# Supplementary Materials

**Bayesian Probabilistic Principal Components Model**

Let denote the -dimensional vector of neurocognitive measures for the th subject, for , with denoting the total sample size. We modeled the covariance structure of using a standard latent variable formulation

where is a matrix, is the number of latent variables, is the -dimensional vector of latent scores for the th subject, and is the -dimensional vector of residuals. We assumed that were marginally normal with zero mean and unit variance, indicated by , where denotes a -dimensional normal distribution with mean and variance-covariance matrix , is a D-dimensional vector of zeros and is the identity matrix. We further assumed that the residuals were marginally distributed as . This model forms the basis for Probabilistic PCA87,88.

We incorporated the study design of ABCD into the analysis via random effects for data collection site and for family for subjects with one or more siblings included in the study. Random effects thus accounted for correlation among the responses between subjects caused by nesting within site and within family. Random effects were included in both the latent scores and the residuals , with variances constrained to meet the identifiability assumptions of the BPPCA model.

First, we describe the random effects for the latent scores. For singletons (subjects without siblings in the study) we modeled the latent score as

where and are independent, denotes the site of collection of the th subject, , and . The overall variance of each component of is thus . As indicated, this quantity was constrained to equal one, necessary for identifiability. For subjects with one or more siblings, we modeled the latent scores as

where , , and are mutually independent, denotes the family of the th subject, , is distributed as before, and . We again made the constraint that . Thus, marginally in all cases, but with random effects and capturing the correlation of latent scores within sites and within families, respectively.

The random effects structure of the residuals was similar and captures the correlation within site and family in the responses not accounted for by the latent scores. For singleton subjects

where independently of . Finally, for subjects with one or more siblings in the study

where all three random variables are mutually independent, is distributed as before, , and . We placed the constraint that , ensuring that the marginal distribtion of remains constant across subjects.

After selecting the number of the latent factors, the BPPCA was rotationally invariant. To address this issue, we performed *post hoc* orientation of the loading matrix and latent scores using the method described in 93.

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**Supplementary Table 1A: Unrotated BPPCA Factor Loadings**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **PC1** |  |  | **PC2** |  |  | **PC3** |  |
|  | .025 | 0.50 | .975 | .025 | 0.50 | .975 | .025 | 0.50 | .975 |
| Pic Vocab | 0.58 | 0.614 | 0.651 | -0.412 | -0.347 | -0.272 | -0.405 | -0.336 | -0.26 |
| Flanker | 0.533 | 0.571 | 0.611 | 0.421 | 0.468 | 0.516 | -0.177 | -0.094 | -0.005 |
| List | 0.611 | 0.643 | 0.676 | -0.309 | -0.258 | -0.207 | 0.005 | 0.078 | 0.149 |
| Card Sort | 0.617 | 0.655 | 0.691 | 0.365 | 0.413 | 0.457 | -0.038 | 0.038 | 0.114 |
| Pattern | 0.47 | 0.513 | 0.554 | 0.587 | 0.633 | 0.678 | -0.055 | 0.046 | 0.136 |
| Picture | 0.503 | 0.543 | 0.583 | -0.302 | -0.195 | -0.084 | 0.598 | 0.653 | 0.707 |
| Reading | 0.613 | 0.651 | 0.686 | -0.378 | -0.306 | -0.226 | -0.491 | -0.429 | -0.363 |
| RAVLT | 0.606 | 0.642 | 0.679 | -0.35 | -0.281 | -0.21 | 0.283 | 0.351 | 0.415 |
| LMT | 0.49 | 0.521 | 0.556 | -0.069 | 0.004 | 0.075 | -0.359 | -0.27 | -0.173 |

