

## 6 Supplementary Material

### 6.1 Optimization procedure of ICQF

Recall that the Lagrangian  $\mathcal{L}_\rho$  of ICQF is:

$$\mathcal{L}_\rho(W, Q, Z, \alpha_Z) = \frac{1}{2} \|\mathcal{M} \odot (M - Z)\|_F^2 + \mathcal{I}_W(W) + \beta \|W\|_{1,1} + \mathcal{I}_Q(Q) + \beta \|Q\|_{1,1} \quad (13)$$

$$+ \langle \alpha_Z, Z - [W, C]Q^T \rangle + \frac{\rho}{2} \|Z - [W, C]Q^T\|_F^2 + \mathcal{I}_Z(Z) \quad (14)$$

Following the ADMM approach, we alternately update primal variables  $W, Q$  and the auxiliary variable  $Z$ , instead of updating them jointly. In particular, we iteratively solve the following sub-problems:

$$W^{(i+1)} = \arg \min_{W \in \mathcal{W}} \frac{\rho}{2} \left\| Z^{(i)} - [W, C]Q^{(i),T} + \frac{1}{\rho} \alpha_Z^{(i)} \right\|_F^2 + \beta \|W\|_{1,1} \quad (\text{Sub-problem 1})$$

$$Q^{(i+1)} = \arg \min_{Q \in \mathcal{Q}} \frac{\rho}{2} \left\| Z^{(i)} - [W^{(i+1)}, C]Q^T + \frac{1}{\rho} \alpha_Z^{(i)} \right\|_F^2 + \beta \|Q\|_{1,1} \quad (\text{Sub-problem 2})$$

$$Z^{(i+1)} = \arg \min_{Z \in \mathcal{Z}} \frac{1}{2} \|\mathcal{M} \odot (M - Z)\|_F^2 + \frac{\rho}{2} \left\| Z - [W^{(i+1)}, C]Q^{(i+1),T} + \frac{1}{\rho} \alpha_Z^{(i)} \right\|_F^2 \quad (\text{Sub-problem 3})$$

for some penalty parameter  $\rho$ . We denote the Hadamard product as  $\odot$ . The vector of Lagrangian multipliers  $\alpha_Z$  is updated via

$$\alpha_Z^{(i+1)} \leftarrow \alpha_Z^{(i)} + \rho(Z^{(i+1)} - [W^{(i+1)}, C](Q^{(i+1)})^T) \quad (15)$$

#### Sub-problems 1 and 2 (Equations 2 and 3)

Note that equation 2 (and similarly equation 3 by taking the transpose) can be split into row-wise constrained Lasso problem. Specifically, the  $r^{\text{th}}$  row problem can be simplified into:

$$x^* = \arg \min_{0 \leq x_i \leq 1} \frac{\rho}{2} \|b - Ax\|_2^2 + \beta \|x\|_1, \quad A = Q^{(i)}, \quad b = \left[ Z^{(i)} - CQ^{(i),T} + \frac{1}{\rho} \alpha_Z^{(i)} \right]_{[r,:]} \quad (16)$$

Here we use the Matlab matrix notation  $[\cdot]_{[r,:]}$  to represent row extraction operation. As suggested in Gaines et al. (2018) one can also use ADMM to solve equation 16:

$$x^{(i+1)} = \arg \min \frac{\rho}{2} \|b - Ax\|_2^2 + \frac{\tau}{2} \|x - y^{(i)} + \frac{1}{\tau} \mu^{(i)}\|_2^2 + \beta \|x\|_1 \quad (17)$$

$$y^{(i+1)} = \text{Proj}_{[0,1]}(x^{(i+1)} + \frac{1}{\tau} \mu^{(i)}) \quad (18)$$

$$\mu^{(i+1)} \leftarrow \mu^{(i)} + \tau(x^{(i+1)} - y^{(i+1)}) \quad (19)$$

Similarly,  $\mu$  is the vector of Lagrangian multipliers and  $\tau$  is the penalty parameter.  $\text{Proj}_{[0,1]}$  refers to the orthogonal projection into  $[0, 1]$  (inherited from the box-constraints of  $W$ ). Equation 17 can be solved via the well-established FISTA algorithm (Beck & Teboulle, 2009). Consider the following optimization problem

$$\arg \min_x \lambda \|x\|_1 + \frac{1}{2} f(x) \quad (20)$$

The FISTA algorithm for solving 20 is summarized as follows:

To solve equation 17 with FISTA algorithm, using the notation as introduced in equation 16, we have

$$f(x) = \rho \|b - Ax\|_2^2 + \tau \|x - y^{(i)} + \frac{1}{\tau} \mu^{(i)}\|_2^2 \quad (21)$$

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**Algorithm 1:** FISTA for equation 20

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**Initialize:**  $\delta = 1e-6$ ;  $x_{-1} = \mathbf{0}$ ,  $x_0 = t_0 = \mathbf{1}$

**Input:**  $L$ , Lipschitz constant of  $\nabla f$

**Result:** Solution  $x$  of equation 20

**while**  $\|x_i - x_{i-1}\|_2 > \delta$  **do**  
     $\tilde{x}_{i+1} = z \left\{ \frac{\lambda}{L} \|z\|_1 + \frac{1}{2} \left\| z - \left( x_i - \frac{1}{L} \nabla f(x_i) \right) \right\| \right\}$ ;  
     $t_{i+1} = \frac{1 + \sqrt{1 + 4t_i^2}}{2}$ ;  
     $x_{i+1} = \tilde{x}_{i+1} + \frac{t_i - 1}{t_{i+1}} (\tilde{x}_{i+1} - x_i)$ ;  
**end**

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519 To compute  $L$ , the Lipschitz constant of  $\nabla f$ , we have

$$\begin{aligned} \nabla f(x) &= 2\rho (A^T A(x - b) + \tau(x - c)) \\ &= 2(\rho A^T A + \tau I)x - 2(\rho A^T A b + \tau c) \end{aligned} \quad (22)$$

520 where  $c = y^{(i)} - \frac{1}{\tau} \mu^{(i)}$ . Thus,  $L$  is just equal to the largest eigenvalue of  $2(\rho A^T A + \tau I)$ .

521 As recommended in Huang et al. (2016), ADMM provides flexibility to use various types of loss  
522 functions and regularizations without changing the procedure. For example, we can simply change to  
523  $L_{2,1}$  norm and equation 16 becomes a constrained ridge-regression problem, which can be efficiently  
524 solved by non-negative quadratic programming algorithms. For most clinical usage, the size of  
525 questionnaire data is manageable on a single machine. However, if optimal computational and  
526 memory efficiency is required, various stochastic optimization approaches such as Mairal et al. (2010)  
527 can replace the ADMM procedure. Yet, an unbiased sampling scheme for generating random batches  
528 that handles missing responses is also needed. Such a scheme is non-trivial to obtain, especially  
529 under the multi-questionnaires scenario.

