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Contents

Introduction

Imagine, for a moment, that you are transported in time to 10th-century Europe. It is Sunday, and the weekly mass is just starting. Look around yourself. The tall ceilings of the impressive church were built so to bring you closer to God. The stained glass windows let through just enough light so that it is not completely dark. Can you smell the incense? Everything in the environment around you reminds you that you are taking part in a sacred ritual. Listen to the priest; when he recites the prayers, his speech does not flow in a natural way. Instead, the entire text is intoned on a single note, except for the slightly inflected ends of clauses. Sometimes, the choir replaces the priest, singing more elaborate monophonic melodies. The words they are singing are Latin, but even if you do not understand them, you know what their purpose is: to celebrate the deity. Their voices echo in the stone church, creating an otherwordly experience.

What you are hearing is called Gregorian chant. It is one of the earliest forms of music preserved in written form, and the largest preserved body of medieval music. The earliest preserved fragments of written notes date back to the 9th century, although texts from as early as the eighth century have been found.. Its name, Gregorian, references Pope Gregory the Great, however, his relation to the chant is not entirely clear.

Gregorian chant is not the only type of chant. In the early centuries after Christianity spread across Western and Eastern Roman Empire, new forms of worship started being developed. The most obvious differences were between the West and the East, which had multiple cultural centers such as Constantinople, Jerusalem, or Alexandria. However, liturgies varied in the West as well, from Rome to Milan to the Iberian peninsula to Gaul. Each center developed their own tradition, including their own type of chant.

(TODO: why is the Roman tradition everywhere now?)

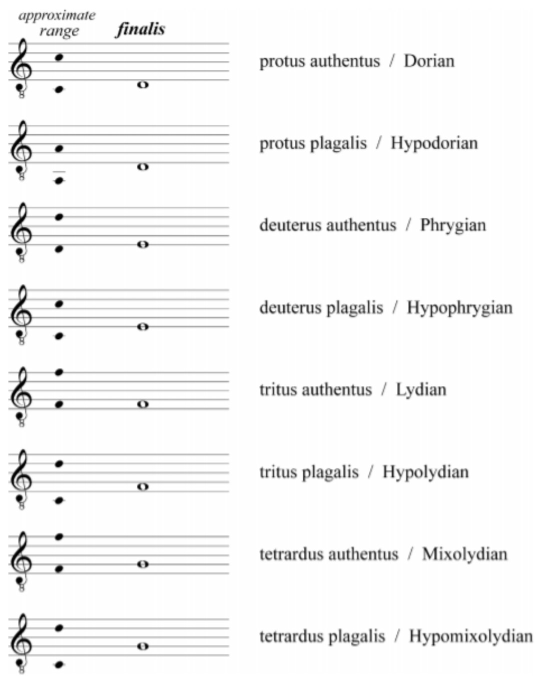
Gregorian chant is an integral part of the Roman church, and has been so for centuries. It is the monophonic music (i.e. single-voice) sung during liturgies. Here, liturgy means chant sung during Christian worship. Unlike in the Eastern churches, where the term is reserved for the Eucharist, liturgy includes both the Mass and the Divine Office in the Roman church.

Mass is the service most familiar to most believers. It can be divided into several parts, all leading up to the most important one, the act of communion. This act commemorates the Last Supper, Jesus's last meal with his disciples before his execution. During the communion, bread, representing Christ's body, and wine, representing his blood, are given out. During the course of the Mass, multiple different chants are sung. *Introitus*, meaning 'entrance', is sung at the beginning of the service while the priest and his assistants are walking to the altar. *Tractus* is a chant that is sung during Lent, i.e. the period between Ash Wednesday and the Saturday before Easter. Outside of this period, *alleluia* replaces *tractus* and is followed by *sequentia* on the most important feast days.

The other part of the liturgy, besides the Mass, is the Divine Office, also called Liturgy of the Hours or canonical hours. It is the set of chants sung during services at different times of the day, for example *Vespers* in the evening or *Lauds* in the morning. The office consists largely of singing psalms, of which there are 150, all sung on different days and hours. Psalms were usually preceded and followed by antiphons, which differ not only by the day of the week, but also depending on the place. Each day of the week had an allocated set of antiphons, hymns and responsories, while responsories were assigned to the different Sundays. Additionally, important feasts had their own set of chants to be sung.

The liturgical year contains several feasts. Some feasts are fixed on a specific date. Feasts associated with a specific saint are an example of those. For example, John the Baptist is celebrated on the 24th of June, Michael on the 29th of September, and All Saints on the 1st of November. Other fixed-date feasts include Christmas Day (25 December), Epiphany (6 January), and others. Such feasts can fall on any day of the week, and if they fall on a Sunday, they will take precedence over it. On the other hand, there are also feasts that are fixed to a specific day of the week, the most important of them being Easter Sunday, the day when Christ rose from the dead. Each feast has a different set of chants that can be completely original.

The individual chants differ in several criteria, the first one being the mode. Mode is the system of pitch organization, somewhat similar to modern-day scales. Melodies are classified into one of eight modes according to their last note, called *finalis*, and their range. Most chants end on one of the notes *D*, *E*, *F*, or *G*. These four notes determine four pairs of modes. The melodies were further classified depending on whether they moved mostly in the range above the *finalis*, in which case it would be classified as the *authentic* mode of the pair, or in the range around the *finalis*, which means it is classified as the *plagal* mode. Some types of chant tend to occur mostly in a specific mode.



approximate range
finalis
protus authentus / Dorian
protus plagalis / Hypodorian
deuterus authentus / Phrygian
deuterus plagalis / Hypophrygian
tritus authentus / Lydian
tritus plagalis / Hypolydian
tetrardus authentus / Mixolydian
tetrardus plagalis / Hypomixolydian

Figure 1: List of modes, their ranges and finalis. [Hiley, 2009, p. 44]

Another criterion is the complexity of chants, that is, how elaborate the melody is. On the one side of the spectrum, there is a one-to-one syllable to note correspondence. Antiphons and some hymns are genres close to this text-setting. The other extreme is melismatic style. Melisma is a long vocalization of a single syllable, therefore melismatic melodies are more ornate. Some of the more melismatic genres are the gradual, tract and offertory.

We have already mentioned several different genres of chant. Antiphons are chants sung to frame a psalm during the Office hours. They are relatively short and simple, somtimes consisting of only two phrases. Responsories are sung during the Night Office. Each has a main section and a verse. They are melodically very rich and are on of the most impressive forms of chant. The number of chants sung during the Mass is lower, as there will usually only be one introit, one gradual, etc. during a service.

It is important to note that text and melody do not form unique pairs. Instead, each text can be sung to multiple different melodies and multiple texts can be sung to one melody.

It is clear that the annual cycle is very complex and the amount of chants is abundant. Therefore, it is not surprising that while the chants during the services themselves were sung from memory, they were written down in books. Each church and each convent had their own manuscripts, which is the reason of their abundance.

