“Difficult” datasets

Feature selection, evaluation metrics, and class imbalance

Quick detour: MONAI

MONAI (https://monai.io)

- “A set of open-source, freely available collaborative frameworks built for accelerating research and clinical collaboration in Medical Imaging”
- Support for handling medical imaging formats (DICOM, etc.)
- Support for data anonymization
- Integration with tools, used by clinicians, for manual segmentation and labelling of images
- Support for distributed processing
- "Model Zoo": an incredibly broad and up-to-date of pre-trained (on public datasets) models (often, winners of specific challenges)

Feature selection

So many features

- In business, companies now collect large amounts of information on their customers and products
- In pharmaceutical research, thousands of features for each compound using quantitative structure-activity relationship (QSAR) methodology
- In biology, a vast array of biological predictors can be measured - *e.g.*, the “Omics” (genomics, proteomics, metabolomics, metagenomics, phenomics and transcriptomics)

What is feature selection?

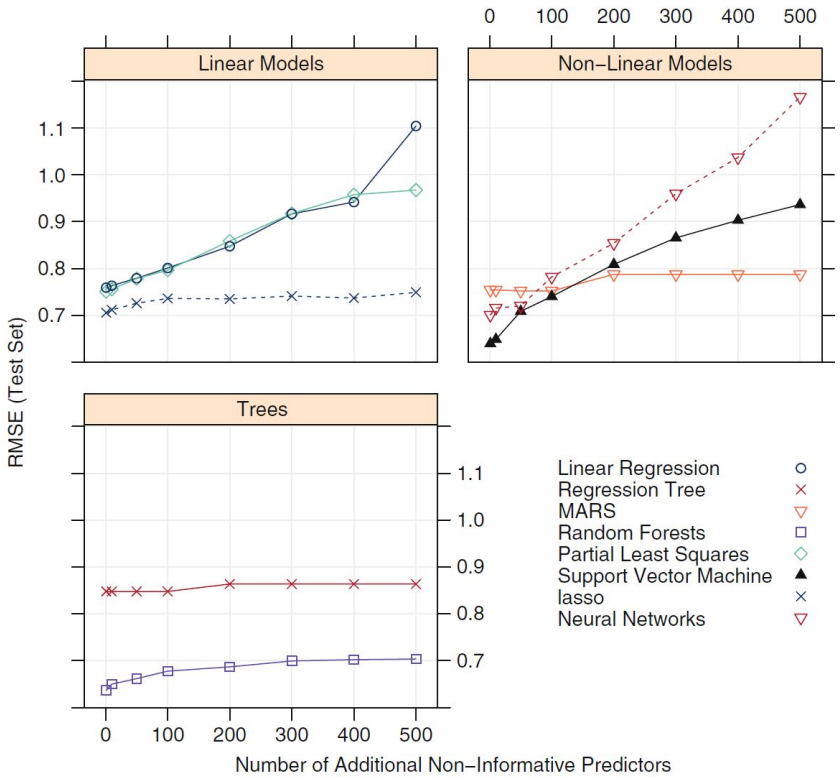
Choose the “best” subset of features (among the 2^P - P is the total number of features) for fitting our model

Types of “useless” features

- Non-informative features
  - Basically, such features do not “correlate” with what you want to predict (*e.g.*, the number of your credit card is probably useless to determine your cancer risk)
  - In your model, they would act as “pure noise”
- Redundant features
  - Some features are highly correlated (*e.g.*, weight and height)
  - Redundancy leads to more complex models (more parameters) yet adds little information
  - Highly unstable models, numerical errors, and degraded predictive performance
- We want to sort features according to their usefulness
  - Almost always, we can’t say: “this is non-informative/redundant. Period.”
  - We can try to say: this is more informative than this
  - Or, better: this is the set of features that work best together
- Many features + little data means discarding even very good features
  - In exchange, hopefully, for even better ones