### 530 Sub-problem 3 (Equation 4)

531 Since both terms in equation 4 are in Frobenius-norm,  $Z$  can be optimized entry-wise. In particular,  
532 we have the following closed-form solution for  $Z^{(i+1)}$ :

$$Z^{(i+1)} = \underset{[\min(M), \max(M)]}{Proj} \left( \mathcal{M} \odot M + \rho[W^{(i+1)}, C](Q^{(i+1)})^T - \alpha_Z^{(i)} \right) \odot (\rho \mathbb{1} + \mathcal{M}) \quad (23)$$

533 where  $\mathbb{1}$  is a 1-matrix with appropriate dimension and  $\odot$  is the Hadamard division.

## 534 6.2 Details and proof of Proposition 3.1

535 In the following, we provide a self-contained convergence proof and show that, under an appropriate  
536 choice of the penalty parameter  $\rho$ , the ADMM optimization scheme discussed in Section 3.2 converges  
537 to a local minimum. To simplify notation, we denote  $\mathbb{V}^{(i,j,k)} = \{W^{(i)}, Q^{(j)}, Z^{(k)}\}$  to be the tuple  
538 of variables  $W, Q$  and  $Z$  during iteration  $(i), (j)$  and  $(k)$  respectively. If  $i = j = k$ , we abbreviate  
539 it as  $\mathbb{V}^{(i)}$ . We also denote  $R^{(i)} = [W^{(i)}, C](Q^{(i)})^T$  and for any matrices  $A, B$  with appropriate  
540 dimensions,  $\langle A, B \rangle = \text{Trace}(A^T B)$ . In the following, we are going to show that the Lagrangian  
541 is decreasing across iterations. Particularly, we consider the difference of Lagrangian between  
542 consecutive iterations:

$$\begin{aligned} &\mathcal{L}_\rho(\mathbb{V}^{(i+1)}, \alpha_Z^{(i+1)}) - \mathcal{L}_\rho(\mathbb{V}^{(i)}, \alpha_Z^{(i)}) \\ &= \underbrace{\mathcal{L}_\rho(\mathbb{V}^{(i+1)}, \alpha_Z^{(i+1)}) - \mathcal{L}_\rho(\mathbb{V}^{(i+1)}, \alpha_Z^{(i)})}_{(I)} + \underbrace{\mathcal{L}_\rho(\mathbb{V}^{(i+1)}, \alpha_Z^{(i)}) - \mathcal{L}_\rho(\mathbb{V}^{(i)}, \alpha_Z^{(i)})}_{(II)} \end{aligned} \quad (24)$$

543 Expanding term (I), we have

$$\begin{aligned} \mathcal{L}_\rho(\mathbb{V}^{(i+1)}, \alpha_Z^{(i+1)}) - \mathcal{L}_\rho(\mathbb{V}^{(i+1)}, \alpha_Z^{(i)}) &= \left\langle \alpha_Z^{(i+1)} - \alpha_Z^{(i)}, Z^{(i+1)} - R^{(i+1)} \right\rangle \\ &= \frac{1}{\rho} \|\alpha_Z^{(i+1)} - \alpha_Z^{(i)}\|_F^2 \end{aligned} \quad (25)$$

544 Expanding term (II), we have

$$\begin{aligned}
& \mathcal{L}_\rho(\mathbb{V}^{(i+1)}, \alpha_Z^{(i)}) - \mathcal{L}_\rho(\mathbb{V}^{(i)}, \alpha_Z^{(i)}) \\
&= \underbrace{\mathcal{L}_\rho(\mathbb{V}^{(i+1)}, \alpha_Z^{(i)}) - \mathcal{L}_\rho(\mathbb{V}^{(i+1, i+1, i)}, \alpha_Z^{(i)})}_{(\mathcal{A})} + \underbrace{\mathcal{L}_\rho(\mathbb{V}^{(i+1, i+1, i)}, \alpha_Z^{(i)}) - \mathcal{L}_\rho(\mathbb{V}^{(i+1, i, i)}, \alpha_Z^{(i)})}_{(\mathcal{B})} \\
&+ \underbrace{\mathcal{L}_\rho(\mathbb{V}^{(i+1, i, i)}, \alpha_Z^{(i)}) - L(S^{(k)}, \alpha_Z^{(i)})}_{(\mathcal{C})} \quad (26)
\end{aligned}$$

545 Expanding (A) by the definition, we have

$$\begin{aligned}
& \frac{1}{2} \|\mathcal{M} \odot (M - Z^{(i+1)})\|_F^2 - \frac{1}{2} \|\mathcal{M} \odot (M - Z^{(i)})\|_F^2 + \langle \alpha_Z^{(i)}, Z^{(i+1)} - R^{(i+1)} \rangle \\
& - \langle \alpha_Z^{(i)}, Z^{(i)} - R^{(i+1)} \rangle + \frac{\rho}{2} \|Z^{(i+1)} - R^{(i+1)}\|_F^2 - \frac{\rho}{2} \|Z^{(i)} - R^{(i+1)}\|_F^2 \\
&= \langle \mathcal{M} \odot (Z^{(i+1)} - M), \mathcal{M} \odot (Z^{(i+1)} - Z^{(i)}) \rangle - \|\mathcal{M} \odot (Z^{(i+1)} - Z^{(i)})\|_F^2 \\
&+ \langle \alpha_Z^{(i)}, Z^{(i+1)} - Z^{(i)} \rangle + \rho \langle Z^{(i+1)} - R^{(i+1)}, Z^{(i+1)} - Z^{(i)} \rangle - \rho \|Z^{(i+1)} - Z^{(i)}\|_F^2 \\
&= \langle \mathcal{M} \odot (Z^{(i+1)} - M) + \rho \cdot Z^{(i+1)} + \alpha_Z^{(i)} - \rho R^{(i+1)}, Z^{(i+1)} - Z^{(i)} \rangle \\
&- \|\mathcal{M} \odot (Z^{(i+1)} - Z^{(i)})\|_F^2 - \rho \|(Z^{(i+1)} - Z^{(i)})\|_F^2 \\
&- \langle \mathcal{M} \odot (Z^{(i+1)} - M), (1 - \mathcal{M}) \odot (Z^{(i+1)} - Z^{(i)}) \rangle
\end{aligned}$$

