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Machine Learning 2: advanced

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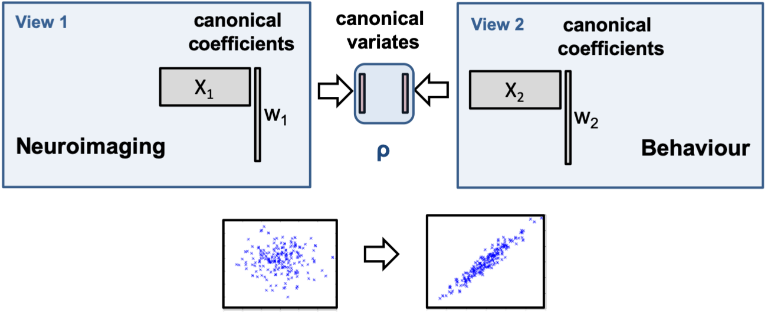
Outline

Outline

Finding mappings between brain and behaviour

- **Canonical Correlation Analysis** is a standard statistical tool for finding multivariate relationships between datasets
- Generalises Pearson correlation to multiple variables
- Finds projections of the data that maximise the correlation between "views" of the data



Canonical Correlation Analysis

- CCA is related to techniques such as partial least squares
- Formally, CCA solves the following objective function:

$$\max_{w_1, w_2} corr(X_1 w_1, X_2 w_2)$$

$$\text{subject to } ||w_1^T X_1^T X_1 w_1|| \leq 1 \text{ and } ||w_2^T X_2^T X_2 w_2|| \leq 1$$

where the constraint is sometimes amended to:

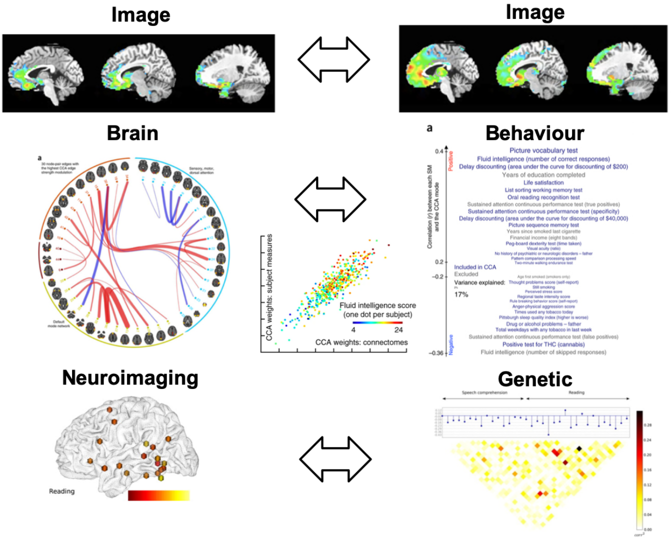
$$\text{subject to } ||w_1||^2 \leq 1 \text{ and } ||w_2||^2 \leq 1$$

...and other constraints can be added (e.g. to promote sparsity)

$$P(w_1) < c_1 \text{ and } P(w_2) < c_2$$

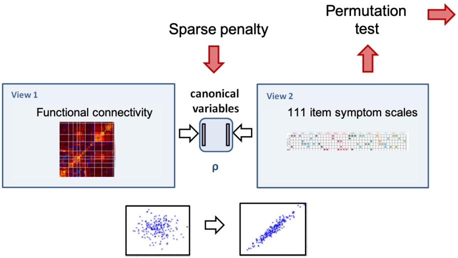
- if $n > p_1$ and p_2, an analytical solution is available
- There are many variants (kernel, Bayesian, deep CCA...)

Applications of CCA

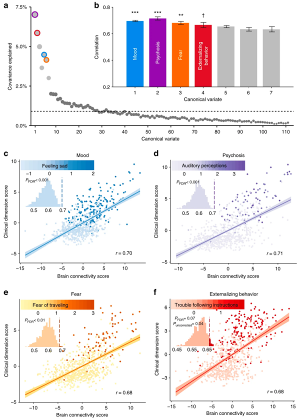


Smith et al. (2015); Floch et al. (2012)

Applications of CCA

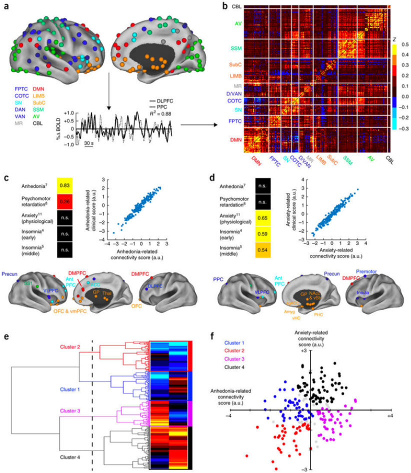


4 Linked dimensions

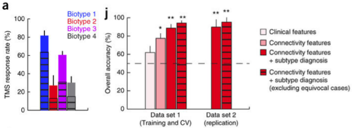


Xia et al. (2018)

