ed. Jaynes (the greatest proponent of Bayesian methods) argued that we could answer this using symmetry arguments

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Uninformative Priors for Scale Parameter

- Why did we choose $a_0 = b_0 = 0$ implying a prior $p(\mu) = 1/\mu$?

- That is, we have no idea on what scale to measure μ

$$\int_A^B p(\mu)\,\mathrm{d}\mu = \int_{A/c}^{B/c} p(\mu)\,\mathrm{d}\mu$$

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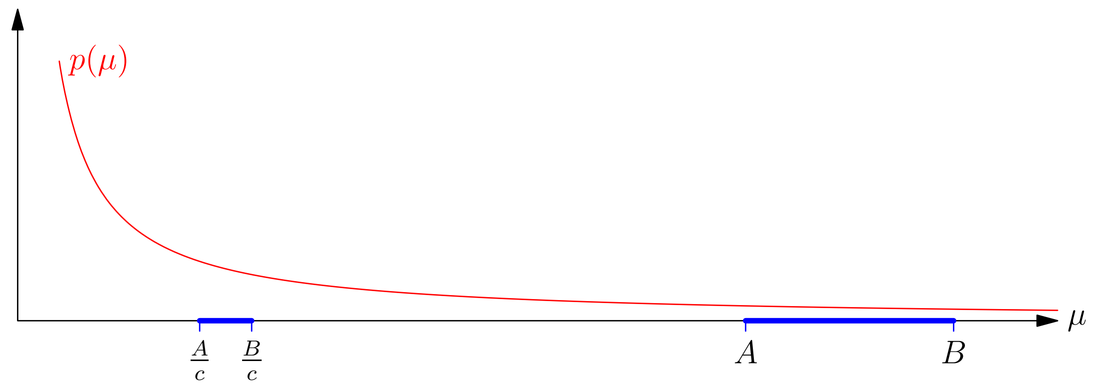

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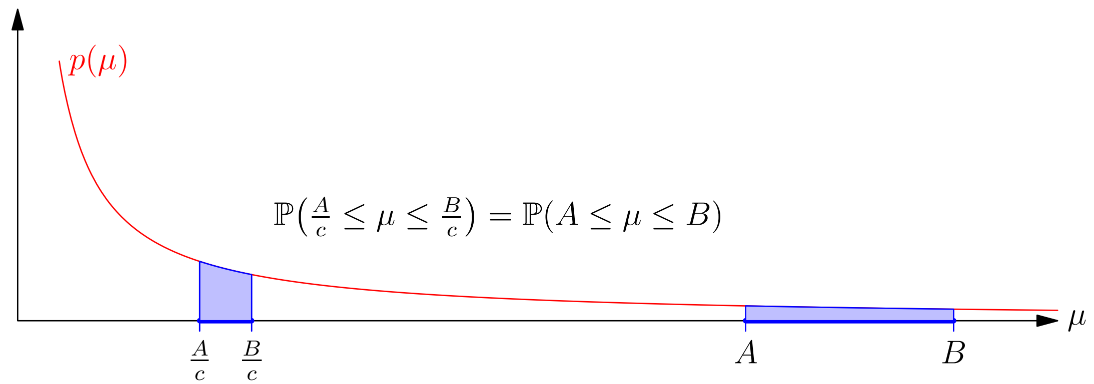

