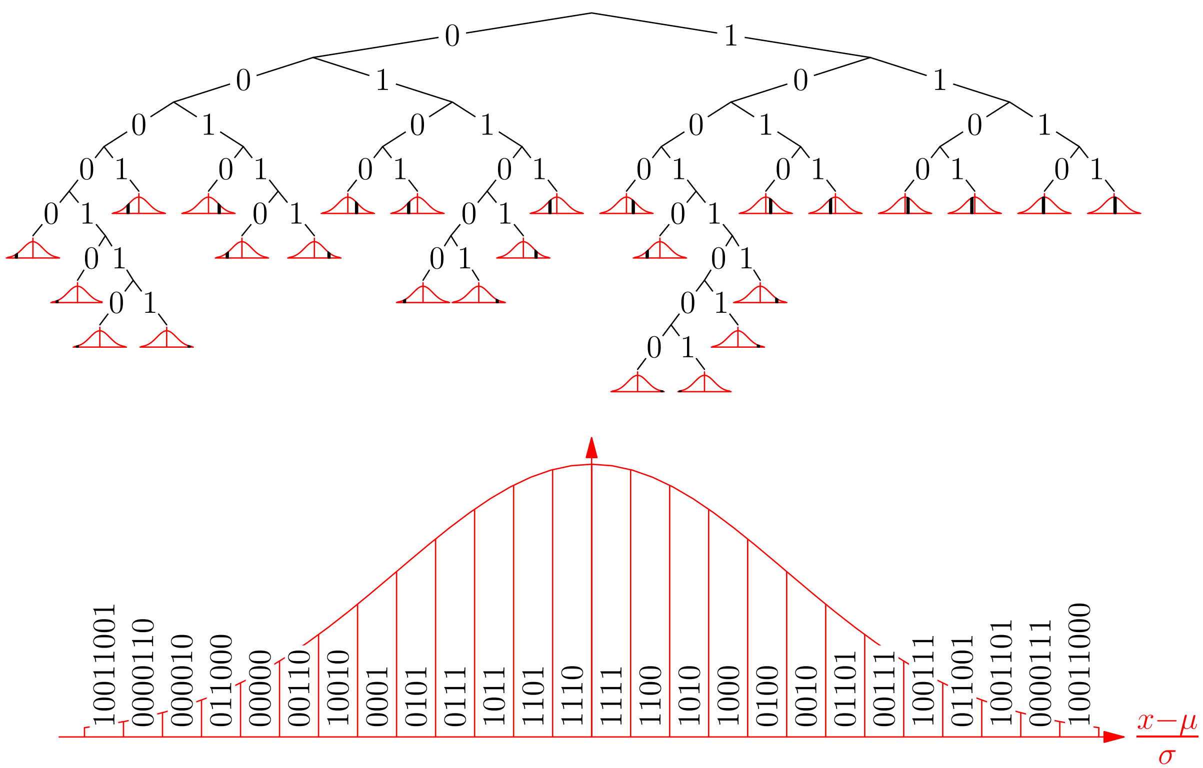
Advanced Machine Learning

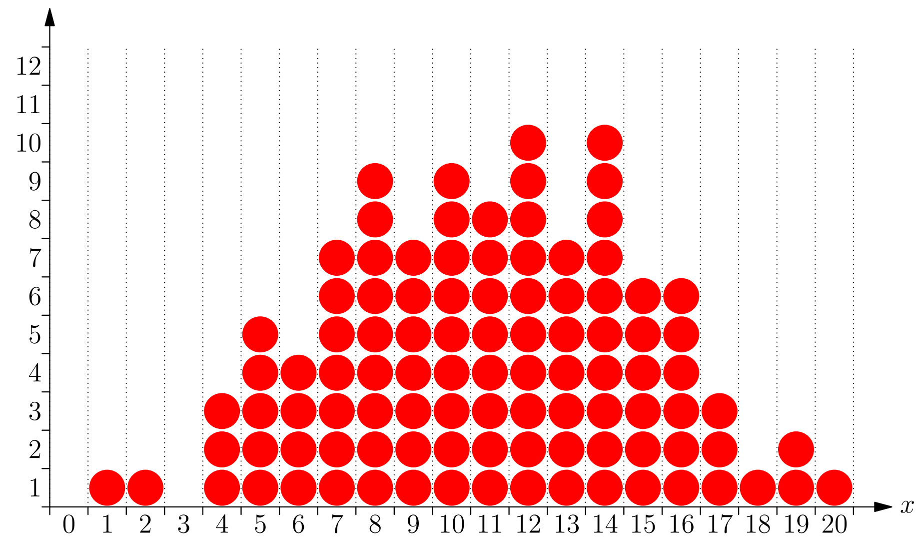
Entropy



Entropy, Coding, Maximum Entropy

Outline

1. **Measuring Uncertainty**
2. Code Length
3. Maximum Entropy



Measuring Uncertainty

- What is more uncertain tossing a coin three times or throwing a dice
- The answer depends on whether you care about the order of the coin tosses
- But, how do we answer such a question?
- Let X be a random variable denoting the possible outcomes
- Interestingly, Shannon entropy give a precise answer

