Stat 315c: Transposable Data Clustering

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Stanford Statistics

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- A form of unsupervised learning. Unsupervised because there is no response.
- Has a long history, at least as old as taxonomy.
- Raises all the vexing issues of an exploratory method.
- We'll look at it as a precursor to 'bi-clustering' of objects and attributes.

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- In the best case, a clustering can reveal the presence of a new categorical variable, e.g. types of diabetes.
- Other times there are no clusters, just a 'smear'
- Or we find clusters but not their meanings.

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Key idea

Items within a cluster are more similar (less distant) to each other than items from different clusters.

k-means

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Algorithm

1. Pick k points $z_1, \ldots, z_k \in \mathbb{R}^d$, then repeat
   - For $i = 1, \ldots, n$ put $g(i) = \min_{1 \le j \le k} \|x_i - z_j\|^2$
   - For $j = 1, \ldots, k$ put $z_j = \text{avg}\{x_i \mid g(i) = j\}$

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Issues

- Handle averaging over empty set
- Pick stopping rule (it must converge, or at worst cycle)
- Answer depends on starting points
- Hard to pick k (at least 30 methods proposed by 1985)

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Properties

- Usually rapid convergence
- An iteration can be done in $O(nkd)$ time. No n^2 or d^2 or k^2. ($k \log(k)$ to sort negligible)

k-means ctd

There's a criterion

- Each step minimizes

$$\sum_{i=1}^{n} \|x_i - z_{g(i)}\|^2$$

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Defining true k problematic (galaxies in clusters in super-clusters)

Variations

Change dist

- Change the distance L^2 to L^1 to $\cdots$ L^p
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Change z

- k medoids
- Require $z_k = x_{i(k)}$ for some $i(k)$
- Avoids using z with 2.3 kids, 30% pregnant, 10% male
- PAM "partitioning around medoids"
- Minimize $\sum_i \min_j D(x_i, z_j)$
- Slow. Uses only D_{ij} values.

What is a cluster?

Defining issues

- Scale of variables matters
- Subset of variables matters too
  Do whales go with penguins or with elephants?
  Why does my breakfast cereal cluster with pure sugar?
- # Density bumps $\neq$ # mixture components

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Scaling data

$$z_{ij} = \frac{x_{ij} - m_j}{s_j}$$

- m, s are mean & stdev (so $z_{\cdot j} \sim (0, 1)$)
- or min & range (so $0 \leq z_{ij} \leq 1$)
- or median & MAD (for robustness)
- NB: transformation defined column-wise [vs row-wise or simultaneous]

Weighting

Weight variables via $w_j \geq 0$

$$d_{ii'} = \sum_{j=1}^{d} w_j |x_{ij} - x_{i'j}| = \sum_{j=1}^{d} |\widetilde{x}_{ij} - \widetilde{x}_{i'j}|$$

with

$$\widetilde{x}_{ij} = x_{ij} \times w_j$$

Weighting and scaling are equivalent (for L^p distances)

Automatic scaling not always sensible. Variables in the same units should sometimes get the same scaling even if they have different variances.

Distances

$n(n-1)/2$ interpoint distances

- $d_{ii'} = \text{dist}(x_i, x_{i'})$
- Usually
  1. $d_{ii'} \geq 0$
  2. $d_{ii} = 0$
  3. $d_{ii'} = d_{i'i}$
- A metric distance has $d_{ij} \leq d_{ik} + d_{jk}$ (Triangle inequality)
- A 'Euclidean' distance $d_{ij} = \|z_i - z_j\|$ for some points $z_i = z(x_i)$
- An ultra-metric distance has $d_{ij} \leq \max(d_{ik}, d_{jk})$ (More later)

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Other distances

- Canberra distance $\sum_{j=1}^{d} \frac{|x_{ij} - x_{i'j}|}{|x_{ij}| + |x_{i'j}|}$ (with $0/0 = 0$)
- Angular or cosine distance (dogs‖cats, wolves‖tigers)

