Exploring Zstandard user-provided dictionary compression for FASTA files

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Abstract

Background

Zstandard (Zstd) represents a universal, lossless data compression standard and implementation that is highly configurable and is aimed at coupling high compression ratios with fast compression/decompression performance. Previous studies have paired specific Zstd configurations with various file formats in bioinformatics to reduce total data volume. This paper presents a primitive "training mode" model, written in the Julia programming language, wherein a custom compression dictionary is generated from a sample FASTA set in order to explore further compression improvements and compare them to the compression performance of Xz, Zlib, Bzip2, and Lz4 universal compressors.

Results

Conclusions

Introduction

The explosion of biological data has represented a significant topic of research, with a number of challenges presented over subsequent generations of technological development in regards to the management of the increasing volume and complexity of data[1, 2]. In response, emerging trends in data management have lead to the development of novel, scalable methods for the efficient transmission and storage of large amounts of data[3]. With a potentially exponential quantity of files, datasets, and other data resources to be handled, data compression represents a method for reducing overall resource size by encoding the original data into a compact form, thus helping to ease storage requirements [4]. Research into data compression in the context of biological data began to pick up near the turn of the 21st century as universal compression algorithms at the time were not considered ideal for compressing DNA or RNA sequence data well, which led to the introduction of purpose-built algorithms that addressed the unique peculiarities of genomic data[5]. At the same time, new file formats were introduced, either text-based or binary-based, for more accurate structuring and representation of biological data, complementing new software tools[6, 7].

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The FASTA file format is a legacy of the original FASTA program for finding sequence similarities with a query sequence[6]. Each file can possess multiple sequences, each paired with a description line distinguished by a ">" symbol followed by arbitrary text, usually a name and/or summary description, on the same line. It is a commonly supported file format in bioinformatics and has been the target for optimized data compressors with competing claims for performance. The DELIMINATE lossless algorithm was first proposed in 2012, wherein header and sequence data are separated into DELIM-1 and DELIM-2 variants and a two-phase process is pursued involving delta encoding, progressive elimination of nucleotide characters, and 7-Zip archiving[8]. The claims of better compression/decompression performance of FASTA files were soon rivaled by the introduction of the MFCompress tool, again separating headers and sequence data but instead relying on probabilistic models to encode the data[9], which was then countered by the Nucleotide Archival Format, a novel file format noteworthy in this context for the inclusion of a Zstandard compression step[10].

IETF RFC 8878, introduced by engineers at Facebook, defines Zstandard as a lossless data compression/decompression format[11]. It is often abbreviated as "Zstd", though such can also refer to Facebook's own implementation of the algorithm written mostly in C[12]. Content is sliced and packaged into "frames" that are independent of one another defined as either compressed data Zstandard frames or Skippable frames containing custom user metadata[11]. Zstd's backbone is the use of Finite State Entropy and Huffman entropy encoding schemes that replace data with coded forms independently of the medium[13, 14], with the former compressing all symbols, though header information is first encoded by the latter[11]. Zstd, for small data compression improvements, also functions as a dictionary coder, meaning that although the algorithm is universal in the sense of being applicable to a number of both text-based and binary-based data files, it can be optimized for compacting characteristic data by "training" Zstd with a collection of sample files to build a set of common patterns that allow for substitutions when compressing/decompressing, allowing for further gains for similar data[15].

Common bioinformatics file formats often include a set structure with the express purpose of representing specific kinds of biological data composed of repeating elements, as is the case with FASTA files with either nucleotide or amino acid sequences. In this work is described a pipeline for building Zstd dictionaries via FASTA datasets along with a comparison of Zstd compression/decompression performance with that of several alternative lossless compressors for select datasets.

Materials and methods

All resources for the paper are included in the public Github repository at github.com/M-PERSIC/Persico2022.git.

