Supplementary Material

SUPPLEMENTARY METHODS

Mixed effect model

A mixed-effects model (MEM) was utilised to evaluate the variation in neuronal signal power recorded from adjacent contacts. Patients and hemispheres (nested into patients), were explored as random effects. Hemisphere was a significant random effect in the ERNA model (patient Akaike Information Criterion (AIC) 344.6 vs patient and hemisphere AIC 332.6, $p<0.001$), though not the beta model and ultimately incorporated only into the ERNA model. The ranking of contacts according to ERNA power and beta power were assigned as fixed-effects to build the final MEM. The log-transformed ERNA power and beta power were assigned as the response variable. The log-transformation was applied to ensure the MEM residuals were normally distributed.

Simple-ranking Method

A simple-ranking method was employed to determine the predictive value of each factor alone (ERNA power, beta oscillations power and Euclidean distance from the ideal anatomical location) in identifying the clinician-chosen contact (Supplementary Figure 1). The method was validated using a 10-fold nested cross-validation (CV), repeated 10 times (see model validation below).

Machine Learning Method

Three machine learning techniques – Logistic Regression (LR)[1], Support Vector Machine (SVM)[2] and Random Forest (RF)[3] – were used to predict the probability of a contact being selected by the clinician for chronic DBS when using a combination of factors (Supplementary Figure 2).

The performance of these learning algorithms was validated using a 10-fold nested CV, repeated 10 times (Supplementary Figure 3a, see model validation below). The dataset was imbalanced due to the unequal class distribution between selected and non-selected electrodes (one selected, three unselected in each hemisphere). Thus, balanced class weight was applied during training to reduce bias in the classification model (Supplementary Figure 3b). The hyperparameter selections used in our grid search are shown in Supplementary Table 2.

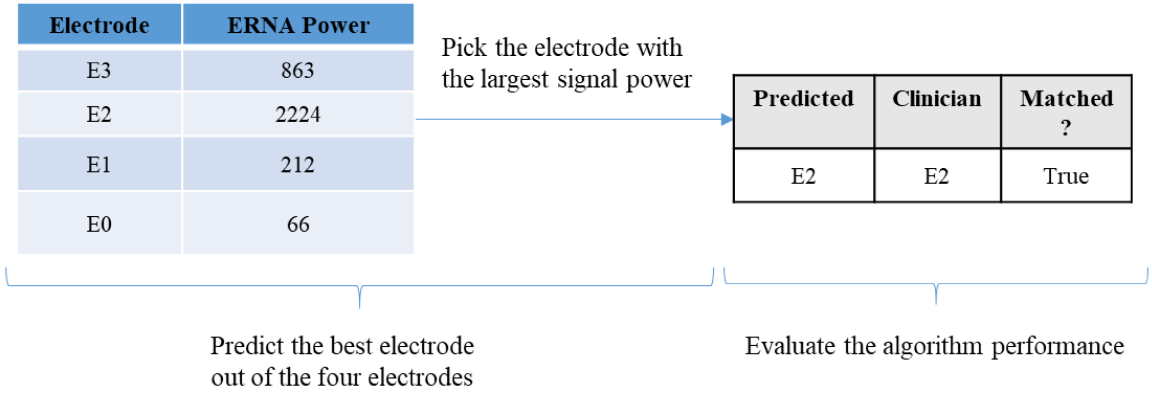
The RF classifier delivered the highest mean predictive value and was employed to evaluate all possible combinations of factors in a model (Supplementary Figure 4).

