Towards running complex models on big data

Working with ‘all the genomes in the world’ without changing the model (too much)

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Motivation

For Large datasets

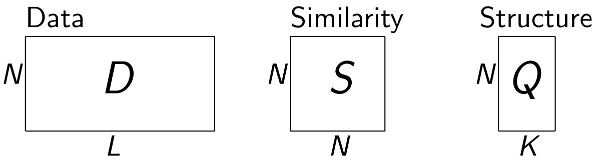
- "Statistics doesn't work" – estimates get worse as we get more data! (for linear compute)
- Simple analytics can extract many useful features
  - e.g. PageRank [Page 1999], K-medians clustering, etc
- Informative in practice - and still hard to get working!
- *Exploit averaging* over lots of data
- But many interesting quantities are subtle...
- or local, so we only have a small amount of data about them
- Always a place for models closer matching reality

Example applications

- 1. Genetics: Model-based clustering for ‘all the genomes in the world’
- (2. Cyber security: finding timing coincidences in event processes a large graph)
- ... In both cases we have a complex model per pair of objects
- but can use a simpler model to find out whether they are at all ‘close’
- Linked by use of a similarity model
- Other applications exist

Similarity: a worked example

$$p(D|S)p(S|Q)p(Q)$$



- Compare N items about which we have a large amount of data D (trivial extension: to $M = O(N)$ other items).
- Similarity $S(i,j)$ is computationally costly to evaluate
- S structured by a model Q
- i.e. Similarity model $p(D|S)$ separates the data D from the structure model $p(S|Q)$
  - If rows of Q sum to 1 this is a mixture model
  - if only 1 element is non-zero it is a partitioning

Random or convenience filtering

- See 'big data'[1] as better sampling of 'data'
- Why not throw away elements from D?
  - Convenience sampling - what can we actually measure?
  - Systematic sampling - retain every n-th data point
  - Simple random sampling - retain fraction p
  - Stratified sampling
  - etc
- For example:
  - Use $L' \ll L$
  - Use $N' \ll N$
- Inference shouldn't get worse with more data!

1: *Big data: any data that can't be processed in memory on a single high spec computer*

Emulated Likelihood Models (ELMs)

Fundamental idea: Replace $p(D|S,\theta)$ in

$$p(D|S,\theta)p(\theta)p(S|Q,\phi)p(Q,\phi)$$

using S^* computed and $S^\dagger$ emulated similarities, s.t. $S = S^* \cup S^\dagger$:

$$\hat{p}(D|S,\theta) = p(D|S^* \cup S^\dagger,\theta) = \int p(D|S^* \cup S^\dagger,\theta,\psi)p(S^\dagger|S^*,\psi)d\psi$$

- S_{ij} is costly to compute, and needed for $S|Q$
- But are highly structured (e.g. clusters)
- So can emulate S_{ij} rather than computing
- Choose S^* to be approximately sufficient for $p(D|S,\theta)$

The oracle

Which NT elements S^* of S should we evaluate?
Natural solution using oracle knowledge of the true S.

- Use a loss function $\mathcal{L}(S^*)$
- Seek $\mathrm{argmin}_{S^*(T)}\mathcal{L}(S^*(T))$
- Choices for $\mathcal{L}$ might be:
  - KL divergence between the true and the emulated posterior
  - A loss based on model usage (e.g. is the clustering correct? Control the false positive rate, etc)
- Choose T based on acceptable loss

Building blocks of a real Emulated Likelihood Model

The oracle is too costly. We instead must:

- Iteratively choose the next S_{ij} to add to S^*
- From a limited set produced by a restriction operator $\mathcal{R}(S^*)$
- Construct an estimator $\hat{\mathcal{L}}$ for $\mathcal{L}$
- Decide on the next point to evaluate using $\operatorname{argmin}_{S_{ij}} \mathbb{E}\left(\hat{\mathcal{L}}(S^* \cup S_{ij}) | S^*\right)$
  - We can consider different histories to evaluate performance
- Stopping rule: convergence of $\hat{\mathcal{L}}$

