Advanced machine learning for neuroimaging

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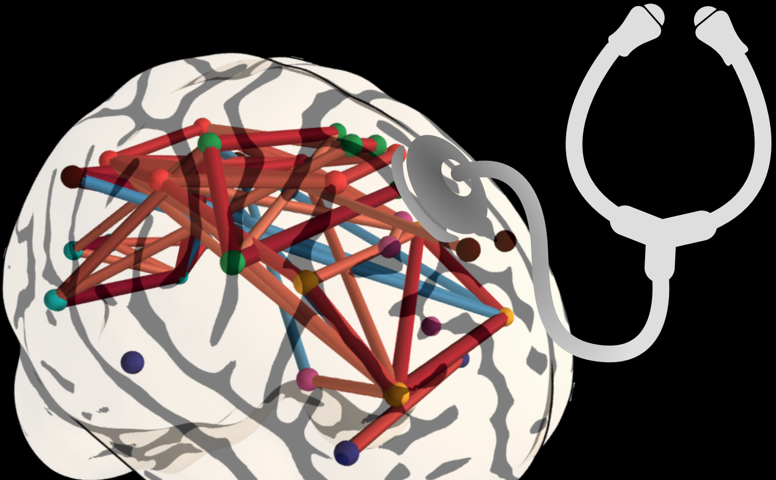
McGill Inria



1. Large scale
2. Some advanced estimators
3. Advanced learners on brain images
4. Machine learning principles

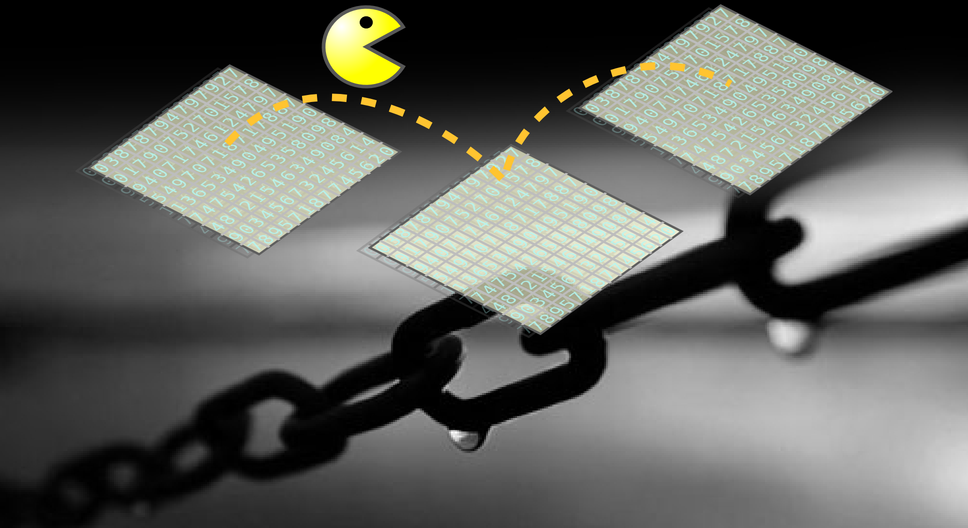
1 Large scale

Difficulty: the data do not fit in memory

See also: http://www.slideshare.net/GaelVaroquaux/processing-biggish-data-on-commodity-hardware-simple-python-patterns

1 On-line algorithms

```
estimator.partial_fit(X_train, Y_train)
```



1 On-line algorithms

```
estimator.partial_fit(X_train, Y_train)
```

Linear models

```
sklearn.linear_model.SGDRegressor
sklearn.linear_model.SGDClassifier
```

SGD = Stochastic gradient descent

Different losses, different penalties   learning rate ☹

1 On-line algorithms

```
estimator.partial_fit(X_train, Y_train)
```

Linear models

sklearn.linear_model.SGDRegressor
sklearn.linear_model.SGDClassifier

Clustering

sklearn.cluster.MiniBatchKMeans
sklearn.cluster.Birch (new in 0.16)

PCA (new in 0.16)

sklearn.decompositions.IncrementalPCA

1 On-the-fly data reduction

Many features

⇒ Reduce the data as it is loaded

```
X_small = estimator.transform(X_big, y)
```

1 On-the-fly data reduction

Random projections (will average features)

```
sklearn.random_projection
```

random linear combinations of the features

Fast clustering of features

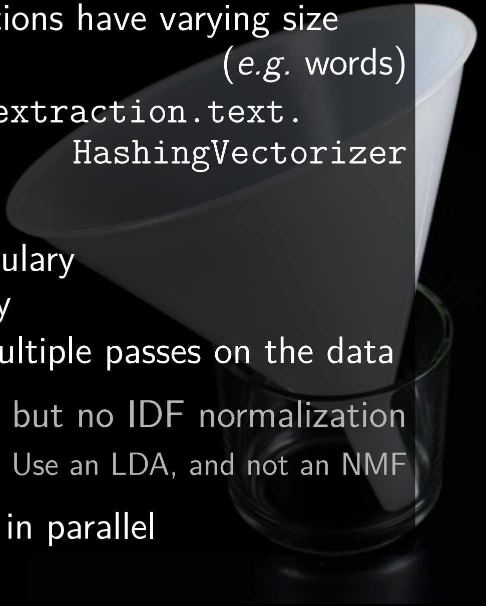
```
sklearn.cluster.FeatureAgglomeration
```

on images: super-pixel strategy

Hashing when observations have varying size (*e.g.* words)

```
sklearn.feature_extraction.text.
    HashingVectorizer
```

1 On-the-fly data reduction



Hashing when observations have varying size (*e.g.* words)

`sklearn.feature_extraction.text.HashingVectorizer`

TF-IDF needs

- to know the vocabulary
- to count everybody

$\Rightarrow$ multiple passes on the data

Hashing avoids that but no IDF normalization

Use an LDA, and not an NMF

\+ stateless: can be used in parallel

2 Some advanced estimators

[Neurosynth, Neuroquery]

Linear estimators

- Can handle large number of features
- Typically a logistic regression

`sklearn.linear_model.LogisticRegression`
`sklearn.linear_model.LogisticRegressionCV`