Similarities

Opposite of distance: $d \leftrightarrow S$

Eg $S_{ii'} = 1 - d_{ii'}$ or $1/d_{ii'}$ or $d_{ii'} = S - S_{ii'}$

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Correlation type similarities

$$S_{ii'} = \frac{\sum_{j=1}^{d} x_{ij}x_{i'j}}{\sqrt{\sum_{j=1}^{d} x_{ij}^2 \sum_{j=1}^{d} x_{i'j}^2}}, \quad \text{or,}$$

$$= \left| \frac{\sum_{j=1}^{d} x_{ij}x_{i'j}}{\sqrt{\sum_{j=1}^{d} x_{ij}^2 \sum_{j=1}^{d} x_{i'j}^2}} \right|, \quad \text{or,}$$

$$= \left| \frac{\sum_{j=1}^{d} (x_{ij} - \bar{x}_j)(x_{i'j} - \bar{x}_j)}{\sqrt{\sum_{j=1}^{d} (x_{ij} - \bar{x}_j)^2 \sum_{j=1}^{d} (x_{i'j} - \bar{x}_j)^2}} \right|, \quad \text{or, } \cdots$$

Similarities

Some equalities are more equal than others

1. i and i' are both Nobel laureates (unusually strong similarity)
2. i and i' are both over 21 years old (mild similarity)
3. i and i' are both not Nobel laureates (barely similar at all)

We can handle 1 vs 2 by weighting the variables.
But 1 vs 3 is trickier (same variable).

Binary similarity measures $d = 1 - S$

p features 2×2 table

	1	0
1	a	b
0	c	d

We want to count a more than d

Generic measure: $\alpha > 0$, $\delta \geq 0$

$$S_{ii'} = \frac{\alpha a + \delta d}{\alpha a + b + c + \delta d}$$

(α, δ) and (α', δ') give the same ranking if $\alpha\delta' = \alpha'\delta$

Janowitz recommends Jaccard or Russel-Rao

Specific measures

$$S_{ii'} = \frac{a+d}{a+b+c+d}$$ Simple matchin

$$S_{ii'} = \frac{a}{a+b+c}$$ Jaccard-Tanimoto

$= 1$ when $a + b + c = 0$

$$S_{ii'} = \frac{a}{a+b+c+d}$$ Russel-Rao

$$S_{ii'} = \frac{2(a+d)}{2(a+d)+b+c}$$ Sokal-Sneath

$$S_{ii'} = \frac{a}{a+2(b+c)}$$ Sokal-Sneath II

Agglomerative clustering

General

- Start with n clusters of one element each
- Repeat
  1. Find closest two clusters
  2. Merge them into a new cluster
- Until only one cluster remains
- We need point to cluster and cluster to cluster distances

Flavors of agglomerative clustering

Single linkage

$$d(C_1, C_2) = \min_{i \in C_1} \min_{j \in C_2} d_{ij}$$

Get 'chaining'; friends of friends

Complete linkage

$$d(C_1, C_2) = \max_{i \in C_1} \max_{j \in C_2} d_{ij}$$

Get dense nearly spherical clusters

Average linkage

$$d(C_1, C_2) = \frac{1}{|C_1|} \frac{1}{|C_2|} \sum_{i \in C_1} \sum_{j \in C_2} d_{ij}$$

