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2 **Supplementary Materials for**
3 **Decoding brain states on the intrinsic manifold of human brain dynamics across**
4 **wakefulness and sleep**

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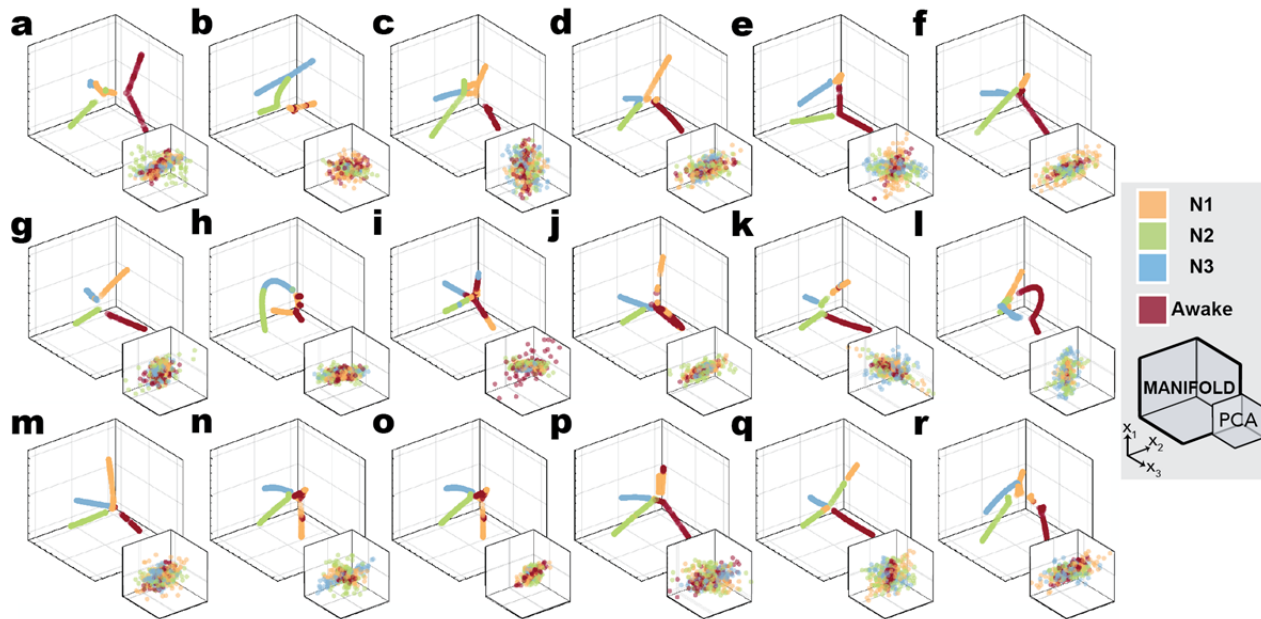
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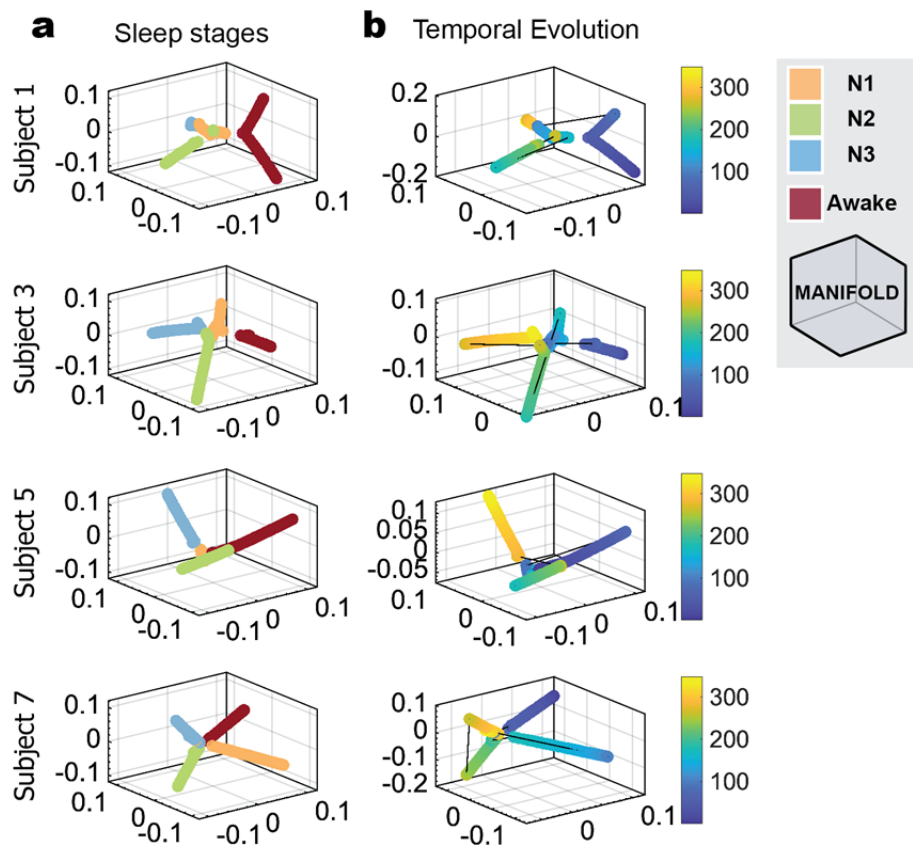
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31 **Supplementary Figure 1.** *Representation of the individual subjects' fMRI BOLD data during*
 32 *wakefulness and sleep embedded into the lower dimensional spaces.* The plots show the fMRI BOLD data
 33 embedded into the three first dimensions of the *intrinsic manifold* (large coordinate system) and into the three
 34 principal components derived from PCA (small coordinate system shown at each corner). Each separate
 35 coordinate system corresponds to the data of eighteen different participants, embedded individually.

