

Radiomic-Based Prediction of Lesion-Specific Systemic Treatment Response in Metastatic Disease

Supplementary Material

Caryn Geady^{1,2}, Farnoosh Abbas-Aghababazadeh¹, Andres Kohan¹, Scott Schuetze³, David Shultz, Benjamin Haibe-Kains^{1,2,4,5,6,7}

¹Princess Margaret Cancer Centre, University Health Network, Toronto, Canada

²Medical Biophysics, University of Toronto, Toronto, Canada

³Department of Medicine, University of Michigan, Ann Arbor, MI, USA

⁴Vector Institute for Artificial Intelligence, Toronto, Canada

⁵Ontario Institute for Cancer Research, Toronto, Canada

⁶Department of Computer Science, University of Toronto, Toronto, Canada

⁷Department of Biostatistics, Dalla Lana School of Public Health, Toronto, Canada

Selected Features

Table S1: Summary of radiomic features included in best performing models for the prediction of pulmonary lesion-specific systemic treatment response to DM.

Group	Radiomic Feature		
	Filter	Class	Name
All lesions	Wavelet-LHL	First Order	Variance (exterior rim)
	LOG ($\sigma = 3\text{mm}$)	GLDM	Grey Level Variance (lesion core)
	-	Shape	Voxel Volume
Z ≤ 3	Wavelet-LHL	First Order	Variance (exterior rim)
	LOG ($\sigma = 3\text{mm}$)	GLDM	Grey Level Variance (lesion core)
	LOG ($\sigma = 3\text{mm}$)	First Order	10th Percentile (exterior rim)
	-	Shape	Voxel Volume

Table S2: Summary of radiomic features included in best performing models for the prediction of pulmonary lesion-specific systemic treatment response to DE.

Group	Radiomic Feature		
	Filter	Class	Name
All lesions	LOG ($\sigma = 4\text{mm}$)	GLDM	Grey Level Variance (interior rim)
	Logarithm	GLCM	Sum of Squares (lesion core)
	-	Shape	Voxel Volume
$ Z \leq 3$	Wavelet-HHL	First Order	Variance (lesion core)
	Wavelet-LLH	First Order	Mean (lesion core)
	Logarithm	First Order	Mean (lesion core)
	Wavelet-LHL	GLCM	Cluster Tendency (lesion core)
	-	Shape	Voxel Volume
$ Z > 3$	Logarithm	GLCM	Sum of Squares (lesion core)
	Logarithm	First Order	Minimum (interior rim)
	Wavelet-HHL	First Order	Variance (lesion core)
	Wavelet-LHL	GLCM	Cluster Tendency (lesion core)
	-	Shape	Voxel Volume

Hyperparameter Tuning

Hyperparameter tuning was performed with GridSearchCV in Python. This process systematically explores optimal hyperparameters for machine learning models. It involves cross-validation, where the dataset is divided into folds, and each hyperparameter combination is assessed using a separate fold. GridSearchCV automates this process by exhaustively searching through a predefined grid of hyperparameter values to select the best-performing combination based on a specified evaluation metric. The predefined grid of hyperparameters used for this study are in **Table S3**.

Table S3: *Predefined grid of hyperparameters used for GridSearchCV used in this study.*

Hyperparameter	Options
'penalty'	['l1', 'l2', 'elasticnet', None]
'solver'	['lbfgs', 'liblinear', 'newton-cg', 'newton-cholesky', 'sag', 'saga']
'tol'	[1e-4, 1e-5, 1e-6, 1e-7, 1e-8, 1e-9]
'max_iter'	[50,100,150,200]