R^2s for Correlated Data: Phylogenetic Models, LMMs, and GLMMs

Anthony R. Ives, Department of Integrative Biology, UW-Madison, Madison, WI 53706

arives@wisc.edu

SUPPLEMENTARY SECTION 1: MORE COMPARISONS AMONG THE R^2S.

To give a comprehensive assessment of the R^2s, this supplement discusses and plots a complete set of simulations, from which a subset was presented in the main text. The different models (LMM, PGLS, GLMM, and PLOG) are presented in turn. In the comparisons for LMMs and GLMMs, I compare the partial R^2s of R^2_{resid}, R^2_{lik} and R^2_{pred} for the fixed effect to $R^2_{glmm(m)}$ and the partial R^2s for the random effect to $R^2_{glmm(r)}$. This illustrates the differences between using partial R^2s and marginal R^2s.

FIGURE CAPTIONS

Figure S1: Simulation results for a Linear Mixed Model (LMM) giving R^2_{resid}, R^2_{lik}, R^2_{pred}, R^2_{glmm}, and R^2_{ols} versus the log likelihood ratio (LLR) between full and reduced models. The simulation model (equation 18) contained both a fixed effect β for a continuous variable x and a random effect b for a categorical variable u. For (a), (b) and (c), data were simulated without the random effect ($\beta = 1$, $\sigma = 0$), and for (d), (e) and (f), data were simulated without the fixed effect ($\beta = 0$, $\sigma = 1.5$). Simulations for (g), (h), and (i) contained both fixed and random effects. Columns give different partial R^2s for each method. Specifically, (a), (d), and (g) give the partial R^2s in which the reduced model removes the fixed effect for x: therefore, these give partial R^2s for the fixed effect. Panels (b), (e), and (h) give the partial R^2s in which the reduced model removes the random effect for u: therefore, these give partial R^2s for the random effect. In panels (c), (f) and (i), the reduced model removes both fixed and random effects, giving the total R^2s. Each data set consisted of 100 simulated points, x was simulated as a normal (0, 1) random variable, and u had

10 levels with b is simulated as a normal (0, σ). All analyses were performed with the function lmer().

Figure S2: Simulation results for a Linear Mixed Model (LMM) giving associations between R^2_{resid}, R^2_{lik}, R^2_{pred}, R^2_{glmm}, and R^2_{ols}. Data are the same as presented in figure S1.

Figure S3: Simulation results for a Linear Mixed Model (LMM) showing means and standard deviations of R^2_{resid}, R^2_{lik}, R^2_{pred}, R^2_{glmm}, and R^2_{ols} versus sample size. The simulation model (equation 18) contained both a fixed effect β for a continuous variable x and a random effect b for a categorical variable u. For each level of u, from 4 to 16 replicates were simulated. (a), (b), and (c) give means of each R^2 were calculated for 500 simulations at each sample, and (d), (e), and (f) give standard deviations. Columns give different partial R^2s, with (a) and (d) giving the partial R^2s for the fixed effect, (b) and (e) giving the partial R^2s for the random effect, and (c) and (f) giving the total R^2s. In the simulations, x is simulated as a normal (0, 1) random variable with $\beta = 1$; u has 10 levels and b is simulated as a normal (0, $\sigma = 1.5$) random variable; and residuals e are independent (0, 1) random variables. All analyses were performed with the function lmer().

Figure S4: Simulation results for the phylogenetic model with a continuous predictor variable x giving R^2_{resid}, R^2_{lik}, and R^2_{pred} versus the log likelihood ratio (LLR) between full and reduced models. For each simulation, a phylogenetic tree was first simulated, and the values of x were simulated up the phylogeny assuming Brownian Motion evolution. Data were simulated using equation (18) with $b = 0$, and residuals e_i were simulated from a multivariate normal distribution with mean zero and covariance matrix $\mathbf{\Sigma}(\lambda) = (1 - \lambda)\mathbf{I} + \lambda\mathbf{\Sigma}_{BM}$. For (a), (b) and (c), data were simulated without phylogenetic signal ($\lambda = 0$, $\beta = 1$), and for (d), (e) and (f), data were simulated without the fixed effect ($\lambda = 0.5$, $\beta = 0$). Simulations for (g), (h), and (i) contained both fixed and phylogenetic effects ($\beta = 1$, $\lambda = 0.5$). (a), (d), and (g) give the partial R^2s for the fixed effect. Panels (b), (e), and (h) give the partial R^2s for the phylogenetic effect. In panels (c), (f) and (i), the reduced model removes both fixed and phylogenetic effects, giving the total R^2s. All analyses were performed with the function phylolm().

Figure S5: Simulation results for a PGLS model giving associations between R^2_{resid}, R^2_{lik}, and R^2_{pred}. Data are the same as presented in figure S3.

Figure S6: Simulation results for the phylogenetic model with a continuous response variable showing means and standard deviations of R^2_{resid}, R^2_{lik}, and R^2_{pred} versus sample size. For each simulation, a phylogenetic tree was first simulated, and the values of the predictor variable x were simulated up the phylogeny assuming Brownian Motion evolution. Residuals e_i were simulated from a multivariate normal distribution with mean zero and covariance matrix $\mathbf{\Sigma}(\lambda) = (1 - \lambda)\mathbf{I} + \lambda\mathbf{\Sigma}_{BM}$, and the parameter values were $\lambda = 0.5$, $\beta = 1$, and $b = 0$. (a), (b), and (c) give means of each R^2 were calculated for 500 simulations at each sample, and (d), (e), and (f) give standard deviations. Columns give different partial R^2s, with (a) and (d) giving the partial R^2s for x, (b) and (e) giving the partial R^2s for phylogenetic signal λ, and (c) and (f) giving the total R^2s. All analyses were performed with the function phylolm().

