Tropical time series, iterated-sums signatures and quasisymmetric functions

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October 1st, Datasig Slides at: https://diehlj.github.io

Overview

Motive

Algebraic setting

Outlook

Convolutional Neural Networks

Why they work so well (probably ...)

- Weight sharing.
- 2 Structure compatible with image data ("receptive field", approximate translation invariance).

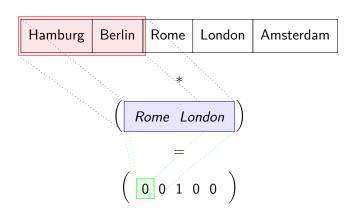
CNNs can, of course, be applied to sequential data.

Does it make sense?

- Weight sharing.
- 2 Structure compatible with time-series data ?

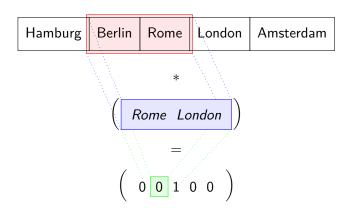
Using a CNN to answer:

"Did a person visit Rome directly before visiting London?"



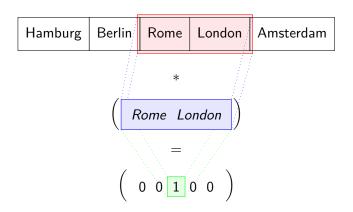
Using a CNN to answer:

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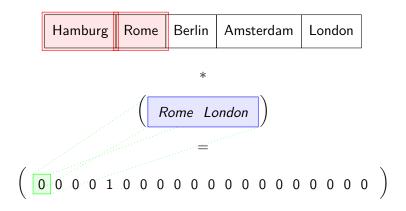
"Did a person visit Rome directly before visiting London?"

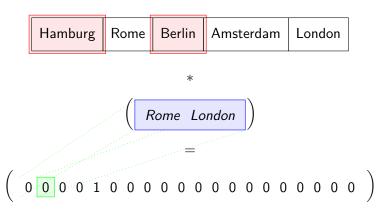


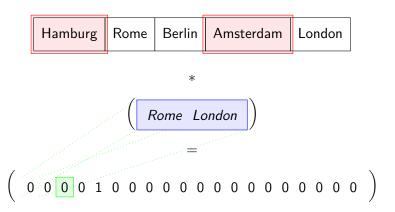
But what if the person visits Rome some time before visiting London?

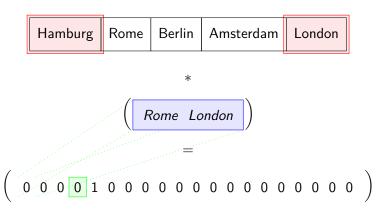
Hamb	ourg Rome	Berlin	Amsterdam	London
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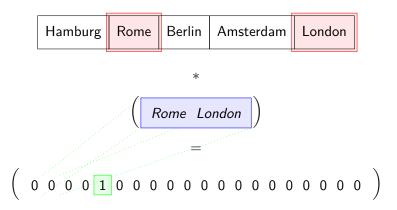
A (one-layer) CNN has difficulties detecting this (unless the kernel is large enough).











More formal

Let

$$\begin{split} \textit{K}: \mathsf{Cities} \times \mathsf{Cities} & \rightarrow \{\mathtt{true}, \mathtt{false}\} \\ & \left(\mathsf{cityA}, \mathsf{cityB}\right) \mapsto \left(\mathsf{cityA} = \bigoplus\right) \ \land \left(\mathsf{cityB} = \bigoplus\right) \end{split}$$

$$\mathsf{pool}: \{\mathsf{true}, \mathsf{false}\}^{\binom{n_\mathsf{in}}{2}} \to \{\mathsf{true}, \mathsf{false}\}$$

$$z \mapsto z_1 \ \lor \ z_2 \ \lor \ \dots \ \lor \ z_{\binom{n_\mathsf{in}}{2}}.$$

Then

$$\operatorname{pool}\left(K(x_I): I \in \binom{[n_{\operatorname{in}}]}{2}\right) = \bigvee_{0 < i_1 < i_2 < n_{\operatorname{in}}} \left(x_{i_1} = \bigcap_{i_1 < i_2 < n_{\operatorname{in}}}\right) \wedge \left(x_{i_2} = \bigcap_{i_1 < i_2 < n_{\operatorname{in}}}\right),$$

is true if and only if Rome was visited some time before London.

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(There is nothing "learnable" here yet, we'll come to this later.)