Model Validation

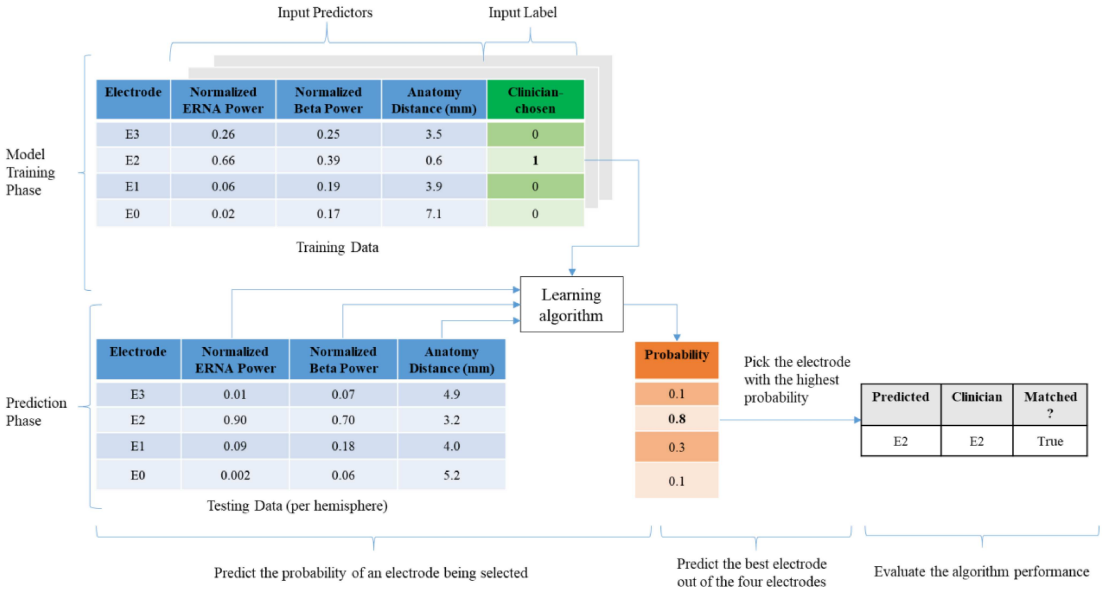
The simple-ranking and machine learning models were validated using a 10-fold nested CV method, repeated 10 times. The dataset was separated into training and testing sets to ensure that data from the same patient was not used for both model development and model evaluation[4] (Supplementary Figure 3a).

SUPPLEMENTARY FIGURES

Supplementary Figure 1: Simple-ranking method. Each contact on the DBS lead is ranked according to ERNA power, beta oscillations power or proximity to the ideal anatomical location. In this example, the contact measuring the largest ERNA power (E2) is predicted to be the best contact and coincides with the clinician-chosen chosen for chronic DBS.

