Correlating topology and performance of membrane filter pore networks

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Abstract

We investigate the correlation of the filtration performance of membrane filters, as influenced by their internal pore network structure (see Fig. 1), 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 key features of a network's pores are represented by a collection of two-dimensional points known as a *persistence diagram* (PD). The data encoded in these PDs are then statistically correlated with certain performance metrics, particularly with total throughput of filtrate over the filter lifetime.

Under random pore-size variations, the number of loops in a pore network (a particular topological feature) is found to be correlated with total throughput. Topological features are also found to be important even for fixed geometric features.

Motivation

Identification of optimal pore network structures that optimize membrane filter performance, based on measures of their topological features.

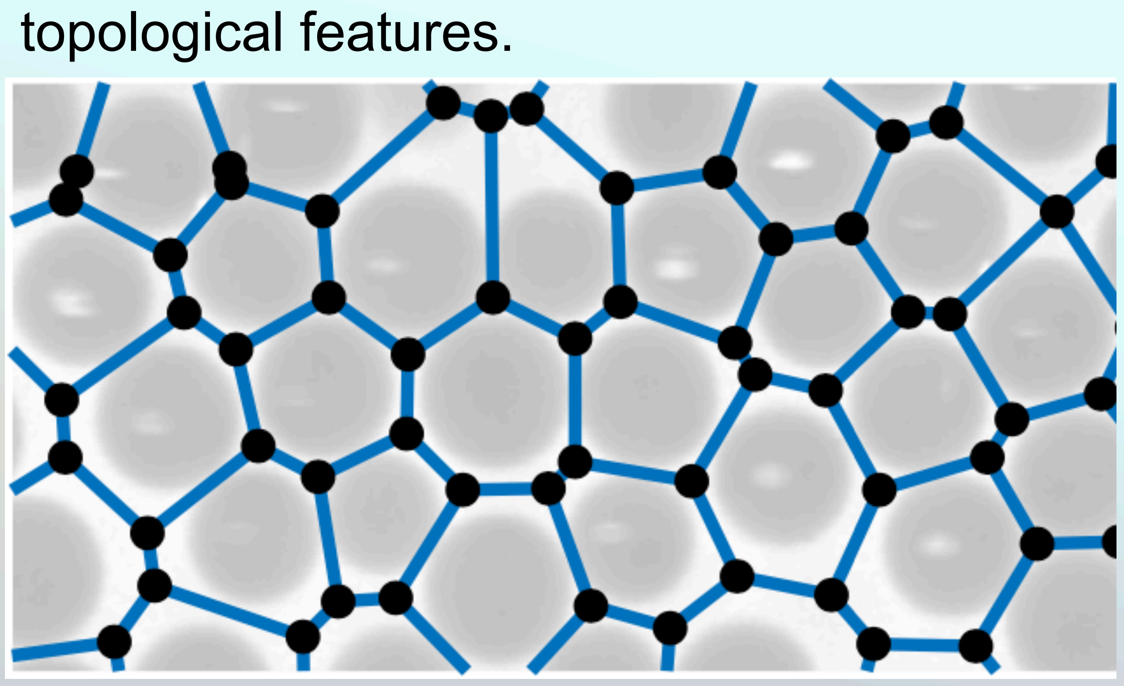

Fig. 1: Illustration showing how the internal pore structure of a real porous medium can be represented by a network of pores (circular cylinders) [1].

Persistence Diagrams

- An increasingly popular tool in topological data analysis.
- PDs depict the *birth* and *death* (i.e. the appearance and disappearance, resp.) of features under thresholding.
- Here we threshold on the pore radii: as the thresholding parameter θ decreases from ∞ down to 0, topological features are born and die.
- The topological features of interest are *connected components* (sets of connected pores in a network), and *loops* (cycles of network pores).
- Features that live longer under thresholding are more significant than shorter-lived ones.

