

Extensions to Local Estimation

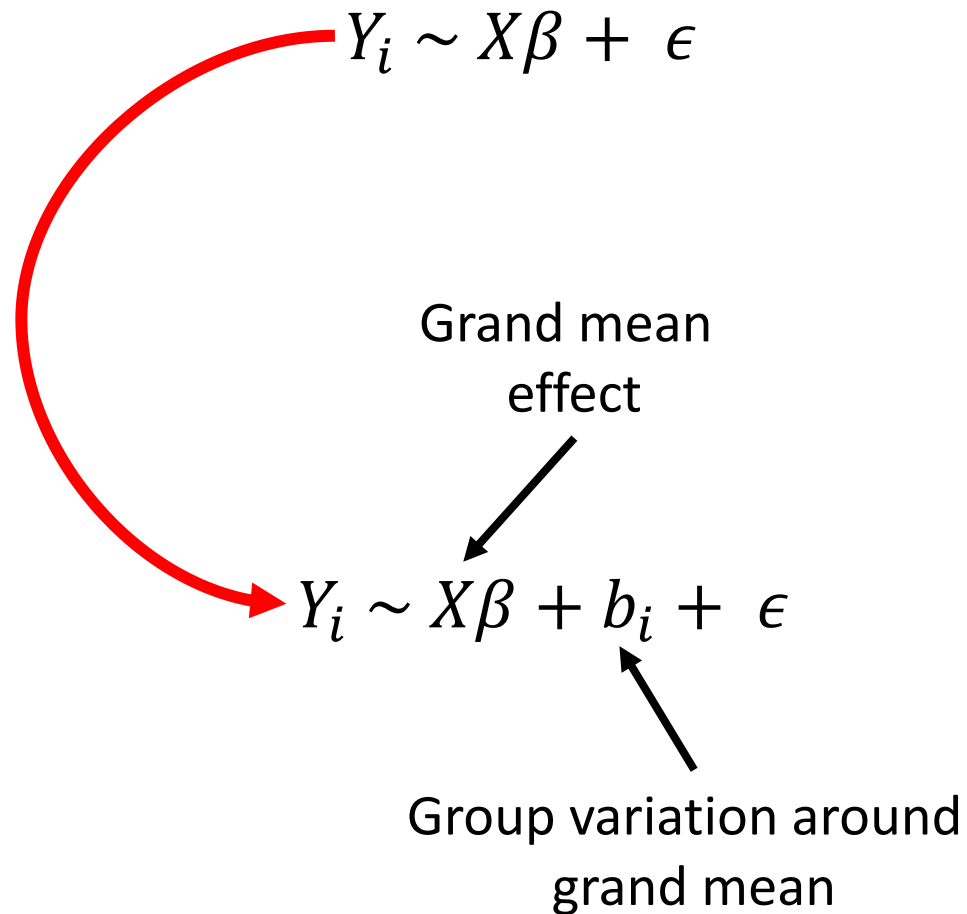
Overview

1. Mixed effects models
2. Pseudo- R^2 s
3. GLMM Example
4. GAM Example

1.1. Fixed vs. Random. Comparison

Fixed	Random
Interested in drawing inferences / making predictions	Not particularly interested in any particular value or level
Represent values from the entire 'universe' of interest	A (random) sample from a larger pool of potential values
Levels not interchangeable	Levels interchangeable (could swap / relabel levels without any change in meaning)
Directly manipulated	Introduces incidental error (e.g., between subjects, blocks, sites, etc.)
Few levels / worth sacrificing d.f. to fit model	Many levels / cannot sacrifice d.f. to fit model

1.1. Fixed vs. Random. From LM to LME



1.1. Fixed vs. Random. Why mixed models?

- More power than modeling the means of groups
- Reduces degrees of freedom necessary to fit model and estimate parameters (vs. modeling as a fixed effect)
- Accounts for uneven sampling within groups by using information across groups to inform the individual group means
- Can account for *non-independence* of observations by explicitly modeling their covariances (e.g., among sites, years, individuals, etc.)

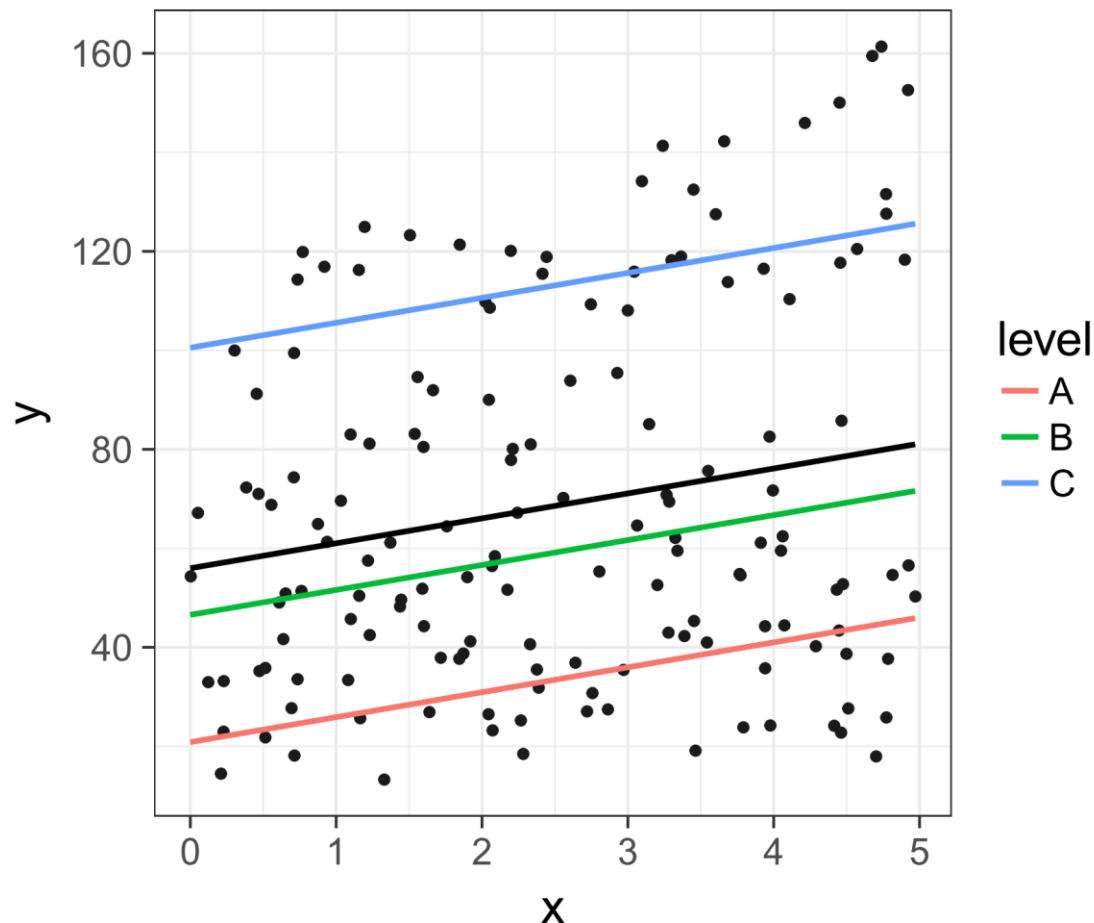
1.1. Fixed vs. Random. Random structure

Different configurations of random structure:

