Multidimensional and Heterogeneous Models

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Outline

Yesterday

- Models of trait evolution.
- The phylogenetic regression.
- Application: HIV virulence heritability.

Today

- Multivariate and heterogeneous models.
- Bayesian inference.
- Application: phylogeography.

Complex Traits

Multidimensional Models

2 Heterogeneous Evolution

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Outline

1 Multidimensional Models

- Multivariate BM
- Multivariate Ornstein-Uhlenbeck
- General Gaussian Model

2 Heterogeneous Evolution

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

BM on a Tree



Multidimensional Models

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

BM on a Tree



Variance: $\mathbb{C}\text{ov}[Y_4;Y_5] = \sigma^2 \times V_{45}$ shared evolution timeExpectation: $\mathbb{E}[Y_i] = \mu$ ancestral root value

Multidimensional Models

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

BM on a Tree



Distribution: Normal

$$\mathbf{Y} \sim \mathcal{N}(\mu \mathbf{1}_n, \sigma^2 \mathbf{V})$$

Multivariate BM



Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Data: Vectors of p traits

$$\mathbf{Y}_i^T = (Y_{i1}, \ldots, Y_{ip})$$

Multivariate BM



Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Data: Vectors of *p* traits

$$\mathbf{Y}_i^T = (Y_{i1}, \ldots, Y_{ip})$$

SDE:d $\mathbf{X}_t = \mathbf{\Sigma} d \mathbf{B}_t$ $\mathbf{R} = \mathbf{\Sigma}^T \mathbf{\Sigma}$ Variance: $\mathbb{C}ov [Y_{ik}; Y_{jl}] = R_{kl} \times V_{ij}$ shared evolution timeExpectation: $\mathbb{E} [\mathbf{Y}_{\cdot k}] = \mu_k$ ancestral root value

Multivariate BM



Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Data: Vectors of *p* traits

$$\mathbf{Y}_i^T = (Y_{i1}, \ldots, Y_{ip})$$

Distribution: Matrix Normal

$$\mathbf{Y} \sim \mathcal{MN}(\mathbf{1}_n \boldsymbol{\mu}^T, \mathbf{V}, \mathbf{R})$$

$$\mathbb{V}$$
ar [vec (\mathbf{Y})] = $\mathbf{R} \otimes \mathbf{V}$

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Vectorisation: stack columns on top of each other

$$\operatorname{vec}(\mathbf{Y}) = \operatorname{vec}\begin{pmatrix} Y_{11} & Y_{12} & \cdots & Y_{1p} \\ Y_{21} & Y_{22} & \cdots & Y_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ Y_{n1} & Y_{n2} & \cdots & Y_{np} \end{pmatrix} = \begin{pmatrix} Y_{11} \\ Y_{21} \\ \vdots \\ Y_{22} \\ \vdots \\ Y_{n2} \\ \vdots \\ Y_{1p} \\ Y_{2p} \\ \vdots \\ Y_{np} \end{pmatrix} = \begin{pmatrix} \mathbf{Y}_{.1} \\ \mathbf{Y}_{.2} \\ \vdots \\ \mathbf{Y}_{.p} \\ \vdots \\ Y_{.p} \end{pmatrix}$$

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Kronecker Product

$$\mathbf{R} \otimes \mathbf{V} = \begin{pmatrix} R_{11}\mathbf{V} & \cdots & R_{1p}\mathbf{V} \\ \vdots & \ddots & \vdots \\ R_{p1}\mathbf{V} & \cdots & R_{pp}\mathbf{V} \end{pmatrix}$$

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

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 $\mathbb{C} \text{ov} \left[Y_{ik}; Y_{jl} \right] = R_{kl} \times V_{ij} \qquad \mathbb{C} \text{ov} \left[\mathbf{Y}_{\cdot k}; \mathbf{Y}_{\cdot l} \right] = R_{kl} \times \mathbf{V}$

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Kronecker Product

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$$\mathbb{C}$$
ov $[Y_{ik}; Y_{jl}] = R_{kl} \times V_{ij}$ \mathbb{C} ov $[\mathbf{Y}_{\cdot k}; \mathbf{Y}_{\cdot l}] = R_{kl} \times \mathbf{V}$

$$\mathbb{V}\operatorname{ar}\left[\begin{pmatrix}\mathbf{Y}_{\cdot 1}\\ \vdots\\ \mathbf{Y}_{\cdot p}\end{pmatrix}\right] = \begin{pmatrix} \mathbb{C}\operatorname{ov}\left[\mathbf{Y}_{\cdot 1}; \mathbf{Y}_{\cdot 1}\right] & \cdots & \mathbb{C}\operatorname{ov}\left[\mathbf{Y}_{\cdot 1}; \mathbf{Y}_{\cdot p}\right]\\ \vdots & \ddots & \vdots\\ \mathbb{C}\operatorname{ov}\left[\mathbf{Y}_{\cdot p}; \mathbf{Y}_{\cdot 1}\right] & \cdots & \mathbb{C}\operatorname{ov}\left[\mathbf{Y}_{\cdot p}; \mathbf{Y}_{\cdot p}\right] \end{pmatrix}$$