'l2' and 'l1' penalties different solvers

`sklearn.linear_model.SGDClassifier`

For on-line estimator

Naive Bayes

- Very good for many classes
- On-line estimator

+ chi2 feature selection

2 For heterogeneous columnar data

Priceless for tabular data *eg* socio-demographics

- Tree methods are good:

  robust to strange data distributions

- Ensemble methods: need to combine many trees

Random forests

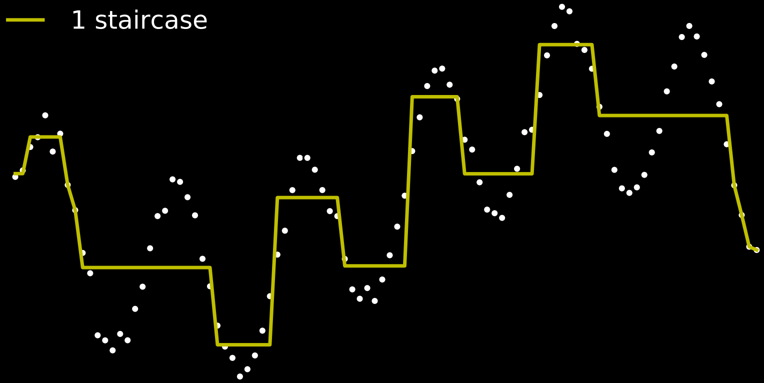
```
sklearn.ensemble.RandomForestClassifier
sklearn.ensemble.ExtraTreesClassifier
```

Boosted trees

```
sklearn.ensemble.HistGradientBoostingClassifier
```

Native support for missing values

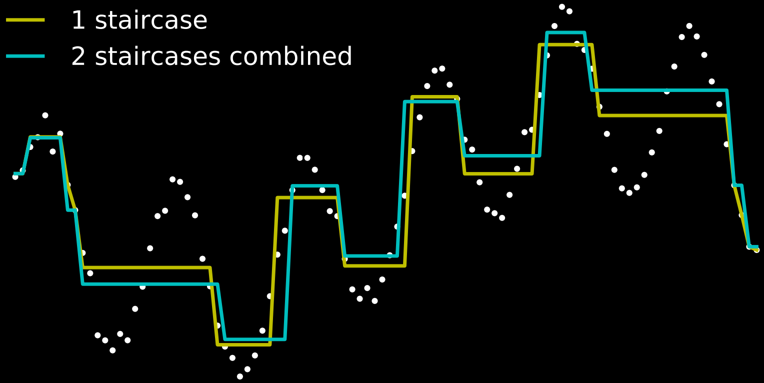
2 Gradient-boosted regression trees



- Fit with a tree of depth 10

staircase of 10 constant values

2 Gradient-boosted regression trees



- Fit with a tree of depth 10

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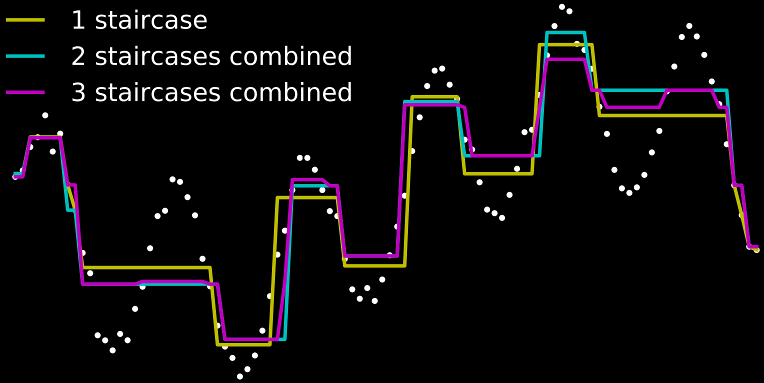
- Fit a new tree on errors

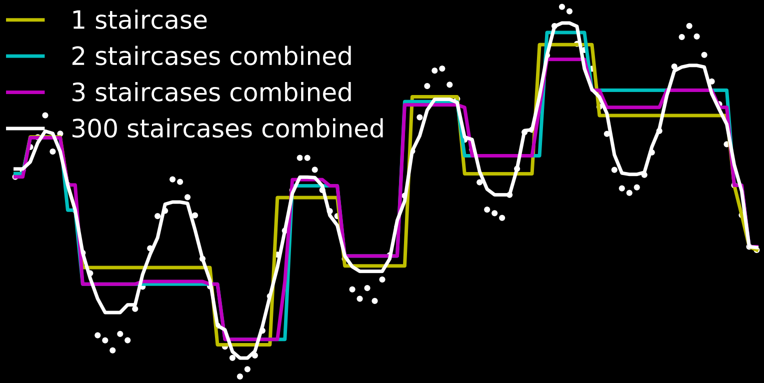
Gradient-boosted regression trees



- Fit with a tree of depth 10

  staircase of 10 constant values

- Fit a new tree on errors
- Keep going



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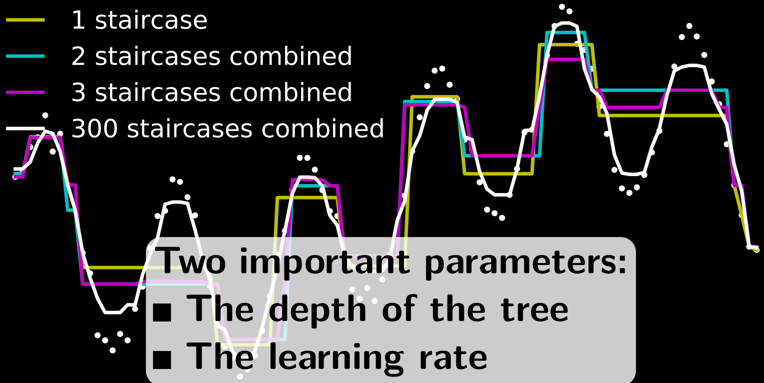
Boosted regression trees



