Transition path theory: diagnosing random systems

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MSN Tech Talk
April 18, 2024

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(this version of the slides has some embedded images removed)

Random Systems

Definition (sort of)

A process is random when identical conditions can lead to different outcomes.

Intrinsic: That's just how it is, and we like it that way. E.g. Quantum mechanics (some interpretations).

Parameterized ignorance: Something is going on under the hood, but it's difficult or impossible to take it into account. E.g. flipping a coin. (but, see Diaconis et al., 2007)

Existential dread: Maybe there's no such thing as "identical conditions" in the first place? E.g. (possibly) everything.

Why we care about randomness: Random processes provide a tool to model arbitrarily complicated phenomenon without having to "really" know what's going on.

Why we care about TPT: it's a measurement and diagnostic tool that acts on random processes.

Markov Chains: Background I

Definition

A discrete time Markov Chain is a sequence of random variables $\{X_n\}_{n\geq 0}$ such that $P(X_{n+1} = x_{n+1}|X_1 = x_1, X_2 = x_2 \ldots X_n = x_n)$ is equal to $P(X_{n+1} = x_{n+1}|X_n = x_n)$. This is the "Markov property" or "memorylessness.".

Idea: A Markov chain is when something is happening randomly and what happens *next* only depends on what is happening *now*.

A Markov chain is a good model for everything.

Well, okay, not *everything*, but a lot.

Markov Chains: Background II

https://en.wikipedia.org/wiki/Snakes_and_ladders

Figure: The board game *Snakes and Ladders* is a discrete-time Markov chain on the location of the player's piece, $\{1, 2 \ldots 100\}$.

Example: The probability of landing on square 10 if you are at square 8 is $1/6$ regardless of how you ended up at square 8.

Transition Path Theory: Motivation

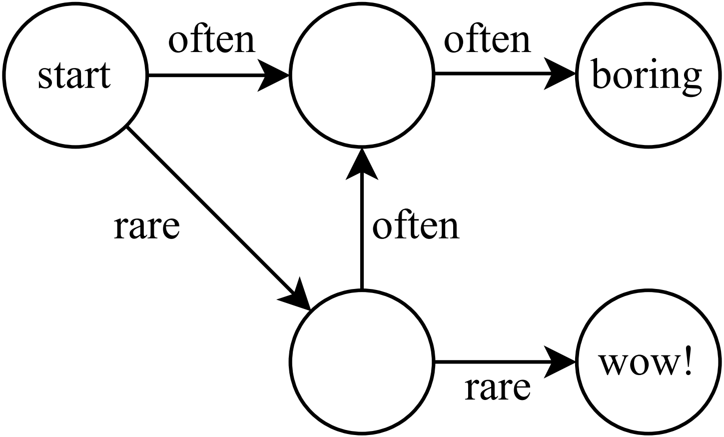

Figure: The boring state will be reached very often. But we aren't interested in that.

Transition Path Theory: Motivation

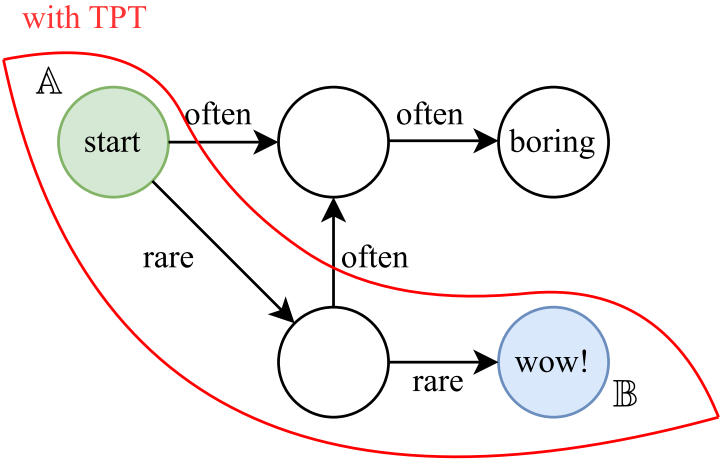

Figure: TPT allows us to look at paths between specific sources $\mathbb{A}$ and targets $\mathbb{B}$.

Transition Path Theory: Reactive Trajectories

Definition

A trajectory through a Markov chain is called reactive if it starts in a source state $\mathbb{A}$, ends in a target state $\mathbb{B}$ and doesn't enter $\mathbb{A}$ or $\mathbb{B}$ at any other time.

