Data compression

Probabilistic models

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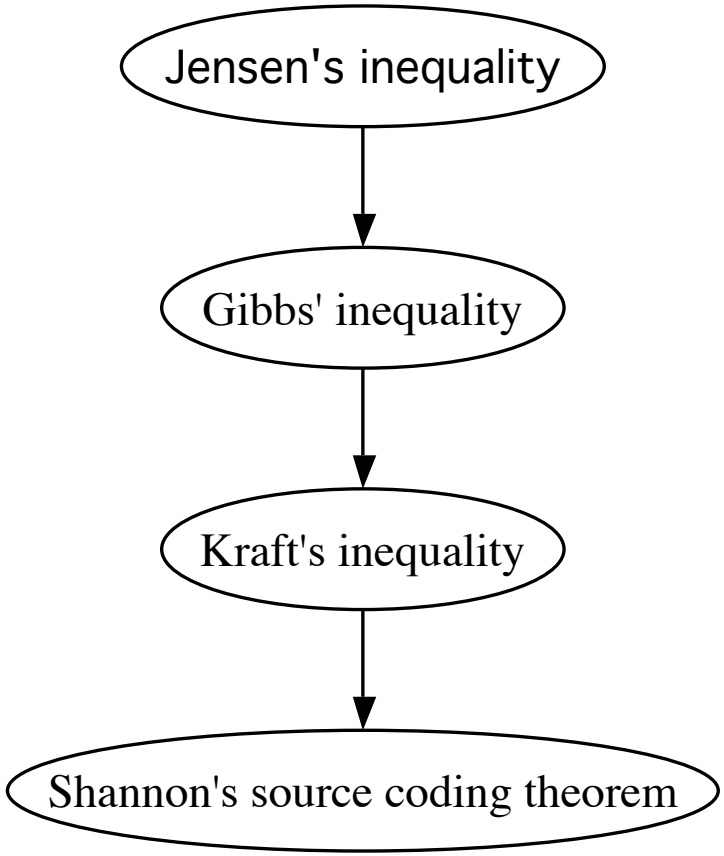
Outline

Information-theoretic quantities

Shannon information:	$h(x)$	$=$	$-\log_2 p(x)$
Shannon entropy:	H_p	$=$	$\langle h(x) \rangle_p$
Relative entropy:	$D(p\|\|q)$	$=$	$\langle \log \frac{p(x)}{q(x)} \rangle_p$
Mutual information:	$I(x;y)$	$=$	$D\left(p(x,y)\|\|p(x)p(y)\right)$
Kolmogorov complexity:	$K(\mathbf{x})$	$=$	size of smallest program that outputs $\mathbf{x}$

Theorems



Information Theory, Inference and Learning Algorithms.
MacKay (2003)

Jensen's Inequality

- A function $f(x)$ is convex over (a, b) if every chord lies above the function.
  - $f''(x) \geq 0$ is sufficient.
- Jensen's inequality:

  If x is an rv and $f(x)$ is convex, then $\langle f(x) \rangle \geq f(\langle x \rangle)$
- If $f(x)$ is concave, then inequality is reversed.

Jensen's Inequality

If x is an rv and $f(x)$ is convex, then $\langle f(x) \rangle \geq f(\langle x \rangle)$

- Physical version:
  - Let $p(x)$ be x-distribution of masses on curve $y = f(x)$.
  - Then center of gravity $(\langle x \rangle, \langle f(x) \rangle)$ lies above curve.

Bounds on the Shannon entropy

$$H_p \leq \log |\Omega|$$

Proof: apply Jensen's inequality to $u = 1/p(x)$, $f(u) = -\log u$

$$\langle f(u) \rangle \geq f(\langle u \rangle)$$

Gibbs' Inequality

$$\boxed{D(p||q) \geq 0 \qquad \text{with equality iff } p = q}$$

where p, q are probability distributions over the same set Ω, and

$$D(p||q) = \sum_x p(x) \log \frac{p(x)}{q(x)}$$

is the relative entropy or Kullback-Leibler divergence.
Proof: apply Jensen to $u = q(x)/p(x)$, $f(u) = -\log u$

$$\langle f(u) \rangle \geq f(\langle u \rangle)$$

Symbol codes

- Let Ω^+ be the set of all finite-length strings over Ω
- A binary symbol code C is a mapping from Ω to $\{0,1\}^+$
- The extended code C^+ is a mapping from Ω^+ to $\{0,1\}^+$ obtained by concatenating codewords:

$$c^+(x_1 x_2 \ldots x_N) = c(x_1)c(x_2)\ldots c(x_N)$$

- Side note: it's common to add an End Of File symbol to the alphabet, so the decoder knows when to stop
  - although it's usually more efficient to send the length of your message first, followed by the symbols