Two important parameters:
- **The depth of the tree**
- **The learning rate**

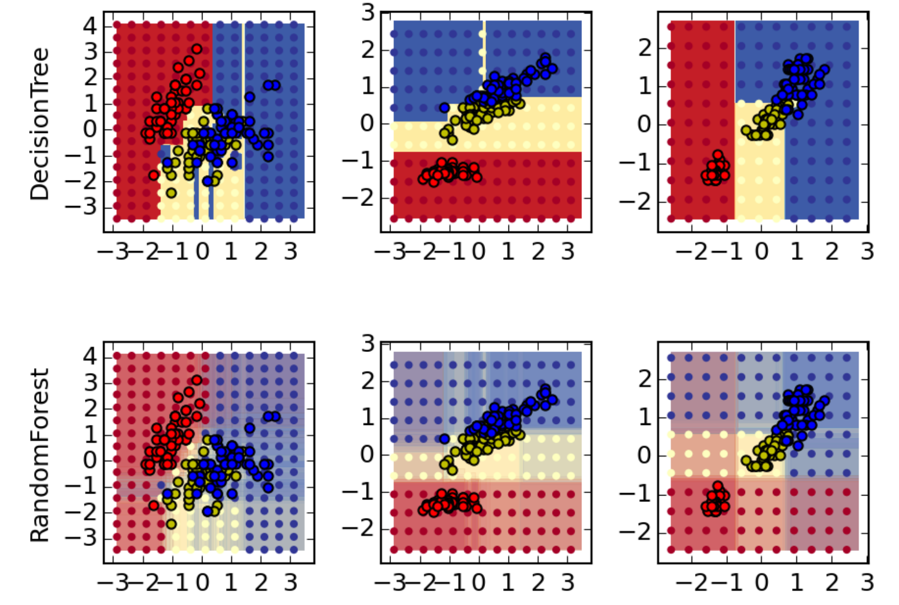
- Fit with a tree of depth 10

staircase of 10 constant values

- Fit a new tree on errors
- Keep going

Boosted regression trees

2 2D intuitions & model averaging



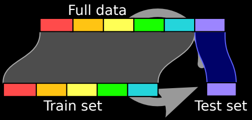
$$x \xrightarrow{\text{model}_1} z \xrightarrow{\text{model}_1} y$$

Learn model$_1$ separately

Directly supervising z:

$z = \hat{y}$ for a (simple) predictive model

Trick: "cross-fit" during training



obtain $\hat{y}$ by splitting the training data

Just use `sklearn.ensemble.StackingRegressor`

Useful to assemble non-linear models from simple ones

Gender	Date Hired	Employee Position Title
M	09/12/1988	Master Police Officer
F	NA	Social Worker IV
M	07/16/2007	Police Officer III
M	01/13/2014	Electrician I
M	04/28/2002	Bus Operator
M	NA	Bus Operator
F	06/26/2006	Social Worker III
F	01/26/2000	Library Assistant I
M	NA 2014	Library Assistant I

Model a) a complete data-generating process
b) a random process occluding entries

Missing at random situation (MAR)

Theorem [Rubin 1976], if for non-observed values, the probability of missingness does not depend on this non-observed value. maximizing likelihood for observed data while **ignoring** the unobserved values gives maximum likelihood of model a).

MCAR: Missing Completely At Random:
missingness independent of **X**

Missing Not at Random situation (MNAR)
Missingness **not ignorable**

Model a) a complete data-generating process
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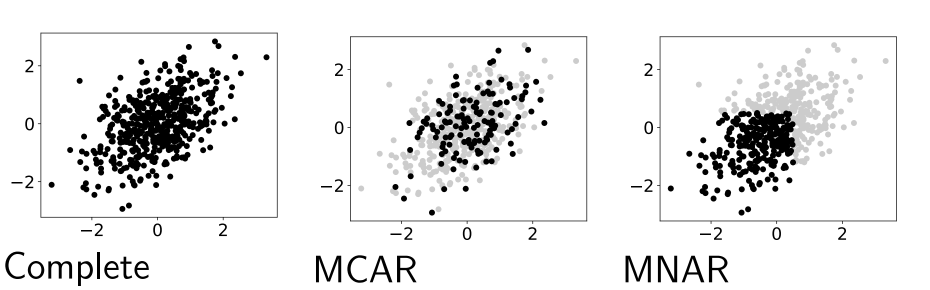

MCAR: Missing Completely At Random:
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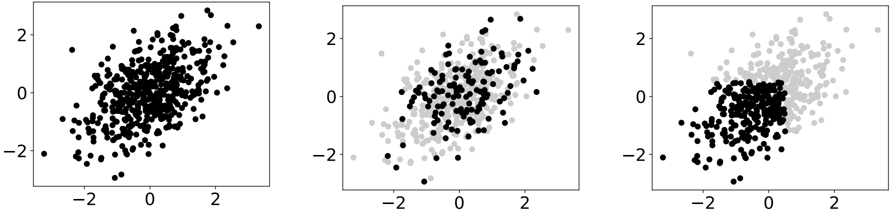
Missing Not at Random situation (MNAR)
Missingness **not ignorable**

2 Classic statistics on missing values

Model a) a complete data-generating process

b) a random process occluding entries



Complete MCAR MNAR

MCAR: Missing Completely At Random

But

- MAR is not frequent
- Machine learning is not about maximizing likelihoods

Missingness **not ignorable**

Fill in information

Gender	Date Hired	Employee Position Title
M	09/12/1988	Master Police Officer
F	~~NA~~ 2000	Social Worker IV
M	07/16/2007	Police Officer III
M	01/13/2014	Electrician I
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Mean imputation special case of univariate imputation

Replace `NA` by the mean of the feature

`sklearn.impute.SimpleImpute`

Mean imputation special case of univariate imputation

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`sklearn.impute.SimpleImpute`

Conditional imputation

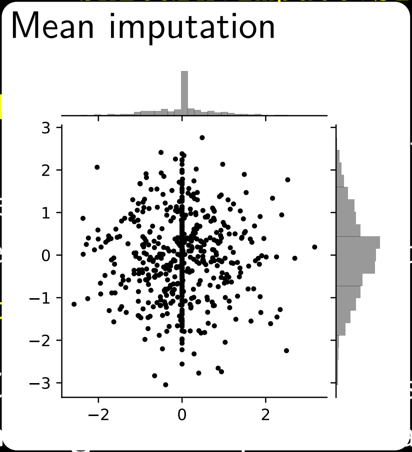
- Modeling one feature as a function of others
- Possible implementation:
  iteratively predict one feature as a function of other
  `sklearn.impute.IterativeImputer`

Statistics: Conditional imputation considered richer
Machine learning mean imputation can be detected by non-linear learners [Josse... 2019]

