## Mixed models in R using the Ime4 package Part 5: Generalized linear mixed models

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## Generalized Linear Mixed Models

- When using linear mixed models (LMMs) we assume that the response being modeled is on a continuous scale.
- Sometimes we can bend this assumption a bit if the response is an ordinal response with a moderate to large number of levels. For example, the Scottish secondary school test results in the mlmRev package are integer values on the scale of 1 to 10 but we analyze them on a continuous scale.
- However, an LMM is not suitable for modeling a binary response, an ordinal response with few levels or a response that represents a count. For these we use generalized linear mixed models (GLMMs).
- To describe GLMMs we return to the representation of the response as an n-dimensional, vector-valued, random variable,  $\mathcal{Y}$ , and the random effects as a q-dimensional, vector-valued, random variable,  $\mathcal{B}$ .



#### Parts of LMMs carried over to GLMMs

- Random variables
  - ${oldsymbol{\mathcal{Y}}}$  the response variable
  - ${\cal B}$  the (possibly correlated) random effects
  - ${\cal U}$  the orthogonal random effects
- Parameters
  - $oldsymbol{eta}$  fixed-effects coefficients
  - $\sigma$  the common scale parameter (not always used)
  - $m{ heta}$  parameters that determine  $\mathrm{Var}(m{\mathcal{B}}) = \sigma^2 m{\Lambda} m{\Lambda}'$
- Some matrices
  - $\boldsymbol{X}$  the  $n \times p$  model matrix for  $\boldsymbol{\beta}$
  - ${m Z}$  the n imes q model matrix for  ${m b}$
  - P fill-reducing  $q \times q$  permutation (from Z)
  - ${f \Lambda}({m heta})$  relative covariance factor, s.t.  ${\sf Var}({m {\cal B}}) = \sigma^2 {f \Lambda} {f \Lambda}'$

$$U(\theta) = Z\Lambda(\theta)$$

## The conditional distribution, $\mathcal{Y}|\mathcal{U}$

- For GLMMs, the marginal distribution,  $\mathcal{B} \sim \mathcal{N}\left(\mathbf{0}, \mathbf{\Sigma}(\boldsymbol{\theta})\right)$  is the same as in LMMs except that  $\sigma^2$  is omitted. We define  $\mathcal{U} \sim \mathcal{N}(\mathbf{0}, I_q)$  such that  $\mathcal{B} = \mathbf{\Lambda}(\boldsymbol{\theta})\mathcal{U}$ .
- For GLMMs we retain some of the properties of the conditional distribution

$$(\mathcal{Y}|\mathcal{U}=u)\sim\mathcal{N}\left(\mu_{\mathcal{Y}|\mathcal{U}},\sigma^2I
ight)$$
 where  $\mu_{\mathcal{Y}|\mathcal{U}}(u)=Xeta+Z\Lambda u$  Specifically

- The distribution  $\mathcal{Y}|\mathcal{U}=u$  depends on u only through the conditional mean,  $\mu_{\mathcal{Y}|\mathcal{U}}(u)$ .
- Elements of  ${\cal Y}$  are conditionally independent. That is, the distribution of  $\mathcal{Y}|\mathcal{U}=u$  is completely specified by the univariate, conditional distributions,  $\mathcal{Y}_i | \mathcal{U}, i = 1, \dots, n$ .
- These univariate, conditional distributions all have the same form. They differ only in their means.
- GLMMs differ from LMMs in the form of the univariate. conditional distributions and in how  $\mu_{\mathcal{Y}|\mathcal{U}}(u)$  depends on u.