Decodability

- The code C is uniquely decodable if, under the extended code C^+, no two strings have the same encoding.
- If no codeword is a prefix of any other codeword, then C is a prefix code.
- All prefix codes are uniquely decodable...

Block codes

- A block code is a code over the alphabet Ω^N
- That is, it divides an Ω-string into blocks of size N
- A common efficiency trick in information theory
  - e.g. if $|\Omega| = 5$, then Shannon info $\sim$2.32 bits/symbol
  - Naive encoding would require 3 bits/symbol: 0.7 bits/symbol wasted
  - Block code with $N = 3$ requires 7/3 $\simeq$2.33 bits/symbol
- For any symbol code C there is a trivial block code C^N

- Let $l(x)$ be the length of the codeword $C(x)$
- Let $p(x)$ be the probability distribution over symbols
- Define the *expected codeword length* of C:

$$L_p(C) = \langle l(x) \rangle_p$$

- Shannon's Source Coding Theorem states that

$$L_p(C) \geq H_p$$

for any uniquely decodable code C.
(Technically, this is the *converse* of the SCT; the SCT itself states that the equality is asymptotically achievable.)

- The equality holds if $l(x) = h(x) \quad \forall x$

Insight into Source Coding Theorem

- Given a unique code C, is it optimal for anything?
- Maybe... if there's a distribution $q(x)$ such that $L_q(C) = H_q$
- This would require that $l(x) = h_q(x) \quad \forall x$, i.e.

$$q(x) = 2^{-l(x)}/z$$

where

$$z = \sum_{x \in \Omega} 2^{-l(x)}$$

is a partition function

- We use these "implicit probabilities" to prove the inequality
  - Note that $l(x) = \log(1/q(x)) - \log z$

Partition function for block code

- Partition function for symbol code C is

$$z = \sum_{x \in \Omega} 2^{-l(x)}$$

- Partition function for block code C^N is

$$\begin{aligned} z^N &= \left[\sum_{x \in \Omega} 2^{-l(x)} \right]^N \\ &= \sum_{x_1 \in \Omega} \sum_{x_2 \in \Omega} \cdots \sum_{x_N \in \Omega} 2^{-(l(x_1)+l(x_2)+\ldots+l(x_N))} \end{aligned}$$

Rearranging the partition function

$$z^N = \sum_{x_1 \in \Omega} \sum_{x_2 \in \Omega} \cdots \sum_{x_N \in \Omega} 2^{-(l(x_1)+l(x_2)+\ldots+l(x_N))}$$

- The quantity $l(x_1) + l(x_2) + \ldots + l(x_N)$ is the length of the C^+-encoding of the string $\mathbf{x} = x_1 x_2 \cdots x_N$.
- For every string $\mathbf{x} \in \Omega^N$, there is one term in the above sum for z^N.
- Let
  - A_l be the number of strings $\mathbf{x}$ having encoded length l
  - $l_{\text{min}} = \min_x l(x)$
  - $l_{\text{max}} = \max_x l(x)$

$$z^N = \sum_{l=Nl_{\text{min}}}^{Nl_{\text{max}}} 2^{-l} A_l$$

The Kraft-McMillan inequality

- A_l is number of strings with encoded length l:

$$z^N = \sum_{l=Nl_{\min}}^{Nl_{\max}} 2^{-l} A_l$$

- If C is uniquely decodable, then $A_l \leq 2^l$. Therefore

$$z^N = \sum_{l=Nl_{\min}}^{Nl_{\max}} 2^{-l} A_l \leq \sum_{l=Nl_{\min}}^{Nl_{\max}} 1 \leq Nl_{\max}$$

