

eXplainable Artificial Intelligence Application in Metrology

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XMANAI
MAKING AI UNDERSTANDABLE

UNIMETRIK
METROLOGY AND CALIBRATION

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Industrial Quality Control

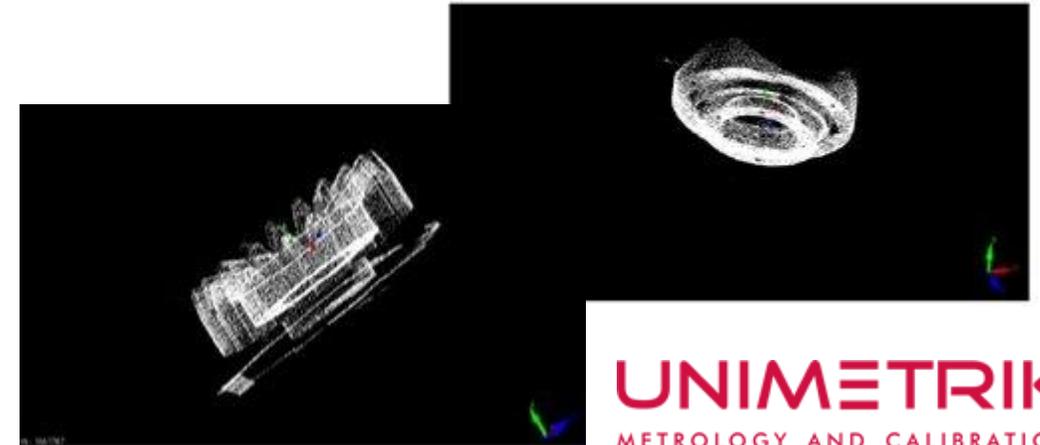
- Manufactured parts for automotive, aeronautic, energy sectors
- Dimensional/positional measurements: Definition of dimension/position & tolerance

Instrument: 3D laser scanner

- User-defined parametrization of scanning conditions
- Point Cloud generation

Software: M3 metrological software

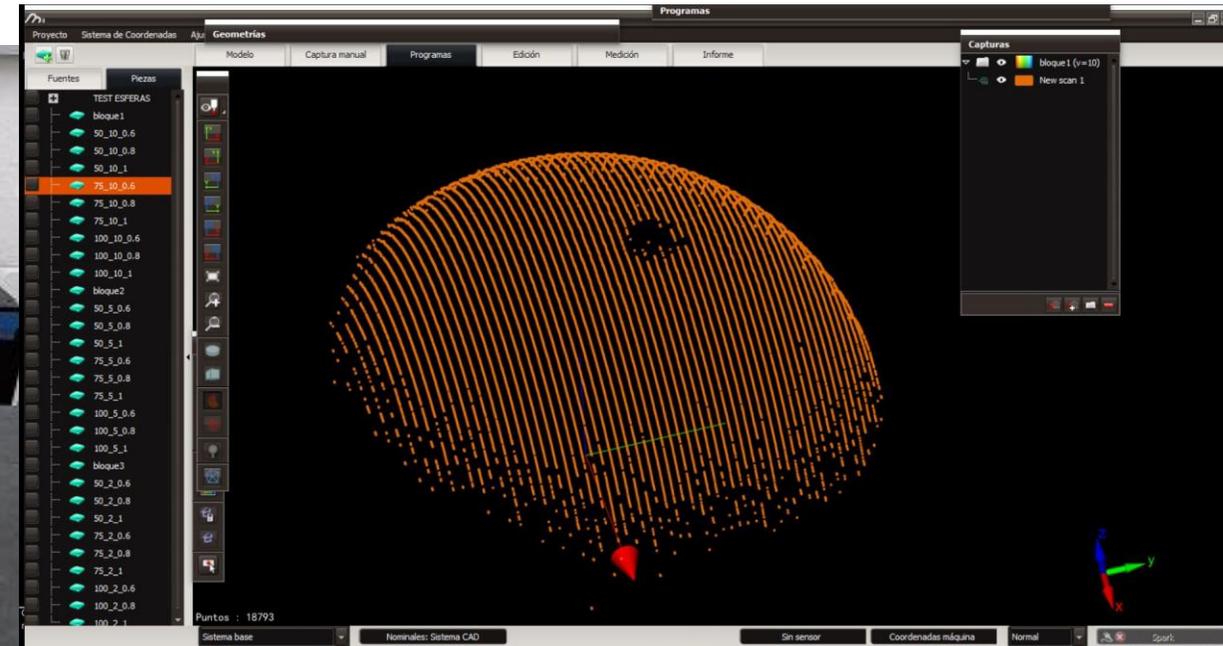
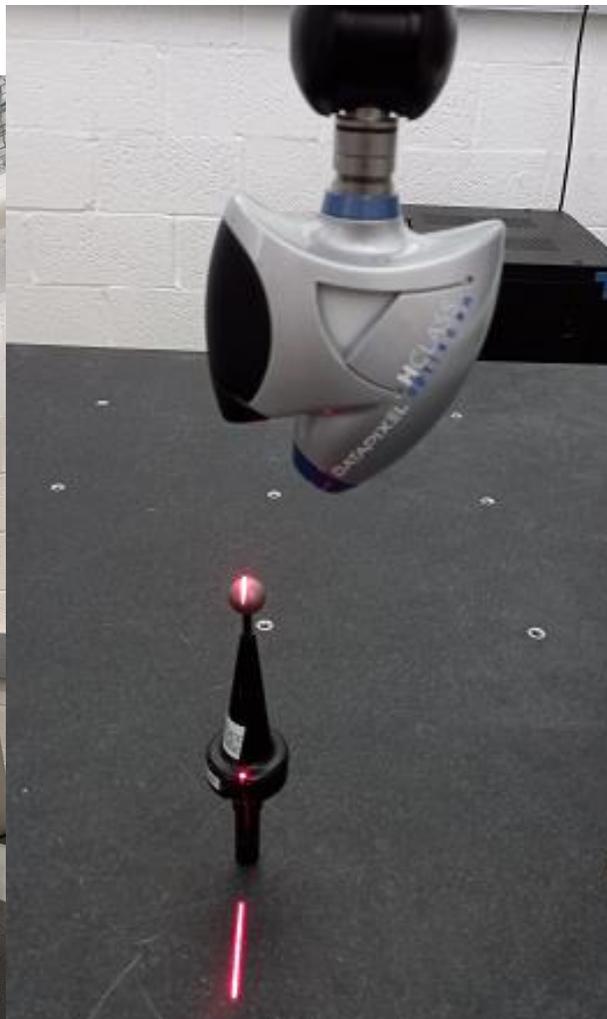
- Point cloud processing
- Measurement using two methods (complete Point Cloud / geometry definition points)



Measurement Workflow

Step 1: Preliminary analysis of the object under study & selection of laser setup

- scanning parameters & laser orientation



Step 2: Configuration of scanning conditions & generation of Point Cloud

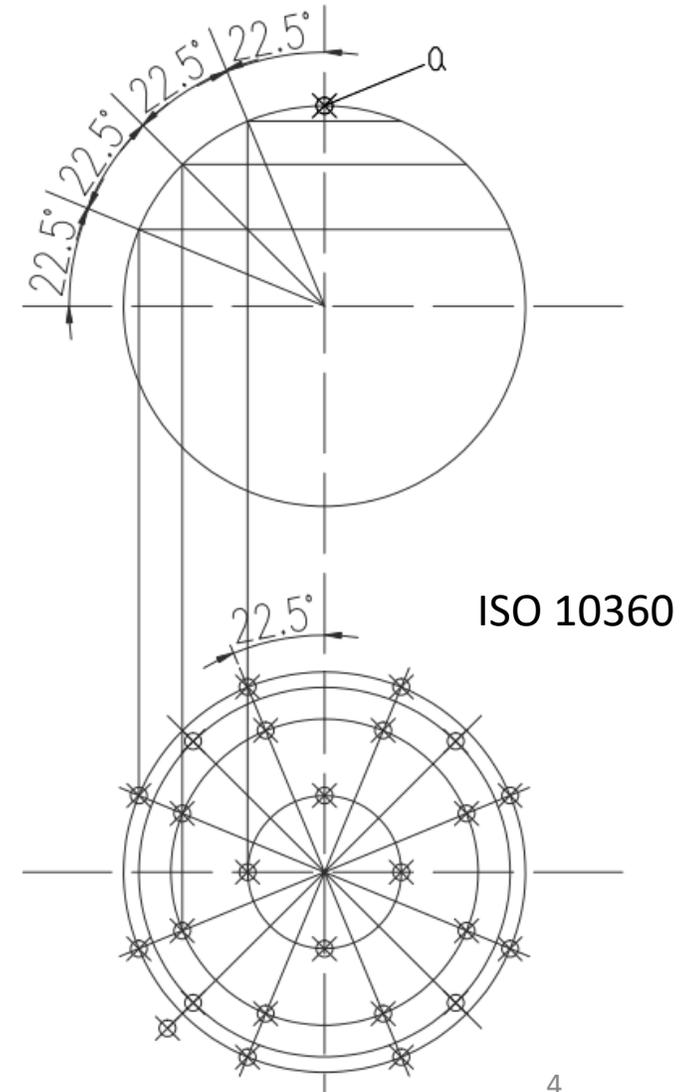
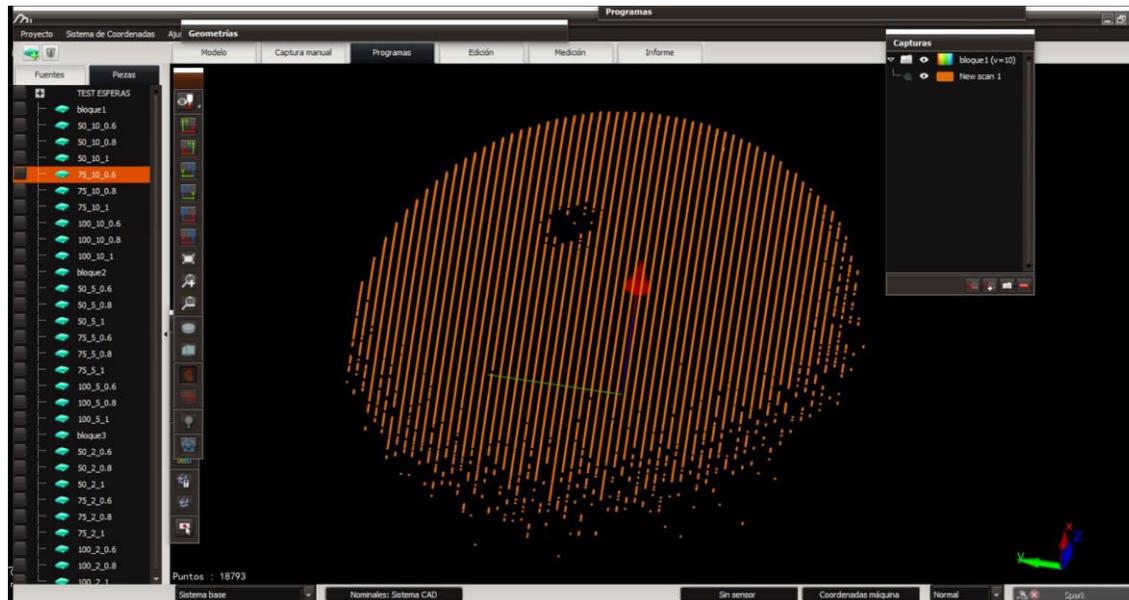
Measurement Workflow

Step 3: Point cloud preprocessing

- Outlier removal
- Noise filtering
- Surface Segmentation

Step 4: Dimensional/positional measurement

- Method#1 (CONSTRUCT) (Geometry definition points)
- Method#2 (EXTRACT) complete Point Cloud

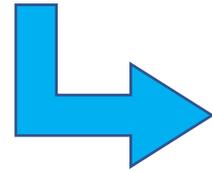


Issues:

- Results depend on metrologist's experience (inconsistency of results)
- Wasted time on iterative analysis, each project from scratch

Use Case 1: Measurement plan parameter optimization

Objective: Optimization of scanning parameters, to achieve **minimum error/uncertainty** in dimensional measurement

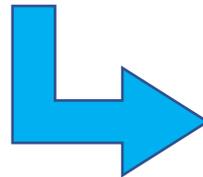


Accelerate/Facilitate
Step 1: Preliminary analysis

Use Case 2: Point Cloud optimization

Objective: Optimization of the 3D point cloud in terms of **quality & size**

- **Size:** minimum # of points sufficient to perform accurate measurement, & preserve shape/geometry information
- **Quality:** Point cloud denoising / filtering / segmentation



Accelerate/Facilitate *Steps 3&4:*
Point Cloud pre-processing & Dimensional measurement

Initial Approach: Supervised Learning Setting

Objective: Model instrument's anisotropic accuracy

- in response to *different surface orientations*
- in relation to *scanning parameters*

Approach: Supervised Regression task

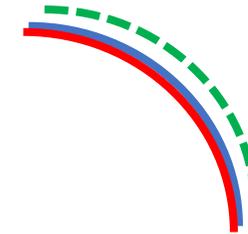
- Prediction of error in Point capturing
- Access to *Ground Truth* needed

Method: Use measurements of *Calibrated artifacts*

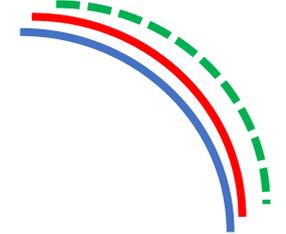
- Actual dimensions precisely known ($\sim 1\mu\text{m}$), i.e.
actual \approx **nominal**
- Validated shape perfection
- Ground Truth: actual Point positions located on artifact's nominal surface

target variable

calibrated



non-calibrated



Nominal => dimension in CAD design

Actual => true dimension

Measured => dimension estimated by measurement

Point Measurement deviation (error):

$$\text{PointDev} = \text{measured} - \text{nominal}$$

Data Sources Description

Geometries

Sphere

Cylinder

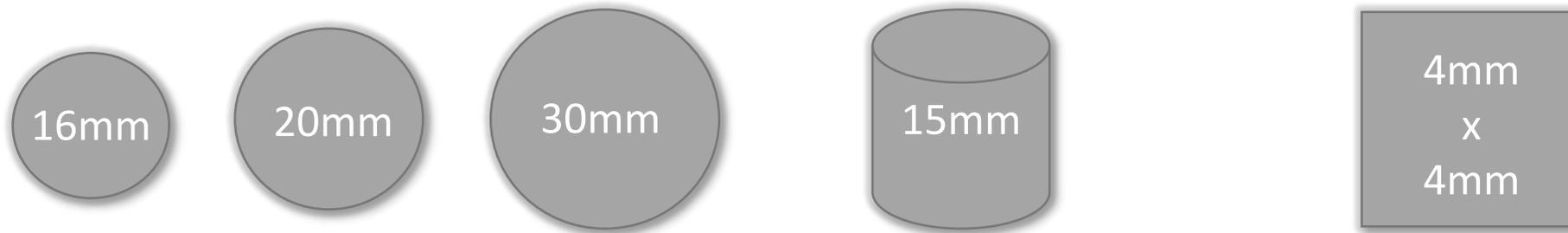
Plane

Ground truth

Diameter

Diameter

Distance to laser



Scanning parameters

1. *Lateral Density*
2. *Scan Direction Density*
3. *Exposure time*

low (50), medium (75), high (100)
 low (2), medium (5), high (10)
 low (0.6), medium (0.8), high (1.0)