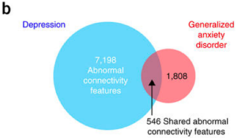
Stratification of major depression



- Extensive validation
- Predict treatment response (TMS)

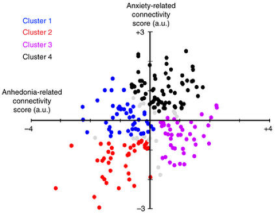


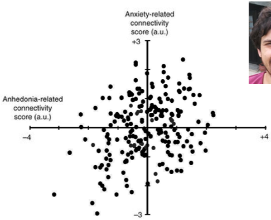
- Cut across diagnoses

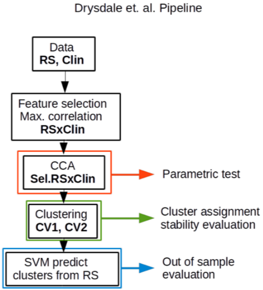


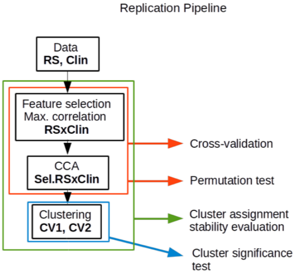
Drysdale et al. (2017)

Stratification of major depression



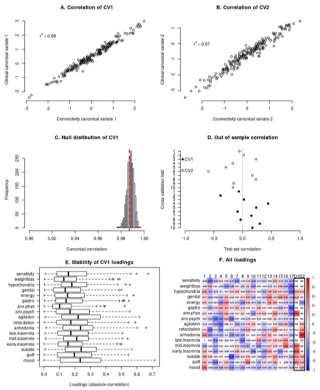


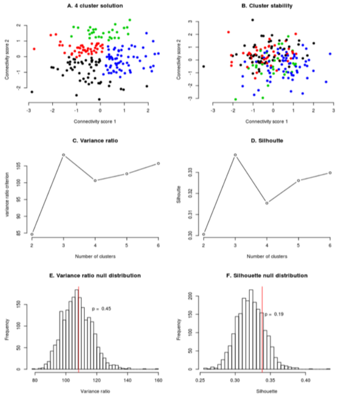




Dinga et al. (2019)

Stratification of major depression

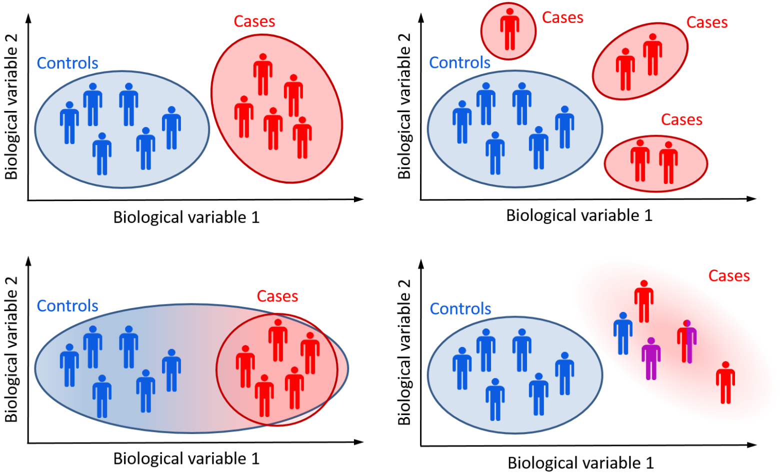




- CCA easily overfits, even when $N > p$
- In-sample canonical correlation is often high under the null!
- Regularization and/or feature selection is very important
- Statistical evaluation should include the whole pipeline

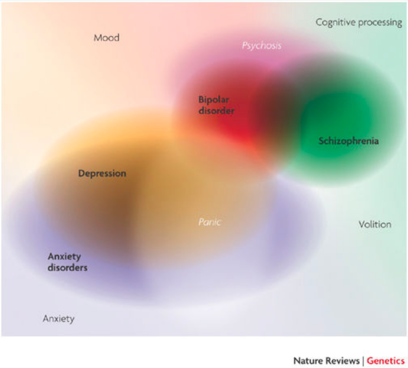
Dinga et al. (2019)

Many types of heterogeneity



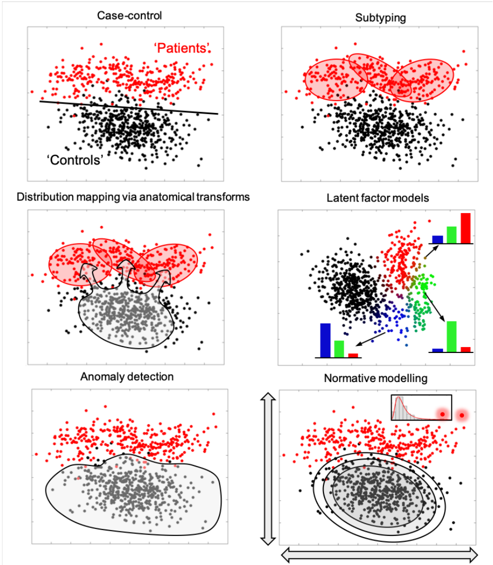
Marquand et al. (2016)