546 Since  $Z^{(i+1)}$  is the minimizer of equation 4, we have

$$\begin{aligned}
& \left\| \mathcal{M} \odot (M - Z^{(i+1)}) \right\|_F^2 + \rho \left\| Z^{(i+1)} - R^{(i+1)} + \frac{1}{\rho} \alpha_Z^{(i)} \right\|_F^2 \\
& \leq \left\| \mathcal{M} \odot (M - Z^{(i)}) \right\|_F^2 + \rho \left\| Z^{(i)} - R^{(i+1)} + \frac{1}{\rho} \alpha_Z^{(i)} \right\|_F^2
\end{aligned}$$

547 which gives

$$\begin{aligned}
& 2 \langle \mathcal{M} \odot (Z^{(i+1)} - M), \mathcal{M} \odot (Z^{(i+1)} - Z^{(i)}) \rangle - \|\mathcal{M} \odot (Z^{(i+1)} - Z^{(i)})\|_F^2 \\
& \leq -2 \langle \rho \cdot Z^{(i+1)} + \alpha_Z^{(i)} - \rho R^{(i+1)}, Z^{(i+1)} - Z^{(i)} \rangle + \rho \|Z^{(i+1)} - Z^{(i)}\|_F^2
\end{aligned}$$

548 It further implies

$$\begin{aligned}
& \langle \rho \cdot Z^{(i+1)} + \alpha_Z^{(i)} - \rho R^{(i+1)}, Z^{(i+1)} - Z^{(i)} \rangle \\
& \leq - \langle \mathcal{M} \odot (Z^{(i+1)} - M), \mathcal{M} \odot (Z^{(i+1)} - Z^{(i)}) \rangle + \frac{1}{2} \|\mathcal{M} \odot (Z^{(i+1)} - Z^{(i)})\|_F^2 \\
& + \frac{\rho}{2} \|Z^{(i+1)} - Z^{(i)}\|_F^2
\end{aligned}$$

549 By direct substitution, we have

$$\begin{aligned}
(\mathcal{A}) & \leq \langle \mathcal{M} \odot (Z^{(i+1)} - M), Z^{(i+1)} - Z^{(i)} \rangle \\
& - \langle \mathcal{M} \odot (Z^{(i+1)} - M), \mathcal{M} \odot (Z^{(i+1)} - Z^{(i)}) \rangle \\
& + \frac{1}{2} \|\mathcal{M} \odot (Z^{(i+1)} - Z^{(i)})\|_F^2 + \frac{\rho}{2} \|Z^{(i+1)} - Z^{(i)}\|_F^2 - \|\mathcal{M} \odot (Z^{(i+1)} - Z^{(i)})\|_F^2 \\
& - \rho \|(Z^{(i+1)} - Z^{(i)})\|_F^2 - \langle \mathcal{M} \odot (Z^{(i+1)} - M), (1 - \mathcal{M}) \odot (Z^{(i+1)} - Z^{(i)}) \rangle \\
& = -\frac{1}{2} \|\mathcal{M} \odot (Z^{(i+1)} - Z^{(i)})\|_F^2 - \frac{\rho}{2} \|(Z^{(i+1)} - Z^{(i)})\|_F^2 \leq -\frac{\rho}{2} \|(Z^{(i+1)} - Z^{(i)})\|_F^2 \quad (27)
\end{aligned}$$

550 For the second term  $(\mathcal{B})$ , by definition, we have,

$$\begin{aligned}
(\mathcal{B}) &= \frac{\rho}{2} \left\| Z^{(i)} - R^{(i+1)} + \frac{1}{\rho} \alpha_Z^{(i)} \right\|_F^2 - \frac{\rho}{2} \left\| Z^{(i)} - [W^{(i+1)}, C] Q^{(i),T} + \frac{1}{\rho} \alpha_Z^{(i)} \right\|_F^2 \\
&\quad + \beta \|Q^{(i+1)}\|_{1,1} - \beta \|Q^{(i)}\|_{1,1} \\
&= \rho \left\langle R^{(i+1)} - Z^{(i)} - \frac{1}{\rho} \alpha_Z^{(i)}, [W^{(i+1)}, C] (Q^{(i+1),T} - Q^{(i),T}) \right\rangle \\
&\quad - \frac{\rho}{2} \left\| [W^{(i+1)}, C] (Q^{(i+1),T} - Q^{(i),T}) \right\|_F^2 + \beta (\|Q^{(i+1)}\|_{1,1} - \|Q^{(i)}\|_{1,1})
\end{aligned}$$

551 We recall that  $Q$  is updated via solving constrained Lasso problems for every row  $Q_{[r,:]}^{(i+1)}$ :

$$y = \arg \min_{x, 0 \leq x} \beta \|x\|_1 + \frac{\rho}{2} \|b - Ax\|_2^2, \quad \text{where } A = [W^{(i+1)}, C], b = \left[ Z^{(i)} + \frac{1}{\rho} \alpha_Z^{(i)} \right]_{[r,:]} \quad (28)$$

552 One obtains  $y$  if and only if there exists  $g \in \partial \|y\|_1$ , the sub-differential of  $\|\cdot\|_1$  such that

$$\rho A^T (Ay - b) + \beta g = \mathbf{0}. \quad (29)$$

553 As  $\|\cdot\|_1$  is convex, we have

$$\|x\|_1 \geq \|y\|_1 + \langle x - y, g \rangle \quad (30)$$

554 which gives

$$\|y\|_1 - \|x\|_1 \leq \left\langle y - x, \frac{\rho}{\beta} A^T (Ay - b) \right\rangle = \left\langle A(y - x), \frac{\rho}{\beta} (Ay - b) \right\rangle \quad (31)$$

555 Re-substituting  $x = Q_{[r,:]}^{(i),T}$ ,  $y = Q_{[r,:]}^{(i+1),T}$ ,  $A = [W^{(i+1)}, C]$ ,  $b = \left[ Z^{(i)} + \frac{1}{\rho} \alpha_Z^{(i)} \right]_{[r,:]}$  and sum over  
556  $r$ , we have

$$\beta \|Q^{(i+1)}\|_{1,1} - \beta \|Q^{(i)}\|_{1,1} \leq -\rho \left\langle R^{(i+1)} - Z^{(i)} - \frac{1}{\rho} \alpha_Z^{(i)}, [W^{(i+1)}, C] (Q^{(i+1),T} - Q^{(i),T}) \right\rangle \quad (32)$$

557 Therefore, we have

$$(\mathcal{B}) \leq -\frac{\rho}{2} \left\| [W^{(i+1)}, C] (Q^{(i+1),T} - Q^{(i),T}) \right\|_F^2 \quad (33)$$

558 With similar argument, we can bound  $(\mathcal{C})$  by

$$(\mathcal{C}) \leq -\frac{\rho}{2} \left\| [(W^{(i+1)} - W^{(i)}), C] Q^{(i),T} \right\|_F^2 \quad (34)$$