Figure S7: Simulation results for a binary Generalized Linear Mixed Model (GLMM) giving R^2_{resid}, R^2_{lik}, R^2_{pred}, R^2_{glmm}, and R^2_{ols} versus the log likelihood ratio (LLR) between full and reduced models. The simulation model (equation 18) contained both a fixed effect β for a continuous variable x and a random effect b for a categorical variable u. The scaling $\sigma^2_{d.rNS} = 0.8768809\ \pi^2/3$ was used for R^2_{resid} (see Appendix 1). For (a), (b) and (c), data were simulated without the random effect ($\beta = 1.8$, $\sigma = 0$), and for (d), (e) and (f), data were simulated without the fixed effect ($\beta = 0$, $\sigma = 1.8$). Simulations for (g), (h), and (i) contained both fixed and random effects. (a), (d), and (g) give the partial R^2s for the fixed effect, and panels (b), (e), and (h) give the partial R^2s for the random effect. In panels (c), (f) and (i) give total R^2s. In the simulations, x is simulated as a normal (0, 1) random variable and u has 10 levels and b is simulated as a normal (0, σ). All analyses were performed with the function glmer().

Figure S8: Simulation results for a Generalized Linear Mixed Model (GLMM) giving associations between R^2_{resid}, R^2_{lik}, R^2_{pred}, R^2_{glmm}, and R^2_{ols}. Data are the same as presented in figure S7.

Figure S9: Simulation results for a binary Generalized Linear Mixed Model (GLMM) showing means and standard deviations of R^2_{resid}, R^2_{lik}, R^2_{pred}, R^2_{glmm}, and R^2_{ols} versus sample size. The scaling $\sigma^2_{d.rNS} = 0.8768809\ \pi^2/3$ was used for R^2_{resid} (see Appendix 1). The simulation model (equation 18) contained both a fixed effect β for a continuous variable x and a random effect b for a categorical variable u. For each level of u, from 4 to 16 replicates were simulated. (a), (b), and (c) give means of each R^2 were calculated for 1000 simulations at each sample, and (d), (e), and (f) give standard deviations. Columns give different partial R^2s, with (a) and (d) giving the partial R^2s for the fixed effect, (b) and (e) giving the partial R^2s for the random effect, and (c) and (f) giving the total R^2s. In the simulations, x is simulated as a normal (0, 1) random variable with $\beta = 1.8$ and u has 10 levels and b is simulated as a normal (0, $\sigma = 1.8$) random variable. All analyses were performed with the function glmer().

Figure S10: Simulation results for the phylogenetic model with a continuous predictor variable x giving R^2_{resid}, R^2_{lik}, and R^2_{pred} versus the log likelihood ratio (LLR) between full and reduced models. The scaling $\sigma^2_{d.rNS} = 0.8768809\ \pi^2/3$ was used for R^2_{resid} (see Appendix 1). For each simulation, a phylogenetic tree was first simulated, and the values of x were simulated up the phylogeny assuming Brownian Motion evolution. Data were simulated using equation (18) with $b = 0$, and residuals e_i were simulated from a multivariate normal distribution with mean zero and covariance matrix $\mathbf{\Sigma}(\lambda) = (1 - \lambda)\mathbf{I} + \lambda\mathbf{\Sigma}_{BM}$. For (a), (b) and (c), data were simulated without phylogenetic signal ($\lambda = 0$, $\beta = 1.5$), and for (d), (e) and (f), data were simulated without the fixed effect ($\lambda = 2$, $\beta = 0$). Simulations for (g), (h), and (i) contained both fixed and phylogenetic effects ($\lambda = 2$, $\beta = 1.5$). (a), (d), and (g) give the partial R^2s for the fixed effect. Panels (b), (e), and (h) give the partial R^2s for the phylogenetic effect. In panels (c), (f) and (i), the reduced model removes both fixed and phylogenetic effects, giving the total R^2s. All analyses were performed with the function phylolm().

Figure S11: Simulation results for a phylogenetic logistic regression model giving associations between R^2_{resid}, R^2_{lik}, and R^2_{pred}. Data are the same as presented in figure S10.

Figure S12: Simulation results for the phylogenetic model with a binary response variable showing means and standard deviations of R^2_{resid}, R^2_{lik}, and R^2_{pred} versus sample size. The scaling

$\sigma^2_{d.rNS}$ = 0.8768809 $\pi^2/3$ was used for R^2_{resid} (see Appendix 1). For each simulation, a phylogenetic tree was first simulated, and residuals e_i (equation 18) were simulated from a multivariate normal distribution with mean zero and covariance matrix $\mathbf{\Sigma}(\lambda) = \lambda\mathbf{\Sigma}_{BM}$. Values of the predictor variable x were assumed to be independently distributed by a (0,1) normal distribution, and the parameter values were $\lambda = 2$, $\beta = 1.5$, and $b = 0$. (a), (b), and (c) give means of each R^2 were calculated for 500 simulations at each sample, and (d), (e), and (f) give standard deviations. Columns give different partial R^2s, with (a) and (d) giving the partial R^2s for x, (b) and (e) giving the partial R^2s for phylogenetic signal λ, and (c) and (f) giving the total R^2s. Calculations of R^2_{lik} were performed with a modified version of the function phyloglm() and the function glm(). Calculations of R^2_{resid} and R^2_{pred} were performed with the function binaryPGLMM().