Mean imputation special case of univariate imputation

Replace `NA` by the mean of the feature

`sklearn.impute.SimpleImpute`



Conditional im

- Modeling one ... thers
- Possible imple

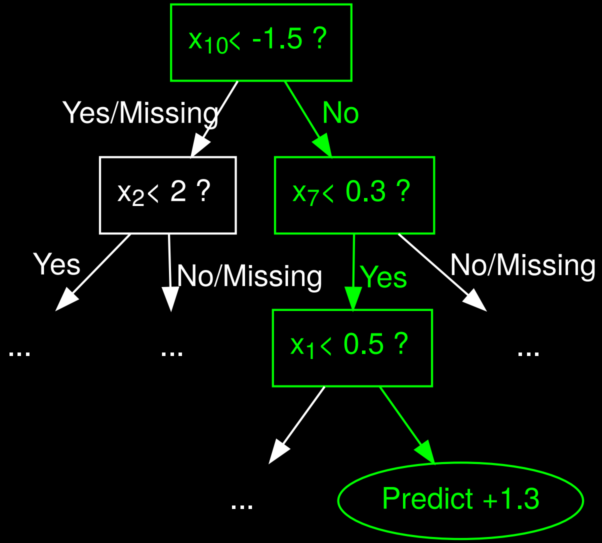
iterately pre ... tion of other

`sklearn.imp`

Statistics: C ... sidered richer

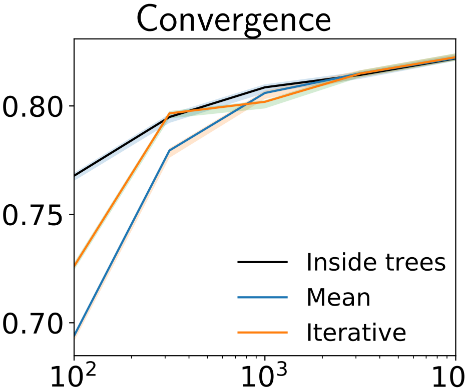
Machine lea ... an be detected by non-linear learners [Josse... 2019]

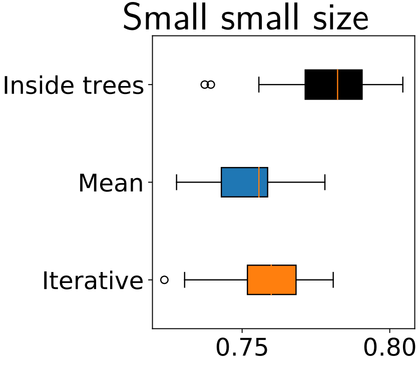
MIA (Missing Incorporated Attribute) [Josse... 2019]



`sklearn.ensemble.HistGradientBoostingClassifier`

Simulation: MCAR + Gradient boosting





Notebook: github – @nprost / supervised_missing

Pathological case [Josse... 2019]

y depends only on wether data is missing or not

eg tax fraud detection

theory: MNAR = “Missing Not At Random”

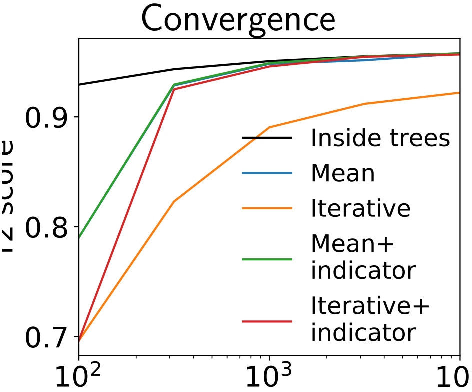
⚠ Imputing makes prediction impossible ⚠

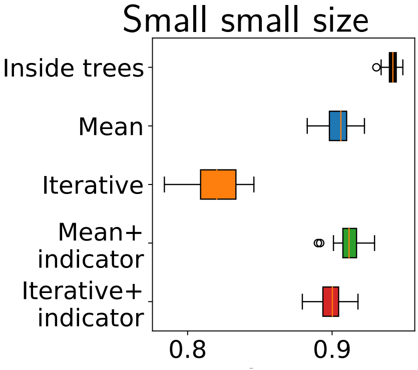
Solution

Add a missingness indicator: extra feature to predict

```
...SimpleImpute(add_indicator=True)
...IterativeImputer(add_indicator=True)
```

Simulation: **y** depends *indirectly* on missingness
censoring in the data





Notebook: github – @nprost / supervised_missing

- **Adding a mask is crucial**
- **Iterative imputation can be detrimental**

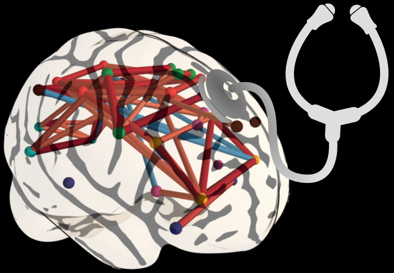
Recommendations

- High-dimensional settings ($p > 1\,000$):
  use linear models
- Lower dimensions, large n ($n > 1\,000$):
  use gradient-boosted trees

- Ensembling reduces variance

- Missing values with linear models: iterative imputer
- Missing values with trees: MIA (native support)

3 Advanced learners on brain images

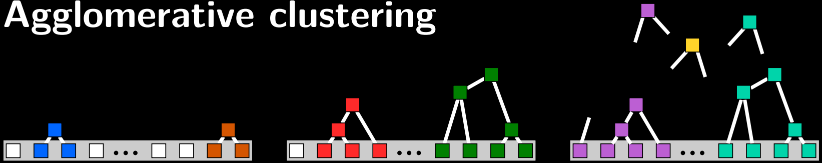


Challenge: many features

Learn feature groups by clustering

- Fast clustering for large k

Agglomerative clustering

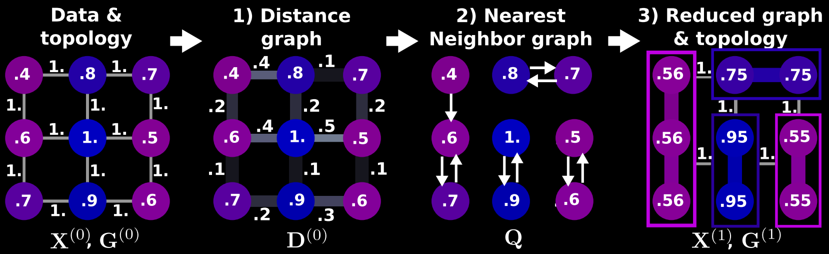


`sklearn.cluster.FeatureAgglomeration`

Choose Ward clustering for best results

[Michel... 2012]