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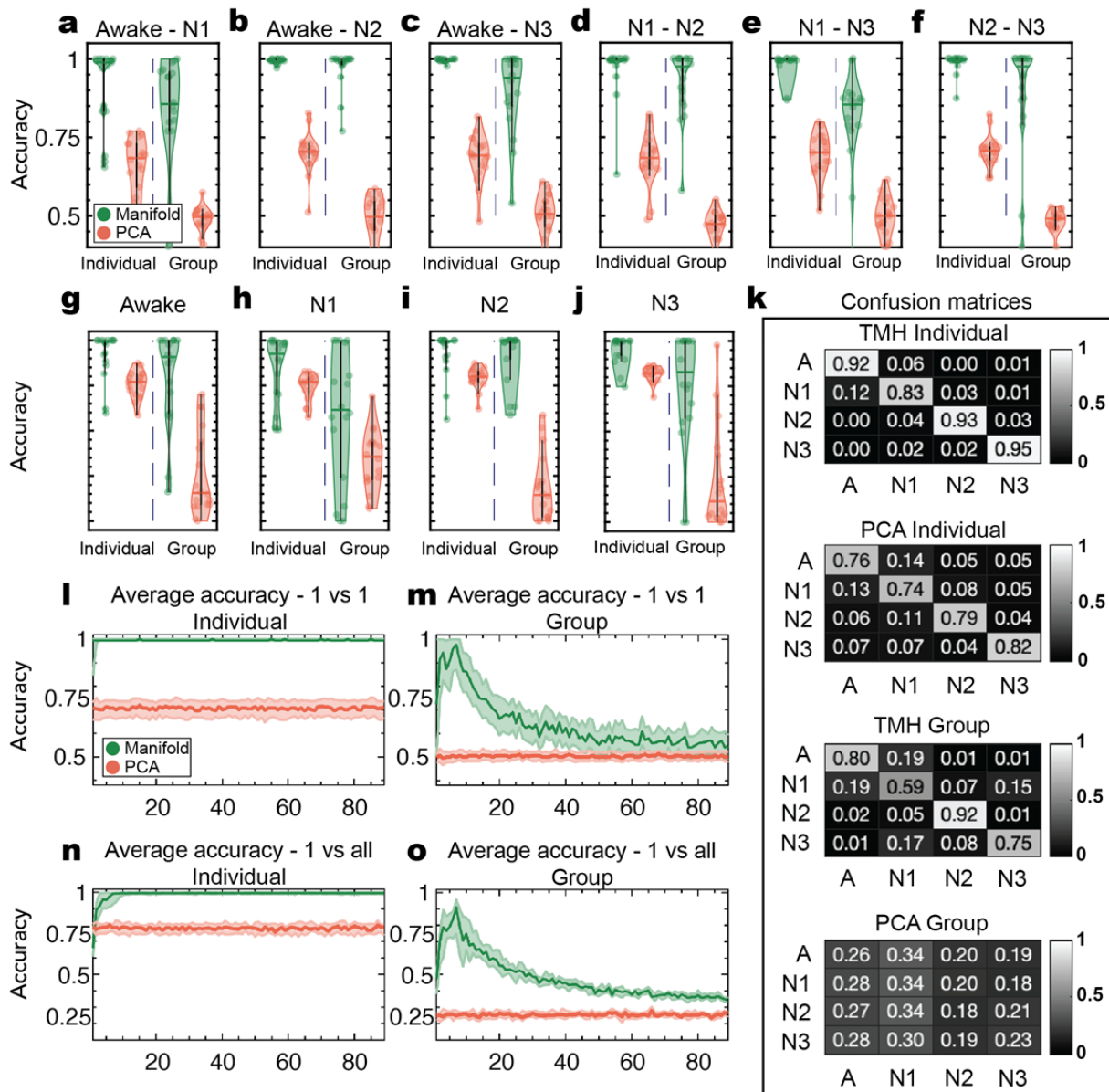
38 **Supplementary Figure 2. Temporal evolution of the fMRI BOLD data during wakefulness and sleep**

39 **embedded in lower dimensional spaces.** The plots show the intrinsic three-dimensional manifolds of four

40 subjects, with color coding for both (a) sleep stage and (b) time-index. For all subjects, fMRI BOLD data

41 shows smooth intra-stage transitions and sharp inter-stage jumps or shortcuts.