Fig. S1

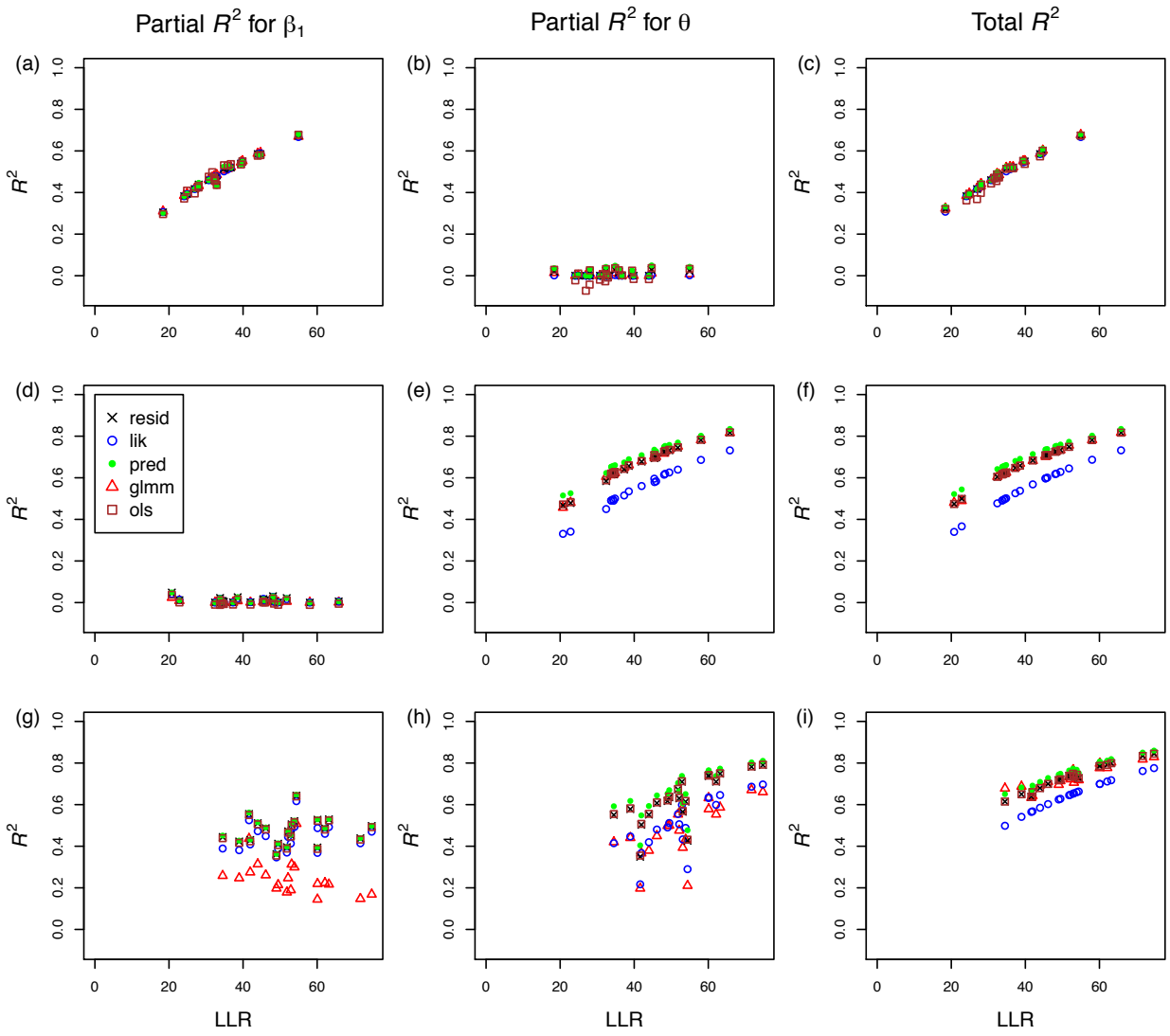

Partial R^2 for β_1
Partial R^2 for θ
Total R^2
(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
(i)
R^2
LLR
resid
lik
pred
glmm
ols