- Since this holds for arbitrarily large N, it must be that

$$z \leq 1$$

- This is the Kraft-McMillan inequality, now for the source coding theorem

Proof of (converse) Source Coding Theorem

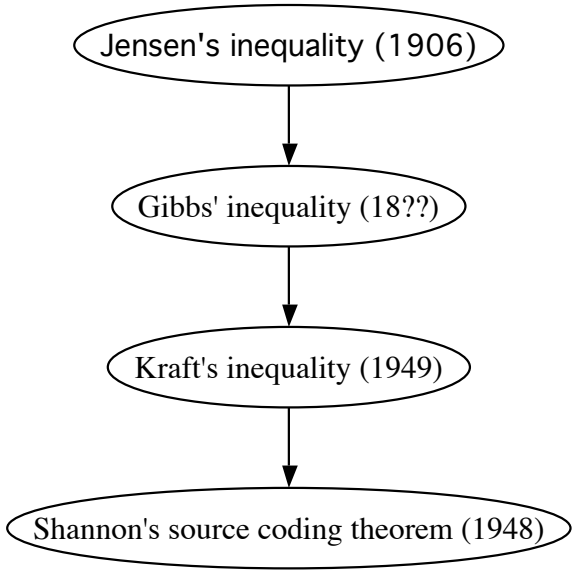
- Recall that

$$\begin{aligned} L_p(C) &= \langle l(x) \rangle_p && \text{(definition of } L_p\text{)} \\ l(x) &= \log(1/q(x)) - \log z && \text{(definition of } q\text{)} \\ \langle \log 1/q(x) \rangle_p &\geq \langle \log 1/p(x) \rangle_p && \text{(Gibbs)} \\ z &\leq 1 && \text{(Kraft-McMillan)} \end{aligned}$$

- It follows that

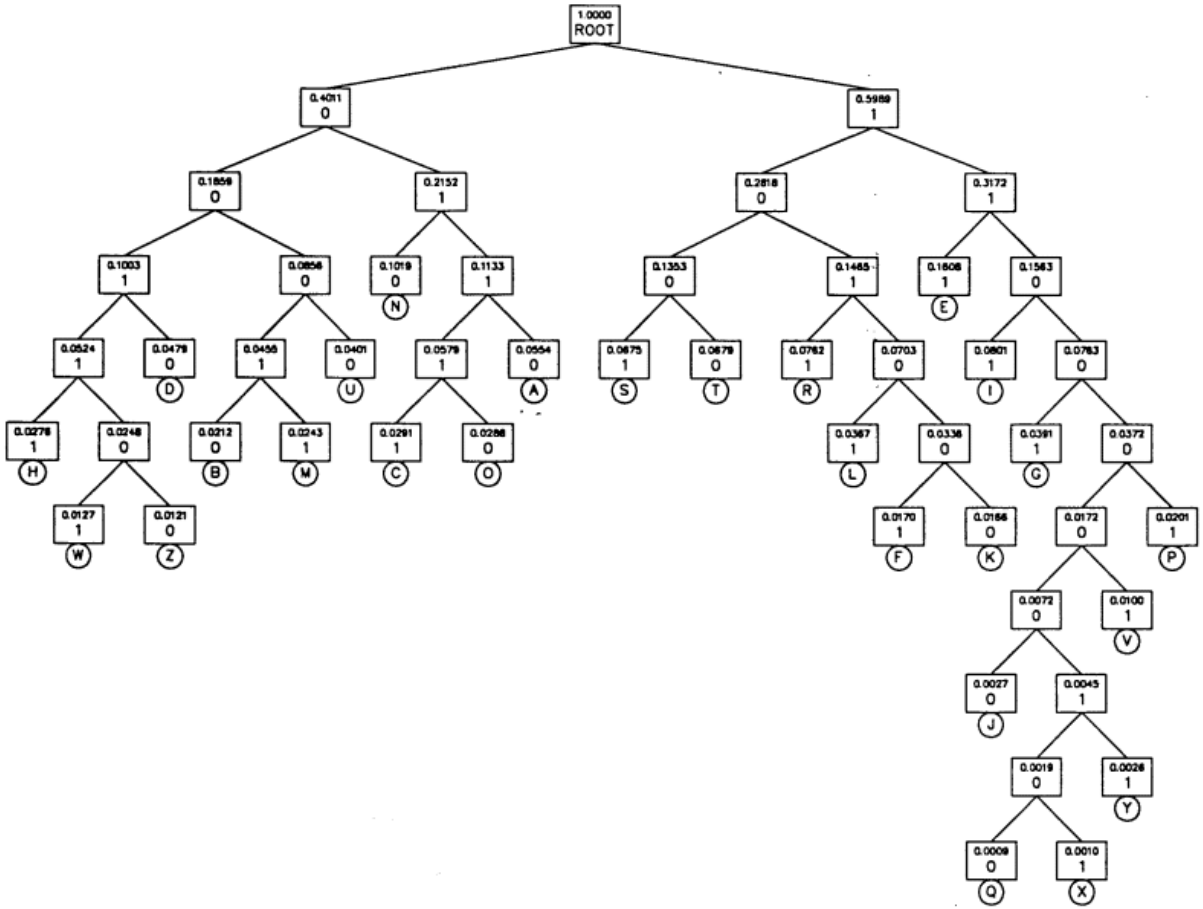
$$\begin{aligned} L_p(C) &= \langle \log 1/q(x) \rangle_p - \log z \\ &\geq \langle \log 1/p(x) \rangle_p - \log z \\ &\geq H_p \end{aligned}$$

