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Principal Component Analysis (PCA) to compute major directions for 3D spatial analysis

November 15, 2023

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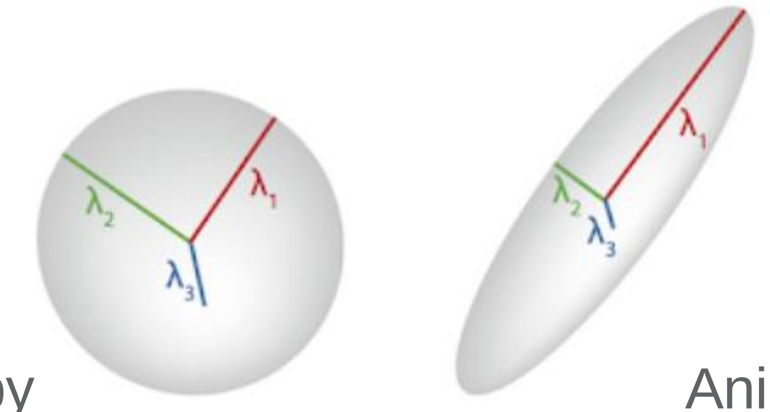
Introduction

- Accurate spatial modeling is crucial for predicting contaminant spread for subsurface environmental clean-up.

- 3D anisotropic models account for variation in a property in three principal directions.



- Traditionally, these directions are chosen through visual inspection of variograms.

- We present an automated method to objectively identify these three principal directions of anisotropy in 3D spatial data.

Principal Component Analysis (PCA)

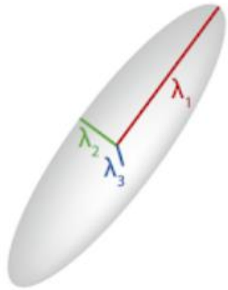
- Uses linear algebra to reduce dimensionality or extract prominent features.
- A covariance matrix is computed to establish the spread of variances between different variables/features.
- Eigenvalue decomposition of the covariance matrix → eigenvector matrix, which would rotate the coordinate system along the principal component.
- Moment of Inertia (MOI) method was explored to establish the spread of variance between the variable and its ‘2D/3D location’

Moment of Inertia (MOI) Method

- An MOI tensor is the sum of the mass distribution occurring in a rigid body rotating about the axes of rotation.
- Calculated by multiplying mass with its distance from the axis of rotation

$$I_{xx} = \sum_i m_i(y_i^2 + z_i^2)$$

- In spatial analysis, the mass is replaced by covariance volume.
- Smallest MOI → Principal direction of the MOI.



- Eigenvalue decomposition of the covariance matrix → eigenvector matrix, which would rotate the coordinate system along the principal component.