Fig. S2

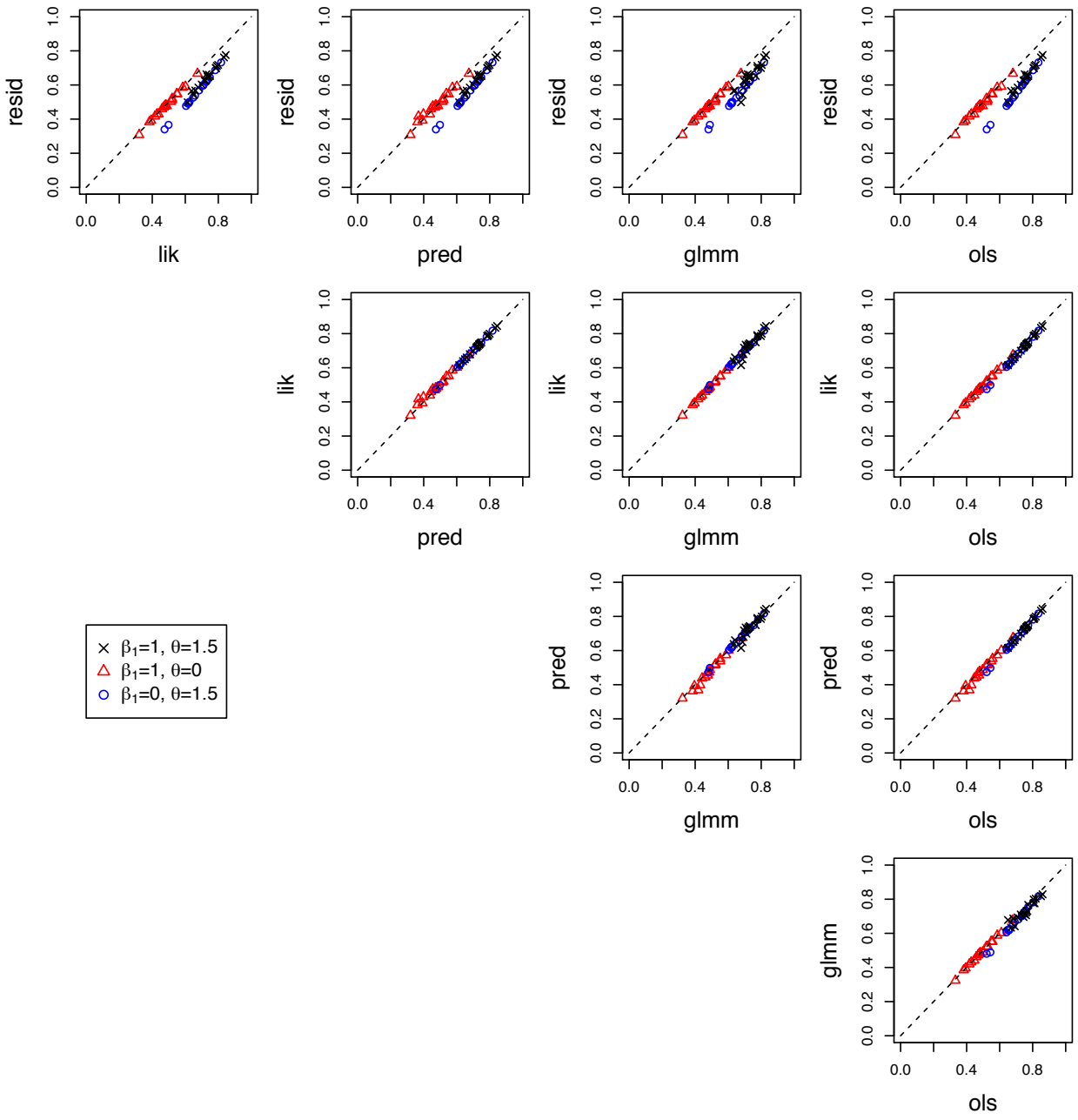


Fig. S3

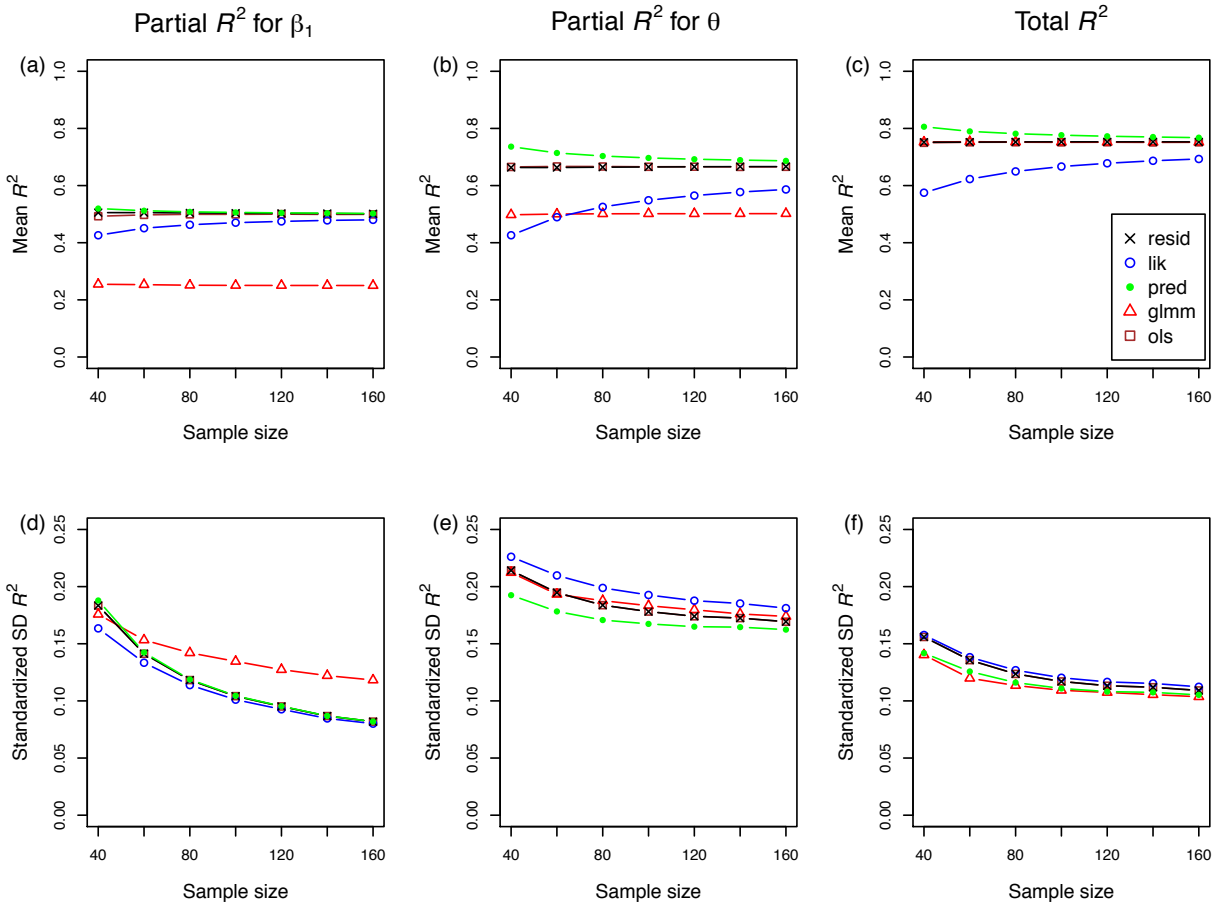

Partial R^2 for β_1
Partial R^2 for θ
Total R^2
(a)
(b)
(c)
(d)
(e)
(f)
Mean R^2
Standardized SD R^2
Sample size
resid
lik
pred
glmm
ols