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#### Some choices of univariate conditional distributions

- Typical choices of univariate conditional distributions are:
  - The Bernoulli distribution for binary (0/1) data, which has probability mass function

$$p(y|\mu) = \mu^y (1-\mu)^{1-y}, \quad 0 < \mu < 1, \quad y = 0, 1$$

- Several independent binary responses can be represented as a binomial response, but only if all the Bernoulli distributions have the same mean.
- The *Poisson* distribution for count  $(0,1,\ldots)$  data, which has probability mass function

$$p(y|\mu) = e^{-\mu} \frac{\mu^y}{y!}, \quad 0 < \mu, \quad y = 0, 1, 2, \dots$$

• All of these distributions are completely specified by the conditional mean. This is different from the conditional normal (or Gaussian) distribution, which also requires the common scale parameter,  $\sigma$ .

## The link function, g

- When the univariate conditional distributions have constraints on  $\mu$ , such as  $0<\mu<1$  (Bernoulli) or  $0<\mu$  (Poisson), we cannot define the conditional mean,  $\mu_{\mathcal{Y}|\mathcal{U}}$ , to be equal to the linear predictor,  $X\beta+U(\theta)u$ , which is unbounded.
- We choose an invertible, univariate *link function*, g, such that  $\eta=g(\mu)$  is unconstrained. The vector-valued link function, g, is defined by applying g component-wise.

$$\eta = g(\mu)$$
 where  $\eta_i = g(\mu_i), i = 1, \dots, n$ 

• We require that g be invertible so that  $\mu=g^{-1}(\eta)$  is defined for  $-\infty < \eta < \infty$  and is in the appropriate range ( $0 < \mu < 1$  for the Bernoulli or  $0 < \mu$  for the Poisson). The vector-valued inverse link,  $\boldsymbol{g}^{-1}$ , is defined component-wise.

#### "Canonical" link functions

- There are many choices of invertible scalar link functions, g, that we could use for a given set of constraints.
- For the Bernoulli and Poisson distributions, however, one link function arises naturally from the definition of the probability mass function. (The same is true for a few other, related but less frequently used, distributions, such as the gamma distribution.)
- To derive the canonical link, we consider the logarithm of the probability mass function (or, for continuous distributions, the probability density function).
- For distributions in this "exponential" family, the logarithm of the probability mass or density can be written as a sum of terms, some of which depend on the response, y, only and some of which depend on the mean,  $\mu$ , only. However, only one term depends on **both** y and  $\mu$ , and this term has the form  $y \cdot g(\mu)$ , where g is the canonical link.



#### The canonical link for the Bernoulli distribution

The logarithm of the probability mass function is

$$\log(p(y|\mu)) = \log(1-\mu) + y \log\left(\frac{\mu}{1-\mu}\right), \ 0 < \mu < 1, \ y = 0, 1.$$

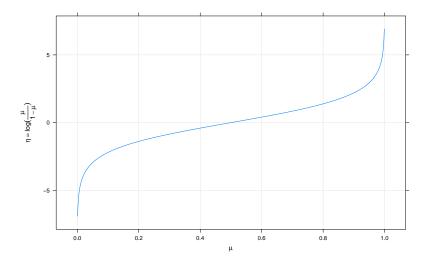
Thus, the canonical link function is the logit link

$$\eta = g(\mu) = \log\left(\frac{\mu}{1-\mu}\right).$$

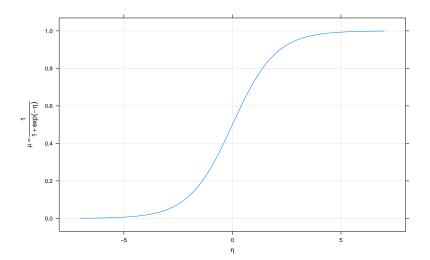
- Because  $\mu=P[\mathcal{Y}=1]$ , the quantity  $\mu/(1-\mu)$  is the odds ratio (in the range  $(0,\infty)$ ) and g is the logarithm of the odds ratio, sometimes called "log odds".
- The inverse link is