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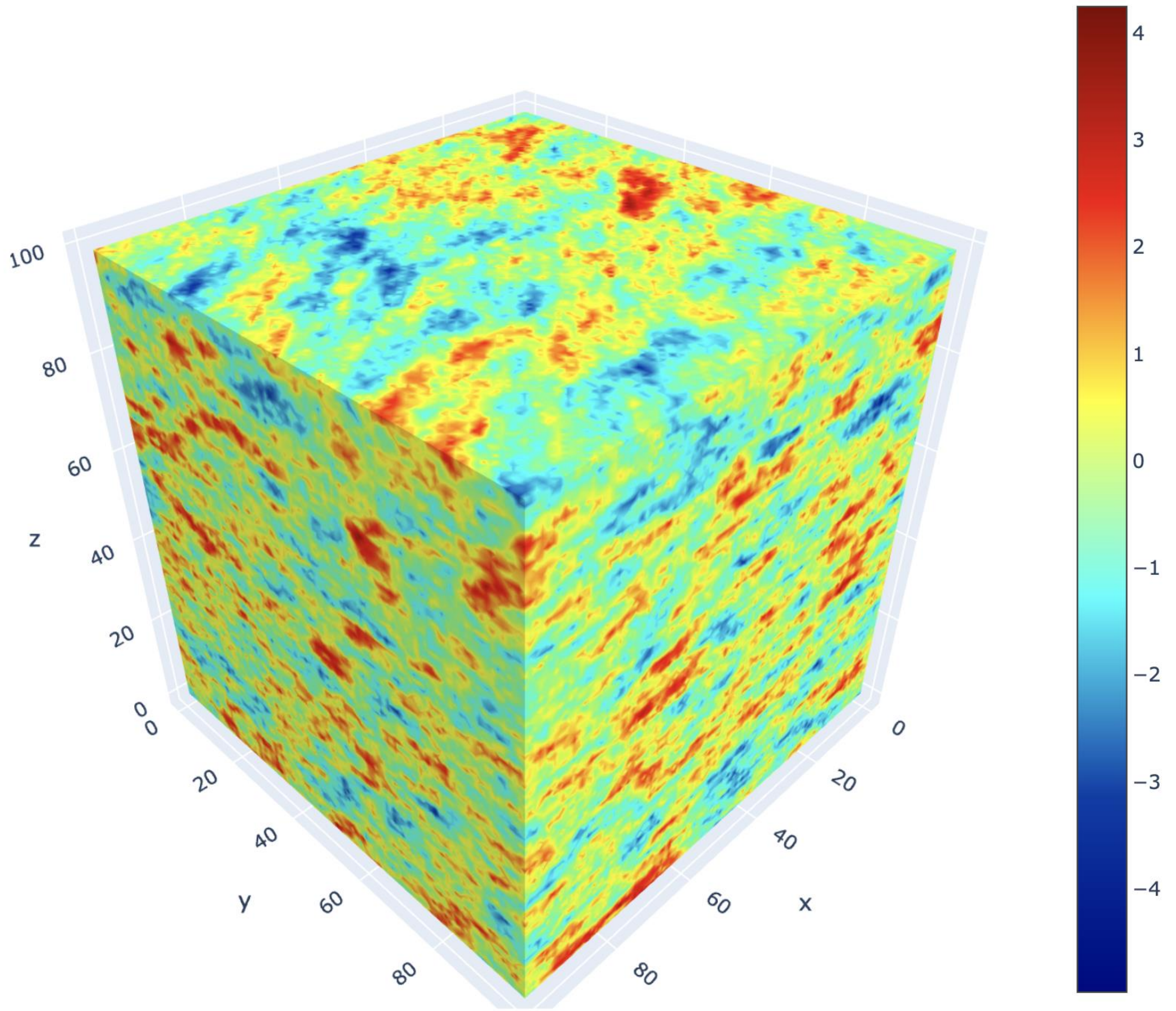
Spatial Data Generated Using GSTools

- GSTools* is a Python library used to create 2D and 3D spatial random field with defined anisotropy in a variogram model.

- Angles of 3D anisotropy are α, β, γ.



*Müller et al., 2022. https://doi.org/10.5194/gmd-15-3161-2022

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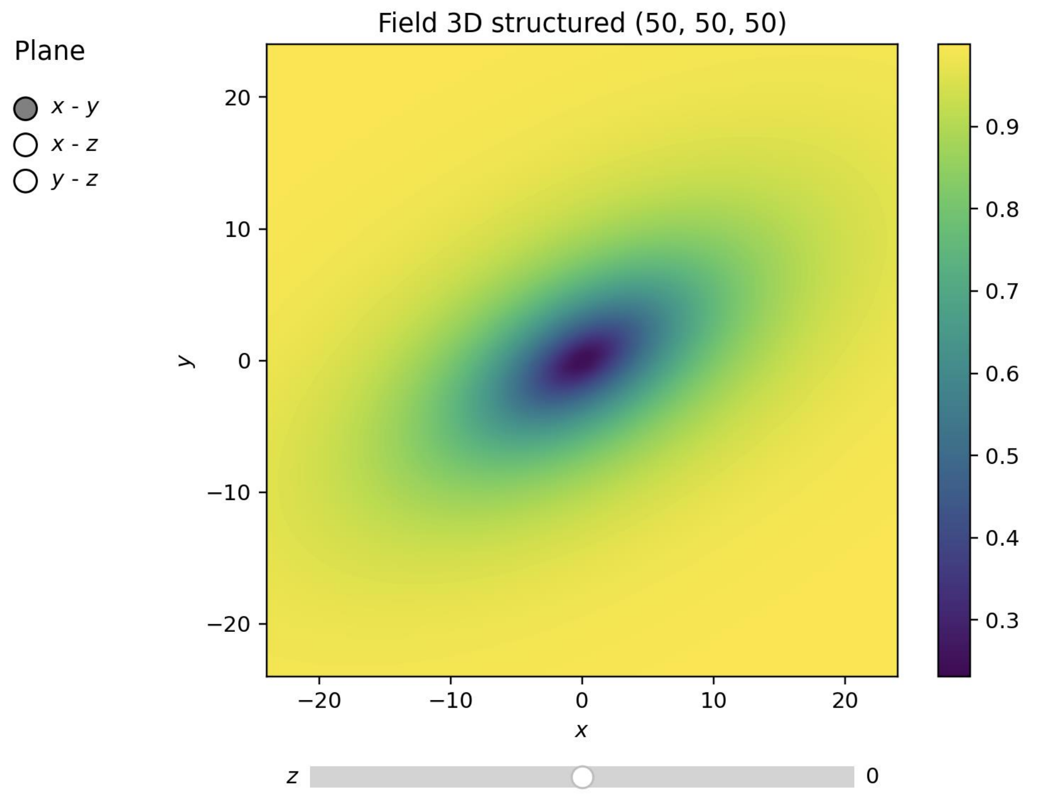
Angles of Anisotropy in 2D and 3D