559 To get an upper bound of  $\|\alpha_Z^{(i+1)} - \alpha_Z^{(i)}\|_F^2$ , we have

$$\begin{aligned}
&\|\alpha_Z^{(i+1)} - \alpha_Z^{(i)}\|_F^2 \\
&\leq \|Z^{(i+1)} - Z^{(i)}\|_F^2 + \|R^{(i+1)} - R^{(i)}\|_F^2 \\
&\leq \|Z^{(i+1)} - Z^{(i)}\|_F^2 + \|[W^{(i+1)}, C] Q^{(i+1),T} - [W^{(i+1)}, C] Q^{(i),T}\|_F^2 \\
&\quad + \|[W^{(i+1)}, C] Q^{(i),T} - [W^{(i)}, C] Q^{(i),T}\|_F^2 \\
&\leq \|Z^{(i+1)} - Z^{(i)}\|_F^2 + \|[W^{(i+1)}, C] (Q^{(i+1),T} - Q^{(i),T})\|_F^2 + \|[W^{(i+1)} - W^{(i)}], C] Q^{(i),T}\|_F^2
\end{aligned} \quad (35)$$

560 Combining equation 25, 35, 26, 27, 33 and 34 with equation 24, we have

$$\begin{aligned}
&\mathcal{L}_\rho(\mathbb{V}^{(i+1)}, \alpha_Z^{(i+1)}) - \mathcal{L}_\rho(\mathbb{V}^{(i)}, \alpha_Z^{(i)}) \\
&\leq \frac{1}{\rho} \left\| \alpha_Z^{(i+1)} - \alpha_Z^{(i)} \right\|_F^2 - \frac{\rho}{2} \left\| Z^{(i+1)} - Z^{(i)} \right\|_F^2 - \frac{\rho}{2} \left\| [W^{(i+1)}, C] (Q^{(i+1),T} - Q^{(i),T}) \right\|_F^2 \\
&\quad - \frac{\rho}{2} \left\| [(W^{(i+1)} - W^{(i)}), C] Q^{(i),T} \right\|_F^2 \\
&\leq \left( \frac{1}{\rho} - \frac{\rho}{2} \right) \cdot \left( \|Z^{(i+1)} - Z^{(i)}\|_F^2 + \|[W^{(i+1)}, C] (Q^{(i+1),T} - Q^{(i),T})\|_F^2 \right. \\
&\quad \left. + \|[W^{(i+1)} - W^{(i)}], C] Q^{(i),T}\|_F^2 \right).
\end{aligned} \quad (36)$$

561 We set  $\rho = 3$  in all experiments for sufficiency.

### 6.3 Details and proof of Proposition 3.2

Assume that there is a ground-truth factorization  $(\mathbf{W}^*, \mathbf{Q}^*)$  of the given  $\mathbf{M} = \mathbf{W}^*(\mathbf{Q}^*)^T$ , with latent dimension  $k^*$ , where  $\mathbf{W}^*$  and  $\mathbf{Q}^*$  are matrix-valued random variables with entries sampled from some bounded distributions. With high probability, the error  $\|\mathbf{M} - \mathbf{W}\mathbf{Q}^T\|_F^2$  we are minimizing is star-convex towards  $(\mathbf{W}^*, \mathbf{Q}^*)$  whenever  $k = k^*$  (Bjorck et al., 2021). To demonstrate the importance of the choice of  $k$ , we consider the scenario when  $k \neq k^*$  below.

First, a more precise assumption for ICQF is to model  $\mathbf{W}$  as *row-independent bounded random matrices*. Recall that  $\mathbf{W}$  is generated by arranging  $n$  participants' latent representation as rows of  $n \times k$  matrix, where the  $n$  participants are assumed to be independent from each other and their corresponding latent representations follow a high-dimensional bounded distribution.

Second, let  $(\mathbf{W}_1, \mathbf{Q}_1)$  and  $(\mathbf{W}_2, \mathbf{Q}_2)$  be two factorizations with dimensions  $k_1$  and  $k_2$  respectively. Consider that there exists two factorizations which achieve the same critical point, i.e. **(a)**: equivalent mismatching loss in expectation, and **(b)**: equivalent expectation approximation to data matrix  $\mathbf{M}$ :

$$\textbf{(a)} : \mathbb{E} [\|\mathbf{M} - \mathbf{W}_1 \mathbf{Q}_1^T\|_F^2] = \mathbb{E} [\|\mathbf{M} - \mathbf{W}_2 \mathbf{Q}_2^T\|_F^2] \quad \text{and} \quad \textbf{(b)} : \mathbb{E} [\mathbf{W}_1 \mathbf{Q}_1^T] = \mathbb{E} [\mathbf{W}_2 \mathbf{Q}_2^T]$$

We also assume **(c)**:  $\mathbb{E} [\sum_{j=1}^n (\mathbf{W}_i)_{j\kappa}^2] := \sigma_{\mathbf{W}_i}^2$  and  $\mathbb{E} [\sum_{j=1}^m (\mathbf{Q}_i)_{j\kappa}^2] := \sigma_{\mathbf{Q}_i}^2$  for all  $\kappa = k_i$ ,  $i = 1, 2$ .

Expanding **(a)**, we have

$$\mathbb{E} [\text{Trace} ((\mathbf{M} - \mathbf{W}_1 \mathbf{Q}_1^T)^T (\mathbf{M} - \mathbf{W}_1 \mathbf{Q}_1^T))] = \mathbb{E} [\text{Trace} ((\mathbf{M} - \mathbf{W}_2 \mathbf{Q}_2^T)^T (\mathbf{M} - \mathbf{W}_2 \mathbf{Q}_2^T))]$$

This gives

$$\mathbb{E} [\text{Trace} (\mathbf{W}_1^T \mathbf{W}_1 \mathbf{Q}_1^T \mathbf{Q}_1 - 2\mathbf{M}^T \mathbf{W}_1 \mathbf{Q}_1^T)] = \mathbb{E} [\text{Trace} (\mathbf{W}_2^T \mathbf{W}_2 \mathbf{Q}_2^T \mathbf{Q}_2 - 2\mathbf{M}^T \mathbf{W}_2 \mathbf{Q}_2^T)]$$

