Transition path theory: diagnosing random systems

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Random Systems

Definition

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.

Markov Chains: Background III

What kinds of things do we calculate?

Distributions: What are the chances of being in a particular state after a set amount of time?

Long-term behavior: Where do things "settle" after a long time?

First passage: When does the *first* visit to a state tend to happen?

Problems:

Paths: It's not entirely clear how individual trajectories "actually" travel between a given initial and final states, or at least it might be hard to simulate.

Rare events: What if the behavior you're interested in is very unlikely to happen?

Enter TPT.

Transition Path Theory: Background

Definition

Let $\mathbb{A}$ and $\mathbb{B}$ be some non-intersecting subsets of the state space of a Markov chain. We will call $\mathbb{A}$ the source and $\mathbb{B}$ the target.

Definition

A trajectory through a Markov chain $(X_n, X_{n+1} \ldots X_{n+\ell})$ is called reactive if $X_n \in \mathbb{A}$, $X_{n+\ell} \in \mathbb{B}$ and $\mathbb{A}$ and $\mathbb{B}$ are not visited at any other time.

Definition

Transition Path Theory is a framework which allows us to calculate various statistics related to reactive trajectories.

Transition Path Theory: Reactive Trajectories

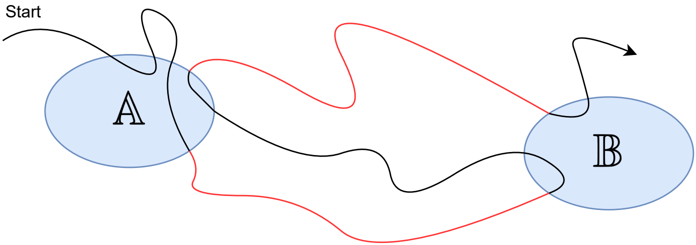

Figure: Schematic of paths through a Markov chain with reactive trajectories highlighed in red.

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, t^{AB}.

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

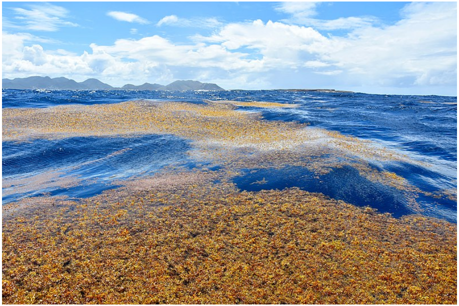

Figure: Rafts of *Sargassum* floating in the Carribean Sea.

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

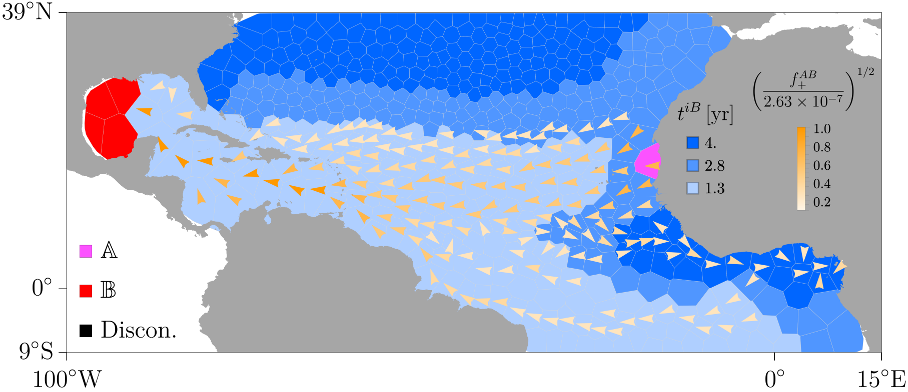

Figure: *Sargassum* transport in the North Atlantic [Bonner et al., 2023].

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 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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