$$\mu = g^{-1}(\eta) = \frac{e^{\eta}}{1 + e^{\eta}} = \frac{1}{1 + e^{-\eta}}$$

#### Plot of canonical link for the Bernoulli distribution



## Plot of inverse canonical link for the Bernoulli distribution



#### The canonical link for the Poisson distribution

• The logarithm of the probability mass is

$$\log(p(y|\mu)) = \log(y!) - \mu + y\log(\mu)$$

• Thus, the canonical link function for the Poisson is the *log* link

$$\eta = g(\mu) = \log(\mu)$$

The inverse link is

$$\mu = g^{-1}(\eta) = e^{\eta}$$

#### The canonical link related to the variance

- For the canonical link function, the derivative of its inverse is the variance of the response.
- For the Bernoulli, the canonical link is the logit and the inverse link is  $\mu=g^{-1}(\eta)=1/(1+e^{-\eta}).$  Then

$$\frac{d\mu}{d\eta} = \frac{e^{-\eta}}{(1+e^{-\eta})^2} = \frac{1}{1+e^{-\eta}} \frac{e^{-\eta}}{1+e^{-\eta}} = \mu(1-\mu) = \text{Var}(\mathcal{Y})$$

• For the Poisson, the canonical link is the log and the inverse link is  $\mu=g^{-1}(\eta)=e^{\eta}$ . Then

$$\frac{d\mu}{dn} = e^{\eta} = \mu = \text{Var}(\mathcal{Y})$$

## The unscaled conditional density of $\mathcal{U}|\mathcal{Y}=y$

 As in LMMs we evaluate the likelihood of the parameters, given the data, as

$$L(\boldsymbol{\theta}, \boldsymbol{\beta} | \boldsymbol{y}) = \int_{\mathbb{R}^q} [\boldsymbol{\mathcal{Y}} | \boldsymbol{\mathcal{U}}](\boldsymbol{y} | \boldsymbol{u}) [\boldsymbol{\mathcal{U}}](\boldsymbol{u}) d\boldsymbol{u},$$

- The product  $[\mathcal{Y}|\mathcal{U}](y|u)[\mathcal{U}](u)$  is the unscaled (or unnormalized) density of the conditional distribution  $\mathcal{U}|\mathcal{Y}$ .
- The density  $[\mathcal{U}](u)$  is a spherical Gaussian density  $\frac{1}{(2\pi)^{q/2}}e^{-\|u\|^2/2}$ .
- The expression  $[\mathcal{Y}|\mathcal{U}](y|u)$  is the value of a probability mass function or a probability density function, depending on whether  $\mathcal{Y}_i|\mathcal{U}$  is discrete or continuous.
- The linear predictor is  $g(\mu_{\mathcal{Y}|\mathcal{U}}) = \eta = X\beta + U(\theta)u$ . Alternatively, we can write the conditional mean of  $\mathcal{Y}$ , given  $\mathcal{U}$ , as

$$\mu_{\mathcal{Y}|\mathcal{U}}(u) = g^{-1}\left(Xeta + U( heta)u
ight)$$

## The conditional mode of $\mathcal{U}|\mathcal{Y}=y$

• In general the likelihood,  $L(\boldsymbol{\theta}, \boldsymbol{\beta}|\boldsymbol{y})$  does not have a closed form. To approximate this value, we first determine the conditional mode

$$ilde{m{u}}(m{y}|m{ heta},m{eta}) = rg \max_{m{u}} [m{\mathcal{Y}}|m{\mathcal{U}}](m{y}|m{u}) \, [m{\mathcal{U}}](m{u})$$

using a quadratic approximation to the logarithm of the unscaled conditional density.

 This optimization problem is (relatively) easy because the quadratic approximation to the logarithm of the unscaled conditional density can be written as a penalized, weighted residual sum of squares,

$$ilde{m{u}}(m{y}|m{ heta},m{eta}) = rg \min_{m{u}} \left\| egin{bmatrix} m{W}^{1/2}(m{\mu}) \left(m{y} - m{\mu}_{m{\mathcal{Y}}|m{\mathcal{U}}}(m{u}) 
ight) \\ -m{u} \end{bmatrix} 
ight\|^2$$

where  $W(\mu)$  is the diagonal weights matrix. The weights are the inverses of the variances of the  $\mathcal{Y}_i$ .