1. Varying intercept, fixed slope
2. Fixed intercept, varying slope
3. Varying intercept, varying slope

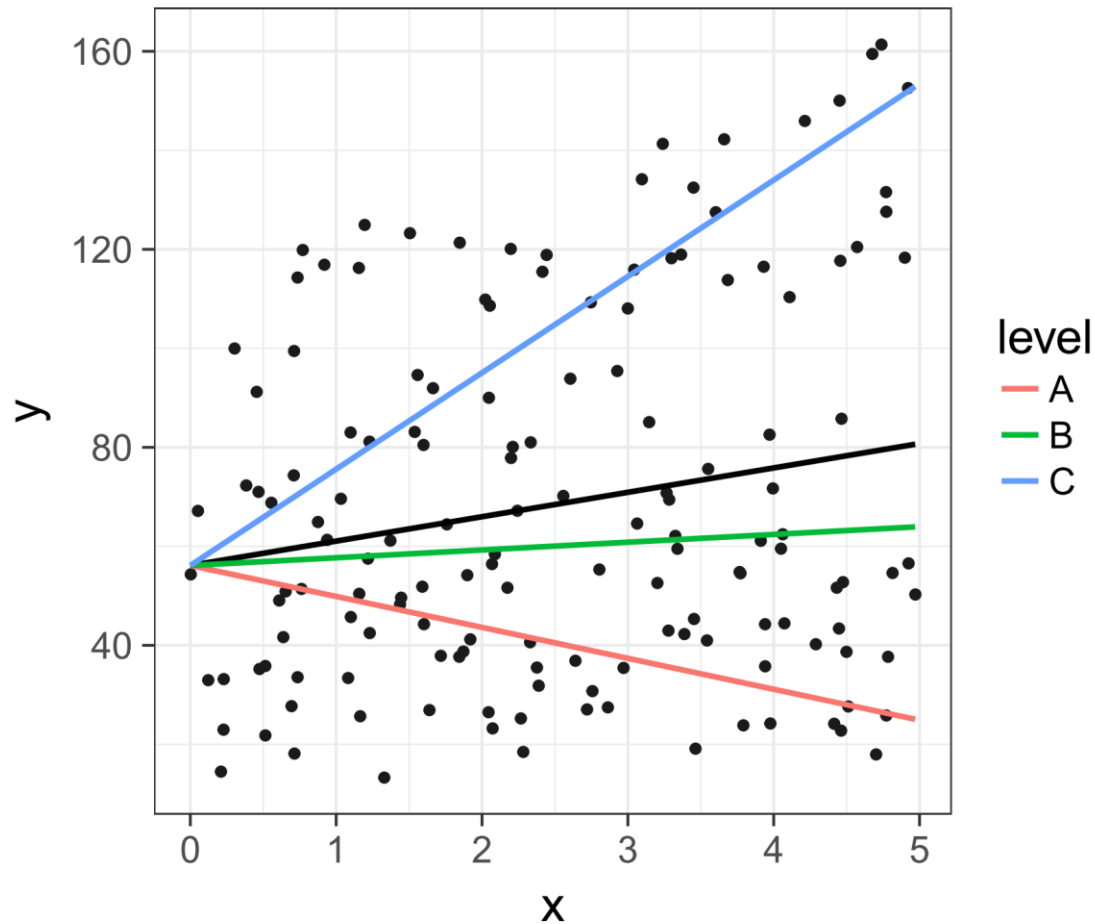
1.1. Fixed vs. Random. Varying intercept

- Estimates different intercept, same slope for all levels of the random effect (Good for block designs, repeated measures)



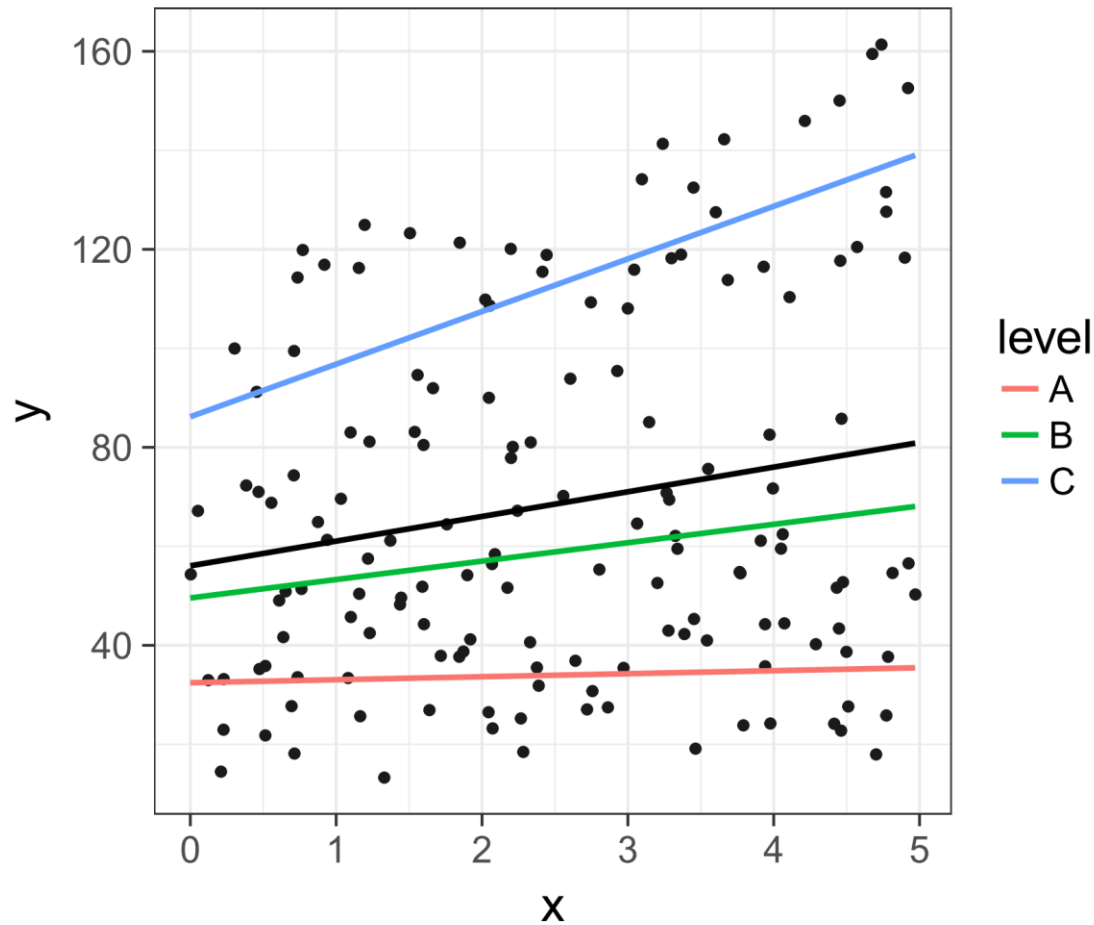
1.1. Fixed vs. Random. Varying slope

- Estimates different slope, same intercept for all levels



1.1. Fixed vs. Random. Varying intercept AND slope

- Estimates different slope, different intercept for all levels



1.1. Fixed vs. Random. Varying intercept AND slope

- Addresses multiple sources of non-independence of within and between levels, leading to lower Type I *and* Type II error
- Random slopes can be extracted and used in other analyses (lacks error)
- Computationally intensive, may lead to non-convergence

1.1. Fixed vs. Random. Nesting

- Hierarchical models represent nested random terms (e.g., site within region)
- Nesting further addresses non-independence by modeling correlations within *and* between levels of the hierarchy
- Good for stratified sampling designs (varying intercept) and split-plot designs (varying slope, varying intercept)

1.1. Fixed vs. Random. Random structures

$(1 group)$	random group intercept
$(x group) = (1+x group)$	random slope of x within group with correlated intercept
$(0+x group) = (-1+x group)$	random slope of x within group: no variation in intercept
$(1 group) + (0+x group)$	uncorrelated random intercept and random slope within group
$(1 site/block) = (1 site)+(1 site:block)$	intercept varying among sites and among blocks within sites (nested random effects)
$site+(1 site:block)$	<i>fixed</i> effect of sites plus random variation in intercept among blocks within sites
$(x site/block) = (x site)+(x site:block) = (1 + x site)+(1+x site:block)$	slope and intercept varying among sites and among blocks within sites
$(x1 site)+(x2 block)$	two different effects, varying at different levels
$x*site+(x site:block)$	fixed effect variation of slope and intercept varying among sites and random variation of slope and intercept among blocks within sites
$(1 group1)+(1 group2)$	intercept varying among crossed random effects (e.g. site, year)