$$H_X = -\sum_{x \in \mathcal{X}} \mathbb{P}(X = x) \log_2(\mathbb{P}(X = x))$$

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Let's Calculate

- For an honest dice $D \in \{1,2,3,4,5,6\}$ and $\mathbb{P}(D=i) = 1/6$ so

$$H_D = -\sum_{i=1}^{6} \frac{1}{6} \log_2\left(\frac{1}{6}\right) = -\log_2\left(\frac{1}{6}\right) = \log_2(6) \approx 2.584\,\text{bits}$$

- For an honest coin where we care about the order so $C \in \{000,001,\ldots,111\}$ the $\mathbb{P}(C=i) = \frac{1}{8}$ and

$$H_C = -\sum_{i=0}^{7} \frac{1}{8} \log_2\left(\frac{1}{8}\right) = -\log_2\left(\frac{1}{8}\right) = \log_2(8) = 3\,\text{bits}$$

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Unordered Coin Toss

- What if we don't care about the order of the out-come then $\mathbb{P}(HHH) = \mathbb{P}(TTT) = 1/8$, $\mathbb{P}(HHT) = \mathbb{P}(HTT) = 3/8$ so

$$H_U = -\frac{1}{4}\log_2\left(\frac{1}{8}\right) - \frac{3}{4}\log_2\left(\frac{3}{8}\right) \approx 1.811\,\text{bits}$$

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- But why Shannon entropy?

Additive Entropy

- If H_X and H_Y is the uncertainty of two independent random variable X and Y, what is the uncertainty of the combined event (X,Y)?

$$\begin{aligned}
H_{(X,Y)} &= -\sum_{X,Y} \mathbb{P}(X,Y) \log_2(\mathbb{P}(X,Y)) \\
&= -\sum_{X,Y} \mathbb{P}(X)\mathbb{P}(Y) \log_2(\mathbb{P}(X)\mathbb{P}(Y)) \\
&= -\sum_{X,Y} \mathbb{P}(X)\mathbb{P}(Y) \left(\log_2(\mathbb{P}(X)) + \log_2(\mathbb{P}(Y))\right) \\
&= -\sum_{X} \mathbb{P}(X) \log_2(\mathbb{P}(X)) - \sum_{Y} \mathbb{P}(Y) \log_2(Y) = H_X + H_Y
\end{aligned}$$

- Shannon's entropy is one of the few functions that satisfy this condition

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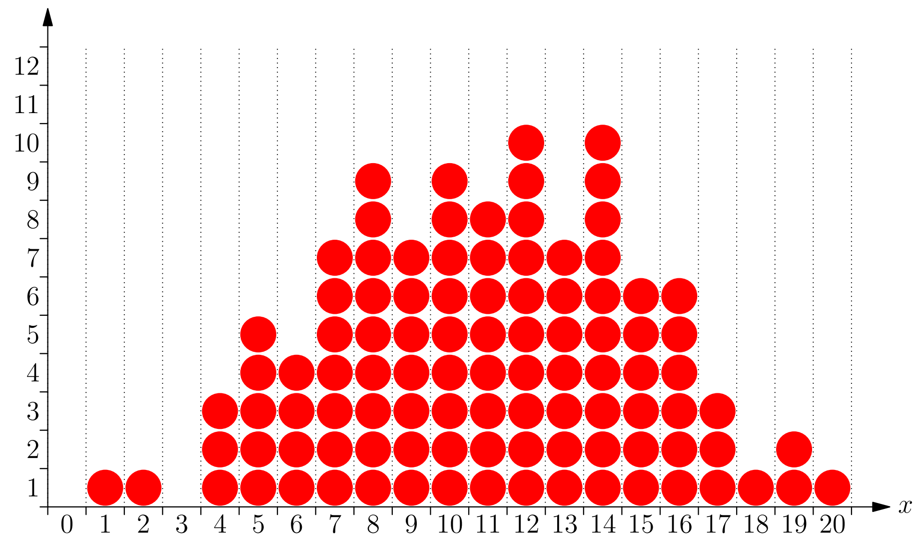

Why Measure Entropy in Bits

- Suppose we had to communicate a message with 2^n equally likely outputs (e.g. the result of n-coin tosses)
- We can do this with a binary string with n bits (011..0)
- If there were 5 possible outcomes I could do this with 3 bits, but waste 3/8 of the message
- However if we have a batch of 3 independent messages each with 5 outcomes then there are 125 possible outcomes
- By batching together enough messages with N outcomes then we asymptotically need just $\log_2(N)$ bits