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

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 $\mathbb{V}\mathsf{ar}\left[\mathsf{vec}(\mathbf{Y})\right]=\mathbf{R}\otimes\mathbf{V}$

Multivariate BM



Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Data: Vectors of *p* traits

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Distribution: Matrix Normal

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Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Estimators

 $\mathsf{vec}(\mathbf{Y}) \sim \mathcal{MN}(\mathsf{vec}(\mathbf{1}_n \boldsymbol{\mu}^{\mathsf{T}}), \mathbf{R} \otimes \mathbf{V}) \qquad \text{with } \mathbf{V} \text{ known}$

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Estimators

$$\operatorname{vec}(\mathbf{Y}) \sim \mathcal{MN}(\operatorname{vec}(\mathbf{1}_n \boldsymbol{\mu}^T), \mathbf{R} \otimes \mathbf{V}) \qquad \text{with } \mathbf{V} \text{ known}$$

Cholesky Decomposition:

 $\mathbf{V} = \mathbf{L}\mathbf{L}^{T}$ vec $(\mathbf{L}^{-1}\mathbf{Y}) \sim \mathcal{MN}(\mathsf{vec}(\mathbf{L}^{-1}\mathbf{1}_{n}\boldsymbol{\mu}^{T}), \mathbf{R} \otimes \mathbf{I}_{n})$

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Estimators

$$\mathsf{vec}(\mathbf{Y}) \sim \mathcal{MN}(\mathsf{vec}(\mathbf{1}_n \boldsymbol{\mu}^T), \mathbf{R} \otimes \mathbf{V}) \qquad \text{with } \mathbf{V} \text{ known}$$

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vec $(\mathbf{L}^{-1}\mathbf{Y}) \sim \mathcal{MN}(ext{vec}(\mathbf{L}^{-1}\mathbf{1}_n oldsymbol{\mu}^{\mathcal{T}}), \mathbf{R} \otimes \mathbf{I}_n)$

Maximum Likelihood Estimators:

$$\hat{\boldsymbol{\mu}}^{T} = (\mathbf{1}_{n}^{T} \mathbf{V}^{-1} \mathbf{1}_{n})^{-1} \mathbf{1}_{n}^{T} \mathbf{V}^{-1} \mathbf{Y}$$
 $\hat{\mathbf{R}} = \frac{1}{n-1} (\mathbf{Y} - \mathbf{1}_{n} \hat{\boldsymbol{\mu}}^{T})^{T} \mathbf{V}^{-1} (\mathbf{Y} - \mathbf{1}_{n} \hat{\boldsymbol{\mu}}^{T})^{T}$

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Phylogenetic Principal Component Analysis

(Revell, 2009)

Diagonalisation of the BM estimated variance:

 $\hat{\boldsymbol{\mathsf{R}}} = \hat{\boldsymbol{\mathsf{W}}} \hat{\boldsymbol{\mathsf{D}}}^2 \hat{\boldsymbol{\mathsf{W}}}^{\mathcal{T}}$

- $\hat{\mathbf{W}}_i$: principal axis *i* (eigenvectors, $\hat{\mathbf{W}}$ is $p \times p$ orthogonal)
- $\hat{\mathbf{D}}_{i}^{2}$: variance explained by $\hat{\mathbf{W}}_{i}$ (eigenvalues, $\hat{\mathbf{D}}^{2}$ diagonal)

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Scores: Data coordinates in the new system.

$$\hat{\mathbf{S}} = (\mathbf{Y} - \mathbf{1}_n \hat{\boldsymbol{\mu}}^T) \hat{\mathbf{W}}$$

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(Revell, 2009)

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- $\hat{\mathbf{W}}_i$: principal axis *i* (eigenvectors, $\hat{\mathbf{W}}$ is $p \times p$ orthogonal)
- \hat{D}_i^2 : variance explained by \hat{W}_i (eigenvalues, \hat{D}^2 diagonal)

Scores: Data coordinates in the new system.