1.1. Fixed vs. Random. A warning

- Assumes fixed and random effects are *uncorrelated*
- If possible, fit random effects as fixed effects and compare parameter estimates of other predictors
- Need to ensure appropriate replication at *lowest* level of nested factors (5-6 levels, *minimum*) – otherwise, fit as fixed effects

1.1. Fixed vs. Random. Different distributions

- *lme4* can fit many kinds of different distributions using `glmer`
- Does not provide *P*-values (d.d.f uncertain, see: <https://stat.ethz.ch/pipermail/r-help/2006-May/094769.html>)
 - *piecewiseSEM* uses *pbkrtest* package which estimates d.d.f. using the Kenward-Rogers approximation (less finicky than *lmerTest*)
 - *piecewiseSEM* does this for you automatically using `coefs`

1.1. Fixed vs. Random. Different distributions

- *nlme* can only handle normal distributions
 - Ives (2015): “For testing the significance of regression coefficients, go ahead and log-transform count data”
- `glmmPQL` in the *MASS* package uses penalized quasi-likelihood to fit models, can incorporate many different distributions and their quasi- equivalents (e.g., quasi-Poisson)
 - Quasi-distributions estimate a separate term for how the variance scales with the mean, so ideal for over/under-dispersed data
 - Quasi-likelihood means no likelihood based statistics (e.g., AIC, LRT, etc.) for any models fit with `glmmPQL`

1.1. Fixed vs. Random. Testing significance

- No matter what reviewers insist, you cannot test significance of random effects
- If you want to assess significance, model them as fixed effects
- Alternatives:
 - Drop random effects and compare to mixed model using AIC/BIC
 - Examine variance components using `varcomp`
 - If they are sufficiently large relative to residual variance probably worth keeping them in
 - Compare conditional and marginal R^2 s
 - Defend yourself philosophically: these are known sources of variation, why not account for them, even if they don't contribute, better safe than sorry!

1.1. Fixed vs. Random. Testing significance

- R has the most infuriating error messages
- Can sometimes solve by switching to a different optimizer
 - `lmeControl(opt = "optim")` usually works
- Reduce tolerance for convergence
 - `lmeControl(tol = 1e-4)`
- Respecify random structure
 - Optimizer constrained to have $\text{cov} > 0$, can sometimes get stuck bouncing around when random components are very close to 0
- <https://stackoverflow.com/>

1.2. Pseudo- R^2 s

1.2. Pseudo- R^2 s. Omnibus test

- Fisher's C/χ^2 is the global fit statistic for local estimation but has many shortcomings:
 - Sensitive to the number of d-sep tests and the complexity of the model (harder to reject as the complexity increases)
 - Sensitive to the size of the dataset (e.g., high n leads to low P)
 - Fails symmetry when dealing with unlinked non-normal intermediate variables
 - Cannot be computed for saturated models

1.2. Pseudo- R^2 s. Local tests

- How do we infer the confidence in our SEM?
 - Examine standard errors of individual paths, qualitatively assess cumulative precision
 - Explore variance explained (i.e., R^2), qualitatively assess cumulative precision

1.2. Pseudo- R^2 s. General linear regression

- Coefficient of determination (R^2) = proportion of variance in response explained by fixed effects
- For OLS regression, simply $1 -$ the ratio of unexplained (error) variance (e.g., SS_{error}) over the total explained variance (e.g., SS_{total})
- Ranges $(0, 1)$, independent of sample size
- Not good for model comparisons since R^2 monotonically increases with model complexity (go to AIC which is penalized for complexity)

1.2. Pseudo- R^2 s. Generalized linear regression

- Likelihood estimation is not attempting to minimize variance but instead obtain parameters that maximize the likelihood of having observed the data
- In a likelihood framework, equivalent $R^2 = 1 - \frac{\text{log-likelihood of the null (intercept-only) model}}{\text{log-likelihood of the full model}}$
- Leads to identical R^2 as OLS for normal (Gaussian) distributions, not so for GLM – need to use likelihood-based pseudo- R^2 (e.g., McFadden, Nagelkerke)

1.2. Pseudo-R²s. Generalized mixed models

- Becomes even worse for mixed models because variance is partitioned among levels of the random factor, so what is the error variance?
- Need a new formulation of R²:
 - Marginal R² = variance explained by fixed effects only

$$R_{\text{GLMM}(m)}^2 = \frac{\sigma_f^2}{\sigma_f^2 + \sum_{l=1}^u \sigma_l^2 + \sigma_e^2 + \sigma_d^2}$$

The diagram illustrates the components of the Marginal R-squared formula for Generalized Linear Mixed Models (GLMMs). The formula is $R_{\text{GLMM}(m)}^2 = \frac{\sigma_f^2}{\sigma_f^2 + \sum_{l=1}^u \sigma_l^2 + \sigma_e^2 + \sigma_d^2}$. Four orange arrows point from text labels to specific terms in the formula:

- An arrow from "Fixed effects variance" points to the σ_f^2 in the numerator.
- An arrow from "Fixed effects variance" also points to the σ_f^2 in the denominator.
- An arrow from "Random effects variance" points to the summation term $\sum_{l=1}^u \sigma_l^2$ in the denominator.
- An arrow from "Residual variance" points to the σ_e^2 term in the denominator.
- An arrow from "Distribution-specific variance" points to the σ_d^2 term in the denominator.

1.2. Pseudo-R²s. Generalized mixed models

- Conditional R² = variance explained by both the fixed and random effects

The diagram illustrates the formula for the conditional R-squared value in a Generalized Linear Mixed Model (GLMM). The formula is:

$$R_{\text{GLMM}(c)}^2 = \frac{\sigma_f^2 + \sum_{l=1}^u \sigma_l^2}{\sigma_f^2 + \sum_{l=1}^u \sigma_l^2 + \sigma_e^2 + \sigma_d^2}$$

Orange arrows point from descriptive labels to the corresponding terms in the formula:

- Fixed effects variance** points to σ_f^2 in the numerator.
- Random effects variance** points to $\sum_{l=1}^u \sigma_l^2$ in the numerator.
- Fixed effects variance** points to σ_f^2 in the denominator.
- Random effects variance** points to $\sum_{l=1}^u \sigma_l^2$ in the denominator.
- Residual variance** points to σ_e^2 in the denominator.
- Distribution-specific variance** points to σ_d^2 in the denominator.

1.2. Pseudo- R^2 s. Generalized mixed models

- Comparison of marginal and conditional R^2 can lead to roundabout assessment of 'significance' of the random effects (e.g., if conditional R^2 is larger relative to marginal R^2)
- Best to report both and allow readers to determine how their magnitude affects the inferences

1.3. GLMM Example

1.3. SEM Example. Shipley 2009

- Hypothetical dataset: predicting latitude effect on survival of a tree species
- Repeated measures on 5 subjects at 20 sites from 1970-2006
- Survival (0/1) influenced by phenology (degree days until bud break, Julian days until bud break), size (stem diameter growth)



1.3. SEM Example. Shipley 2009

- Two distributions: normal, binary (survival)
- Random effects:
 - Site-only: latitude
 - Site and year: degree days, date
 - Site, year, and subject: diameter, survival



1.3. SEM Example. What is the basis set?



- $\text{Date} \perp \text{Lat} \mid (\text{Degree days})$
- $\text{Growth} \perp \text{Lat} \mid (\text{Date})$
- $\text{Survival} \perp \text{Lat} \mid (\text{Growth})$
- $\text{Growth} \perp \text{Degree days} \mid (\text{Date}, \text{Lat})$
- $\text{Survival} \perp \text{Degree days} \mid (\text{Growth}, \text{Lat})$
- $\text{Survival} \perp \text{Date} \mid (\text{Growth}, \text{Degree days})$