Denote  $\mathbb{E} [\mathbf{W}_i] = \mu_{\mathbf{W}_i}$ ,  $\mathbb{E} [\mathbf{Q}_i] = \mu_{\mathbf{Q}_i}$  for  $i = 1, 2$ , we have  $\mathbf{W}_i = \bar{\mathbf{W}}_i + \mu_{\mathbf{W}_i}$  and  $\mathbf{Q}_i = \bar{\mathbf{Q}}_i + \mu_{\mathbf{Q}_i}$ , where  $\bar{\mathbf{W}}_i$  and  $\bar{\mathbf{Q}}_i$  denote the corresponding centered variables. Note that by the independence of  $\mathbf{W}_i$  and  $\mathbf{Q}_i$  and linearity of trace and expectation operator,

$$\begin{aligned} & \mathbb{E} [\text{Trace} (\mathbf{M}^T \mathbf{W}_1 \mathbf{Q}_1^T)] \\ &= \mathbb{E} [\text{Trace} (\mathbf{M}^T \bar{\mathbf{W}}_1 \bar{\mathbf{Q}}_1^T + \mathbf{M}^T \bar{\mathbf{W}}_1 \mu_{\mathbf{Q}_1}^T + \mathbf{M}^T \mu_{\mathbf{W}_1} \bar{\mathbf{Q}}_1^T + \mathbf{M}^T \mu_{\mathbf{W}_1} \mu_{\mathbf{Q}_1}^T)] \\ &= \text{Trace} (\mathbf{M}^T \mathbb{E} [\mathbf{W}_1] \mathbb{E} [\mathbf{Q}_1^T]) = \text{Trace} (\mathbf{M}^T \mathbb{E} [\mathbf{W}_2] \mathbb{E} [\mathbf{Q}_2^T]) = \mathbb{E} [\text{Trace} (\mathbf{M}^T \mathbf{W}_2 \mathbf{Q}_2^T)] \end{aligned} \quad (37)$$

which yields

$$\mathbb{E} [\text{Trace} (\mathbf{W}_1^T \mathbf{W}_1 \mathbf{Q}_1^T \mathbf{Q}_1)] = \mathbb{E} [\text{Trace} (\mathbf{W}_2^T \mathbf{W}_2 \mathbf{Q}_2^T \mathbf{Q}_2)] \quad (38)$$

Consider  $\mathbb{E} [\text{Trace} (\mathbf{W}_1^T \mathbf{W}_1 \mathbf{Q}_1^T \mathbf{Q}_1)]$  via definition, we have

$$\begin{aligned} & \mathbb{E} [\text{Trace} (\mathbf{W}_1^T \mathbf{W}_1 \mathbf{Q}_1^T \mathbf{Q}_1)] \\ &= \text{Trace} (\mathbb{E} [\mathbf{W}_1^T \mathbf{W}_1] \mathbb{E} [\mathbf{Q}_1^T \mathbf{Q}_1]) \\ &= \text{Trace} \left( \mathbb{E} \left[ \begin{pmatrix} \left( \sum_{j=1}^n (\mathbf{W}_1)_{j1}^2 \right) & & * \\ & \ddots & \\ * & & \left( \sum_{j=1}^n (\mathbf{W}_1)_{jk_1}^2 \right) \end{pmatrix} \right] \right. \\ & \quad \left. \times \mathbb{E} \left[ \begin{pmatrix} \left( \sum_{j=1}^m (\mathbf{Q}_1)_{j1}^2 \right) & & 0 \\ & \ddots & \\ 0 & & \left( \sum_{j=1}^m (\mathbf{Q}_1)_{jk_1}^2 \right) \end{pmatrix} \right] \right) \\ &= \sum_{\kappa=1}^{k_1} \mathbb{E} \left[ \sum_{j=1}^n (\mathbf{W}_1)_{j\kappa}^2 \right] \mathbb{E} \left[ \sum_{j=1}^m (\mathbf{Q}_1)_{j\kappa}^2 \right] \end{aligned} \quad (39)$$

Incorporating assumption **(c)**, we have

$$\mathbb{E} [\text{Trace} (\mathbf{W}_1^T \mathbf{W}_1 \mathbf{Q}_1^T \mathbf{Q}_1)] = k_1 \sigma_{\mathbf{W}_1}^2 \sigma_{\mathbf{Q}_1}^2 \quad (40)$$

Consider equation 38 with  $k_2 > k_1$ . For  $\mathbf{W}_1, \mathbf{Q}_1$ , W.L.O.G. we pad  $k_2 - k_1$  columns of zeros. Moreover, let  $\mathbf{P}$  be an optimal  $k_2 \times k_2$  permutation matrix, we also have

$$\mathbb{E} [\text{Trace} ((\mathbf{W}_2 \mathbf{P})^T \mathbf{W}_2 \mathbf{P} (\mathbf{Q}_2 \mathbf{P})^T \mathbf{Q}_2 \mathbf{P})] = \mathbb{E} [\text{Trace} (\mathbf{W}_2^T \mathbf{W}_2 \mathbf{Q}_2^T \mathbf{Q}_2)] = k_2 \sigma_{\mathbf{W}_2}^2 \sigma_{\mathbf{Q}_2}^2 \quad (41)$$

Combining with equation 38, it is equivalent to

$$k_1 \sigma_{\mathbf{W}_1}^2 \sigma_{\mathbf{Q}_1}^2 = k_2 \sigma_{\mathbf{W}_2}^2 \sigma_{\mathbf{Q}_2}^2 \quad (42)$$

which gives

$$\mathbb{E} [\|\mathbf{W}_1\|_F^2] = \frac{\sigma_{\mathbf{Q}_2}^2}{\sigma_{\mathbf{Q}_1}^2} \mathbb{E} [\|\mathbf{W}_2\|_F^2] = \frac{\sigma_{\mathbf{Q}_2}^2}{\sigma_{\mathbf{Q}_1}^2} \mathbb{E} [\|\mathbf{W}_2 \mathbf{P}\|_F^2] \quad (43)$$

To evaluate the impact of interpretability of latent representation under different latent dimension, we consider  $\mathbb{E} [\|\mathbf{W}_1 - \mathbf{W}_2 \mathbf{P}\|_F^2]$ :

$$\begin{aligned} \mathbb{E} [\|\mathbf{W}_1 - \mathbf{W}_2 \mathbf{P}\|_F^2] &= \mathbb{E} [\text{Trace} ((\mathbf{W}_1 - \mathbf{W}_2 \mathbf{P})^T (\mathbf{W}_1 - \mathbf{W}_2 \mathbf{P}))] \\ &= \mathbb{E} [\|\mathbf{W}_1\|_F^2] + \frac{\sigma_{\mathbf{Q}_1}^2}{\sigma_{\mathbf{Q}_2}^2} \mathbb{E} [\|\mathbf{W}_1\|_F^2] - 2 \mathbb{E} [\text{Trace} (\mathbf{W}_1^T \mathbf{W}_2 \mathbf{P})] \end{aligned} \quad (44)$$