- GSTools follows the Tait-Bryan convention of angular rotations.
- Sequential rotations are made about Z, Y, and X axes, respectively.
- The first rotation about the Z-axis (X-Y plane), α, is the first major direction of anisotropy.
- In 3D anisotropy, β and γ are angular rotations about Y and X axes, respectively.



Metrics Computed to Ascertain Accuracy of Angular Estimates

- We calculate the following metrics to ascertain the accuracy of estimates of α, β, and γ -

  - Mean, $\mu = \frac{\sum_{i=1}^{n} x_i}{n}$

  where n is the total number of estimates (realizations) and x_i are individual predicted values.

  - Mean absolute deviation, MAD $= \frac{\sum_{i=1}^{n} \lfloor x_i - \hat{x} \rfloor}{n}$

  where $\hat{x}$ are the true values.

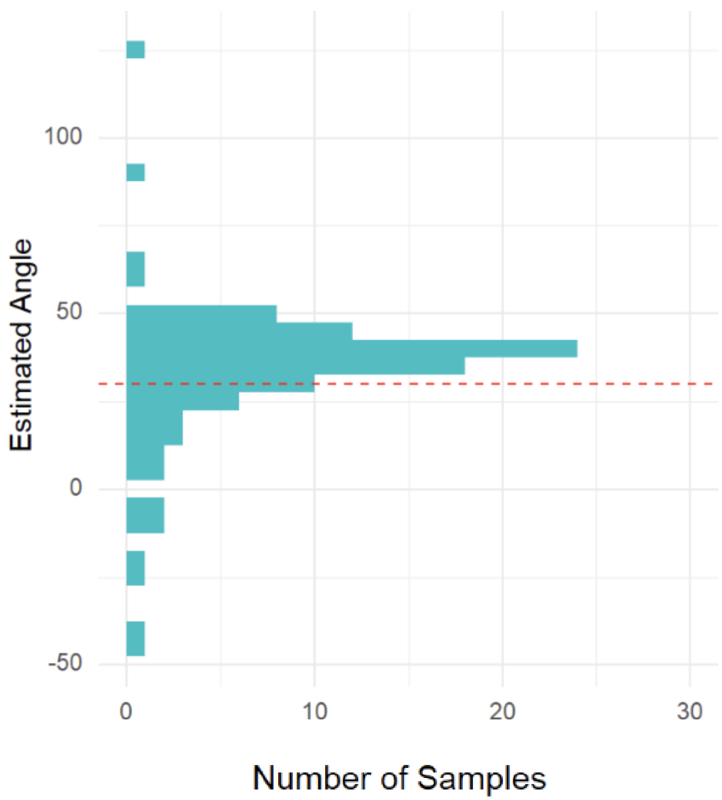
MOI Applied to 2D Dataset

- One hundred realizations of spatial random field are generated based on the following variogram model:
  - model type: Exponential
  - dimensions: 2
  - nugget: 0.0
  - variance: 1.0
  - length scales: 8, 4
  - anisotropy: 0.5

