

Albert Einstein

Eine neue Bestimmung der Moleküldimensionen

Diss. ETH No. ?

PESHO IVANOV

OPTIMAL PAIRWISE ALIGNMENT USING A*

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A dissertation submitted to attain the degree of

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(Dr. sc. ETH Zurich)

presented by

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2022

With gratitude to Vipassana meditation

ABSTRACT

Sequence alignment is the process of detecting similarities between biological sequences, such as DNA, RNA and proteins. For the last half a century, variations of this problem have been of central importance for molecular biology. Alignment is usually a building block for a wide range of applications, include evolutionary biology, genome assembly, read mapping, variation detection aComputational methods are crucial for the correctness of the analyses and the practical applicability to the vast amounts of biological data.

The usual way to represent the similarities between sequences is by a base-to-base correspondence between them which that minimizes general edit distance. Biological sequences do not generally align perfectly due to biological differences and technical errors. Instead, desired are the best imperfect alignments according to a similarity metric, such as *edit distance*.

A good alignment algorithm should ① find accurate alignments of ② a wide range of data, in ③ little time and memory. We consider a principled shortest path formulation of alignment and argue that the A* algorithm fullfils the desired properties better than current methods. In particular it can ① provide optimality guarantees according to edit distance, ② tolerate long and noisy sequences, and ③ scale subquadratically with sequence length.

The classical dynamic programming (DP) algorithms run in quadratic time, even though the resulting alignment is linear. This gap has motivated the development of various faster but approximate algorithms. Moreover, theoretical results suggest that it is impossible to solve any reasonable alignment problem in strongly subquadratic time in the worst case.

In this thesis we argue that the A* informed search algorithm radically improving the runtime scaling (up to linear) in the average case while can provide optimality guarantees while. On real data, this approach reaches orders of magnitude of speedup compared to existing approaches.

In this thesis, we consider the alignment as a shortest path problem that we approach via A*. The A* algorithm naturally encompasses the existing approaches but extends them with the possibility for informed search which is capable of using information from the whole sequences to direct the search. In practice, while achieving polynomial speed ups on real

data. Our A* approach is applicable to various settings of the alignment problem.

To scale to large reference sequences, we extend the graph with a trie index. To scale to long queries, we introduce design an admissible *seed heuristic*, which is provably-optimal also efficient to compute. To scale to high error rates, we design

Informed search. Admissibility. Seed heuristic.

Many tools do not have a well-stated problem they optimize.

Probabilistic approach. Focus on the metric. Extend to MSA, local, affine. Prorotype implementations No asymptotics.

ZUSAMMENFASSUNG

Deutsche Zusammenfassung hier.

ACKNOWLEDGEMENTS

I would like to thank ...

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NOTATION

FREQUENTLY USED SYMBOLS

E energy

m rest mass

p impulse

PHYSICAL CONSTANTS

c speed of light in vacuum, $c = 299\,792\,458\,\text{m s}^{-1}$

(CODATA 2014 [1])

INTRODUCTION

*Sapere aude! Habe Mut, dich deines eigenen
Verstandes zu bedienen!*

— Immanuel Kant

The number of possible alignments grow exponentially with length. The usual underlying question to finding “correct” alignments. Regarding the precision of alignment, one is usually interested in base-to-base (aka letter-to-letter) correspondence between the sequences, even though for some applications a less detailed solution is sufficient: only the similarity between sequences or the location where a read maps to a reference. Exact alignment is only useful for very short sequences (often kmers), and for all other cases the optimized metric may be hamming distance, edit distance (unit costs), Levenshtein distance, affine costs, convex and concave costs, general costs and others.

Depending on the the number of aligned sequences, there is pairwise alignment and multiple sequence alignment (MSA). Depending on the parts of the sequences that are aligned to each other, we differentiate global, local and various semi-global alignemnts. There are generalizations to sequence-to-sequence alignment, including aligning to nonlinear structures, such as directed acyclic graphs, DAGs, general graphs and others. These structures are nowadays becoming more common as a compressed form of representing a set of references to which a sequence can be aligned. Often, one best alignment is sufficient but finding several best (top-K) alignments. In the context of read mapping, a set of reads is aligned to the same reference sequence so an indexing procedure is often useful for the performance.