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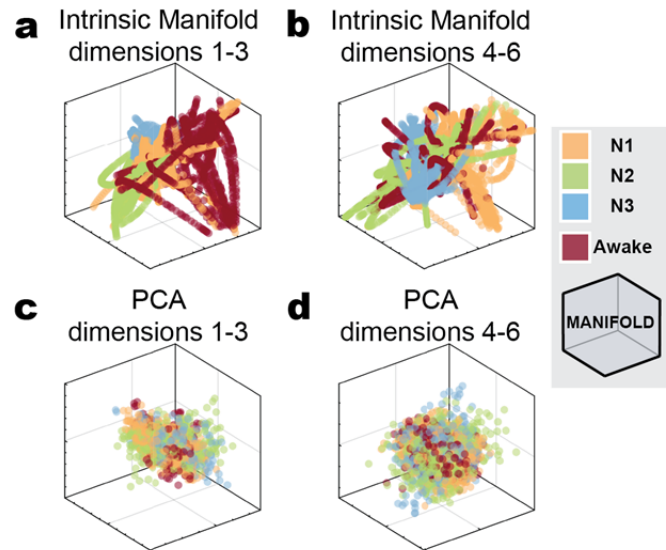


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44 **Supplementary Figure 3. Accuracy of brain state decoding on the intrinsic manifold of brain**
 45 **dynamics and on PCA for 3 dimensions using a linear SVM. A-F)** The accuracies of the SVM 1-vs-1
 46 classification between **a)** wakefulness and N1, **b)** wakefulness and N2, **c)** wakefulness and N3, **d)** N1 and
 47 N2, **e)** N1 and N3, and **f)** N2 and N3. **g-j)** The accuracies of the SVM 1-vs-all classification for each stage:
 48 **g)** wakefulness, **h)** N1, **i)** N2 and **j)** N3. The accuracy is defined as the ratio between the number of true
 49 positives and the total number of tested time points. The boxplots' centrality is indicated by the median,
 50 and the boxes extend between 25-th and 75-th percentiles. Each colored circle corresponds to the
 51 classification accuracy for each single subject (in the case of individual analysis, left of the central dashed
 52 line) and to the accuracy of each leave-one-subject-out round (in the case of group analysis, right to the

53 central dashed line). The classification accuracies on the intrinsic manifold and in PCA space are shown in
54 green and red dots, respectively. Classifications are performed in spaces of dimensionality $d=3$. For all
55 classifications, intrinsic manifold classification yields significantly better accuracies (for all comparisons,
56 $p\text{-value}<.001$, Wilcoxon Rank-sum two-sided test, corrected for multiple comparisons via FDR). **k**)
57 Confusion matrices obtained from the 1-vs-all classification experiments (shown in **g-j**)). **l-m**) show the
58 average accuracy across all stage-to-stage classifications for varying dimensionality of the embedding
59 spaces for individual participants (**l**) and for group analysis (**m**)), respectively. **n-o**) show the average
60 accuracy across all stage (1-vs-all) classifications for varying dimensionality of the embedding spaces for
61 individual participants (**n**) and for group analysis (**o**)), respectively. The solid lines indicate the median of
62 the distribution across classifications and shaded areas indicate 25-th and 75-th percentiles.

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66 **Supplementary Figure 4. Representation of the fMRI BOLD data during wakefulness and sleep at**
 67 **the group level embedded in lower dimensional spaces.** The plots show the intrinsic manifolds aligned
 68 to a common reference for 18 participants. The six first dimensions of the intrinsic manifold (big
 69 coordinate system) and into the six principal components derived from PCA (small coordinate system).
 70 For all cases, nonlinear embedding of the data into their intrinsic manifold led to well-structured intrinsic
 71 manifolds with a clearer separation of different sleep stages (as defined through polysomnography)
 72 compared to the PCA linear embedding.

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74 **Supplementary Table 1. SVM accuracy medians comparison through Wilcoxon Ranksum two-sided**
 75 **test. *p*-values corrected for multiple comparisons via FDR.** All reported accuracies for the SVM
 76 classification are higher in the intrinsic manifold, and significant differences are marked with asterisks (**
 77 $p < .005$, * $p < .05$, Monte-Carlo phase-randomized simulations, corrected for multiple comparisons via
 78 FDR).