Compromise

Example

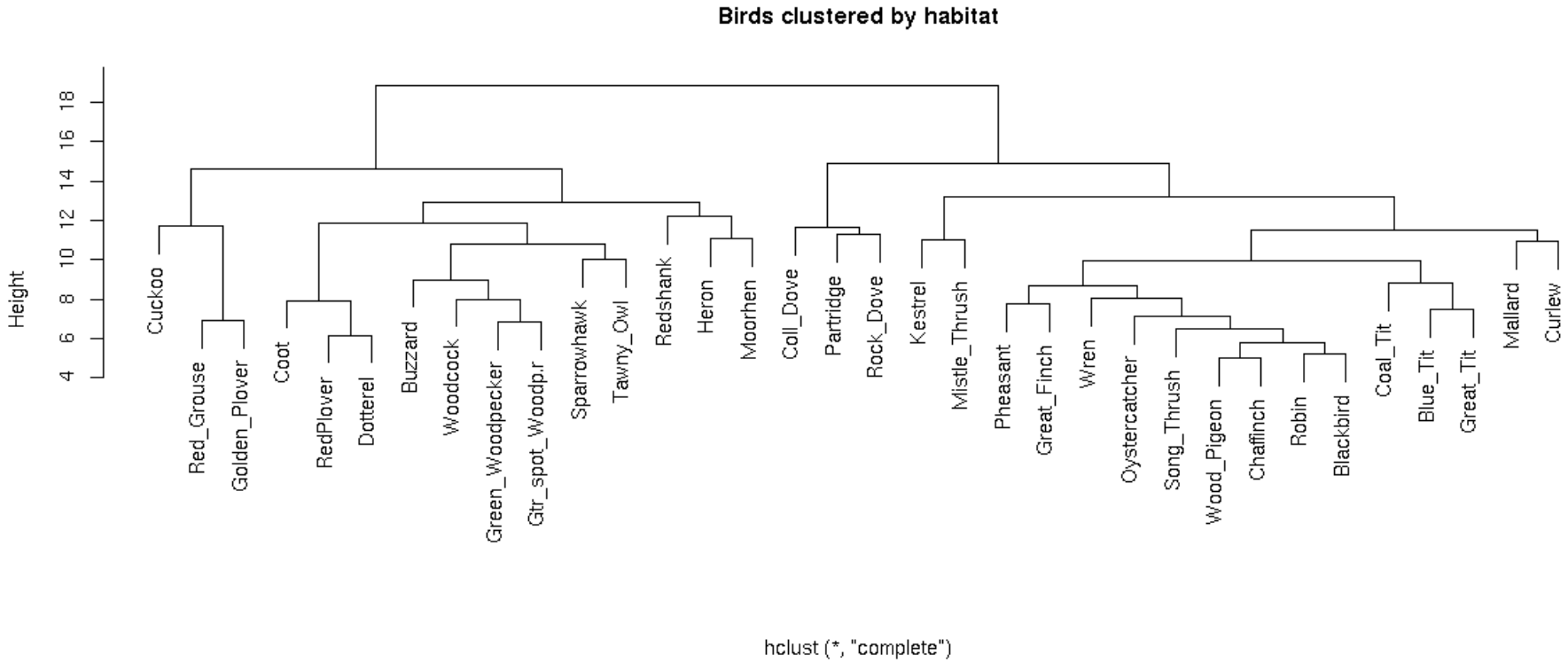
Bird data

```
> dim(voeg)
[1] 395  34
> voeg[1:5,1:5]
  Heron Mallard Sparrowhawk Buzzard Kestrel
1     0       0           0       0       1
2     1       0           0       0       0
3     0       0           1       0       0
4     0       0           1       0       0
5     1       1           0       0       0
```