## The PIRLS algorithm

- Parameter estimates for generalized linear models (without random effects) are usually determined by iteratively reweighted least squares (IRLS), an incredibly efficient algorithm. PIRLS is the penalized version. It is iteratively reweighted in the sense that parameter estimates are determined for a fixed weights matrix  $\boldsymbol{W}$  then the weights are updated to the current estimates and the process repeated.
- For fixed weights we solve

$$\min_{oldsymbol{u}} \left\| \begin{bmatrix} oldsymbol{W}^{1/2} \left( oldsymbol{y} - oldsymbol{\mu}_{oldsymbol{\mathcal{Y}} | oldsymbol{\mathcal{U}}}(oldsymbol{u}) 
ight) \end{bmatrix} 
ight\|^2$$

as a nonlinear least squares problem with update,  $\delta_u$ , given by

$$P\left(UMWMU'+I\right)P'\delta_{m{u}}=UMW(m{y}-m{\mu})-m{u}$$

where  $M=d\mu/d\eta$  is the (diagonal) Jacobian matrix. Recall that for the canonical link,  $M={\rm Var}({\cal Y}|{\cal U})=W^{-1}$ .

## The Laplace approximation to the deviance

ullet At convergence, the sparse Cholesky factor,  $oldsymbol{L}$ , used to evaluate the update is

$$oldsymbol{L} oldsymbol{L}' = oldsymbol{P} \left( oldsymbol{U} oldsymbol{M} oldsymbol{W} oldsymbol{M} oldsymbol{U}' + oldsymbol{I} 
ight) oldsymbol{P}'$$

or

$$oldsymbol{L} oldsymbol{L}' = oldsymbol{P} \left( oldsymbol{U} M oldsymbol{U}' + oldsymbol{I} 
ight) oldsymbol{P}'$$

if we are using the canonical link.

- The integrand of the likelihood is approximately a constant times the density of the  $\mathcal{N}(\tilde{\pmb{u}}, \pmb{L} \pmb{L}')$  distribution.
- On the deviance scale (negative twice the log-likelihood) this corresponds to

$$d(\boldsymbol{\beta}, \boldsymbol{\theta}|\boldsymbol{y}) = d_g(\boldsymbol{y}, \boldsymbol{\mu}(\tilde{\boldsymbol{u}})) + ||\tilde{\boldsymbol{u}}||^2 + \log(|\boldsymbol{L}|^2)$$

where  $d_g(\boldsymbol{y}, \boldsymbol{\mu}(\tilde{\boldsymbol{u}}))$  is the GLM deviance for  $\boldsymbol{y}$  and  $\boldsymbol{\mu}$ .



## Modifications to the algorithm

- Notice that this deviance depends on the fixed-effects parameters,  $\boldsymbol{\beta}$ , as well as the variance-component parameters,  $\boldsymbol{\theta}$ . This is because  $\log(|\boldsymbol{L}|^2)$  depends on  $\mu_{\boldsymbol{\mathcal{Y}}|\boldsymbol{\mathcal{U}}}$  and, hence, on  $\boldsymbol{\beta}$ . For LMMs  $\log(|\boldsymbol{L}|^2)$  depends only on  $\boldsymbol{\theta}$ .
- It is likely that modifying the PIRLS algorithm to optimize simultaneously on u and  $\beta$  would result in a value that is very close to the deviance profiled over  $\beta$ .
- Another approach, which is being implemented as a Google Summer of Code project, is adaptive Gauss-Hermite quadrature (AGQ). This has a similar structure to the Laplace approximation but is based on more evaluations of the unscaled conditional density near the conditional modes. It is only appropriate for models in which the random effects are associated with only one grouping factor

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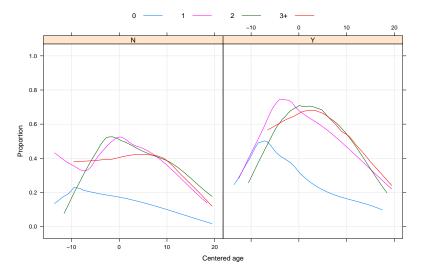
Model building



