Supplementary

Descriptions of the extracted features

(I) 107 radiomics features are extracted with the help of Pyradiomics toolbox 3.0 which follows the Image Biomarker Standardisaion Initiative (IBSI) guidelines. The definitions of the features are detailed at https://pyradiomics.readthedocs.io/. The name list is as follows.

[1]original_shape_VoxelVolume
[2]original_shape_Sphericity
[3]original_shape_Maximum2DDiameterSlice
[4]original_shape_Maximum2DDiameterColumn
[5]original_shape_Maximum3DDiameter
[6]original_shape_Flatness
[7]original_shape_MeshVolume
[8]original_shape_SurfaceArea
[9]original_shape_MinorAxisLength
[10]original_shape_SurfaceVolumeRatio
[11]original_shape_Maximum2DDiameterRow
[12]original_shape_MajorAxisLength
[13]original_shape_LeastAxisLength
[14]original_shape_Elongation
[15]original_glcm_ClusterProminence
[16]original_glcm_SumSquares
[17]original_glcm_DifferenceVariance
[18]original_glcm_JointAverage
[19]original_glcm_Contrast
[20]original_glcm_ClusterShade
[21]original_glcm_Idm
[22]original_glcm_Idmn
[23]original_glcm_Id
[24]original_glcm_MCC
[25]original_glcm_Autocorrelation
[26]original_glcm_JointEnergy
[27]original_glcm_JointEntropy
[28]original_glcm_SumAverage
[29]original_glcm_InverseVariance
[30]original_glcm_Imc2
[31]original_glcm_ClusterTendency
[32]original_glcm_DifferenceAverage
[33]original_glcm_DifferenceEntropy
[34]original_glcm_SumEntropy
[35]original_glcm_Idn
[36]original_glcm_MaximumProbability
[37]original_glcm_Imc1
[38]original_glcm_Correlation
[39]original_ngtdm_Contras
[40]original_ngtdm_Strength
[41]original_ngtdm_Coarseness
[42]original_ngtdm_Busyness
[43]original_ngtdm_Complexity

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[44]original_glszm_SmallAreaEmphasis
[45]original_glszm_LargeAreaEmphasis
[46]original_glszm_ZonePercentage
[47]original_glszm_GrayLevelVariance
[48]original_glszm_ZoneEntropy
[49]original_glszm_LargeAreaLowGrayLevelEmphasis
[50]original_glszm_GrayLevelNonUniformityNormalized
[51]original_glszm_SizeZoneNonUniformityNormalized
[52]original_glszm_GrayLevelNonUniformity
[53]original_glszm_SmallAreaHighGrayLevelEmphasis
[54]original_glszm_SizeZoneNonUniformity
[55]original_glszm_SmallAreaLowGrayLevelEmphasis
[56]original_glszm_ZoneVariance
[57]original_glszm_LowGrayLevelZoneEmphasis
[58]original_glszm_HighGrayLevelZoneEmphasis
[59]original_glszm_LargeAreaHighGrayLevelEmphasis
[60]original_glrlm_RunVariance
[61]original_glrlm_RunLengthNonUniformity
[62]original_glrlm_LongRunLowGrayLevelEmphasis
[63]original_glrlm_HighGrayLevelRunEmphasis
[64]original_glrlm_ShortRunEmphasis
[65]original_glrlm_GrayLevelNonUniformityNormalized
[66]original_glrlm_ShortRunLowGrayLevelEmphasis
[67]original_glrlm_ShortRunHighGrayLevelEmphasis
[68]original_glrlm_GrayLevelVariance
[69]original_glrlm_GrayLevelNonUniformity
[70]original_glrlm_RunPercentage
[71]original_glrlm_LowGrayLevelRunEmphasis
[72]original_glrlm_LongRunHighGrayLevelEmphasis
[73]original_glrlm_RunEntropy
[74]original_glrlm_LongRunEmphasis
[75]original_glrlm_RunLengthNonUniformityNormalized
[76]original_gldm_SmallDependenceEmphasis
[77]original_gldm_SmallDependenceHighGrayLevelEmphasis
[78]original_gldm_LargeDependenceHighGrayLevelEmphasis
[79]original_gldm_GrayLevelVariance
[80]original_gldm_SmallDependenceLowGrayLevelEmphasis
[81]original_gldm_LargeDependenceLowGrayLevelEmphasis
[82]original_gldm_GrayLevelNonUniformity
[83]original_gldm_LowGrayLevelEmphasis
[84]original_gldm_DependenceEntropy
[85]original_gldm_DependenceNonUniformity
[86]original_gldm_HighGrayLevelEmphasis
[87]original_gldm_LargeDependenceEmphasis
[88]original_gldm_DependenceNonUniformityNormalized
[89]original_gldm_DependenceVariance
[90]original_firstorder_InterquartileRange
[91]original_firstorder_10Percentile

