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A model ensemble generator to explore structural uncertainty in karst systems with unmapped conduits

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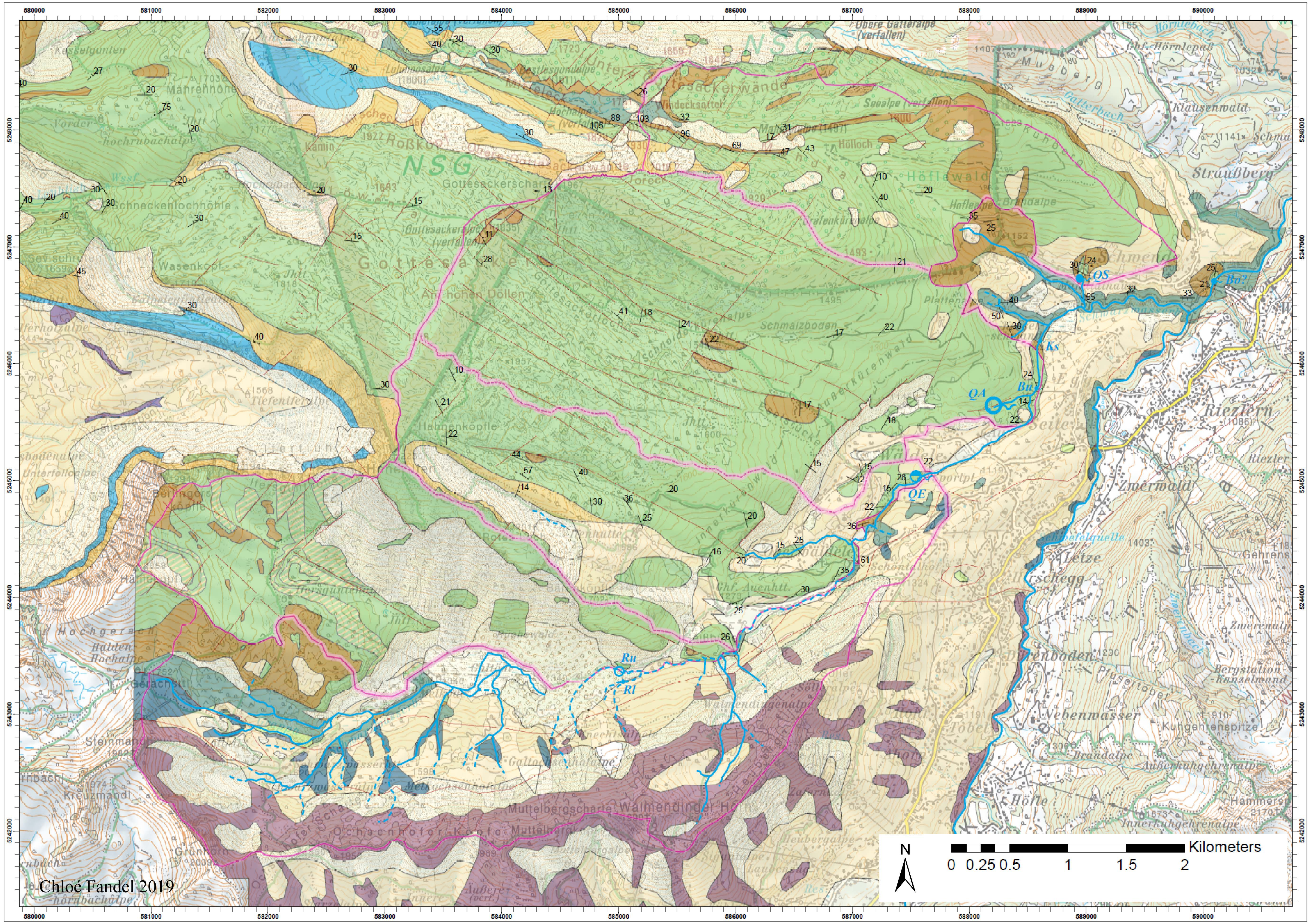
Text S1:
Links to GitHub repositories for GemPy, Karstnet, pyKasso, pysheds, and the code used for this paper.

GemPy: https://github.com/cgre-aachen/gempy
karstnet: https://github.com/UniNE-CHYN/karstnet
pyKasso: https://github.com/randlab/pyKasso
pysheds: https://github.com/mdbartos/pysheds
Gottesacker system ensemble generator & viewer: https://github.com/cfandel/gottesacker

Figure S1: Hydrogeologic map of the Gottesacker/Schwarzwasser valley area (and inset indicating original sources for different map areas) (next page)

Gottesacker karst system hydrogeology



Legend

Hydrology

- stream (permanent)
- stream (intermittent)
- spring (permanent)
- spring(intermittent)
- estavelle

Catchment boundaries

- major
- minor
- major (uncertain)
- minor (uncertain)

Geology

- strike & dip
- fault
- wetland
- alluvium
- scree
- rockfall
- glacial deposits
- Wang
- Amdener
- Garschella
- Schrattenkalk
- marl (transition)
- Drusberg
- Kieselkalk
- Palfris
- Liebensteiner
- Feuerstaetter
- Flysch

Data sources

- catchment boundaries
- Goldscheider 1997
- Huth 1998
- Tomsu 1998
- Sinreich 1998
- Geological Survey of Austria

Coordinate system: WGS 1984 UTM Zone 32N
Projection: Transverse Mercator
False easting: 500,000.000
Central meridian: 9.0000
Latitude of origin: 0.0000
Datum: WGS 1984
False Northing: 0.000
Scale Factor: 0.9996
Units: meter

Text S2: Explanation of k-means clustering.