$$\hat{\mathsf{S}} = (\mathsf{Y} - \mathbf{1}_n \hat{\boldsymbol{\mu}}^{\mathsf{T}}) \hat{\mathsf{W}}$$

Scores are empirically phylogenetically un-correlated:

$$\begin{split} \hat{\mathbf{S}}^{\mathsf{T}} \mathbf{V}^{-1} \hat{\mathbf{S}} &= \hat{\mathbf{W}}^{\mathsf{T}} (\mathbf{Y} - \mathbf{1}_n \hat{\boldsymbol{\mu}}^{\mathsf{T}})^{\mathsf{T}} \mathbf{V}^{-1} (\mathbf{Y} - \mathbf{1}_n \hat{\boldsymbol{\mu}}^{\mathsf{T}}) \hat{\mathbf{W}} \\ &= \hat{\mathbf{W}}^{\mathsf{T}} [(n-1)\hat{\mathbf{R}}] \hat{\mathbf{W}} \\ &= (n-1) \hat{\mathbf{D}}^2 \end{split}$$

Phylogenetic Principal Component Analysis

(Revell, 2009)

Diagonalisation of the BM estimated variance:

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Scores: Data coordinates in the new system.

$$\hat{\mathsf{S}} = (\mathsf{Y} - \mathbf{1}_n \hat{\mu}^{\mathsf{T}}) \hat{\mathsf{W}}$$

Scores are empirically phylogenetically un-correlated:

$$\langle \mathbf{S}_i, \mathbf{S}_j \rangle_{\mathbf{V}^{-1}} = 0 \quad \forall \ i \neq j$$

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Phylogenetic Principal Component Analysis

(Revell, 2009)

Simulation according to an uncorrelated BM.



Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Phylogenetic Principal Component Analysis

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Simulation according to an uncorrelated BM.



Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Phylogenetic Principal Component Analysis

(Revell, 2009)

Simulation according to an uncorrelated BM.



Multivariate BM **Multivariate Ornstein-Uhlenbeck** General Gaussian Model

Ornstein-Uhlenbeck Modeling

(Hansen, 1997)



$$d X_t = \alpha [\beta - X_t] d t + \sigma d B_t$$

Deterministic part:

- β : primary optimum (mechanistically defined).
- $\ln(2)/\alpha$: phylogenetic half live.

Stochastic part:

- X_t: trait value (actual optimum).
- $\sigma dB(t)$: Brownian fluctuations.

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

OU on a Tree



Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

OU on a Tree



SDE:
$$d X_t = \alpha [\beta - X_t] d t + \sigma d B_t$$

Variance: $\mathbb{C}ov [Y_4; Y_5] = \frac{\sigma^2}{2\alpha} e^{-\alpha (V_4 + V_5)} (e^{2\alpha V_{45}} - 1)$
Expectation: $\mathbb{E} [Y_i] = \mu e^{-\alpha V_i} + \beta (1 - e^{-\alpha V_i})$

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

$$d \mathbf{X}_t = \mathbf{A}[\boldsymbol{\beta} - \mathbf{X}_t] d t + \mathbf{\Sigma} d \mathbf{B}_t$$

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

d
$$\mathbf{X}_t = \mathbf{A}[\boldsymbol{\beta} - \mathbf{X}_t] \, \mathrm{d} \, t + \mathbf{\Sigma} \, \mathrm{d} \, \mathbf{B}_t$$

Scalar: $\mathbf{A} = \begin{pmatrix} 0.1 & 0 \\ 0 & 0.1 \end{pmatrix} \qquad \boldsymbol{\beta} = \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix}$



Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model



Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model





Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

$$\mathrm{d}\,\mathbf{X}_t = \mathbf{A}[\boldsymbol{\beta} - \mathbf{X}_t]\,\mathrm{d}\,t + \boldsymbol{\Sigma}\,\mathrm{d}\,\mathbf{B}_t$$

Diagonalizable in
$$\mathbb{R}$$
: $\mathbf{A} = \begin{pmatrix} -0.02 & -0.04 \\ 0.2 & 0.2 \end{pmatrix}$ $\boldsymbol{\beta} = \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix}$



Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Multivariate OU

$$d \mathbf{X}_t = \mathbf{A}[\boldsymbol{\beta} - \mathbf{X}_t] d t + \mathbf{\Sigma} d \mathbf{B}_t$$

Diagonalizable: $\mathbf{A} = \mathbf{P} \mathbf{A} \mathbf{P}^{-1}$ $\lambda_k > 0$