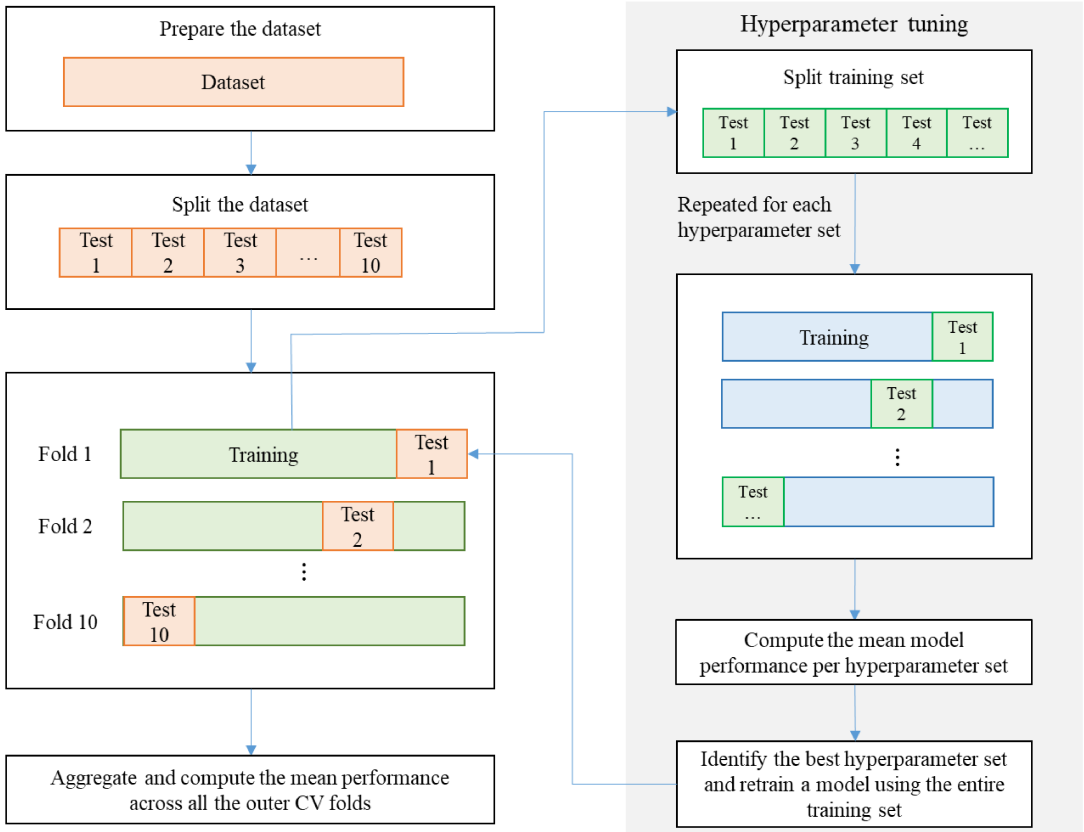


Supplementary Figure 2: In the model training phase, a combination of factors is used to determine the optimal contact prediction through a learning algorithm. In the testing data, within each hemisphere, the probability that a given contact coincides with the clinician-chosen contact is calculated using the learning algorithm. Finally, the contact with the highest probability is compared to the clinician-chosen contact.

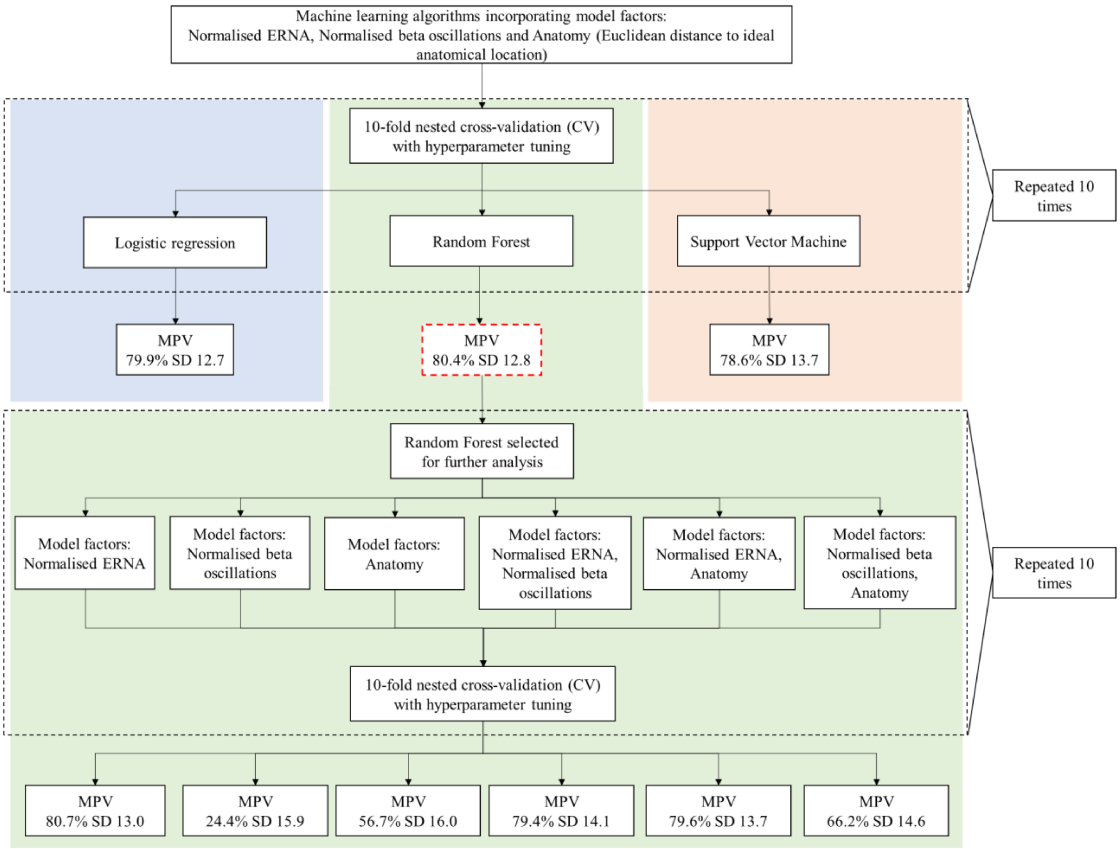


Supplementary Figure 3: Nested cross-validation (CV) for algorithm training and testing. (a) illustrates the 10-fold nested outer CV used for evaluating the algorithm performance, which was repeated 10 times. (b) illustrates the inner CV used for hyperparameter tuning to find the optimal hyperparameters for each algorithm (Logistic Regression, Support Vector Machine and Random Forest). After identification of the optimal hyperparameter set, the algorithm was applied to the outer CV testing set to generate the predictive value of the model.