Fig. S4

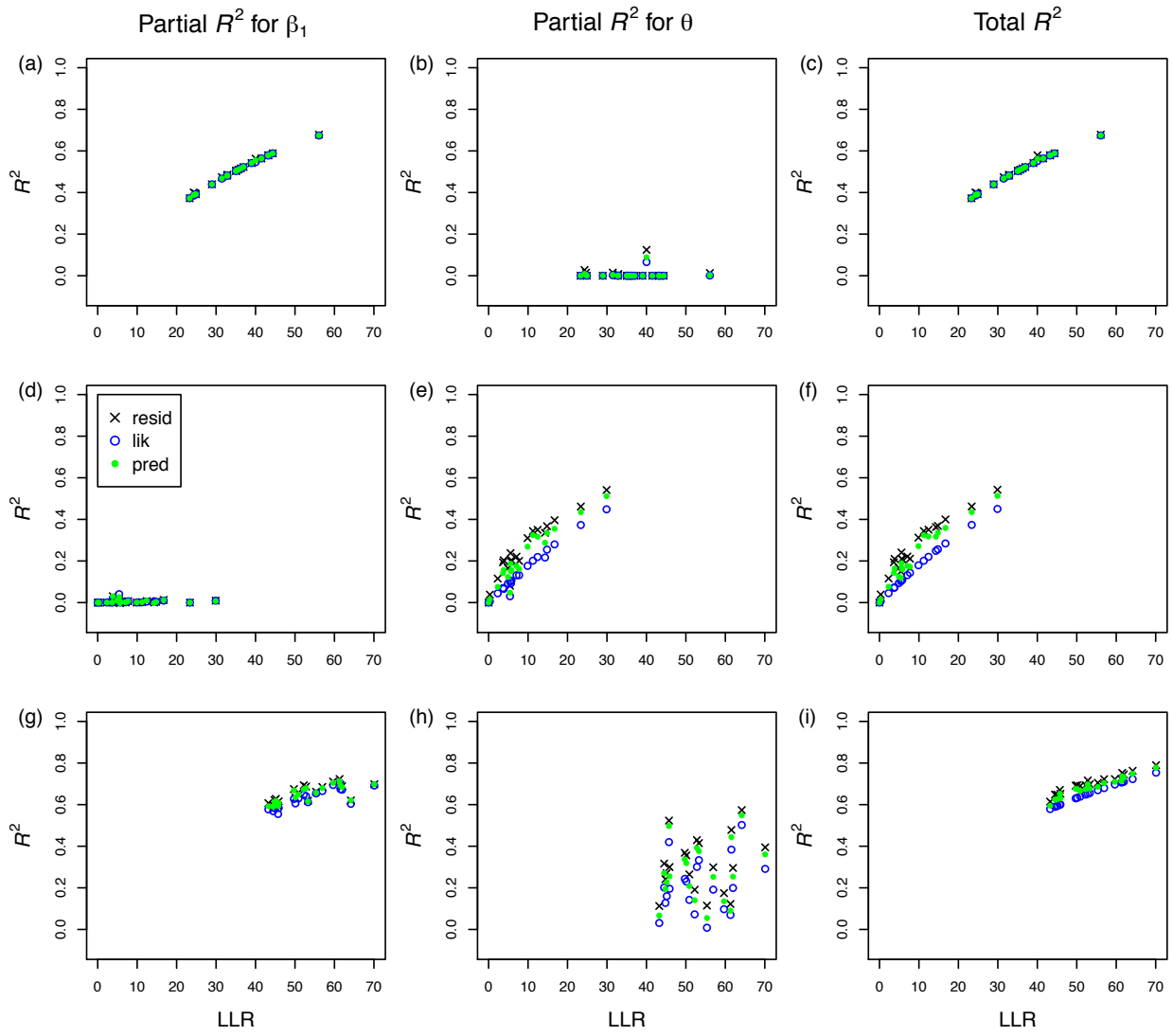

Partial R^2 for β_1
Partial R^2 for θ
Total R^2
(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
(i)
R^2
LLR
resid
lik
pred