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**Supplementary Table 1B: Promax Rotated BPPCA Factor Loadings**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | PC1 |  |  | PC2 |  |  | PC3 |  |
|  | .025 | 0.50 | .975 | .025 | 0.50 | .975 | .025 | 0.50 | .975 |
| Pic Vocab | 0.763 | 0.831 | 0.894 | -0.155 | -0.108 | -0.063 | -0.088 | -0.017 | 0.062 |
| Flanker | 0.01 | 0.08 | 0.142 | 0.678 | 0.732 | 0.785 | -0.141 | -0.07 | 0.002 |
| List | 0.314 | 0.405 | 0.495 | -0.049 | -0.001 | 0.052 | 0.305 | 0.398 | 0.492 |
| CardSort | -0.024 | 0.031 | 0.094 | 0.656 | 0.709 | 0.759 | 0.056 | 0.118 | 0.185 |
| Pattern | -0.24 | -0.18 | -0.124 | 0.829 | 0.881 | 0.93 | -0.063 | -0.002 | 0.058 |
| Picture | -0.263 | -0.219 | -0.174 | -0.012 | 0.028 | 0.07 | 0.895 | 0.954 | 1.012 |
| Reading | 0.86 | 0.912 | 0.966 | -0.093 | -0.051 | -0.004 | -0.181 | -0.12 | -0.058 |
| RAVLT | 0.095 | 0.163 | 0.241 | -0.068 | -0.022 | 0.026 | 0.626 | 0.697 | 0.762 |
| LMT | 0.405 | 0.507 | 0.6 | 0.158 | 0.219 | 0.289 | -0.193 | -0.107 | -0.008 |

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**Supplementary Table 2a: Unrotated NIH Toolbox BPPCA Factor Loadings**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **PC1** |  |  | **PC2** |  |  | **PC3** |  |
|  | .025 | 0.50 | .975 | .025 | 0.50 | .975 | .025 | 0.50 | .975 |
| Pic Vocab | 0.579 | 0.617 | 0.656 | -0.502 | -0.451 | -0.398 | -0.35 | -0.287 | -0.223 |
| Flanker | 0.596 | 0.634 | 0.67 | 0.338 | 0.385 | 0.437 | -0.239 | -0.167 | -0.093 |
| List | 0.611 | 0.646 | 0.681 | -0.378 | -0.328 | -0.277 | 0.113 | 0.18 | 0.246 |
| Card Sort | 0.657 | 0.695 | 0.733 | 0.331 | 0.373 | 0.416 | -0.081 | -0.019 | 0.048 |
| Pattern | 0.529 | 0.569 | 0.609 | 0.547 | 0.59 | 0.628 | -0.124 | -0.047 | 0.029 |
| Picture | 0.476 | 0.517 | 0.555 | -0.235 | -0.132 | -0.025 | 0.755 | 0.792 | 0.825 |
| Reading | 0.616 | 0.655 | 0.693 | -0.484 | -0.429 | -0.372 | -0.373 | -0.313 | -0.242 |

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**Supplementary Table 2b: Promax-rotated NIH Toolbox BPPCA Factor Loadings**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **PC1** |  |  | **PC2** |  |  | **PC3** |  |
|  | .025 | 0.50 | .975 | .025 | 0.50 | .975 | .025 | 0.50 | .975 |
| Pic Vocab | 0.82 | 0.864 | 0.907 | -0.078 | -0.043 | -0.008 | -0.132 | -0.087 | -0.042 |
| Flanker | 0.065 | 0.12 | 0.171 | 0.681 | 0.733 | 0.784 | -0.15 | -0.086 | -0.017 |
| List | 0.404 | 0.482 | 0.555 | -0.046 | 0 | 0.045 | 0.322 | 0.403 | 0.493 |
| Card Sort | 0.018 | 0.068 | 0.115 | 0.679 | 0.726 | 0.772 | 0.031 | 0.09 | 0.152 |
| Pattern | -0.197 | -0.153 | -0.108 | 0.827 | 0.868 | 0.91 | -0.063 | -0.006 | 0.053 |
| Picture | -0.165 | -0.132 | -0.091 | -0.027 | 0 | 0.026 | 0.972 | 1.003 | 1.032 |
| Reading | 0.837 | 0.881 | 0.924 | -0.036 | 0.003 | 0.04 | -0.151 | -0.108 | -0.062 |