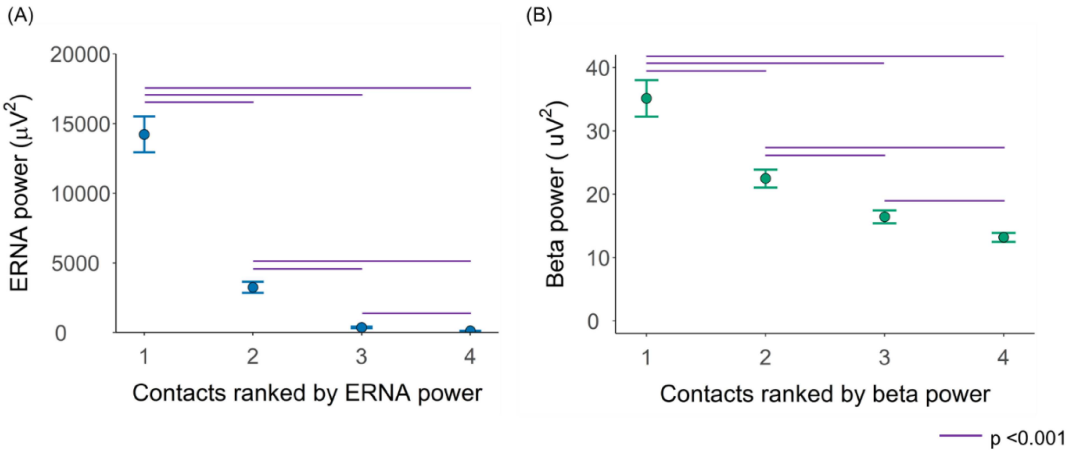
Note: Simple-ranking method does not require hyperparameter tuning.



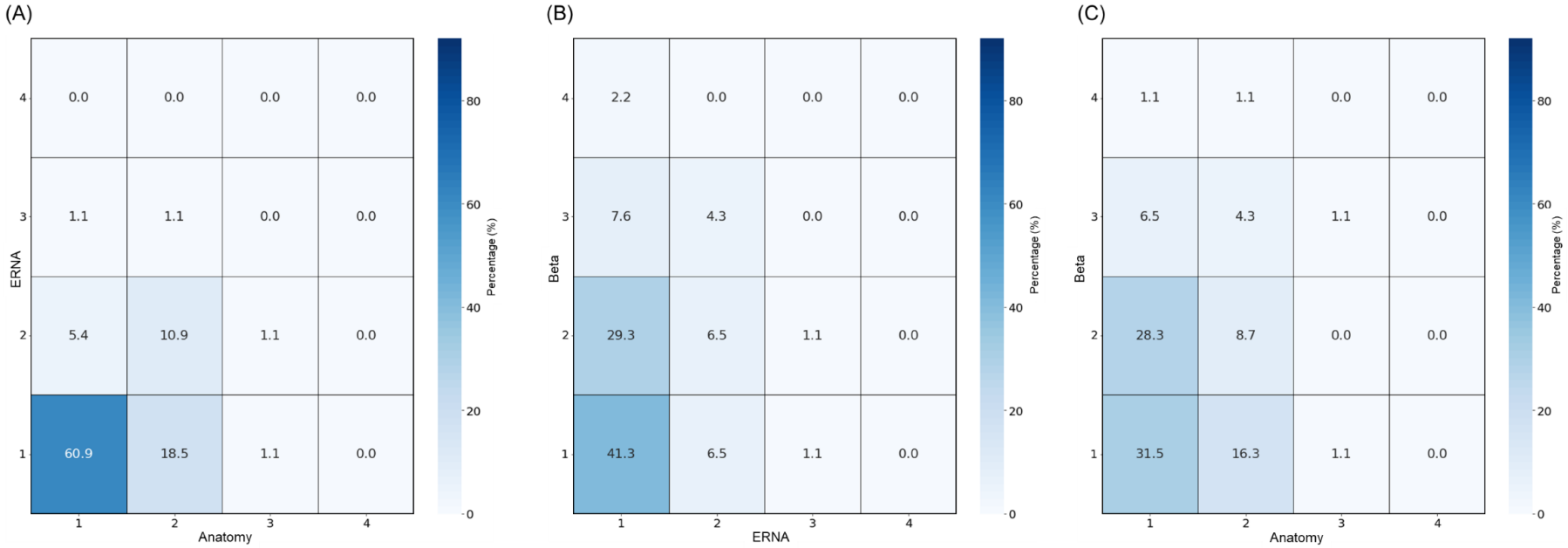
Supplementary Figure 4: Machine learning algorithms. Three machine learning algorithms were evaluated to assess the mean predictive value of models employing a combination of factors. The Random Forest model produced the highest predictive value and was employed for further analysis of factor combinations. MPV = mean predictive value, SD = standard deviation