First, we want to deal with a problem: $\binom{n_{in}}{2}$ gets large real quick!

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To clarify, let us do 3 cities whose ordered visit we want to detect:

$$\mathcal{K}(\dots) := (\mathsf{cityA} = \bigcirc) \land (\mathsf{cityB} = \bigcirc) \land (\mathsf{cityC} = \bigcirc)$$

$$\operatorname{pool}\left(K(x_I): I \in \binom{[n_{\operatorname{in}}]}{3}\right) := \bigvee_{I \in \binom{[n_{\operatorname{in}}]}{3}} K(x_I).$$

This needs $O(n_{\rm in}^3)$ evaluations of K.

But! There is a better way.

$$\bigvee_{I \in \binom{[n_{in}]}{3}} K(x_I) = \bigvee_{i_1 < i_2 < i_3} (x_{i_1} = \bigcirc) \land (x_{i_2} = \bigcirc) \land (x_{i_3} = \bigcirc) \land (x_{i_3$$

Only n_{in} evaluations!

Further

$$\mathsf{pool}'_{i_3} = \bigvee_{i_1 < i_2 < i_3} (x_{i_1} = \bigcirc) \land (x_{i_2} = \bigcirc)$$

$$= \bigvee_{i_2 < i_3} \left(\bigvee_{i_1 < i_2} (x_{i_1} = \bigcirc) \right) \land (x_{i_2} = \bigcirc)$$

$$=: \bigvee_{i_2 < i_3} \mathsf{pool}''_{i_2} \land (x_{i_2} = \bigcirc).$$

Only n_{in} evaluations (to calculate all of pool_•)! Finally,

$$pool''_{i_2} = \bigvee_{i_1 < i_2} (x_{i_1} = i_2)$$

Only n_{in} evaluations (to calculate all of pool.")!

total amount of evaluations: $O(3n_{in}) = O(n_{in})$

What have we achieved?

We calulated

$$\begin{aligned} &\operatorname{pool}\left(K(x_I): I \in \binom{[n_{\operatorname{in}}]}{3}\right) \\ &= \bigvee_{I \in \binom{[n_{\operatorname{in}}]}{3}} K(x_I) \\ &= \bigvee_{i_1 < i_2 < i_3} (x_{i_1} = \bigotimes) \wedge (x_{i_2} = \bigotimes) \wedge (x_{i_3} = \bigotimes) , \end{aligned}$$

which, on paper, costs $O(n_{\rm in}^3)$, in only $O(n_{\rm in})$ time !

What did we use?

- ∧ distributes over ∨
- ∧ and ∨ are associative

And that's it

What have we achieved?

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And that's it.

Definition

The tuple $(\mathbb{S}, \oplus_s, \odot_s, \mathbf{0}_s, \mathbf{1}_s)$ is a commutative **semiring** if

- \blacksquare $\left(\mathbb{S}, \oplus_{\text{\tiny S}}, \mathbf{0}_{\text{\tiny S}}\right)$ is a commutative monoid with unit $\mathbf{0}_{\text{\tiny S}}$
- \blacksquare $\left(\mathbb{S},\odot_{_{\mathbb{S}}},\mathbf{1}_{_{\mathbb{S}}}\right)$ is a commutative monoid with unit $\mathbf{1}_{_{\mathbb{S}}}$
- $\bullet \mathbf{0}_{\scriptscriptstyle \mathbb{S}} \odot_{\scriptscriptstyle \mathbb{S}} \mathbb{S} = \{ \mathbf{0}_{\scriptscriptstyle \mathbb{S}} \}$
- multiplication distributes over addition, i.e.

$$a \odot_{s} (b \oplus_{s} c) = (a \odot_{s} b) \oplus_{s} (a \odot_{s} c)$$

Examples of semirings

- any commutative ring
- boolean semiring

$$(\{\mathtt{false},\mathtt{true}\},ee,\wedge,\mathtt{false},\mathtt{true})$$

- min-plus ("tropical") semiring $(\mathbb{R} \cup \{+\infty\}, \min, +, +\infty, 0)$
- possibilistic (or Viterbi or Bayesian) semiring $([0,1], \max, \cdot, 0, 1)$

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 ({false, true}, ∨, ∧, false, true)
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Examples of semirings $(\mathbb{S}, \oplus_s, \odot_s, \mathbf{0}_s, \mathbf{1}_s)$

- semiring of subsets of a set M $(2^M, \cup, \cap, \emptyset, M)$
- any distributive lattice (with minimal and maximal element)
- ...