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	<i>Individual manifold</i>			<i>Group manifold</i>		
	Intrinsic manifold accuracy	PCA accuracy	Median comparison <i>p</i> -value	Intrinsic manifold accuracy	PCA accuracy	Median comparison <i>p</i> -value
<i>1 vs 1</i>	0.99±0.03 **	0.69±0.07 **	<.001	0.92±0.13 **	0.50±0.03	<.001
<i>1 vs all</i>	0.96±0.04 **	0.78±0.03 **	<.001	0.85±0.09 **	0.25±0.07	<.001

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84 **Supplementary Table 2. SVM accuracy medians comparison for each class, through Wilcoxon**85 **Ranksum two-sided test. *p*-values corrected for multiple comparisons via FDR.** All reported accuracies

86 for the SVM classification are higher in the intrinsic manifold, and all differences are significant (**

87 *p*<.005, * *p*<.05, Ranksum two-sided test, corrected for multiple comparisons via FDR).

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		<i>Individual manifold</i>			<i>Group manifold</i>		
		Intrinsic manifold accuracy	PCA accuracy	Median comparison <i>p</i> -value	Intrinsic manifold accuracy	PCA accuracy	Median comparison <i>p</i> -value
<i>1 vs 1</i>	<i>Awake – N1</i>	0.96±0.07	0.67±0.09	**	0.82±0.20	0.50±0.03	**
	<i>Awake – N2</i>	0.99±0.01	0.71±0.06	**	0.91±0.14	0.51±0.03	**
	<i>Awake – N3</i>	0.99±0.01	0.69±0.07	**	0.96±0.06	0.49±0.03	**
	<i>N1 – N2</i>	0.99±0.01	0.70±0.07	**	0.90±0.15	0.49±0.03	**
	<i>N1 – N3</i>	0.99±0.01	0.69±0.07	**	0.97±0.05	0.51±0.04	**
	<i>N2 – N3</i>	0.99±0.01	0.70±0.04	**	0.94±0.09	0.52±0.03	**
<i>1 vs all</i>	<i>Awake</i>	0.95±0.07	0.76±0.07	**	0.81±0.21	0.20±0.16	**
	<i>N1</i>	0.91±0.13	0.76±0.07	**	0.76±0.23	0.35±0.16	**
	<i>N2</i>	0.98±0.03	0.80±0.05	**	0.88±0.19	0.21±0.12	**
	<i>N3</i>	0.99±0.01	0.80±0.05	**	0.96±0.09	0.24±0.18	**

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90 **Supplementary Table 3. AUC medians comparison through *Wilcoxon Ranksum* two-sided test.**
 91 **p-values corrected for multiple comparisons via FDR.** All AUC are significantly higher for the
 92 intrinsic manifold than for the projection into the PCA space.
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	<i>Individual manifold</i>		
	Intrinsic manifold AUC	PCA AUC	Median comparison <i>p</i> -value
<i>Awake – N1</i>	0.99±0.04	0.51±0.01	<.001
<i>Awake – N2</i>	0.98±0.04	0.51±0.01	<.001
<i>Awake – N3</i>	0.99±0.04	0.51±0.01	<.001
<i>N1 – N2</i>	0.99±0.04	0.51±0.01	<.001
<i>N1 – N3</i>	1.00±0.01	0.51±0.01	<.001
<i>N2 – N3</i>	0.94±0.10	0.52±0.02	<.001

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96 **Supplementary Table 4. Decoding accuracy compared to Tagliazucchi 2012 Neuroimage.** This table
 97 reports the results of *Tagliazucchi et al. Neuroimage 2012*, in comparison to our results on group
 98 manifolds, and on individual manifolds. We believe that the comparison between our accuracies on
 99 individual manifolds and previous efforts is the fairest comparison, as in both these cases, data from the
 100 same subjects are included in both training and testing sets.

	Tagliazucchi 2012 (TW: 1 min; max accuracy out of 6-fold – see their TABLE 5)	Intrinsic manifold (GROUP, single time-points; mean accuracy out of leave-one-subject-out)	Intrinsic manifold (INDIVIDUAL, single time-points; mean accuracy out of 6-fold cross-validation)
<i>Awake – N1</i>	0.76	0.82	0.96
<i>Awake – N2</i>	0.88	0.91	0.99
<i>Awake – N3</i>	0.89	0.96	0.99
<i>N1 – N2</i>	0.83	0.90	0.99
<i>N1 – N3</i>	0.93	0.97	0.99
<i>N2 – N3</i>	0.87	0.94	0.99

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