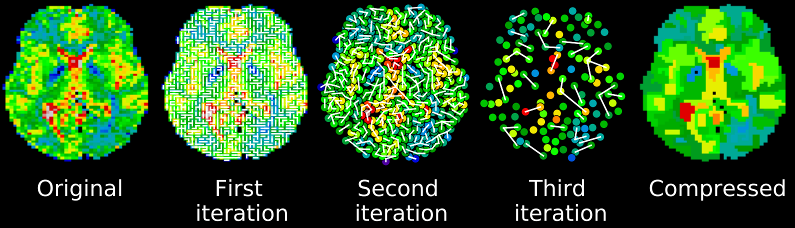
3 ReNA: fast spatial clustering



Very fast with spatial constraints

[Hoyos-Idrobo... 2018a]

ReNA: fast spatial clustering



1. Compute distance on neighborhood graph
2. Assign each vertex to its nearest neighbor on the graph
3. Connect components of graph are next features

Rinse and repeat

`nilearn.regions.Parcellations`

[Hoyos-Idrobo... 2018a]

3 **Fast spatial penalties** (FREM) [Hoyos-Idrobo... 2018b]

- Very fast sub optimal models
- Average many of them

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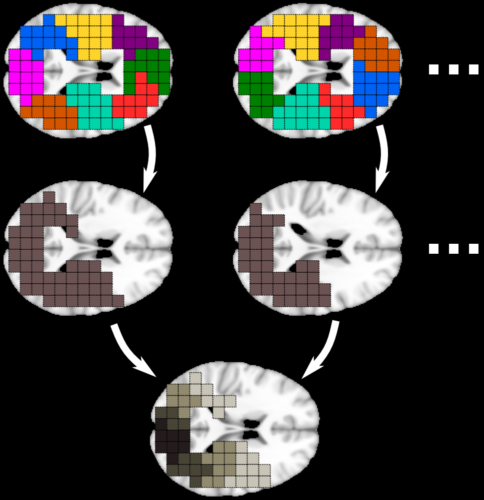
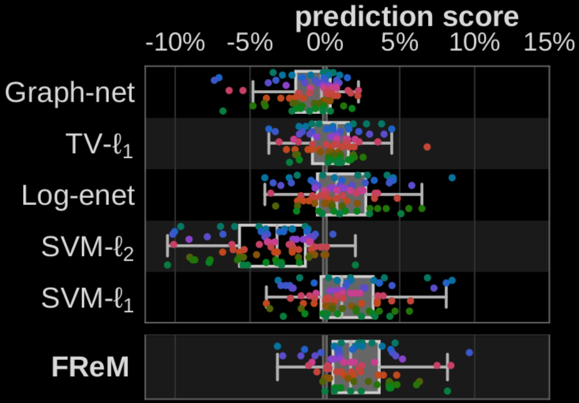


- Learn parcellation on perturbed data
- Estimate linear models

Average the results

- Very fast sub optimal models
- Average many of them



3 Fast spatial penalties (FREM) [Hoyos-Idrobo... 2018b]

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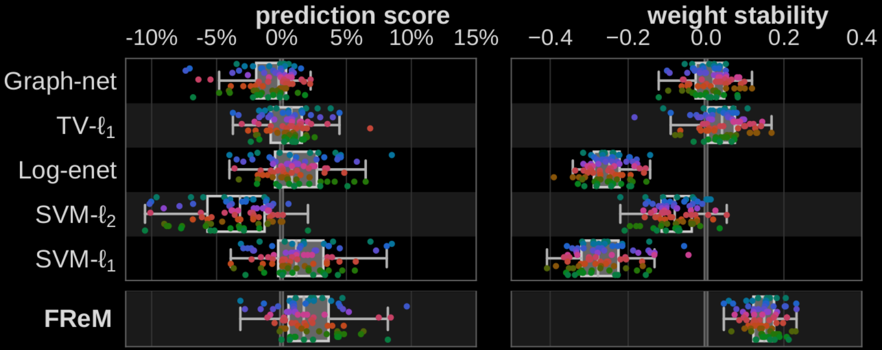

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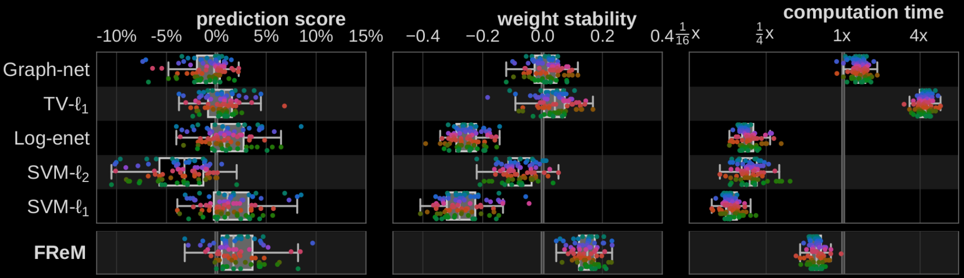


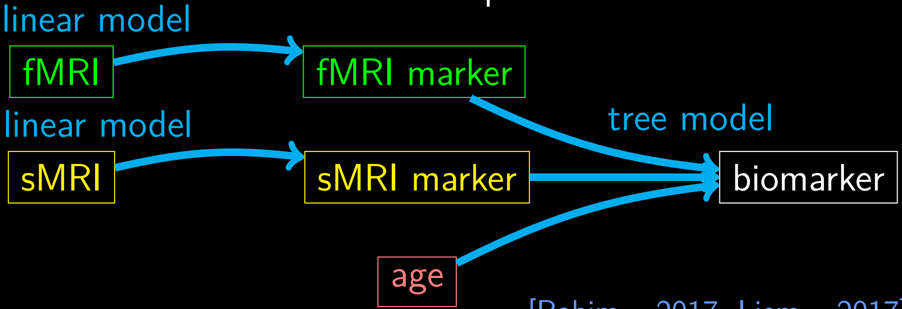
3 Stacking, multimodal non-linear models

Modality-specific linear models

- On each imaging modality fit a linear model

Non-linear model stacking

- Combine the **predicted** outcome values with other clinical variables as the input of tree-based model



[Rahim... 2017, Liem... 2017]

