Supplemental Material

- **Figure S1** Identification of the linear part of the bouton cloud. A: Shown is the proportion of boutons in the set *L* versus the fractal dimension of *L* for a layer 2/3 pyramidal cell. Kernel width ρ is indicated along the curve. The linear part of the bouton cloud is *L* with ρ such that its fractal dimension is in the range 0.95-1.05. **B** and **C**: Coronal view (B) and top view (C) of the bouton cloud of the layer 2/3 pyramidal cell. Boutons belonging to the linear part are shown in gray, the remaining boutons are indicated in black. The proportion of boutons in the linear part is 25%.
- Figure S2 Testing the cluster performance. A: Clustering of an artificial example of a patchy distribution of points in 3-D. 3000 points are drawn from a mixture of 10 trivariate gaussian distributions. Left: Top view of the point cloud. Recovered clusters are indicated by different colors and by the associated 2-ellipsoids. For comparison, the 2-ellipsoids of the theoretical tri-variate mixture are also indicated (gray stippled lines). Gray crosses and open circles indicate points which were ignored for various reasons, including a small volume or a large elongation. Right: Similarity index between consecutive partitions as a function of the kernel width *h*. Red rectangle indicates the first stable regime where a change of the kernel width causes only minute differences (similarity index >0.99) between partitions. The effective width for detecting the clusters was chosen from this interval. B: Clustering a random uniform distribution of points showing that spurious clusters are not detected. 2000 points are distributed randomly in a box of 2*mm* side length. Left: Shown is the top view of the point cloud. Right: Similarity index between consecutive partitions as a

function of kernel width *h*. Merging spurious clusters resulted in the only stable regime (red rectangle) with the trivial solution of one cluster containing all points.

- Figure S3 Choice of effective kernel width h^{*} for the example bouton clouds shown in figure 1. Shown is the similarity index between consecutive pairs of partitions as a function of kernel width h. Red rectangles indicate the stable regimes from which the kernel width h^{*} was selected for the detection of the clusters in the bouton cloud. A: layer 2/3 pyramidal cell, B and D: layer 6 pyramidal cells, C: layer 2/3 basket cell, E: layer 4 pyramidal cell.
- **Figure S4** Straightening the cortical layers. Depicted is the coronal view of a cortical layer which contains a cluster (gray shaded 2-ellipsoid, shown here as an ellipse) from a neuron whose cell body is indicated (large gray dot) before (left) and after (right) the flattening operation. The flattening operation straightens the layer and maps the cluster center and the cluster orientation correspondingly. Left: *A* and *B* indicate intersection points of the upper and lower cortical border of the layer (curved gray lines) with the vertical axis (stippled gray line) through the cell soma. *P* and *Q* indicate the closest points between the upper and lower border of the layer with the cluster center *O*. Based on these four points we determine d(A,P), the distance between *A* and *P* along the upper border, d(B,Q) the distance between *B* and *Q* along the lower border, the vector *OP* from *O* to *P*, the vector *QO* from *Q* to *O*, the vector n=OP+QO, and the coefficient $\alpha=|OP|/(|OP|+|OQ|)$ which is a (normalised) measure of the distance between the point *O* and the lower border. **Right**: Cortical layers and cluster in the flattened cortex. The location of the soma, and the points *A* and *B* remain unchanged. The new origin of the cluster is given by

O' with $O'_x = B_x + \alpha d(A, P) sign(P_x) + (1 - \alpha) d(B, Q) sign(Q_x)$, $O'_y = O_y$, and $O'_z = B_z + \alpha |AB|$. The 2-ellipsoid and the vector *n* are rotated in the xz-plane about *O*' until *n* points vertically upwards (*n*').

Figure S5 The largest of the three cluster diameter scales with the shortest diameter. Shown is for each cluster (closed circles from excitatory neurons, open circles from inhibitory neurons) the scatterplot of the largest diameter of the 2-ellipsoid with the smallest diameter. Stippled line indicates the regression line (a=0.04, b=0.37, r^{2} =0.48, p<0.05,).

Figure S6 Density of boutons in clusters. A and B: Individual (dots) and cell type averages (bars) of bouton densities in the cluster of rank 1 (A) and rank 2 (B). C: For each excitatory neuron and inhibitory neuron (inset) the bouton density is shown as a function of cluster rank *k*. Black lines indicate neurons with 2 clusters, dark gray lines indicate neurons with 5 clusters, and light gray lines are neurons forming neither 2 nor 5 clusters.