Worse than useless

Adding non-informative features (predictors) degrades performance in many models



Classes of feature selection methods

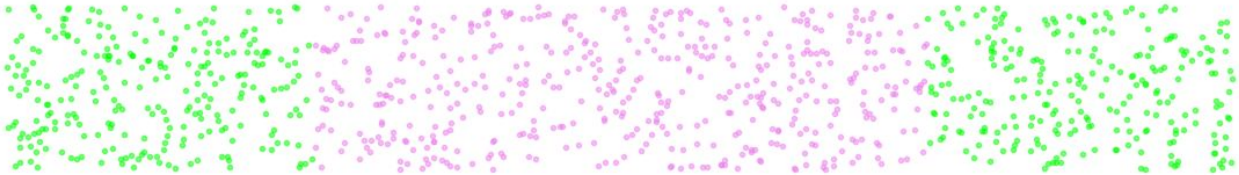
- Model agnostic methods (filters)
  - Computationally efficient
  - Many drawbacks
  - Basically, they are **no longer used** (except for exploratory analysis)
- Regularization methods (embedded)
  - Based on simple models
  - Computationally efficient
  - Yet quite powerful
- Model-based methods (wrappers)
  - Powerful, but computationally demanding
  - Higher risk of overfitting

“Unsupervised” filters

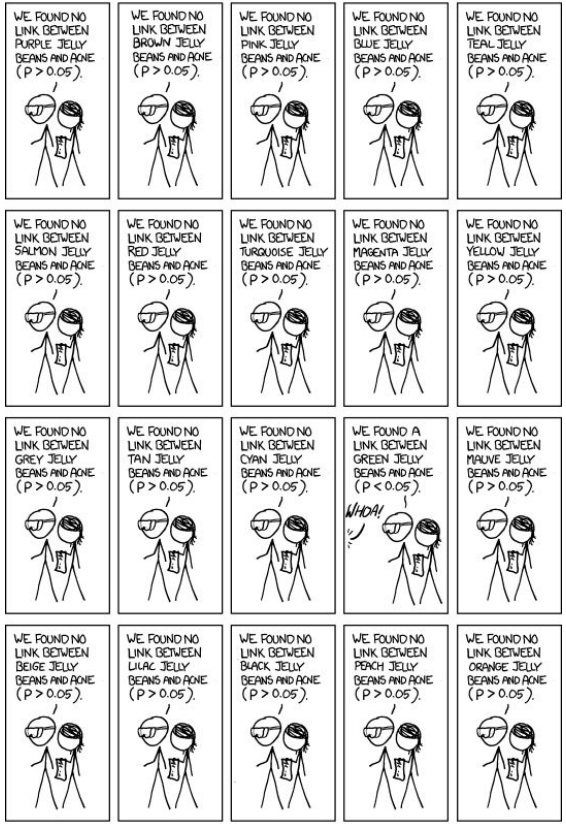
- “Near-zero variance” features
  - Attribute “male” is not very useful if we want to predict heart attacks in males (“zero variance”)
  - Near-zeros can be problematic (numerical problems, “pure” batches)
  - Yet: rare genetic profiles could be very useful (for a minority of cases)
- Correlated features
  - A and B: the two most correlated features (absolute value)
  - cA (cB) < correlation of feature A (B) with all the remaining features
  - If cA > cB: discard A; else: discard B
  - Repeat
  - **Or: Good ol’ PCA**
  - Yet: “fatness” is weight - α height…

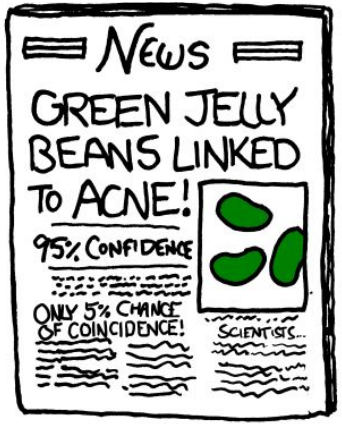
“Supervised” filters

- Feature x, prediction y
- Measure how strong the relationship between x and y is
  - Pearson correlation, ANOVA, chi-squared test, t-test, mutual information, etc.
- Several problems
  - When to discard a feature? P-test? (see next slide!)
  - We can keep the “best” k — how to choose k?
  - Significant is NOT (necessarily) “important” (“car lighter” and “price”)
  - What about “non-linear” features?