Many types of heterogeneity



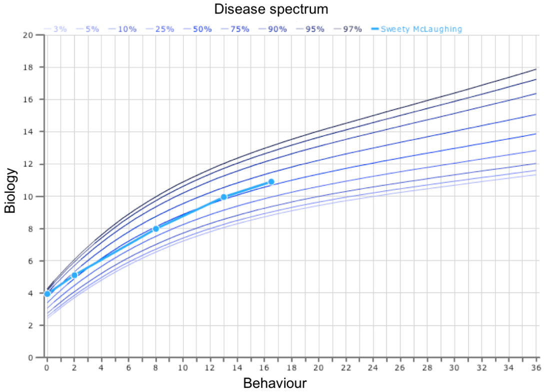
Burmeister et al. (2008)

Methods for addressing heterogeneity



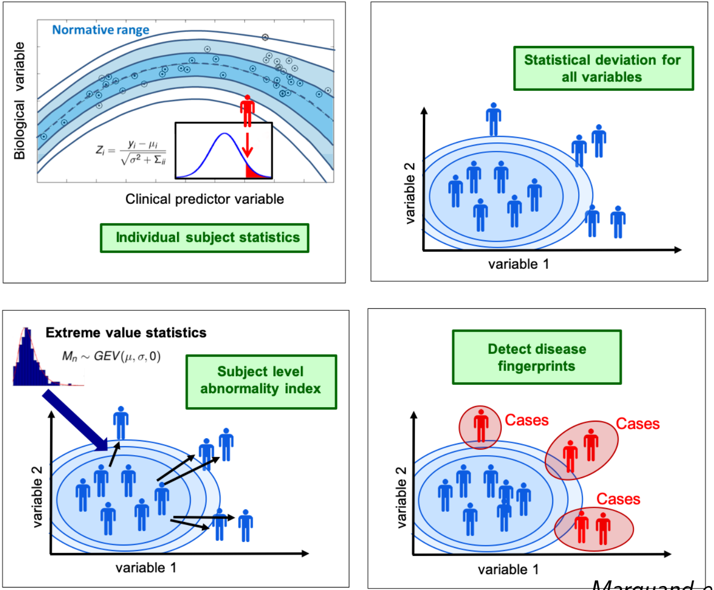
Dong et al. (2016); Zhang et al. (2016); Mourao-Miranda et al. (2011)

Normative modelling



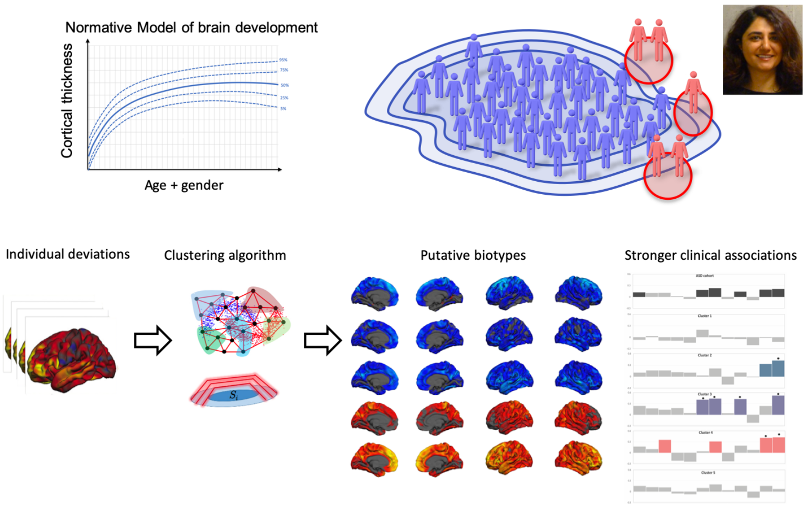
Marquand et al. (2016)

Normative modelling



Marquand et al. (2016)

Normative modelling of autism



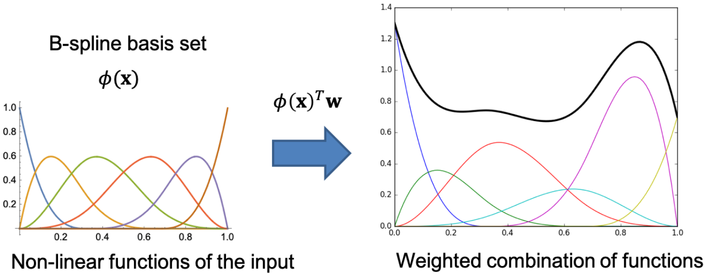
Zabihi et al. (2019)