The model contains two pipelines, one for Zstd custom dictionary generation and another for generating transcoded compression data using Bzip2, Xz, zLib, and Zstd compressors, with a general overview in Fig 1. Julia was chosen as there is package support for working with sequence data as well as for trivial transcoding of compressed or decompressed data via TranscodingStreams.jl wherein compression algorithm implementations are loaded as codecs[16]. A list of all direct dependencies can be found in the repository's Project.toml file. The Julia implementation operates by first unloading a tarball containing the set of FASTA training files into a Julia artifact, or life-cycled datastore. The files are plugged into Zstd's training mode, via the Zstd command line interface –train option, to generate a custom dictionary specific to that

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dataset. Subsequent dictionary manipulation in Julia is based on an experimental CodecZstd.jl branch that includes functions that wrap the Zstd Dictionary API[17]. Random FASTA data is generated using BioSequences.jl[18] and FASTX.jl[19] APIs which is then transcoded into compressed formats via the CodecBzip2.jl[20], CodecXz.jl[21], CodecZlib.jl[22], and CodecZstd.jl[23] codecs for comparative analysis. Both dictionary-based and default Zstd compression are applied to determine if the former desmontrates a significant reduction in data size.

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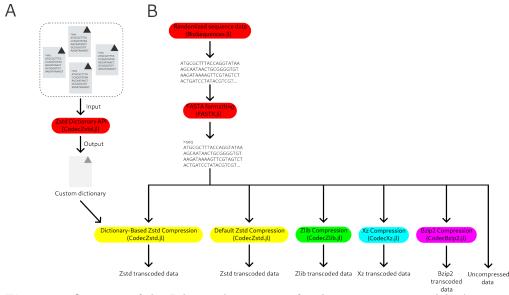


Figure 1. Overview of the Julia implementation for the compression model. **A**, Custom dictionary generation via an Julia artifact of FASTA files plugged into the Zstd Dictionary API. **B**, Transcoding randomly generated FASTA formatted data using TranscodingStreams.jl[16] compression codecs.

Results

Discussion

The provided FASTA training dataset was retrieved from a set of *E.coli* MS 200-1 strain genomic scaffolds from a whole genome shotgun run[24]. Sampling a single organism may allow for additional compression/decompression improvements as the sequence data could possess repeating patterns unique to that individual's or species' genome that are recognized and added to the Zstd dictionary during training. The FASTA files themselves may bear similarity with one another in the same set, such as each file being of similar length. Simultaneously, the Zstd dictionary may not achieve comparable compression/decompression performance when attempted on more dissimilar sequence data. Portability of Zstd dictionaries, in the sense of being universally applicable across all sequence data, could be weighed against generating dedicated dictionaries for specific datasets depending on the storage requirements. Zstd parameters were kept default, though they can be manually altered, including advanced compression options like compression job size or selecting from 22 predefined compression levels[12].

Zstd's multifarious design warrants further research in how tuning the implementation by altering available options (block size, compression level,...) that might influence compression performance. The development of novel data toolsets have

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utilized Zstd in unique ways. Aside from the Nucleotide Archival Format, FASTAFS was recently introduced as a filesystem in userspace (FUSE) toolkit wherein FASTA files are pooled into a virtualization abstraction layer that archives the set of data synced with its metadata, generating a high-level interface for accessing and storing FASTA data[25]. The zstd-seekable compression library is an embedded component that keeps the FASTAFS archive compressed for storage reduction purposes, and it represents an alternative compressed data format that deviates from Zstandard, albeit in a compatible manner, that allows for partial decompression of subranges of data[12]. This is achieved via independently compressed/decompressed Zstd frames, which FASTAFS exploits for fast random access to FASTA files by decompressing only data of interest. Further areas of research for general lossless data compression in the context of biological data could include exploring other properties like compression/decompression speed performance, meaning how fast data transcoding occurs, or piloting proof-of-concept algorithms that attempt novel strategies.

Supporting information

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