1.3. SEM Example. List of equations



```
library(piecewiseSEM)
library(nlme)
library(lme4)

# Load data
data(shipley); shipley <- na.omit(shipley)

# Create list of structural equations
shipley.sem <- psem(
  lme(DD ~ lat, random = ~1|site/tree, na.action = na.omit,
    data = shipley),
  lme(Date ~ DD, random = ~1|site/tree, na.action = na.omit,
    data = shipley),
  lme(Growth ~ Date, random = ~1|site/tree, na.action = na.omit,
    data = shipley),
  glmer(Live ~ Growth + (1|site) + (1|tree),
    family = binomial(link = "logit"), data = shipley)
)
```



1.3. SEM Example. D-sep tests



```
# Get summary  
summary(shipley.sem)
```

```
Structural Equation Model of shipley.sem
```

```
Call:  
  DD ~ lat  
  Date ~ DD  
  Growth ~ Date  
  Live ~ Growth
```

```
      AIC  
21745.782
```

```
---
```



1.3. SEM Example. D-sep tests



Tests of directed separation:

Independ.Claim	Test.Type	DF	Crit.Value	P.Value
Date ~ lat + ...	coef	18	-0.0798	0.9373
Growth ~ lat + ...	coef	18	-0.8929	0.3837
Live ~ lat + ...	coef	1431	1.0280	0.3039
Growth ~ DD + ...	coef	1329	-0.2967	0.7667
Live ~ DD + ...	coef	1431	1.0046	0.3151
Live ~ Date + ...	coef	1431	-1.5617	0.1184

--

Global goodness-of-fit:

Chi-Squared = NA with P-value = NA and on 6 degrees of freedom

Fisher's C = 11.536 with P-value = 0.484 and on 12 degrees of freedom

Warning message:

check model convergence: log-likelihood estimates lead to negative chi-squared!



1.3. SEM Example. D-sep tests



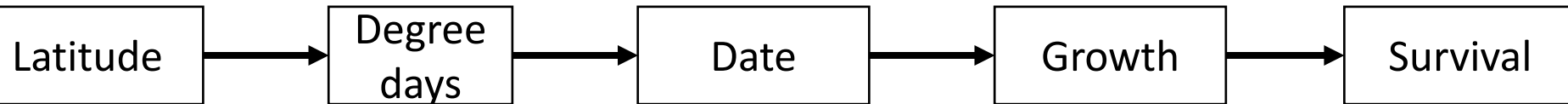
```
# Look at problematic model & variance components
Live.model <- glmer(Live ~ Growth + Date + DD + lat + (1|site) +
(1|tree), family = binomial(link = "logit"), data = shipley)
boundary (singular) fit: see ?issingular
```

```
VarCorr(Live.model)
```

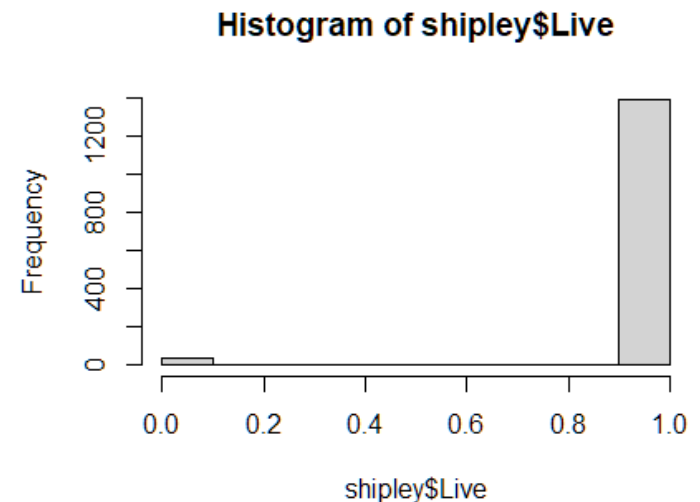
Groups	Name	Std.Dev.
tree	(Intercept)	0
site	(Intercept)	0



1.3. SEM Example. D-sep tests



- Re-specify random structure
- Still no positive χ^2 statistic ☹️
- Consider other distributions (e.g., negative binomial)
- Revert to d-sep test



1.3. SEM Example. D-sep tests



Coefficients:

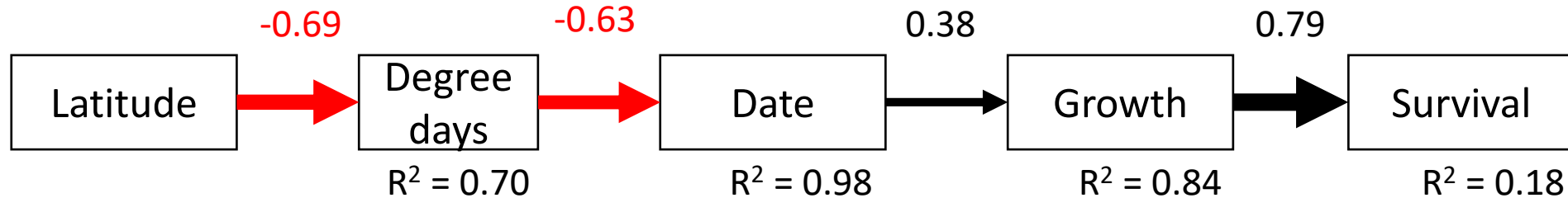
Response	Predictor	Estimate	Std.Error	DF	Crit.Value	P.Value	Std.Estimate
DD	lat	-0.8355	0.1194	18	-6.9960	0	-0.6877 ***
Date	DD	-0.4976	0.0049	1330	-100.8757	0	-0.6281 ***
Growth	Date	0.3007	0.0266	1330	11.2.917	0	0.3824 ***
Live	Growth	0.3479	0.0584	1431	5.9552	0	0.7866 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05

Individual R-squared:

Response	method	Marginal	Conditional
DD	none	0.49	0.70
Date	none	0.41	0.98
Growth	none	0.11	0.84
Live	delta	0.16	0.18

1.3. SEM Example. Populate final model



Coefficients:

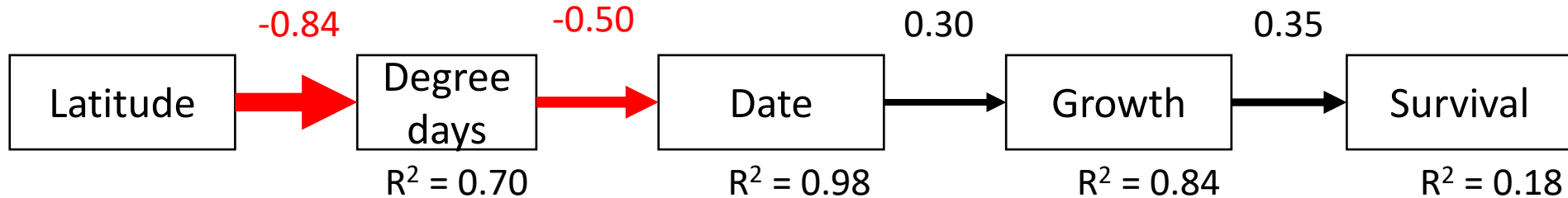
Response	Predictor	Estimate	Std.Error	DF	Crit.Value	P.Value	Std.Estimate
DD	lat	-0.8355	0.1194	18	-6.9960	0	-0.6877 ***
Date	DD	-0.4976	0.0049	1330	-100.8757	0	-0.6281 ***
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Individual R-squared:

Response	method	Marginal	Conditional
DD	none	0.49	0.70
Date	none	0.41	0.98
Growth	none	0.11	0.84
Live	delta	0.16	0.18

1.3. SEM Example. Refit using *lavaan*



...