Laser setup

Source orientation \vec{L}

$\vec{L} = \text{constant}$ (Sphere & Plane)

$\vec{L}1, \vec{L}2 = \text{constant}$ & symmetrical wrt axis (Cylinder)

Detector (CMOS) viewing direction \vec{V}
 Vertical distance $Z_l \approx 90\text{mm}$

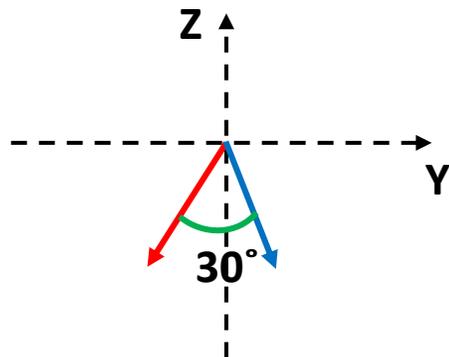
\vec{V} at 30° wrt \vec{L} (rotate over axis of movement)
 $Z_l = \text{constant}$ for all measurements

Data Sources Description

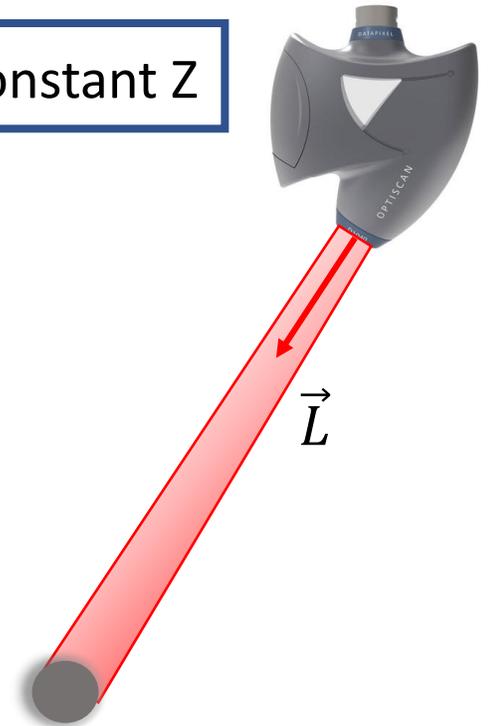
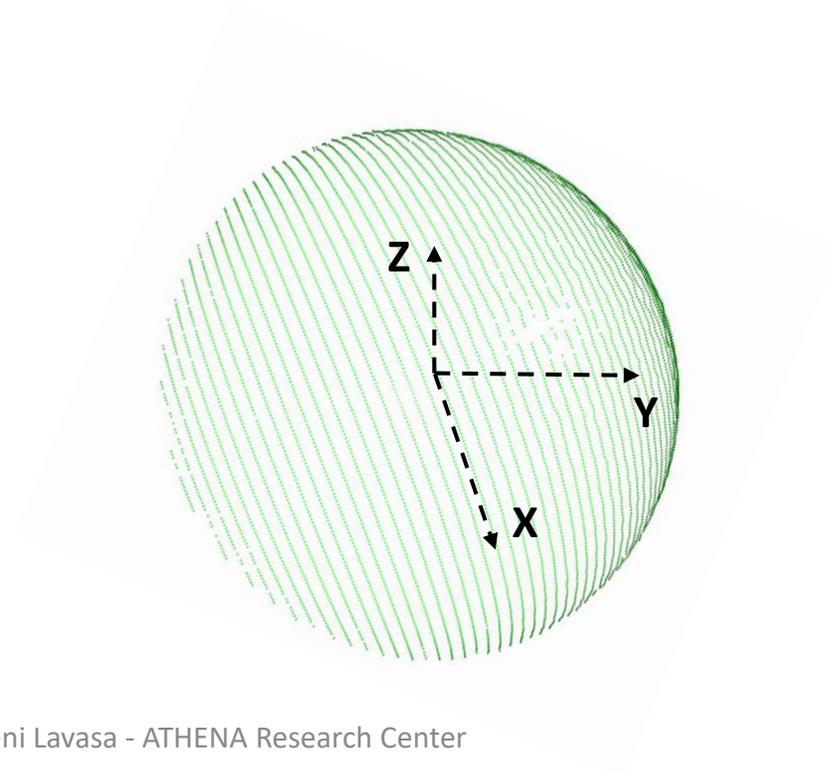
Rotary Head of Optical System



\vec{L} = Laser Source orientation vector
 \vec{V} = Detector (CMOS) viewing direction



Head moves along Y-axis at constant Z

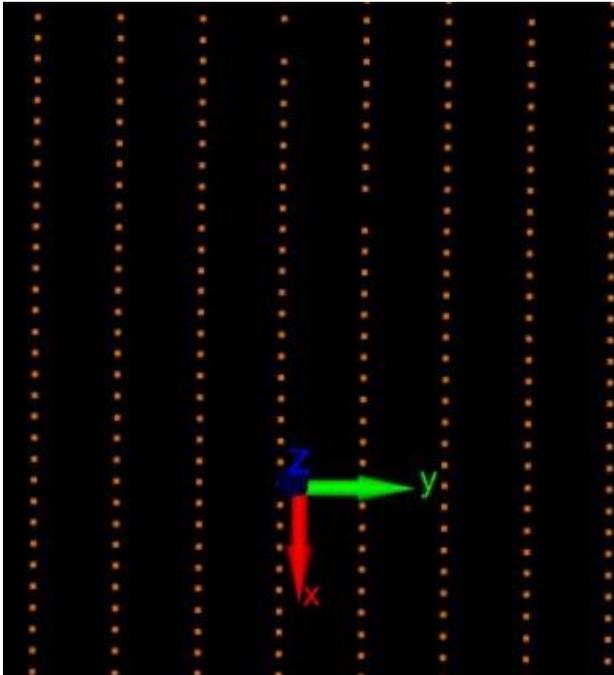


Data Sources Description

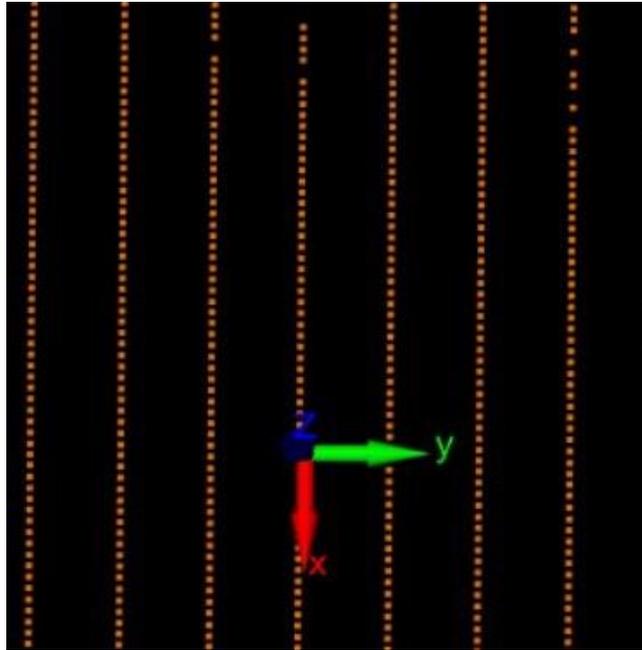
Scanning Parameters: *Lateral Density*

Increasing point density along each line (lateral direction)

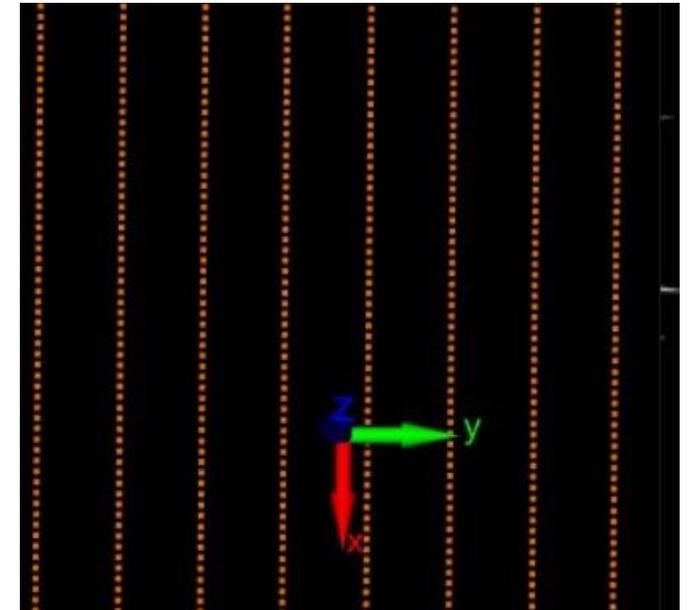
50



75



100



Data Sources Description

Scanning Parameters: *Scan Direction Density*

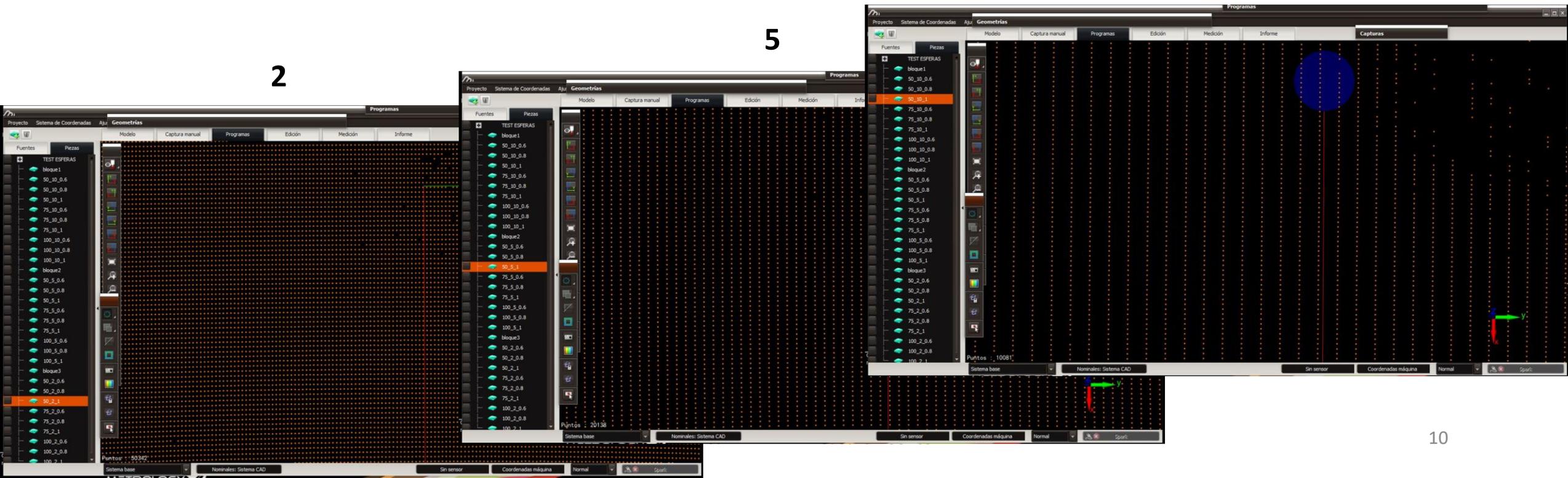
Decreasing point density in the direction of movement (sparse lines)

..increasing velocity of rotary head movement

10

2

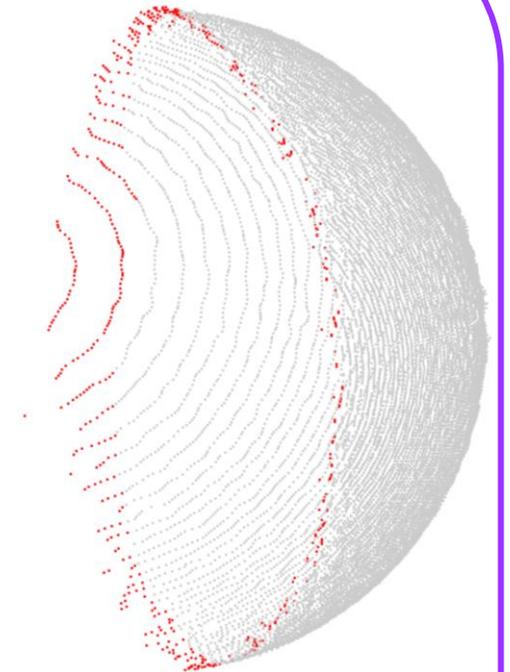
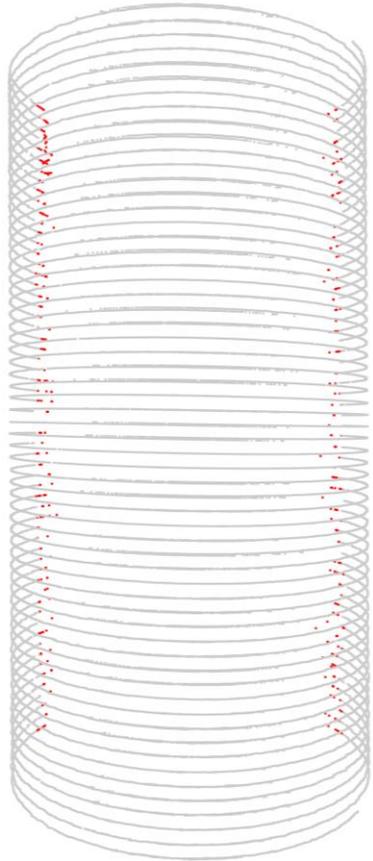
5





Statistical outlier removal

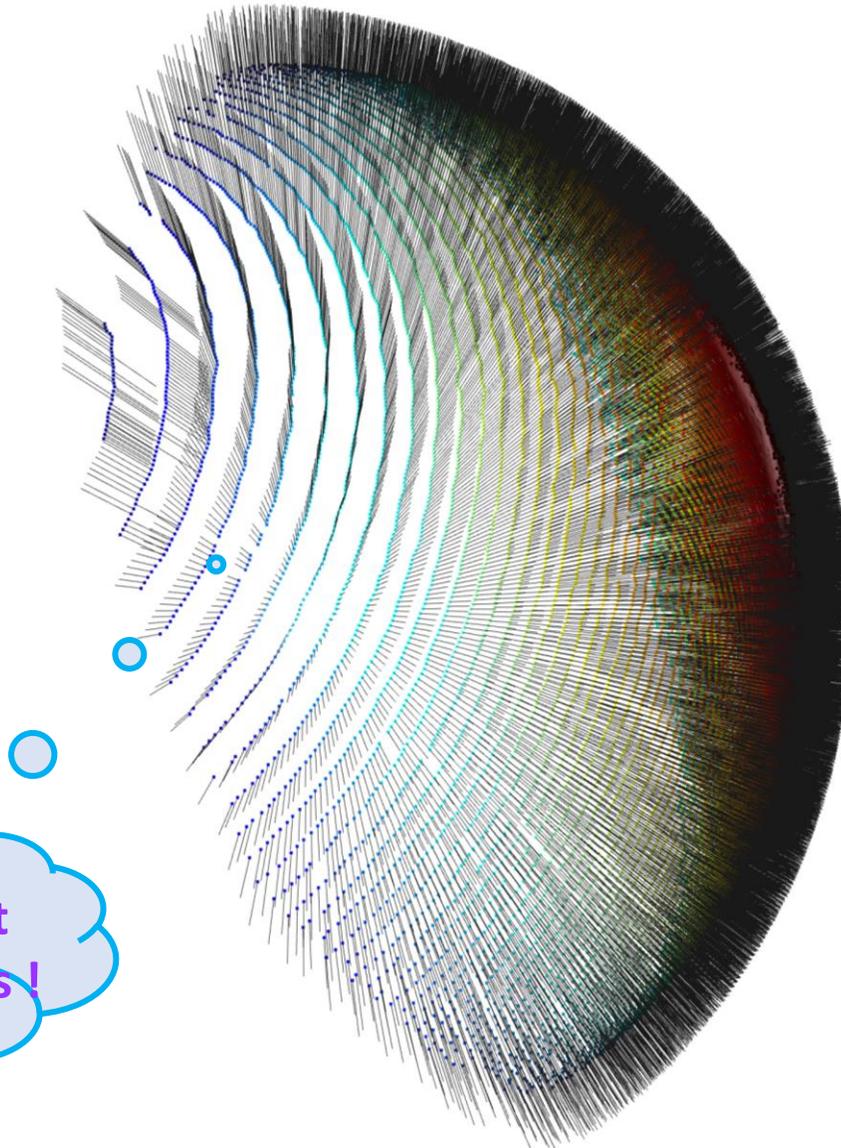
- Based on distance to nearest neighbors (number of NN, std)
- inliers: red
- outliers: grey



Estimation of normal vectors $\vec{N} = [N_x, N_y, N_z]$

- **surface orientation** at each point
- Based on nearest neighbors within a given radius (number of NN, radius)

Ensure alignment of normal vectors!