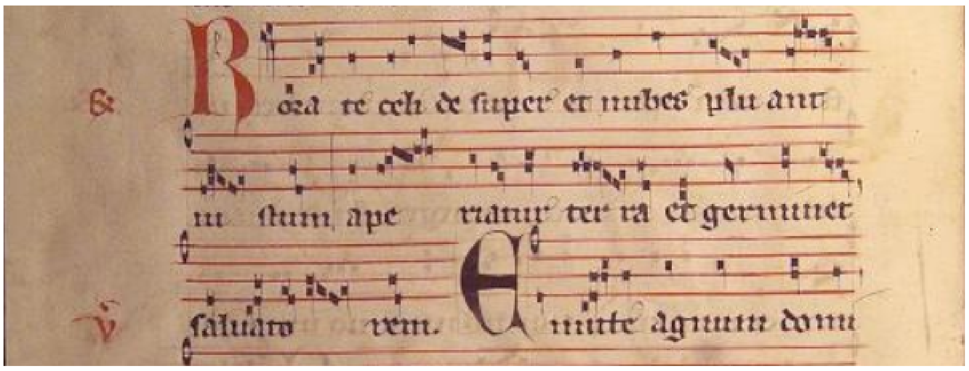


Figure 2: Example of a chant in a manuscript. [Lacoste et al., id 007553]

1. Related work

With the advent of computers, the field of Music Information Retrieval (MIR) emerged. Research in this interdisciplinary field focuses on extracting information from musical notation using computer science methods, such as signal processing or machine learning. Its applications vary widely, from recommender systems, to automatic audio transcription, to music generation. MIR encompasses all different kinds of music, regardless of their location, age, or function. Researchers have developed a multitude of software tools that facilitate music analysis, irrespective of what type of music it is. One of such toolkits is *music21* [Cuthbert and Ariza, 2010], a Python package able to encode musical notation as Python objects and perform analysis on large datasets.

The study of plainchant using computational methods has not been done extensively. The main research tool for musicologists in this field is the Cantus Index [Lacoste and Koláček]. It is an online index of chants from several different chant databases, providing researchers with a common API for all of them. The entries in Cantus Index only contain four data fields: full-text, genre, feast (not required), and Cantus ID, which is automatically assigned to newly added chants. The tool is also able to search for melodies in the original source and even provides search-by-melody functionality. There are ten databases indexed in the catalogue, the largest of which is the Cantus database [Lacoste et al.].

Cornelissen et al. [2020a] developed *chant21*, a Python package able to convert two standard melodic notations, *volpiano* and *gabc* to a *music21* object, therefore making it easier to study Gregorian chant computationally. The data they used were scraped from Cantus database [Lacoste et al.] and GregoBase [Berten and contributors] and released as CantusCorpus and GregoBaseCorpus, respectively. Finally, they performed two case studies using the package. In the first one, they confirmed the melodic arch hypothesis [Huron, 1996], which had previously only been studied manually. Second, they analyzed the relation between differentiæ and antiphon openings [Shaw, 2018] and found that it differs accross modes.

Some of the computational research into plainchant has been centered on mode classification. Huron and Veltman [2006] used pitch class profiles to classify modes. They created a pitch-class distribution for each of the eight modes, and used these classes to classify previously unseen data. Cornelissen et al. [2020b] compared three approaches to mode classification: classical approach, which classifies chants based on the final pitch, range, and the initial pitch; profile approach, which was largely inspired by Huron and Veltman [2006]; and distributional approach, which focuses on the melodic aspect of mode. The authors chose various segmentations and representations of chants and used a tf-idf vector model to classify mode. The study found that we can accurately classify mode even when we discard all absolute pitch information, the melody contour contains enough information on its own.

A considerable amount of research has been done into the evaluation of melodic similarity, albeit not for Gregorian chant specifically. Wickland [2017] provides an overview of the methods. He mentions edit distance, Markov chains, and geometric measurements as the most widely used ones. Park et al. [2019] used an adapted edit distance metric to calculate the similarity of two melodic sequences by first calculating the similarity for all segments of each of the sequences and then scaling them by a weight function depending on the segment length, which yielded them what they call a multi-scale similarity stack. The overall similarity was obtained by averaging its values. Then they used the MSS stack to create a visualization that takes on the shape of a trapezoid that shows which segments of two sequences are the most similar.

Bountouridis et al. [2017] argue that methods originally developed for bioinformatics have a great potential to be applied to music. They offer analogies for bioinformatics concepts found in musicology. For example, they liken DNA and proteins to melodic sequences, homologues (proteins that have the same ancestor) to song covers, evolution to oral transmission, etc. They claim that despite the similarities, MRI has not leveraged the full potential of bioinformatics methods. In their article, they focus on modelling melodic similarity using multiple-sequence alignment (MSA) algorithms, therefore not relying on heuristics, as opposed to previous works. Their results revealed that the MAFFT algorithm yields the best alignemnt, which can be attributed to the algorithm using gap-free segments as anchor points, therefore partitioning melodies into more meaningful segments than other algorithms.

The general algorithm for calculating pairwise sequence alignment is the Needleman-Wunsch algorithm [Needleman and Wunsch, 1970]. It uses dynamic programming to break down the problem into smaller problems. Given two sequences, it starts aligning them from the beginning. At each point, the algorithm checks whether the two sequences match in the current position, and if not, whether it will leave the elements mismatched or insert a space. In essence, all possible alignments are computed and scored and the best one is chosen. The algorithm always yields an optimal alignment, therefore it is used when the quality of the alignment is important. However, because of its time complexity, it is unsuitable for many applications.

Unlike pairwise sequence alignment, multiple sequence alignment has been shown to be NP-complete [Wang and Jiang, 2009]. As such, there is no practical way of computing an optimal MSA and we must instead rely on heuristics to obtain a sufficiently good alignment.

Notredame [2007] provides an overview of modern multiple sequence alignment algorithms. According to him, the most frequently used algorithms use the progressive approach, where a guide tree is estimated from unaligned sequences and then pairwise alignment algorithms are used to find the MSA following the tree. He notes that the scoring methods of the pairwise algorithm are essential. There are two main groups of scoring methods: matrix-based algorithms, where a substitution matrix is used to determine the cost of replacing one symbol with another, and the consistency-based methods, which use a collection of global and local alignments to calculate a position-specific substitution matrix. The author claims that the best methods yield indistinguishable results, except for remote homologs with less than 25% identity.

T-Coffee [Notredame et al., 2000] uses the progressive approach described above. It was the first algorithm that used a preprocessed collection of alignments to create a library that helps create the guide tree. The library is generated using both global and local pairwise alignments. Thanks to this approach, T-Coffee minimizes the errors made in the first stages of building the MSA, which is a shortcoming of many previous algorithms, as these errors tend to persist. They combined precomputed local and global alignments and create a function that assigns a weight to each pairwise alignment depending on how consistent the pair of residues is with the residue pairs from all other alignments. This process leads to a significant improvement of the results.

MAFFT [Katoh et al., 2002] further improves on other methods by using Fast Fourier transform to identify homologues fast. In addition, the authors propose a simplified scoring system that reduces CPU time while maintaining its accuracy. The authors' results showed a performance 100 times better than that of T-Coffee.

2. Data

Our main source of data is the Cantus database [Lacoste et al.], one of the databases indexed in the Cantus Index. The database serves as a digital archive of chants, each entry containing information about its source, liturgical occasion, mode, and others. Work on the project started in the late 1980s, and to date, around 500,000 individual chants from approximately 150 manuscripts have been indexed. Each entry is transcribed manually and undergoes a thorough examination before publishing [Lacoste, 2012].

