## Data supplement

## Modified partial correlation algorithm

In this study the structural connections of the cortical network are defined as statistical connections between pairs of average grey matter thickness extracted from 34 regions of interest from each hemisphere. A structural connection was considered to be present if the correlation coefficient for a pair of brain area thicknesses was statistically significant. The interregional correlation matrix $(68 \times 68)$ was obtained for each group by calculating the partial correlation coefficients using a partial correlation ( $\mathrm{PC}^{\star}$ ) algorithm modified from Li \& Wang ${ }^{14}$ (Wheland et al ${ }^{15}$ ). The $\mathrm{PC}^{\star}$ algorithm improves performance over the typical partial correlation method by leveraging connection sparsity. Whereas an edge is typically checked by calculating the partial correlation between the two corresponding random variables conditioned on all others, $\mathrm{PC}^{*}$ seeks to test the same edge using partial correlation conditioned on an equivalent, yet more optimal, smaller data-set. Because fewer conditioning variables are used, the $\mathrm{PC}^{\star}$ estimates require fewer data samples and generally include less variance, making it a better estimate of the true partial correlations and consequently more sensitive for determining connectivity. Furthermore, the PC ${ }^{*}$ algorithm used the Benjamini-Hochberg (BH) procedure
for controlling the false detection rate (FDR) instead of the original type 1 error hypothesis test in which an edge is accepted if its $P$ value is below some target. Unlike the type 1 test, which is applied to one edge at a time, the BH procedure is applied to the $P$ values of all edges simultaneously. Because the PC algorithm generates multiple $P$ values for a single edge by conditioning on a number of sets, there is a question of which value to use with the BH procedure for each edge. In this case the maximum value over all conditioning sets is used for each edge, as doing so has been shown to result in convergence to the true underlying graph.

## Additional references

14 Li J, Wang ZJ. Controlling the false discovery rate of the association/causality structure learned with the PC algorithm. J Mach Learn Res 2009; 10: 475-514.

15 Wheland D, Joshi AA, McMahon K, Hansell NK, Martin NG, Wright MJ, et al. Robust identification of partial-correlation based networks with applications to cortical thickness data. IEEE 9th International Symposium on Biomedical Imaging, 2-5 May 2012; pp. 1551-4 (doi: 10.1109/ISBI.2012.6235869).

Table DS1 Topological graph theory metrics obtained for the whole brain, the frontal network and its nodes for psychopathy and control groups

|  | Betweenness |  | Characteristic path length |  | Clustering coefficient |  | Local efficiency |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Control | Psychopathy | Control | Psychopathy | Control | Psychopathy | Control | Psychopathy |
| Whole brain | 2106 | 2056 | 0.14 | 0.13 | 0.12 | 0.11 | 0.22 | 0.49 |
| Frontal cortex | 46 | 47 | 0.22 | 0.19 | 0.21 | 0.18 | 0.36 | 0.33 |
| Left | 45 | 63 | 0.19 | 0.20 | 0.17 | 0.20 | 0.23 | 0.4 |
| Frontal pole | 66 | 90 |  |  |  |  |  |  |
| SFG | 14 | 216 |  |  |  |  |  |  |
| Rostral MFG | 0 | 58 |  |  |  |  |  |  |
| Caudal MFG | 24 | 44 |  |  |  |  |  |  |
| Pars orbitalis | 140 | 0 |  |  |  |  |  |  |
| Pars triangularis | 74 | 54 |  |  |  |  |  |  |
| Pars opercularis | 0 | 8 |  |  |  |  |  |  |
| Lateral OFG | 0 | 0 |  |  |  |  |  |  |
| Medial OFG | 132 | 86 |  |  |  |  |  |  |
| Rostral ACC | 40 | 138 |  |  |  |  |  |  |
| Caudal ACC | 8 | 0 |  |  |  |  |  |  |
| Right | 46 | 31 | 0.25 | 0.17 | 0.25 | 0.16 | 0.48 | 0.26 |
| Frontal pole | 0 | 0 |  |  |  |  |  |  |
| SFG | 88 | 158 |  |  |  |  |  |  |
| Rostral MFG | 0 | 16 |  |  |  |  |  |  |
| Caudal MFG | 0 | 0 |  |  |  |  |  |  |
| Pars orbitalis | 0 | 0 |  |  |  |  |  |  |
| Pars triangularis | 144 | 44 |  |  |  |  |  |  |
| Pars opercularis | 0 | 78 |  |  |  |  |  |  |
| Lateral OFG | 74 | 0 |  |  |  |  |  |  |
| Medial OFG | 212 | 0 |  |  |  |  |  |  |
| Rostral ACC | 0 | 40 |  |  |  |  |  |  |
| Caudal ACC | 0 | 2 |  |  |  |  |  |  |

[^0]

Fig. DS1 Connectivity analyses based on interregional correlations matrices, showing significant differences between psychopathy and normal control groups for the whole brain (a) and frontal sub-networks (b). The blocks in the matrix are color coded in white to indicate non-significant group difference and red/blue to indicate significant group difference surviving false detection rate (FDR) correction (set to $q=0.01$, with an equivalence to $P<0.0005$ ). ACC, anterior cingulate cortex; MFC, middle frontal cortex; OFC, orbitofrontal cortex; SFC, superior frontal cortex.
(a)

(b)


Frontal Temporal Parietal Occipital Frontal Temporal Parietal Occipital Correlation
LEFT HEMISPHERE
RIGHT HEMISPHERE

Fig. DS2 Whole-brain interregional correlations matrix for the normal control (a) and psychopathy groups (b). The colour bar indicates positive (red) and negative (blue) partial correlation coefficients between the average thickness of two regions. The boxes highlighted indicate intrahemisphere (red, left-left; blue, right-right) and interhemisphere (green, left-right) interregional correlations within the frontal sub-network.


[^0]:    ACC, anterior cingulate cortex; MFG, middle frontal gyrus; OFG, orbitofrontal gyrus; SFG, superior frontal gyrus.