Theorems (with dates)

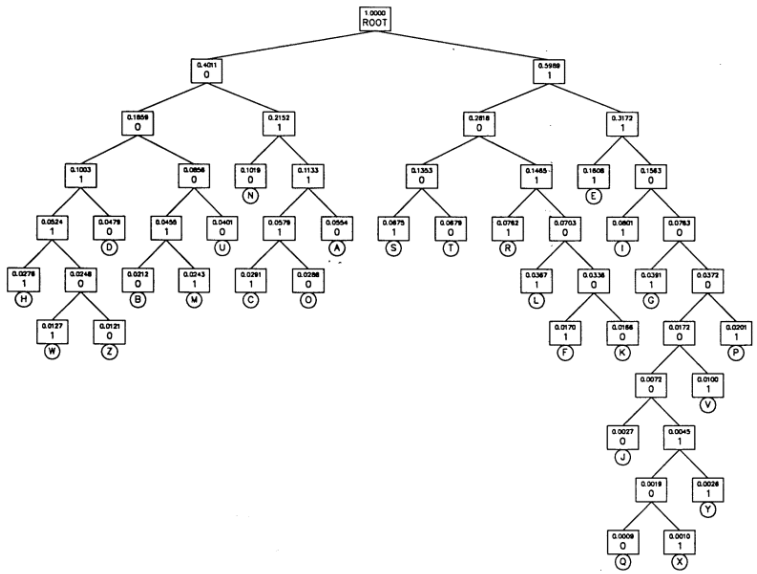


- Gibbs worked extensively on statistical mechanics.
  Where/when was Gibbs' inequality published?
- McMillan independently rediscovered Kraft's result in 1956.
- Kraft & McMillan cited (respectively) Redheffer & Doob.
- Shannon's formulation of his theorem was slightly different (asymptotic error rate of general block code).