## Contraception data

- One of the data sets in the "mlmRev" package, derived from data files available on the multilevel modelling web site, is from a fertility survey of women in Bangladesh.
- One of the responses is whether or not the woman currently uses artificial contraception (i.e. a binary response)
- Covariates included the woman's age (on a centered scale), the number of live children she had, whether she lived in an urban or rural setting, and the district in which she lived.
- Instead of plotting such data as points, we use the 0/1 response to generate scatterplot smoother curves versus age for the different groups.

## Contraception use versus age by urban and livch



## Comments on the data plot

- These observational data are unbalanced (some districts have only 2 observations, some have nearly 120). They are not longitudinal (no "time" variable).
- Binary responses have low per-observation information content (exactly one bit per observation). Districts with few observations will not contribute strongly to estimates of random effects.
- Within-district plots will be too imprecise so we only examine the global effects in plots.
- The comparisons on the multilevel modelling site are for fits of a model that is linear in age, which is clearly inappropriate.
- The form of the curves suggests at least a quadratic in age.
- The urban versus rural differences may be additive.
- It appears that the livch factor could be dichotomized into "0" versus "1 or more".



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## Preliminary model using Laplacian approximation

```
Generalized linear mixed model fit by maximum likelihood ['merMod']
 Family: binomial
Formula: use ~ age + I(age^2) + urban + livch + (1 | district)
  Data: Contraception
     AIC
              BIC logLik deviance
 2388.774 2433.313 -1186.387 2372.774
Random effects:
 Groups Name Variance Std.Dev.
 district (Intercept) 0.2253 0.4747
Number of obs: 1934, groups: district, 60
Fixed effects:
            Estimate Std. Error z value
(Intercept) -1.019342 0.174010 -5.858
          0.003516 0.009212 0.382
age
I(age^2) -0.004487 0.000723 -6.205
urbanY
         0.684625 0.119691 5.720
livch1 0.801901 0.161899 4.953
```

livch2 0.901037 0.184801 4.876

0.899413 0.185435 4.850

livch3+

#### Comments on the model fit

- This model was fit using the Laplacian approximation to the deviance.
- There is a highly significant quadratic term in age.
- The linear term in age is not significant but we retain it because the age scale has been centered at an arbitrary (and unknown) value.
- The urban factor is highly significant (as indicated by the plot).
- Levels of livch greater than 0 are significantly different from 0 but may not be different from each other.

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#### Reduced model with dichotomized livch

```
Generalized linear mixed model fit by maximum likelihood ['merMod']
Family: binomial
Formula: use ~ age + I(age^2) + urban + ch + (1 | district)
  Data: Contraception
              BIC logLik deviance
2385.231 2418.635 -1186.615 2373.231
Random effects:
Groups Name Variance Std.Dev.
district (Intercept) 0.2242 0.4734
Number of obs: 1934, groups: district, 60
Fixed effects:
             Estimate Std. Error z value
(Intercept) -0.9913326 0.1675636 -5.916
          0.0061720 0.0078273 0.789
age
I(age^2) -0.0045584 0.0007142 -6.382
urbanY 0.6804429 0.1194818 5.695
chY
           0.8462275 0.1470584 5.754
```



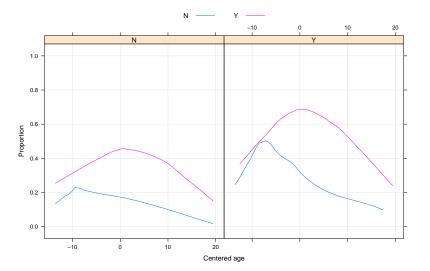
## Comparing the model fits

 A likelihood ratio test can be used to compare these nested models.