Outline

Modelling non-linearity using Bayesian 'linear' regression

- A simple way to model non-linearity is to use a pre-specified basis expansion Φ (e.g. polynomials, RBF, B-spline)

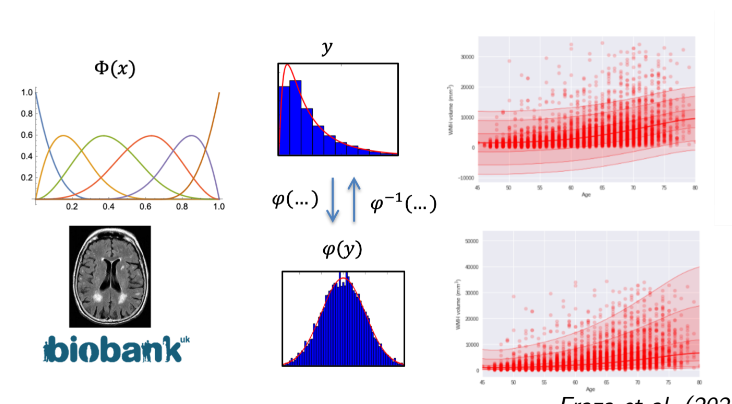
$$p(y|\boldsymbol{w}, \phi(\boldsymbol{x}), \sigma) \propto \mathcal{N}(y|\boldsymbol{\phi}(\boldsymbol{x})^T \boldsymbol{w}, \sigma)\mathcal{N}(\boldsymbol{w}|0, \boldsymbol{\Sigma_\theta})$$



Modelling non-Gaussianity

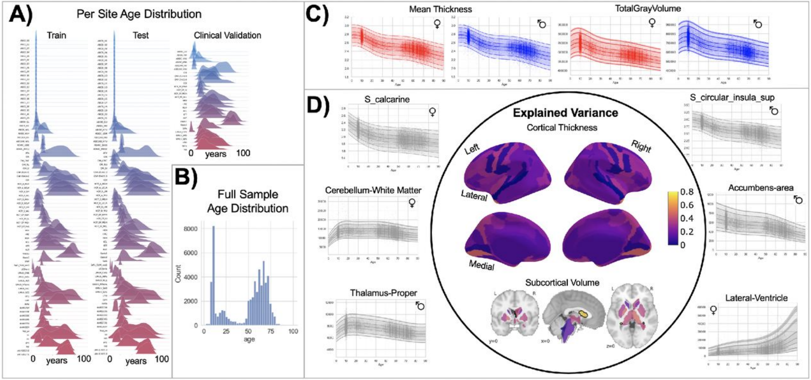
- One way to model non-Gaussian data is to 'warp' the data to a Gaussian space using a non-linear function $\varphi()$

$$p(\varphi(y)|\boldsymbol{w}, \phi(\boldsymbol{x}), \sigma) \propto \mathcal{N}(\varphi(y)|\phi(\boldsymbol{x})^T \boldsymbol{w}, \sigma)\mathcal{N}(\boldsymbol{w}|0, \boldsymbol{\Sigma_\theta})$$



Fraza et al. (2021)

Braincharts across the lifespan

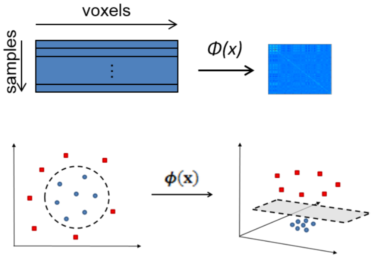


Tutorial: https://github.com/saigerutherford/CPC_ML_tutorial

Rutherford et al. (2021a,b)

Kernels

- Kernel methods (e.g. SVM, GPs) use the "kernel trick" to turn a linear model into a non-linear one



$$\max_{\alpha} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j \mathrm{x}_i^T \mathrm{x}_j$$

$$\text{s.t.:} \sum_i \alpha_i y_i = 0$$

$$0 \leq \alpha_i \leq C$$

- In the dual form, the data appear as an inner product, which can be substituted with a kernel function (e.g. RBF, linear)

$$\mathrm{x}_i^T \mathrm{x}_j \Rightarrow k(\mathrm{x}_i, \mathrm{x}_j) \Rightarrow \phi(\mathrm{x}_i)^T \phi(\mathrm{x}_j)$$

- linear operations on kernels also yield valid kernels, e.g.

$$k(\mathrm{x}, \mathrm{x}') = k_1(\mathrm{x}, \mathrm{x}') + 2k_2(\mathrm{x}, \mathrm{x}')k_3(\mathrm{x}, \mathrm{x}') + \dots$$