Huffman coding



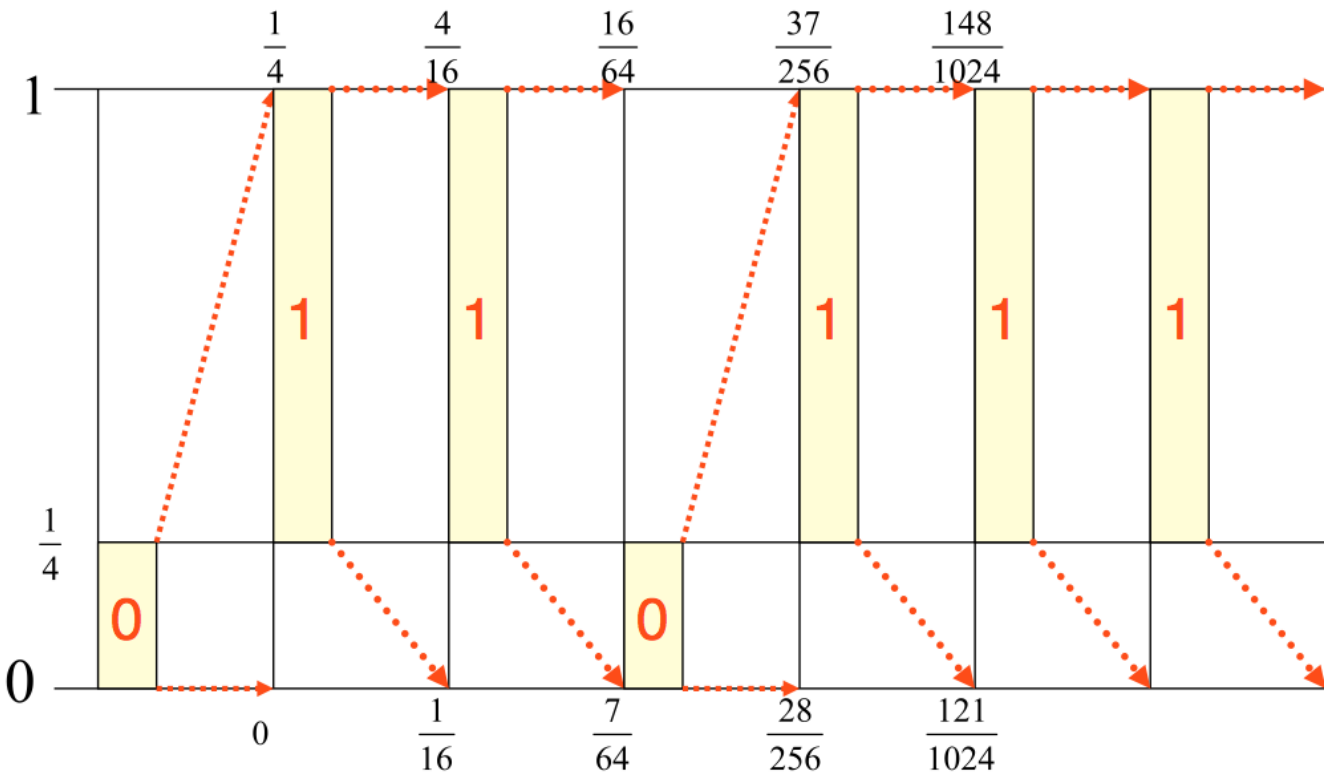
Huffman coding algorithm



- **Huffman tree** generates optimal prefix codes with $L_p(C) < H_p + 1$ (but NB overhead of 1 bit/symbol).
  - Bottom-up tree construction algorithm: combine the two least frequent symbols into a single symbol, and repeat.

Arithmetic coding

$$f_X(0) = \frac{1}{4} \qquad f_X(1) = \frac{3}{4}$$



Arithmetic coding

- **Arithmetic coding** is a block (not symbol) compression scheme that achieves asymptotically perfect efficiency.
- The message **x** is represented as a subinterval of $[0, 1)$
  - Subinterval found by recursive subdivision
  - Width of subinterval $\simeq$ probability of message $P(\mathbf{x})$
- Represent message as shortest binary fraction in subinterval
  - Guaranteed to be expressible in $\sim -\log_2 P(\mathbf{x})$ bits

Arithmetic coding: the adaptive model

- Represent the alphabet numerically: $\Omega = \{1, 2 \ldots N\}$
- Suppose we have encoded $k-1$ characters of message **x**
- Let $k-1$'th interval be $[a, a+b)$
- Next (k'th) interval is $[a', a'+b')$ where

$$\begin{aligned} a' &= a + b \sum_{\omega=1}^{x_k - 1} p_k(\omega) \\ b' &= b p_k(x_k) \\ p_k(\omega) &= P(x_k = \omega | x_1 \ldots x_{k-1}) \end{aligned}$$

- Note that p_k is adaptive — it has a "memory" of the last $k-1$ encoded/decoded characters