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[92]original_firstorder_RootMeanSquared
[93]Original_firstorder_MeanAbsoluteDeviation
[94]original_firstorder_TotalEnergy
[95]original_firstorder_Range
[96]original_firstorder_Entropy
[97]original_firstorder_Variance
[98]original_firstorder_Minimum
[99]original_firstorder_Skewness
[100]original_firstorder_Energy
[101]original_firstorder_RobustMeanAbsoluteDeviation
[102]original_firstorder_Median
[103]original_firstorder_Maximum
[104]original_firstorder_Kurtosis
[105]original_firstorder_Uniformity
[106]original_firstorder_Mean
[107]original_firstorder_90Percentile

(II) 84 CoLIAGe (Co-occurrence of Local Anisotropic Gradient Orientations) features

The detailed descriptions of the 84 GoLIAGe features are in the paper "Co-occurrence of Local Anisotropic Gradient Orientations (CoLlAGe): A new radiomics descriptor" (17). First of all, gradient orientations for every voxel in X, Y, Z dimensions are computed. Then, the 2-Dimension local dominant orientations (theta) and the 3-Dimension local dominant orientations (fai) for every voxel within a 3*3*3 neighborhood using singular value decomposition (SVD) are calculated. Then based on the "thetas" and "fais", with the help of Pyradiomics toolbox 3.0 which follows the Image Biomarker Standardisaion Initiative (IBSI) guidelines, 84 radiomics features are extracted. The name list is as follows.

[1]theta_SumSquares
[2]theta_DifferenceAverage
[3]theta_DifferenceEntropy
[4]theta_MCC
[5]theta_ClusterTendency
[6]theta_ClusterProminence
[7]theta_Idmn
[8]theta_Imc1
[9]theta_Autocorrelation
[10]theta_Correlation
[11]theta_Idn
[12]theta_JointEntropy
[13]theta_ClusterShade
[14]theta_Contrast
[15]theta_MaximumProbability
[16]theta_Id
[17]theta_SumAverage
[18]theta_Imc2
[19]theta_InverseVariance
[20]theta_JointAverage
[21]theta_JointEnergy
[22]theta_Idm
[23]theta_DifferenceVariance
[24]theta_SumEntropy

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[25]fai_SumSquares
[26]fai_DifferenceAverage
[27]fai_DifferenceEntropy
[28]fai_MCC
[29]fai_ClusterTendency
[30]fai_ClusterProminence
[31]fai_Idmn
[32]fai_Imc1
[33]fai_Autocorrelation
[34]fai_Correlation
[35]fai_Idn
[36]fai_JointEntropy
[37]fai_ClusterShade
[38]fai_Contrast
[39]fai_MaximumProbability
[40]fai_Id
[41]fai_SumAverage
[42]fai_Imc2
[43]fai_InverseVariance
[44]fai_JointAverage
[45]fai_JointEnergy
[46]fai_Idm
[47]fai_DifferenceVariance
[48]fai_SumEntropy
[49]theta_first_Maximum
[50]theta_first_Entropy
[51]theta_first_RootMeanSquared
[52]theta_first_Median
[53]theta_first_Minimum
[54]theta_first_MeanAbsoluteDeviation
[55]theta_first_Energy
[56]theta_first_90Percentile
[57]theta_first_RobustMeanAbsoluteDeviation
[58]theta_first_InterquartileRange
[59]theta_first_Variance
[60]theta_first_TotalEnergy
[61]theta_first_Range
[62]theta_first_Skewness
[63]theta_first_10Percentile
[64]theta_first_Kurtosis
[65]theta_first_Uniformity
[66]theta_first_Mean
[67]fai_first_Maximum
[68]fai_first_Entropy
[69]fai_first_RootMeanSquared
[70]fai_first_Median
[71]fai_first_Minimum
[72]fai_first_MeanAbsoluteDeviation