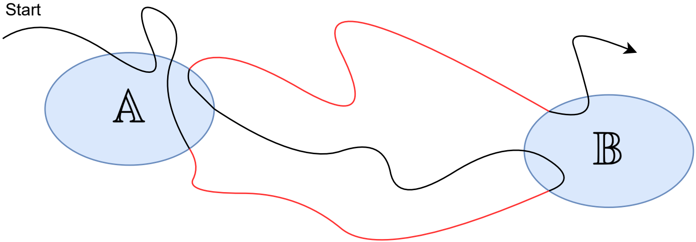

Figure: Reactive trajectory segments highlighted in red.

Basic quantities (see Helfmann et al., 2020 for a detailed review) are

- The reactive density, showing where reactive trajectories spend the most time.
- The forward current, showing where reactive trajectories "flow."
- The transition time.

Transition Path Theory: Summary

Punchline: If we have a Markov chain, we can apply TPT to see how trajectories move from a given source to a given target in the chain.

Applications:

- Markov Decision Processes
- Ocean drifters
- Molecular dynamics
- Extreme weather events
- many more ...

Application 1: MDPs

See notebook.

Application 2: *Sargassum* I

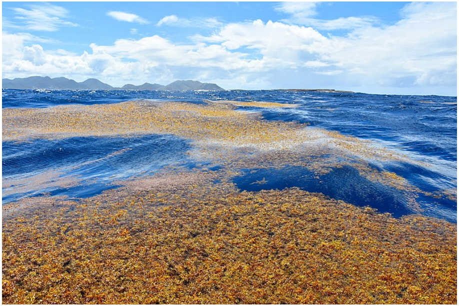

Figure: Rafts of *Sargassum* floating in the Carribean Sea.

Observation: Since 2011, islands in the Caribbean Sea and beaches in South Florida were inundated with abnormally large quantities *Sargassum*

Problem: To understand the transport of *Sargassum* by the ocean.

Application 2: *Sargassum* II

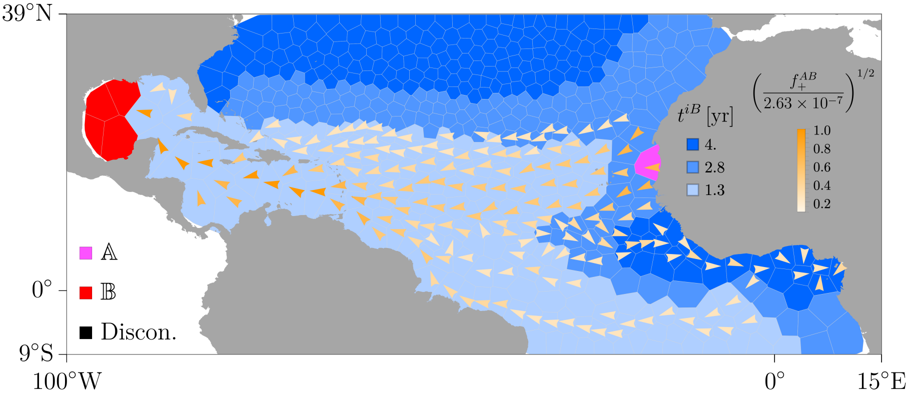

Figure: *Sargassum* transport in the North Atlantic [Bonner et al., 2023].

Application 3: Molecular dynamics

Figure 5 of Lorpaiboon et al., 2022

Figure: Overdamped Langevin dynamics. (a) Traditional TPT, (b) TPT with intermediate states [Lorpaiboon et al., 2022].

Application 4: Rare weather events

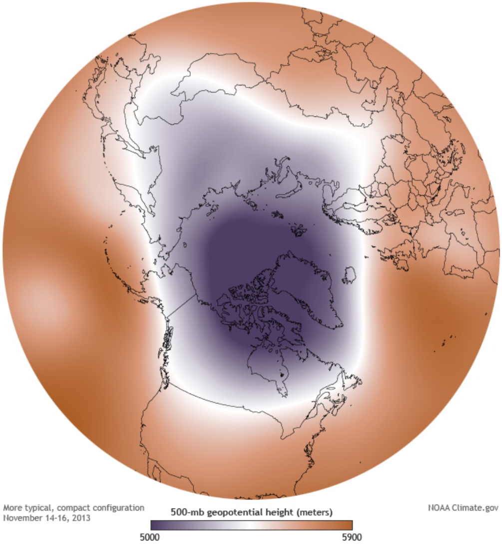

Figure: Polar vortex in the Northern hemisphere.

Application 4: Rare weather events

Figure 4 of Finkel et al., 2023

Figure: Sudden stratospheric warming. [Finkel et al., 2023].

Summary

TPT: A number of applications across diverse fields.

Computation: The basic statistics are easily calculated in a fast and efficient manner.

SCAN ME

https://github.com/70Gage70/TPTApplications

References

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