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Multivariate OU

$$d \mathbf{X}_t = \mathbf{A}[\boldsymbol{\beta} - \mathbf{X}_t] d t + \mathbf{\Sigma} d \mathbf{B}_t$$

Diagonalizable: $\mathbf{A} = \mathbf{P} \mathbf{A} \mathbf{P}^{-1}$ $\lambda_k > 0$

Expectation:

$$\mathbb{E}\left[\mathbf{Y}_i
ight] = \mu e^{-\mathbf{A}V_i} + eta(1-e^{-\mathbf{A}V_i})$$
Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Multivariate OU

$$d \mathbf{X}_t = \mathbf{A}[\boldsymbol{\beta} - \mathbf{X}_t] d t + \mathbf{\Sigma} d \mathbf{B}_t$$

Diagonalizable: $\mathbf{A} = \mathbf{P}$

$$\mathbf{A} = \mathbf{P} \mathbf{\Lambda} \mathbf{P}^{-1} \quad \lambda_k > \mathbf{0}$$

Expectation:

$$\mathbb{E}\left[\mathbf{Y}_{i}
ight]=\mu e^{-\mathbf{A}V_{i}}+eta(1-e^{-\mathbf{A}V_{i}})$$

Variance:

$$\mathbb{C} \text{ov} \left[\mathbf{Y}_{i}; \mathbf{Y}_{j} \right] = \mathbf{P} \left[\mathbf{W}_{ij} \odot \mathbf{P}^{-1} \mathbf{R} \mathbf{P}^{-T} \right] \mathbf{P}^{T}$$
$$\mathbf{W}_{ij} = \left[\frac{1}{\lambda_{q} + \lambda_{r}} e^{-\lambda_{q} V_{i}} e^{-\lambda_{r} V_{j}} \left(e^{(\lambda_{q} + \lambda_{r}) V_{ij}} - 1 \right) \right]_{1 \le q, r \le p}$$

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Multivariate OU

$$d \mathbf{X}_t = \mathbf{A}[\boldsymbol{\beta} - \mathbf{X}_t] d t + \mathbf{\Sigma} d \mathbf{B}_t$$

Diagonalizable: $\mathbf{A} = \mathbf{P} \mathbf{A} \mathbf{P}^{-1}$ $\lambda_k > 0$

Expectation:
$$\mathbb{E}[\mathbf{Y}_i] = \mu e^{-t}$$

$$\mathbb{E}\left[\mathbf{Y}_{i}\right] = \mu e^{-\mathbf{A}V_{i}} + \beta(1 - e^{-\mathbf{A}V_{i}})$$

Variance:

$$\mathbb{C}\text{ov}\left[\mathbf{Y}_{i};\mathbf{Y}_{j}\right] = \mathbf{P}\left[\mathbf{W}_{ij} \odot \mathbf{P}^{-1}\mathbf{R}\mathbf{P}^{-T}\right]\mathbf{P}^{T}$$
$$\mathbf{W}_{ij} = \left[\frac{1}{\lambda_{q}+\lambda_{r}}e^{-\lambda_{q}V_{i}}e^{-\lambda_{r}V_{j}}\left(e^{(\lambda_{q}+\lambda_{r})V_{ij}}-1\right)\right]_{1 \le q, r \le p}$$

Distribution:

Still Gaussian.

No nice Kronecker product.

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

General Model

 $\mathsf{BM},\,\mathsf{OU}:$ Instance of a general Gaussian propagation model.

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

General Model

BM, OU: Instance of a general Gaussian propagation model.



BM:
$$\mathbf{q}_j = \mathbf{I}_p$$
, $\mathbf{r}_j = \mathbf{0}_p$, $\mathbf{\Sigma}_j = \ell_j \mathbf{R}$.

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

General Model

BM, OU: Instance of a general Gaussian propagation model.



BM:
$$\mathbf{q}_j = \mathbf{I}_p$$
, $\mathbf{r}_j = \mathbf{0}_p$, $\mathbf{\Sigma}_j = \ell_j \mathbf{R}$.
OU: $\mathbf{q}_j = e^{-\mathbf{A}\ell_j}$, $\mathbf{r}_j = (\mathbf{I}_p - e^{-\mathbf{A}\ell_j})\beta_j$, $\mathbf{\Sigma}_j = \mathbf{S} - e^{-\mathbf{A}\ell_j}\mathbf{S}e^{-\mathbf{A}^T\ell_j}$.

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

General Model

BM, OU: Instance of a general Gaussian propagation model.