- This is the basis for *multi-kernel learning*

Multi-Kernel Learning

- Kernels can represent different modalities, different views or different regions

$$k(\mathrm{x}, \mathrm{x}') = \sum_{m=1}^{M} d_m k_m(\mathrm{x}, \mathrm{x}') \text{ with } d_m \geq 0 \text{ and } \sum_m d_m = 1$$

- Optimisation problem is a convex combination of kernels

$$\min_{\mathrm{w}} \frac{1}{2} \sum_{m=1}^{M} ||\mathrm{w}_m||^2 + C \sum_{i=1}^{n} \xi_i$$

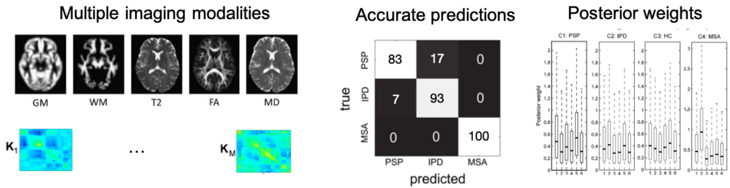
$$\text{subject to: } y_i\left(\sum_m (\mathrm{x}_i^T \mathrm{w}_m + b)\right) \geq 1 - \xi_i, \xi_i \geq 0 \; \forall i$$

$$\sum_m d_m = 1 \text{ and } d_m \geq 0$$

Applications of MKL in neuroscience

Multimodal data fusion for predicting brain disorders

$$p(y_{ic}|\mathrm{x}_1 \ldots \mathrm{x}_M) = \frac{\exp f_{ic}}{\sum_d \exp f_{id}} \qquad p(\mathrm{y}|\mathrm{x}_1 \ldots \mathrm{x}_M) = \mathcal{GP}(0, \mathrm{K}(\theta))$$

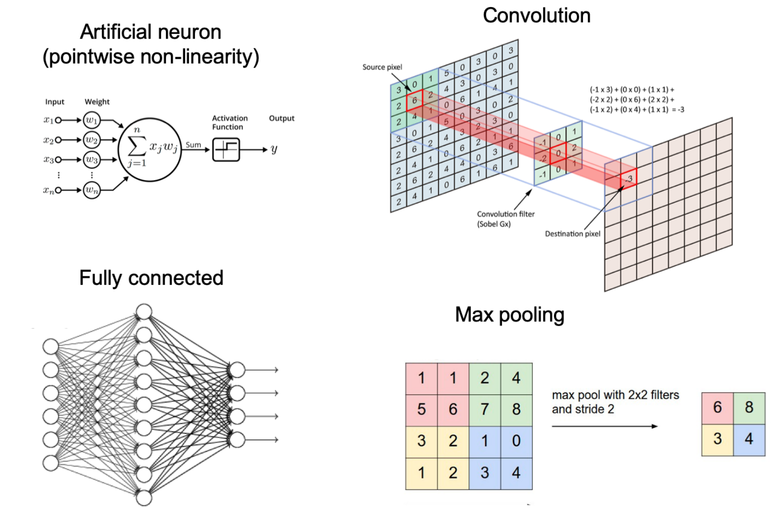


Filippone et al. (2012)

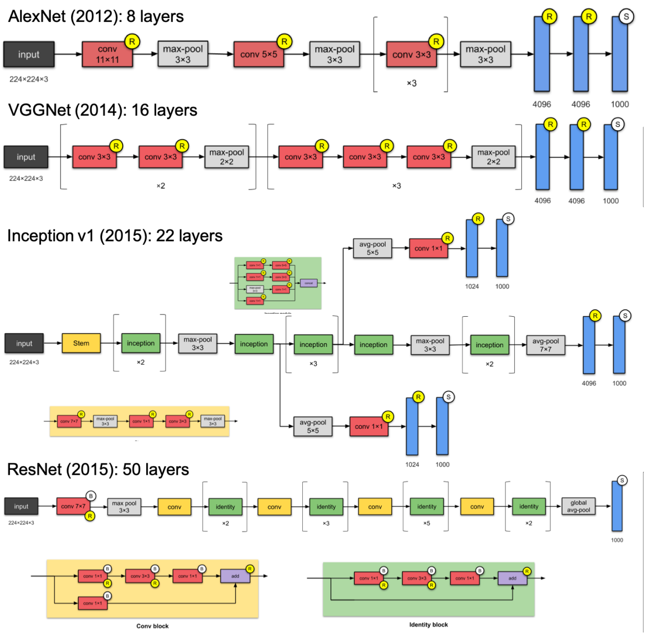
Deep Learning

It is helpful to think of deep learning as combining matix products with point-wise linearity, e.g.:

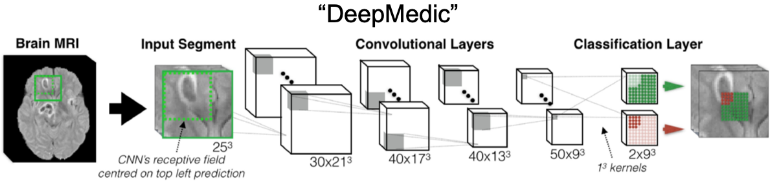
$$f(x) = \sigma(xW_1 + b_1)W_2$$

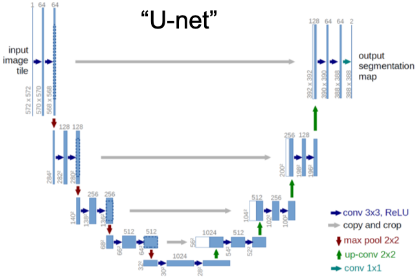


Convolutional Neural Networks



Deep Learning for Segmentation

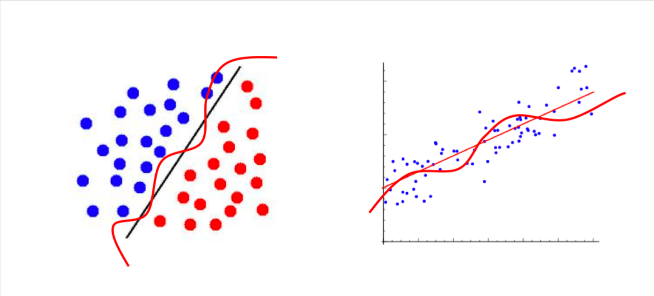




Kamnitsas et al. (2017); Ronneberger et al. (2015)

Overfitting (again)

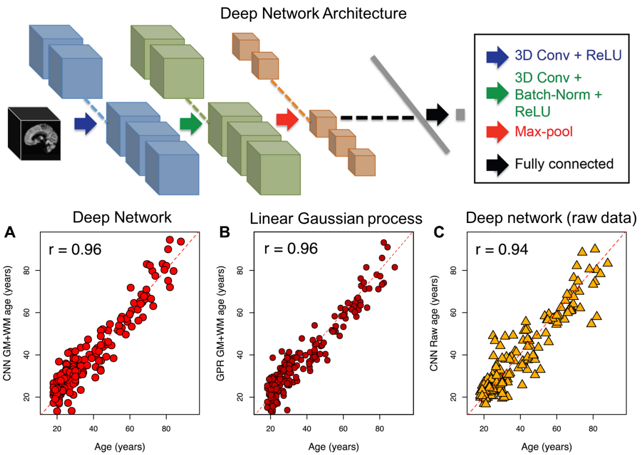
- But if your problem is linear, your fancy nonlinear algorithm will just overfit



- The more complex the model, the easier it is to overfit
- In complex (deep) models it is often not possible to properly optimise all parameters
- This makes validation extremely important!

Deep Learning in Neuroscience?

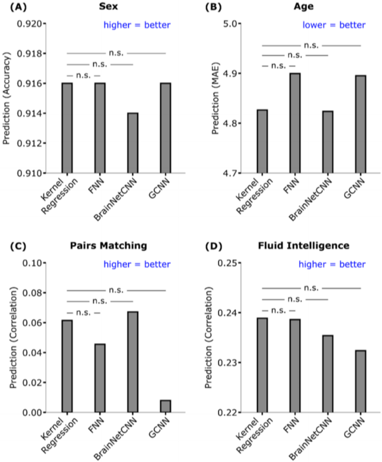
- Predict age from N= 2001 structural MRI images



- Similar performance to a linear model on preprocessed data
- Better performance on minimally processed data

Cole et al. (2017)

Deep Learning in Neuroscience?



He et al. (2019)

Deep Learning in Neuroscience?

New Results

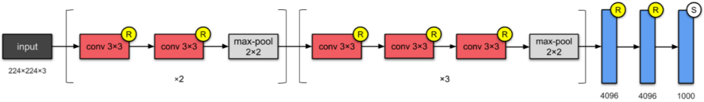
Comment on this paper

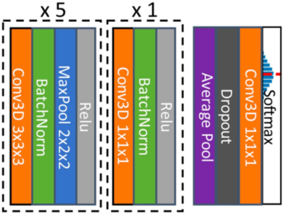
Accurate brain age prediction with lightweight deep neural networks

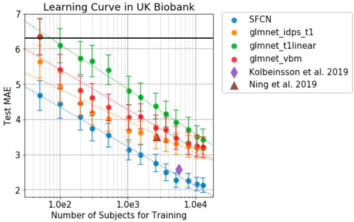
Han Peng, Weikang Gong, Christian F. Beckmann, Andrea Vedaldi, Stephen M. Smith

doi: https://doi.org/10.1101/2019.12.17.879346

This article is a preprint and has not been certified by peer review [what does this mean?].