They are of huge interest in computer science / automata theory.

Corollary (DEFT '20)

Let $(S, \oplus_s, \odot_s, \mathbf{0}_s, \mathbf{1}_s)$ be a commutative semiring. Then

$$\operatorname{\mathsf{pool}}\left(z_I:I\in\binom{[n_{\mathsf{in}}]}{k}\right):=\bigoplus_{\substack{i_1<\dots< i_k\leq n_{\mathsf{in}}}}z_{i_1}^{\odot_{\mathbb{S}}\alpha_1}\odot_{\mathbb{S}}\dots\odot_{\mathbb{S}}z_{i_k}^{\odot_{\mathbb{S}}\alpha_k},$$

is calculable in $O(n_{in})$ -time.

Examples

■ Over the ring ℝ

$$\sum_{i_1 < \dots < i_k} z_{i_1}^{\alpha_1} \dots z_{i_k}^{\alpha_k},$$

→ iterated-sums signature (quasisymmetric functions)
This has a long history.

- Graham '13 "Sparse arrays of signatures for . . . ".
- Lyons, Ni, Oberhauser '14 "A feature set for streams . . . "
- various works by L Jin et al '15 on Chinese character recognition.
- Kiraly, Oberhauser '16 "Kernels for sequentially ordered data".
- Lyons, Oberhauser '17 "Sketching the order of events".
- D '13, D, Reizenstein '19 on invariant features.
- D,Ebrahimi-Fard, Tapia '19 "Time warping invariants".
- Kidger, Bonnier, Arribas, Salvi, Lyons '19 "Deep Signature Transforms".
- Toth, Bonnier, Oberhauser '20 "Seq2Tens".

In these works it progressively emerged that it is helpful to learn the signature-type features.

Paraphrasing

$$\rightsquigarrow \sum_{i_1 < \dots < i_k} f_{\theta_1}(z_{i_1}) \cdot \dots \cdot f_{\theta_k}(z_{i_k}).$$

with $f_{\theta}: \mathbb{R}^d \to \mathbb{R}$.

We propose to boil this down to the bare minimum needed, namely

distributivity and associativity,

to arrive at a richer set of features

$$\leadsto \bigoplus_{i_1 < \dots < i_k} f_{\theta_1}(z_{i_1}) \odot_{\mathbf{s}} \dots \odot_{\mathbf{s}} f_{\theta_k}(z_{i_k})$$

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Examples

Over the tropical semiring

$$\min_{i_1 < \dots < i_k} \left\{ \alpha_1 \cdot \mathbf{z}_{i_1} + \dots + \alpha_k \cdot \mathbf{z}_{i_k} \right\}$$

Leaving the strict setting of tropical-sums, we can do a learnable version of the visiting-cities example:

- Fix some embedding z_i of the visited cities in \mathbb{R}^d (e.g. one-hot-encoding).
- Introduce parametrized functions $f_{\theta}: \mathbb{R}^d \to \mathbb{R} \cup \{-\infty\}$,

$$\rightsquigarrow \max_{i_1 < i_2} \left\{ f_{\theta_1}\left(z_{i_1}\right) + f_{\theta_2}\left(z_{i_2}\right) \right\},$$

and learn θ_1, θ_2 .

Non-example

Not all type of sums work. For general nonlinear σ the sum

$$\sum_{i_1<\dots< i_k} \sigma(x_{i_1}+\dots+x_{i_k}),$$

cannot be efficiently computed, since one can frame NP-complete problems in this form:

Subset sum problem: Given $x_1, \ldots, x_n \in \mathbb{Z}$ is there a subset which sums to 0?

Sub-problem: Is there a k-subset that sums to 0?

$$\sum_{i_1 < \cdots < i_k} 1_{\{0\}} (x_{i_1} + \cdots + x_{i_k}).$$

If this would only cost $O(k \cdot n)$ we would get an $O(n + 2n + \cdots + nn) = O(n^2)$ algorithm.

Summary

Expressions of the from

$$\operatorname{pool}\left(K(x_I):I\subset\binom{n_{\operatorname{in}}}{k}\right)$$

extract meaningful, chronological information of time series. In this generality they are computationally untractable.