Fig. S5

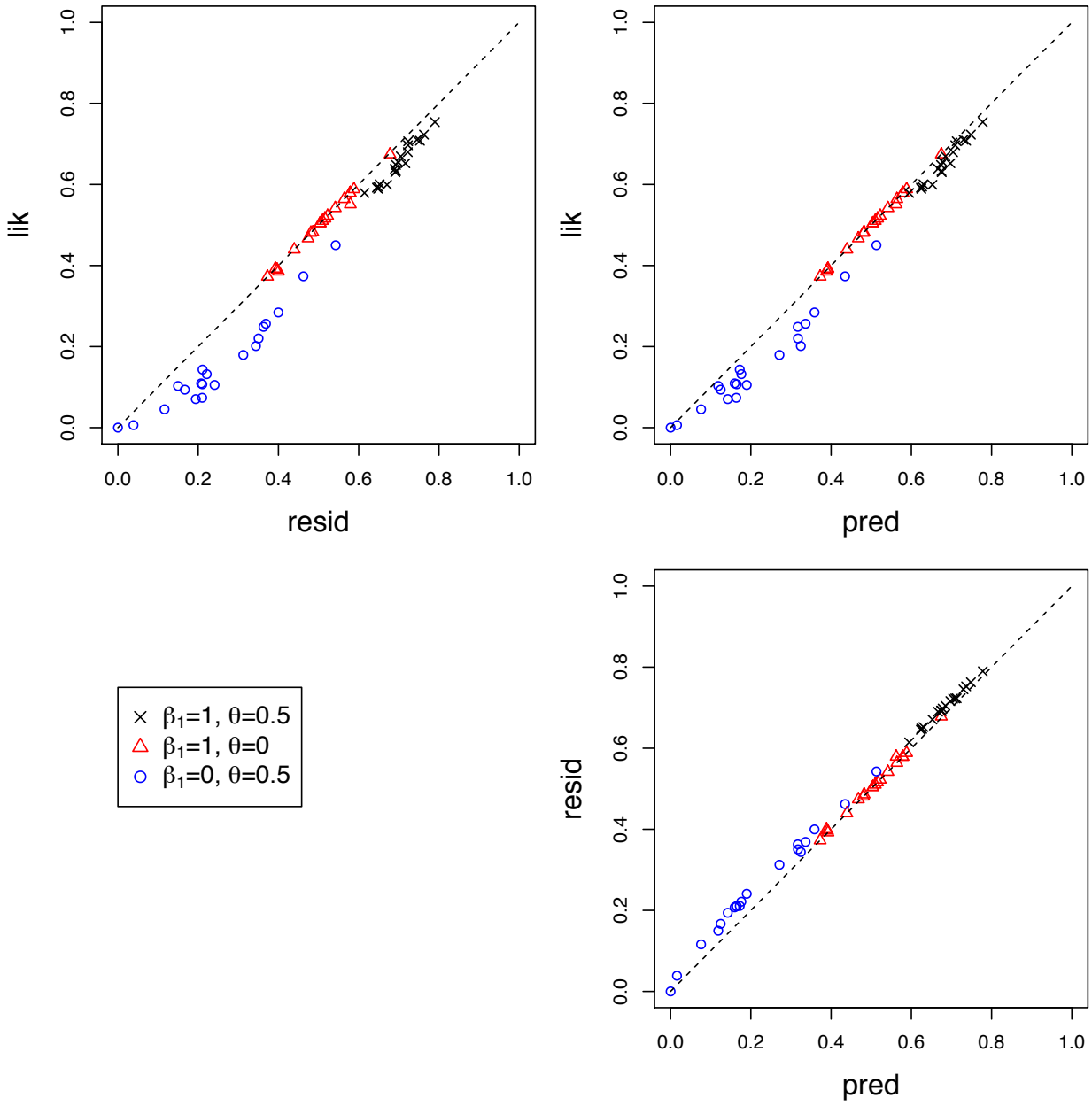

lik
resid
0.0
0.2
0.4
0.6
0.8
1.0
lik
pred
resid
pred
β1=1, θ=0.5
β1=1, θ=0
β1=0, θ=0.5

Fig. S6

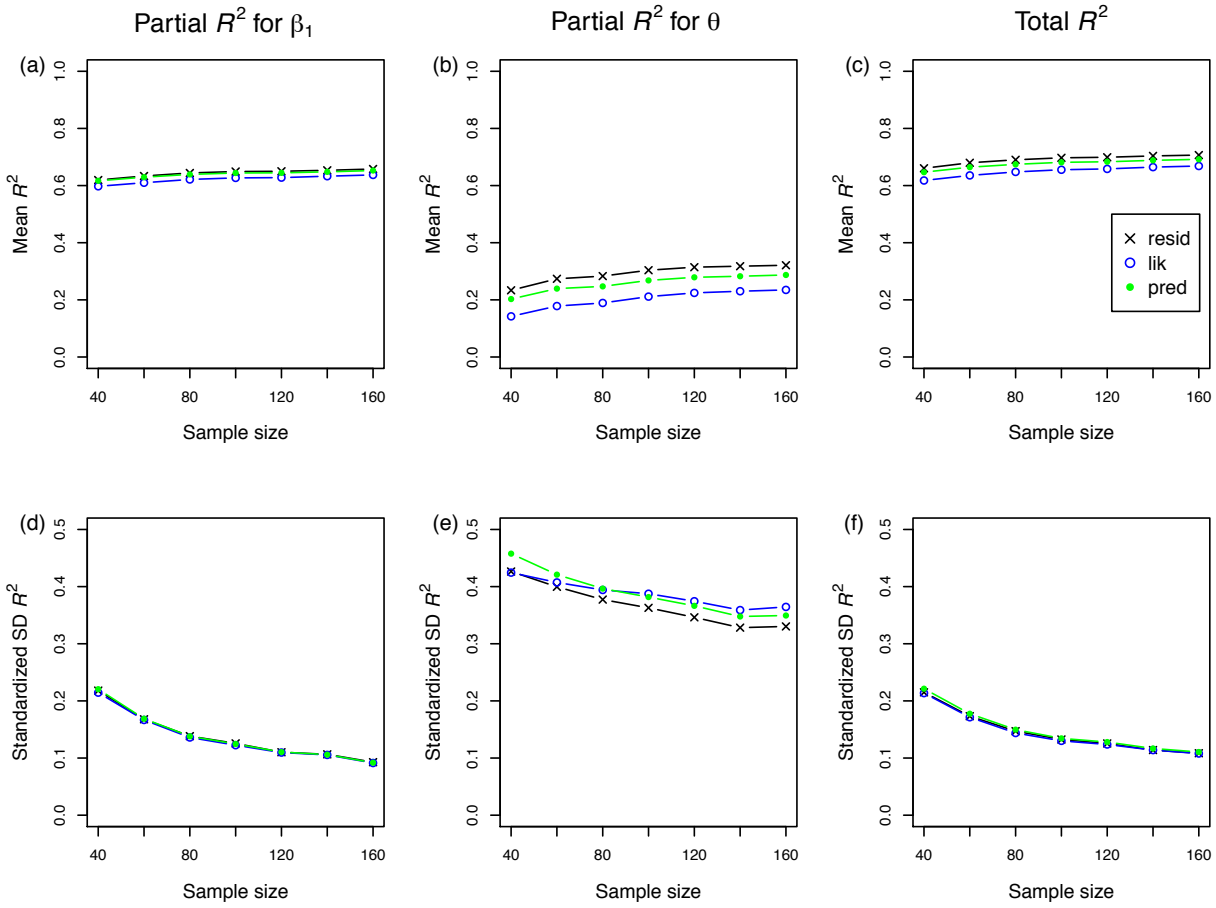

Partial R^2 for β_1
Partial R^2 for θ
Total R^2
(a)
(b)
(c)
(d)
(e)
(f)
Mean R^2
Standardized SD R^2
Sample size
resid
lik
pred