BM: $\mathbf{q}_j = \mathbf{I}_p$, $\mathbf{r}_j = \mathbf{0}_p$, $\mathbf{\Sigma}_j = \ell_j \mathbf{R}$. OU: $\mathbf{q}_j = e^{-\mathbf{A}\ell_j}$, $\mathbf{r}_j = (\mathbf{I}_p - e^{-\mathbf{A}\ell_j})\beta_j$, $\mathbf{\Sigma}_j = \mathbf{S} - e^{-\mathbf{A}\ell_j}\mathbf{S}e^{-\mathbf{A}^T\ell_j}$. Drift, shifts, Integrated OU...

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

General Model

BM, OU: Instance of a general Gaussian propagation model.



BM: $\mathbf{q}_j = \mathbf{I}_{\rho}$, $\mathbf{r}_j = \mathbf{0}_{\rho}$, $\mathbf{\Sigma}_j = \ell_j \mathbf{R}$. OU: $\mathbf{q}_j = e^{-\mathbf{A}\ell_j}$, $\mathbf{r}_j = (\mathbf{I}_{\rho} - e^{-\mathbf{A}\ell_j})\beta_j$, $\mathbf{\Sigma}_j = \mathbf{S} - e^{-\mathbf{A}\ell_j}\mathbf{S}e^{-\mathbf{A}^T\ell_j}$. Drift, shifts, Integrated OU...

Easy computations (Kalman filter)

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Intra-species variations Model



$$egin{array}{lll} {\sf Z}^r &\sim \mathcal{N}\left({m \mu}, {\sf F}
ight) & ext{root} \ {\sf Z}^j & \left| ~ {\sf Z}^{{\sf pa}(j)} &\sim \mathcal{N}\left({m q}_j {\sf Z}^{{\sf pa}(j)} + {m r}_j, ~ {m \Sigma}_j
ight) & ext{nodes} \end{array}$$

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Intra-species variations Model



Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Intra-species variations Model



Measurement Errors, Non phylogenetic variations, intra-species variations, ...

Multivariate BM Multivariate Ornstein-Uhlenbeck General Gaussian Model

Intra-species variations Model



Measurement Errors, Non phylogenetic variations, intra-species variations, ...

"Heritability":
$$\mathbf{h}^2 = \frac{V(\mathbf{Z}_{tips})}{V(\mathbf{Y})}$$

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Outline

1 Multidimensional Models

2 Heterogeneous Evolution

- Phylogenetic ANOVA
- Regime Painting
- Automatic Shift Detection

Heterogeneous Evolution

Regime Painting Automatic Shift Detection

Monkey Brain Example



Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Reminder: One way ANOVA

K groups, each with n_k data points:

$$y_{ki} = \mu_k + \sigma \epsilon_{ik}, \quad \epsilon_{ik} \sim \mathcal{N}(0, 1), \quad 1 \leq k \leq K, \quad 1 \leq i \leq n_k$$

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Reminder: One way ANOVA

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 $y_{ki} = \mu_k + \sigma \epsilon_{ik}, \quad \epsilon_{ik} \sim \mathcal{N}(0, 1), \quad 1 \leq k \leq K, \quad 1 \leq i \leq n_k$ One-way ANOVA:

 $\mathcal{H}_{0}: \mu_{k} = \mu_{l}, \ \forall 1 \leq k, l \leq K \quad vs \quad \mathcal{H}_{1}: \exists k, l \mid \mu_{k} \neq \mu_{l}$

Reminder: One way ANOVA

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 $\mathcal{H}_{0}: \mu_{k} = \mu_{I}, \ \forall 1 \leq k, I \leq K \quad \textit{vs} \quad \mathcal{H}_{1}: \exists k, I \mid \mu_{k} \neq \mu_{I}$

Group 1 as reference:

$$y_{ki} = \mu_1 + \beta_k + \sigma \epsilon_{ik}$$
, with $\beta_1 = 0$

Reminder: One way ANOVA

K groups, each with n_k data points:

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Group 1 as reference:

$$y_{ki} = \mu_1 + \beta_k + \sigma \epsilon_{ik}$$
, with $\beta_1 = 0$

One-way ANOVA:

$$\mathcal{H}_0: \beta_k = 0, \ \forall 2 \leq k \leq K \quad vs \quad \mathcal{H}_1: \exists k \mid \beta_k \neq 0$$

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Reminder: One way ANOVA

Group 1 as reference:

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Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Reminder: One way ANOVA

