Correlating topology and performance of membrane filter pore networks

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Abstract

We investigate the correlation between the performance of membrane filter pore networks and their topological properties, in order to discover optimal pore topologies for membrane filter design.

We use persistent homology as our principal tool for quantifying topological features, where the radii of a network's pores are represented by a collection of points in two-dimensional space known as a *persistence diagram*. The data encoded in these persistence diagrams are then statistically correlated with certain performance metrics, particularly with total throughput of filtrate.

Under random pore-size variations, total persistence (one particular topological measure) is found to be positively correlated with total throughput and membrane porosity.

Motivation

Identification of optimal pore network structures that optimize membrane filter performance, based on measures of their topological features. Such measures include *total persistence*, *persistence landscapes*, and *Euler characteristics.*

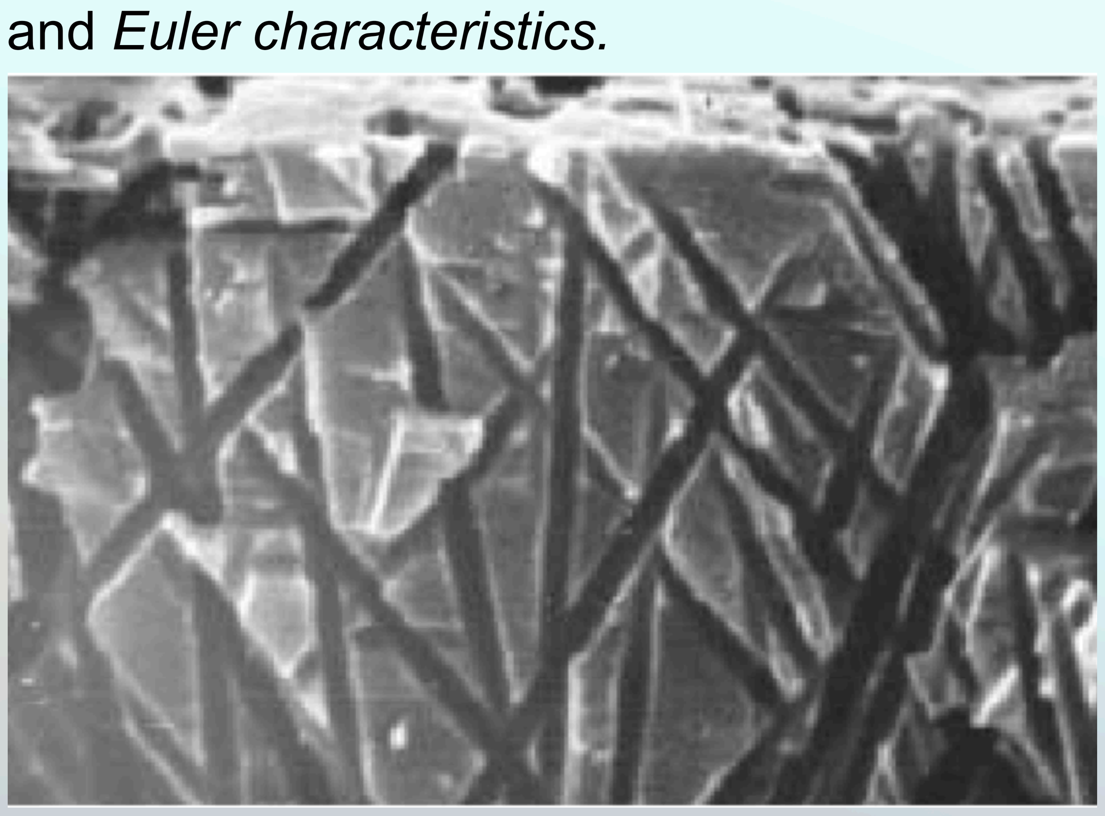

Fig. 1: Two-dimensional cross-section of a membrane filter with network-type pore structure [1].

Persistence Diagrams

- An increasingly popular tool in topological data analysis.
- Persistence diagrams (PDs) depict the *birth* and *death* (i.e. the appearance and disappearance, respectively) of topological features.
- Birth and death occur as a *thresholding parameter* θ decreases from ∞ down to 0. Here, θ ranges over values of the pore radii.
- The topological features of interest are *connected components* (sets of connected pores in a network), and *loops* (cycles of network pores).
- The longer-lived features are considered to be more significant than shorter-lived features.