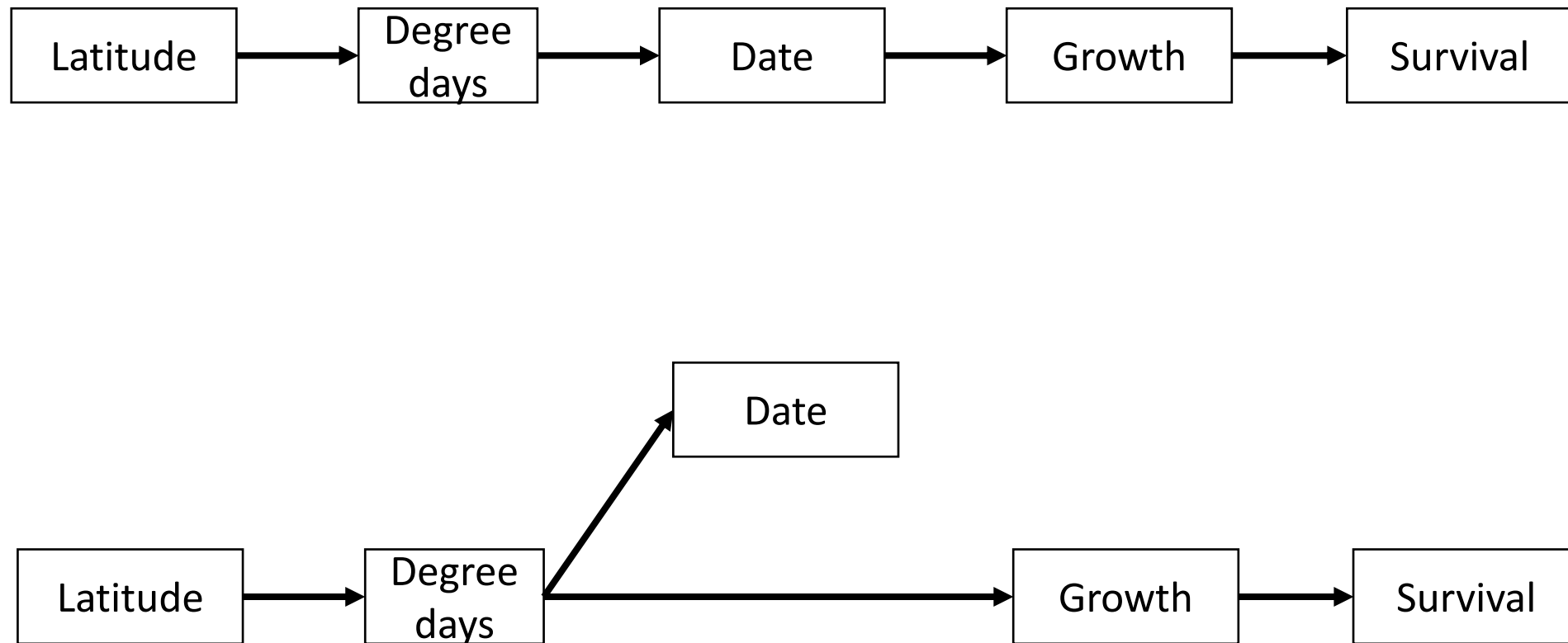
Estimator	ML
Model Fit Test Statistic	38.433
Degrees of freedom	6
P-value (Chi-square)	0.000

...

Regressions:

	Estimate	Std.Err	z-value	P(> z)
DD ~				
lat	-0.860	0.023	-37.923	0.000
Date ~				
DD	-0.517	0.016	-32.525	0.000
Growth ~				
Date	0.173	0.020	8.508	0.000
Live ~				
Growth	0.006	0.001	9.854	0.000