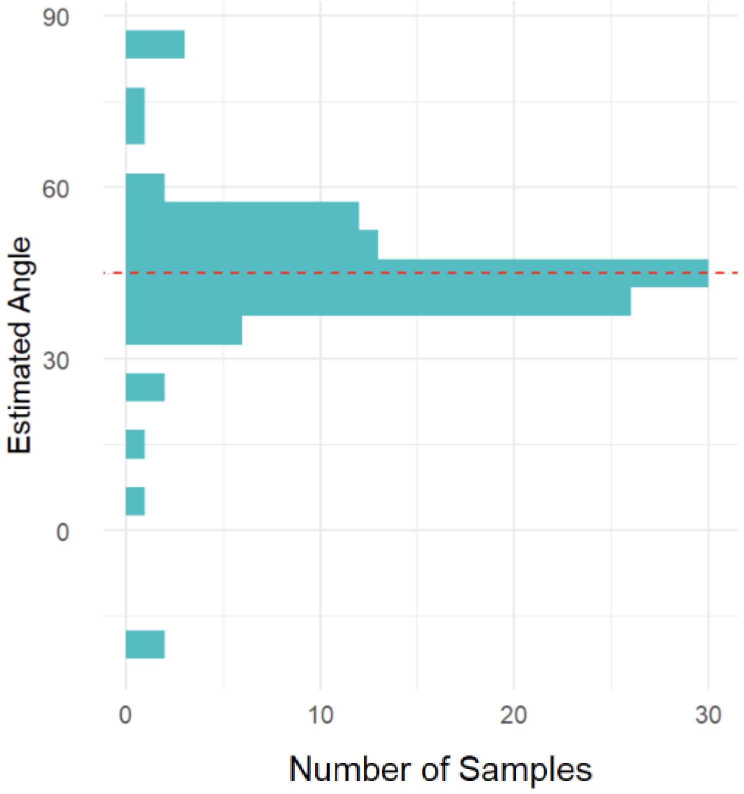
- Angle of anisotropy (α) tested were 30°, 45°, 60°.

- MOI method was applied to each dataset to estimate α.