As  $\text{Trace} (\mathbf{W}_1^T \mathbf{W}_2 \mathbf{P}) \leq \|\mathbf{W}_1\|_F \|\mathbf{W}_2 \mathbf{P}\|_F$ , we also have

$$\begin{aligned} \mathbb{E} [\text{Trace} (\mathbf{W}_1^T \mathbf{W}_2 \mathbf{P})] &\leq \mathbb{E} [\|\mathbf{W}_1\|_F] \cdot \mathbb{E} [\|\mathbf{W}_2 \mathbf{P}\|_F] \\ &\leq \sqrt{\mathbb{E} [\|\mathbf{W}_1\|_F^2] \cdot \mathbb{E} [\|\mathbf{W}_2\|_F^2]} = \sqrt{\frac{\sigma_{\mathbf{Q}_1}^2}{\sigma_{\mathbf{Q}_2}^2} \mathbb{E} [\|\mathbf{W}_1\|_F^2]} \end{aligned} \quad (45)$$

which implies

$$\mathbb{E} [\|\mathbf{W}_1 - \mathbf{W}_2 \mathbf{P}\|_F^2] \geq \left(1 - 2 \sqrt{\frac{\sigma_{\mathbf{Q}_1}^2}{\sigma_{\mathbf{Q}_2}^2}} + \frac{\sigma_{\mathbf{Q}_1}^2}{\sigma_{\mathbf{Q}_2}^2}\right) \mathbb{E} [\|\mathbf{W}_1\|_F^2] = \left(1 - \sqrt{\frac{\sigma_{\mathbf{Q}_1}^2}{\sigma_{\mathbf{Q}_2}^2}}\right)^2 \mathbb{E} [\|\mathbf{W}_1\|_F^2] \quad (46)$$

Since  $\mathbf{W}_i$  is generated from row-wise independent bounded distribution, if we add a mild assumption that  $\sigma_{\mathbf{W}_i}^2 := \sigma_{\mathbf{W}}^2$  for all  $i$  through re-scaling, Equation 42 implies  $k_1 \sigma_{\mathbf{Q}_1}^2 = k_2 \sigma_{\mathbf{Q}_2}^2$  and therefore

$$\mathbb{E} [\|\mathbf{W}_1 - \mathbf{W}_2\|_F^2] \geq \left(1 - 2 \sqrt{\frac{k_2}{k_1}} + \frac{k_2}{k_1}\right) \mathbb{E} [\|\mathbf{W}_1\|_F^2] = \left(\sqrt{\frac{k_2}{k_1}} - 1\right)^2 \mathbb{E} [\|\mathbf{W}_1\|_F^2] \quad (47)$$

If we substitute  $k_1 = k^*$ ,  $(\mathbf{W}_1, \mathbf{Q}_1) = (\mathbf{W}^*, \mathbf{Q}^*)$ , we have

$$\mathbb{E} [\|\mathbf{W}^* - \mathbf{W}_2\|_F^2] \geq \left(\sqrt{\frac{k_2}{k^*}} - 1\right)^2 \mathbb{E} [\|\mathbf{W}^*\|_F^2] \quad (48)$$

which means the relative expected difference between  $\mathbf{W}^*$  and  $\mathbf{W}_2$  is bounded below by  $\left(\sqrt{\frac{k_2}{k^*}} - 1\right)^2$ .

To prove that equation 48 holds in general, we consider the matrix concentration inequalities and show that large deviations from their means are exponentially unlikely. Benefitting from the model constraints, we can further assume that  $\mathbf{W}$  is generated from some high dimensional bounded distribution. In the following, we make use of the main theorem proposed in Meckes & Szarek (2012) on concentration of non-commutative random matrices polynomials. As  $\mathbf{W}_i$  are generated from bounded distributions,  $\|\mathbf{W}_i - \mathbb{E}[\mathbf{W}_i]\|_F$  is uniformly bounded. Therefore, it satisfies the convex concentration properties. The theorem achieves the following results:

$$\mathbb{P} \{ \|\mathbf{W}\|_F^2 - \mathbb{E} [\|\mathbf{W}\|_F^2] > t k n^2 \} \leq C_1 \exp \left( -C_2 \min(t^2, t^{1/2}) n \right) \quad (49)$$

Recall that  $\mathbb{E} [\|\mathbf{W}_1 - \mathbf{W}_2 \mathbf{P}\|_F^2] = \mathbb{E} [\|\mathbf{W}_1\|_F^2] + \frac{\sigma_{\mathbf{Q}_1}^2}{\sigma_{\mathbf{Q}_2}^2} \mathbb{E} [\|\mathbf{W}_1\|_F^2] - 2 \mathbb{E} [\text{Trace} (\mathbf{W}_1^T \mathbf{W}_2 \mathbf{P})]$ . By padding  $\mathbf{W}_1$  and  $\mathbf{W}_2$  with zeros columns, we assume that  $\mathbf{W}_i$  are all  $n \times n$  matrices. Then the probability that the any one of the terms is deviating from their mean by a relative factor  $\epsilon$  is less than  $C_1 \exp(-C_2 \epsilon^2 n)$  for some small  $\epsilon$ . By the union bound, the probability that the either of them does is less than or equal to  $C_3 \exp(-C_4 \epsilon^2 n)$ .