Arithmetic coding: issues

- Underflow #1: finite precision
  - Range delimiters $[a, b)$ may reach hardware precision limit
  - Solution: while a and b have same top digit: output, shift, add padding digits
    - e.g. $[.436, .437) \rightarrow [.600, .799)$ and output "43"
    - NB we pad a with 0's and b with 9's, to maximize range
- Underflow #2: delimiters straddle boundary
  - Decimal equivalent: ranges like [0.49999995,0.50000005)
  - Top digits don't converge before underflow occurs
  - Solution: extract next most significant digits, output them later (when top digits converge)
- Floating-point math: don't trust reproducibility of FPU
  - No room for vagaries of floating-point math
  - Solution: truncate all probabilities to some finite fraction
  - Use integers throughout code (e.g. discretized log-probs)

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Other symbol and number codes

- Encoding symbols from finite alphabets
  - Binary encoding: use $k = \log_2 n$ bits to encode n symbols
  - Truncated binary encoding: let $b = n - 2^k$.
    - First $2^k - b$ symbols use first $2^k - b$ codewords of length k
    - Remaining $2b$ symbols use **last** codewords of length $k + 1$
- Encoding arbitrary integers, n
  - Unary encoding: transmit number n as n 1's, followed by a 0
  - Golomb encoding: choose parameter m
    - transmit n/m using unary encoding
    - transmit $n\%m$ using truncated binary encoding

Each of these is optimal for some probability distribution:
can you see which?

Codes based on repetition

- Each of these has a shorthand for some repetition
  - Run-length encoding: repeated characters
  - Dictionary (Lempel-Ziv) encoding: repeated words
    - LZ77: sliding window
    - LZ78: adaptive dictionary
- Which probability distribution is each optimal for?
  - Imagine a process that generates such patterns....

Probabilistic models used with arithmetic coding

- "Adaptive arithmetic coding": updated frequency tables
- Order-N Markov chain
- PPM: Prediction by Partial Matching
  - Attempts to predict using the previous n characters
  - If previous n not seen before, drops to $n-1$, then $n-2$, etc.
  - If no context seen, uses a flat (or, in PPMd, adaptive) prior
- PAQ: uses a mixture of several prediction models
  - PPM-like n-gram contexts
    - Various sparse and bit-twiddled subsets of such contexts
  - Periodic contexts (period is heuristically estimated)
  - Customized models for specific file formats
    - .BMP, .TIFF. .JPEG, .EXE, etc.