OPEN3D

Data Sources Description

Calculation of the target variable

at point P:

$P(X, Y, Z) =$ *measured point coordinates*

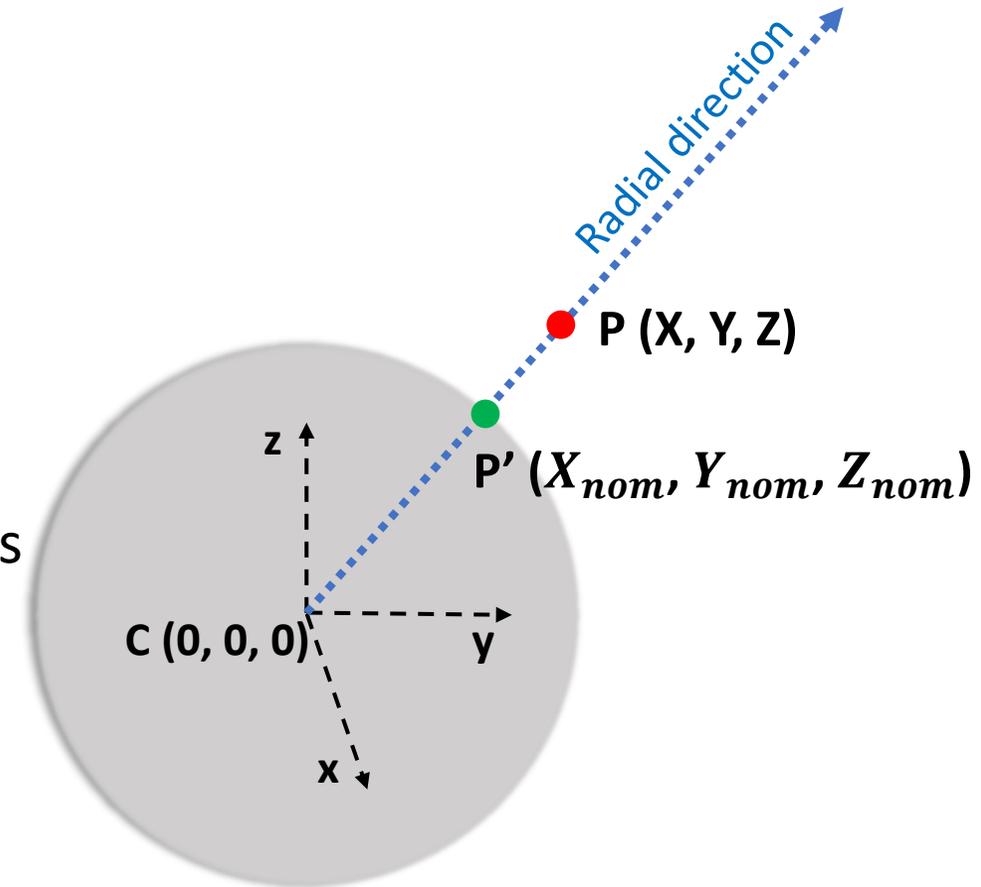
$P'(X_{nom}, Y_{nom}, Z_{nom}) =$ *projected point coordinates*
(nominal surface)

$|CP| = R =$ **measured** point radial distance (spheres)
(cylinder: axial, plane: vertical)

$|CP'| = R_{nom} =$ **nominal** radial distance = Nominal Radius

PointDev = $|P'P| = R - R_{nom}$

= **point deviation from nominal surface**



Data Sources Description

\vec{L} = Laser Source orientation vector
 \vec{V} = Detector (CMOS) viewing direction

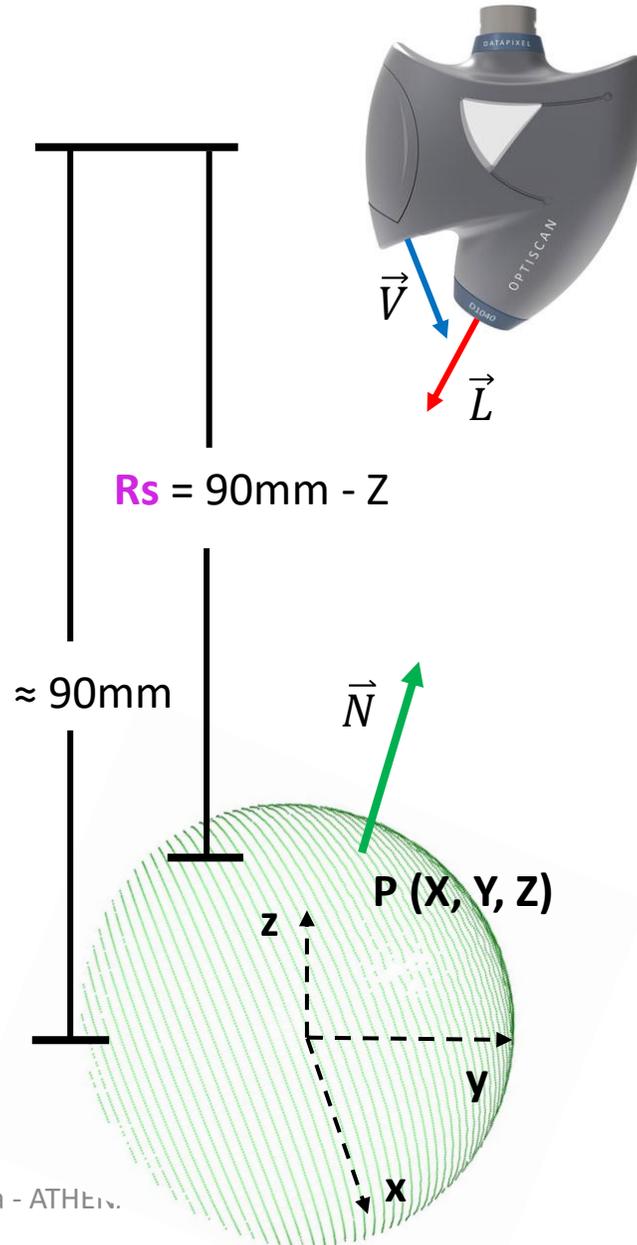
at point P:

$\vec{N} = [Nx, Ny, Nz]$ = surface orientation

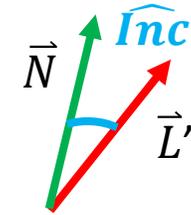
\widehat{Inc} = incidence angle of light on surface

$\widehat{ViewAng}$ = viewing angle from CMOS

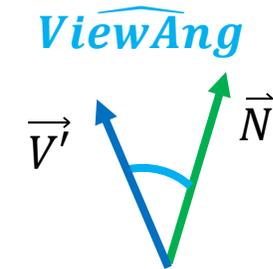
R_s = Vertical distance to laser source



$$\widehat{Inc} = \arccos \left(\frac{\vec{N} \cdot \vec{L}'}{\|\vec{N}\| \cdot \|\vec{L}'\|} \right)$$



$$\widehat{ViewAng} = \arccos \left(\frac{\vec{N} \cdot \vec{V}}{\|\vec{N}\| \cdot \|\vec{V}\|} \right)$$



Data Sources Description

\vec{L} = Laser Source orientation vector = $[I, J, K]$

\vec{V} = Detector (CMOS) viewing direction = $[I', J', K']$

at point P:

\vec{N} = $[N_x, N_y, N_z]$ = surface orientation

\vec{Ori} = $\vec{N} - \vec{L} = [OriX, OriY, OriZ]$

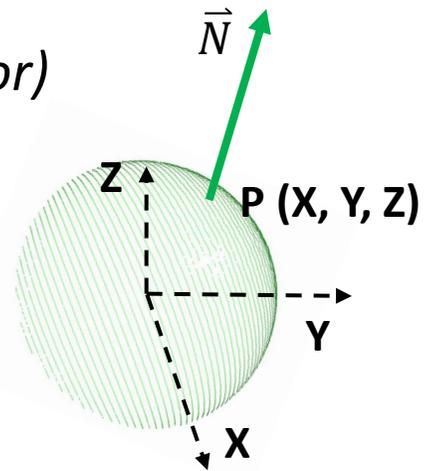
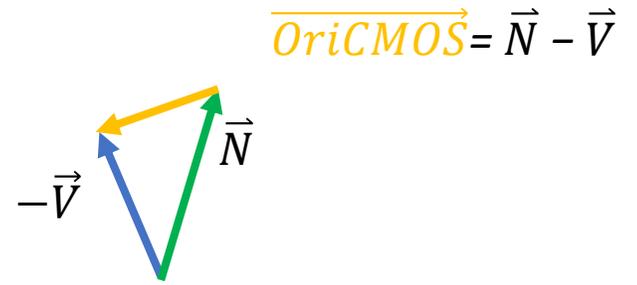
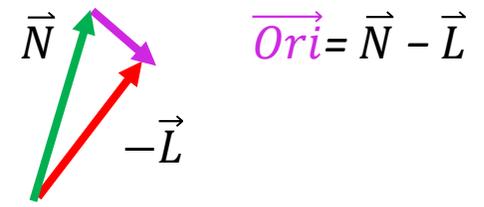
= Orientation difference vector (surface & laser)

$\vec{OriCMOS}$ = $\vec{N} - \vec{V}$ = Orientation difference vector

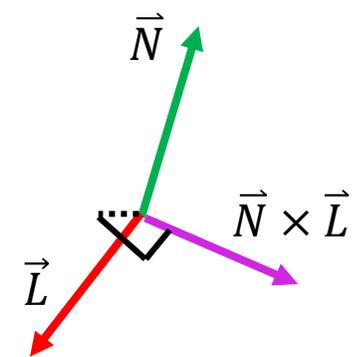
(surface & CMOS sensor)

$OriY_{cmos} = N_y - J'$

\widehat{Ang} = 4-quadrant angle



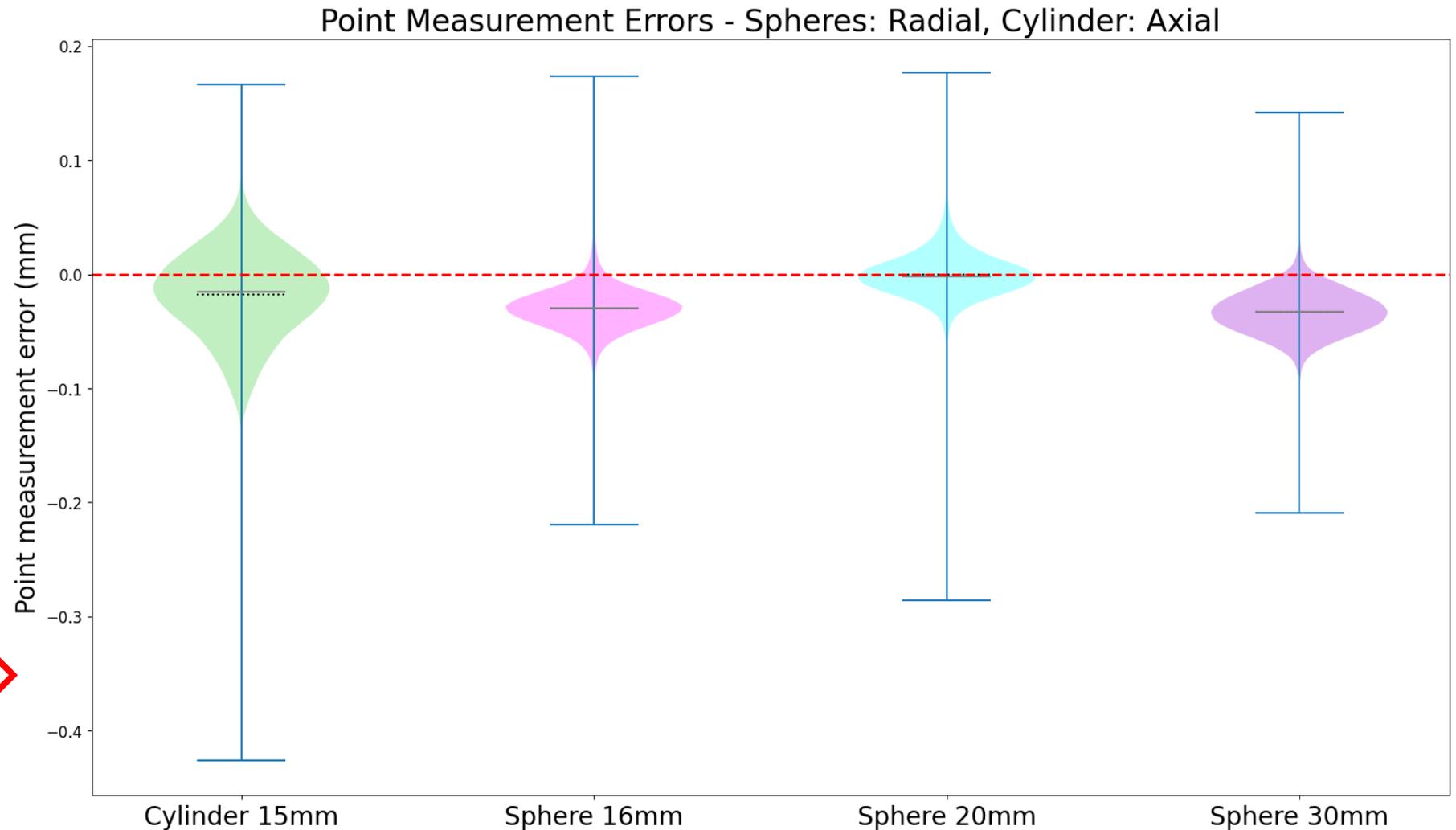
$$\widehat{Ang} = \text{arctan2d}(\vec{N} \times \vec{L}, \vec{N} \cdot \vec{L})$$