Fig. S7

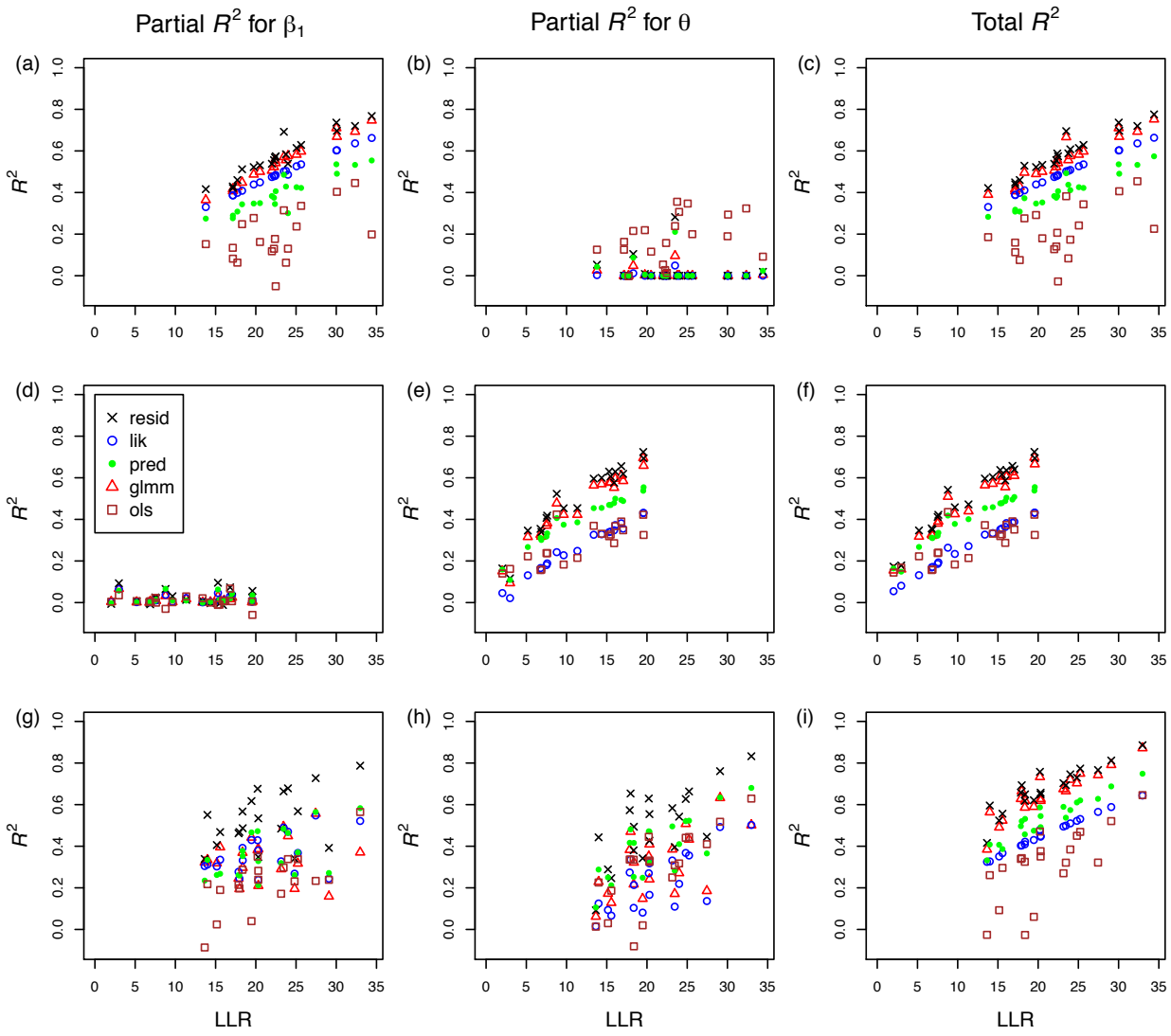

Partial R^2 for β_1
Partial R^2 for θ
Total R^2
(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
(i)
R^2
LLR
resid
lik
pred
glmm
ols

