

Supplemental S1 Multimodal Variational AutoEncoders

This appendix presents details on the multiview variational autoencoder (mVAE) models, used to perform the Digital Avatar Analysis, once they are trained.

Multimodal (or multiview) VAEs are extensions of the well-established VAE [15] that allows joint integration and reconstruction of two or more views. These two VAE models are themselves derived from AEs which attempt to find a compressed representation that contains as much information as possible about the input data. They are based on the assumption that the input data can be generated from a lower dimensional space [93]. AEs have been extensively studied [94] and used in various applications such as medical image segmentation [95]. In the variational version of an AE, the main idea is to learn a probability distribution over the low dimensional latent space. Finally, multimodal VAEs allow the construction of view-specific and shared latent spaces via the different modeling schemes. This is of great interest in medicine, for example to separate common sources of variability from disease-specific one [8, 9, 10].

The selected model

Let $x = \{x_1, \dots, x_K\}$ be an observation of K views, where each x_k can have different dimensions J_k . We assume that there exist $K + 1$ latent variables underlying the data generation process, one latent variable specific to each view, and one joint, expressing the shared variability across views. The general form of the latent variables is $\{z, z_1, \dots, z_k, \dots, z_K\}$ with z denoting the d -dimensional latent variable shared by all x_k , and z_k the view-specific d_k -dimensional latent variables. We assume the following generative process for the observation set:

$$\begin{aligned} z &\sim p(z) \\ z_k &\sim p(z_k) \\ x_k &\sim p_\theta(x_k|z, z_k) \end{aligned}$$

where $p(z), p(z_k)$ are prior distributions for the latent variables and $p_\theta(x_k|z, z_k)$ is a likelihood distribution of the observations conditioned on the latent variable. The generative process $p_\theta(x)$ is approximated by its Evidence Lower Bound (ELBO). The bottleneck of this approximation problem comes to computing the posterior $p_\theta(z, z_k|x)$. A first usual assumption about $p_\theta(z|x)$ considers that it contains all the shared information between the views, and we can write $p_\theta(z, z_k|x) = p_\theta(z|x) \times p_\theta(z_k|x_k)$. Other assumptions are needed since these posteriors are not analytically tractable. The posterior distributions are classically approximated by parametrised distributions $q_\phi(z|x)$ (the so-called joint variational posterior) and $q_\phi(z_k|x_k)$ respectively.

State-of-the-art models solve this problem with different ways of modeling the joint variational posterior distribution $q_\phi(z|x)$. These approaches compose $q_\phi(z|x)$ using the Gaussian experts $q_\phi(z|x_k)$ unimodal posteriors, which may be combined in various ways. In Product of Experts (PoE) approach [8], $q_\phi(z|x)$ is defined as a product of individual Gaussian experts, assuming the conditional independence of the experts, hence remains Gaussian. The product operator used in PoE may dampen the specific variability of a given block described by gaussian unimodal posterior, and other work proposes to model [9] $q_\phi(z|x)$ using a Mixture of Experts (MoE), assuming each unimodal experts contributes equally to the joint posterior. MoPoE approaches defines $q_\phi(z|x)$ as a Mixture of Product of Experts. Each product of experts is computed over the different subsets of views [10]. We use the latter strategy, referred to as MoPoE-VAE, as it is a generalisation of the two previous approaches. Each strategy has different ways of handling missing views, that may differ between train and test time. The MoPoE-VAE simply uses the subsets of available views for each observation. As regards to the unimodal posteriors $q_\phi(z_k|x_k)$, we classically use Gaussian distributions.

The MoPoE-VAE optimises a generalised multimodal ELBO objective for learning view-specific and a joint distribution of multiple views x with potential missing data, defined as:

$$\begin{aligned} L_{MoPoE}(\theta, \phi; x) = & \sum_{k=1}^K E_{q_\phi(z, z_k|x)} [\log(p_\theta(x_k|z, z_k))] \\ & - \sum_{k=1}^K D_{KL}(q_\phi(z_k|x_k) || p_\theta(z_k)) - D_{KL} \left(\underbrace{\frac{1}{2^K} \sum_{x_p \in \mathcal{P}(x)} \tilde{q}_\phi(z|x_p)}_{=q_\phi(z|x)} || p_\theta(z) \right) \end{aligned}$$

There are 2^K different subsets contained in the powerset $\mathcal{P}(x)$, and $\tilde{q}_\phi(z|x_p) = \prod_{x_k \in x_p} q_\phi(z|x_k)$ is the product of Gaussian expert posteriors $q_\phi(z|x_k)$, defined for the subset of views in x_p .