Studying the behavior of the instrument

- Errors in point capture tend to be negative
- Instrument tends to under-estimate the dimension of objects

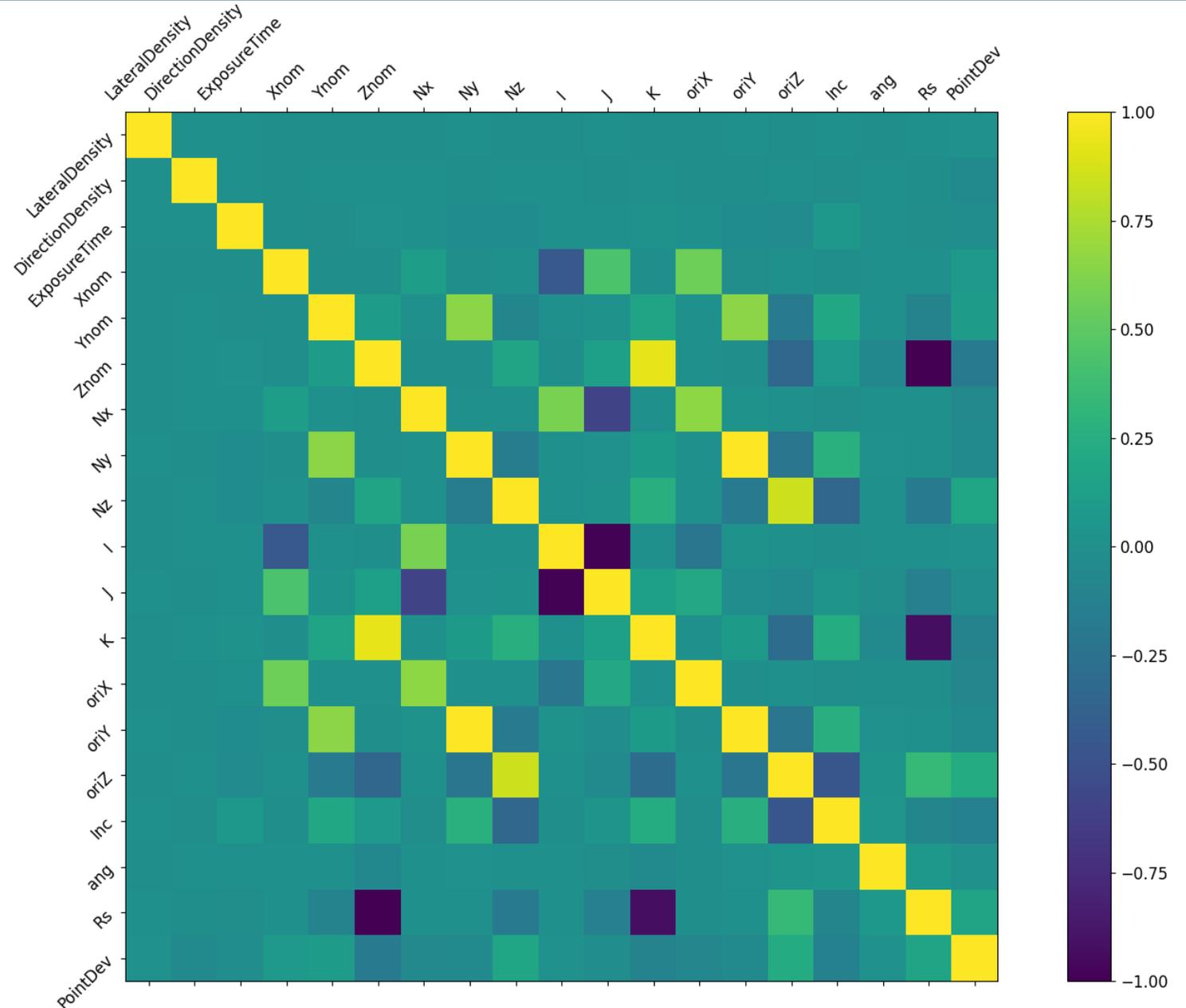
Mean Point Error
 -0.024 ± 0.053 mm



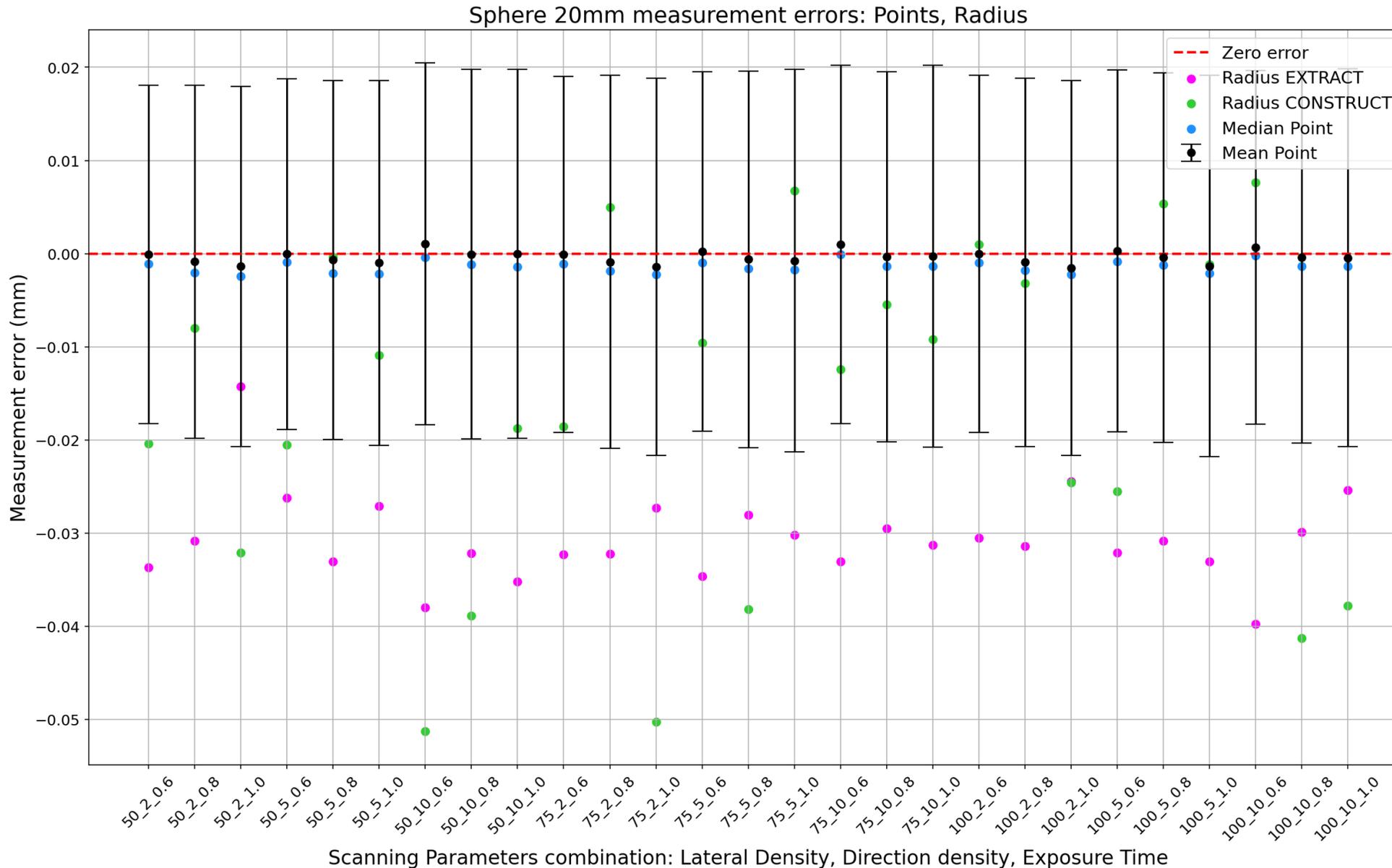
Data exploration & Analysis

Investigating (anti)correlations amongst features

- Scanning parameters (Lateral Density, Direction Density, Exposure Time) are not related to the target variable, Point measurement error (PointDev)
- The z-component of the normal vector (Nz) and the orientation difference vector (oriZ) show minor correlation to PointDev
- Strong correlations are due to calculation formulas or bias induced by specific geometries (sphere & cylinder)



Data exploration & Analysis



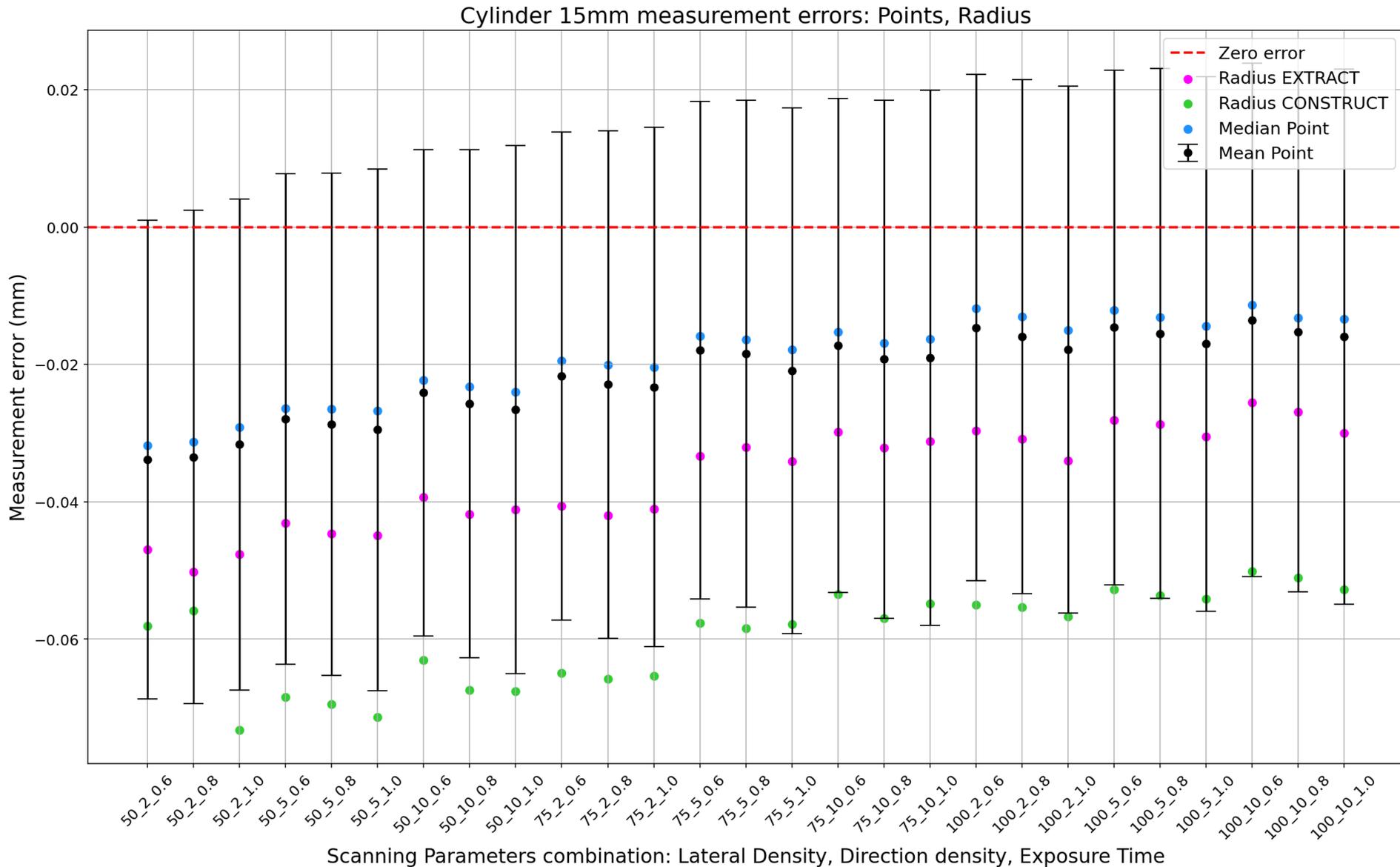
- Statistical distribution of points: captures well actual surface
- Mean of radial distribution: good estimate of actual radius
- Both methods under-estimate sphere radius, method EXTRACT (Point Cloud) performs worse

Data exploration & Analysis



- Statistical point distribution: well below actual surface
- Mean of distribution: bad estimate of radius
- Method EXTRACT (Point Cloud) under-estimates radius
- Method CONSTRUCT (Geometry Definition points) performs better

Data exploration & Analysis



- Statistical point distribution: below actual surface
- Mean of point radial distribution: good estimate of radius
- Both methods consistently underestimate radius, Method EXTRACT (Point Cloud) performs better
- Cylinder captured better with high Lateral Density

Machine Learning Pipeline

Step 1

- Random selection of N points/point cloud
- Feature & target scaling to [0, 1] interval

Step 2

- Selection of algorithms (SVM, MLP, Decision Tree, Random Forest)
- Wide hyper-parameter grid