The p-value fallacy





Bonferroni correction helps…
but probably too rigid

Embedded methods

- LASSO (basically, L1 regularization)
  - Fit a simple model (like linear regression, logistic regression)
  - Discard all the features whose weight is very small (normalized features!)
  - The larger λ, the fewer features will survive
- Random Forest
  - Discard all the features not selected by the random forest
  - Or use average decrease of impurity
  - Or Shapley values
    - Different teams = different values. How much does each player contribute on average across all possible teams?
    - They can be efficiently computed for a tree

L1 sparsifies (and L2 rescales)

L2

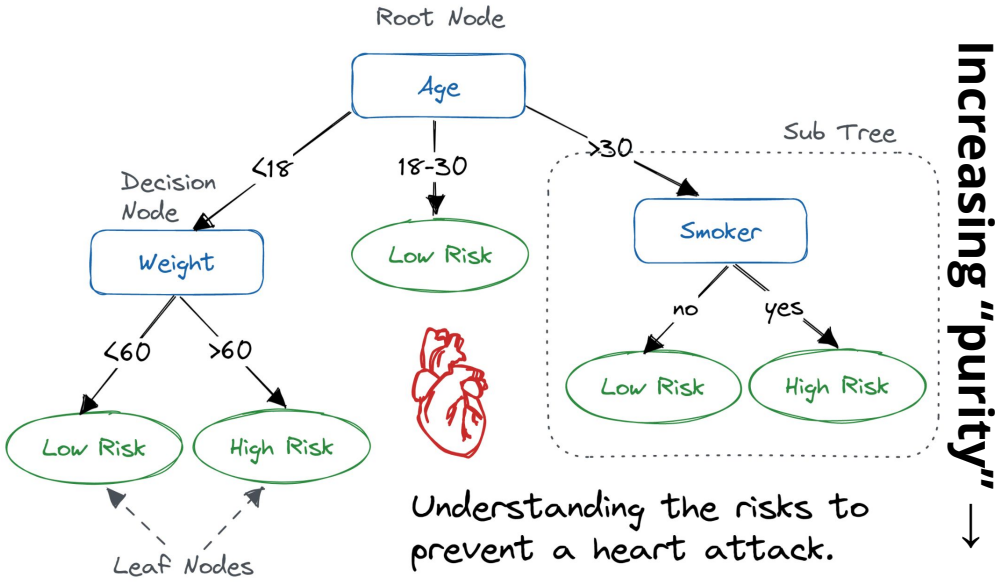
$$f(\theta) \simeq \frac{(\theta - \overline{\theta})^2}{2} + \lambda\,\theta^2 \qquad \theta = \frac{\overline{\theta}}{1 + 2\,\lambda}$$

L1

$$f(\theta) \simeq \frac{(\theta - \overline{\theta})^2}{2} + \lambda\,|\theta| \qquad \theta = \overline{\theta} - \lambda\,\mathrm{sign}(\theta)$$

$$\text{If } |\overline{\theta}| < \lambda \implies \theta = 0$$

Decision trees and random forests



https://www.datacamp.com/tutorial/decision-tree-classification-python

Random forest

- Many shallow trees
- At each node, only a subset of features is considered

$$\hat{y}(x) = \frac{1}{T}\sum_{i}^{T} \text{tree}_i(x)$$

Wrappers

- Basic algorithm
  - Start with a subset of features
  - Add or subtract one of these features and fit the model (“**proposed change**”)
  - Check if the new model is “better-enough” or “not-too-worse”
  - Accept or discard the **proposed change**
  - Repeat until we have to stop
- Add=”forward selection”, subtract=”backward selection”, both=”stepwise”
  - We can add and subtract in various combinations
  - Simulated annealing, genetic algorithms
- How to measure “better-enough”
  - Performance (RMSE, cross entropy, etc.) + Complexity penalization (Akaike Information Criterion — AIC, Bayesian Information Criterion — BIC)
- Permutation importance
  - Take your model; shuffle the values of a feature; see how your performance is impacted