These formulae show our specific implementation of the MoPoE-VAE which handles multi-views by modelling view-specific latent space posterior distributions, and a joint posterior distribution shared between views as a mixture of the products of their marginal posteriors (experts). This implementation differs from the one benchmarked in [21, 96] which consider only one joint latent (MoPoE-VAE with its initial formulation [10]). These benchmarks also favor the generative abilities when we essentially consider its representation space in our interpretation framework.

Model specification and training

In our work, the encoders with parameters ϕ are each defined as multilayer perceptrons (MLPs), each with one hidden layer of 256 units and a ReLU activation. The decoders with parameters θ are linear (a single fully connected layer). Note that every decoder has a learnable variance parameter for each reconstructed feature that does not depend on the input observation. This allows the decoders to learn a population-level variability. To handle inputs of different sizes, the dimensions of the view-specific latent spaces were set individually. Based on a previous study [97], we chose $d_{eCRF} = 1$ and $d_{ROI} = 20$. Defining the dimension of the shared latent space jointly with the dimensions $(J_1, \dots, J_K)$ of the input views seems to be a reasonable criterion, we use the following rule:

$$d < \min_{k \in \{1, \dots, K\}} \{J_k - d_k\}$$

To spread the variability of the observations across the view-specific and shared latent representations, we choose $d = 3$. All data are z-scored before being fed into the network. The model is trained with an Adam optimisation, an initial learning rate of 2×10^{-3} and a batch size of 256.

Supplemental S2 Representational Similarity Analysis

Assessing model quality in an unsupervised setting remains an open issue. To investigate the learned latent representations, we derive a Representational Similarity Analysis (RSA) [47] between these representations and some target measures on subjects (in our case clinical scores). Note that the considered seven scores are correlated (see Fig. S2-1). We compute the subject-pairwise dissimilarity matrices in the latent space (modality-specific and joint) using the euclidean distance. We derive the same subject-pairwise dissimilarity matrices for the target measures. Finally, the Kendall rank correlation coefficient (Kendall τ) enables the comparison of these dissimilarity matrices emphasising the captured information. RSA is used twice in the present work. First we use it as a component of our framework to weight the contribution of a model when aggregating its extracted associations in the regularised digital avatar analysis (r-DAA) (see Section 2.3 and Alg. Supplemental S5.2). Second we consider it to evaluate the information contained in the different latent representations (see Section 3.1).

Model quality scoring used in r-DAA

We hypothesise that the latent representations of a good model to understand eCRF symptom scores should contain some amount of symptoms-related variability. We evaluate each trained MoPoE-VAE using RSA output Kendall τ between the model’s joint latent space and each eCRF score (τ_s), defined as $\boldsymbol{\tau} = (\tau_1, \dots, \tau_{|S|}) \in [-1, 1]^{|S|}$. For each of the n_E models, we use it’s average Kendall $\hat{\tau} = \frac{1}{|S|} \sum_{s=1}^{|S|} \tau_s$ across eCRF scores as its quality score, used to weight the aggregation function in the ensembling of the n_E corresponding DAAs (see section 2.3). This is detailed in the Alg. Supplemental S5.2 as well.

Assessing the latent representation spaces with RSA

We report in Table 1 aggregated results from RSAs applied to each split and corresponding models. We report the average $N \times n_E$ Kendall τ between each different measure and latent space. In the table we report the significance of these correlations. We compute it by considering the p -values of the Kendall τ statistics (corresponding to the rejection of the null hypothesis). We correct them for multiple testing using the Hommel [98] correction for multiple dependent tests and multiple independent test using Bonferroni. Then we consider the median of the corrected p -values. We chose the value of 1% for the significance threshold.