$\hat{\mathcal{L}}$ can be implicit from $\mathcal{R}$, if it returns points ordered by $\mathbb{E}(\hat{\mathcal{L}})$

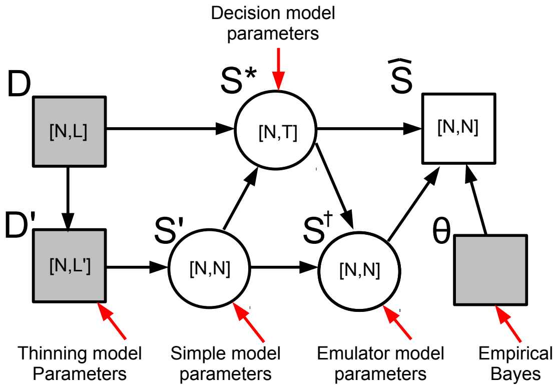
The emulator

'Machine learning' emulator with the usual caveats:

- Rarely optimal, rarely unbiased
- Prediction error estimated using online cross validation
- Respects computational constraints:
  - $L \gg N$: Consider $O(N^2 + LN)$ algorithms
  - $N \gg L$: Consider $O(LN)$ algorithms
  - Massive data: Consider $O(LN^\alpha + N)$ algorithms with $\alpha < 1$.

Fast finestructure - outline

Emulator:

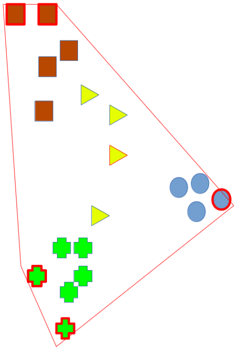


S becomes the data for inferring *Q*:

$$\left[p(D|\hat{S},\hat{\theta})\right] p(S|Q,\phi)p(Q,\phi)$$

Fast finestructure - decision and emulation

- Decision $\mathcal{R}$: Choose item to evaluate i_t^* using the *point most distant to all evaluated points*
- We are evaluating S^* in entire rows
- Emulation: Predict $S_{\cdot i}^{\dagger}$: mixture model $S_i^* = \mathrm{MM}(S_{i*}^*)$, and regression on $\hat{S}_{ij} = \mathrm{LM}(S_{ij}^*, S_{ij}')$
- Implicit loss function $\mathcal{L}$:
  - Minimise the *maximum* prediction error
  - Finds outliers and clusters
  - S^* form convex hull of S



Fast finestructure - in practice

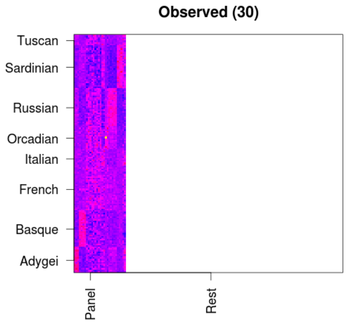
- Computation of S costs $O(N^2L' + NT^2L) \ll O(N^2L)$
- Current datasets: $L = 10,000,000$, $N = 5000$, $L' = 10,000$ $T = 100$, predicted saving ratio is 100

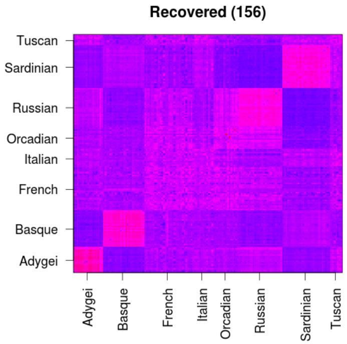
We can save up to factor 10000 by reducing T, the cost of the linearised model on the reduced dataset. L will not grow beyond this, but N will - can introduce an emulation step for S'