Step 3

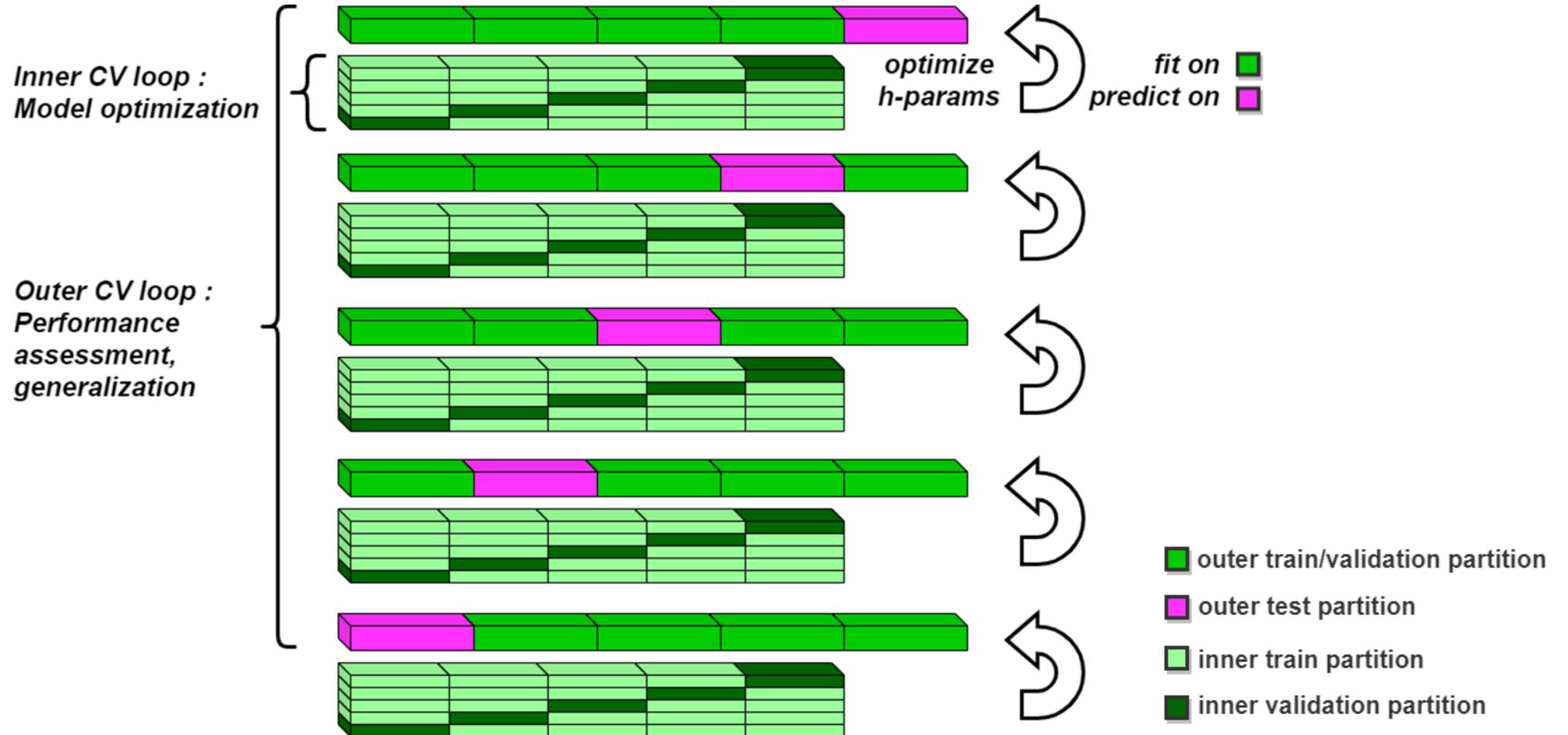
- Randomized Grid search cross-validation
- Nested Cross-Validation scheme (10 fold)

Step 4

- Optimal model retrieval based on mean validation scores

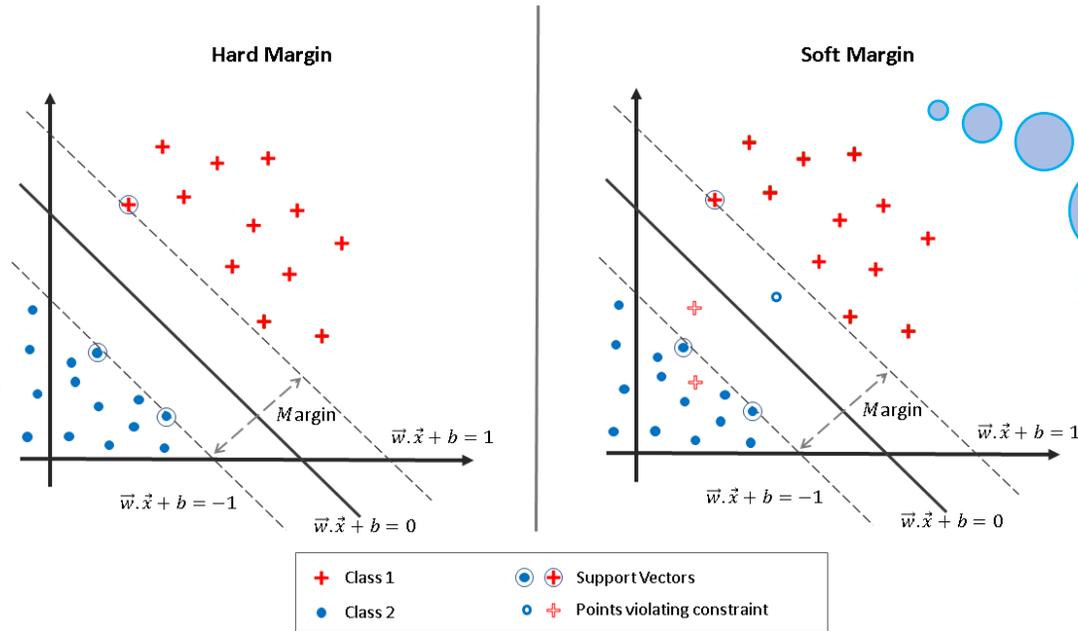
Nested Cross-Validation scheme

Self-consistent methodology to train/optimize models & assess their performance

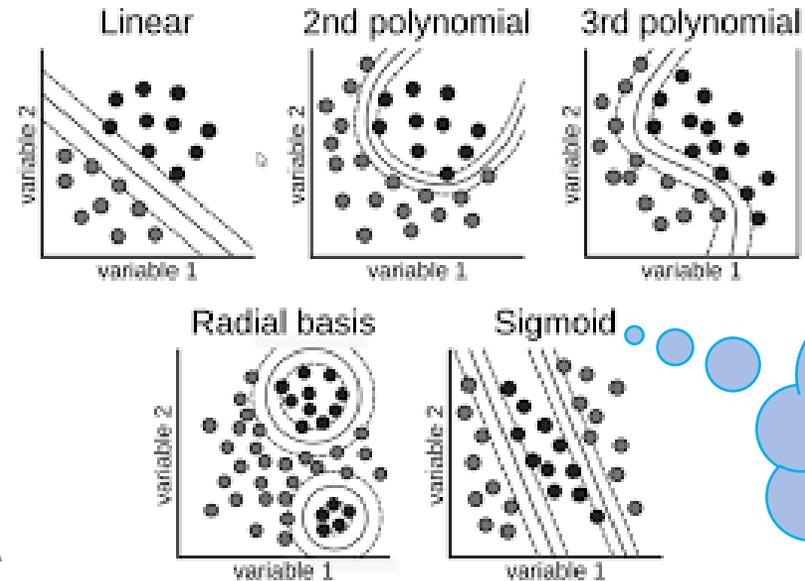
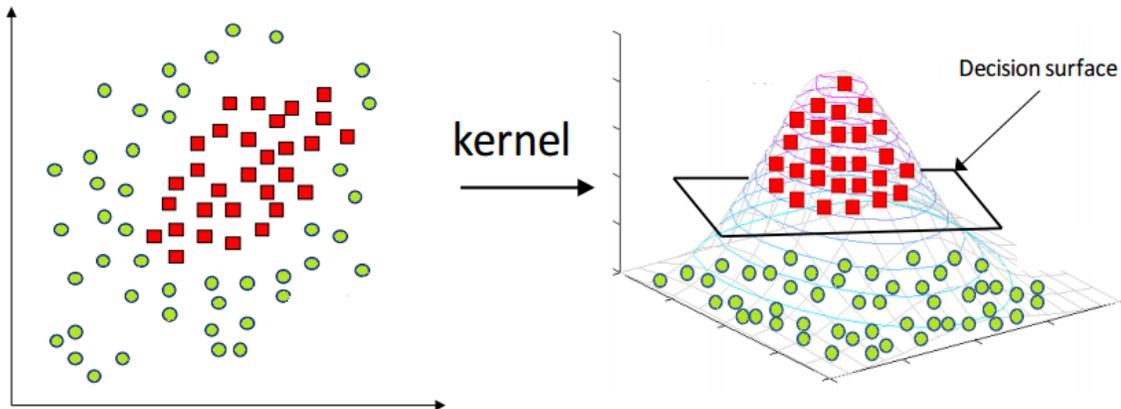


Model intuition – Support Vector Machine (SVM)

- Finds **Optimal separating hyperplane** (decision surface) for linearly separable patterns
- **Optimal Hyperplane** => maximum margin
- **Support vectors** => data points closest to the decision surface (points most difficult to discriminate – specify optimum location of decision surface)
- Extend to not linearly separable patterns: **transformations of original data into new space** – Kernel function



Hyper-parameter **C** controls margin
Large C => small margin



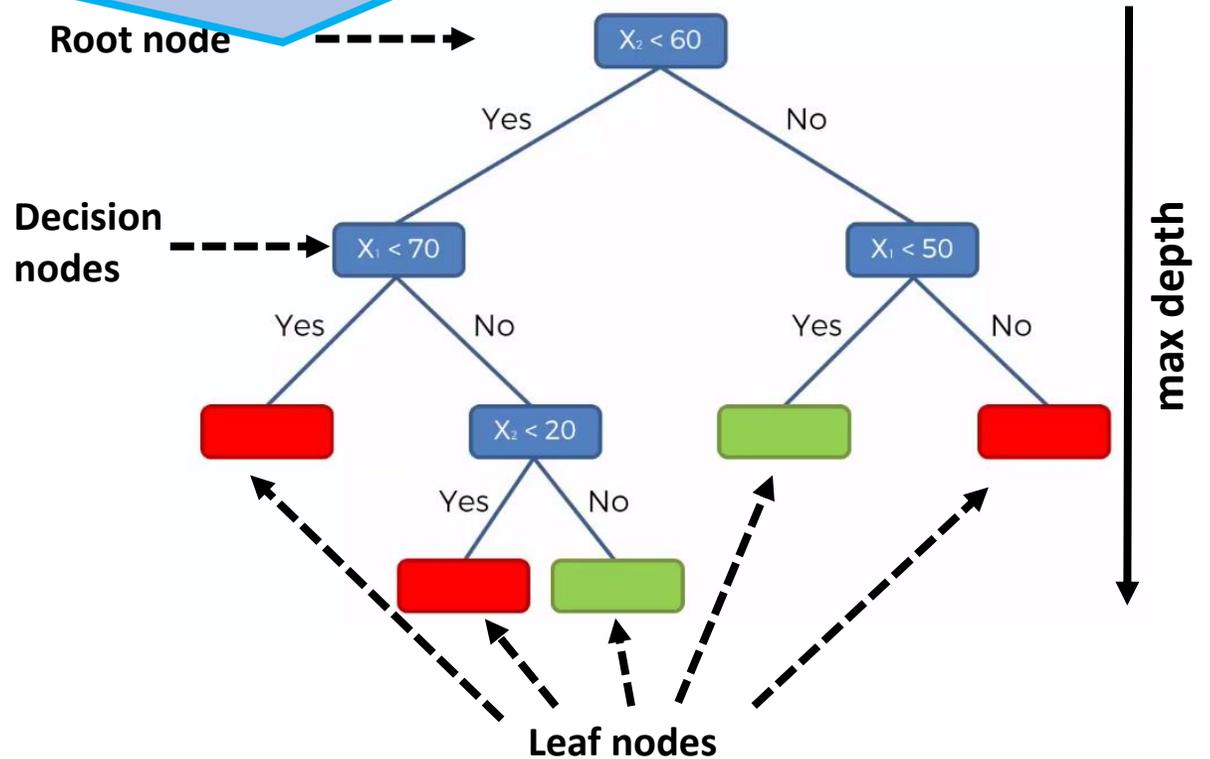
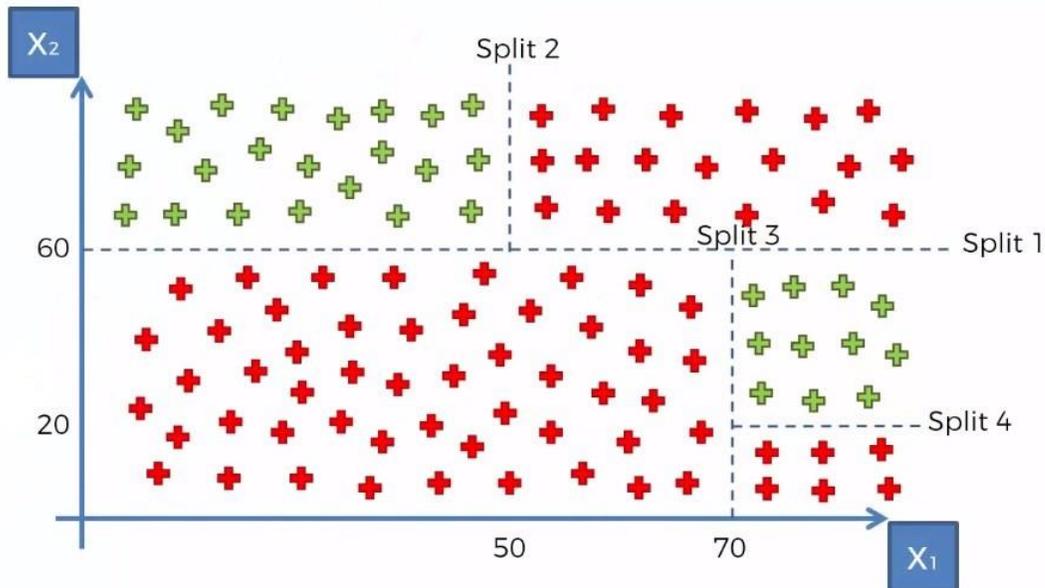
H-parameter **kernel** controls kernel function

Model intuition - Decision Tree

- Splits data points to **maximize information gain** (minimize impurity) in the resulting data partitions
- Optimal partitions contain as much as possible information and less randomness

Hyper-parameters (regression)

- *max_depth*: maximum depth of the tree (max # of decision levels)
- *splitter*: strategy to perform splits (“best”, “random”)
- *split_criterion*: function to measure quality of split (“squared_error”, ...)
- *min_samples_split*: minimum # of samples to split decision nodes
- *min_samples_leaf*: minimum # of samples at leaf nodes