We are using a scraped version of the Cantus database released as CantusCorpus [Cornelissen et al., 2020a]. Unlike the Cantus database which is continuously being updated and is therefore unsuitable for computational study, the corpus is versioned, therefore each version always contains the same data. We are using version 0.2 released in July 2020 which contains 497,071 entries. However, a majority of the data is not suitable for this application, as they do not contain both melodic and textual data in full, therefore we are only using a subset of size around 13,000. The corpus is available for download in CSV format.

2.1 CSV

CSV is one of the most common formats for tabular data. The abbreviation stands for *comma-separated values*. As the name suggests, the format uses commas to separate columns (although other separators, such as a semicolon, can be used as well to allow for simpler parsing in case that the data frequently contains commas that would otherwise need to be escaped), while the individual rows are separated by a line break. The data is stored as plaintext, which makes it easily readable. Parsing CSV files becomes more complicated when the data contains column and row separators inside fields; in that case quotation marks or esape sign has to be used. There exist many well-designed parsers, one such parser is the Python module simply called *csv*. This application uses the module *pandas* to parse CSV files, which in turn uses the *csv* module.

2.2 Database fields

The following table represents the data fields in the database.

Data field	Description
id	automatically generated id in the database
corpus_id	human-readable id identifying the chant in the CantusCorpus
incipit	incipit (the first few words) of chant
cantus_id	id identifying the chant in the Cantus Index
mode	mode of the chant
finalis	the final note of the chant
differentia	the melodic ending of psalms
siglum	manuscript in which the chant is found
position	liturgical role of the chant

folio	page of the manuscript where the chant is found
sequence	order in which the chant is found in the folio
marginalia	clarification about the location of the chant
cao_concordances	references to older literature
feast_id	feast of the year during which the chant was sung
genre_id	genre of the chant, e.g. *antiphon*, *responsory*
office_id	office of the day during which the chant was sung, e.g. *Laudes*, *Vespers*
source_id	id of the manuscript in which the chant is found
melody_id	id of melody by which it can be found in the Cantus Index
drupal_path	URL of the chant on the Cantus database website
full_text	full text in a standardized spelling
full_text_manuscript	full text in the manuscript spelling
volpiano	transcription of the melody in volpiano format
notes	indexing notes

Table 2.1: List of database fields

2.3 User-defined data

The application enables user to upload their own dataset. The following table specifies the fields in the database. Validation of the file is not implemented; it is left up to the user to upload a valid file. The meaning of the individual fields is as described in the previous section unless said otherwise.

Column name	Type	Can be empty	Notes
none or Unnamed: 1	any	yes	the column will be dropped
id	string	yes	equivalent to *corpus_id* in the database
incipit	string	no	
cantus_id	string	yes	should be a valid Cantus ID
mode	string	yes	list of modes is in attachment
finalis	string	yes	
differentia	string	yes	
siglum	string	no	
position	string	yes	
folio	string	yes	
sequence	string	yes	
marginalia	string	yes	
cao_concordances	string	yes	
feast_id	string	yes	list of feasts is in attachment
genre_id	string	yes	list of genres is in attachment
office_id	string	yes	list of offices is in attachment
source_id	string	yes	
melody_id	string	yes	

drupal_path	string	yes	should be a valid URL
full_text	string	no	
full_text_manuscript	string	yes	
volpiano	string	no	has to be in Volpiano format
notes	string	yes	

Table 2.2: Fields in the user-uploaded CSV

2.4 Volpiano

The melodies in the volpiano fields are encoded as strings of alphanumeric characters and dashes. These can be rendered as musical notation using the volpiano font. Each character represents either a pitch, empty space, or other musical characters, such as a clef.

Volpiano was developed as a research tool optimized for databases and word processors. There are strict rules concerning the transcription, which leads to all volpiano-encoded melodies having a standardized format. Each transcription begins with a treble clef. Gaps between words are encoded as three dashes, while two dashes represent gaps between syllables (Helsen and Lacoste [2011]).

2.5 Data cleaning

As mentioned earlier, not the entire dataset is usable. Since we are analysing melodies, it is necessary that each data point contains information about the chant's melody.

As one of the application's main features is melody alignment, it is necessary that we only use those data points whose *volpiano* field is not empty. Moreover, some visualizations compare text length to melody length, therefore we require the data points to have both. Additionally, text and melody should be able to be aligned, i.e. they contain the same number of words and syllables.

Removing the data that does not adhere to the conditions, we are left with 13,397 usable data points.

```
,id,incipit,cantus_id,mode,finalis,differentia,siglum,
    position,folio,sequence,marginalia,cao_concordances
    ,feast_id,genre_id,office_id,source_id,melody_id,
    drupal_path,full_text,full_text_manuscript,volpiano
    ,notes
621,chant_000622,A Christo de caelo vocatus
    ,001188,8,,1,F–Pn lat. 12044,3.,053v,5.0,,,
    feast_0287,genre_a,office_m,source_014,,http://
    cantus.uwaterloo.ca/chant/399542/,A Christo de
    caelo vocatus et in terram prostratus ex
    persecutore effectus est vas electionis,A xpisto de
     caelo vocatus et in terram prostratus ex
    persequutore effectus est vas electionis,1−−−g——g–
    kk—h——g——h—g——f—gh—g——g——g——hgf—g——gh—
    f—f7——g——f—h—j—kl—kj–klk——h—kj—hg——g——h
    ——gf—gh—h—g—g−−−4,
635,chant_000636,A Christo de caelo vocatus,007123a
    ,1,,,US–CHNbcbl 097,01,035r,2.0,,,feast_1321,
    genre_v,office_m,source_069,,http://cantus.
    uwaterloo.ca/chant/665425/,A Christo de caelo
    vocatus,,1−−h——h—hghgf——g——g—g——g—gh—g−−−,
645,chant_000646,A Christo de caelo vocatus,007123a
    ,1,,,D–KA Aug. LX,01,125r,2.0,,,feast_1321,genre_v,
    office_m,source_414,,http://cantus.uwaterloo.ca/
    chant/617583/,A Christo de caelo vocatus et in
    terram prostratus ex persecutore effectus est vas
    electionis,A xpisto de celo vocatus et in terram
    prostratus ex persecutore effectus est vas
    electionis | ~Vere,1−−−h–h——hg—hg–gf7——g——g—g
    ——g—gh—g——g——g——hG—gh——gh—hjh—h——hf——gh
    —h—h—hk—h——h—hk—h——h——h——hg–hg—hf—fghg
    —hkh–hgfe—fgh–gf7−−−3,
667,chant_000668,A Christo de caelo vocatus,007123a
    ,1,,,A–KN 1018,01,071v,3.0,,,feast_1321,genre_v,
    office_m,source_265,,http://cantus.uwaterloo.ca/
    chant/293103/,A Christo de caelo vocatus et in
    terram prostratus ex persecutore effectus est vas
    electionis,A christo de celo vocatus et in terram
    prostratus ex persecutore efectus est vas
    eleccionis,1−−−dh——h—hg–hgg——g——g—g——g—gh—g
    ——g——g——hF—gh7——gh—hijh—h——h——gH—h—h—hk
    —h——h—hk—h——h——hghgfed–efg——gh—fe7—ef—
    fghgh—gf−−−3,
923,chant_000924,A deo praelectus*,600006,8,,,NL–Uu
    406,,196r,8.0,,,feast_1814,genre_r,office_v2,
    source_573,,http://cantus.uwaterloo.ca/chant
    /497010/,A deo praelectus*,A deo preelectus,1−−−g
    ——g—ffg——gge−−−3,
```