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Different Probabilities

- We "showed" that if we had N events, X_i, each with probability, $\mathbb{P}(X_i) = 1/N$, we can code the outcomes with a message of length $-\log_2(\mathbb{P}(X_i))$
- With a shorter message we would not be able to distinguish all possible outcomes from the message
- What happens if some of outcomes occur with a different probability

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\begin{array}{rcccccc}
X_i: & 1 & 2 & 3 & 4 & 5 & 6 \\
p(X_i): & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{4} & \frac{1}{4} \\
\text{Code:} & 000 & 001 & 010 & 011 & 10 & 11 \\
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Shannon's Entropy

- If the probabilities are not equal to 2^{-n} we can still find a code with a length very close to $-\log_2(\mathbb{P}(X))$ per message by transmitting a large number of messages

- The length of the message measures the amount of **surprise** on receiving the message

- Shannon's entropy is the expected length of the message to communicate a random variable X

$$H_X = \mathbb{E}_X[-\log_2(\mathbb{P}(X))] = -\sum_{x \in \mathcal{X}} \mathbb{P}(X = x) \log_2(\mathbb{P}(X = x))$$

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- The expected length is a measure of the uncertainty (how much information on average we need to convey the outcome)

Real Codes

- Those of you with some computer science background will realise that we can't actually use different length strings in a code without paying some price
- We won't know where a code word ends so we can't decode the message
- An optimal solution is to use Huffman encoding where we associate the leaf of a tree with each code word
- Using the tree we can decode any message constructed using the tree
- There is a greedy algorithm for constructing the optimal tree