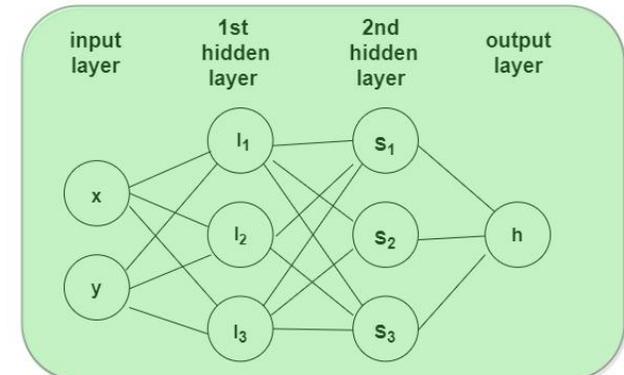
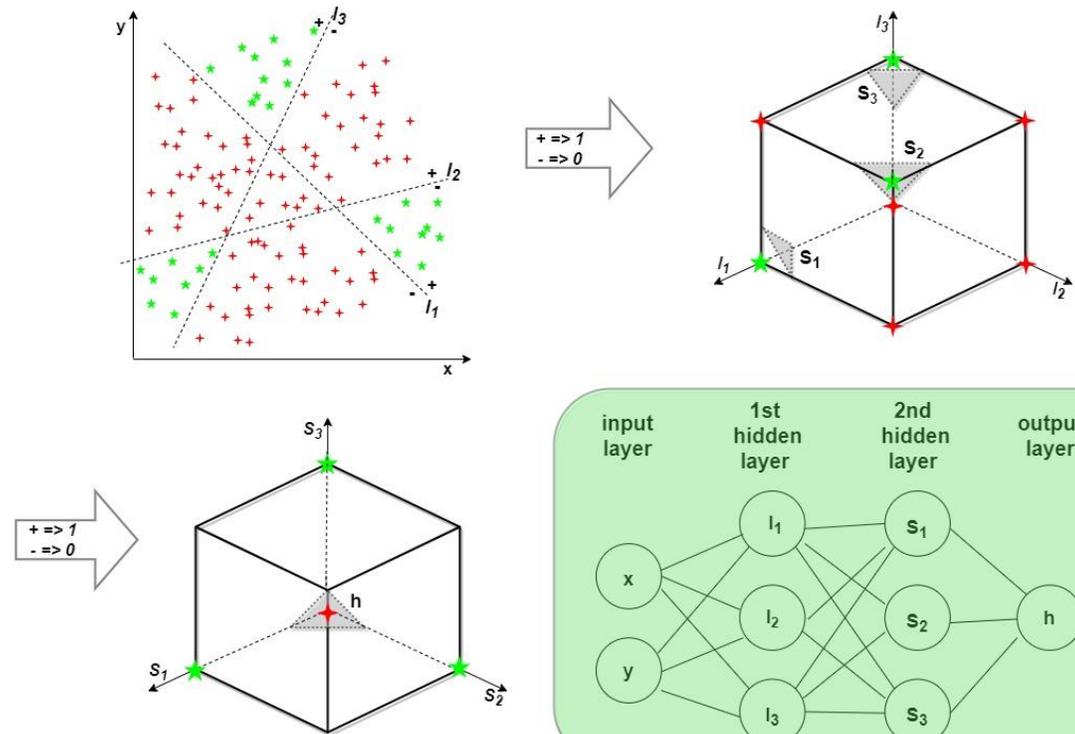
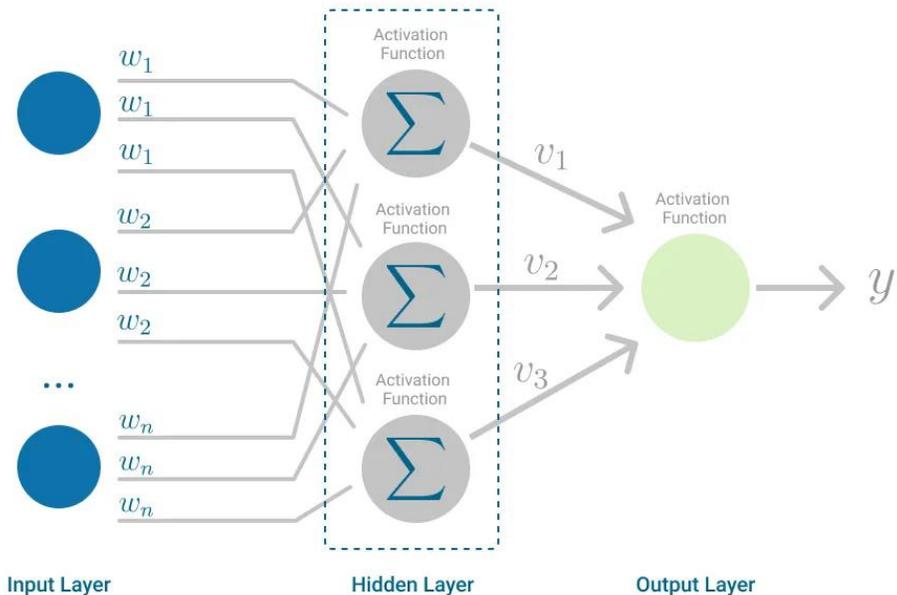


Model intuition - Multi-layer Perceptron (MLP)

- Sequentially transforms input into higher dimensional spaces: samples can be discriminated
- Neuron: basic unit of computation, receives inputs & weights (for each input)
- At each neuron: inputs combined in a weighted sum
- If weighted sum exceeds predefined threshold: neuron activation, output production
- Threshold represented by activation function

Hyper-parameters

- *hidden_layer_sizes*: the number of neurons in each hidden layer
- *activation*: Activation function (“logistic”, “relu” ...)
- *solver*: the algorithm for weight optimization (“sgd”, “adam”, ...)



ML Experimental results – Model performance

Optimal SVM model

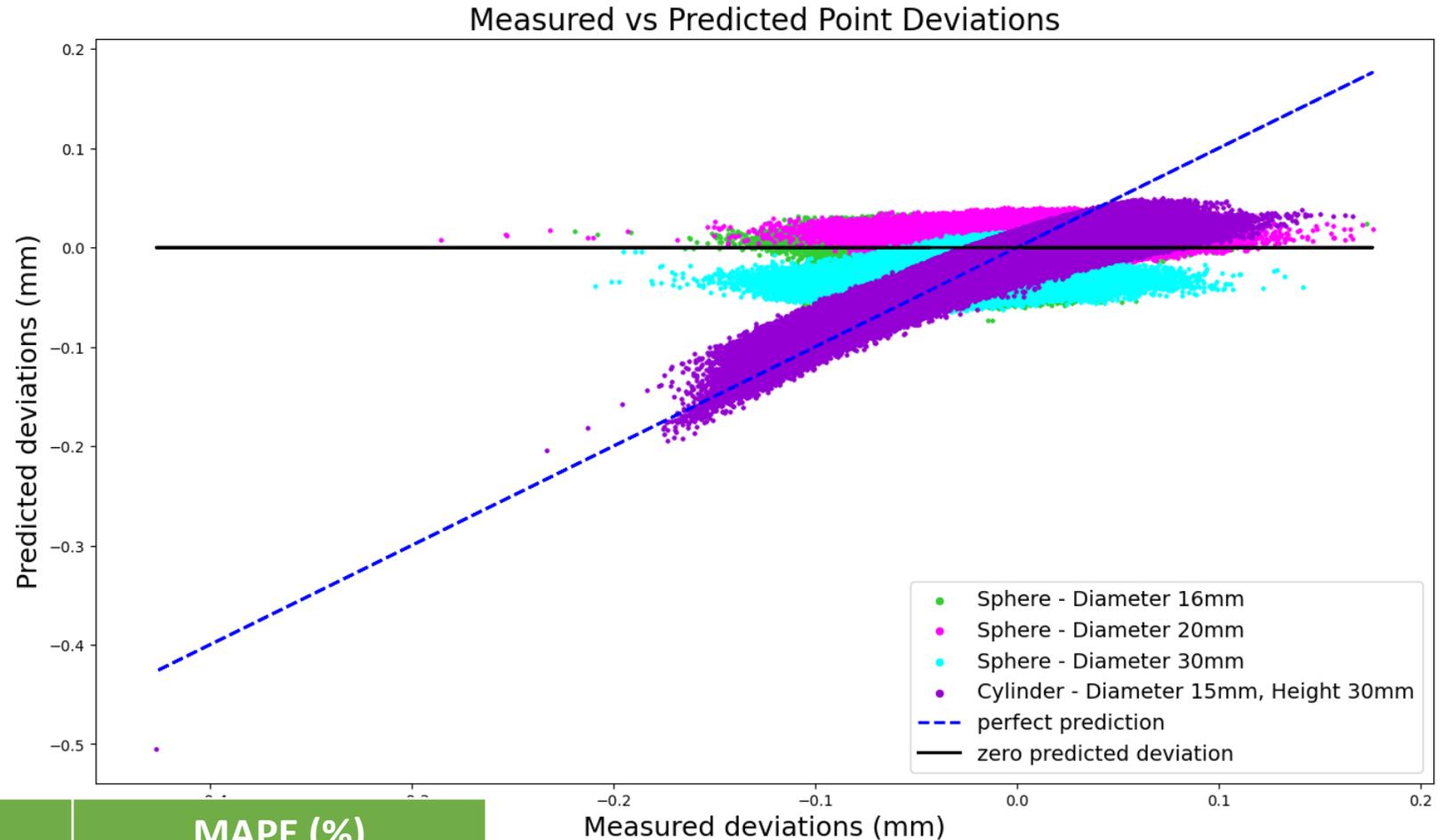
Hyperparameters = {
kernel: RBF,
C: 10.0}

Predictions on spheres

Large deviations from actual
Flat distribution

Predictions on cylinder

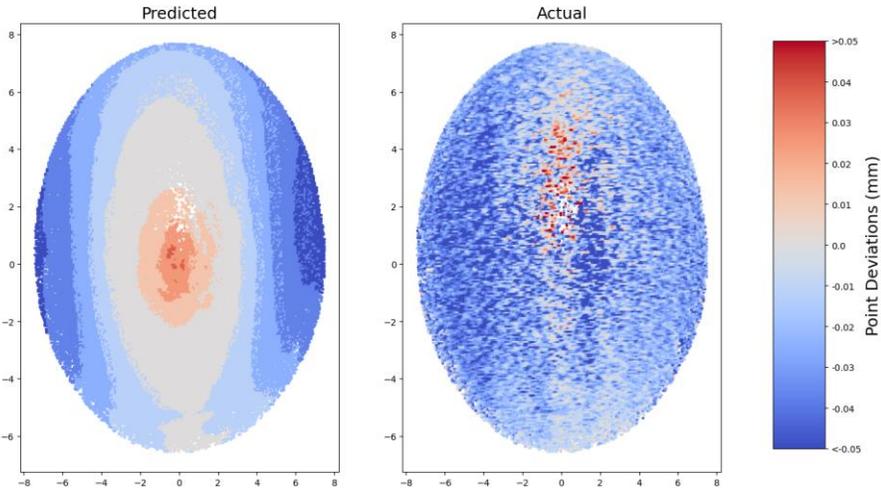
better approximation of truth



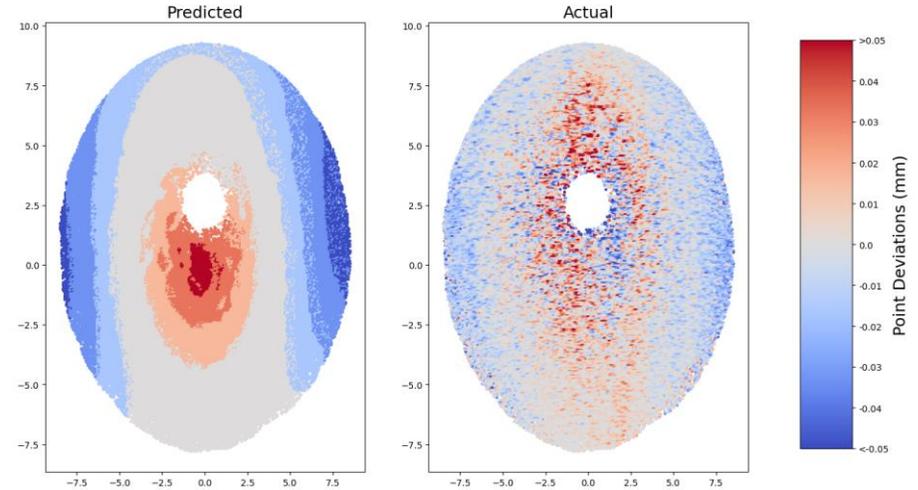
	MAE (mm)	MAPE (%)
Mean Validation score	0.026 ± 0.002	3.24 ± 0.03
Mean Test score	0.028 ± 0.004	3.4 ± 0.1

ML Experimental results – Visualize predictions

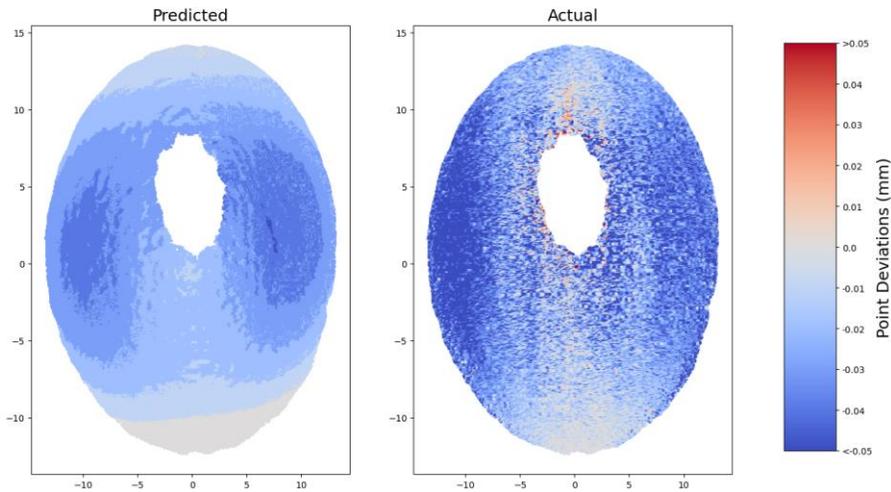
Sphere 16.0026mm, Lateral Density=50, Direction Density=2, Exposure Time=1.0



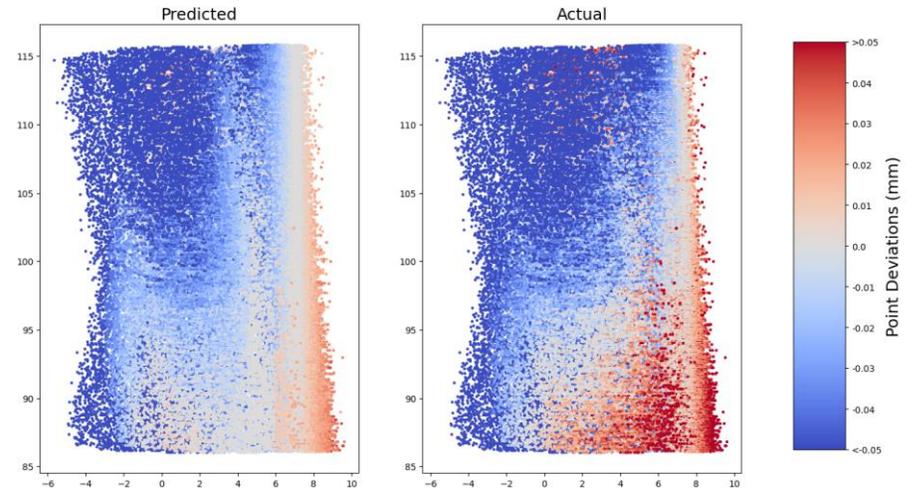
Sphere 20.0118mm, Lateral Density=50, Direction Density=2, Exposure Time=1.0