 Semirings provide a large class of examples that <u>are</u> tractable, namely

$$\bigoplus_{i_1 < \dots < i_k} f_{\theta_1}(x_{i_1}) \odot_{\scriptscriptstyle S} \dots \odot_{\scriptscriptstyle S} f_{\theta_k}(x_{i_k}).$$

Overview

Motive

Algebraic setting

Outlook

Algebraic setting

For $z_1, z_2, \dots \in \mathbb{S}$, s < t, we define a collection of values in \mathbb{S} , indexed by words in the alphabet \mathbb{N} ,

$$\left\langle \mathsf{ISS}^{\mathbb{S}}_{\mathsf{s},\mathsf{t}}(z), \mathsf{w} \right\rangle := \bigoplus_{\substack{\mathsf{s} < i_1 < \dots < i_k < t+1}} z_{i_1}^{\odot_{\mathsf{s}} \mathsf{w}_1} \odot_{\mathsf{s}} \dots \odot_{\mathsf{s}} z_{i_k}^{\odot_{\mathsf{s}} \mathsf{w}_k}.$$

For example

$$\left\langle \mathsf{ISS}_{s,t}^{\mathbb{S}}(z), 537 \right\rangle = \bigoplus_{s < h < \dots < h_3 < t+1} z_{i_1}^{\odot_s 5} \odot_s z_{i_2}^{\odot_s 3} \odot_s z_{i_3}^{\odot_s 7}$$

which in min-plus equals

$$\min_{s < i_1 < i_2 < i_3 < t < t+1} \{ 5 \cdot z_{i_1} + 3 \cdot z_{i_2} + 7 \cdot z_{i_3} \}.$$

$$\text{Recall: } z_1,z_2,\dots \in \mathbb{S}; \left\langle \mathsf{ISS}_{s,t}^{\mathbb{S}}(z),\mathbf{537} \right\rangle := \bigoplus\nolimits_{s < i_1 < i_2 < i_3 < t+1} z_{i_1}^{\odot,\mathfrak{s}} \odot_{\mathbf{s}} z_{i_2}^{\odot,\mathfrak{s}} \odot_{\mathbf{s}} z_{i_3}^{\odot,\mathfrak{s}}^{\mathsf{T}}.$$

 $\mathsf{ISS}^{\mathbb{S}}_{s,t}(z)$ is an element of $\mathbb{S}\langle\langle\mathbb{N}\rangle\rangle$, the space of formal, infinite sums of words (in the alphabet \mathbb{N}) with coefficients in \mathbb{S} :

$$\mathsf{ISS}_{s,t}^{\mathbb{S}}(z) = \sum_{w} c_{w} \ w,$$

with

$$c_{\mathsf{w}} := \bigoplus_{\mathsf{s} < i_1 < \dots < i_k < t+1} \mathsf{z}_{i_1}^{\odot_{\mathsf{s}} \mathsf{w}_1} \odot_{\mathsf{s}} \dots \odot_{\mathsf{s}} \mathsf{z}_{i_k}^{\odot_{\mathsf{s}} \mathsf{w}_k}.$$

$$\text{Recall: } z_1, z_2, \dots \in \mathbb{S}; \ \left\langle \mathsf{ISS}_{s,t}^{\mathbb{S}}(z), \mathbf{537} \right\rangle := \bigoplus\nolimits_{s < i_1 < i_2 < i_3 < t+1} z_{i_1}^{\odot_{\mathfrak{z}} 5} \odot_{\mathfrak{z}} \ z_{i_2}^{\odot_{\mathfrak{z}} 3} \odot_{\mathfrak{z}} \ z_{i_3}^{\odot_{\mathfrak{z}} 7}.$$

Theorem (DEFT '20)

(Quasi-shuffle identity)

$$\left\langle \mathsf{ISS}_{s,t}^{\mathbb{S}}(z), w \right\rangle \odot_{\scriptscriptstyle{\mathbb{S}}} \left\langle \mathsf{ISS}_{s,t}^{\mathbb{S}}(z), u \right\rangle = \left\langle \mathsf{ISS}_{s,t}^{\mathbb{S}}(z), w \star u \right\rangle$$

2 (Chen's identity) For s < t < u,

$$\left\langle \mathrm{ISS}_{s,u}^{\mathbb{S}}(z),w\right\rangle = \bigoplus_{w'\cdot w''=w}^{\mathbb{S}} \left\langle \mathrm{ISS}_{s,t}^{\mathbb{S}}(z),w'\right\rangle \odot_{\mathbb{S}} \left\langle \mathrm{ISS}_{t,u}^{\mathbb{S}}(z),w''\right\rangle$$