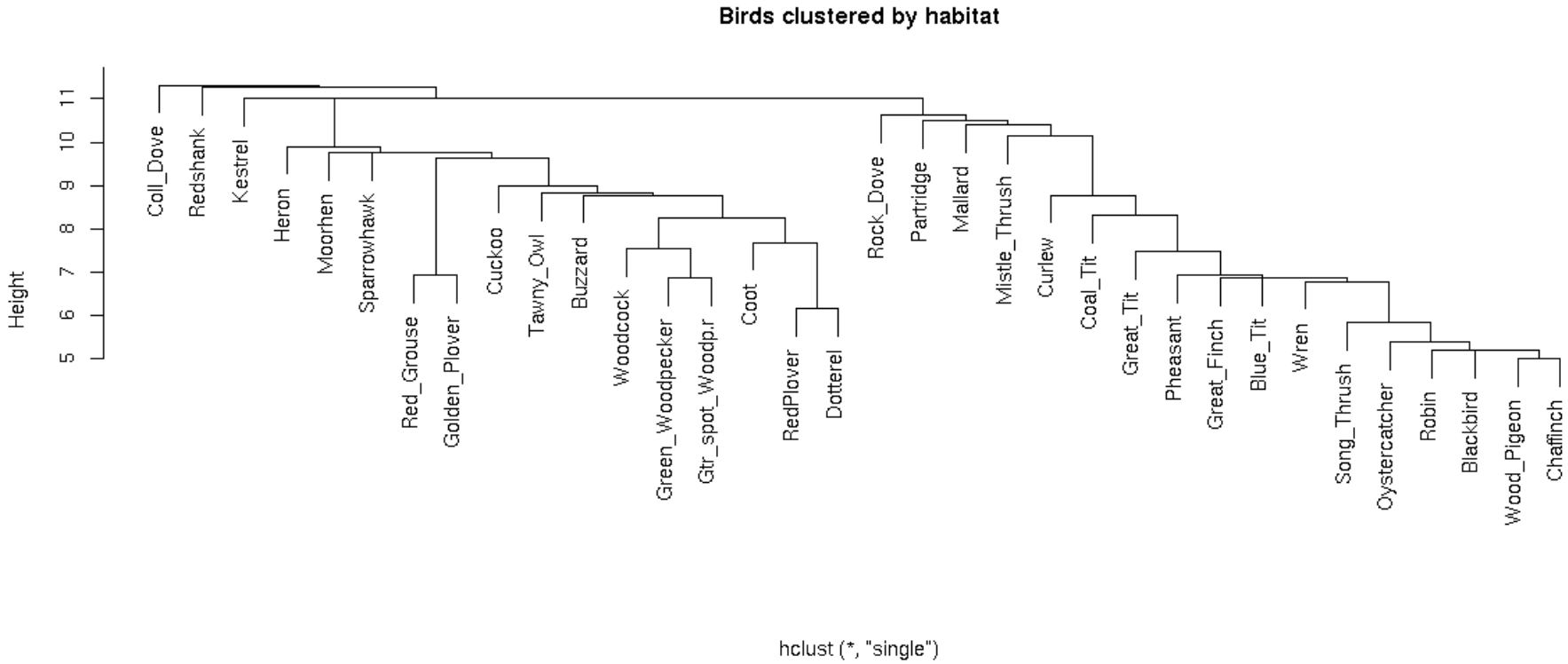
1 means that place i has bird j

Place names not present

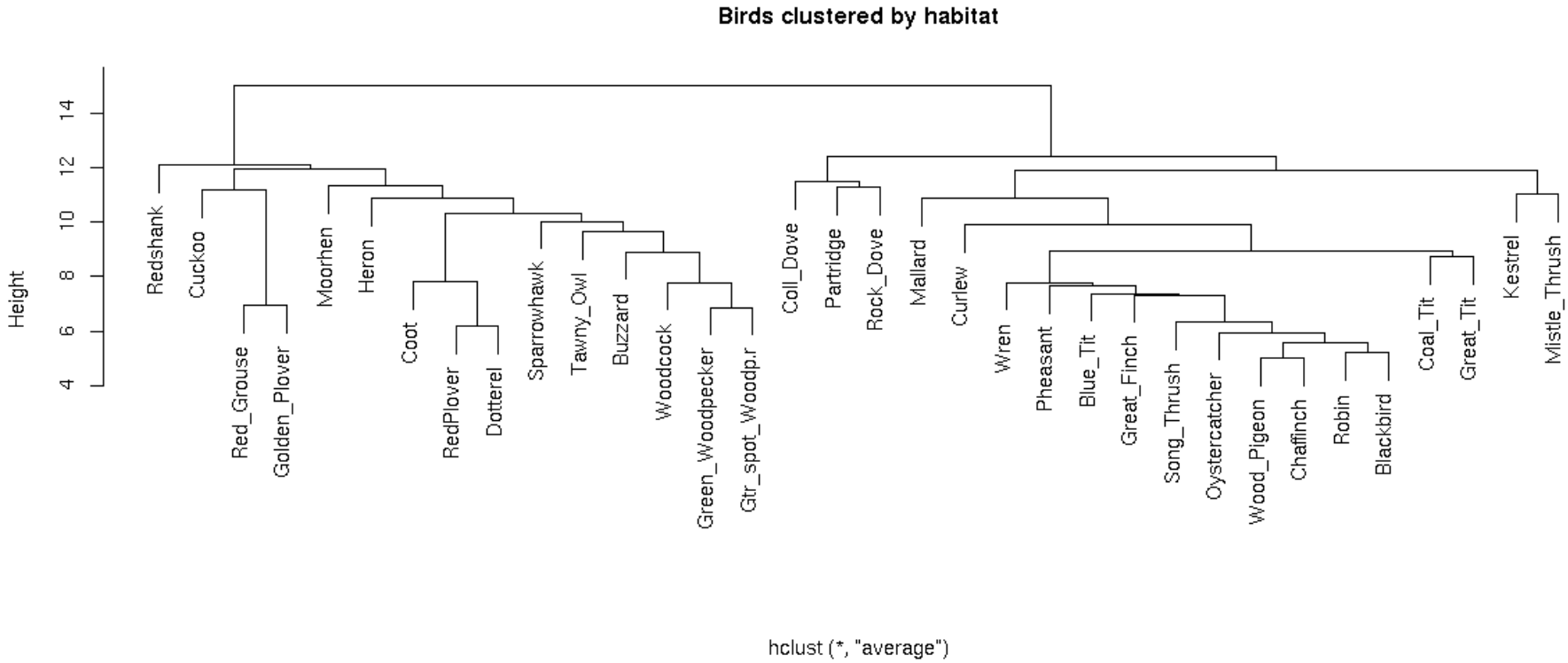
Complete linkage dendrogram



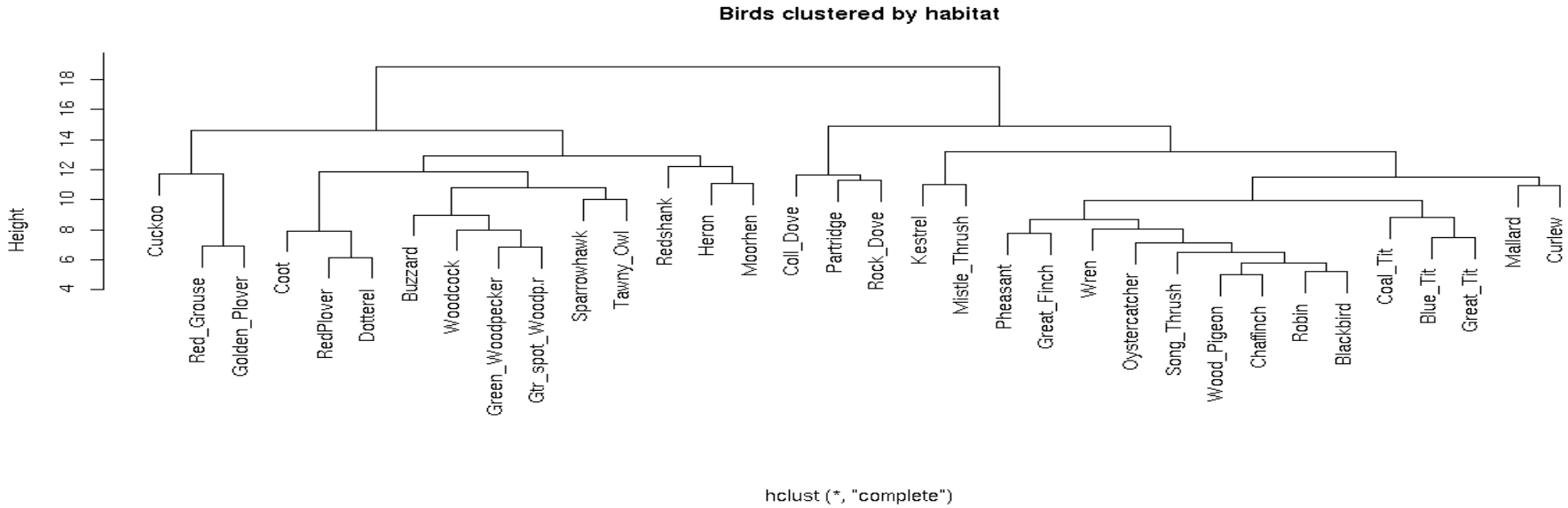
Single linkage dendrogram

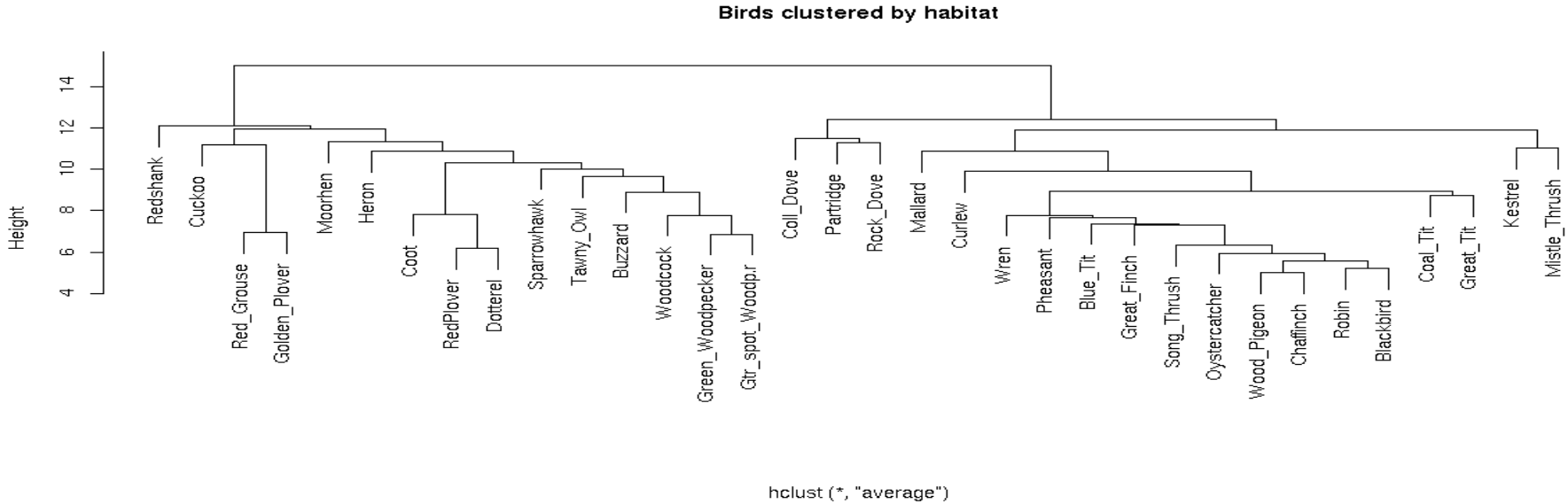


Average linkage dendrogram

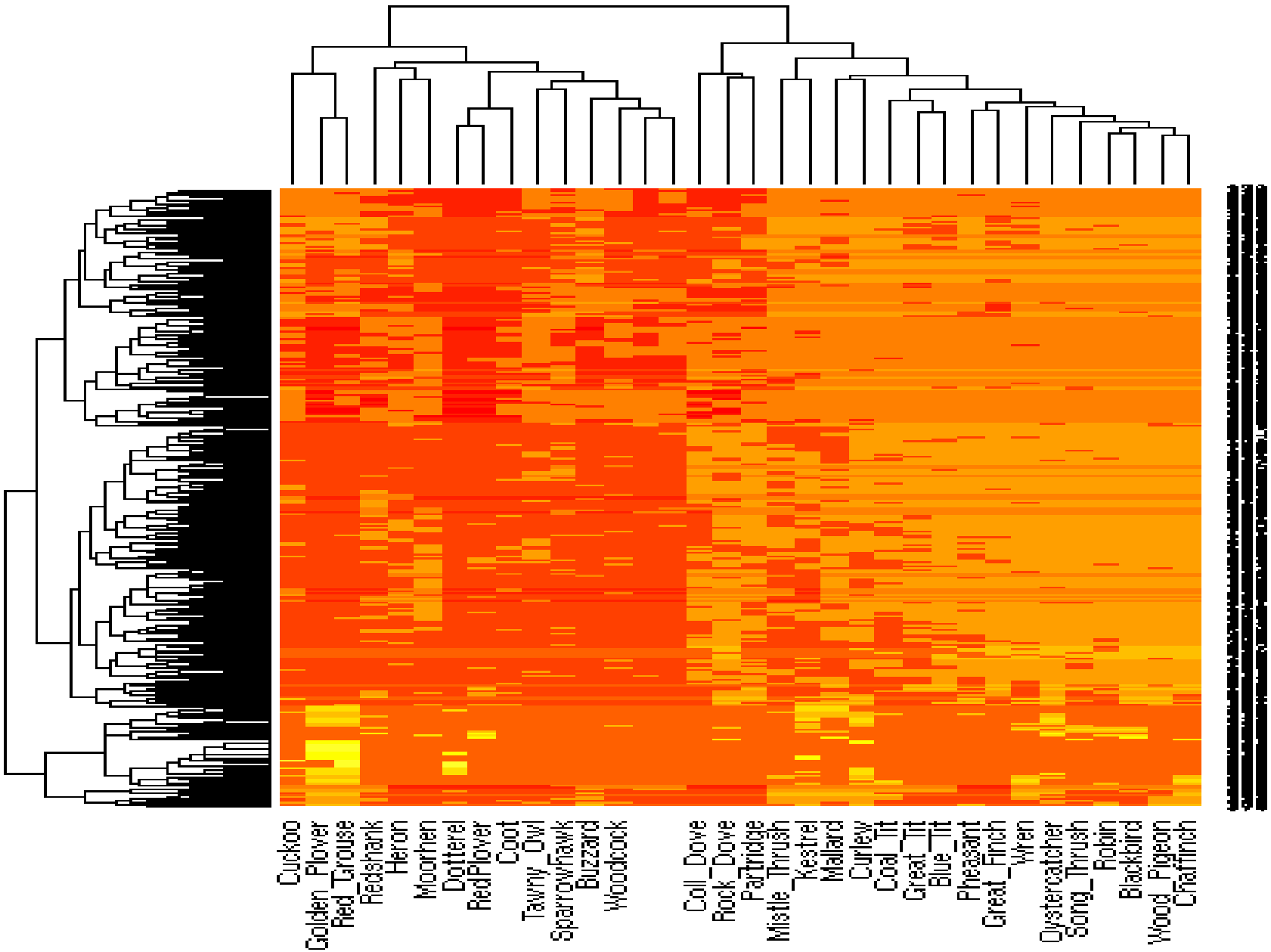


Complete vs Average linkage dendrograms





Heatmap


Cuckoo
Golden_Plover
Red_Grouse
Redshank
Heron
Moorhen
Dotterel
RedPlover
Coot
Tawny_Owl
Sparrowhawk
Buzzard
Woodcock
Coll_Dove
Rock_Dove
Partridge
Mistle_Thrush
Kestrel
Mallard
Curlew
Coal_Tit
Great_Tit
Blue_Tit
Pheasant
Great_Finch
Wren
Oystercatcher