## 6.4 Visualization of the experimental setup for diagnostic prediction evaluation

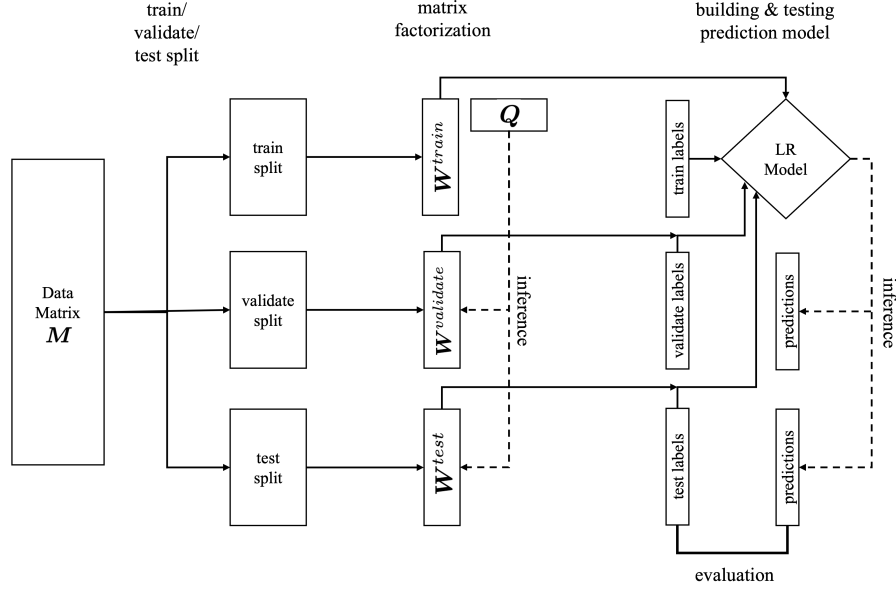


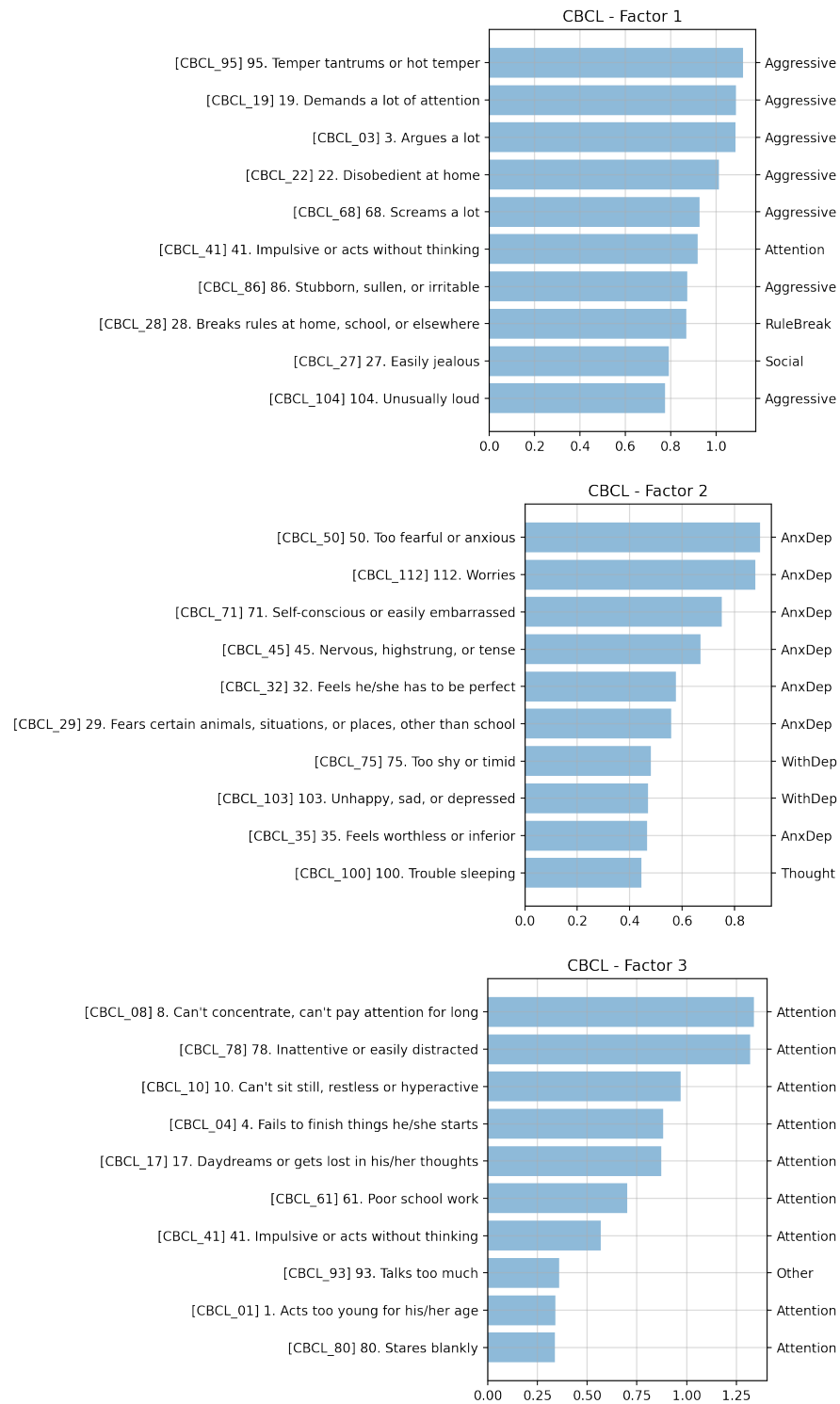
Figure 4: Setup for diagnostic prediction experiments.

## 6.5 Table of the 21 questionnaires used in HBN dataset

Table 3: Optimal  $(k, \beta)$  of all 21 questionnaires.