3 ISS $_{0}^{\mathbb{S}}(z)$ is invariant to inserting $\mathbf{0}_{\mathbb{S}}$ into z.

$$\text{Recall: } z_1, z_2, \dots \in \mathbb{S}; \ \left\langle \mathsf{ISS}_{\mathfrak{s}, \mathfrak{t}}^{\mathbb{S}}(z), \mathbf{537} \right\rangle := \bigoplus\nolimits_{\mathfrak{s} < i_1 < i_2 < i_3 < \mathfrak{t} + 1} \underbrace{z_{i_1}^{\circlearrowleft_{\mathfrak{s}} 5} \odot_{\mathfrak{s}} \ z_{i_2}^{\circlearrowleft_{\mathfrak{s}} 3} \odot_{\mathfrak{s}} \ z_{i_3}^{\circlearrowleft_{\mathfrak{s}} 7}}.$$

Quasi-shuffle:

$$32 \star 4 = 324 + 36 + 342 + 72 + 432$$

Theorem (DEFT '20)

1 (Quasi-shuffle identity)

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ISS $_{0,\infty}^{\mathbb{S}}(z)$ is invariant to inserting $\mathbf{0}_{\mathbb{S}}$ into z.

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Quasi-shuffle:

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32 * 4 = 324 + 36 + 342 + 72 + 432

2 (Chen's identity) For s < t < u,

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ISS $_{0,\infty}^{\mathbb{S}}(z)$ is invariant to inserting $\mathbf{0}_{\mathbb{S}}$ into z.

Concatenation:

$$32 \cdot 4 = 324$$

Quasisymmetric functions

Using formal variables Z_1, Z_2, \ldots , the expressions

$$\bigoplus_{s < i_1 < \dots < i_k < t+1} Z_{i_1}^{\odot_s w_1} \odot_s \dots \odot_s Z_{i_k}^{\odot_s w_k}$$

are quasisymmetric expressions.

This is the monomial basis.

Over a ring there are many bases (monomial, fundamental, ..). This does not work over a semiring (there is no additive inverse).

In the monomial basis, the product is given by the quasi-shuffle.

Summary

■ In the special case of monomial f, we are led to the iterated-sums signature over a semiring

$$\left\langle \mathsf{ISS}^{\mathbb{S}}_{\mathsf{s},t}(\mathsf{z}), \mathsf{w} \right\rangle = \bigoplus_{\mathsf{s} < i_1 < \dots < i_k < t+1} \mathsf{z}_{i_1}^{\odot_{\mathtt{S}} \mathsf{w}_1} \odot_{\mathtt{s}} \dots \odot_{\mathtt{s}} \mathsf{z}_{i_k}^{\odot_{\mathtt{S}} \mathsf{w}_k}.$$

■ This is the evaluation of quasisymmetric function expressions on the time series. Almost all properties of the classical setting survive (they mostly depend on the structure of the index set ..).

Motive

Algebraic setting

Outlook

Structure of quasisymmetric functions Log signature Multidimensional time series Controlled systems Dynamic programming

Structure of quasisymmetric functions

Over a ring, polynomial expressions correspond to polynomial functions. This is in general not true over semirings.

Example

On the tropical semiring we have that the different polynomial expressions

$$X_1^{\odot 2} \oplus X_2^{\odot 2}$$
 and $X_1^{\odot 2} \oplus X_2^{\odot 2} \oplus (X_1 \odot X_2)$,

yield the same functions, since for all $x_1, x_2 \in \mathbb{S}$

$$\min\{2 \cdot x_1, 2 \cdot x_2\} = \min\{2 \cdot x_1, 2 \cdot x_2, x_1 + x_2\}.$$

Q: To what extend can we identify quasisymmetric expressions with quasisymmetric functions?

(compare Kalisnik, Lesnik - 2019 - Symmetric polynomials in tropical algebra semirings)

Log signature

There is no log signature, since there is no minus.

More concretely, over the tropical semiring

$$\left(\left\langle \mathsf{ISS}^{\mathbb{S}}(z), 1 \right\rangle\right)^{\odot_{\mathbb{S}} 2} = \left\langle \mathsf{ISS}^{\mathbb{S}}(z), 11 \right\rangle \oplus_{\mathbb{S}} \left\langle \mathsf{ISS}^{\mathbb{S}}(z), 2 \right\rangle$$

But knowing both

$$\left(\left\langle \mathsf{ISS}^{\mathbb{S}}(z), 1 \right\rangle\right)^{\odot_{\mathbb{S}} 2} = 2 \min_{i} z_{i}$$
$$\left\langle \mathsf{ISS}^{\mathbb{S}}(z), 2 \right\rangle = 2 \cdot \min_{i} z_{i},$$

we can clearly not deduce the value of

$$\langle \mathsf{ISS}^{\mathbb{S}}(z), \frac{11}{2} \rangle = \min_{i_1 < i_2} \{ z_{i_1} + z_{i_2} \}.$$

Q: How to extract the "minimal" information contained in the signature?