Group 1 as reference:

$$y_{ki} = \mu_1 + \beta_k + \sigma \epsilon_{ik}$$
, with $\beta_1 = 0$

Linear Model:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \sigma \mathbf{E}$$
 $\mathbf{X} = (\mathbf{1}, \mathbf{1}_2, \dots, \mathbf{1}_K)$ $\boldsymbol{\beta} = (\mu_1, \beta_2, \dots, \beta_K)^T$

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Reminder: One way ANOVA

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$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \sigma \mathbf{E}$$
 $\mathbf{X} = (\mathbf{1}, \mathbf{1}_2, \dots, \mathbf{1}_K)$ $\boldsymbol{\beta} = (\mu_1, \beta_2, \dots, \beta_K)^T$

One-way ANOVA is a Fisher global F test

$$\begin{aligned} \mathcal{H}_0 : \beta_k &= 0, \ \forall 2 \le k \le K \quad vs \quad \mathcal{H}_1 : \exists k \mid \beta_k \neq 0 \\ F &= \frac{\|\hat{\mathbf{y}} - \bar{\mathbf{y}}\|^2 / (K - 1)}{\|\mathbf{y} - \hat{\mathbf{y}}\|^2 / (n - K)} \underset{\mathcal{H}_0}{\sim} \mathcal{F}_{n - K}^{K - 1}. \end{aligned}$$

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Simulated Example

```
set.seed(18300718)
n <- 90
# Noise
eps <- rnorm(n, mean = 0, sd = 1)
# Groups
group <- as.factor(rep(c(1, 2, 3), each = n/3))
# Response variable
mu1 <- 2; mu2 <- -5; mu3 <- 2
y <- mu1 * (group == 1) + mu2 * (group == 2) + mu3 * (group == 3)
y <- y + eps</pre>
```

$$\mathbf{X} = \begin{pmatrix} 1 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 0 \\ 1 & 1 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 1 \end{pmatrix} \qquad \beta = \begin{pmatrix} \mu_1 \\ \mu_2 - \mu_1 \\ \mu_3 - \mu_1 \end{pmatrix}$$

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Simulated Example

plot(y, col = group)



Simulated Example

```
fitanova <- lm(y ~ group)
summary(fitanova)
##
## Call:
## lm(formula = y ~ group)
##
## Residuals:
##
      Min
              10 Median 30
                                    Max
## -2.8389 -0.6950 0.2115 0.6247 2.0544
##
## Coefficients:
##
             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 1.92023 0.17258 11.127 <2e-16 ***
## group2 -6.59378 0.24406 -27.017 <2e-16 ***
## group3 -0.02984 0.24406 -0.122 0.903
## ----
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.9452 on 87 degrees of freedom
## Multiple R-squared: 0.9176, Adjusted R-squared: 0.9157
## F-statistic: 484.4 on 2 and 87 DF, p-value: < 2.2e-16
```

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Phylogenetic One way ANOVA

Linear Model:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \sigma \mathbf{E}$$
 $\mathbf{X} = (\mathbf{1}, \mathbf{1}_2, \dots, \mathbf{1}_K)$ $\boldsymbol{\beta} = (\mu_1, \beta_2, \dots, \beta_K)^T$

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Phylogenetic One way ANOVA

Linear Model:

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Phylogenetic Errors (θ assumed to be known)

 $\mathbf{E} \sim \mathcal{N}(\mathbf{0}_n, \mathbf{V}(\boldsymbol{\theta}))$

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

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One-way ANOVA is a Fisher global F test

$$\begin{aligned} \mathcal{H}_0 : \beta_k &= 0, \ \forall 2 \le k \le K \quad \text{vs} \quad \mathcal{H}_1 : \exists k \mid \beta_k \neq 0 \\ F &= \frac{\|\hat{\mathbf{y}} - \bar{\mathbf{y}}\|_{\mathbf{V}(\theta)^{-1}}^2 / (K - 1)}{\|\mathbf{y} - \hat{\mathbf{y}}\|_{\mathbf{V}(\theta)^{-1}}^2 / (n - K)} \underset{\mathcal{H}_0}{\sim} \mathcal{F}_{n-K}^{K-1}. \end{aligned}$$

Simulated Example

```
set.seed(18300718)
n <- 90
# Tree
tree <- rphylo(n, 0.1, 0)</pre>
# Noise
eps <- rTrait(1, tree, "BM",</pre>
              parameters = list(ancestral.state = 0, sigma2 = 2))
# Groups
group <- as.factor(rep(c(1, 2, 3), each = n/3))
# Response variable
mu1 <- 2; mu2 <- -5; mu3 <- 2
y <- mu1 * (group == 1) + mu2 * (group == 2) + mu3 * (group == 3)
y <- y + eps
```