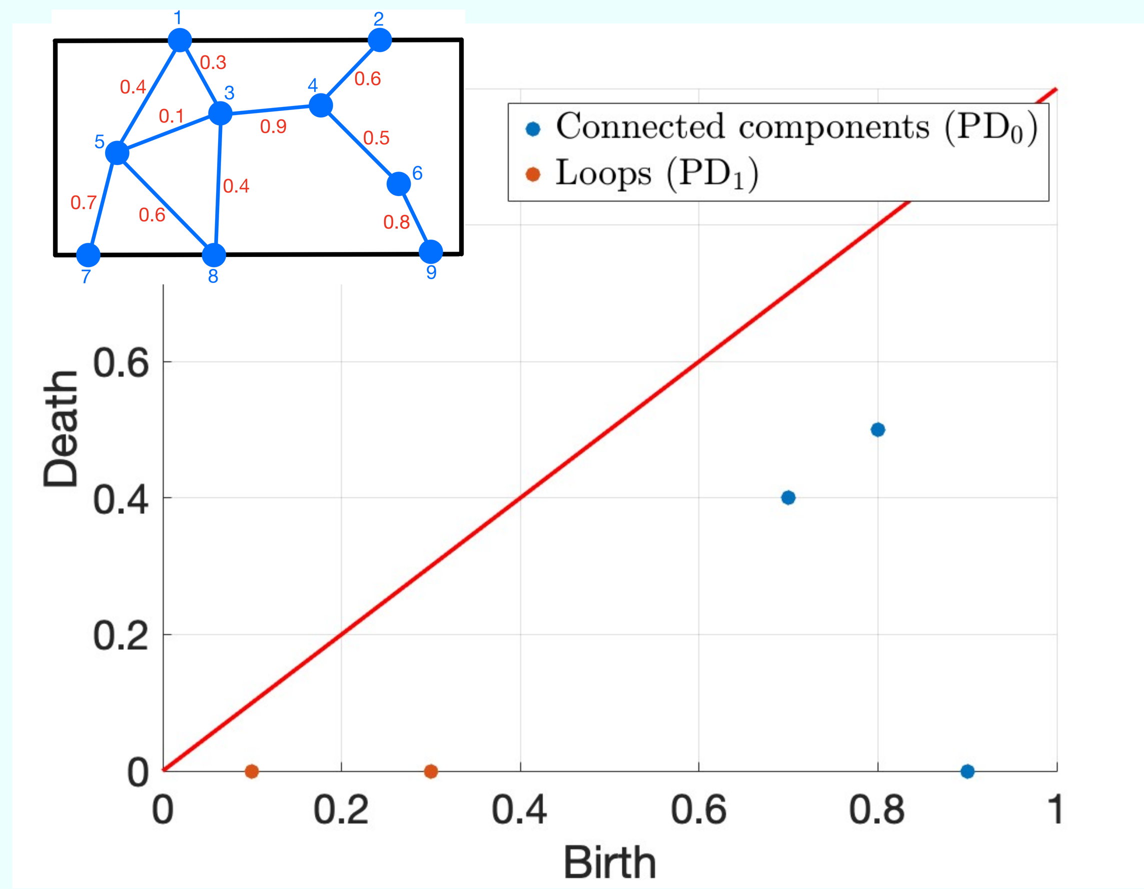

Fig. 2: Example of the persistence diagrams for a simple network (top left; pore radii shown in red).

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 variations is investigated by generating 1000 different networks and perturbing their radii independently, using the log-normal distribution.

The key measure of performance is *total throughput* h, given by:

$$h = \int_0^{t_{final}} q_{out}(t')dt', \quad q_{out}(t) = \sum_{v_j \in V_{out}} \sum_{v_i:(v_i,v_j)\in E} q_{ij}(t)$$

t_{final} : *The lifetime of the filter*

$v_j \in V_{out}$: *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*

The key topological measure is *the number of generators* in PD_1, NG_1 (*or the number of loops*).

The key geometric measures are:

NP : *Number of pores in a network*

$\bar{r}$: *Mean of pore radii at* $t = 0$.