Figure 2.1: Example of a valid CSV file

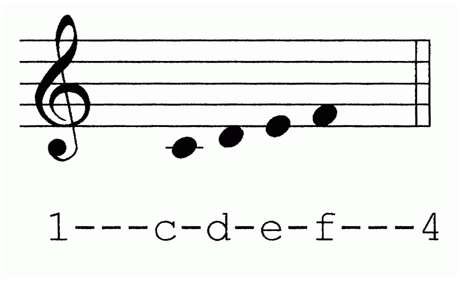


Figure 2.2: Example of volpiano as stored in the database and how it is rendered as musical notation. [Lacoste, 2012, Figure 2]

3. Multiple sequence alignment

Sequence alignment, in general, is a task whose purpose is to arrange two or more sequences with a common alphabet to identify similar and different regions within them. A set of sequences being *aligned* in this case can be understood as each being extended by spaces in such a way that if they are arranged in a matrix, each sequence occupying one row and each column containing one character, it can be seen what had to happen for one sequence to change into another on a character-by-character basis: insertion (or deletion), character substitution, or nothing if the characters in the given position are identical. A good sequence alignment algorithm is one that does not perform unnecessary insertions (deletions) or substitutions.

The problem of multiple sequence alignment is most studied in bioinformatics. Since DNA was first sequenced in the 1970s, there has been a need to compare various genomes to determine similarity. As organisms mutate and evolve, their DNA or RNA changes. Aligning their genomes reveals similar and different regions, which facilitates the tracking of these mutations and makes it possible to determine the order in which they happened.

However, the applications of sequence alignment are not limited to biology. Every task that makes use of determinig the similarity of some sequences, where the emphasis is put on finding regions where they do not diverge, can make use of the existing methods.

Melody alignment of Gregorian chant can be considered as such. As the tradition spread across Europe, each place changed some of the existing melodies by a little, thereby creating new melodies that can change further as they travel through time and space. This is akin to the mutations in DNA caused by environmental factors. Finding well-conserved regions in many instances of chant provides great insight into which parts of a melody are unlikely to change, and, on the other hand, which ones tend to vary a lot. It can also reveal the ancestors of a melody and the path which it traveled to transform into its final form. This is in line with the focus of philology shifting not to merely reconstructing an earliest layer of a text (with the unspoken assumption that this is the “real” text), but to map the entire tradition of text transmission and evolution, taking the later layers to be as valid within their cultural environment as the older layers.

In this chapter, we will first give the definition of the problem of sequence alignment. We will mention some important considerations, as well as theoretical limitations. Then we will provide an overview of the methods developed for bioinformatics that attempt to solve the problem. Finally, we will show how we applied the existing methods and technologies on Gregorian chant melodies.

3.1 The problem of sequence alignment

Assume that we have an alphabet $\mathcal{A}$ and a character σ such that $\sigma \notin \mathcal{A}$. Then let us have a set of sequences $S = \{s_1, s_2, ..., s_k\}$ with $s_i \in \mathcal{A}^{l_i}$. The output of a sequence alignment algorithm is the set of aligned sequences $A = \{a_1, a_2, ..., a_k\}$, where $a_k \in (\mathcal{A} \cup \{\sigma\})^L$, $L \geq l_i \, \forall i \in \{1, 2, ..., k\}$. Each original sequence s_i can be obtained from the aligned sequence a_i by removing all σ.

Given two aligned sequences a_i and a_j and an index $p \leq L$, we define the following operations:

- *Identity*: $(a_i)_k = (a_j)_k$
- *Insertion*: $(a_i)_k = \sigma \wedge (a_j)_k \in \mathcal{A}$
- *Deletion*: $(a_i)_k \in \mathcal{A} \wedge (a_j)_k = \sigma$
- *Substitution*: $(a_i)_k \in \mathcal{A} \wedge (a_j)_k \in \mathcal{A} \wedge (a_i)_k \neq (a_j)_k$

Each of the operations has an associated cost. The cost of substitution can further vary depending on which characters are being substituted. We can then define the overall cost of the alignment A in different ways, e.g. as the sum of costs over all triples (i, j, p) $\forall i, j \in \{1, 2, ..., k\}$ $\forall p \leq L$ or as the sum of costs for unordered pairs $\{i, j\}$ and indices p, in which case insertion and deletion are considered the same operation. The goal of a sequence alignment algorithm is to minimize the cost. There are other, more complicated ways of defining the cost function, and the performance of an algorithm is highly dependent on which one it uses.

3.1.1 Pairwise and multiple sequence alignment

Depending on the number of sequences to align, we distinguish between pairwise alignment for pairs of sequences and multiple sequence alignment for more than two. Despite the similarity in their outcomes, the two problems are fundamentally different from a computational perspective.

Pairwise alignment is relatively easy to solve. The Needleman-Wunsch algorithm, which is a dynamic programming algorithm, can find an optimal solution in the asymptotic time of $\mathcal{O}(mn)$, where m and n are the respective lengths of the sequences. This means that it is possible to find an optimal alignment even for longer sequences.

Needleman-Wunsch algorithm can be extended to more than two sequences. However, with each additional sequence, its complexity increases, and it quickly becomes impractical or even practically impossible to align multiple sequences this way. In fact, it has been proven that multiple sequence alignment is an NP-complete problem [Wang and Jiang, 2009]. It is therefore necessary to use various heuristics to generate alignments. Current algorithms do not aim at finding the optimal alignment; instead, they try to produce one that is good enough.

3.1.2 Local and global sequence alignment

There is a distinction to be made between local and global sequence alignment.

The problem description above is the definition of global alignment. Aligning sequences globally means aligning the entire sequences end-to-end. (This does not mean, however, that there cannot be gaps at the beginning or at the end of the generated alignment.) All characters from all sequences must be present in the final alignment. Global alignment is used to compare relatively similar sequences, such as protein homologues or versions of the same chant sung at different points in time.

On the other hand, the goal of local alignment is to find similar regions in divergent sequences, while the rest of the sequences is disregarded. The output of local alignment algorithms contains only a substring of both sequences. Local alignment is suitable for finding conserved patterns.

Both methods are useful in their own way. Local alignment provides a slightly different insight than global alignment, however, they can be combined to extract more information. In fact, the best current multiple sequence alignment algorithms use local alignment for pairs of sequences to generate a better overall global alignment. [Notredame, 2007]

3.2 Sequence alignment methods

The methods used to find sequence alignments depend on how many sequences there are and whether they should be aligned globally or locally. Dynamic programming can used for finding pairwise alignment, both local and global. For many sequences, other methods have been developed. They do not compute the optimal alignment, however, by using appropriate heuristics, their output is good enough.

3.2.1 Pairwise alignment: dynamic programming

Dynamic programming techniques are useful for pairwise alignment. The Needleman-Wunsch algorithm [Needleman and Wunsch, 1970] computes the global alignment of two sequences. A variation of the algorithm, the Smith-Waterman algorithm [Smith and Waterman, 1981], computes the local alignment of two sequences.