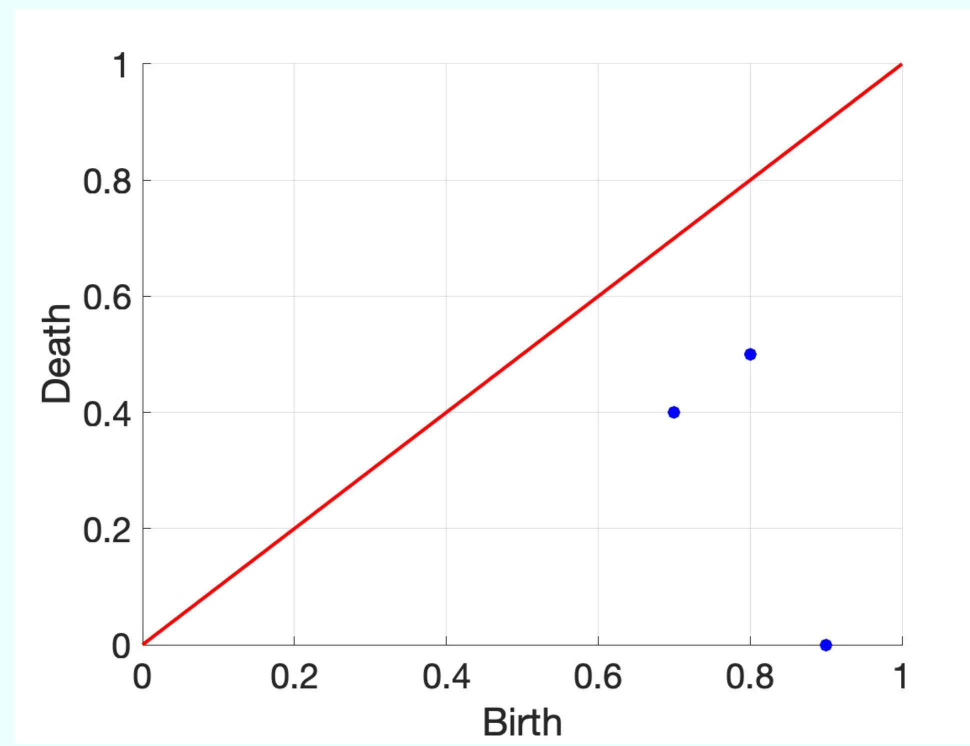

Fig. 2: Example of the persistence diagram for a simple network.

Definitions

A feed solution is driven by a fixed pressure through the pore network, carrying impurities at a certain concentration. The foulant particles adhere to the inner pore walls, shrinking them until the fluid can no longer pass through the filter.

The effect of random (log-normal) pore size variations is investigated by choosing a "typical" network and perturbing its pore radii 1000 times. We refer to this approach as "*noise variation*".

Key quantities of interest are:

$$h(t) = \frac{1}{\lambda}\int_0^t q_{out}(t')dt', \quad q_{out}(t) = \sum_{v_j \in V_{out}} \sum_{v_i:(v_i,v_j)\in E} \boldsymbol{q}_{ij}(t)$$

$$\phi = \pi \sum_{(v_i,v_j)\in E} r_{ij}^2 l_{ij}, \quad \mathrm{TP}_i = \left[\sum_{k=1}^{B_i} (b_k - d_k)^p\right]^{1/p}$$

$h(t)$: *Total throughput* (flux through the filter up to time *t*)

λ : Foulant adsorption rate at pore walls

$v_i \in V_{out}$: Network nodes in the lower membrane surface

$(v_i, v_j) \in E$: Network edges (filter pores)

$q_{ij}(t)$: Flux through pore (v_i, v_j) at time *t*

ϕ : *Porosity* (normalized sum of the pores' volumes).

r_{ij}, l_{ij} : Radius and length of pore (v_i, v_j)

