**Supplementary Figure S1. Cortical ensembles as a representation of multidimensional population vectors obtained with two-photon calcium imaging**

(A) Schematic representation of active neurons at different frames. Black dots represent active neurons at different times (left). Binary raster plot representing the overall network activity of observed neurons (right). Population vectors capture the coordinated activity of a given neuronal ensemble. (B) Population vectors can be understood as a multidimensional array in which clusters of population vectors taken from different times define network states.

**Supplementary Figure S2. Added nodes does not affect graph properties**

(A) CRF graphs of baseline model (no added nodes) and hidden node model, trained with the same experiment. Edge color represents ; node color represents node strength. Node size represents the node degree. Scale bar represents 50μm. (B) Graph densities, (C) node strength, (D) node degrees, (E) clustering coefficients and (F) centrality do not differ significantly between the two models (n = 101 neurons; paired *t*-test; n.s. p>0.05).

**Supplementary Figure S3. Comparison of prediction performance with CRF, SVD ensembles and high OSI cells**

(A) Examples of core neurons identified using SVD (green) and CRFs (orange). Circles represent core neurons of horizontal (left) and vertical (right) visual stimuli, respectively. Neurons shared between CRFs and SVD methods are represented by green and orange dots. Scale bar represents 50μm. (B) Percentage from the total population size representing core neurons for SVD and CRFs methods. (C) Percentage of shared neurons identified by SVD and CRFs methods. Percentage is calculated by number of cells that belong to both methods divided by the total number of unique cells in both methods. (D) Cosine similarity between population vectors that belong to given visual stimuli (color) compared with population vectors from different visual stimuli (black). (E) ROC curve of the classification result with SVD, CRF and high OSI cells. Dashed line represent random chance. (F) Area under curve (AUC) of ROC curves. (G) Accuracy, (H) precision and (I) recall of predictions for each visual stimuli using both methods. (J) Cosine similarity between population vectors representing optimal cortical ensembles identified with SVD for a given visual stimuli. Each SVD ensemble was randomly down-sampled (dark green). The cosine similarity of population vectors belonging to different visual stimuli is shown in light green. (K) Accuracy, (L) precision and (M) recall of predictions from randomly down-sampled SVD ensembles. (N) Cosine similarity between population vectors of high OSI cells. (O) Accuracy, (P) precision and (Q) recall of predictions from randomly down-sampled high OSI cells.

**Supplementary Figure S4. Minimum dataset size to obtain stable performance**

(A) Cosine similarity between ensemble population vectors of the given visual stimuli (orange) compared with population vectors from different visual stimuli (gray). (B) Accuracy, (C) precision and (D) recall of CRF ensemble prediction reach stable with a minimum of 200 frames training data. The data used in this experiment contains 101 neurons.

**Supplementary Figure S5. CRF ensembles are able to predict multiple stimuli**

(A) An example of constructed CRF graph from the Paul Allen dataset, with four orientations of drifting grating stimuli (squares). Edge color indicates the strength of inferred connections; node size indicates the node degrees. (B) Temporal course of ensemble classification for four drifting-gratings. Colored stripes indicate visual stimuli. Scale bar represents 200 frames. (C) Accuracy, (D) precision and (E) recall of prediction with CRF model trained with temporal frequency 1Hz, on dataset of temporal frequency 2, 4, 8, and 15Hz.