- The large p-value indicates that we would not reject cm2 in favor of cm1 hence we prefer the more parsimonious cm2.
- The plot of the scatterplot smoothers according to live children or none indicates that there may be a difference in the age pattern between these two groups.



## Contraception use versus age by urban and ch

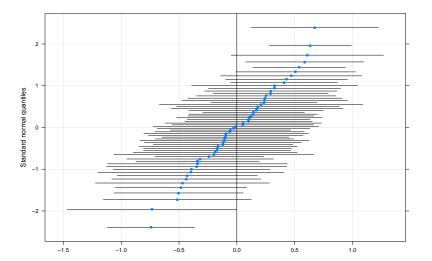


## Allowing age pattern to vary with ch

```
Generalized linear mixed model fit by maximum likelihood ['merMod']
Family: binomial
Formula: use ~ age * ch + I(age^2) + urban + (1 | district)
  Data: Contraception
     AIC
              BIC logLik deviance
2379.227 2418.198 -1182.613 2365.227
Random effects:
Groups Name Variance Std.Dev.
district (Intercept) 0.2225 0.4717
Number of obs: 1934, groups: district, 60
Fixed effects:
           Estimate Std. Error z value
(Intercept) -1.304583 0.213473 -6.111
age -0.046526 0.021701 -2.144
chY 1.190985 0.205945 5.783
I(age^2) -0.005660 0.000833 -6.795
urbanY 0.700970 0.120055 5.839
```

age:chY 0.067224 0.025293 2.658

#### Prediction intervals on the random effects



## Extending the random effects

 We may want to consider allowing a random effect for urban/rural by district. This is complicated by the fact the many districts only have rural women in the study

```
district
urban
                                 6
                                                    10
                                                         11
                                                              12
                                                                                 16
        54
             20
                       19
                            37
                                58
                                     18
                                          35
                                               20
                                                    13
                                                         21
                                                              23
                                                                  16
                                                                       17
                                                                            14
                                                                                 18
                       11
                                      0
                                           2
                                                3
                                                               6
                                                     0
                                                          0
                                                                      101
                                                                             8
      district
                                               25
                                                         27
                                                                       30
                                                                                 32
urban
        17
             18
                  19
                       20
                            21
                                22
                                     23
                                          24
                                                    26
                                                              28
                                                                  29
                                                                            31
             33
                                     15
                                          14
                                               49
                                                    13
                                                         39
                                                             45
    N
        24
                       15
                            10
                                20
                                                                  25
                                                                       45
                                                                                 24
```

## Including a random effect for urban by district

Generalized linear mixed model fit by maximum likelihood ['merMod']

Family: binomial

Formula: use ~ age \* ch + I(age^2) + urban + (urban | district)

Data: Contraception

AIC BIC logLik deviance 2371.636 2421.742 -1176.818 2353.636

Random effects:

Groups Name Variance Std.Dev. Corr

district (Intercept) 0.3773 0.6142

urbanY 0.5271 0.7260 -0.794

Number of obs: 1934, groups: district, 60

#### Fixed effects:

Estimate Std. Error z value (Intercept) -1.308648 0.221298 -5.914 age -0.045071 0.021729 -2.074 chY 1.182726 0.206610 5.724 I(age^2) -0.005509 0.000839 -6.567 urbanY 0.766746 0.159864 4.796 age:chY 0.064845 0.025348 2.558

## Significance of the additional random effect

```
Data: Contraception

Models:
cm3: use ~ age * ch + I(age^2) + urban + (1 | district)
cm4: use ~ age * ch + I(age^2) + urban + (urban | district)

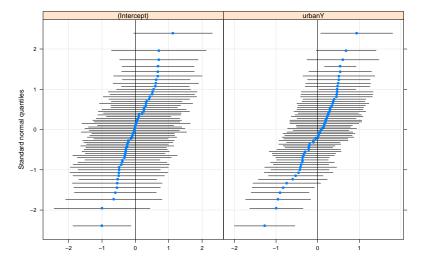
Df AIC BIC logLik deviance Chisq Chi Df Pr(>Chisq)
cm3 7 2379.2 2418.2 -1182.6 2365.2
cm4 9 2371.6 2421.7 -1176.8 2353.6 11.591 2 0.003042
```

- The additional random effect is highly significant in this test.
- Most of the prediction intervals still overlap zero.