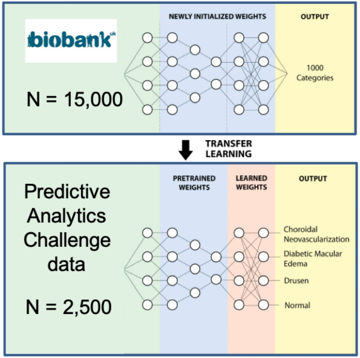




Won the 2019 PAC 'brainage' challenge

Peng et al. (2019)

Transfer Learning



- Basic idea: transfer knowledge (i.e. weights) from a large dataset to a small one (where it is harder to learn)
- Different variants depending on whether the targets are the same, similiar or different

Deep Learning in Medicine?

- Predict mortality from electronic health records

ARTICLE OPEN

Scalable and accurate deep learning with electronic health records

Alvin Rajkomar[1,2], Eyal Oren[1], Kai Chen[1], Andrew M. Dai[1], Nissan Hajaj[1], Michaela Hardt[1], Peter J. Liu[1], Xiaobing Liu[1], Jake Marcus[1], Mimi Sun[1], Patrik Sundberg[1], Hector Yee[1], Kun Zhang[1], Yi Zhang[1], Gerardo Flores[1], Gavin E. Duggan[1], Jamie Irvine[1], Quoc Le[1], Kurt Litsch[1], Alexander Mossin[1], Justin Tansuwan[1], De Wang[1], James Wexler[1], Jimbo Wilson[1], Dana Ludwig[2], Samuel L. Volchenboum[3], Katherine Chou[1], Michael Pearson[1], Srinivasan Madabushi[1], Nigam H. Shah[4], Atul J. Butte[2], Michael D. Howell[1], Claire Cui[1], Greg S. Corrado[1] and Jeffrey Dean[1]

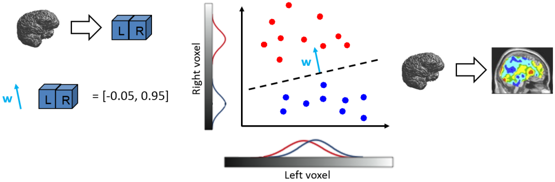
	Hospital A	Hospital B
Inpatient Mortality, AUROC[1](95% CI)		
Deep learning 24 hours after admission	**0.95**(0.94-0.96)	**0.93**(0.92-0.94)
Full feature enhanced baseline at 24 hours after admission	0.93 (0.92-0.95)	0.91 (0.89-0.92)
Full feature simple baseline at 24 hours after admission	0.93 (0.91-0.94)	0.90 (0.88-0.92)
Baseline (aEWS[2]) at 24 hours after admission	0.85 (0.81-0.89)	0.86 (0.83-0.88)
30-day Readmission, AUROC (95% CI)		
Deep learning at discharge	**0.77**(0.75-0.78)	**0.76**(0.75-0.77)
Full feature enhanced baseline at discharge	0.75 (0.73-0.76)	0.75 (0.74-0.76)
Full feature simple baseline at discharge	0.74 (0.73-0.76)	0.73 (0.72-0.74)
Baseline (mHOSPITAL[3]) at discharge	0.70 (0.68-0.72)	0.68 (0.67-0.69)
Length of Stay at least 7 days AUROC (95% CI)		
Deep learning 24 hours after admission	**0.86**(0.86-0.87)	**0.85**(0.85-0.86)
Full feature enhanced baseline at 24 hours after admission	0.85 (0.84-0.85)	0.83 (0.83-0.84)
Full feature simple baseline at 24 hours after admission	0.83 (0.82-0.84)	0.81 (0.80-0.82)
Baseline (mLiu[4]) at 24 hours after admission	0.76 (0.75-0.77)	0.74 (0.73-0.75)

Outline

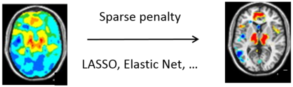
Mapping the discriminative pattern

For clinical applications it is crucial to infer which variables drive the predictions. There are multiple options:

- Regional classification accuracy as a proxy (searchlight)
- For linear models, the weights can be directly visualised ("discriminative mapping")



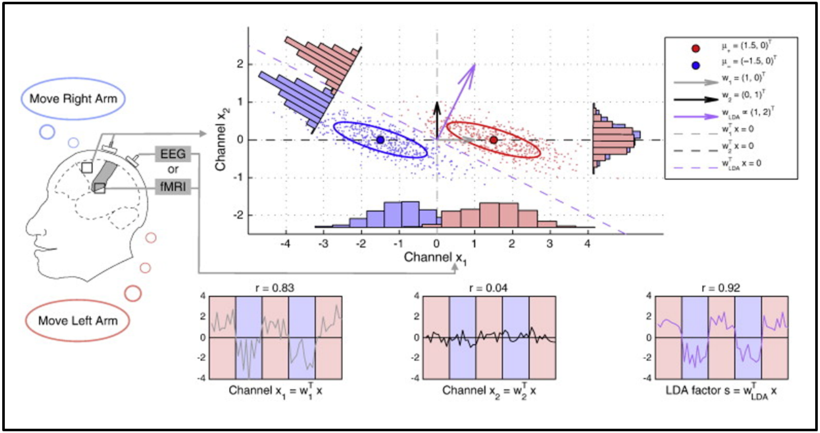
- Can also use regularization to enforce sparse weights