Multidimensional time series

Multidimensional time series can be treated as usual, by projecting the time series to coordinates before calculating the iterated-sums.

In the semiring setting a more interesting approach seems possible, by considering a time series as taking values in a larger semiring.

One example is via the map

$$\mathbb{R}^d o ext{ bounded convex polytopes}$$
 $x \mapsto \{x\}.$

The resulting time series can then be considered in the semiring of polytopes.

Q: In what semirings to embed a time series?

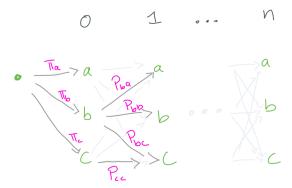
Controlled systems

The iterated-integrals signature has close relation to controlled ODEs, and iterated-sums over a ring appear in discretized dynamic systems.

There is a vast literature on discrete control over semirings.

Q: Is there a relation of the $ISS^{\mathbb{S}}$ to discrete control theory in a semiring?

Consider a time-homogeneous Markov chain X_i on states $\{a, b, c\}$.



A costly way to get the terminal distribution is

$$\mathbb{P}[X_n = a] = \sum_{w \in \{a,b,c\}^{n+1}} \pi_{w_0} p_{w_0 w_1} \dots p_{w_{n-1} w_n} \quad \leadsto O(3^n) \not$$

There is, of course, a more economic way:

$$\mathbb{P}[X_n = a] = \mathbb{P}[X_{n-1} = a] \cdot p_{aa} + \mathbb{P}[X_{n-1} = b] \cdot p_{ca} + \mathbb{P}[X_{n-1} = c] \cdot p_{ba}.$$

Iterating, one gets an O(n) algorithm.

By changing the semiring one gets other quantities. For example, in the possibilistic semiring, the most probable path ending at a:

$$\max_{w \in \{a,b,c\}^{n+1}, w_n = a} \pi_{w_0} \cdot p_{w_0 w_1} \cdot p_{w_1 w_2} \cdot \dots \cdot p_{w_{n-1} w_n}$$

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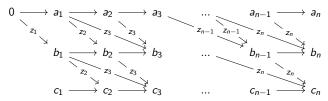
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Iterating, one gets an O(n) algorithm.

By changing the semiring one gets other quantities. For example, in the possibilistic semiring, the most probable path ending at *a*:

$$\max_{w \in \{a,b,c\}^{n+1}, w_n = a} \pi_{w_0} \cdot p_{w_0 w_1} \cdot p_{w_1 w_2} \cdot \dots \cdot p_{w_{n-1} w_n}.$$

We can embed the iterated-sums in such a framework: Let $z_1, ..., z_n$ be a time series in a semiring S. Consider



where all horizontal edges have weight $\mathbf{1}_{s}$.

W(m) := the sum of weight of all paths from 0 to m.

Then

$$\begin{split} W(c_2) &= z_1 \odot_{\scriptscriptstyle S} z_2 \\ W(c_3) &= z_1 \odot_{\scriptscriptstyle S} z_2 \odot_{\scriptscriptstyle S} \mathbf{1}_{\scriptscriptstyle S} \oplus_{\scriptscriptstyle S} z_1 \odot_{\scriptscriptstyle S} z_3 \oplus_{\scriptscriptstyle S} \mathbf{1}_{\scriptscriptstyle S} \odot_{\scriptscriptstyle S} z_2 \odot_{\scriptscriptstyle S} z_3 \\ &= z_1 \odot_{\scriptscriptstyle S} z_2 \oplus_{\scriptscriptstyle S} z_1 \odot_{\scriptscriptstyle S} z_3 \oplus_{\scriptscriptstyle S} z_2 \odot_{\scriptscriptstyle S} z_3 \\ W(c_n) &= \left\langle \mathsf{ISS}^{\mathbb{S}}(z), 11 \right\rangle. \end{split}$$

Note that the "naive" dynamic programming still has superlinear cost (too many paths ..), but one can (ad-hoc) reduce the graph to see the linear cost.

Q: Is there a deeper connection to the dynamic programming?

Thank you!