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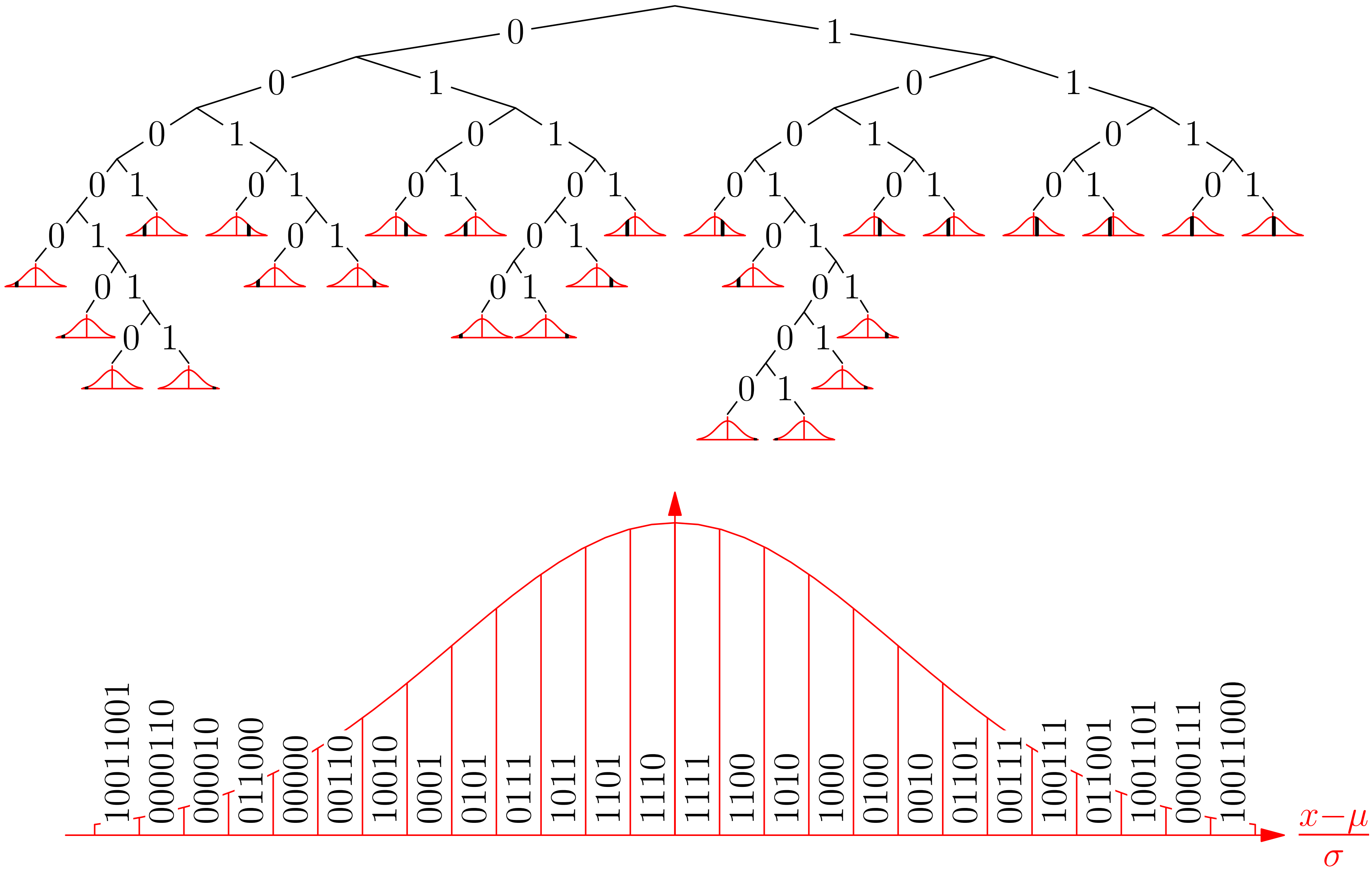
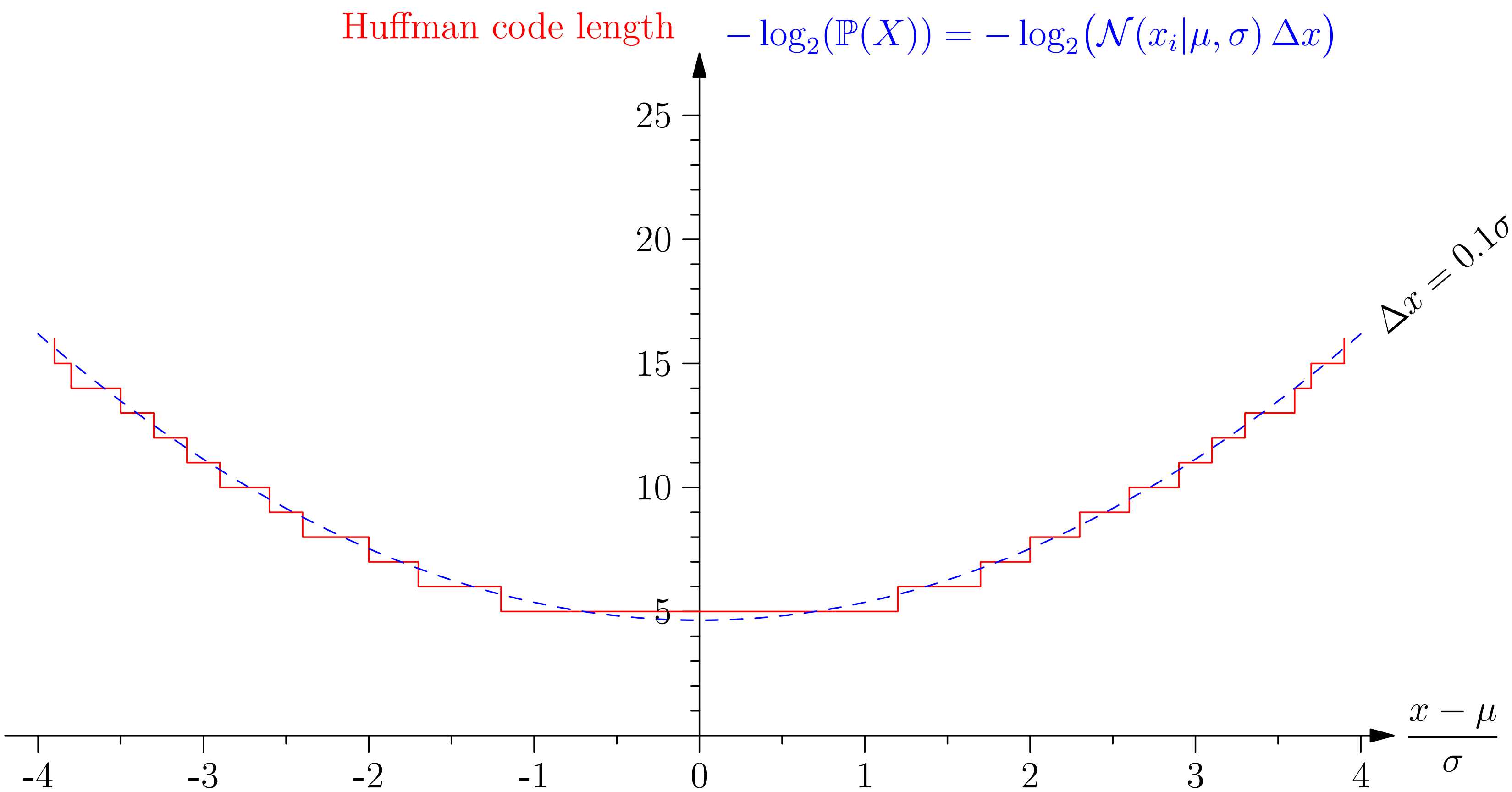
Coding Normals