Sphere 30.0085mm, Lateral Density=50, Direction Density=2, Exposure Time=1.0

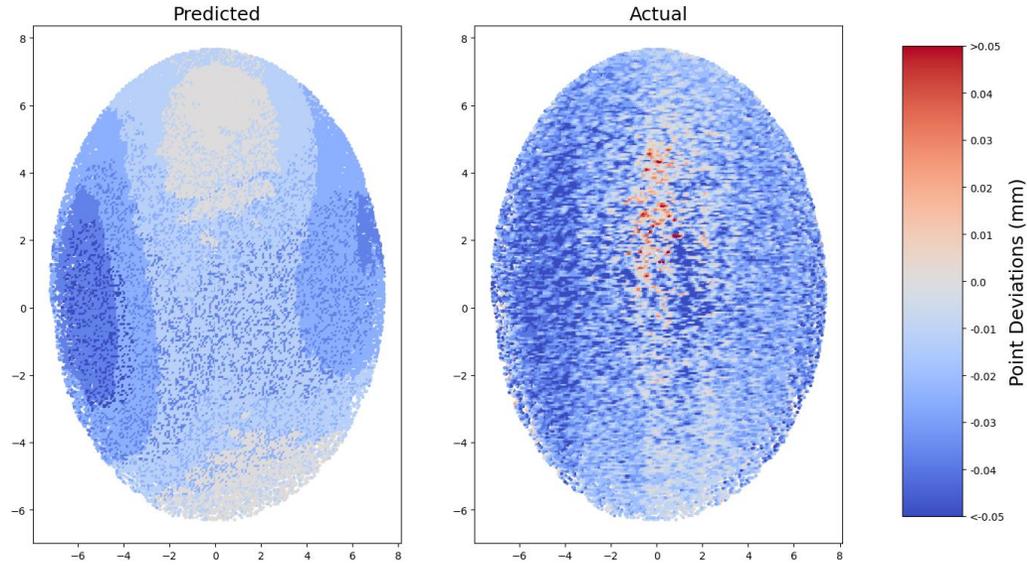


Cylinder 15.0219mm, Lateral Density=50, Direction Density=2, Exposure Time=1.0

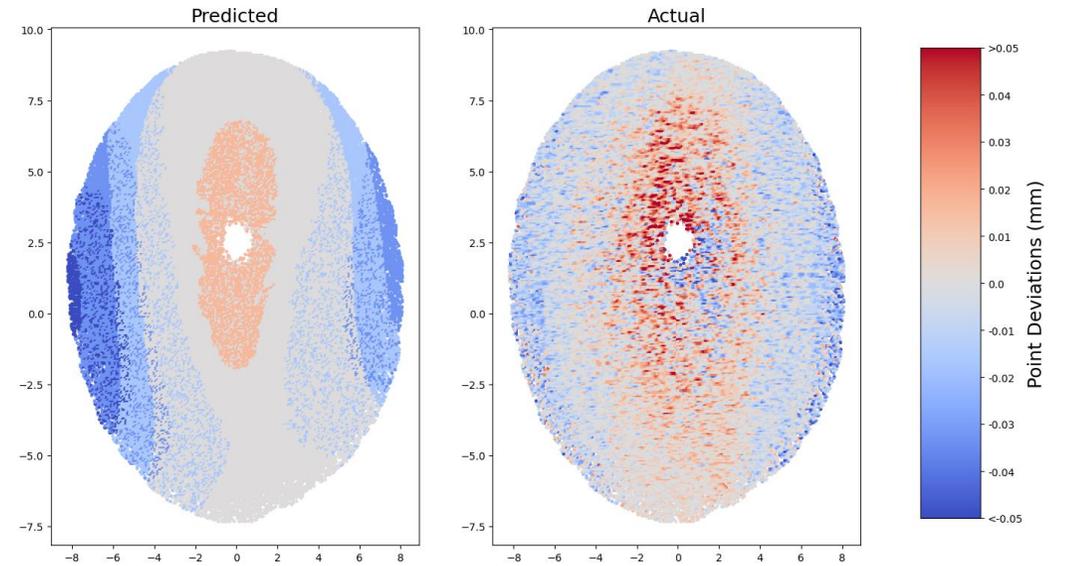


ML Experimental results – Visualize predictions

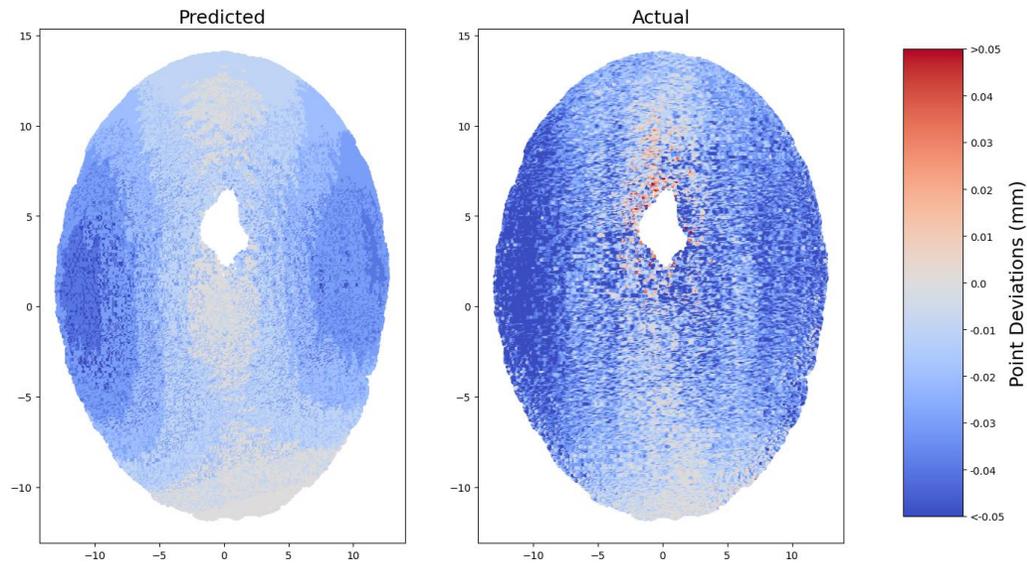
Sphere 16.0026mm, Lateral Density=50, Direction Density=2, Exposure Time=0.6



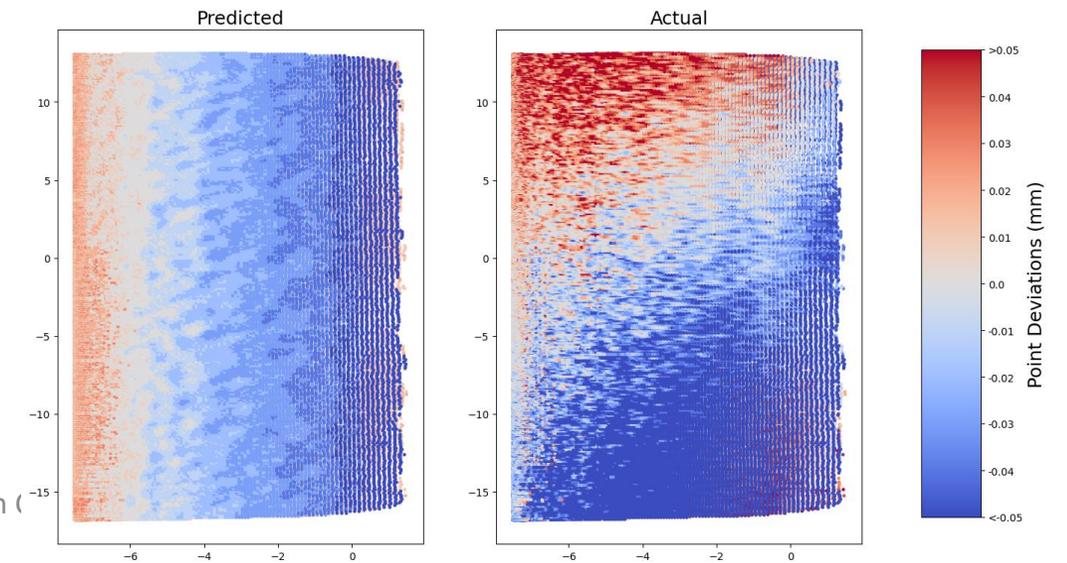
Sphere 20.0118mm, Lateral Density=50, Direction Density=2, Exposure Time=0.6



Sphere 30.0085mm, Lateral Density=50, Direction Density=2, Exposure Time=0.6



Cylinder 15.0219mm, Lateral Density=50, Direction Density=2, Exposure Time=0.6



Model Explanations - Feature Importance methods

Permutation Feature Importance

- Permute each feature by **random shuffle of values**
- Compute the **decrease in model performance** scores
- Repeat N times
- Calculate **mean decrease & std** in performance scores

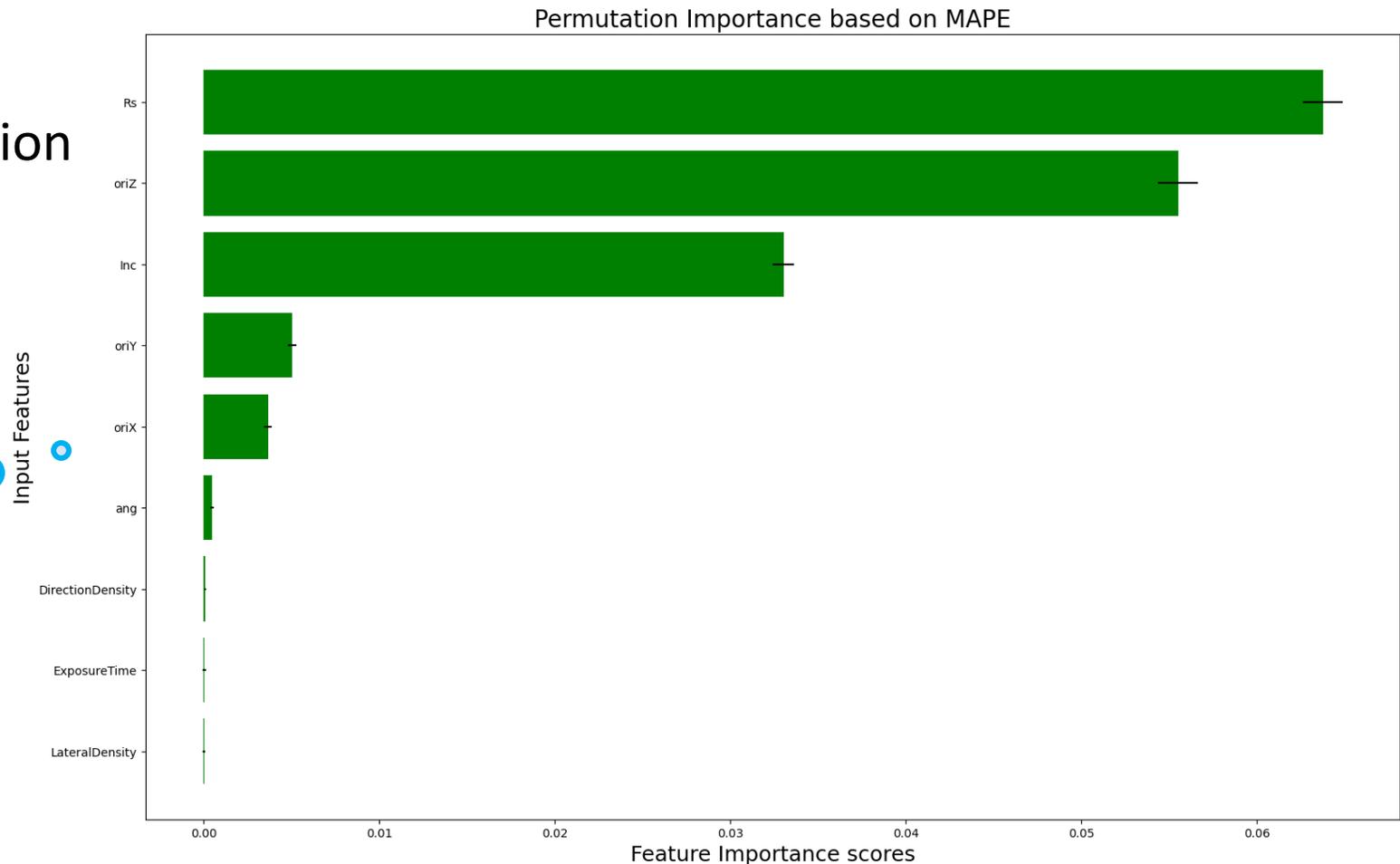
Computed independently for each feature ...
Permutation Importance scores **do not** add up to 1

	TV	Radio	Newspaper	Sales
0	230.1	37.8	69.2	22.1
1	44.5	39.3	45.1	10.4
2	17.2	45.9	69.3	9.1
3	151.5	41.3	58.5	18.5
4	180.8	10.8	58.4	12.9

Features with high effect on model's output:

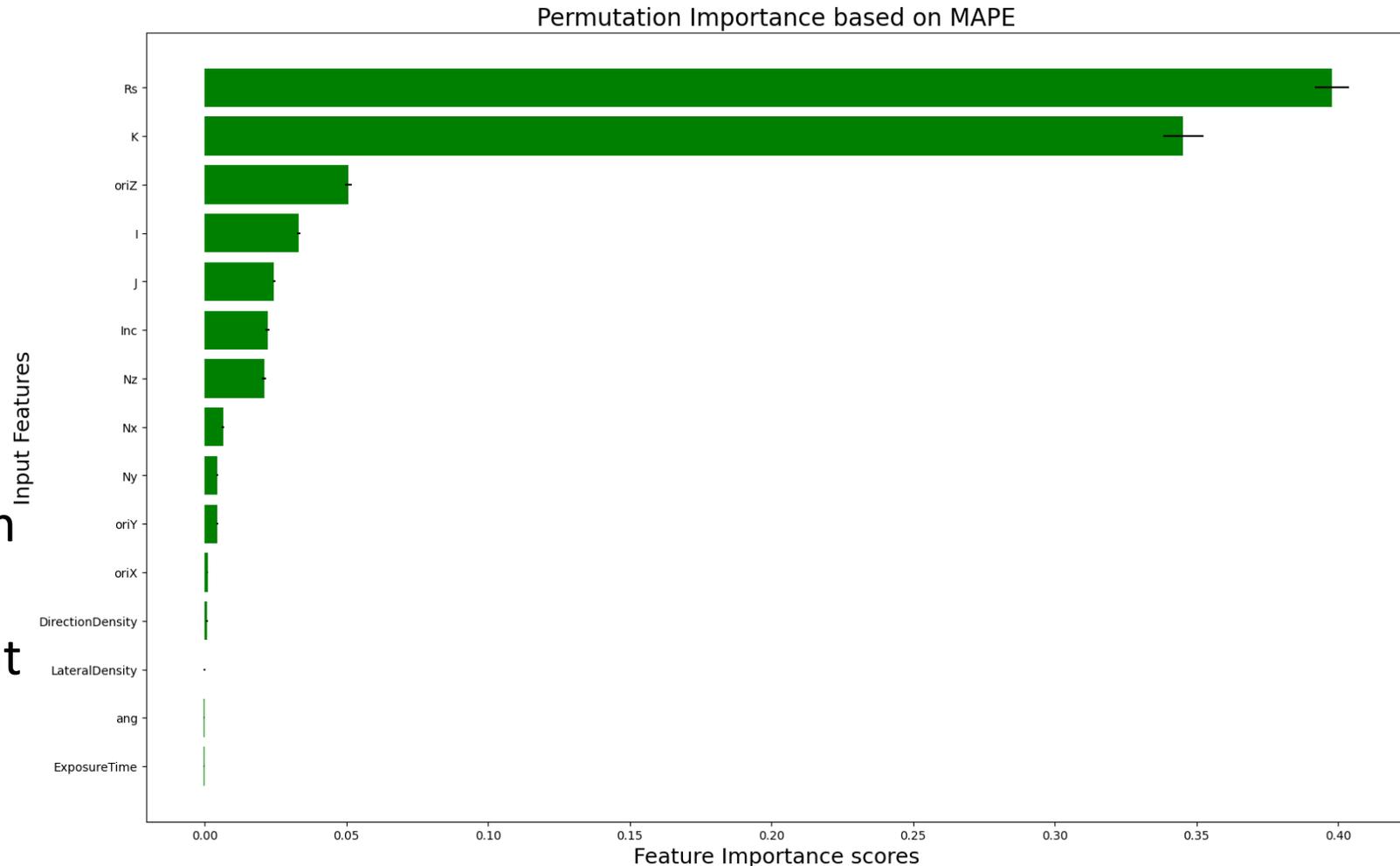
- R_s = Distance to laser source
- $oriZ$ = z-component of Orientation difference vector
- Inc = Incidence angle