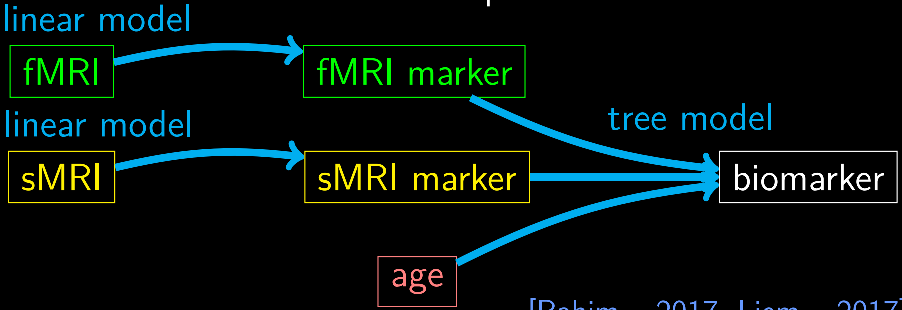
Modality-specific linear models

- On each imaging modality fit a linear model

Non-linear model stacking

[Engemann... 2020]: missing-value support in trees for subjects with only part of the modalities.

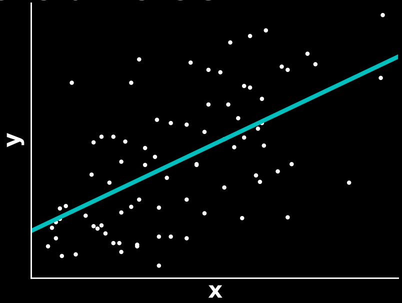
as the input of tree-based model



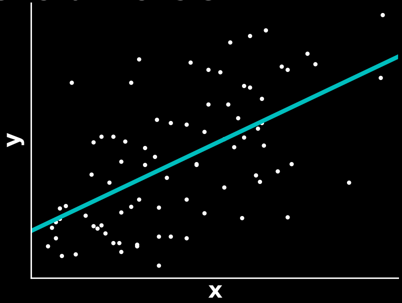
[Rahim... 2017, Liem... 2017]

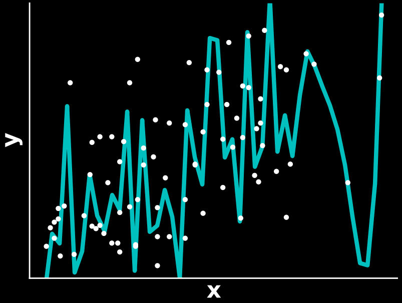
4 Machine learning principles

A single descriptor: one dimension



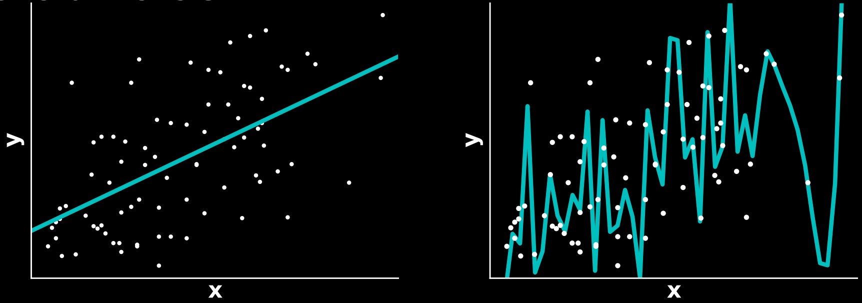
A single descriptor: one dimension





Which model to prefer?

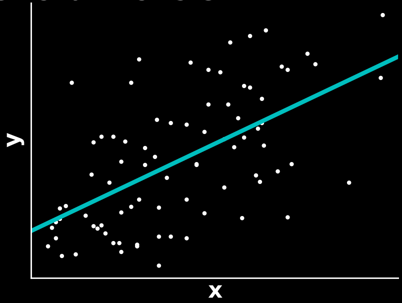
A single descriptor: one dimension

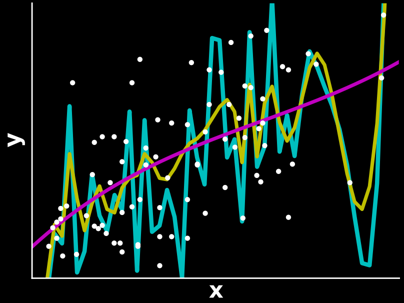


Problem of *"over-fitting"*

- Minimizing error is not always the best strategy (learning noise)
- Test data $\neq$ train data

A single descriptor: one dimension



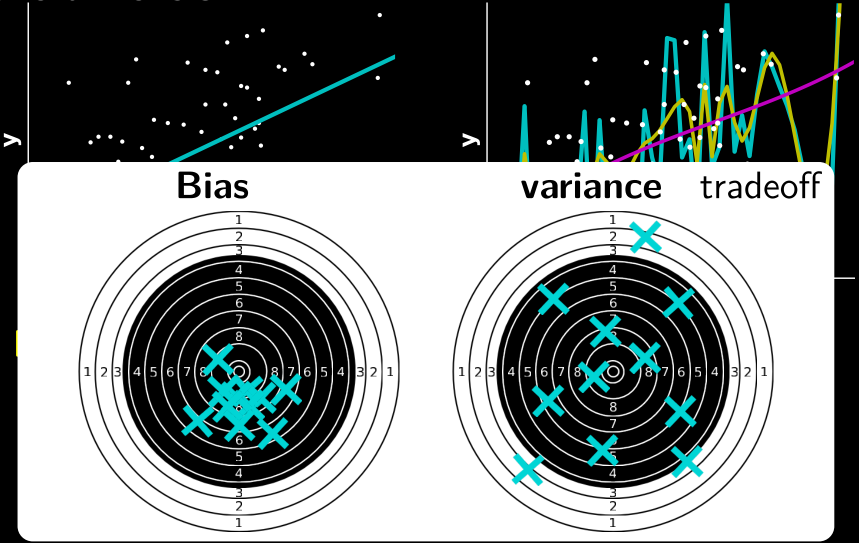


Prefer simple models

= concept of *"regularization"*

Balance the number of parameters to learn with the amount of data

A single descriptor: one dimension



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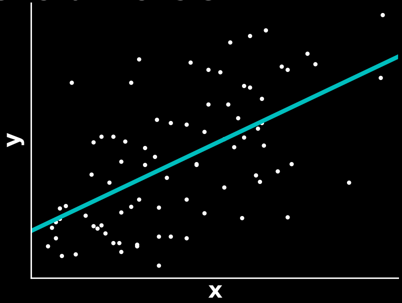
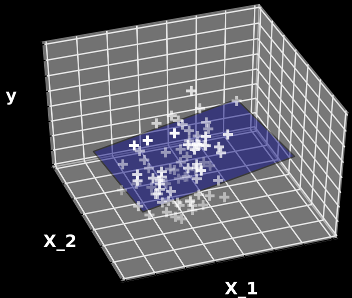
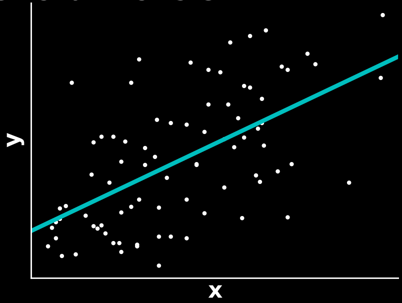