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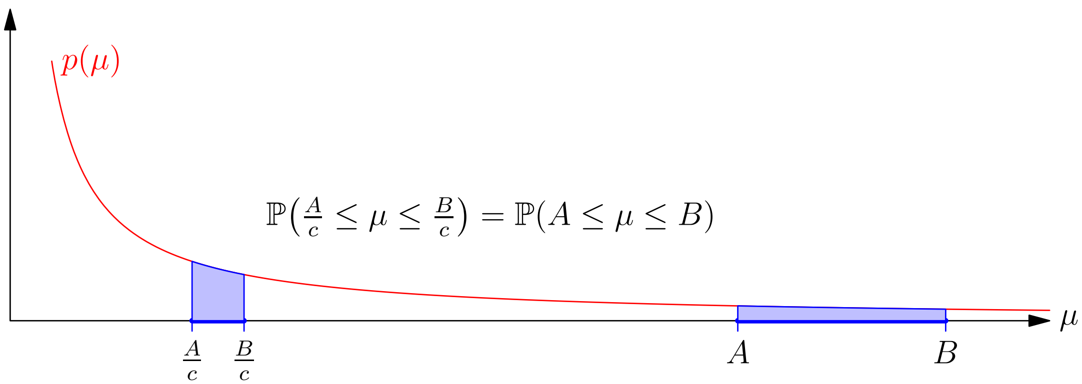

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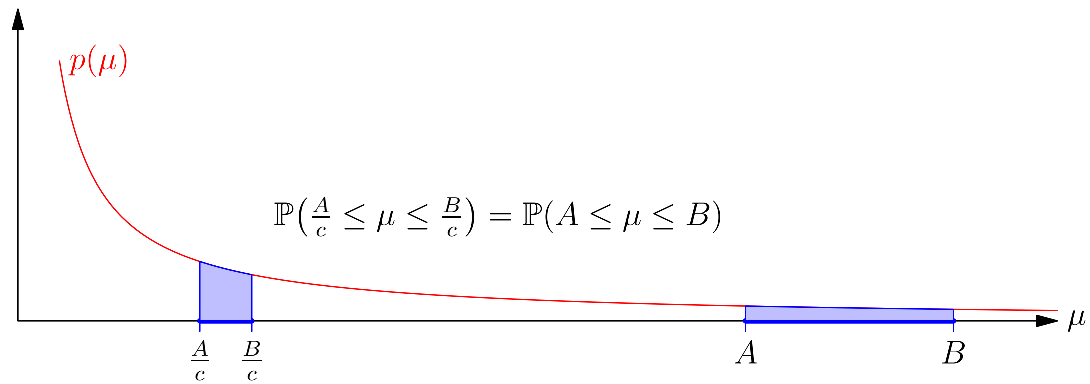

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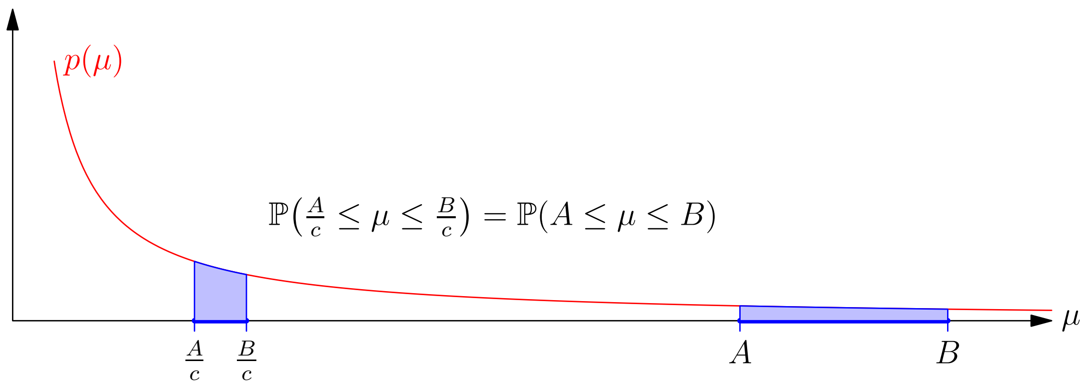

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Benford's Law

- Numbers occurring in life (physical constants, amounts of money) should not depend on the units (scale) measuring them
- They should then be distributed as $p(x) \propto 1/x$
- A curious consequence of this is that the significant figure has a distribution