1.3. SEM Example. Compare these models

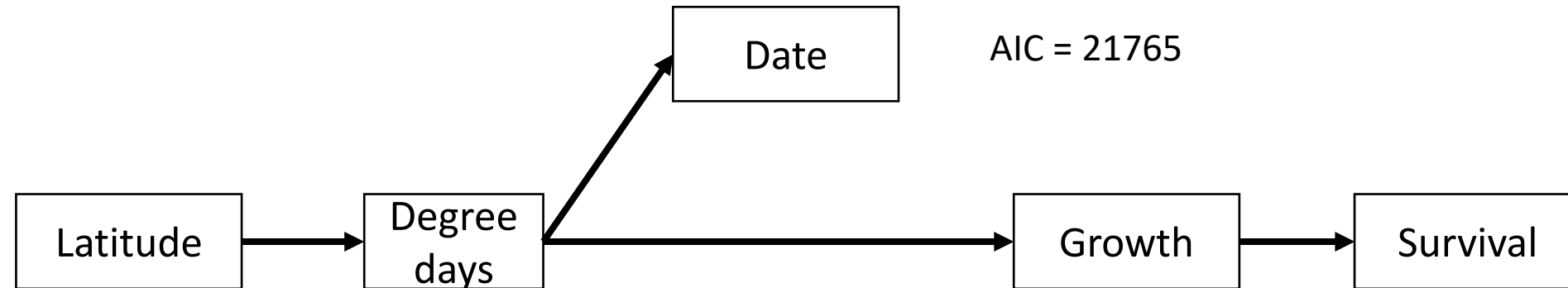


1.3. SEM Example. Compare these models

AIC = 21745



AIC = 21765

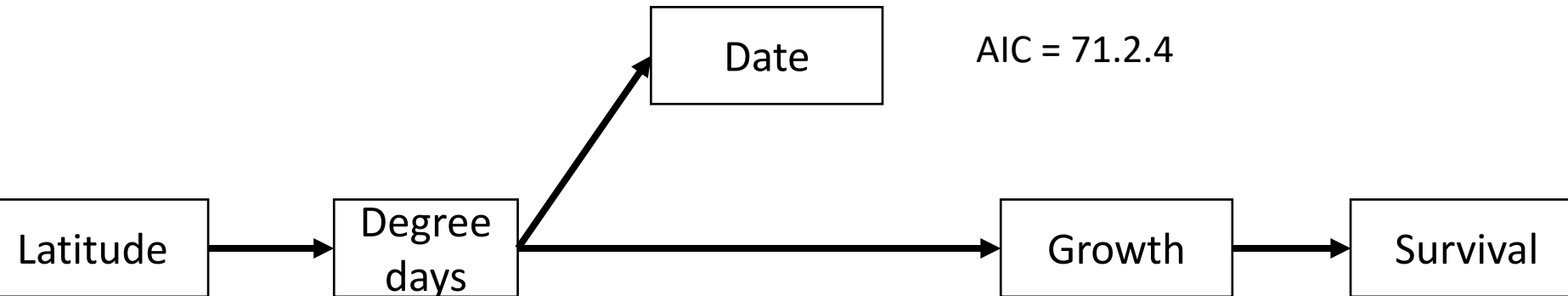


1.3. SEM Example. Compare these models (d-sep)

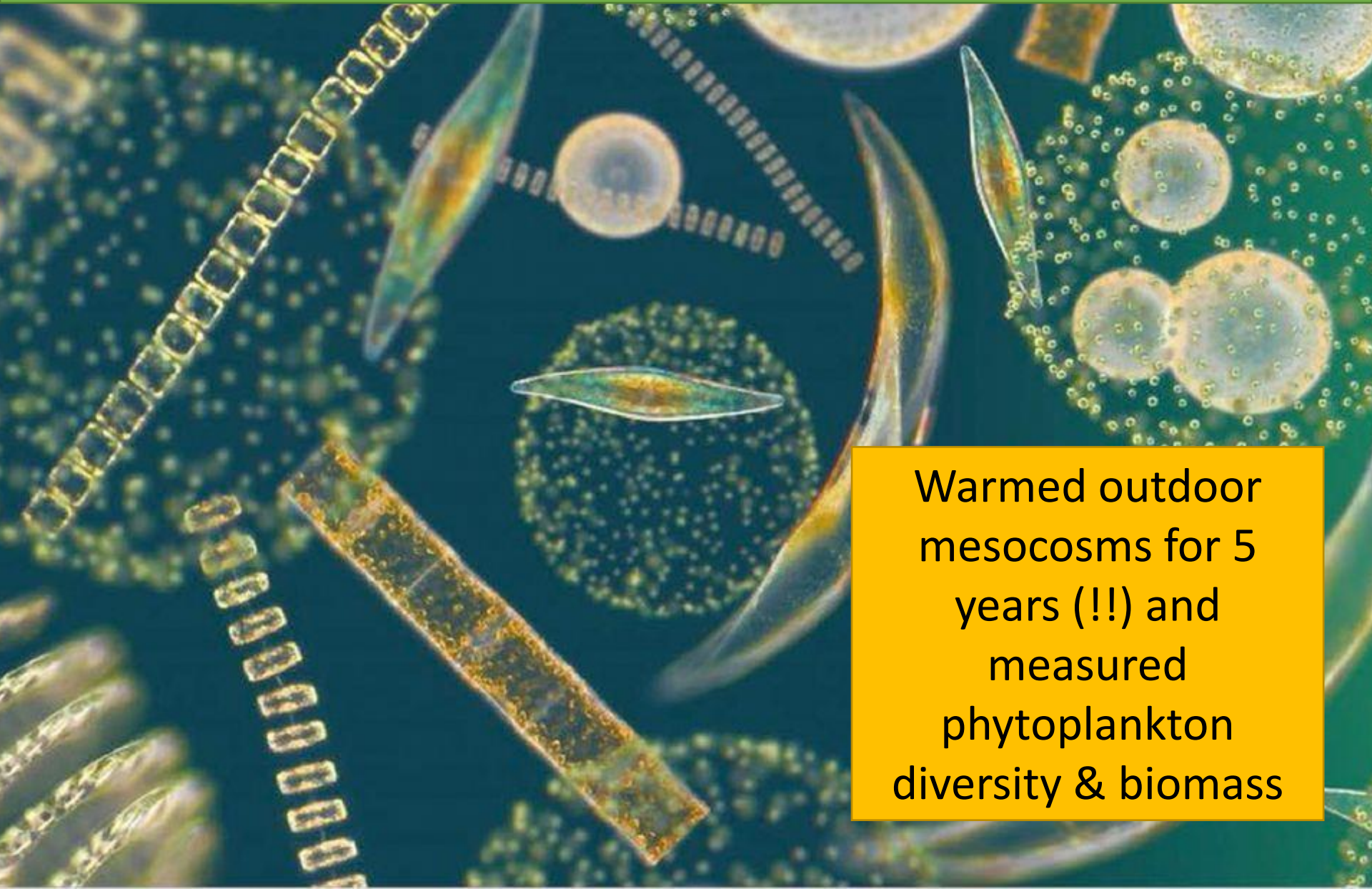
AIC = 49.54



AIC = 71.2.4

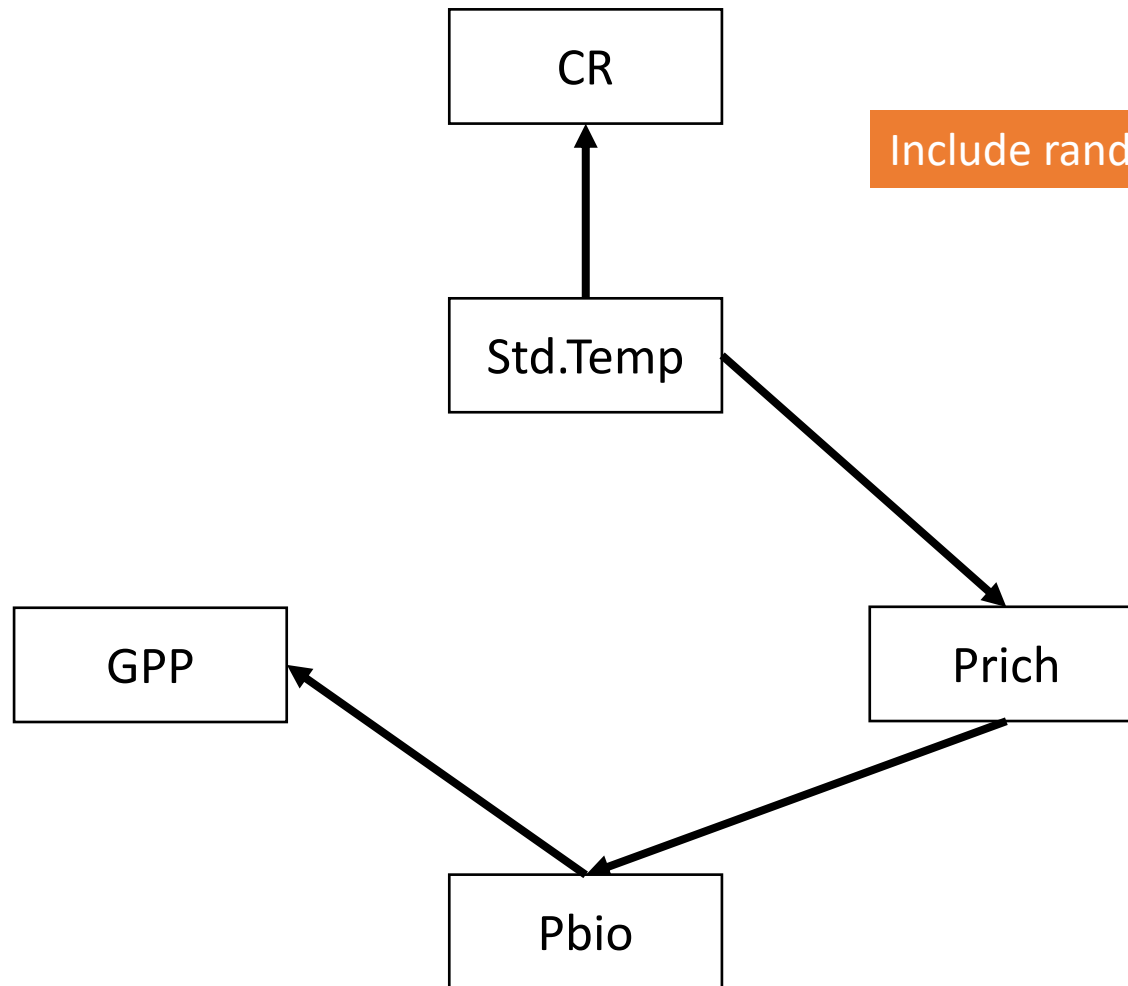


Yvon-Durocher et al (2015): Experimental warming on phytoplankton diversity and biomass



Warmed outdoor mesocosms for 5 years (!!) and measured phytoplankton diversity & biomass