Results

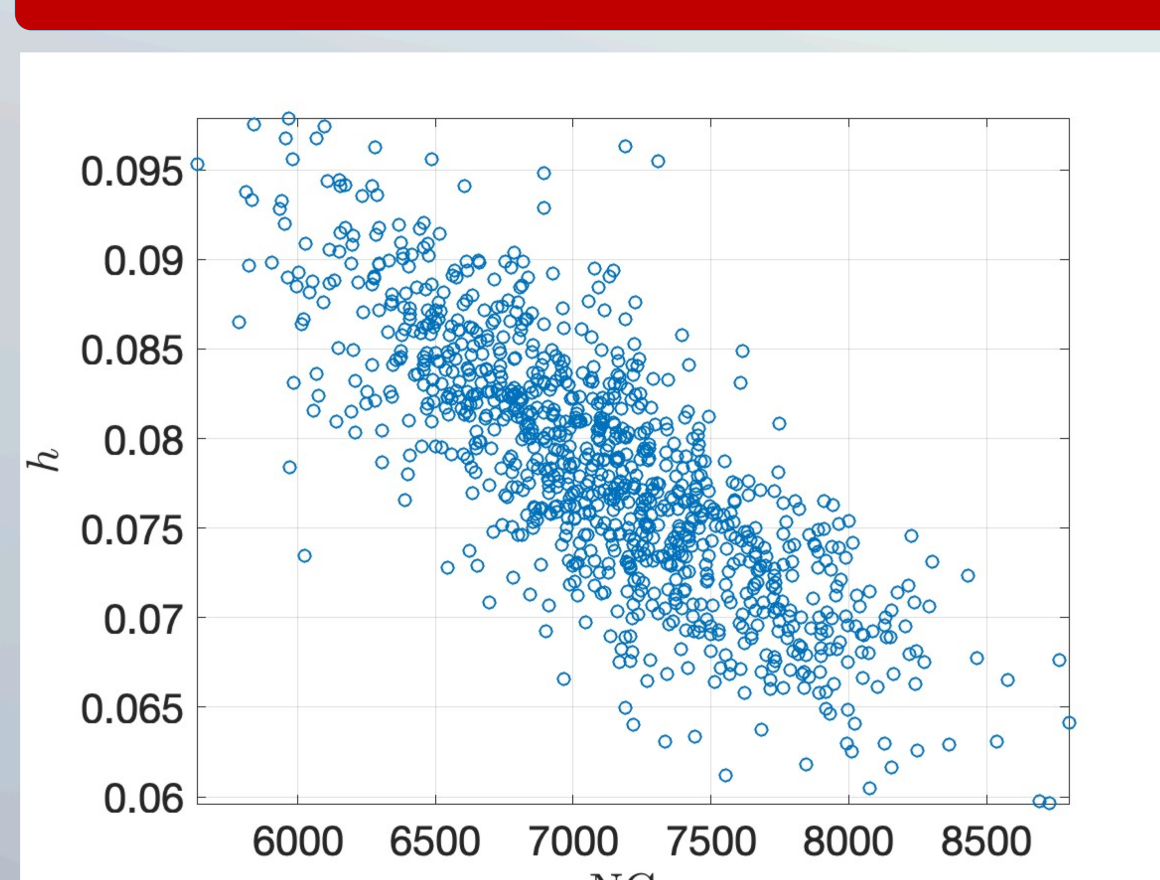

Fig. 3: Total throughput h *vs. number of loops* NG_1.

There is a strong negative correlation between total throughput and number of loops.

NG_1 and h are strongly correlated with geometrical network properties, such as mean radius $\bar{r}$ and number of pores NP. Therefore, to check that NG_1 correlates with h independently of these quantities, we scale h by each, and find that there remains a correlation with NG_1:

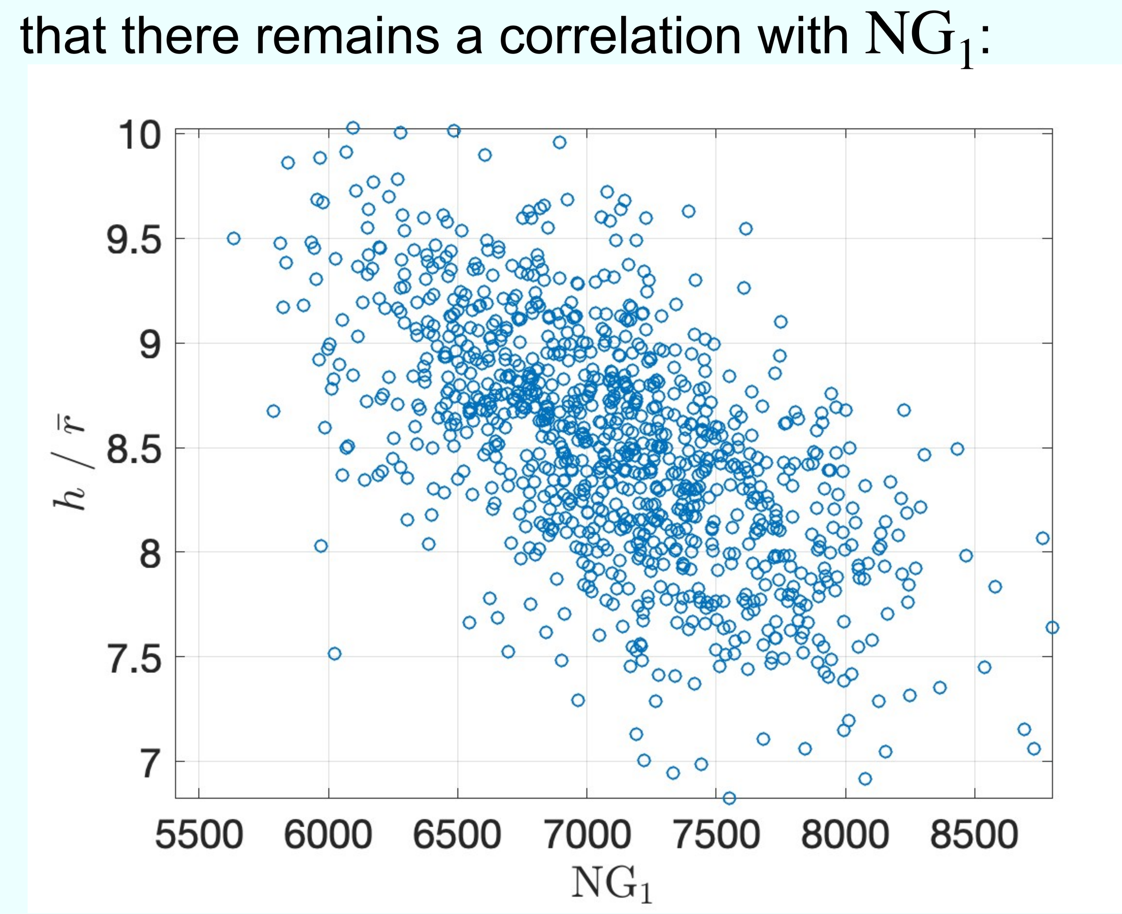

Fig. 4: Total throughput h *(scaled by mean pore radius* $\bar{r}$*) vs. number of loops* NG_1.

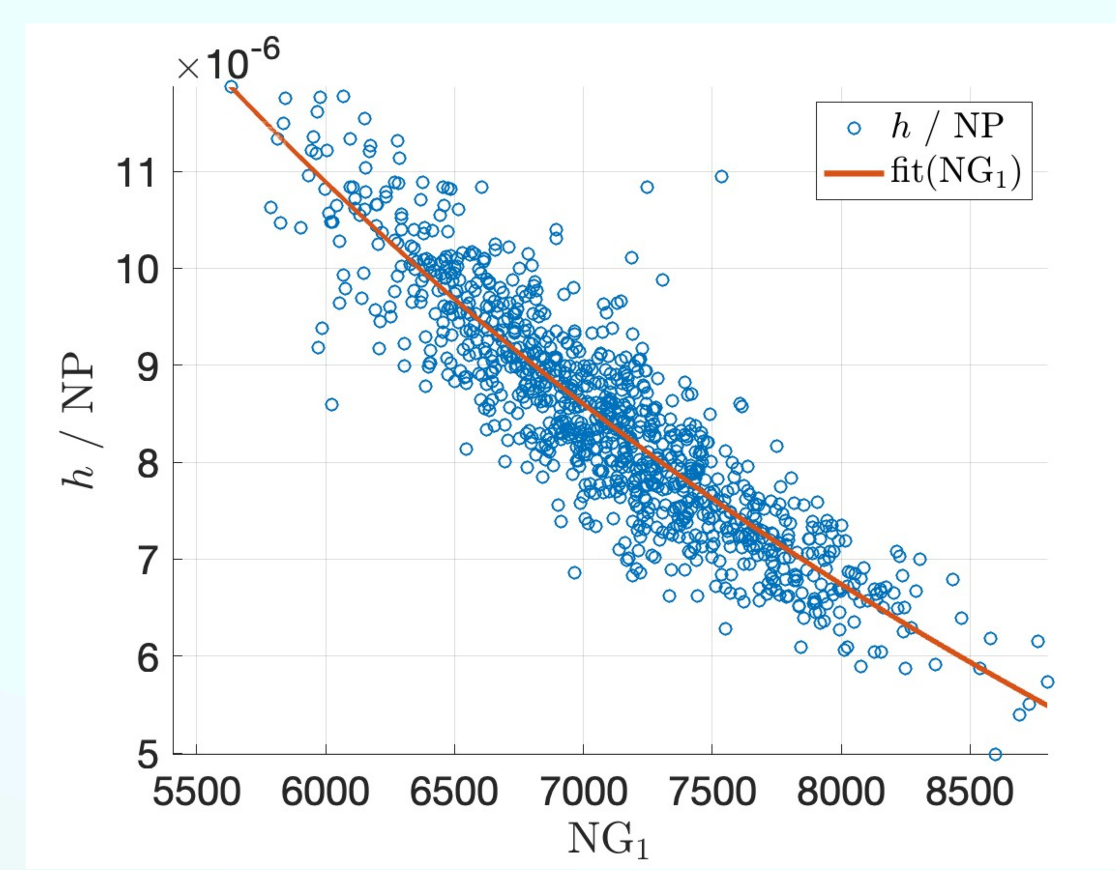

Fig. 5: Total throughput h *(scaled by number of pores* NP*) vs. number of loops* NG_1

Summary

- Loops in the pore network are a strong predictor of filtration performance.
- Network topology is important for filtration, independent of geometrical features.
- Future Work: We will investigate the evolution of topology over time, to further understand the implications of pore network topology for filtration performance.
- This includes the use of other topological measures, such as NG_0 and the Wasserstein distance.
- Further work could explore the effect of NG_1 on h at a fundamental topological level.

References

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