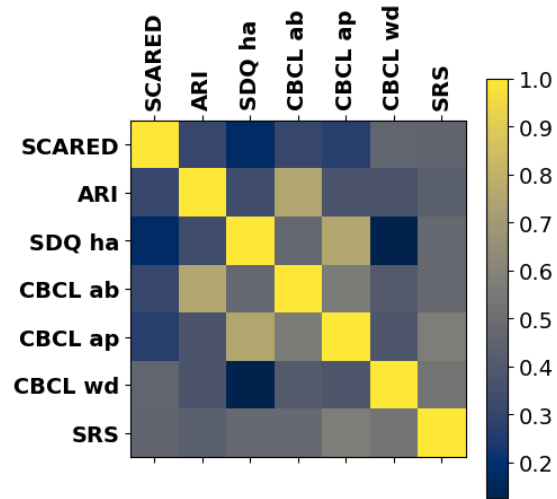


Figure S2-1: Correlations between the 7 eCRF scores.

Supplemental S3 Digital Avatar Analysis

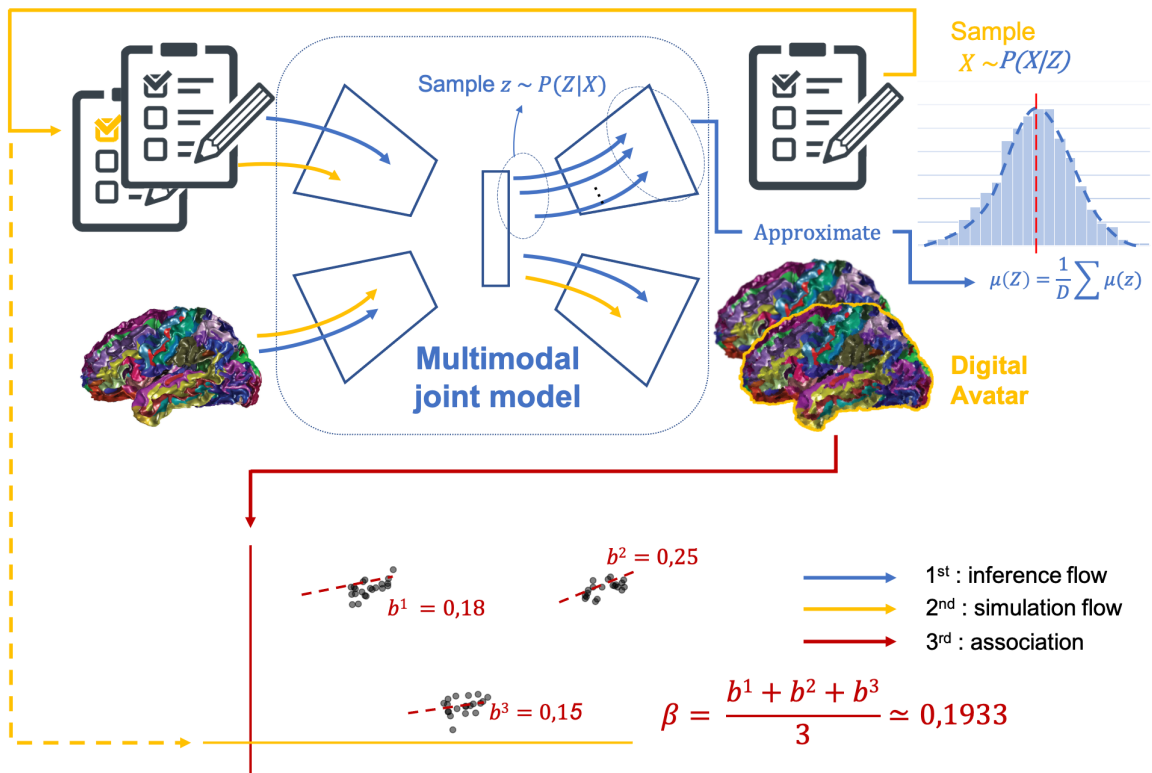


Figure S3-1: Illustration of the DAA interpretation framework in a clinical cohort setting with two modalities: imaging data and clinical questionnaires. First, the inference flow estimates output distributions via sampling in the latent space (blue arrows). Then, the simulation flow generates realistic perturbed samples of the view we want to study against the questionnaires and infer digital avatars through the model (yellow arrows). Finally, meaningful inter-view associations are inspected using hierarchical linear regressions (red arrows).