Needleman-Wunsch algorithm

The idea of the algorithm is to start with two empty sequences and subsequently add characters from either or both of the given sequences so as to obtain an optimal alignment in each step. Namely, suppose that we have two sequence prefixes A and B that have already been aligned optimally and their alignment gives a score of s. Furthermore, suppose that the next characters in the sequences are a and b, respectively. There are three possibilities:

- We append a and b to the respective prefixes. By doing so, we obtain the aligned sequence prefixes Aa and Bb.

```
Aa
Bb
```

- We append a to A and a gap to B. This way, we get the aligned prefixes Aa and B.

```
Aa
B-
```

- We append a gap to A and b to B. Now we have aligned the prefixes A and Bb.

```
A-
Bb
```

Each of the possibilities adds a value to the score s depending on what characters were added. To get the optimal alignment, we choose the one that yields the highest score. We then proceed to the next character, having two optimally aligned prefixes A' and B'. This leads to a recursive algorithm that can be formulated using dynamic programming.

Let us have two input sequences, A and B of lengths m and n with a common alphabet $\mathcal{A}$ and the gap character σ. Let us define the scoring function s as

$$s(a,b) = \begin{cases} 1 & \text{if } a = b \\ -1 & \text{if } a = \sigma \vee b = \sigma \\ -1 & \text{if } a \neq b \end{cases}$$

The algorithm initializes a matrix M of size $(m+1) * (n+1)$. The rows and columns represent the characters of A and B, respectively, except for the first row and the first column, which represent the beginning of a sequence or an empty sequence. That is to say, the row $M_{i,*}$ represents the character A_{i-1} for $i \geq 2$ and analogically, the column $M_{*,j}$ represents the character B_{j-1} for $j \geq 2$.

The algorithm iterates over the rows and columns of the matrix. In each step, it calculates the value of a cell $M_{i,j}$, provided that each of the cells $M_{i-1,j}$, $M_{i,j-1}$ and $M_{i-1,j-1}$ have been filled out, as

$$M_{i,j} = max \begin{cases} M_{i-1,j-1} + s(A_{i-1}, B_{j-1}) \\ M_{i-1,j} + s(A_{i-1}, \sigma) \\ M_{i,j-1} + s(\sigma, B_{j-1}) \end{cases}$$

In other words, the algorithm either aligns the two characters in positions $i-1$ and $j-1$, or it inserts a gap into sequence B, or it inserts a gap into sequence A, and chooses the version which yields the highest score.

The first row and column are apparently special cases, as there is no previous row or column. Therefore, for each cell in the first row or column, there is only one possible choice of score, which is equivalent to inserting a space.

After filling out the entire matrix, the algorithm then finds the optimal alignment by backtracking in the matrix. It starts in the bottom right cell of the matrix, which represents both sequences being aligned. In each iteration, it looks at the cells above, to the left and to the top-left of the current positions and chooses the highest score. If it moves top or left, it means that a gap was inserted. Moving diagonally represents a match or mismatch. By tracing its way back to the top left corner, the algorithm finds the alignment that yielded the highest score.

Let us show the algorithm on an example. Consider two sequences of nucleotide residues:

```
GATTA
GCATG
```

The matrix is initialized without anything filled out.

```
      G  C  A  T  G


G
A
T
T
A
```

We start filling out the matrix in the top left corner. Using the basic scoring scheme (+1 for a match, -1 for everything else), we insert a 0 to the beginning, and, since there is no top cell for the first row and no left cell for the first column, we add -1 to each subsequent cell, representing a gap insertion.

```
      G  C  A  T  G
   0 -1 -2 -3 -4 -5
G -1
A -2
T -3
T -4
A -5
```

The next cell to fill out is the one in the first `G` column and the first `G` row. We have three options:

- Move from the top, represents gap insertion for a score of -1. The final score would be $(-1) + (-1) = -2$.
- Move diagonally, represents match, giving a score of +1. The score in this case would be $0 + 1 = 1$.
- Move from the left, i.e. gap insertion. The score would be -2 as in the first case.

We choose the highest score, which in this case is a diagonal move representing a match. It follows intuition: we are now aligning `G` and `G`, matching them seems logical.

```
      G  C  A  T  G
   0 -1 -2 -3 -4 -5
G -1  1
A -2
T -3
T -4
A -5
```

Now let us look at the cell in the `C` column and the `G` row. Moving from the top yields -3, moving from the left yields 0 and moving diagonally yields -2, as it is a mismatch in this case. The highest of these scores is 0.

```
        G  C  A  T  G
     0 -1 -2 -3 -4 -5
  G -1  1  0
  A -2
  T -3
  T -4
  A -5
```

We continue filling out the table this way until it is complete.

```
        G  C  A  T  G
     0 -1 -2 -3 -4 -5
  G -1  1  0 -1 -2 -3
  A -2  0  0  1  0 -1
  T -3 -1 -1  0  2  1
  T -4 -2 -2 -1  1  1
  A -5 -3 -3 -1  0  0
```

As we have now calculated the scores for all prefixes, we can use backtracking to find the optimal alignment for the two sequences. Starting in the bottom right cell, we choose the cell (top, left or top-left) with the highest score. If multiple cells have the same score, we can choose either. The different alignments the cells represent are all optimal. The cell that we choose gives us the optimal alignment of the sequences before the last character was added. Depending on the direction by which we moved, we know whether this last character was a character of the sequence or a gap.

For example, consider the bottom right corner of the matrix.

```
     T  G
  T  1  1
  A  0  0
```

Starting in the bottom right, we can choose either the top or the top-left cell. Choosing the top-left one, i.e. moving diagonally, means that the last characters in the alignment were `A` and `G` for the respective sequences. We can find the alignment of the prefixes `GATT` and `GCAT` by backtracking from the top-left cell. By contrast, choosing the top cell means inserting a gap in the second sequence, and by backtracking from there we can find the alignment of `GATT` and `GCATG`.

Figure 3.1 shows a path that represents the alignment

```
  G A - T T A
  G C A T - G
```

$$\begin{tikzcd}
 & & G & C & A & T & G \\
 & 0 & -1 & -2 & -3 & -4 & -5 \\
G & -1 & 1 \arrow[ul] & 0 & -1 & -2 & -3 \\
A & -2 & 0 & 0 \arrow[ul] & 1 \arrow[l] & 0 & -1 \\
T & -3 & -1 & -1 & 0 & 2 \arrow[ul] & 1 \\
T & -4 & -2 & -2 & -1 & 1 \arrow[u] & 1 \\
A & -5 & -3 & 3 & -1 & 0 & 0 \arrow[ul]
\end{tikzcd}$$

Figure 3.1: A path representing an optimal alignment.

Smith-Waterman algorithm

The algorithm is similar to Needleman-Wunsch algorithm. As its purpose is to find an optimal local alignment, it does not penalize long regions of mismatches or gaps. Its purpose is to find regions with the most matches. The only difference from the Needleman-Wunsch algorithm is in how new matrix cells are filled out. Namely, when willing out a new cell, we use the formula

$$M_{i,j} = max \begin{cases} 0 \\ M_{i-1,j-1} + s(A_{i-1}, B_{j-1}) \\ M_{i-1,j} + s(A_{i-1}, \sigma) \\ M_{i,j-1} + s(\sigma, B_{j-1}) \end{cases}$$

In other words, all negative values in what would be the matrix from Needleman-Wunsch algorithm are replaced by 0.

3.2.2 Multiple sequence alignment: progressive methods

As has already been mentioned, it is essentially impossible to use dynamic programming to compute the alignment of more than two sequences. Therefore, other methods have been developed. The most successful ones appear to be the so-called progressive methods. In general, they use some heuristics to estimate a guide tree, which is a phylogenetic tree determining how close the sequences are to each other, and then they compute the actual multiple alignment following the order of this tree.