Simulated Example

par(mar = c(5, 0, 0, 0) + 0.1)
plot(tree, show.tip.label = FALSE, x.lim = 45)
phydataplot(y, tree, scaling = 0.1, offset = 4, col = group)



Simulated Example

```
fitanova <- lm(y ~ group)
summary(fitanova)
##
## Call:
## lm(formula = y ~ group)
##
## Residuals:
##
       Min
               10 Median
                                 30
                                         Max
## -15.9379 -4.7827 0.5931 5.0899 15.8830
##
## Coefficients:
##
             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 0.5436 1.2830 0.424 0.67282
## group2 -5.6136 1.8144 -3.094 0.00266 **
## group3 -0.6349 1.8144 -0.350 0.72725
## ----
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 7.027 on 87 degrees of freedom
## Multiple R-squared: 0.1166, Adjusted R-squared: 0.09629
## F-statistic: 5.741 on 2 and 87 DF. p-value: 0.004549
```

Simulated Example

```
fitphyanova <- phylolm(y ~ group, phy = tree)
summary(fitphyanova)
##
## Call:
## phylolm(formula = y ~ group, phy = tree)
##
   AIC logLik
##
  510.4 -251.2
##
##
## Raw residuals:
##
      Min
              10 Median 30
                                     Max
## -18.101 -5.858 -1.062 3.714 15.689
##
## Mean tip height: 26.0683
## Parameter estimate(s) using ML:
## sigma2: 1.911819
##
## Coefficients:
##
               Estimate StdErr t.value p.value
## (Intercept) 1.976426 2.174670 0.9088 0.3659
## group2 -6.852544 0.491231 -13.9497 <2e-16 ***
## group3 0.095371 0.500516 0.1905 0.8493
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## R-squared: 0.9624 Adjusted R-squared: 0.9615
```

Regime Painting

Phylogenetic ANOVA:

- Test for a known group structure (habitat, ...).
- Each group has its own expectation.

Regime Painting

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- Model selection using LRT, AIC, BIC, ...

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Example: OU optima



Regime Painting: Can we test that orange tips have a different optimum than others ?

Example: OU optima

(Butler and King, 2004)

Test of several evolutionary hypotheses for species of *Anolis bimaculatus*.



		-			
	BM	OU(1)	OU(3)	OU(4)	OU(LP)
$-2\log \mathcal{L}$	-34.66	-34.66	-40.21	-47.22	-49.69
AIC	-30.66	-26.66	-28.21	-33.22	-37.69
SIC	-28.39	-22.12	-21.40	-25.27	-30.88
LR		0	5.55	12.56	15.03
P value		1	.24	1028	.0046

Regime Painting

Regime Painting:

- Test for a known group structure (habitat, ...).
- Each group at the tip has its own process parameter (variance, selection strength, ...)
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R packages:

- OUwie (univariate) Beaulieu et al. (2012)
- mvMORPH (multivariate) Clavel et al. (2015)
Regime Painting

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Problem: Shifts (regimes) must be fixed a priori.

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Identifiability



Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Equivalencies



Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Equivalencies



Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Equivalencies



Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Equivalencies



Equivalent allocations *cannot* be distinguished from the data.

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Equivalencies



Equivalent allocations *cannot* be distinguished from the data. Parcimony Keep only solutions with the smallest number of shifts.

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

New World Monkeys

(Aristide et al., 2016)



Callithrix penicillata

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

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Automatic Shift Detection : Optimal Value of an OU

• SURFACE approximate, independent trait (Ingram and Mahler, 2013)

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- SURFACE approximate, independent trait (Ingram and Mahler, 2013)
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- PhylogeneticEM maximum likelihood, correlated traits (Bastide et al., 2017, 2018)

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Automatic Shift Detection : Variance of a BM

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Automatic Shift Detection : Variance of a BM

- RRW Bayesian, no regime (Lemey et al., 2010)
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- BAMM coupled with a birth-death model (Rabosky et al., 2013)

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Thank you for listening



Institut Montpelliérain Alexander Grothendieck

Appendices

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Model Selection: Penalized Likelihood

Idea
$$\hat{K} = \underset{0 \le K \le K_{\max}}{\operatorname{argmax}} \left\{ \log p_{\hat{\theta}_{K}}(Y) - \operatorname{pen}(K) \right\}$$
 (Univariate)



Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Model Selection: Penalized Likelihood

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Phylogenetic ANOVA Regime Painting Automatic Shift Detection

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(Univariate)



Collection of Models

Size of a collection of models Number of Equivalence Classes $|\mathcal{S}_{K}^{Pl}|$

•
$$\left| \mathcal{S}_{K}^{PI} \right| \leq {m+n-1 \choose K} = {\# \text{ of edges} \choose \# \text{ of shifts}}$$



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back

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- $\mapsto\,$ Generally dependent on the topology of the tree.