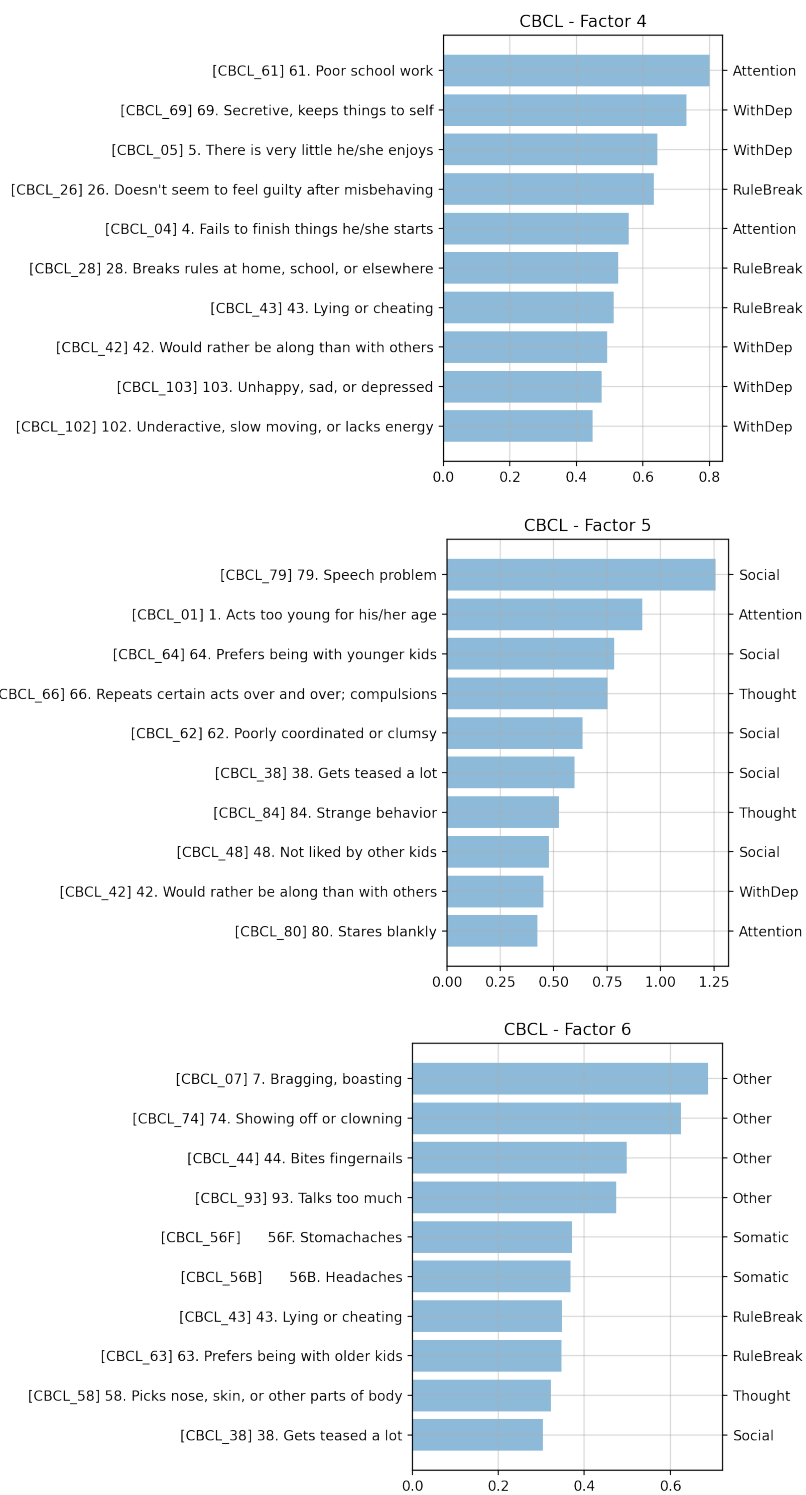
Questionnaire	Abbreviation	$n$ questions	Subscales	$k$	$\beta$
Affective Reactivity Index (Parent-Report)	ARI_P	7	nan	2	0.01
Affective Reactivity Index (Self-Report)	ARI_S	7	nan	2	0.01
Autism Spectrum Screening Questionnaire	ASSQ	27	nan	2	0.01
Conners 3 (Self-Report)	C3SR	9		4	0.05
Child Behavior Checklist	CBCL	119	9	8	0.5
Extended Strengths and Weaknesses Assessment of Normal Behavior	ESWAN	65	nan	13	0.2
Inventory of Callous-Unemotional Traits (Parent-Report)	ICU_P	24	3	4	0.1
Inventory of Callous-Unemotional Traits (Self-Report)	ICU_SR	24	3	3	0.1
Mood and Feelings Questionnaire (Parent-Report)	MFQ_P	34	nan	2	0.1
Mood and Feelings Questionnaire (Self-Report)	MFQ_SR	33	nan	2	0.1
The Positive and Negative Affect Schedule	PANAS	20	2	2	0.05
Repetitive Behaviors Scale	RBS	43	5	3	0.1
Screen for Child Anxiety Related Disorders (Parent-Report)	SCARED_P	41	5	3	0.1
Screen for Child Anxiety Related Disorders (Self-Report)	SCARED_SR	41	5	3	0.3
Social Communication Questionnaire	SCQ	40	nan	4	0.02
Strength and Difficulties Questionnaire	SDQ	33	9	6	0.05
Social Responsiveness Scale (School Age)	SRS	65	7	3	0.5
The Strengths and Weaknesses Assessment of Normal Behavior Rating Scale for ADHD	SWAN	18	2	3	0.02
Symptom Checklist (Parent-Report)	SympChck	63	nan	3	0.1
Teacher Report Form (School Age)	TRF	116	19	8	0.5
Youth Self Report	YSR	119	11	3	0.2

612 **6.6 Full list of Top 10 questions from factorizing CBCL-HBN questionnaire**

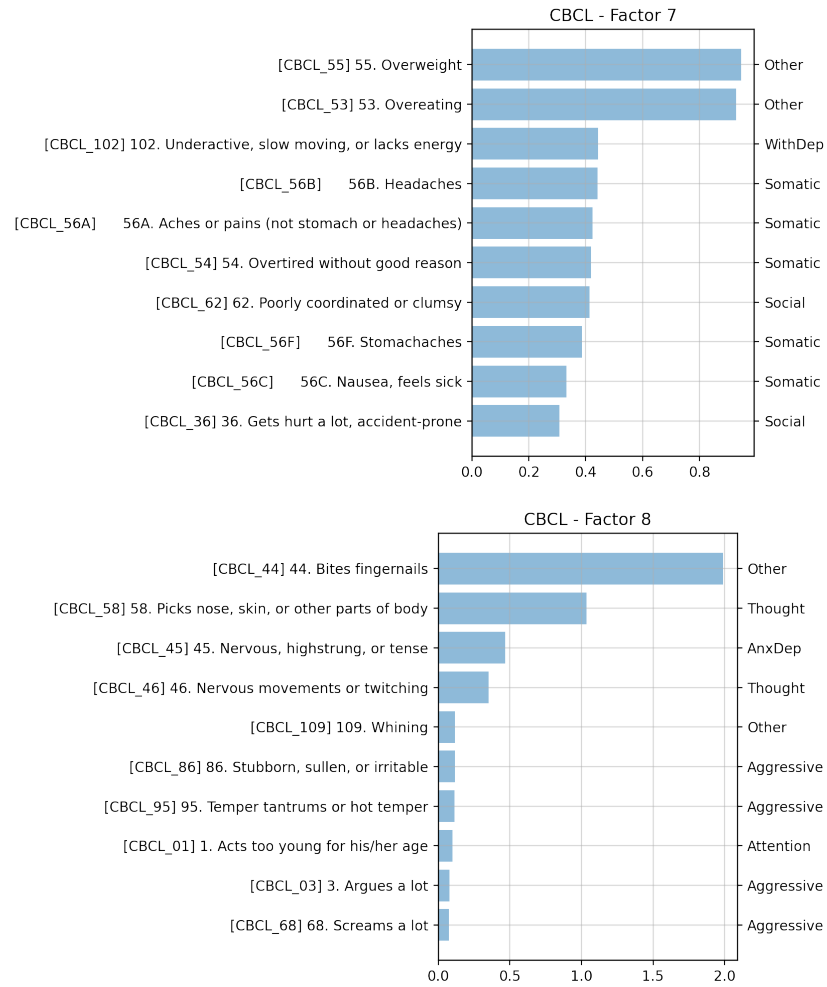


**Figure 5:** Top 10 questions ranked by  $Q$  in *CBCL* using  $Q$  obtained from ICQF (Factor 1-3).





**Figure 6:** Top 10 questions ranked by  $Q$  in *CBCL* using  $Q$  obtained from ICQF (Factor 4-6).



**Figure 7:** Top 10 questions ranked by  $Q$  in  $CBCL$  using  $Q$  obtained from ICQF (Factor 7-8).