Supplemental S4 Detailed graphical abstract

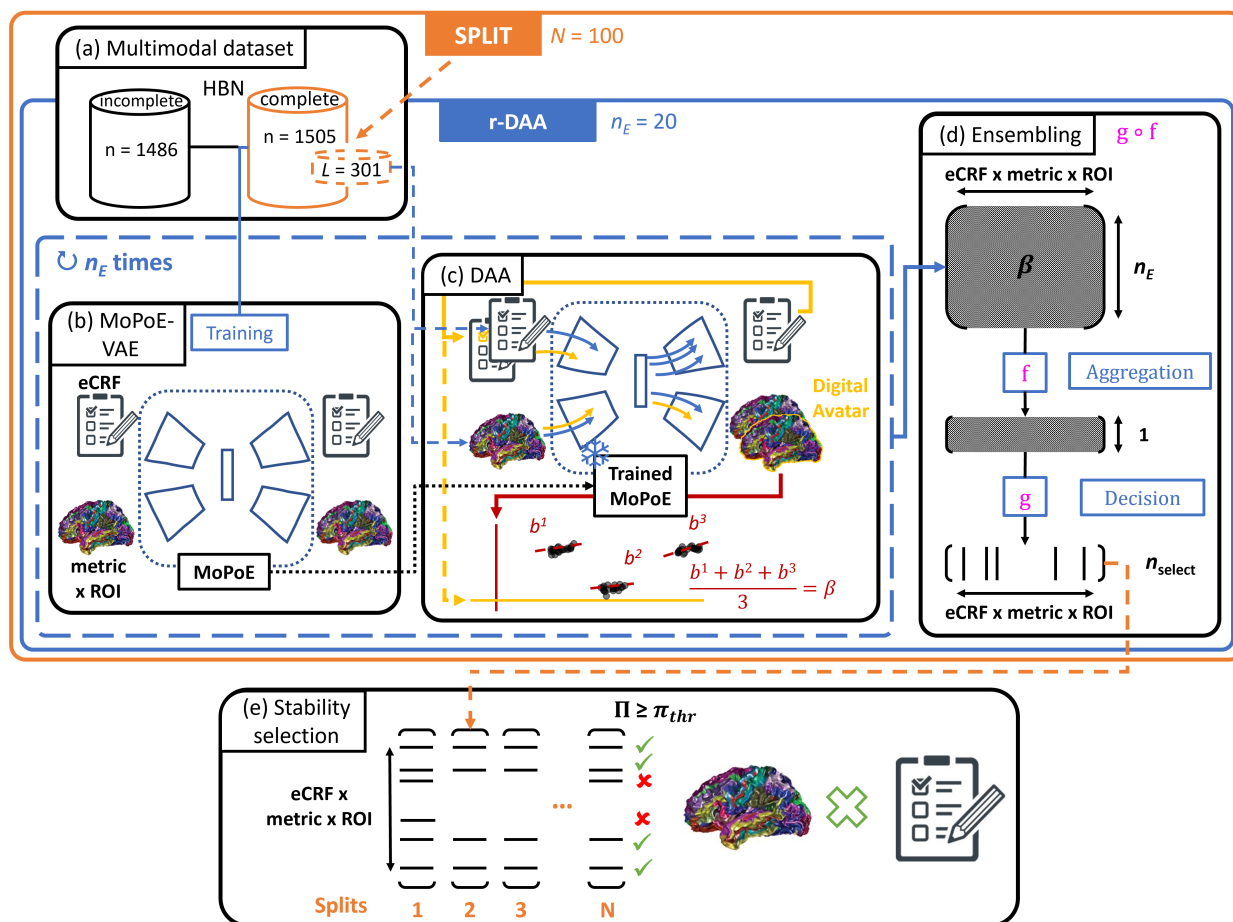


Figure S4-1: Illustration of the interpretation framework based on DAA. In (a) the multi-view dataset is split accounting for missing data. For each split, the complete data is divided N times (plain orange, dotted orange) in order to form a training set (adding the incomplete data) and L left-out subjects. A r-DAA is conducted on each split (blue box) by retraining n_E times a MoPoE-VAE, and conducting the DAA on the left-out subjects (blue dotted box). By subsequently using ensembling in (d), we identify stable associations from n_E DAAs association matrices β using an aggregation function f and a decision function g . In (e), from the generated N binary decision support, a stability selection procedure is used to retain associations with stability path $\Pi \geq \pi_{thr}$.

Supplemental S5 Algorithm pseudocodes

We display below the pseudocode of the two procedures developed for our association discovery pipeline, relying on r-DAA and stability selection. At line 11, for the weights, we either use 1 (quality is assumed to be uniformly correct) or to the Kendall τ coefficients (see Alg. [Supplemental S5.2](#) for details on their computation).

Supplemental S5.1 Finding associations with a non-weighted or weighted r-DAA (DAA + ensembling)

Algorithm 1 Finding associations with a non-weighted or weighted r-DAA

Input R : a set of ROIs
 M : a set of metrics
 S : a set of eCRF scores
 X : a list containing train/left-out subjects splits.

1: $p \leftarrow |R| * |M| * |S|$ ▷ num of features
2: $n_E \leftarrow 20$ ▷ num of models
3: $N \leftarrow 100$ ▷ num of splits
