

Supplementary Material

Table 1. Comparisons between subject(s) and a reference – Combining MRI metrics

MVComp function name	Description
<code>compute_average</code>	To compute the group average maps of each metric (will serve as the reference).
<code>feature_gen</code>	Apply to the reference group average maps to extract the feature matrix (<code>m_f_mat</code> of shape n voxels \times n features), a mask vector (<code>mat_mask</code> of shape n voxels) and a nibabel object of the mask (<code>mask_img</code>).
<code>norm_covar_inv</code>	To compute the covariance matrix (<code>s</code>) and its pseudoinverse (<code>pinv_s</code>) from the reference feature and mask matrices (<code>m_f_mat</code> and <code>mat_mask</code>).
<code>correlation_fig</code>	To generate a correlation matrix figure from the covariance matrix (<code>s</code>). For visualization.
<code>model_comp</code>	To calculate voxel-wise D2 between each subject contained in the provided <code>subject_ids</code> list and the reference (group average). Yields a D2 matrix of size number of voxels \times number of subjects. *For leave-one-out approach, set the <code>exclude_comp_from_mean_cov</code> option to True (the previous steps can be skipped in this case since a new covariance matrix is computed for each subject, within the <code>model_comp</code> function).
<code>dist_plot</code>	To produce D2 maps for every subject from the D2 matrix generated by <code>model_comp</code> .

<code>model_comp</code> with <code>return_raw</code> set to True	To extract features contribution to D2 in a region of interest. When <code>return_raw</code> is set to True, the function returns a 3D array of size (number of voxels) x (number of metrics) x (number of subjects). This information can then be summarized to obtain the % contribution of each metric for a group of subjects.
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Table 2. Comparisons between subject(s) and a reference – Combining spatial dimensions

MVComp function name	Description
<code>spatial_mvcomp</code>	To compute a D2 score between each subject and the reference from a matrix containing the data (e.g., mean FA in each WM tract) of all subjects (n subjects x n tracts). Returns a vector with a single D2 value per subject. *For leave-one-out approach, set the <code>exclude_comp_from_mean_cov</code> option to True.
<code>spatial_mvcomp</code> with <code>return_raw</code> set to True	To extract features contribution to D2. If set to True, a 2D array of size (number of subjects) x (number of tracts) is returned. This information can then be summarized to obtain the relative importance of each tract to D2.

Table 3. Comparisons within a single subject – Voxel-wise D2 resolution

MVComp function name	Description
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<code>feature_gen</code>	Provide the path of the images (i.e., one image per metric) and the reference ROI mask to this function to extract the feature matrix (<code>m_f_mat</code> of shape n voxels \times n features), a mask vector (<code>mat_mask</code> of shape n voxels) and a nibabel object of the mask (<code>mask_img</code>). This function can also be used to extract the data inside the ROI of voxels to be evaluated.
<code>norm_covar_inv</code>	To compute the covariance matrix (<code>s</code>) and its pseudoinverse (<code>pinv_s</code>) from the reference feature and mask matrices (<code>m_f_mat</code> and <code>mat_mask</code>).
<code>correlation_fig</code>	To generate a correlation matrix figure from the covariance matrix (<code>s</code>). For visualization.
<code>mah_dist_mat_2_roi</code>	To compute voxel-wise D2 between all voxels within a mask and a specific reference ROI. The user will need to provide a vector of data for the reference ROI (i.e., mean across voxels in the ROI for each metric), along with the feature matrix containing the data for the voxels to be evaluated.
<code>mah_dist_mat_2_roi</code> with <code>return_raw</code> set to True	To extract features' contributions. The output will be of shape (number of voxels) \times (number of metrics).

Table 4. Comparisons within a single subject – Voxel-voxel matrix D2 resolution

MVComp function name	Description
<code>voxel2voxel_dist</code>	To compute D2 between each voxel and all other voxels in a mask. Yields a symmetric 2-D matrix of size n voxels \times n voxels containing D2 values between each pair of voxels.