Coding Normals to Accuracy Δx



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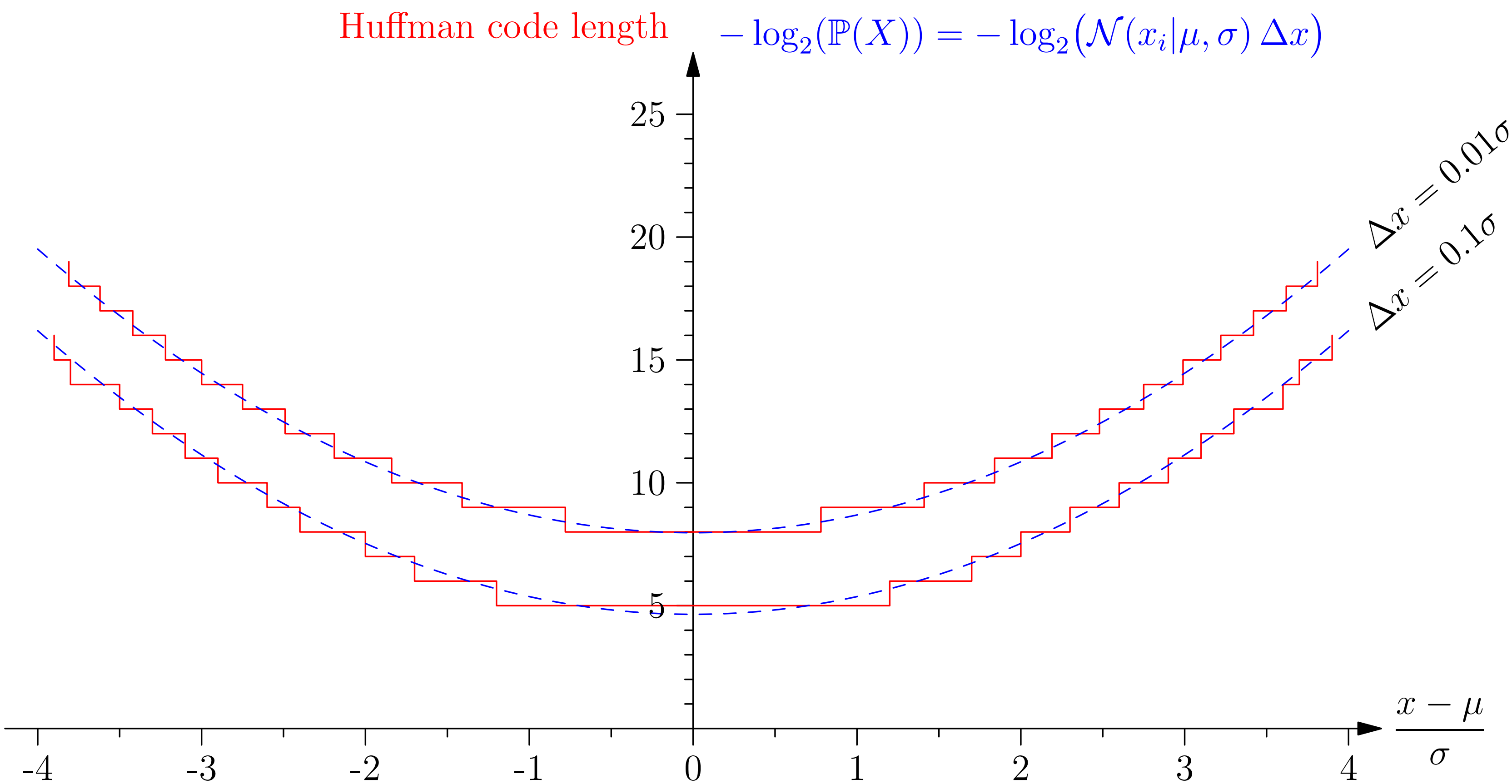