We specifically consider the mapping of a set of reads to a general graph, and the global pairwise alignment.

SAMPLE CHAPTER

The true logic of this world is in the calculus of probabilities.

— James C. Maxwell

Maxwell [2] derived some very useful equations for electromagnetic fields:

$$\nabla \cdot \vec{D} = \rho \quad (2.1)$$

$$\nabla \cdot \vec{B} = 0 \quad (2.2)$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \quad (2.3)$$

$$\nabla \times \vec{H} = \vec{j} + \frac{\partial \vec{D}}{\partial t} \quad (2.4)$$

The energy-momentum relation, eq. (2.5), is one of *my* important results:

$$E^2 = m^2 c^4 + (pc)^2 \quad (2.5)$$

Write units like this: 5 μm .

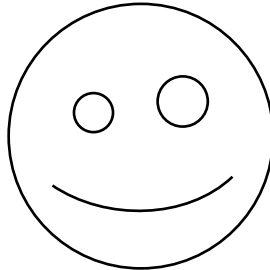


FIGURE 2.1: A lovely face.

HEADING ON LEVEL 0 (CHAPTER)

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

3.1 HEADING ON LEVEL 1 (SECTION)

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And after the second paragraph follows the third paragraph. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information.

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After this fourth paragraph, we start a new paragraph sequence. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

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3.1.1 *Heading on Level 2 (subsection)*

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3.2 LISTS

3.2.1 *Example for list (itemize)*

- Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.
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3.2.1.1 Example for list (4*itemize)

- Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest

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- * Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

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of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

3.2.2 *Example for list (enumerate)*

1. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.
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3.2.2.1 *Example for list (q*enumerate)*

1. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.
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- ii. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and

it should be written in of the original language. There is no need for special content, but the length of words should match the language.

- b) Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.
2. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

3.2.3 *Example for list (description)*

FIRST ITEM IN A LIST Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

SECOND ITEM IN A LIST Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no

information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

THIRD ITEM IN A LIST Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

FOURTH ITEM IN A LIST Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

FIFTH ITEM IN A LIST Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

3.2.3.1 *Example for list (q*description)*

FIRST ITEM IN A LIST Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

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FIRST ITEM IN A LIST Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

FIRST ITEM IN A LIST Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like

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SECOND ITEM IN A LIST Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

SECOND ITEM IN A LIST Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

SUMMARY

I dream my painting and I paint my dream.

— Vincent van Gogh

Summary here.



APPENDIX

Here be dragons.

BIBLIOGRAPHY

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2. Maxwell, J. C. A Dynamical Theory of the Electromagnetic Field. *Philosophical Transactions of the Royal Society of London* **155**, 459 (1865).

CURRICULUM VITAE

PERSONAL DATA

Name	Albert Einstein
Date of Birth	March 14, 1879
Place of Birth	Ulm, Germany
Citizen of	Switzerland

EDUCATION

1896 – 1900	Eidgenössisches Polytechnikum, Zürich, Switzerland <i>Final degree:</i> Diploma
1895 – 1896	Aargauische Kantonsschule (grammar school) Aarau, Switzerland <i>Final degree:</i> Matura (university entrance diploma)
– July 1894	Luitpold-Gymnasium (grammar school) Munich, Germany

EMPLOYMENT

June 1902 –	Technical Expert, III Class <i>Federal Office for Intellectual Property,</i> Bern, Switzerland
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PUBLICATIONS

Articles in peer-reviewed journals:

1. Einstein, A. Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen. *Annalen der Physik* **322**, 549 (1905).
2. Einstein, A. Zur Elektrodynamik bewegter Körper. *Annalen der Physik* **322**, 891 (1905).

Conference contributions:

3. Einstein, A. *Implications of a fixed vacuum speed of light in Relativity* Oct. 2–6, 1905 (1st Conference on Special Relativity, Zurich, Switzerland).