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**Supplementary Table 3: Communalities and Uniquenesses for BPPCA Model**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **Communality** | |  |  | **Uniqueness** | |  |
| Quantiles: | .025 | 0.50 | .975 | | .025 | 0.50 | .975 | |
| Pic Vocab | 0.552 | 0.611 | 0.674 | | 0.326 | 0.389 | 0.448 | |
| Flanker | 0.500 | 0.557 | 0.617 | | 0.383 | 0.443 | 0.500 | |
| List | 0.441 | 0.487 | 0.538 | | 0.462 | 0.513 | 0.559 | |
| Card Sort | 0.546 | 0.601 | 0.662 | | 0.338 | 0.399 | 0.454 | |
| Pattern | 0.604 | 0.668 | 0.732 | | 0.268 | 0.332 | 0.396 | |
| Picture | 0.687 | 0.764 | 0.837 | | 0.163 | 0.236 | 0.313 | |
| Reading | 0.642 | 0.704 | 0.767 | | 0.233 | 0.296 | 0.358 | |
| RAVLT | 0.554 | 0.616 | 0.677 | | 0.323 | 0.384 | 0.446 | |
| LMT | 0.292 | 0.347 | 0.410 | | 0.590 | 0.653 | 0.708 | |

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**Supplementary Table 4: Communalities and Uniquenesses for NIH Toolbox BPPCA Model**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **Communality** | |  |  | **Uniqueness** |  |
| Quantiles: | .025 | 0.50 | .975 | | .025 | 0.50 | .975 |
| Pic Vocab | 0.613 | 0.668 | 0.723 | | 0.277 | 0.332 | 0.387 |
| Flanker | 0.522 | 0.580 | 0.638 | | 0.362 | 0.420 | 0.478 |
| List | 0.506 | 0.559 | 0.612 | | 0.388 | 0.441 | 0.494 |
| Card Sort | 0.569 | 0.624 | 0.681 | | 0.319 | 0.376 | 0.431 |
| Pattern | 0.618 | 0.674 | 0.732 | | 0.268 | 0.326 | 0.382 |
| Picture | 0.851 | 0.914 | 0.976 | | 0.024 | 0.086 | 0.149 |
| Reading | 0.654 | 0.711 | 0.771 | | 0.229 | 0.289 | 0.346 |

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**Supplementary Table 5: Varimax-Rotated Factor Loadings for First Split-Half BPPCA Model**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **PC1** |  |  | **PC2** |  |  | **PC3** |  |
|  | .025 | 0.50 | .975 | .025 | 0.50 | .975 | .025 | 0.50 | .975 |
| Pic Vocab | 0.69 | 0.766 | 0.832 | -0.013 | 0.036 | 0.085 | 0.125 | 0.206 | 0.301 |
| Flanker | 0.115 | 0.191 | 0.266 | 0.64 | 0.7 | 0.756 | 0.052 | 0.128 | 0.216 |
| List | 0.335 | 0.435 | 0.529 | 0.129 | 0.191 | 0.255 | 0.384 | 0.499 | 0.596 |
| Card Sort | 0.12 | 0.184 | 0.255 | 0.67 | 0.729 | 0.785 | 0.145 | 0.22 | 0.3 |
| Pattern | -0.03 | 0.03 | 0.093 | 0.736 | 0.795 | 0.849 | -0.018 | 0.053 | 0.12 |
| Picture | -0.016 | 0.032 | 0.085 | 0.111 | 0.157 | 0.211 | 0.777 | 0.846 | 0.906 |
| Reading | 0.737 | 0.801 | 0.863 | 0.062 | 0.111 | 0.159 | 0.084 | 0.155 | 0.237 |
| RAVLT | 0.206 | 0.277 | 0.364 | 0.05 | 0.1 | 0.149 | 0.66 | 0.737 | 0.807 |
| LMT | 0.418 | 0.53 | 0.635 | 0.205 | 0.284 | 0.368 | -0.047 | 0.056 | 0.167 |