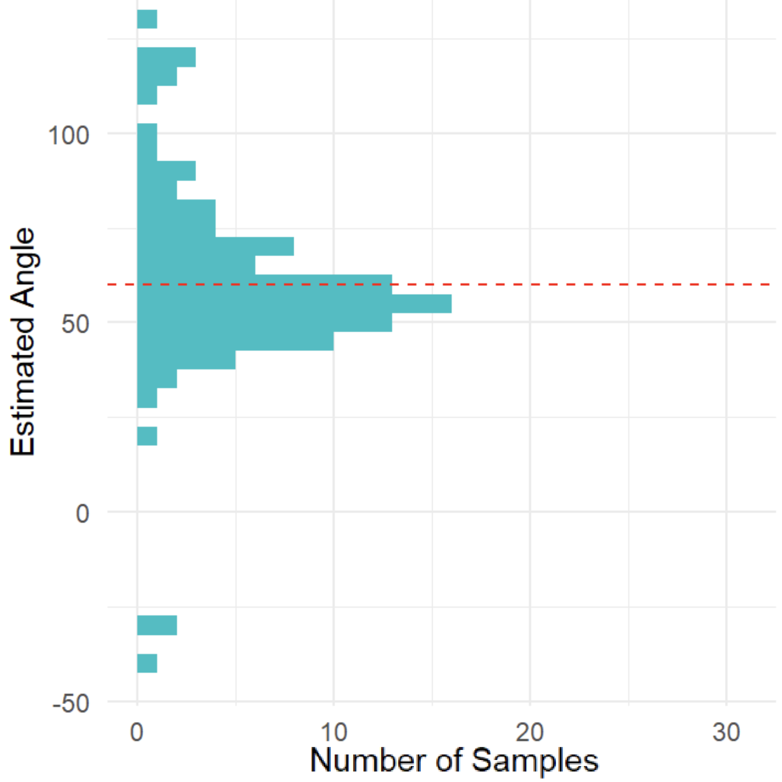
Results for MOI in 2D



α = 30°, Mean = 32.9°, MAD = 9.1°



α = 45°, Mean = 44.3°, MAD = 4.3°

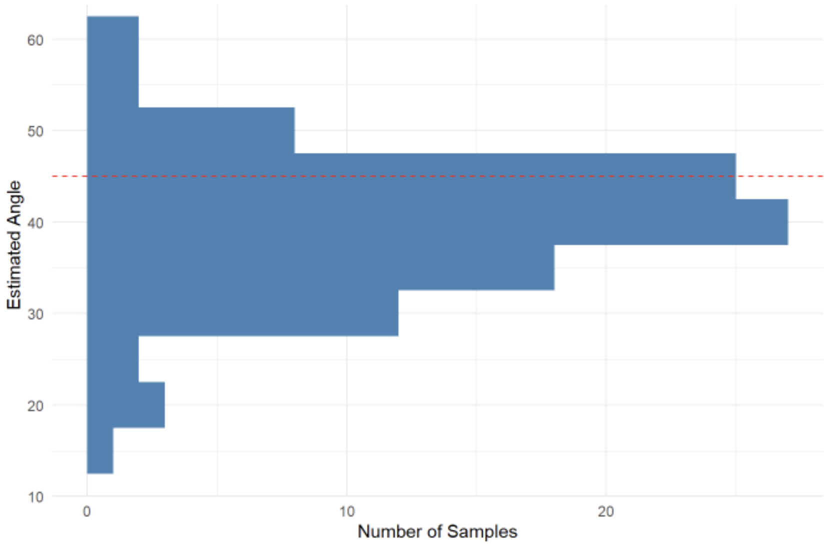


α = 60°, Mean = 59.9°, MAD = 8.6°

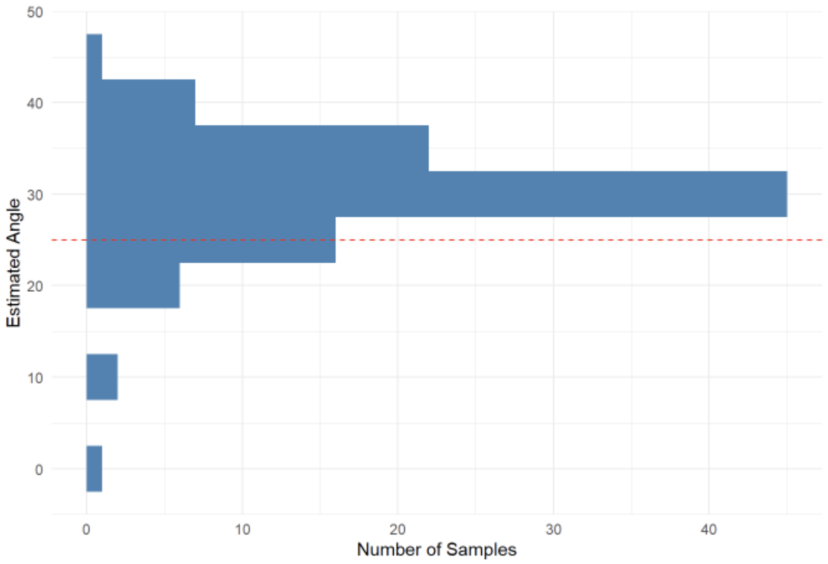
MOI Applied to 3D Dataset

- One hundred realizations of the same variogram model as 2D with the following modifications:
  - length scales: 8, 4, 2
  - anisotropy: 0.5, 0.25
  - angles of anisotropy: α=45°, β=25°, γ=10°

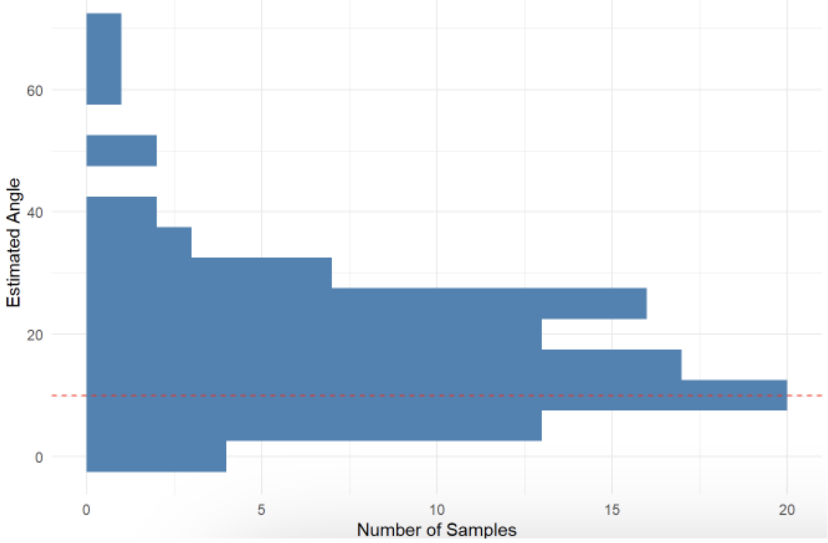
α = 45°, Mean = 39.5°, MAD = 7.4°



β = 25°, Mean = 29.9°, MAD = 6.6°



γ = 10°, Mean = 18.7°, MAD = 10.8°



Conclusions

- MOI method is successful in automating the determination of major angles of anisotropy from a randomly generated spatial field.
- For 2D datasets, the estimated angles are within $\pm 3°$ range and variability is ~4° - 9°.
- For a 3D dataset, the estimated angles are within $\pm$ 9° range and variability is ~6° - 11°.
- We are looking into another approach using the Covariance Tensor Identity (CTI) method to ascertain more accurate automated estimates.
  - In CTI, the covariance function's Hessian matrix is derived from sample derivatives. Anisotropy parameters are determined through solutions of nonlinear equations connecting anisotropic angles with the ratios of the Hessian matrix elements.
- These methods will be applied to real databases to evaluate their practical applications to existing spatial analysis software like the Visual Sample Plan (VSP).

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Questions?

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