- Weights are often regarded as being difficult to interpret, but this is not always true

Weights do not reflect univariate differences

One proposal is to consider the the weights from a forward model



Construct 'forward maps' by premultiplying by the data covariance

$$a = \frac{1}{\sigma_y^2} \Sigma_x w$$

Haufe et al. (2014)

Understanding weights of discriminative models

- The correct interpretation of the weights is the contribution of each feature to the predictions. This is the same as in a GLM
- Difficulty arises only due to multicollinearity between predictor variables which inflates the variance of the weights
- A variable can have a high weight because:
  1. It is associated with the response variable
  2. It acts as a 'supressor' variable that helps to cancel out noise or mismatch in other covariates
- To distinguish between these possibilities, we can compute:

$$\mathrm{a} \propto \Sigma_x \mathrm{w} = \mathrm{cov}\left[\mathrm{X}, \hat{\mathrm{y}}\right] = \mathrm{corr}\left[\mathrm{X}, \hat{\mathrm{y}}\right]$$

- These are **structure coefficients** from multivariate statistics
- These measure the univariate association between covariate p and the predictions, i.e.:

$$\rho(\mathrm{x}_p, \hat{\mathrm{y}})$$

Kraha et al. (2012)

But what about the penalty?

- Collinearity is well-known in classical GLM settings, where advice is often given to avoid collinearity
- It is true that collinearity impacts on efficiency, but models with collinear predictors are still interpretable
- Collinearity also impacts penalised regression. Recall that:

$$f(\mathrm{x}_i, \mathrm{w}) = \mathrm{x}_i^T \mathrm{w} \qquad \Rightarrow \hat{\mathrm{w}} = \min_{\mathrm{w}} \sum_{i=1}^{n} \ell(y_i, f_i) + \lambda J(\mathrm{w})$$

- Considering ridge regression, where the objective function is:

$$\hat{\mathrm{w}} = \min_{\mathrm{w}} \sum_{i=1}^{n} \mathcal{N}(\mathrm{w}^T \mathrm{x}_i, \sigma^2) + \frac{\lambda}{2} ||\mathrm{w}||_2^2$$

- This is eqivalent to:

$$\min_{\mathrm{w}} -\frac{1}{2\sigma^2} \left(\sum_{i=1}^{n} (y_i - \mathrm{x}_i^T \mathrm{w})^2 + \lambda \mathrm{w}^T \mathrm{w} \right)$$

But what about the penalty?

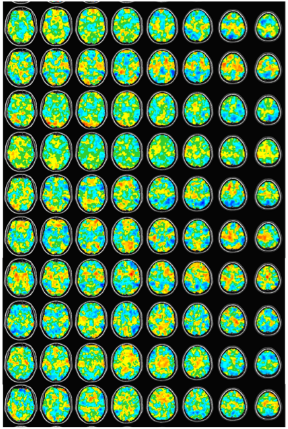
- This is exactly equivalent to finding the MAP estimate of a posterior distribution over w, with prior:

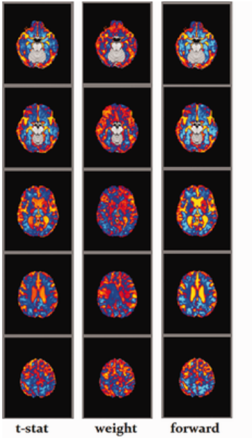
$$\mathcal{N}(0, \sigma^2/\lambda \mathrm{I})$$

So what does this mean?

- Collinearity influence the magnitude and sign of coefficients
- Including/excluding variables can change both magnitude and sign of coefficients
- When $p > n$, the problem is ill-posed (multiple ways the same prediction can be achieved).
- Regularisation helps to stabilise coefficients, but does not eliminate the problem

Examples of weights





Aksman et al. (2016)

Outline

Take home messages

- Machine learning provides powerful tools for single subject inference and detect spatially distributed effects
- Many different approaches beyond simple notions such as ‘classification’ or ‘clustering’

Recommendations

- Linear models are often sufficient: they are fast, interpretable and often perform as well as non-linear methods
- Careful validation is extremely important for all methods to guard agains overfitting
- Machine learning can be easily integrated with neurocognitive models (e.g. to assess candidate models)

Acknowledgments

Mariam Zabihi

Richard Dinga

Thomas Wolfers

Saige Rutherford

Charlotte Fraza

Predictive Clinical Neuroscience Lab

Seyed Mostafa Kia

We are hiring!

Tutorial on Normative modelling:

https://github.com/saigerutherford/CPC_ML_tutorial

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