One of such methods is the Tree-based Consistency Objective Function for alignment Evaluation (T-Coffee) algorithm [Notredame et al., 2000]. Its most important contribution is its extended library generated from both local and global pairwise alignments of all pairs of input sequences. This library enables the algorithm to make fewer mistakes in the initial stages of the guide tree, as these errors propagate throughout the entire tree.

Another method is MAFFT (the name presumably coming from the acronyms for multiple alignment and fast Fourier transform) [Katoh et al., 2002]. The authors focused on finding alignments that are not only optimal, but also biologically correct. They developed a way of rapid identification of homologous regions between two sequences using FFT, and then used the better pairwise alignments to create a better multiple alignment.

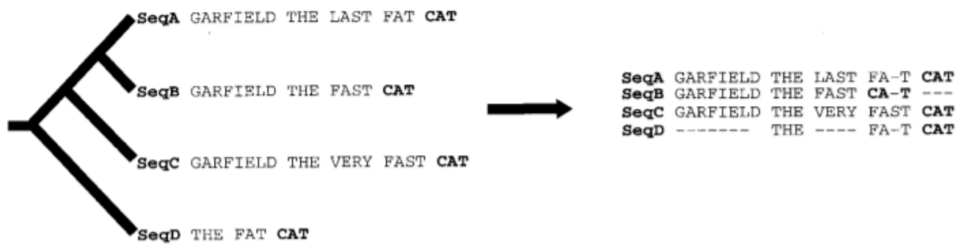

SeqA GARFIELD THE LAST FAT CAT
SeqB GARFIELD THE FAST CAT
SeqC GARFIELD THE VERY FAST CAT
SeqD THE FAT CAT
SeqA GARFIELD THE LAST FA-T CAT
SeqB GARFIELD THE FAST CA-T ---
SeqC GARFIELD THE VERY FAST CAT
SeqD -------- THE ---- FA-T CAT

Figure 3.2: Misalignment of the word CAT using other progressive methods. [Notredame et al., 2000, Figure 2(a)]

T-Coffee

The T-Coffee algorithm consists of various stages. The first one is to compute pairwise alignments for all pairs of input sequences. Two primary libraries are generated, one for global and one for local alignments. Each can contain more than one alignment for each pair.

As some alignments tend to be more correct than others, weighting is then performed. The authors chose sequence identity of two aligned sequences as the weight of each of the aligned residues in the pair. For example, consider the sequences A `GARFIELD THE LAST FAT CAT` and B `GARFIELD THE FAST CAT`. If they are aligned as

```
GARFIELD THE LAST FAT CAT
GARFIELD THE FAST CAT ---
```

then their sequence identity is 88%, as there are two non-equal characters aligned (i.e. there is no gap penalty). Therefore, the weight of each residue pair $W(A(x), B(y))$, where $A(x)$ denotes the character x from sequence A, and analogically for $B(y)$, is equal to 88.

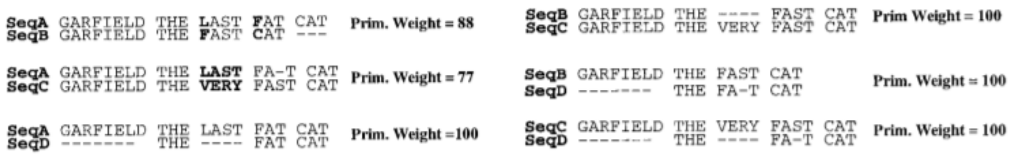

SeqA GARFIELD THE LAST FAT CAT
SeqB GARFIELD THE FAST CAT ---
Prim. Weight = 88
SeqB GARFIELD THE ---- FAST CAT
SeqC GARFIELD THE VERY FAST CAT
Prim Weight = 100
SeqA GARFIELD THE LAST FA-T CAT
SeqC GARFIELD THE VERY FAST CAT
Prim. Weight = 77
SeqB GARFIELD THE FAST CAT
SeqD -------- THE FA-T CAT
Prim. Weight = 100
SeqA GARFIELD THE LAST FAT CAT
SeqD -------- THE ---- FAT CAT
Prim. Weight =100
SeqC GARFIELD THE VERY FAST CAT
SeqD -------- THE ---- FA-T CAT
Prim. Weight = 100

Figure 3.3: Primary library created from 4 sequences. [Notredame et al., 2000, Figure 2(b)]

The two primary libraries are then combined into one by combining all identical residue pairs into one entry and summing their weights, while pairs that are only present once are added with their original weight. Residue pairs that are not present in any alignment have an implicit weight of 0.

Although the information present in the primary library is sufficient to obtain a multiple alignment, it is computationally hard to do so. Instead, the authors chose to generate what they call an extended library using the weights in the primary library.

Library extension is performed by comparing each aligned residue pair with all the others. Consider a residue pair $(A(x), B(y))$ and a sequence C. The initial weight of the pair is then increased by $min(W(A(x), C(z)), W(C(z), B(y)))$, i.e. the minimum weight associated to the alignment of some residue $C(z)$ with both $A(x)$ and $B(y)$. This is done for all residues from all sequences. In practice, most of the weights will be 0, therefore the actual algorithm computes the weights more efficiently. Library extension in effect computes how consistent a residue-pair alignment is.

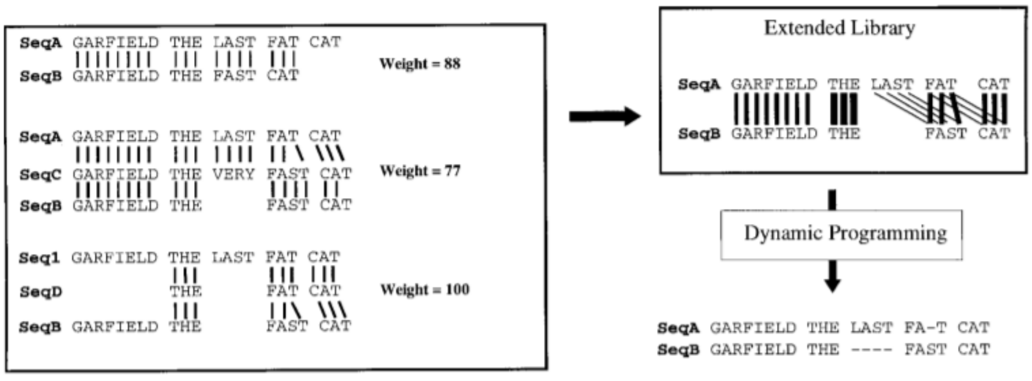

SeqA GARFIELD THE LAST FAT CAT
SeqB GARFIELD THE FAST CAT
Weight = 88
SeqA GARFIELD THE LAST FAT CAT
SeqC GARFIELD THE VERY FAST CAT
SeqB GARFIELD THE FAST CAT
Weight = 77
Seq1 GARFIELD THE LAST FAT CAT
SeqD THE FAT CAT
SeqB GARFIELD THE FAST CAT
Weight = 100
Extended Library
SeqA GARFIELD THE LAST FAT CAT
SeqB GARFIELD THE FAST CAT
Dynamic Programming
SeqA GARFIELD THE LAST FA-T CAT
SeqB GARFIELD THE ---- FAST CAT

Figure 3.4: Extended library weights for two sequences and their alignment recomputed using these weights. [Notredame et al., 2000, Figure 2(c)]

Having obtained the consistency information from the extended library, it is now possible to create the guide tree and the final multiple alignment. Using a distance matrix between all the sequences, the tree is computed as follows. First, we align the closest two sequences using dynamic programming and the weights from the extended library. In each of the following steps, we either add a sequence to an already computed alignment, or we align the next closest sequences. We repeat this step until the alignment of all sequences is complete.