4: $n_{\text{select}} \leftarrow 12$ ▷ num of sel assoc
5: $\pi_{\text{thr}} \leftarrow 0.4$ ▷ stability path thr

(a) DAA { 6: **for** $j \in \{1, \dots, N\}$ **do**
7: $x_{\text{train}}^j, x_{\text{left-out}}^j \leftarrow X[j]$ ▷ a random split
8: **for** $k \in \{1, \dots, n_E\}$ **do**
9: Fit a $MoPoE_k^j$ model on x_{train}^j using init random weights θ^k
10: Compute the DAA association weights $\beta_k^j \in \mathbb{R}^p$ on $x_{\text{left-out}}^j$
11: Compute weights $\alpha_k^j \in \mathbb{R}_+$ assessing the model quality ▷ 1 or coefs as [Supplemental S5.2](#)
12: **end for**
13: $\beta^j \leftarrow [\beta_1^j, \dots, \beta_{n_E}^j]$
14: $\alpha^j \leftarrow [\alpha_1^j, \dots, \alpha_{n_E}^j]$
15: $\alpha^j \leftarrow \frac{1}{\sum_k \alpha_k^j} \alpha^j$ ▷ norm the weights

(b) ensembling { 16: Select an aggregation function f
17: $f \leftarrow$ weighted mean operator ▷ we chose one for simplicity
18: Compute aggregated scores $f(\beta^j, \alpha^j) \in \mathbb{R}^p$
19: $A^j \leftarrow f(\beta^j, \alpha^j)$
20: Compute decision support $g(A^j) \in \{0, 1\}^p$ by selecting the top n_{select} associations
21: $S^j \leftarrow g(A^j)$
22: **end for**

(c) stability selection { 23: Compute the selection probability of each feature $\Pi^{n_E} \in \mathbb{R}^p$
24: $\Pi^{n_E} \leftarrow \frac{1}{N} \sum_{j=1}^N S^j(n_E)$ ▷ function of n_E
25: Compute stable association wrt. the number of models n_E
26: $S^{\text{stable}} \leftarrow \{k : \max_{n_E \in \{1, \dots, 20\}} \Pi^{n_E} > \pi_{\text{thr}}\}$ ▷ stable associations

Output S^{stable}

Supplemental S5.2 Computing the coefficients to weight the model associations using RSA Kendall correlations