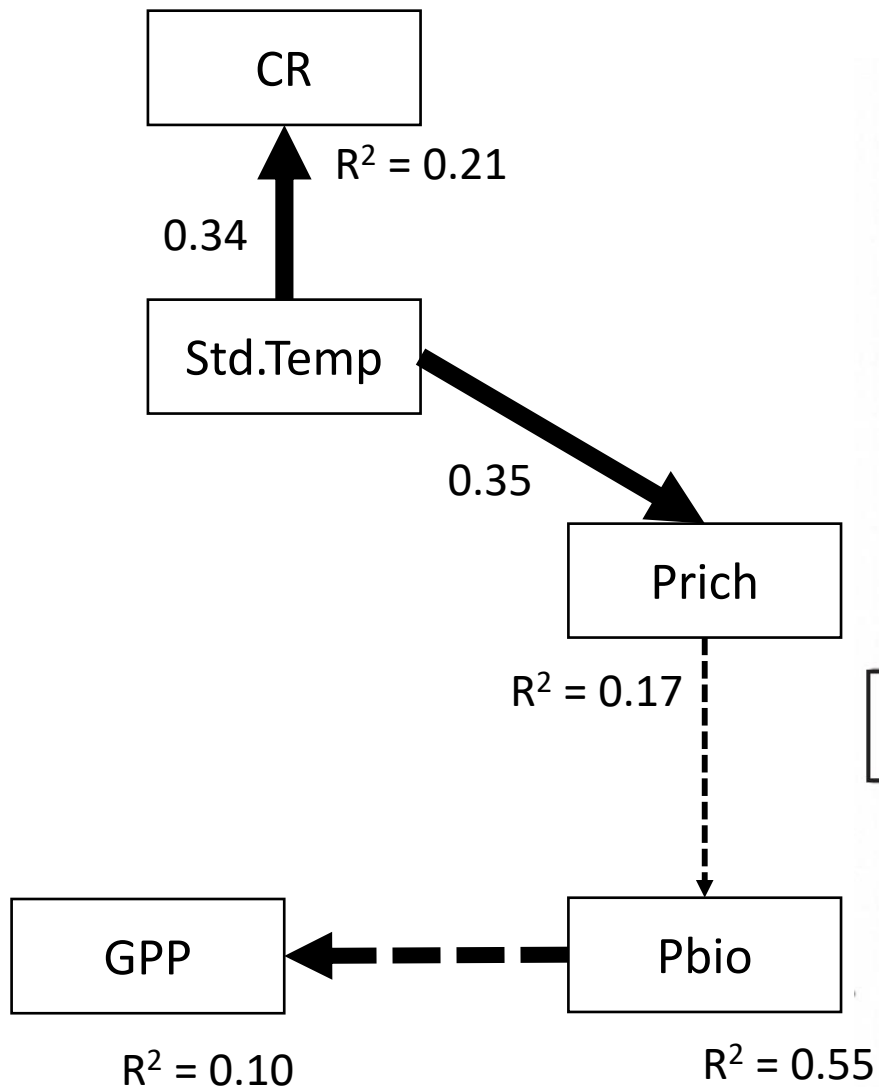
ACTIVITY. Fit Durocher dataset



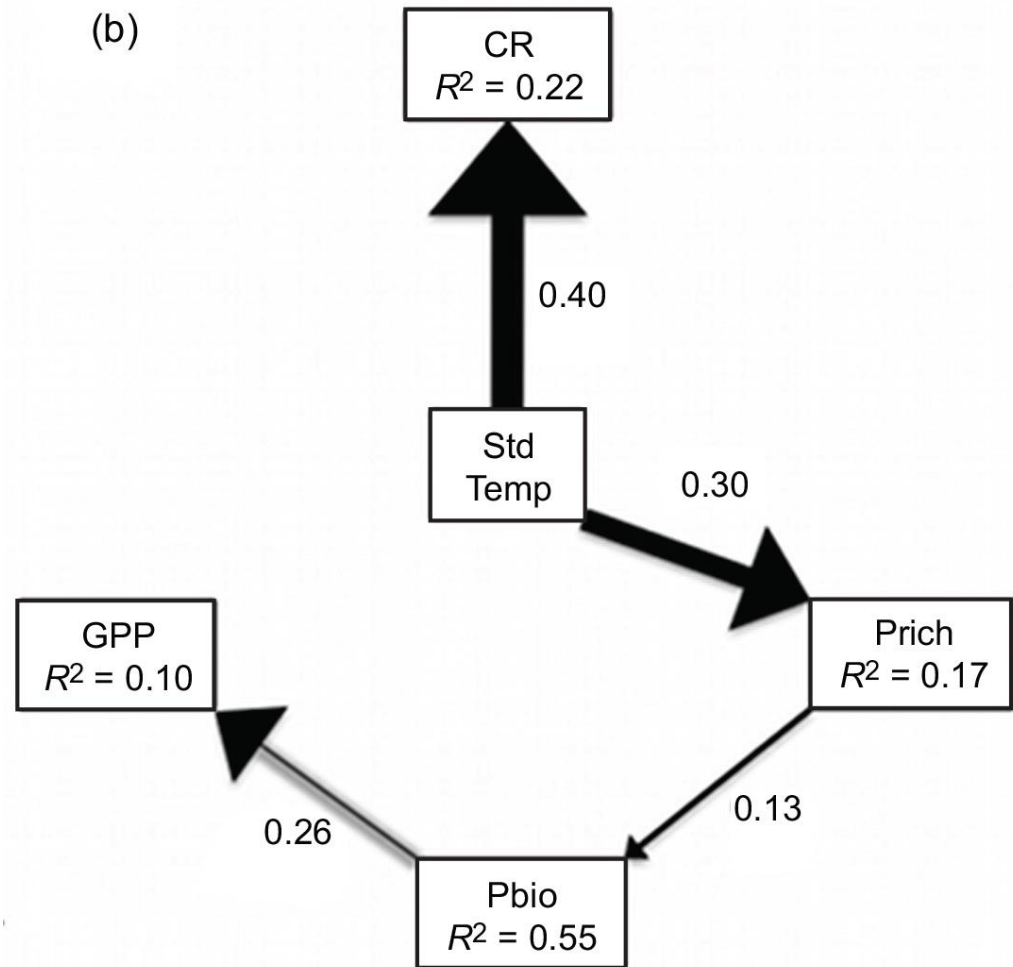
Include random effect of Pond.ID!

1.3. SEM Example. Your turn...

Model-wide $P = 0.063$ or $P < 0.001$



(b)



1.3. SEM Example. Your turn...

- Try removing incomplete cases first: `complete.cases`
 - What is their mistake here?
- Methods state: “with multiple measurements of variables made seasonally, nested within replicate mesocosms,” but then, “a path model as a set of hierarchical linear mixed effects models, each of which included hypothesized relationships between a response variable and a set of predictors as fixed effects and mesocosm ID as a random effect on the intercept.”
 - Play with the random structure?
- What about by treatment (Ambient vs. Heated)?
- Can anyone reproduce this result? Is it time to write a response?

1.4. GAM Example

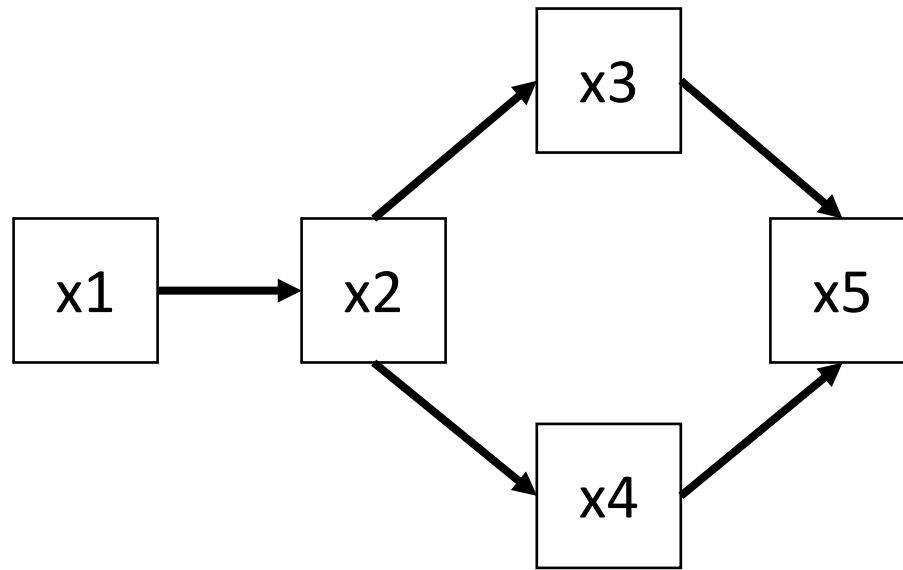
1.4. Generate example data

- Example data from appendix of Shipley and Douma using a mix of non-normal and non-linear variables