Supplementary Figure 5: (A) ERNA power and (B) beta oscillations power at contacts ranked according to the neuronal signal power. The raw means (dots) and standard errors (bars) are presented in the figures, while statistical analyses employed fitted means adjusted for fixed and random effects. ERNA = evoked resonant neural activity.



Supplementary Figure 6: Confusion matrices comparing the ranking of contacts according to each factor of interest (ERNA power, beta oscillation power, anatomy) at the contact chosen by the clinician for chronic DBS at six months post-operatively. A) ERNA power vs Anatomy confusion matrix. B) ERNA power vs beta oscillation power confusion matrix. C) Beta oscillation power vs Anatomy confusion matrix. The number in each square indicates the percentage of hemispheres (of the available 92) in which the corresponding combination of rankings according to the two factors of interest occurred. E.g., In A), square 1,1 (bottom row, left corner) indicates that in 60.9% of hemisphere, the clinician-chosen contact corresponded with both the first-ranked ERNA contact and the first-ranked anatomy contact. Square 2,1 (bottom row, second from the left) indicates that in 18.5% of hemispheres, the clinician-chosen contact corresponded with the first-ranked ERNA contact and the second-ranked anatomy contact. The darker the square, the greater the proportion of hemispheres in the corresponding combination of rankings.



SUPPLEMENTARY TABLES

Supplementary Table 1: The mean predictive value of the features of interest using different modelling techniques.

Analysis method	**Included factors**	**Mean predictive value (%)**	**SD**
Simple ranking method	ERNA	80.3	14.2
	Beta oscillations	49.9	16.5
	Anatomy	66.8	16.5
Logistic regression	Normalised ERNA, normalised beta oscillations, Anatomy	79.9	12.7
Support Vector Machine	Normalised ERNA, normalised beta oscillations, Anatomy	78.6	13.7
Random forest	Normalised ERNA, normalised beta oscillations, Anatomy	80.4	12.8
	Normalised ERNA	80.7	13.0
	Normalised beta oscillations	24.4	15.9
	Anatomy	56.7	16.0
	Normalised ERNA, normalised beta oscillations	79.4	14.1
	Normalised ERNA, Anatomy	79.6	13.7
	Normalised beta oscillations, Anatomy	66.2	14.6

Data is presented as mean and standard deviation (SD).

Supplementary Table 2: The hyperparameter selections used in the grid search for Logistic Regression, Support Vector Machine and Random Forest models.

Model	**Hyperparameters**	**Values**
Logistic Regression	Penalty	Elastic-net
	Tolerance for stopping criteria	10^{-6}
	Inverse of regularization strength, C	0, 10^0, 10^1, 10^3, 10^5
	Ratio of L1 penalty	0, 0.25, 0.50, 0.75, 1.0
	Max iteration number	5000
Support Vector Machine	Kernel	Radial basis function
	Regularization strength, C	0, 10^0, 10^1, 10^3, 10^5
	Tolerance for stopping criteria	10^{-6}
Random Forest	Number of decision trees	100
	Maximum features per tree	Same as number of features
	Quality of split criterion	Gini
	Min samples per leaf	1, 5, 10, 20, 50
	Max samples per tree (%)	50, 80, 100

References

1. Dreiseitl S, Ohno-Machado L. Logistic regression and artificial neural network classification models: a methodology review. *Journal of biomedical informatics* 2002;35(5-6):352-59.
2. Boser BE, Guyon IM, Vapnik VN. A training algorithm for optimal margin classifiers. Proceedings of the fifth annual workshop on Computational learning theory. Pittsburgh, Pennsylvania, USA: Association for Computing Machinery, 1992:144–52.
3. Breiman L. Random Forests. *Machine Learning* 2001;45(1):5-32. doi: 10.1023/A:1010933404324
4. Vabalas A, Gowen E, Poliakoff E, et al. Machine learning algorithm validation with a limited sample size. *PloS one* 2019;14(11):e0224365. doi: 10.1371/journal.pone.0224365