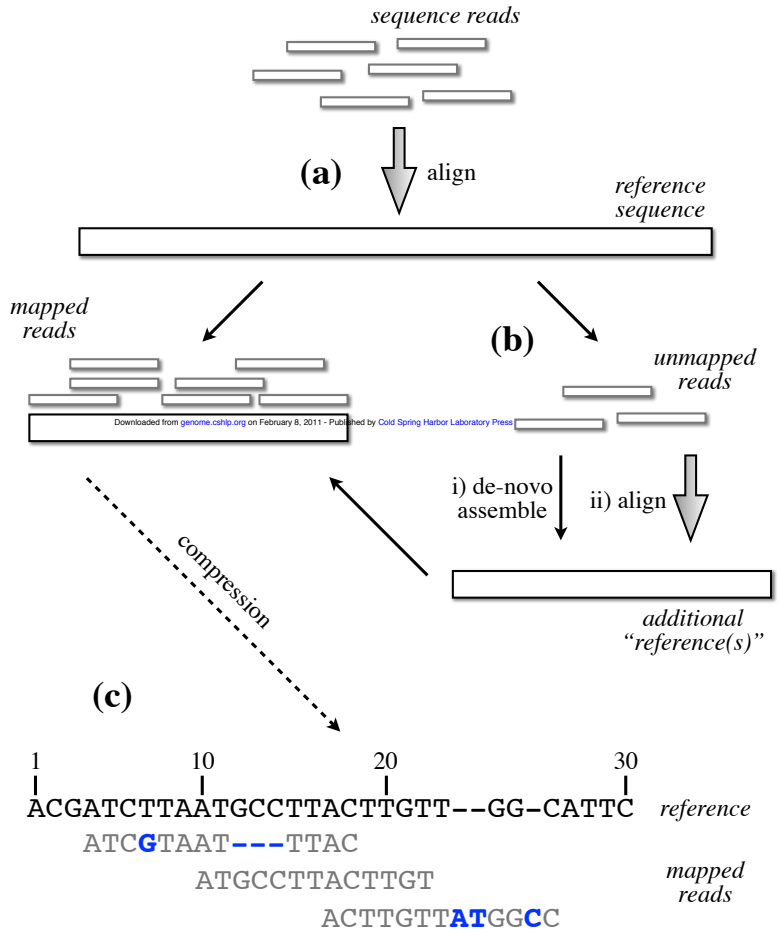
Transformations of the input string

- Idea: invertible operation, makes input easier to compress
  - e.g. aggregates disperse repetitions
- Burrows-Wheeler transform, aka block-sorting
  - Sort all rotations of text, then take last column
    - Invertible permutation of input string
  - Also has some excellent properties as a substring index
    - FM Index — **Opportunistic Data Structures with Applications** Ferragina and Manzini (2000)
- Turns repeated motifs $\leftrightarrow$ repeated characters
  - Can then compress e.g. with run-length encoding or order-N Markov

Motivation: whole genome re-sequencing

- Example: cancer re-sequencing (**International network of cancer genome projects**, ICGC, Nature 2010)
  - At least 10 cancer resequencing projects by 2010 (many more coming)
  - 300-500 samples per tumour
  - Sequencing coverage at least 30X
  - That's about 5×10^{13} bases, per project
  - FASTQ uses 8 bits for the base + 8 bits for the quality score
  - So, 10^{14} bytes $\simeq$ 60 terabytes per project. OUCH
- Could throw the data away after analysis.... unsatisfactory
- Most of the reads are substrings of the reference genome

Compression of reads to reference genome



Birney *et al*. 2011.

Compression of reads to reference genome

- Central idea:
  - Align reads to reference genome.
    - For unaligned reads, do *de novo* assembly, then align to that
  - Store read lengths using Huffman coding.
  - Store distances between reads/differences using Golomb coding (m = expected distance between reads/differences)
  - Read-pairs: use Golomb for separation, plus 3 extra bits to indicate strands & relative orientation of paired reads.
  - Lossy compression of quality scores.
- References:
  - Birney *et al*. **Efficient storage of high throughput sequencing data using reference-based compression.** Genome Research, 2011.
  - Baldi *et al*. **Data structures and compression algorithms for high-throughput sequencing technologies.** BMC Bioinformatics, 2010.

Underlying structure of Baldi/Birney methods

- Augment data before compressing it.
  - Augmented data is easier to compress
    - e.g. as a delta from a known reference genome
  - Augmentation step involves (CPU-intensive) processing
  - In this case augmentation = alignment (+ assembly)
  - Could also imagine phylogenetic placement as augmentation step
- Note that augmentation is theoretically unnecessary—we could marginalize the augmentation and shave off some bits—but this may be impractical, or even impossible due to complexity

Some other compression methods for genomes

- NB these do not involve augmentation *or* short reads. Just "straightforward" compression of genomes
  - Matsumoto *et al*, 2000. **Biological sequence compression algorithms.** Finds repeats, palindromes; c.f. LZ77, LZ78
  - Chen *et al*, 2002. **DNACompress: fast and effective DNA sequence compression.** Finds repeats
  - Christley *et al*, 2009. **Human genomes as email attachments.** James Watson's genome in 4MB

The Right Way To Do It

- Proposal: bio-oriented compression library
  - Arithmetic coding/decoding
  - Handlers for standard file formats
  - Preprocessing: assembly, alignment, annotation, phylogeny
  - Models: phylogenetic factor graphs, HMMs, SCFGs
  - Modular reference dictionaries that are themselves compressed

Summary

- Compressed bits/symbol $\geq$ Shannon entropy/symbol
  - Arithmetic coding approaches limit, given adaptive model:

$$P(\text{next symbol}|\text{previous symbols})$$

  - Other codes (e.g. Golomb, Huffman, Lempel-Ziv) are easier to implement & often run faster
  - All codes have an implicit probability distribution for which they are ideal
- Transformation and preprocessing often useful
  - e.g. aligning high-throughput sequence reads to reference genome