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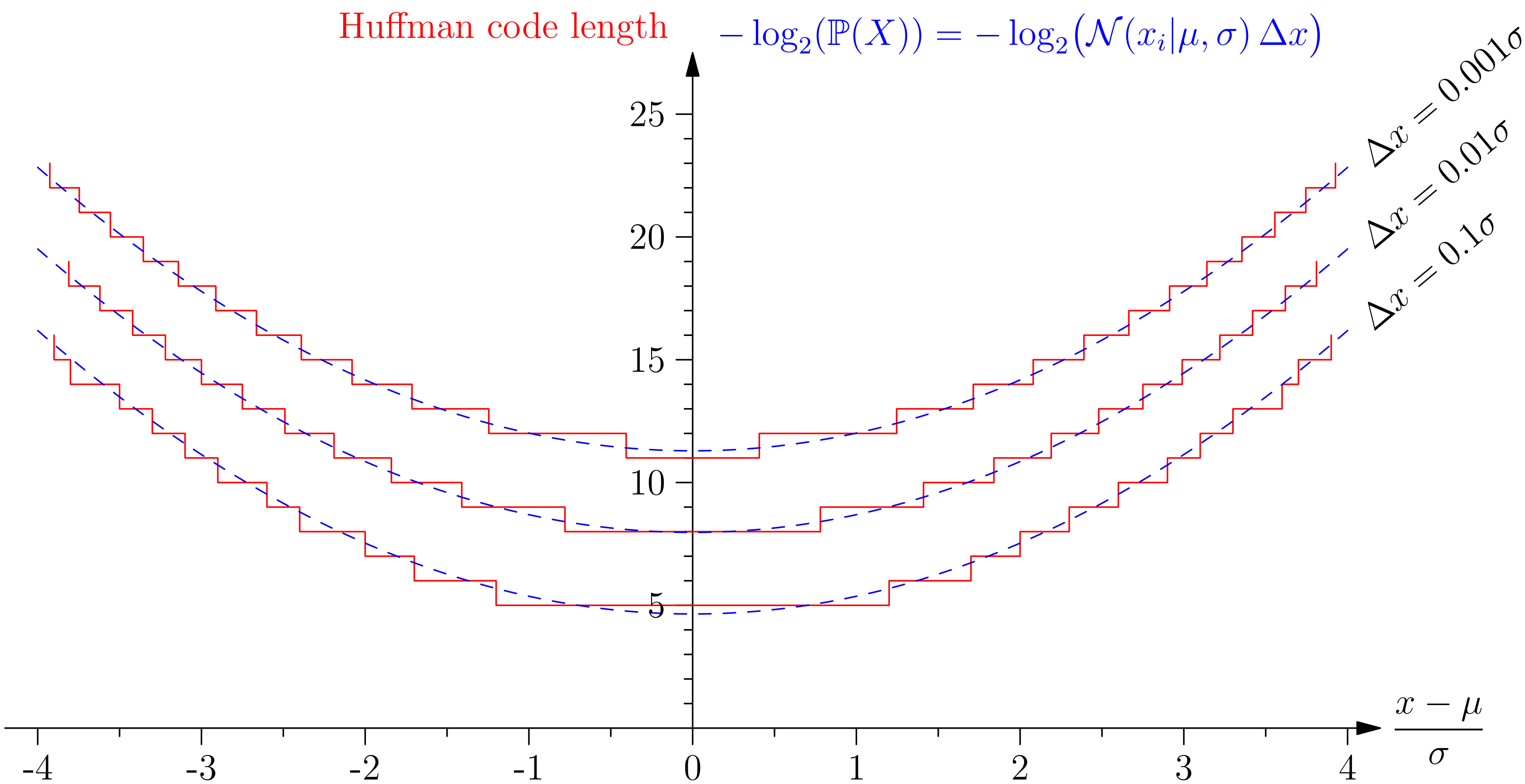

bits and nats

- We have measured entropy in **bits** using

$$H_X = -\sum_{x \in \mathcal{X}} \mathbb{P}(X = x) \log_2\big(\mathbb{P}(X = x)\big)$$

- Sometimes it is easier to use natural logarithms

$$H_X = -\sum_{x \in \mathcal{X}} \mathbb{P}(X = x) \ln\big(\mathbb{P}(X = x)\big)$$