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**Supplementary Table 6: Varimax-Rotated Factor Loadings for Second Split-Half BPPCA Model**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **PC1** |  |  | **PC2** |  |  | **PC3** |  |
|  | .025 | 0.50 | .975 | .025 | 0.50 | .975 | .025 | 0.50 | .975 |
| PicVocab | 0.696 | 0.758 | 0.817 | 0.045 | 0.096 | 0.15 | 0.109 | 0.177 | 0.263 |
| Flanker | 0.151 | 0.212 | 0.272 | 0.66 | 0.722 | 0.779 | -0.043 | 0.027 | 0.094 |
| List | 0.421 | 0.518 | 0.598 | 0.055 | 0.11 | 0.171 | 0.373 | 0.475 | 0.573 |
| CardSort | 0.17 | 0.234 | 0.298 | 0.627 | 0.685 | 0.742 | 0.184 | 0.255 | 0.331 |
| Pattern | -0.048 | 0.009 | 0.066 | 0.77 | 0.823 | 0.875 | 0.049 | 0.106 | 0.17 |
| Picture | -0.038 | 0.01 | 0.06 | 0.067 | 0.113 | 0.159 | 0.818 | 0.873 | 0.93 |
| Reading | 0.774 | 0.827 | 0.881 | 0.081 | 0.131 | 0.183 | 0.031 | 0.095 | 0.164 |
| RAVLT | 0.259 | 0.33 | 0.413 | 0.105 | 0.157 | 0.21 | 0.611 | 0.684 | 0.752 |
| LMT | 0.384 | 0.481 | 0.571 | 0.244 | 0.323 | 0.403 | -0.028 | 0.061 | 0.158 |

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**Supplementary Table 7: Varimax-Rotated Factor Loadings for Imputed BPPCA Model**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **PC1** |  |  | **PC2** |  |  | **PC3** |  |
|  | .025 | 0.50 | .975 | .025 | 0.50 | .975 | .025 | 0.50 | .975 |
| Pic Vocab | 0.709 | **0.754** | 0.795 | 0.033 | 0.067 | 0.099 | 0.127 | 0.177 | 0.232 |
| Flanker | 0.178 | 0.222 | 0.268 | 0.669 | **0.711** | 0.751 | 0.008 | 0.06 | 0.109 |
| List | 0.439 | **0.504** | 0.569 | 0.106 | 0.144 | 0.185 | 0.392 | **0.468** | 0.538 |
| Card Sort | 0.163 | 0.204 | 0.244 | 0.683 | **0.718** | 0.758 | 0.181 | 0.224 | 0.272 |
| Pattern | -0.019 | 0.018 | 0.055 | 0.771 | **0.809** | 0.847 | 0.062 | 0.099 | 0.141 |
| Picture | -0.011 | 0.024 | 0.057 | 0.108 | 0.136 | 0.166 | 0.829 | **0.87** | 0.912 |
| Reading | 0.77 | **0.809** | 0.849 | 0.092 | 0.127 | 0.161 | 0.082 | 0.128 | 0.177 |
| RAVLT | 0.274 | 0.324 | 0.385 | 0.101 | 0.135 | 0.17 | 0.652 | **0.707** | 0.753 |
| LMT | 0.443 | **0.512** | 0.576 | 0.262 | 0.313 | 0.368 | -0.009 | 0.049 | 0.12 |

**Supplementary Figure 1: Density Histograms of Standardized Neurocognitive Measures** 

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**Supplementary Figure 2: Density Histograms of CBCL Outcomes** 

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**Supplementary Figure 3: Trace Plots for BPPCA Variance Components** 