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- Recursive algorithm to compute $|\mathcal{S}_{K}^{PI}|$.
- $\mapsto\,$ Generally dependent on the topology of the tree.
 - Binary tree: $|\mathcal{S}_{K}^{PI}| = {\binom{2n-2-K}{K}} = {\binom{\# \text{ of edges}-\# \text{ of shifts}}{\# \text{ of shifts}}}$

 \mapsto See convex characters: Semple and Steel (2003)

Linking Shifts and Clustering

Assumption "No Homoplasy": 1 shift = 1 new color

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Linking Shifts and Clustering

Assumption "No Homoplasy": 1 shift = 1 new color



The No Homoplasy hypothesis is not respected.

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Linking Shifts and Clustering

Assumption "No Homoplasy": 1 shift = 1 new color



The No Homoplasy hypothesis is not respected.

Proposition "K shifts $\iff K + 1$ clusters"

Phylogenetic ANOVA Regime Painting Automatic Shift Detection

Definitions

- \mathcal{T} a rooted tree with *n* tips
- $N_{K}^{(\mathcal{T})} = |\mathcal{C}_{K}|$ the number of possible partitions of the tips in K clusters
- $A_{K}^{(T)}$ the number of possible *marked* partitions



Partitions in two groups for a binary tree with 3 tips

Difference between $N_2^{(\mathcal{T}_3)}$ and $A_2^{(\mathcal{T}_3)}$:

- $N_2^{(\mathcal{T}_3)} = 3$: partitions 1 and 2 are equivalent
- A₂^(T₃) = 4: one marked color ("white = ancestral state")

General Formula (Binary Case)

If \mathcal{T} is a binary tree, consider T_{ℓ} and \mathcal{T}_r the left and right sub-trees of \mathcal{T} . Then:

$$\begin{cases} N_{K}^{(\mathcal{T})} = \sum_{k_{1}+k_{2}=K} N_{k_{1}}^{(\mathcal{T}_{\ell})} N_{k_{2}}^{(\mathcal{T}_{r})} + \sum_{k_{1}+k_{2}=K+1} A_{k_{1}}^{(\mathcal{T}_{\ell})} A_{k_{2}}^{(\mathcal{T}_{r})} \\ A_{K}^{(\mathcal{T})} = \sum_{k_{1}+k_{2}=K} A_{k_{1}}^{(\mathcal{T}_{\ell})} N_{k_{2}}^{(\mathcal{T}_{r})} + N_{k_{1}}^{(\mathcal{T}_{\ell})} A_{k_{2}}^{(\mathcal{T}_{r})} + \sum_{k_{1}+k_{2}=K+1} A_{k_{1}}^{(\mathcal{T}_{\ell})} A_{k_{2}}^{(\mathcal{T}_{r})} \end{cases}$$

We get:

$$\mathcal{N}_{K+1}^{(\mathcal{T})} = \mathcal{N}_{K+1}^{(n)} = egin{pmatrix} 2n-2-K\ K \end{pmatrix}$$
 and $\mathcal{A}_{K+1}^{(\mathcal{T})} = \mathcal{A}_{K+1}^{(n)} = egin{pmatrix} 2n-1-K\ K \end{pmatrix}$

Recursion Formula (General Case)

If we are at a node defining a tree T that has p daughters, with sub-trees T_1, \ldots, T_p , then we get the following recursion formulas:

$$\begin{cases} N_{K}^{(\mathcal{T})} = \sum_{\substack{k_{1}+\dots+k_{p}=K \\ k_{1},\dots,k_{p}\geq 1}} \prod_{i=1}^{p} N_{k_{i}}^{(\mathcal{T}_{i})} + \sum_{\substack{l\subset [\![1,p]\!] \\ |l|\geq 2}} \sum_{\substack{k_{1}+\dots+k_{p}=K+|l|-1 \\ k_{1},\dots,k_{p}\geq 1}} \prod_{\substack{i\in I \\ k_{i},\dots,k_{p}\geq 1}} N_{k_{i}}^{(\mathcal{T}_{i})} \prod_{\substack{i\notin I \\ k_{i}}} N_{k_{i}}^{(\mathcal{T}_{i})} \end{cases}$$

No general formula. The result depends on the topology of the tree.

back