TP_i : *Total persistence* of i^{th} PD

(b_i, d_i) : Coordinates of a persistence diagram

B_i : Number of generators in i^{th} PD

Results

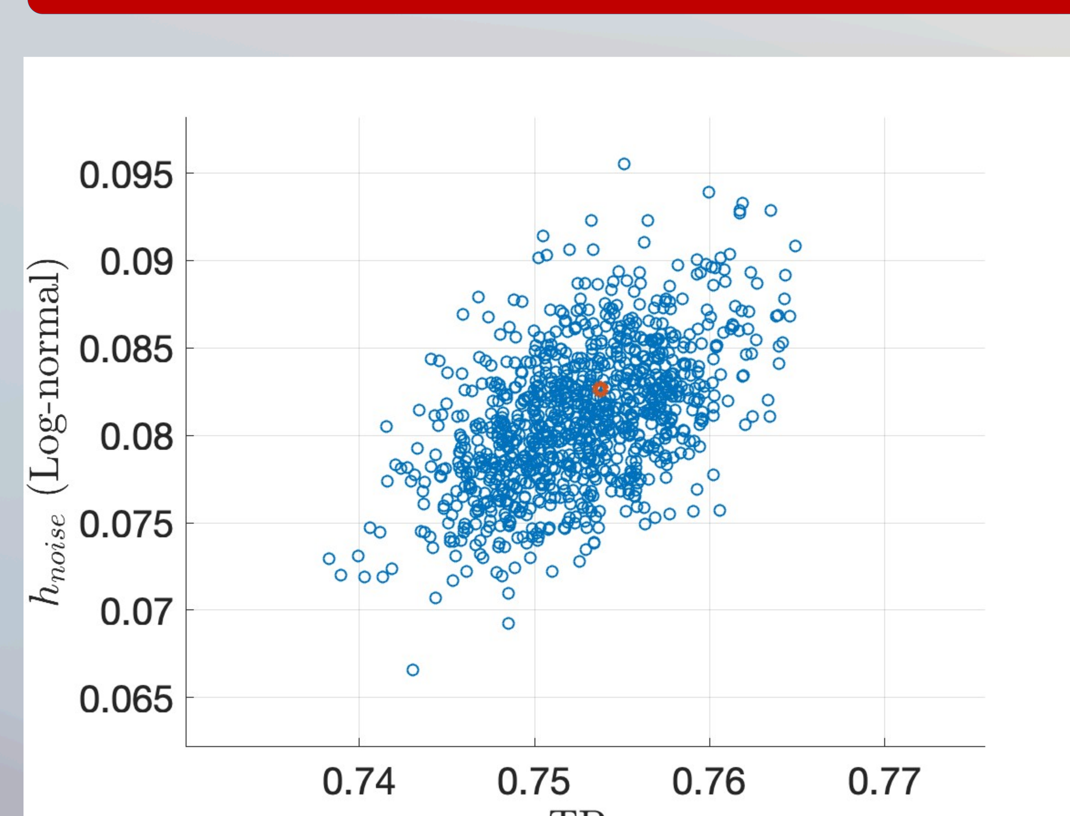

Fig. 3: Total throughput vs. total persistence.

Under noise perturbations and for loops, there is a positive correlation between total throughput and total persistence (TP_1).