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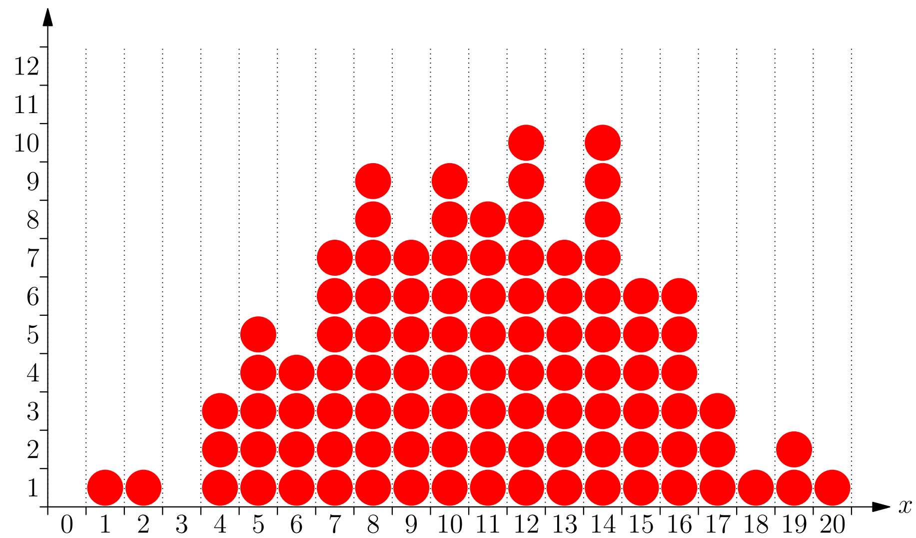
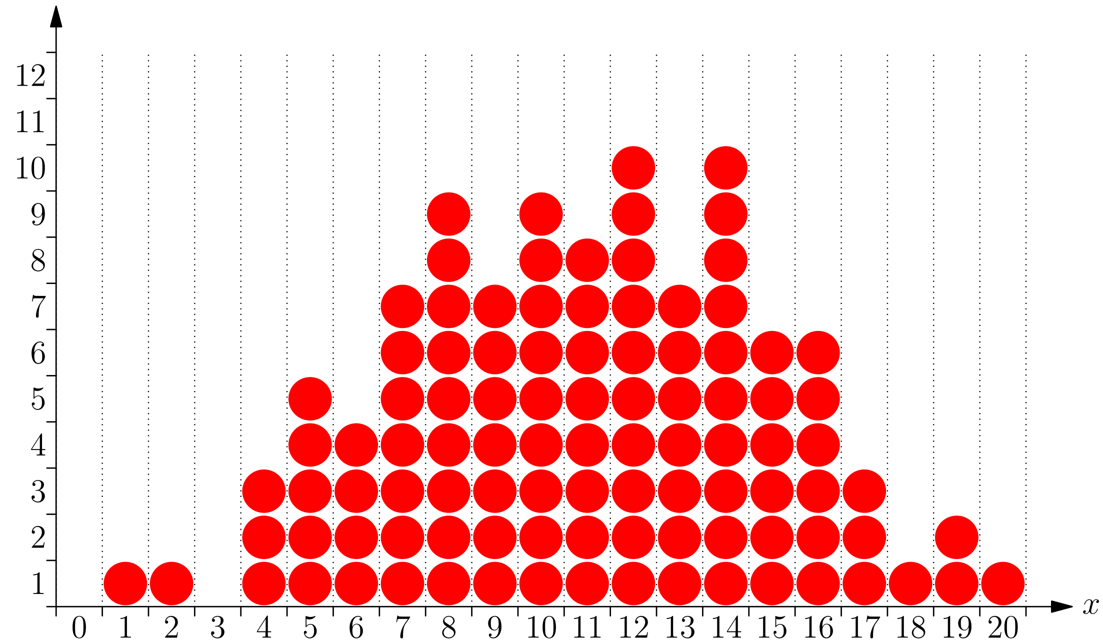
Outline

1. Measuring Uncertainty
2. Code Length
3. **Maximum Entropy**



Number of States

- Suppose I have N balls I them put in K boxes with coordinates x_i such that the mean is μ and variance is σ^2



$$\mathbb{P}(\boldsymbol{n}) \propto \frac{N!}{n_1! n_2! \cdots n_K!} \left[\!\!\left[\sum_i \frac{n_i}{N} x_i = \mu \right]\!\!\right] \left[\!\!\left[\sum_i \frac{n_i}{N} (x_i - \mu)^2 = \sigma^2 \right]\!\!\right]$$

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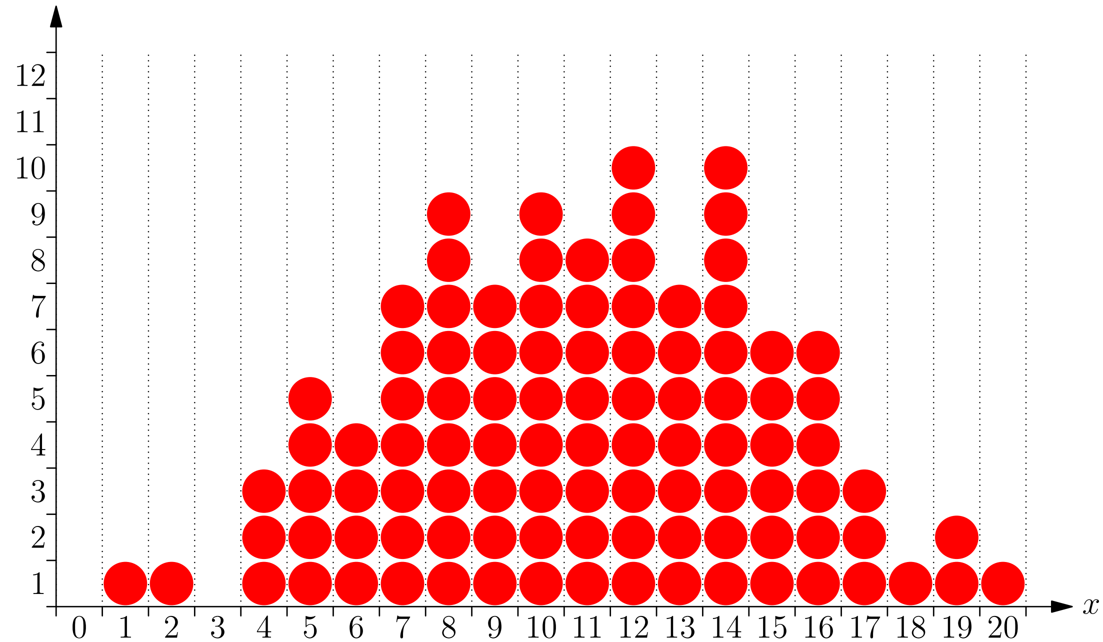