Algorithm 2 Computing the coefficients to weight the model associations

Input $x_{\text{left-out}}^j$: the left-out subjects of split j
 $MoPoE_k^j$: a trained model k on the x_{train}^j set
 S : a set of eCRF scores

- 1: $L \leftarrow |x_{\text{left-out}}^j|$ ▷ num of left-out subj
- 2: $z_k \leftarrow MoPoE_k^j(x_{\text{left-out}}^j) \in \mathbb{R}^{L \times d}$ ▷ joint latent d -dim reps
- 3: Compute the pairwise joint latent dissimilarity matrix $C_k^j \in \mathbb{R}^{L \times L}$
- 4: $C_k^j \leftarrow [\|z_k^m - z_k^n\|_2^2 \text{ for } (m, n) \in \{1, \dots, L\}^2] \in \mathbb{R}^{L \times L}$ ▷ pairwise l_2 dist
- 5: **for** $s \in S$ **do**
- 6: Compute the pairwise eCRF score dissimilarity matrix $S^s \in \mathbb{R}^{L \times L}$
- 7: $S^s \leftarrow [\|s^m - s^n\|_2^2 \text{ for } (m, n) \in \{1, \dots, L\}^2] \in \mathbb{R}^{L \times L}$
- 8: Compute the associated Kendall $\tau_k^{j,s} \in \mathbb{R}$ between C_k^j and S^s
- 9: **end for**
- 10: Average the obtained Kendall $\tau_k^{j,s} \in \mathbb{R}$ across the eCRF scores
- 11: $\tau_k^j \leftarrow \frac{1}{|S|} \sum_{s \in S} \tau_k^{j,s}$