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[73]fai_first_Energy
[74]fai_first_90Percentile
[75]fai_first_RobustMeanAbsoluteDeviation
[76]fai_first_InterquartileRange
[77]fai_first_Variance
[78]fai_first_TotalEnergy
[79]fai_first_Range
[80]fai_first_Skewness
[81]fai_first_10Percentile
[82]fai_first_Kurtosis
[83]fai_first_Uniformity
[84]fai_first_Mean

(III) 3 SUV features
a) SUV peak: the maximum uptake in 1 cm3 area.
b) SUV mean: the mean uptake in the VOI.
c) SUV max: the max uptake in the VOI.

Table S1 Hyperparameters-tuning range of classifiers

Classifiers	hyperparameters-tuning range
SVM-RBF	'C' : [0.001, 0.01, 0.1, 1, 2, 3, 4, 5, 10, 50, 60, 70, 80, 90, 100, 200, 300, 400, 500, 1000, 2000, 2500, 3000, 3500, 4000, 5000, 10000]
	'gamma' : ['scale', 0.0001, 0.001, 0.004, 0.005, 0.01, 0.05 , 0.04, 0.03, 0.02, 0.08, 0.1, 0.15, 0.2, 0.25, 0.5, 1]
SVM linear	'C' : [0.001, 0.01, 0.1, 1, 2, 3, 4, 5, 10, 50, 60, 70, 80, 90, 100, 200, 300, 400, 500, 1000, 2000, 2500, 3000, 3500, 4000, 5000, 10000]
	'gamma' : ['scale', 0.001, 0.004, 0.005, 0.01, 0.05 , 0.04, 0.03, 0.02, 0.08, 0.1, 0.15, 0.2, 0.25, 0.5, 1]
Random forest	'n_estimators' : [5, 50],
	'max_depth' : np.arange (1, 3),
	'min_samples_split': np.arange (2,3),
	'min_samples_leaf': np.arange (1,3),
	'max_features' : ['auto']
Logistic regression	'penalty': ['l1', 'none'],
	'C':[0.1, 0.5, 1, 5, 10]
Gaussian process	'max_iter_predict': [100,150,200]
Linear discriminant	'solver': ['svd', 'lsqr', 'eigen']
Adaboost	'n_estimators': [2, 5, 10]

SVM, support vector machine; RBF, radial basis function kernel; Adaboost, adaptive boosting; l1, lasso or L1 regression; svd, singular value decomposition; lsqr, least square QR dissolution; QR, orthogonal matrix; eigen, eigenvalue decomposition.

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Table S2 The corresponding hyperparameters of SVM-RBF

Folds	3D subregion-based	4D subregion-based	5D subregion-based	Conventional
1	C=10, gamma=scale	C=0.1, gamma=0.25	C=100, gamma=0.01	C=5000, gamma=0.03
2	C=70, gamma=0.004	C=1, gamma=1	C=60, gamma=0.004	C=3000, gamma=0.5
3	C=1, gamma=scale	C=3, gamma=scale	C=60, gamma=0.001	C=10, gamma=0.5
4	C=50, gamma=0.005	C=60, gamma=0.004	C=5, gamma=0.004	C=60, gamma=0.01
5	C=2, gamma = 0.08	C=10000, gamma=0.004	C=2500, gamma=0.02	C=100, gamma=0.5

SVM, support vector machine; RBF, radial basis function kernel; D, dimension.

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