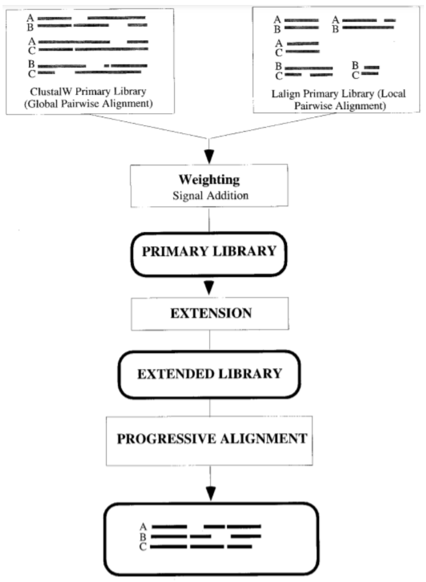

ClustalW Primary Library (Global Pairwise Alignment)
Lalign Primary Library (Local Pairwise Alignment)
Weighting
Signal Addition
PRIMARY LIBRARY
EXTENSION
EXTENDED LIBRARY
PROGRESSIVE ALIGNMENT

Figure 3.5: T-Coffee layout. [Notredame et al., 2000, Figure 1]

MAFFT

The MAFFT method is similar to T-Coffee in that it constructs a library of alignments which it then uses to create the final multiple alignment. The authors developed MAFFT to work in multiple modes, one of which is the progressive method as described above; the other one is the iterative refinement method, which allows for alterations of the multiple alignment obtained from the progressive method.

Pairwise alignment in MAFFT uses the fact that certain amino acids have more similar physico-chemical properties than others. Substitutions tend to preserve the overall structrure of a protein, therefore substitutions of similar amino acids are more frequent than those of different ones. The two properties the authors use are amino acid volume and polarity.

Let us define the correlation of the volume component between two amino acid sequences with the positional lag of k as

$$c_v(k) = \sum_{1\leq n\leq N, 1\leq n+k\leq M} \hat{v}_1(n)\hat{v}_2(n+k)$$

where N and M are the lengths of the sequences and $\hat{v}(a) = [v(a) - \bar{v}]/\sigma_v$ is the normalized volume value with $\bar{v}$ denoting the average volume of all the amino acids and σ_v their standard deviation.

Since the sequences tend to be equal in length, computing $c_v(k)$ using naive methods takes time proportional to N^2. However, applying Fast Fourier transform to the calculation reduces the time to $\mathcal{O}(NlogN)$.

We define the polarity component correlation $c_p(k)$ analogically.

The correlation between two amino acids is then expressed as

$$c(k) = c_v(k) + c_p(k)$$

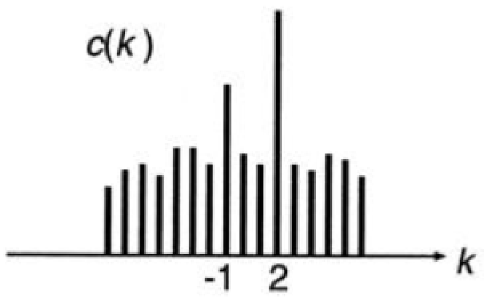


Figure 3.6: Plot of the correlation function $c(k)$. [Katoh et al., 2002, Figure 1A]

If we plot the function $c(k)$, there will be some peaks corresponding to the homologous regions of the two sequences, if there are any (Figure 3.6). However, the FFT analysis only gives us the positional lag of the regions, not their positions. To find the exact positions, we use a sliding window (of size 30 in the article) and calculate the degree of local homologies for the 20 highest peaks in the $c(k)$

function. If a segment exceeding a given homology threshold is identified, we label it as a homologous region.

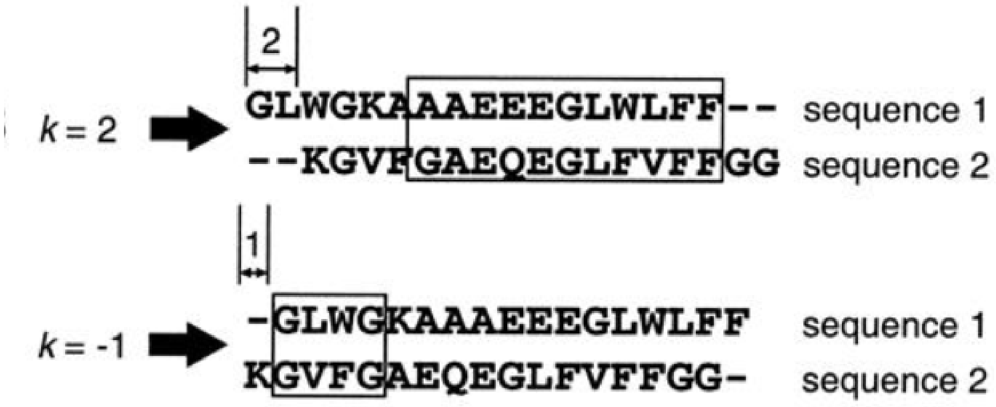


Figure 3.7: Finding homologous regions with different positional lags using a sliding window. [Katoh et al., 2002, Figure 1B]

After finding homologous segments between two sequences, their alignment is obtained by constructing a homology matrix $S \in R^{n*n}$, where n is the number of homologous segments. The cell S_{ij} is assigned a value depending on whether the i-th homologous segments of the first sequence corresponds to the j-th homologous segment of the second sequence. If so, the cell gets a value corresponding to the score of this segment; otherwise it has a value of 0. The optimal arrangment of homologous segments is then obtained using dynamic programming.

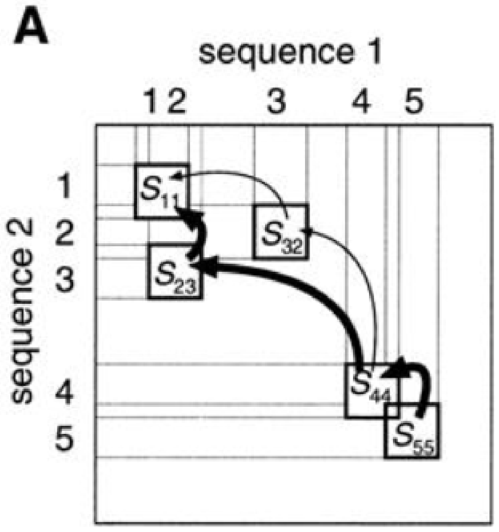


Figure 3.8: Dynamic programming applied on segment arrangement. [Katoh et al., 2002, Figure 2A]

Having arranged homologous segments, the algorithm then computes pairwise alignments for each pair of sequences. As in T-Coffee, it uses the alignments to create the primary and extended libraries, which are in turn used to estimate the guide tree and the final alignment. If MAFFT is configured to perform the progressive method, this alignment is the final one. Otherwise, if iterative refinement is allowed, MAFFT uses the weights from the library to adjust the alignment to get a more optimal one. However, iterative refinement is very slow from a relatively low number of sequences, therefore it is not suitable for a large dataset.