Feature selection and overfitting

Things favouring overfitting

- The data set is small
- The number of feature is large
- Large-variance models (*e.g.*, deep networks)

Never ever use test data for feature selection

Too many levels (high cardinality)

- Categorical features with many possible values
  - Think: diagnosis, “previous employer”, postal codes, brand of a car, *etc*.
  - *Many* must be understood in comparison to the number of data points
- First: avoid one-hot encoding
- Binary encoding (and other forms of encoding)
- “Other” solution
- Grouping for effect (on part of the training set!)
- “Contrastive”-L1
- Expert grouping
- Boosted trees + “Fisher trick” (maximum homogeneity)
- Embedding
  - A priori embedding (for example, using LLM)
  - Learned embedding

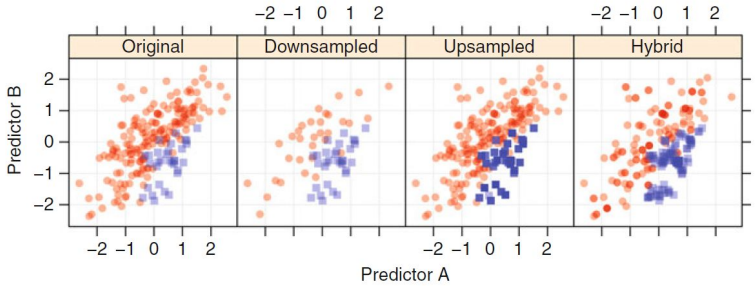
Class imbalance

Class imbalance

- When in our dataset, one or more of the classes are very rare
- Examples
  - Online advertising: will the reader click on the ad? Clicks are like 2% of all visits
  - Drugs: of thousands of compounds, only a few are expected to be active
  - Frauds: we expect only a small fraction of “transactions” to be malicious
- Accuracy not a good metric
  - There is nothing wrong with accuracy. It is our intuition that can get derailed
  - If I say my model gets 99% accuracy, you’d probably say: great! (thank you)
  - Yet: if frauds rate is 1%, the **“blind” model** that always gives a “not-a-fraud” response reaches an accuracy of…? Yes, 99%
- It is difficult to make our model not too “blind”
  - Because in many respects there is too little to be gained (and too little information)
  - The more imbalance, the harder the problem gets

Dealing with imbalance

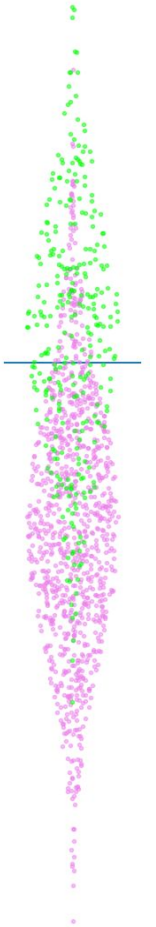
- Tuning hyperparameters
- Adjusting prior probabilities (Bayes)
- **Giving more weight to different classes** in your error function
  - Very effective (akin to up-sampling — see below)
- **Resampling techniques**
  - Up-sampling, down-sampling
  - SMOTE (**synthetic** minority over-sampling technique): down-sampling and up-sampling + K-nearest neighbours
  - All effective, yet no clear winner (different models requires different sampling techniques)



Classes of metrics

Classifier outputs a real value; higher = “belongs more to positive class”

- Threshold metrics
  - Accuracy, precision, recall, *etc.*
  - All the possible compositions of TP, FP, TN, and FN
- Ranking metrics
  - ROC Area Under the Curve (AUC), Precision-Recall AUC
- Probability metrics
  - Log-loss/cross entropy



Receiver Operating Characteristic (ROC) curve

- ROC curve gives a graphical depiction of the diagnostic ability of a binary classifier as its discrimination threshold is varied
- High threshold: no “positives” (TP = 0, FP = 0)
- Low threshold: all “positives” (TP / P = 1, FP / N = 1)
- AUC = Probability that f(positive) > f(negative)
- Changing decision threshold = different tradeoffs along the ROC