Fast finestructure - Parallel MCMC algorithm

A parallel tempering algorithm for when MCMC parallelises poorly

- Evaluate the unlinked model S'
- Master node: perform MCMC clustering to find $\hat{Q}_t$ using $\hat{S}_t$, when there are t rows S^*_t computed
- Worker nodes compute $S^*_{\cdot i}$ in the order chosen by the master
- Stopping rule: posterior distribution of $\hat{Q}$ converges
  - No new information added when increasing t
  - (Or if the MCMC is slower than the evaluation of S, sometime afterwards)


Observed (30)
Tuscan
Sardinian
Russian
Orcadian
Italian
French
Basque
Adygei
Panel
Rest


Recovered (156)
Tuscan
Sardinian
Russian
Orcadian
Italian
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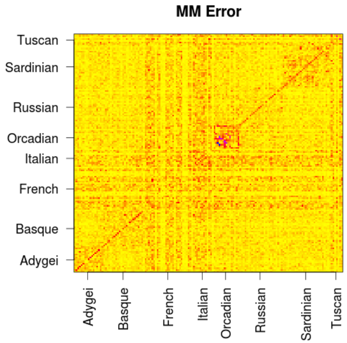
Basque
Adygei
Adygei
Basque
French
Italian
Orcadian
Russian
Sardinian
Tuscan


MM Error
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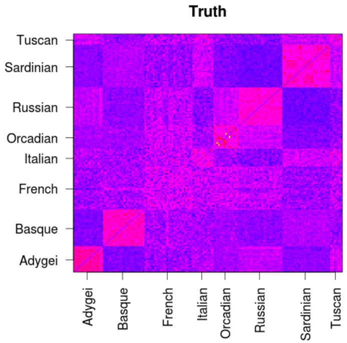
Tuscan


Truth
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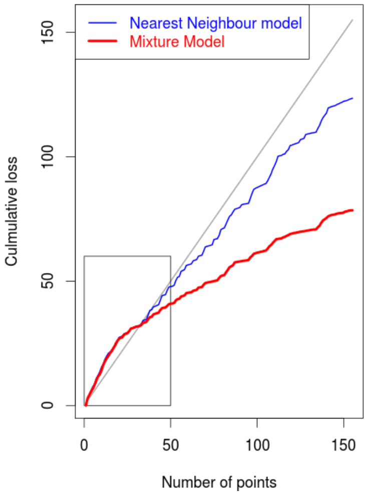
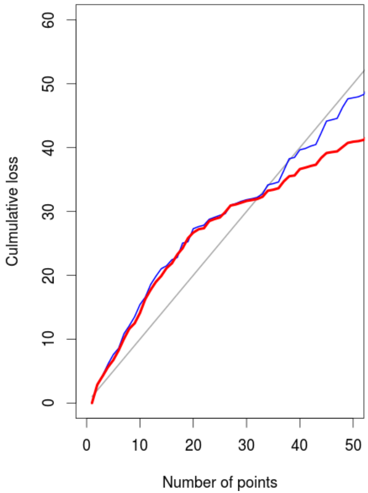
Russian
Sardinian
Tuscan


Nearest Neighbour model
Mixture Model
Culmulative loss
Number of points
0
50
100
150


Culmulative loss
Number of points
0
10
20
30
40
50
60

Emulated Likelihood Models for general Bayesian problems

General emulation for big (but not so big) problems

$$\hat{p}(D|S,\theta) = \int p(D|S^* \cup S^\dagger, \theta) p(S^\dagger|S^*, \theta, \psi) d\psi$$

- i.e. Can use θ to emulate $S^\dagger(\theta)$ - e.g. regression in (S,θ) space
  - Gaussian Process for $S_{ij}(\theta)$ is a natural choice
- If $S^\dagger$ is an unbiased estimator of S^* this is a pseudo-marginal approach (and hence targeting the correct posterior)

Discussion

- Goal: Approximate answers to the right questions using exact answers to the wrong questions
- Machine learning is increasingly important for large datasets
- Statistical modelling still has a place
- Proposed the Emulated Likelihood Model:
  - Full statistical modelling
  - Machine learning algorithms used for the calculation
  - Statistical estimation of parameters is retained but approximated