Output τ_k^j

Supplemental S6 Additional stability plots

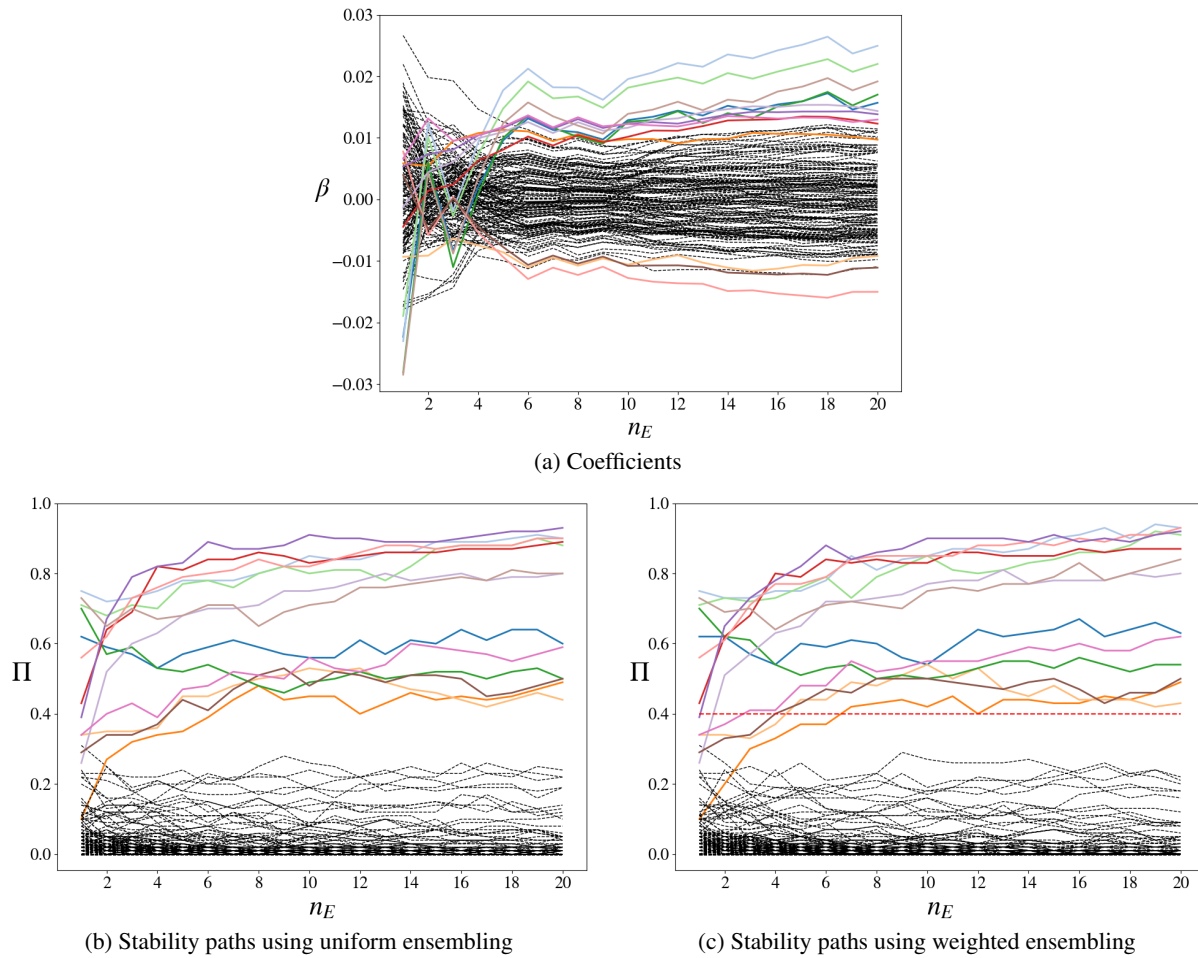


Figure S6-1: Investigation of the ROIs associated with SDQ-ha in area. Dotted black lines are not selected by the stability selection procedure (using a threshold $\pi_{\text{thr}} = 0.4$, represented by a red horizontal dotted line in (c)) when using the RSA weighted mean as an aggregation function. The selected ROIs are coloured consistently across the three plots. The three plots displays (a) the mean coefficients aggregated across models for a given split, (b) the ROIs stability paths Π when using a mean operator to aggregate the DAA coefficients, and (c) the ROIs stability paths Π when using a RSA weighted mean operator to aggregate the DAA coefficients against the number of ensembling models n_E .

Supplemental S7 The retained brain-behaviour associations for each score-metric pair

Supplemental_table.xlsx lists the retained associations for each score-metric pair. The following notations are used: L: left, R: right, S: sulcus, G: gyrus, Lat: lateral, Ci: cingul, Pa: parietal, Ce: central, Oc: occipital, Te: temporal, Fr: front, Orb: orbital, Ins: insula, Post: posterior, Mid: middle, Ant: anterior, Med: medial, Sup: superior, Inf: inferior, Ventr: ventral, Dors: dorsal, PostCe: postcentral, PreCe: precentral, ParaCe: paracentral, PeriCal: pericallosal, Marg: marginal, Pl: plan, Tri: triangular, Circ: circular, Supr: supramarginal, Ang: angular, PH: parahippocampal, SubPa: subparietal, Transv: transverse, FrPole: frontopolar, Pola: polar, SubCal: subcallosal, St: short, Fis: fissure, Olfact: olfactory, Rect: rectus, Precu: precuneus, FrMag: fronto-marginal, FrMarg: frontomargin, Inter: intermedius, Li: lingual, Jens: Jensen, Vert: vertical, Prim: primus.

Data availability

The data is accessible at <https://zenodo.org/records/10987604>, but requires prior authorisation. The data used to prepare this manuscript originate from Healthy Brain Network (HBN) cohort established by the Child Mind Institute (Project: <https://healthybrainnetwork.org/>, data portal: https://fcon_1000.projects.nitrc.org/indi/cmi_healthy_brain_network)

Code availability

The code to reproduce the experiments and results is made publicly available at <https://zenodo.org/records/10987502>.

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Author Contributions

C.A., V.F. and A.G. designed the experiments, C.A. conducted the experiments, V.F. and A.G. provided critical feedback, V.F. supervised the project, A.G. pre-processed the data, C.A., V.F. and A.G. wrote the manuscript, C.A., V.F., A.G. and J.H. reviewed and edited the manuscript. All authors have read and agreed to the submitted version of the manuscript.

Competing interests

The other authors declare no conflict of interest

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