> anova(cm4, cm3)

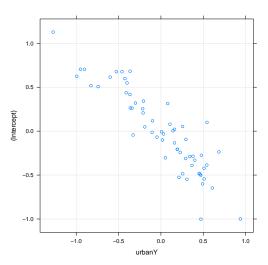
 A scatterplot of the random effects shows several random effects vectors falling along a straight line. These are the districts with all rural women or all urban women.

#### Prediction intervals for the bivariate random effects





## Scatter plot of the BLUPs



# Nested simple, scalar random effects versus vector-valued Generalized linear mixed model fit by maximum likelihood ['merMod']

Family: binomial
Formula: use ~ age \* ch + I(age^2) + urban + (1 | urban:district) + (1
 Data: Contraception

AIC BIC logLik deviance 2371.675 2416.214 -1177.838 2355.675

Random effects:

Groups Name Variance Std.Dev. urban:district (Intercept) 0.3086025 0.55552 district (Intercept) 0.0006808 0.02609

Number of obs: 1934, groups: urban:district, 102; district, 60

#### Fixed effects:

Estimate Std. Error z value (Intercept) -1.3042507 0.2188531 -5.959 age -0.0448232 0.0217800 -2.058 chY 1.1810768 0.2070578 5.704 I(age^2) -0.0054804 0.0008384 -6.537 urbanY 0.7613873 0.1683946 4.521 age:chY 0.0646389 0.0253854 2.546

C I . C D I DCC .

## Using the interaction term only

Generalized linear mixed model fit by maximum likelihood ['merMod']

Family: binomial

Formula: use ~ age \* ch + I(age^2) + urban + (1 | urban:district)

Data: Contraception

AIC BIC logLik deviance 2368.542 2407.514 -1177.271 2354.542

Random effects:

Groups Name Variance Std.Dev. urban:district (Intercept) 0.3218 0.5672

Number of obs: 1934, groups: urban:district, 102

#### Fixed effects:

Estimate Std. Error z value (Intercept) -1.3094337 0.2196438 -5.962 age -0.0448438 0.0218185 -2.055 chY 1.1814379 0.2073624 5.697 I(age^2) -0.0055277 0.0008409 -6.574 urbanY 0.7643086 0.1702630 4.489 age:chY 0.0646063 0.0254321 2.540

Correlation of Fixed Effects:



## Comparing models with random effects for interactions

> anova(cm6, cm5, cm4)

```
Data: Contraception
Models:
cm6: use ~ age * ch + I(age^2) + urban + (1 | urban:district)
cm5: use ~ age * ch + I(age^2) + urban + (1 | urban:district) + (1 |
cm5: district)
cm4: use ~ age * ch + I(age^2) + urban + (urban | district)
Df AIC BIC logLik deviance Chisq Chi Df Pr(>Chisq)
cm6 7 2368.5 2407.5 -1177.3 2354.5
cm5 8 2371.7 2416.2 -1177.8 2355.7 0.0000 1 1.0000
cm4 9 2371.6 2421.7 -1176.8 2353.6 2.0393 1 0.1533
```

- The random effects seem to best be represented by a separate random effect for urban and for rural women in each district.
- The districts with only urban women in the survey or with only rural women in the survey are naturally represented in this model.

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- Again, carefully plotting the data is enormously helpful in formulating the model.
- Observational data tend to be unbalanced and have many more covariates than data from a designed experiment.
   Formulating a model is typically more difficult than in a designed experiment.
- A generalized linear model is fit by adding a value, typically binomial or poisson, for the optional argument family in the call to lmer.
- MCMC sampling is not provided for GLMMs at present but will be added.
- We use likelihood-ratio tests and z-tests in the model building.