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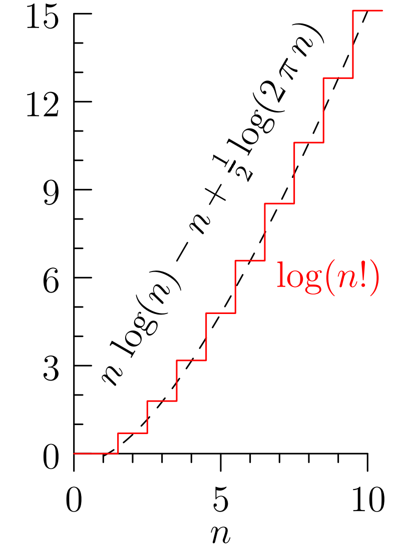
- We can approximate the factorial $n!$ using **Stirling's approximation**

$$n! \approx \sqrt{2\pi n}\, n^n \mathrm{e}^{-n}$$

$$\log(n!) = n\log(n) - n + \frac{1}{2}\log(2\pi n)$$



- Using this in our formula for $\mathbb{P}(\boldsymbol{n})$ we have

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where $(f_1(x_i), v_l) = \{(1,1), (x_i, \mu), ((x_i-\mu)^2, \sigma^2)\}$

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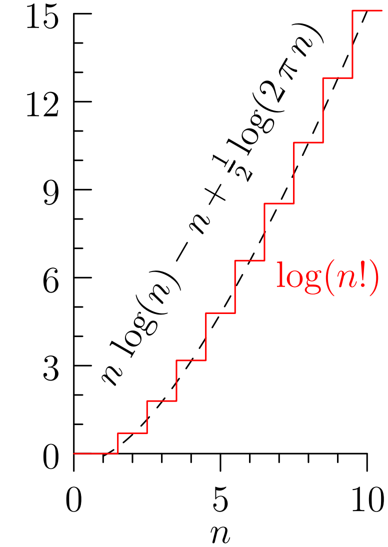

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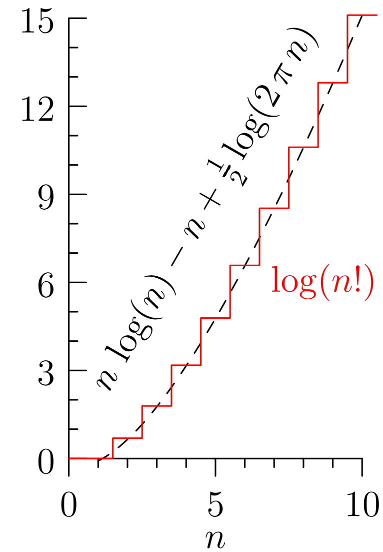

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Number of States and Entropy

- Let $p(x_i) = n_i/N$ be the proportion of balls in bin i then

$$\mathbb{P}(\boldsymbol{n}) \approx C \mathrm{e}^{N H_X} \prod_{l=1}^{3} \left[\!\!\left[\sum_i \frac{n_i}{N} f_l(x_i) = v_l \right]\!\!\right]$$

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Maximum Entropy Method

- When we are trying to infer a distribution given some observations then we can maximise the entropy subject to constraints
- This is known as the **maximum entropy method**
- We can rationalise this as this is by far the most likely set of configurations consistent with the observations
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Knowing the Mean and Variance

- Consider a continuous random variable, X, with a known mean and second moment

$$\mathbb{E}[X] = \mu, \qquad \mathbb{E}\left[X^2\right] = \mu_2 = \mu^2 + \sigma^2$$

- To maximise the entropy subject to constraints consider

$$\mathcal{L}(f) = -\int f_X(x) \log(f_X(x))\, \mathrm{d}x + \lambda_0 \left(\int f_X(x) \mathrm{d}x - 1 \right) + \lambda_1 \left(\int f_X(x)\, x\, \mathrm{d}x - \mu \right) + \lambda_2 \left(\int f_X(x)\, x^2 \mathrm{d}x - \mu_2 \right)$$

- Thus

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- Maximum entropy is often used to infer distributions
- It can be very effective, but it might not work well if there are other constraints that we have not included
- The place that they work superbly well is in statistical physics
- The whole of statistical physics is about inferring distributions making observations of volume, pressure, etc.
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- Its interpretation as the number of states was introduced by Ludwig Boltzmann
- The person who got it all right was Josiah Willard Gibbs (and James Clerk Maxwell)
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Conclusion

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- It forms the basis of information theory which we will look at in the next lecture
- $-\log(\mathbb{P}(X = x))$ can be seen as the minimum length of a message to communication x
- This will be used as the basis of the minimum description length formalism also discussed in the next lecture
- Entropy can be used as a prior, which we often maximise subject to constraints to obtain an unbiased estimate

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