Song_Thrush
Robin
Blackbird
Wood_Pigeon
Chaffinch

Dendrogram details

Ordering

- n points $\implies$ $n-1$ splits $\implies$ 2^{n-1} orderings
- R puts 'tightest' cluster on the left
- heatmap lets you control ordering somewhat

Ultrametric

- H_{ij} height at which clusters containing i and j merge
- It's an ultrametric: for i, j, k top two of H_{ij}, H_{ik}, H_{jk} are equal
- Need $H_{ij} \leq \max(H_{ik}, H_{jk})$
- Non-ultrametric measures yield dendrograms with 'reversals'

More hierarchical

Centroid merging

$$d(C_1, C_2) = \|\bar{X}_{C_1} - \bar{X}_{C_2}\|$$

Requires original points, not just distances

Ward's

$$d(C_1, C_2) = \frac{2|C_1||C_2|}{|C_1| + |C_2|}\|\bar{X}_{C_1} - \bar{X}_{C_2}\|$$

Via within cluster SS (after $-$ before)

Goal is to min

$$\sum_j \sum_{i \in C_j} \|X_i - \bar{X}_{C_j}\|^2$$

Costs of hierarchical splits

- It takes $O(n^2 d)$ to get all pairwise distances
- We have to take $O(n)$ steps
- Naive implementation would be $O(n^3 d)$.

Lance-Williams family of methods

Dist of $i \cup j$ to k

$$\alpha_i d_{ki} + \alpha_j d_{kj} + \beta d_{ij} + \gamma |d_{ki} - d_{kj}|$$

eg: $\alpha = 1/2$, $\beta = 0$, $\gamma = -1/2$ for single linkage.
α_i can depend on n_i.
Updates lead to $O(n^2 d)$ cost.

Divisive clustering

Recipe

- Start with one cluster of n objects
- Repeat
  1. Select one cluster
  2. Split it into two
- Until there are n clusters of size 1

Choices

- Which cluster to split. E.g. largest 'diameter'

$$\arg\max_j \max_{i,i' \in C_j} \|X_i - X_{i'}\|$$

- How to split it. E.g. remove far point, X_i goes with nearer of far point, $\bar{X}_{C_j - \text{far}}$

Apparently no good speedup

Optimization based clustering

E.g. Ward's

Recipe

- Measure quality of a cluster
  - Scale est, like diameter, RMS width, median width
- Combine into quality of clustering
  - Typically the sum (max plausible)
- (Attempt to) optimize

Isolation measures

- Split $\min_{i \in C, j \notin C} d_{ij}$
- Cut $\sum_{i \in C, j \notin C} d_{ij}$