Two descriptors: 2 dimensions



More parameters

A single descriptor: one dimension



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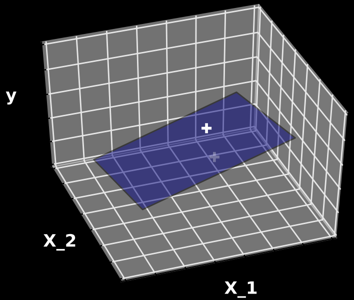

More parameters

⇒ Model with more parameters need much more data

"curse of dimensionality"

- Given n pairs $(x, y) \in \mathcal{X} \times \mathcal{Y}$ drawn *i.i.d.*
  find a function $f : \mathcal{X} \rightarrow \mathcal{Y}$ such that $f(x) \approx y$

  Notation: $\hat{y} \stackrel{\text{def}}{=} f(x)$

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Empirical risk minimization

- Given a “loss” function $l : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$
- Estimation of f: $$f^\star = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \, \mathbb{E}\big[l(\hat{y}, y)\big]$$

Can create f such that $\hat{y} = \mathbb{E}[\mathbf{y}|\mathbf{X}]$

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Empirical risk minimization

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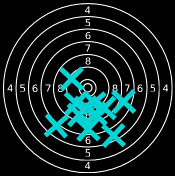
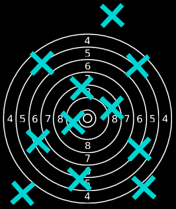
  Can create f such that $\hat{y} = \mathbb{E}[\mathbf{y}|\mathbf{X}]$

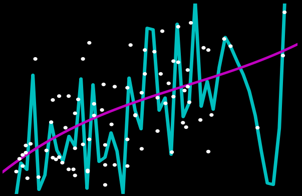
The inference & control is on f, not parameters

In general, f can be anything (choice of $\mathcal{F}$)

4 **Some formalism**: bias and regularization



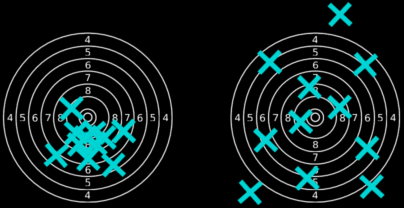


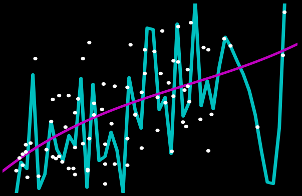


Settings: data $(\mathbf{X}, \mathbf{y})$, prediction $\mathbf{y} \sim f(\mathbf{X}, \mathbf{w})$

Our goal: $\underset{\mathbf{w}}{\text{minimize}} \quad \|\mathbf{y} - f(\mathbf{X}, \mathbf{w})\|$

4 **Some formalism**: bias and regularization





Settings: data $(\mathbf{X}, \mathbf{y})$, prediction $\mathbf{y} \sim f(\mathbf{X}, \mathbf{w})$

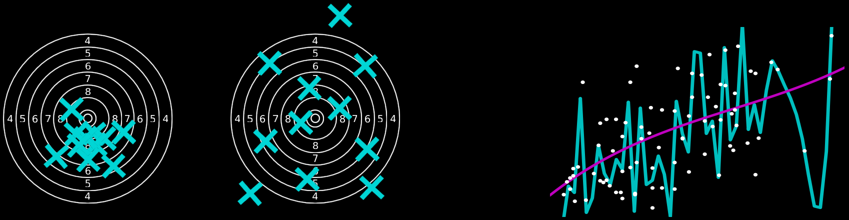
Our goal: $\underset{\mathbf{w}}{\text{minimize}}\ \mathbb{E}\big[\|\mathbf{y} - f(\mathbf{X}, \mathbf{w})\|\ \big]$

We only can measure $\|\mathbf{y} - f(\mathbf{X}, \mathbf{w})\|$

Prediction is very difficult, especially about the future.

Niels Bohr

4 Some formalism: bias and regularization



Settings: data $(\mathbf{X}, \mathbf{y})$, prediction $\mathbf{y} \sim f(\mathbf{X}, \mathbf{w})$

Our goal: $\underset{\mathbf{w}}{\text{minimize}}\ \mathbb{E}[\|\mathbf{y} - f(\mathbf{X}, \mathbf{w})\|\ ]$

We only can measure $\|\mathbf{y} - f(\mathbf{X}, \mathbf{w})\|$

Solution: bias $\mathbf{w}$ to push toward a plausible solution

In a minimization framework:

$$\underset{\mathbf{w}}{\text{minimize}}\ \|\mathbf{y} - f(\mathbf{X}, \mathbf{w})\| + p(\mathbf{w})$$

Going further

- Scipy lecture notes:
  `http://www.scipy-lectures.org`

  In particular chapter on statistics

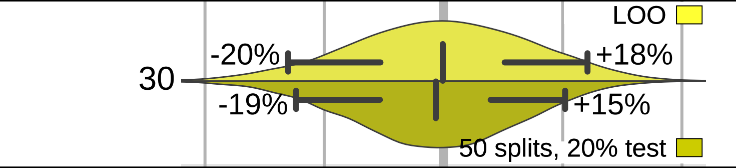
- The scikit-learn documentation:
  `http://scikit-learn.org`