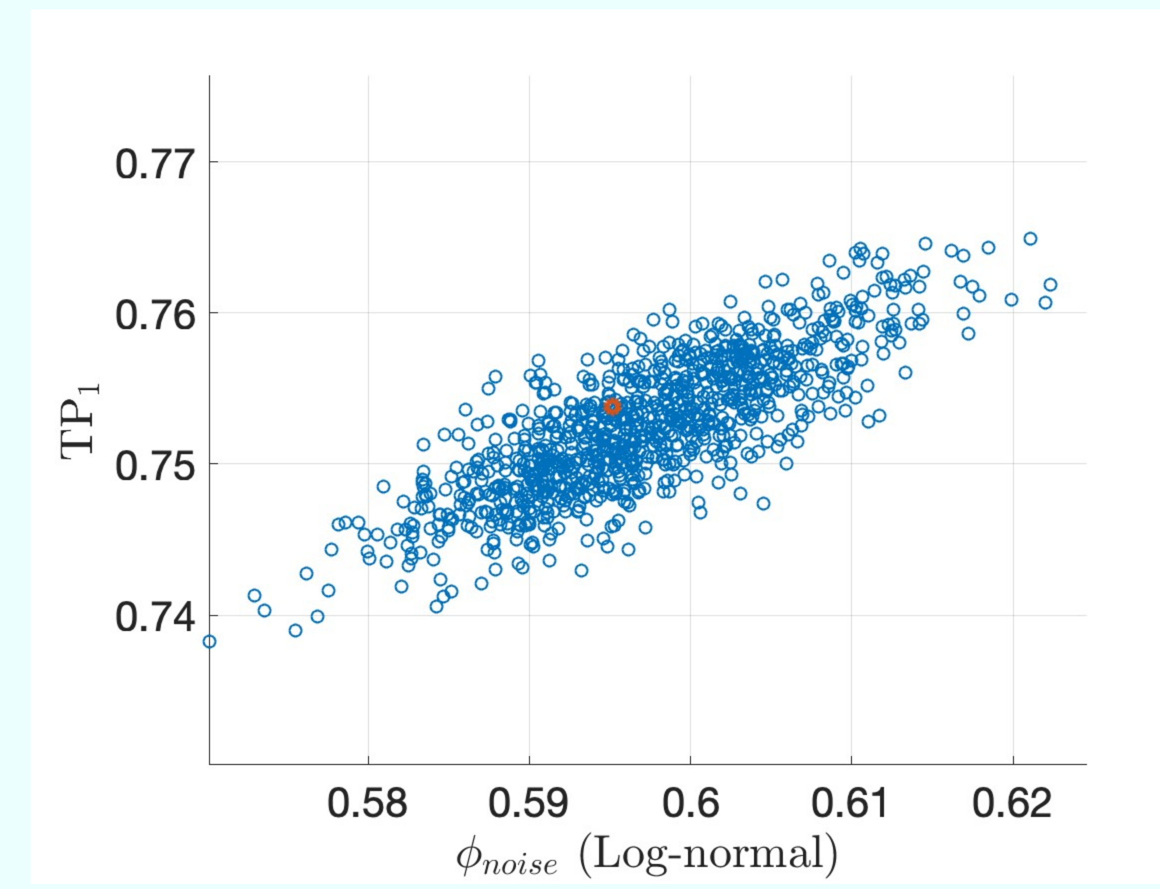

Fig. 4: Total persistence (loops) vs. porosity.

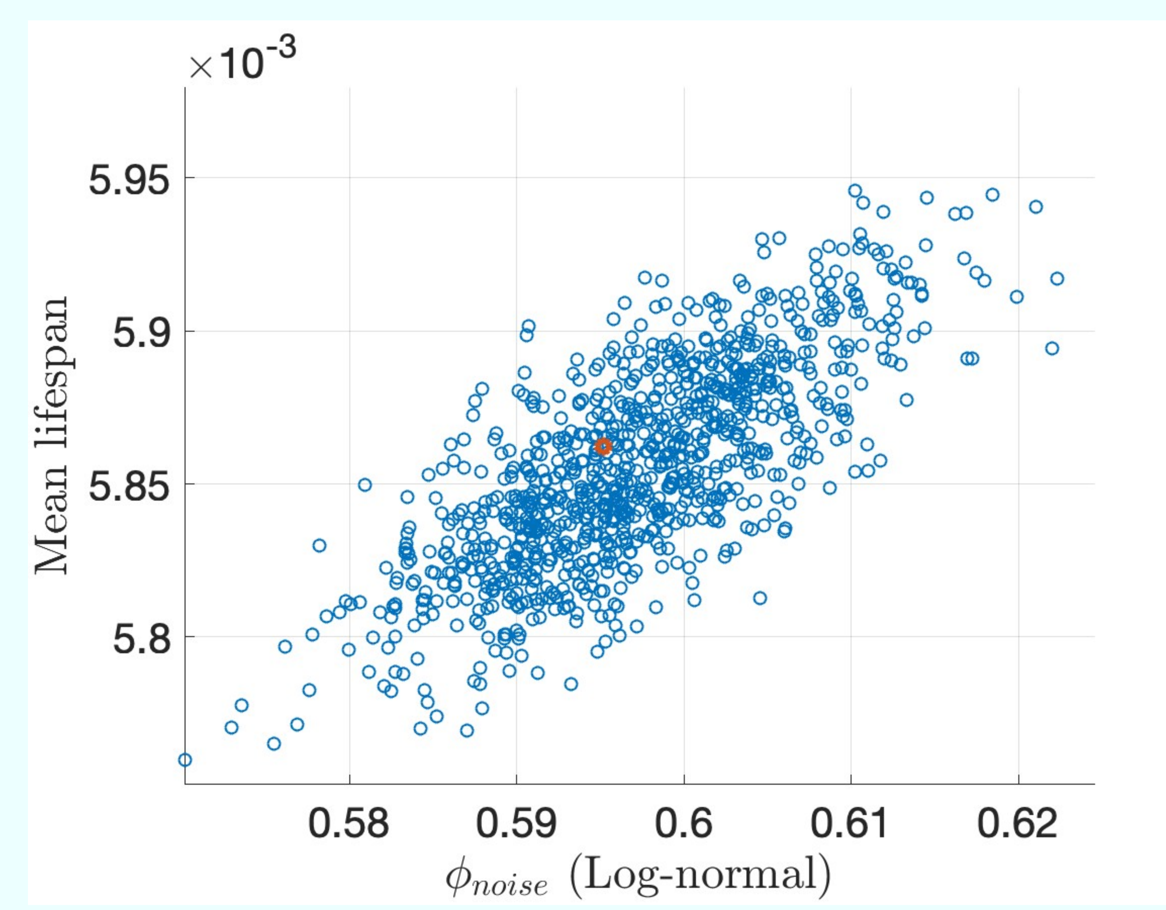

Fig. 5: Mean lifespan $(b_i - d_i)$ *vs. porosity.*

Summary

Total persistence has some predictive power for determining total throughput.

This predictive power is mostly restricted to noise variations and loops.

Correcting for porosity variations due to pore size variations may change the results.

Future Work: We will try other, more complex measures than total persistence. We will also simulate larger systems, to reduce the noise in our results.

References

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