3.3 Sequence alignment for chant melodies

As we have discussed before, melodies of Gregorian chant are in many ways similar to biological sequences. The alphabet is different (instead of 20 amino acids in proteins or 4 nucleotide bases in DNA we have around 40 different characters used in melody representation) and the chants are usually shorter in length. The evolution of both biological and melodic sequences is guided by environmental factors such as migration to other places. Some segments tend to undergo a lot of modifications, while other remain relatively unchanged. Studying the alignment of chant melodies can reveal a lot of information about their relationship.

In the following sections, we describe three approaches to melody alignment used in our application.

The first one is a naive approach. It merely aligns all chants to have the same number of words and each word to have the same number of syllables, filling the extra positions with gaps, if needed.

The other two approaches use MAFFT to perform a proper sequence alignment. They differ in what we are aligning. One of them aligns notes and other symbols as they are; each representing a certain pitch. The other one is more sophisticated: it does not use the absolute value of the pitches, but rather the intervals between the notes. This way, we can see segments that have merely been shifted by a certain interval.

3.3.1 Naive alignment

3.3.2 Multiple alignment using absolute pitches

For this task, we are using the MAFFT software[1]. As the software uses the character `-` for marking gaps, it requires that the input sequences do not contain any, or they will be removed. Since melodies encoded as Volpiano use the character to mark ends of words and ends of syllables, we need to perform some preprocessing. Namely, we replace all contiguous sequences `---` with the end-of-word marking symbol `~` and all contiguous sequences `--` with the end-of-syllable marker `|`. All remaining `-`s are removed, if there are any.

The sequences are then passed to MAFFT with the option `--text`, which indicates that the sequences are not biological. Additionally, we also pass the option `--reorder`, which returns the aligned sequences in order of similarity. We made this choice so as to facilitate the identification of related melodies.

After MAFFT performs the alignment, we retrieve the sequences and attempt to combine them with their text. We do this by splitting both the text and the melody into syllables and mapping them onto each other (Algorithm 1). However, this might not be possible. Due to errors in the original encoded melody

[1]https://mafft.cbrc.jp/alignment/software/

(i.e. a missing or an extra `-`), we may have altered the structure of the chant in preprocessing. In case of such event, we remove the affected sequence from consideration and align the remaining sequences again.

Algorithm 1: Aligning melody and lyric

```
input  : volpiano: melody divided into words and those into syllables,
         and text: lyric divided analogically
output: volpiano and text aligned

set aligned_text_and_melody to be an empty list;
for word at index i do
    open new word in aligned_text_and_melody;
    if i-th word of text has more syllables than i-th word of melody then
        merge the extra syllables into the last one;
    else if i-th word of text has fewer syllables than i-th word of melody
     then
        extend the i-th word of text by empty syllables to match the
         volpiano word
    for syllable at index j of i-th word do
        combine text and melody of the j-th syllable of the i-th word and
         add it to the current word;
    end
    close current word;
end
return aligned_text_and_melody;
```

Once all sequences are successfully aligned without errors in text and melody combination, we can display them to the user. In the application, we use the Volpiano font, so as to maintain consistency. However, the sequences shown are not properly encoded in Volpiano format. First of all, we choose different representations of end of a word (here we use a bar line) and end of a syllable (a single space) so that the number of characters in each sequence remains equal and the alignment is visible. Second of all, after the alignment, MAFFT will have inserted `-`s to represent gaps. In proper Volpiano, these characters represent gaps between words, syllables, and neumes. However, here they just mean empty space.

Algorithm 2: Multiple alignment using absolute pitches

```
input  : a set of volpiano-encoded melodies with their respective lyrics
output: aligned melodies combined with their lyrics

preprocess all melodies to a MAFFT-friendly format;
while melodies have not been aligned without error do
    run MAFFT on all melodies;
    for aligned melody do
        combine melody with its text;
        if melody and text cannot be combined then
            remove melody from list;
            remember to run the while loop again;
        end
    end
end
return list of aligned melodies combined with their texts;
```

3.3.3 Multiple alignment using intervals

The general outline of the algorithm is the same as Algorithm 2. However, as we are not aligning absolute pitches, but rather intervals, we need to compute these intervals.

There are 18 possible pitches, which means 37 possible intervals (17 positive, 17 negative, and one without the change of pitch). We will represent the no-change interval with the character `a`, the positive intervals with the lowercase characters `b-t` and the negative intervals with the uppercase characters `B-T`. The characters `i` and `I` are not used for reasons explained later.

The interval representation is constructed from a Volpiano-encoded melody by replacing the note symbols with the appropriate interval symbol. The i-th note will be replaced with the symbol representing the interval $(i-1, i)$. As the first note has no predecessor, it is left as it is. The non-note symbols also remain unchanged.

Algorithm 3: Converting volpiano-encoded melody into interval representation

```
input  : volpiano-encoded melody
output: interval representation of the input melody

$interval\_representation \longleftarrow$ "";
for character c in volpiano do
    if c is a non-note character then
        append c to interval_representation;
    else if c is a note-representing character and it is the first such one
     then
        append c to interval_representation;
        $last\_seen\_note \longleftarrow c$;
    else
        $interval \longleftarrow (last\_seen\_note, c)$;
        $i \longleftarrow symbol\ for\ interval$;
        append i to interval_representation;
        $last\_seen\_note \longleftarrow c$;
end
return interval_representation;
```

We use the interval representations as inputs to MAFFT. That means that what MAFFT returns are the aligned sequences of intervals. To display them to the user properly, we need to decode the sequences.

Algorithm 4: Converting interval representation back to volpiano

```
output: interval representation of a melody
input  : volpiano-encoded equivalent of the input melody

$volpiano \longleftarrow$ "";
for character c in interval representation do
    if c is a non-interval character then
        append c to volpiano;
    else if c is a note-representing character and it is the first such one
     then
        append c to volpiano;
        $last\_seen\_note \longleftarrow c$;
    else if c is an interval-representing character and we have already
     seen the first note then
        $note \longleftarrow last\_seen\_note +$ interval represented by $i$;
        append note to volpiano;
        $last\_seen\_note \longleftarrow note$;
end
return volpiano;
```

The reason why we are not using `i` and `I` as symbols for an interval is that as we are looking at whether a character is a note or an interval or neither, if they represented an interval, we would choose the appropriate branch in Algorithm 4. However, marking an interval is not the only way how the character could have got there: `i` and `I` represent non-note elements in the Volpiano protocol. Therefore, we could mistakenly shift the melody by an interval, as there is no way of knowing which case it is.

The complete algorithm is similar to Algorithm 2.

Algorithm 5: Multiple alignment using intervals

```
input  : a set of volpiano-encoded melodies with their respective lyrics
output: aligned melodies combined with their lyrics

convert all melodies to interval representations;
preprocess all interval representations to a MAFFT-friendly format;
while melodies have not been aligned without error do
    run MAFFT on all interval representations;
    for aligned interval representation do
        convert interval representation to volpiano-encoded melody;
        combine melody with its text;
        if melody and text cannot be combined then
            remove melody from list;
            remember to run the while loop again;
        end
    end
end
return list of aligned melodies combined with their texts;
```

Conclusion

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A. Attachments

A.1 First Attachment