K-means clustering groups observations (in this case, proposed conduit networks) into a pre-determined number of clusters, in which each observation belongs to the cluster with the nearest mean, minimizing the sum of squared distances from each point in the cluster to the center of the cluster (the within-cluster distance) (Kriegel et al. 2017). In this case, the conduit networks are grouped into ten clusters, over 48 dimensions (3 springs × 4 SKS runs × 4 discharge statistics). The minimum number of clusters needed can be determined by graphing the relationship between the number of clusters and the within-cluster distance, and visually determining at which point an increase in the number of clusters no longer results in a meaningful decrease in the within-cluster distance. This distance simply represents how "clumpy" the clusters are in multi-dimensional space. Lower within-cluster distances indicate more tightly clumped clusters, such that any one model picked from the cluster is likely to be fairly representative of the other models in the cluster. Higher within-cluster distances indicate that the cluster is more spread out, with each model in the cluster potentially quite different from the others, such that a single model picked from the cluster may not adequately represent the other models in the cluster. In this ensemble, based on the plot below, four clusters would have been sufficient, but ten clusters were chosen for a maximum representation of different networks given computational limitations. One conduit network was selected at random from each cluster, yielding a reduced ensemble of ten conduit networks for further flow modeling.

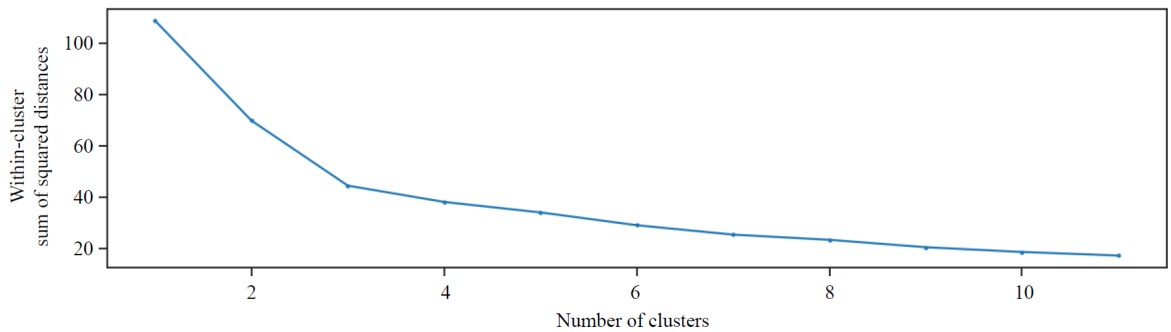


Figure S2: Minimum number of clusters needed to represent initial network ensemble

Text S3: Illustration of sum of squared distances (SSD) matrix calculations.

An example matrix of distance calculations between and across network structures: there are three networks (A, B, C), each with three parameter sets (i,j,k; l,m,n; o,p,q). First the SSD between each flow run on network A and each flow run on network B is calculated. This process is repeated for each possible pairing of networks and flow runs, such that a table of distances between models is produced. Each colored cell contains the sum of squared differences between the two models for that cell.
Taking the mean of the SSDs in the various highlighted zones gives the mean distance between models within versus across networks. The mean distance between flow runs within a network is the mean of the SSDs for all runs on that network.
The distance between network A and network B is the mean of the SSDs for all flow runs on both networks (i,j,k and l,m,n). The mean distance between networks is the mean of all of the distances in the table.

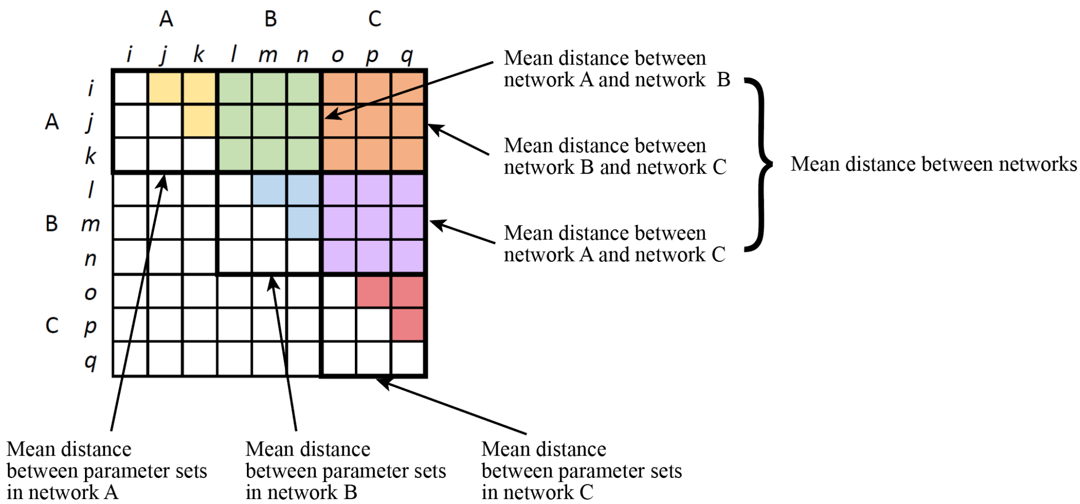


Figure S3: Example matrix of pairings for calculating the sum of squared distances between and across network structures.

ESM Reference

Kriegel, H.-P., Schubert, E., Zimek, A., 2017. The (black) art of runtime evaluation: Are we comparing algorithms or implementations? Knowl Inf Syst 52, 341–378. https://doi.org/10.1007/s10115-016-1004-2