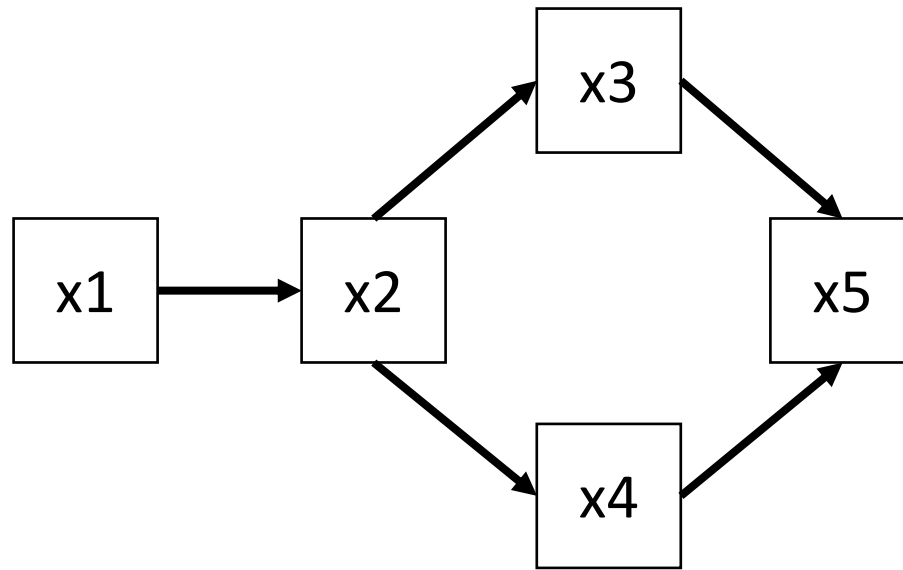
```
# Generate data from paper
set.seed(100)
n <- 100
x1 <- rchisq(n, 7)
mu2 <- 10*x1/(5 + x1)
x2 <- rnorm(n, mu2, 1)
x2[x2 <= 0] <- 0.1
x3 <- rpois(n, lambda = (0.5*x2))
x4 <- rpois(n, lambda = (0.5*x2))
p.x5 <- exp(-0.5*x3 + 0.5*x4)/(1 + exp(-0.5*x3 + 0.5*x4))
x5 <- rbinom(n, size = 1, prob = p.x5)
dat2 <- data.frame(x1 = x1, x2 = x2, x3 = x3, x4 = x4, x5 = x5)
```



1.4. Fit this SEM using `lm` and get GoF

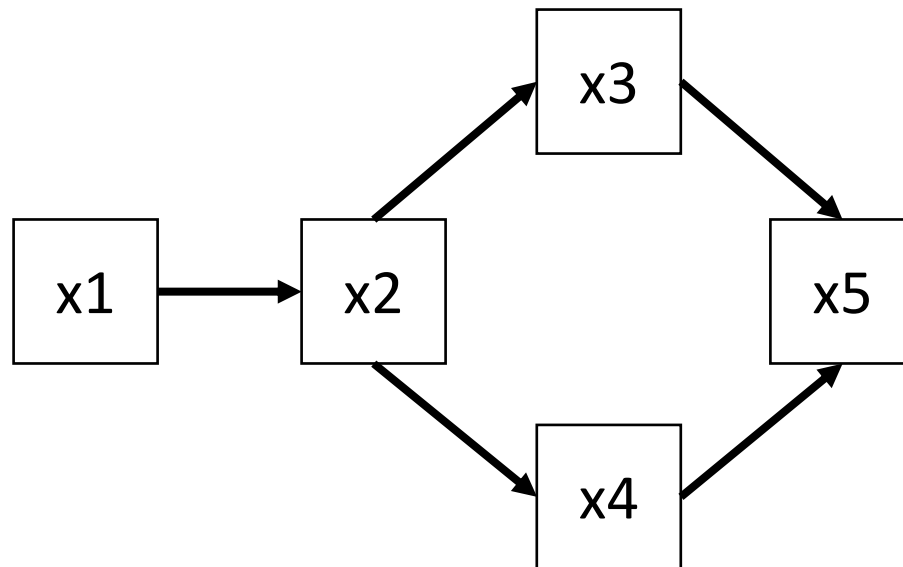


1.4. Fit this SEM using `lm` and get GoF



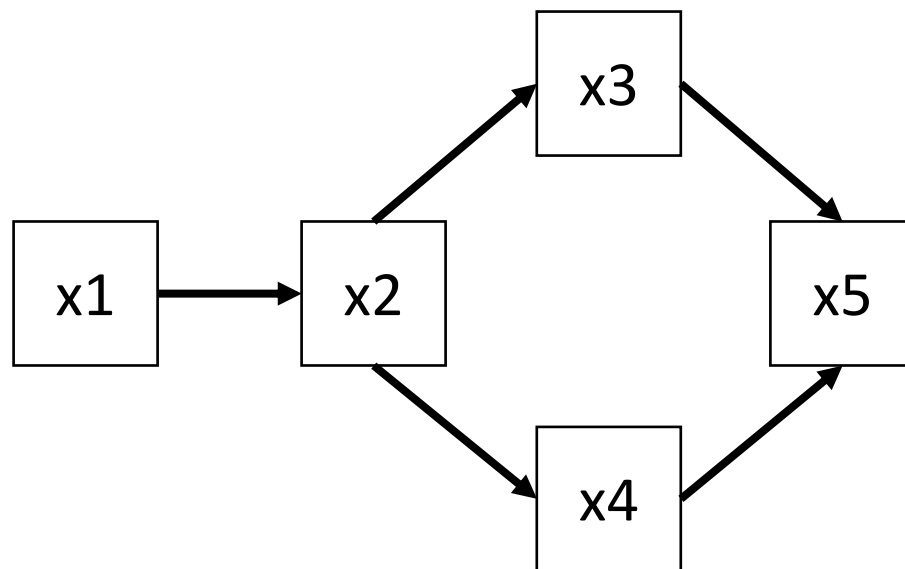
```
LLchisq(shipley_psem2)  
  Chisq df P.value  
1  4.143   5    0.529
```


1.4. Fit using GAM and GLM



```
shipleypsem3 <- psem(  
  gam(x2 ~ s(x1), data = dat2, family = gaussian),  
  glm(x3 ~ x2, data = dat2, family = poisson),  
  gam(x4 ~ x2, data = dat2, family = poisson),  
  glm(x5 ~ x3 + x4, data = dat2, family = binomial)  
)
```

1.4. Fit using GAM and GLM

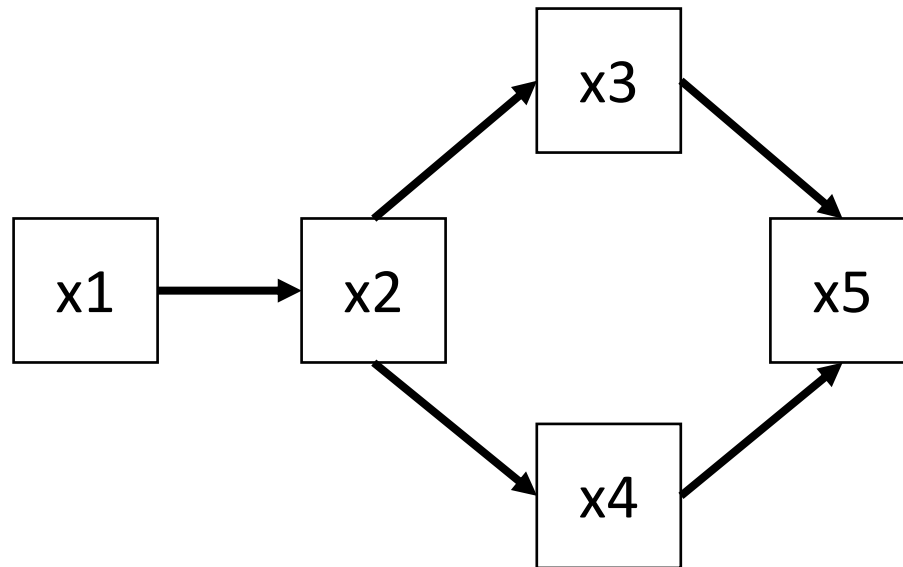


```
# Get goodness-of-fit  
LLchisq(shipley_psem2)
```

	Chisq	df	P.value
1	4.143	5	0.529



1.4. Fit using GAM and GLM



```
# Compare linear and non-linear models  
AIC(shipley_psem2, shipley_psem3)
```

	AIC	K	n
1	1240.20	13.000	100
2	1190.75	11.563	100

1.4. Truly Non-Linear Implementations

- Possible to compare models with the same typology but different ML fitting functions and forms (or nested models)
- Do not get coefficients returned by `coefs` because smoothed terms are non-linear functions
- How to present this path diagram???

1.4. Truly Non-Linear Implementations

- Piecewise SEM can be extended to many different model types: as long as you can get a P -value or compute a log-likelihood, you can estimate fit
 - Matrix regression (Barnes et al. 2016)
 - Spatially-explicit models