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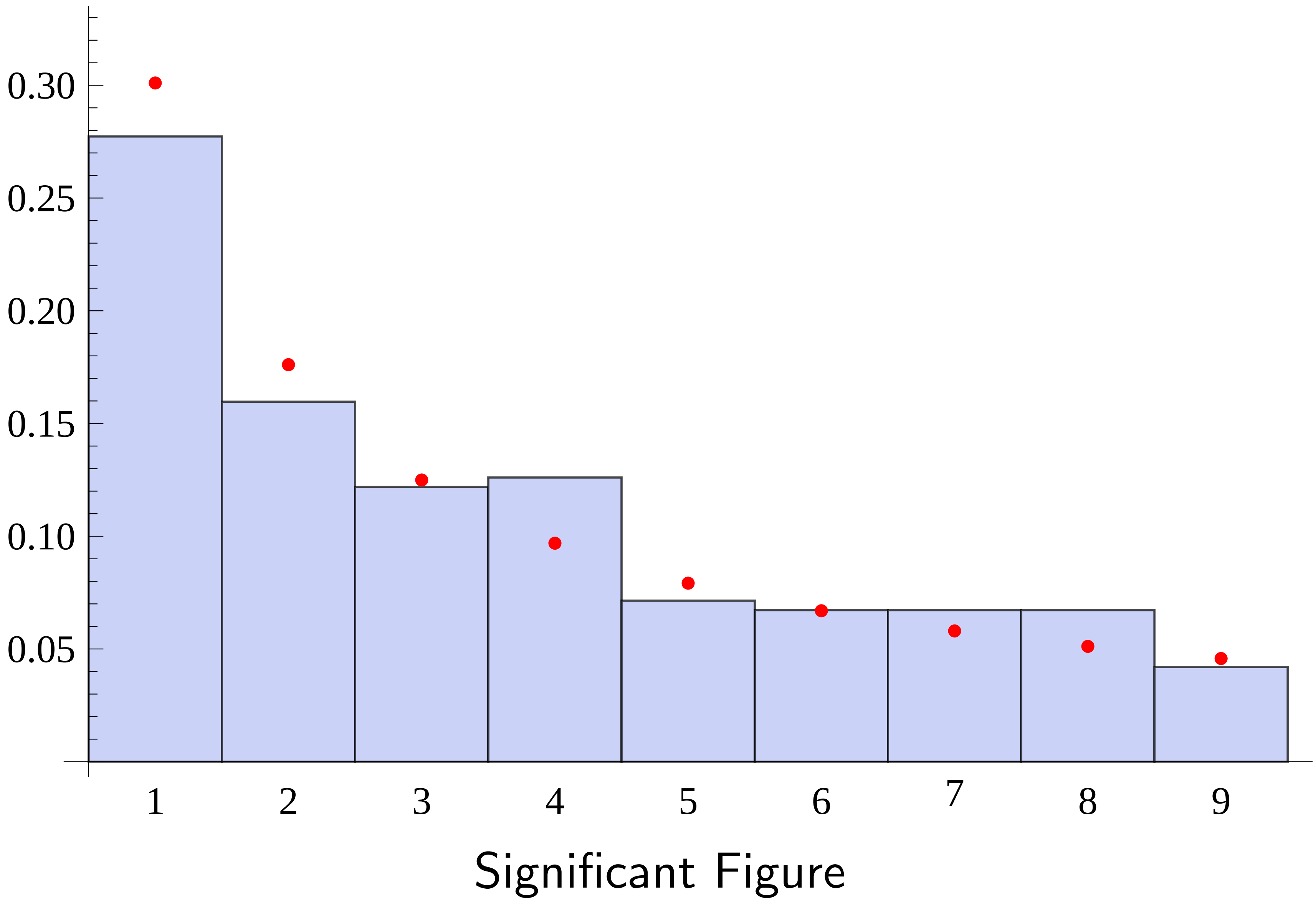
Population Size of 238 Countries



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- However, it requires a model of what is happening
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