  It's a reference on machine learning

- `nilearn`

@GaelVaroquaux

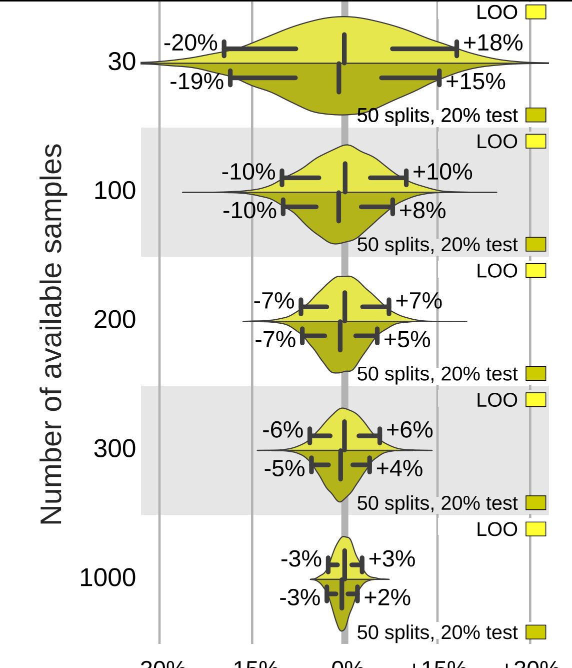
4 Careful with evidence for generalization



Sampling distribution of test error for $n = 30$

[??]

4 Careful with evidence for generalization

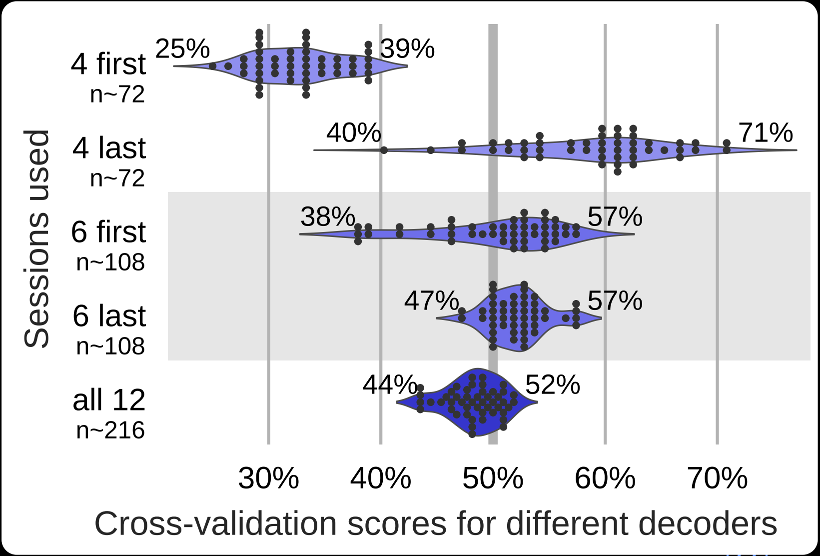


[??]

4 Careful with evidence for generalization

Trivial analytic variations on a permuted data:

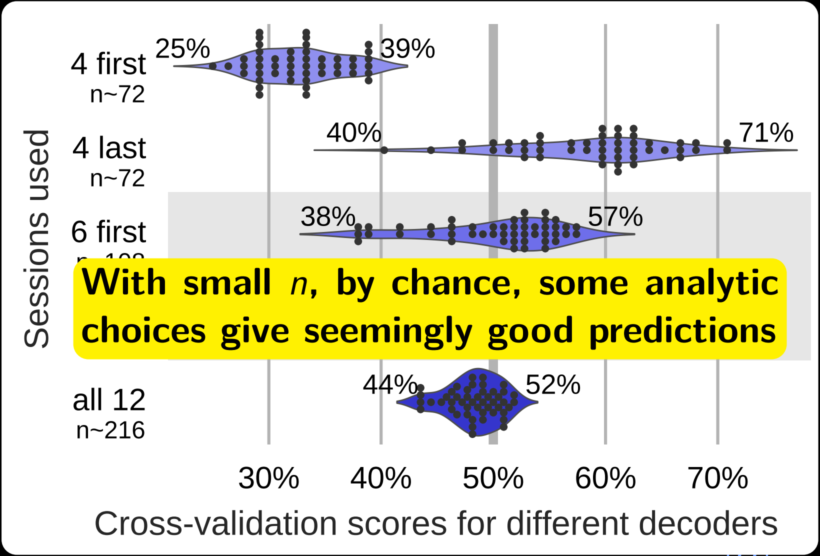
smoothing, SVM vs log-reg, feature selection



4 Careful with evidence for generalization

Trivial analytic variations on a permuted data:

smoothing, SVM vs log-reg, feature selection

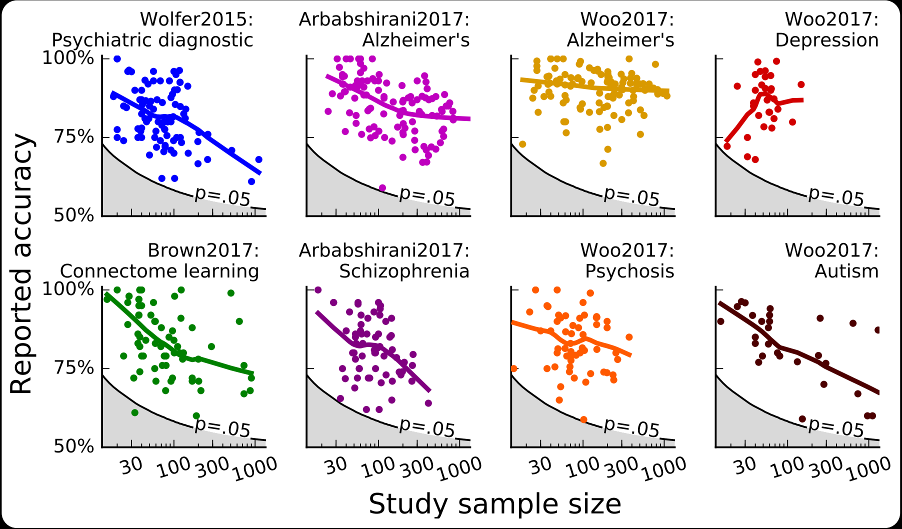


With small *n*, by chance, some analytic choices give seemingly good predictions

[: :]

4 Careful with evidence for generalization

In the literature, effect sizes decrease with sample sizes



[??]

5 References I

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