Very low importance scores < 7%



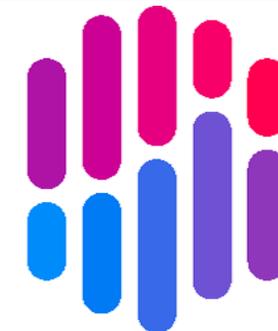
Features with high effect on model's output:

- R_s = Distance to laser source
- K = z-component of laser source direction
- Features R_s , K have ~8-10 times higher importance than the rest
- Features R_s , K have significant impact on model's predictions: 35-40%



Model Explanations - Feature Attribution methods

SHAP – SHapley Additive exPlanations



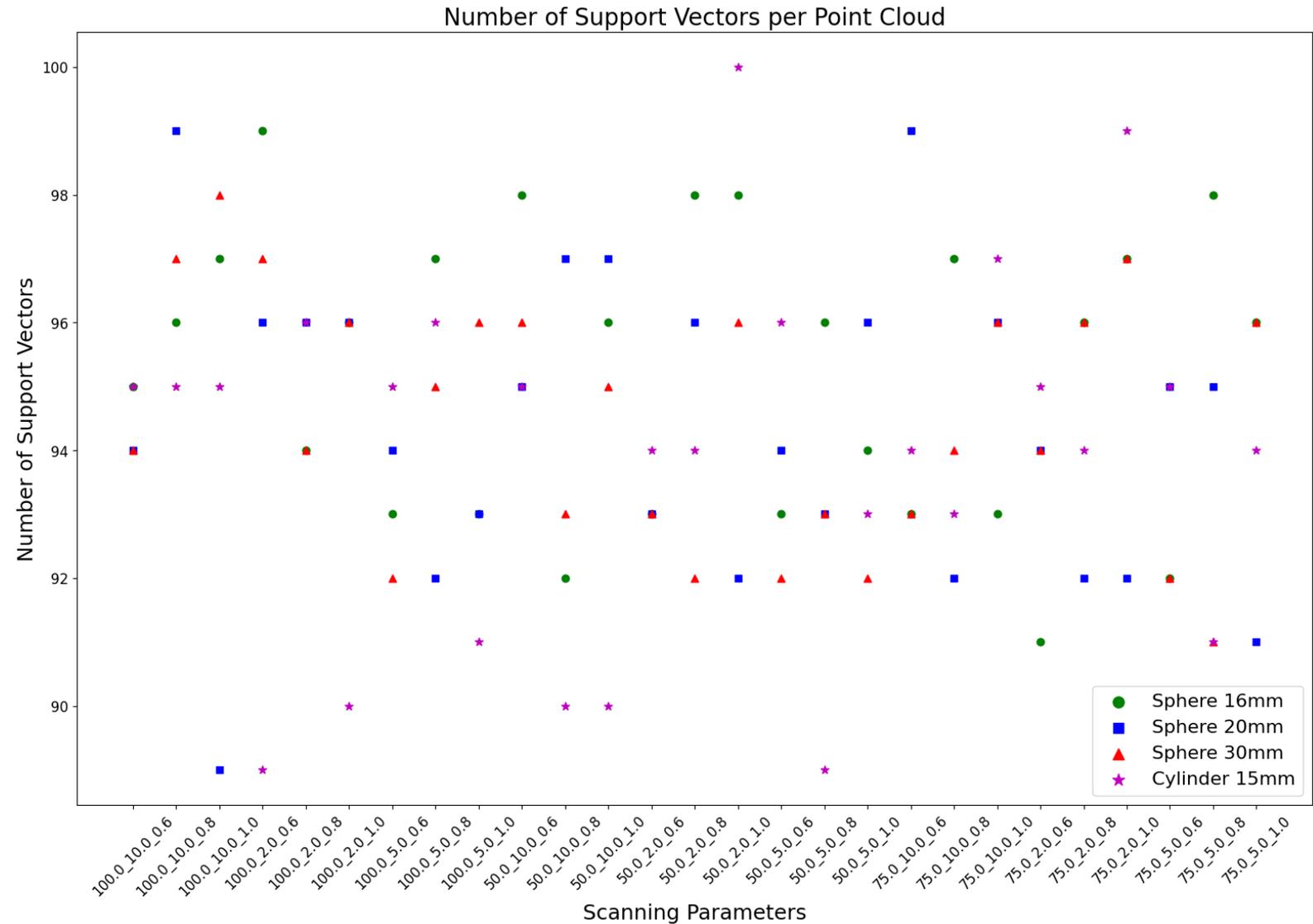
- Based on **Shapley values** from cooperative game theory
- **Shapley** quantifies the **contribution** of each **player** to the outcome of the game, **considering every possible coalition** of players
- **SHAP** quantifies the **contribution** each feature brings to each prediction of the ML model, considering all possible combinations of input features

- Builds **one predictive model per combination of features**, sequentially including more features: estimates the **marginal contribution** of each feature to the final outcome
- Aggregation of local explanations: **global picture!**



Retrieve Support Vectors (SV):

- 90-100 SVs per Point Cloud
- Training samples per Point Cloud = 100
 - SVs \approx training samples!



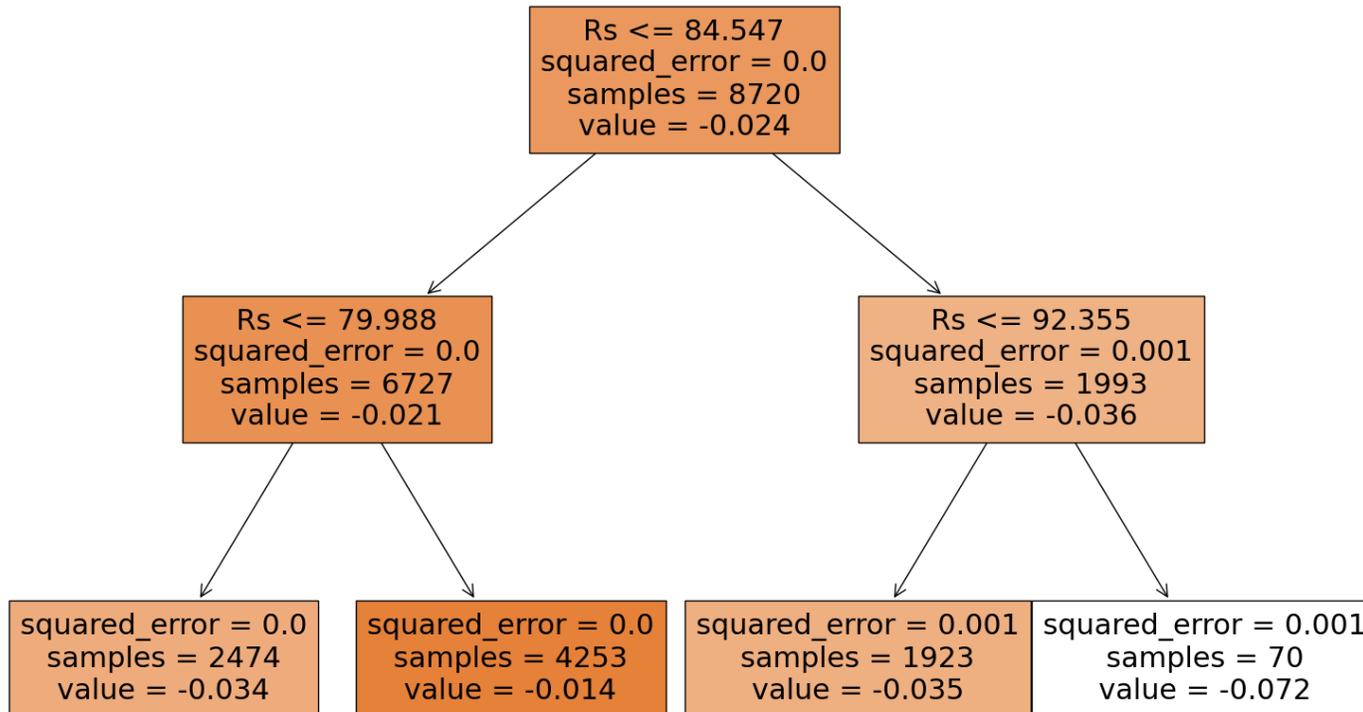
Model Explanations – Global surrogate

Decision Tree to explain trained SVM

- Depth = 2
- MAE = 0.014 (mm)



Decision Rules



```
|--- Rs <= 84.55  
| |--- Rs <= 79.99  
| | |--- value: [-0.03]  
| |--- Rs > 79.99  
| | |--- value: [-0.01]  
|--- Rs > 84.55  
| |--- Rs <= 92.35  
| | |--- value: [-0.03]  
| |--- Rs > 92.35  
| | |--- value: [-0.07]
```

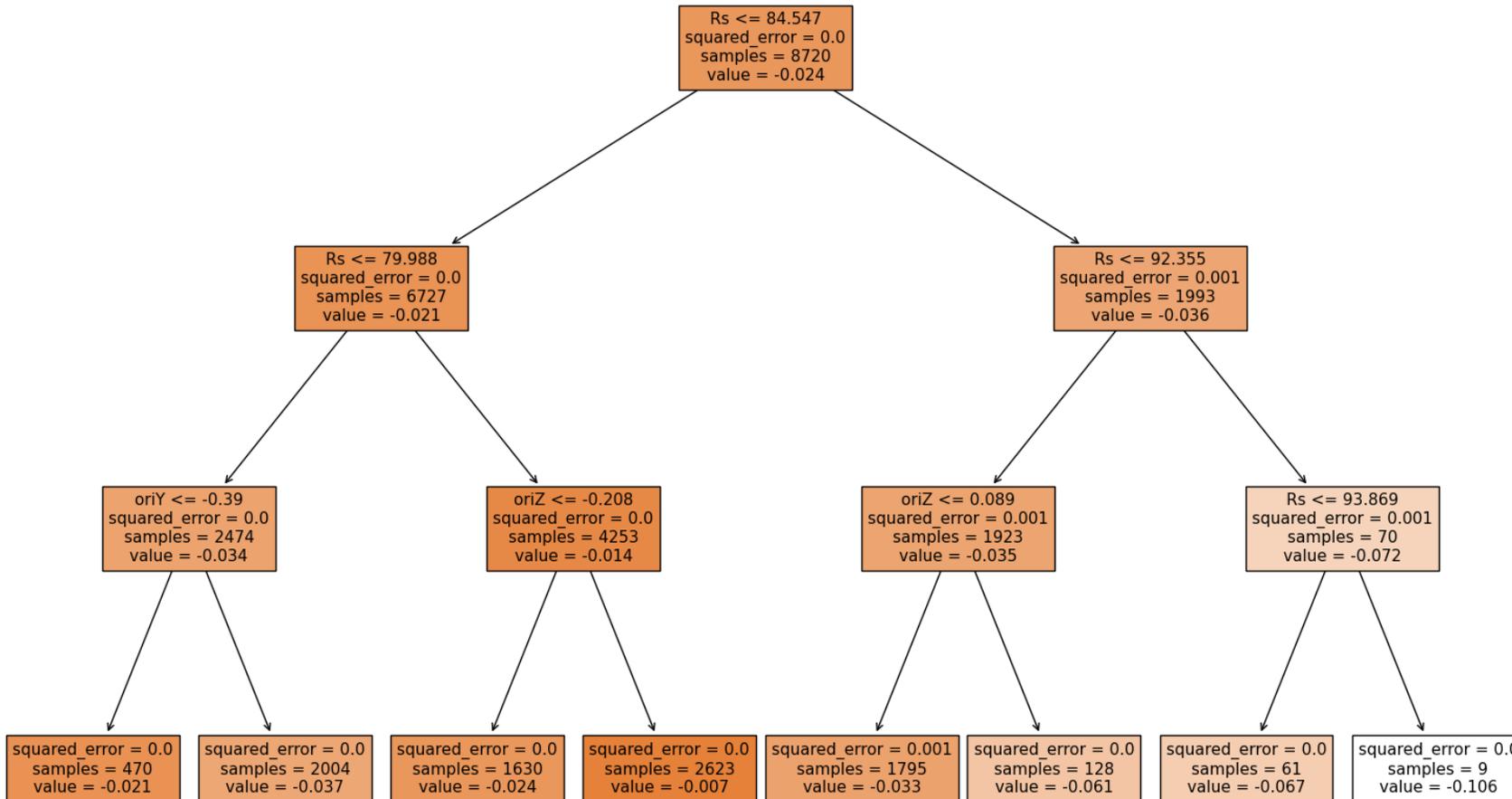
Model Explanations – Global Surrogate

Decision Tree to explain trained SVM

- Depth = 3
- MAE = 0.012 (mm)



Decision Rules



```

|--- Rs <= 84.55
| |--- Rs <= 79.99
| | |--- oriY <= -0.39
| | | |--- value: [-0.02]
| | |--- oriY > -0.39
| | | |--- value: [-0.04]
| |--- Rs > 79.99
| | |--- oriZ <= -0.21
| | | |--- value: [-0.02]
| | |--- oriZ > -0.21
| | | |--- value: [-0.01]
|--- Rs > 84.55
| |--- Rs <= 92.35
| | |--- oriZ <= 0.09
| | | |--- value: [-0.03]
| | |--- oriZ > 0.09
| | | |--- value: [-0.06]
| |--- Rs > 92.35
| | |--- Rs <= 93.87
| | | |--- value: [-0.07]
| | |--- Rs > 93.87
| | | |--- value: [-0.11]
    
```

Prediction of point-wise measurement accuracy

- Extraction of additional features
- More measurements needed (different geometries, fine granulation of scanning parameters)
- Repeat experiments for concave/complex geometries (different laser setup)

Relate point deviations to the target of the measurement

- Use Open3D to fit nominal geometries, calculate dimension & estimate uncertainty

New problem statement

- Unsupervised / semi-supervised learning methods
- Model data on graphs & apply Graph ML techniques

Thank you for your attention!