Fig. S8

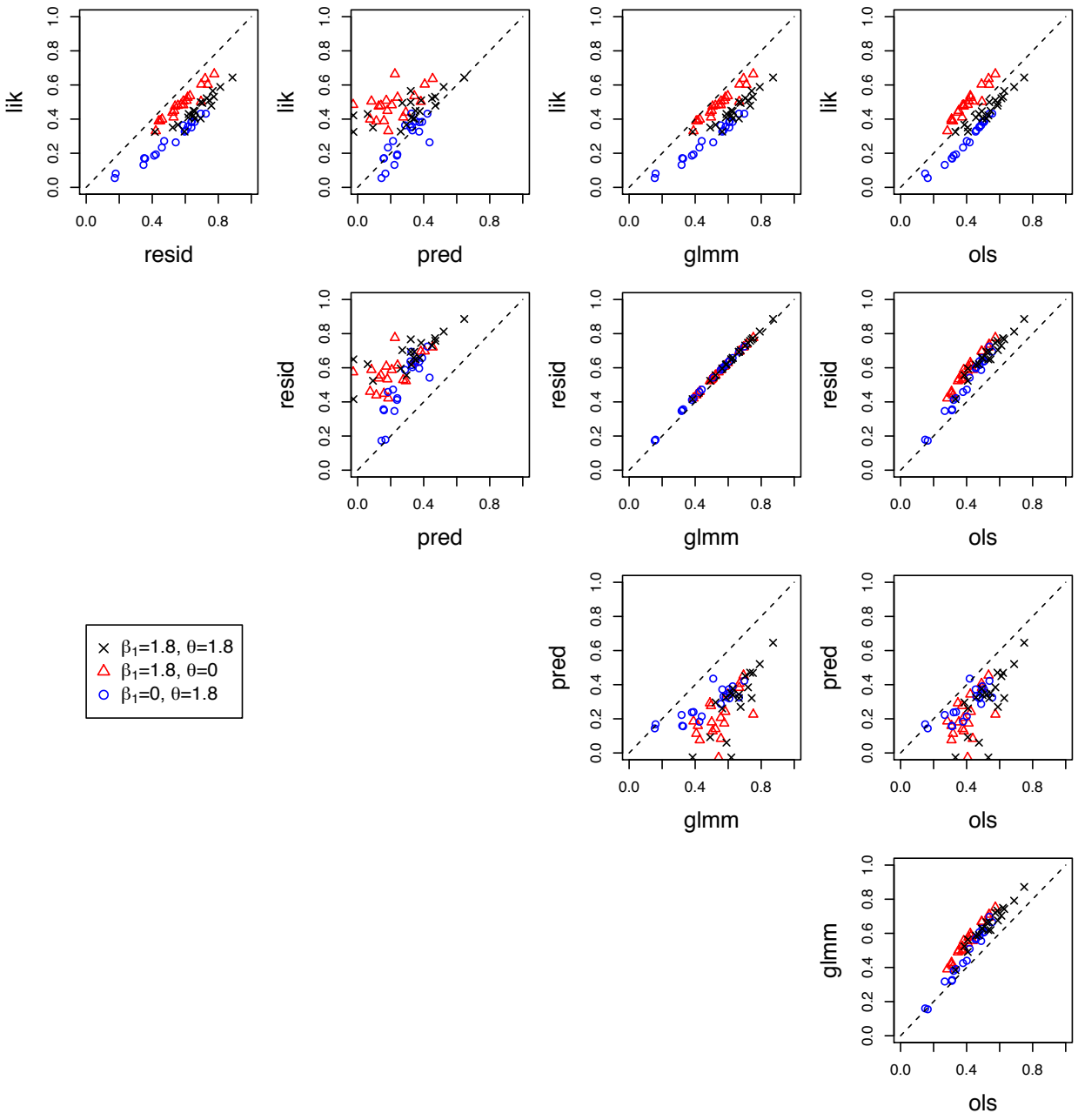


Fig. S9

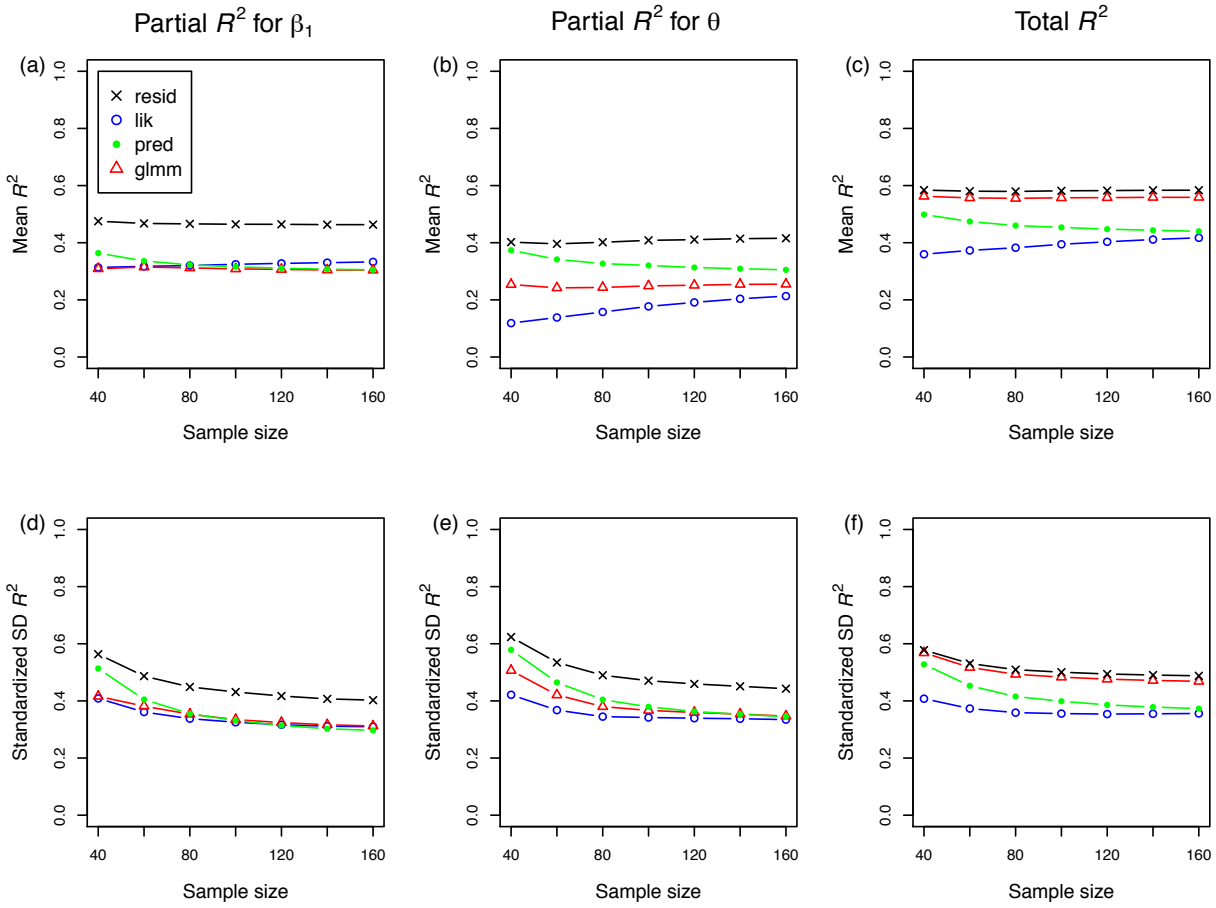

Partial R^2 for β_1
Partial R^2 for θ
Total R^2
(a)
(b)
(c)
(d)
(e)
(f)
resid
lik
pred
glmm
Mean R^2
Standardized SD R^2
Sample size
0.0
0.2
0.4
0.6
0.8
1.0
40
80
120
160

Fig. S10

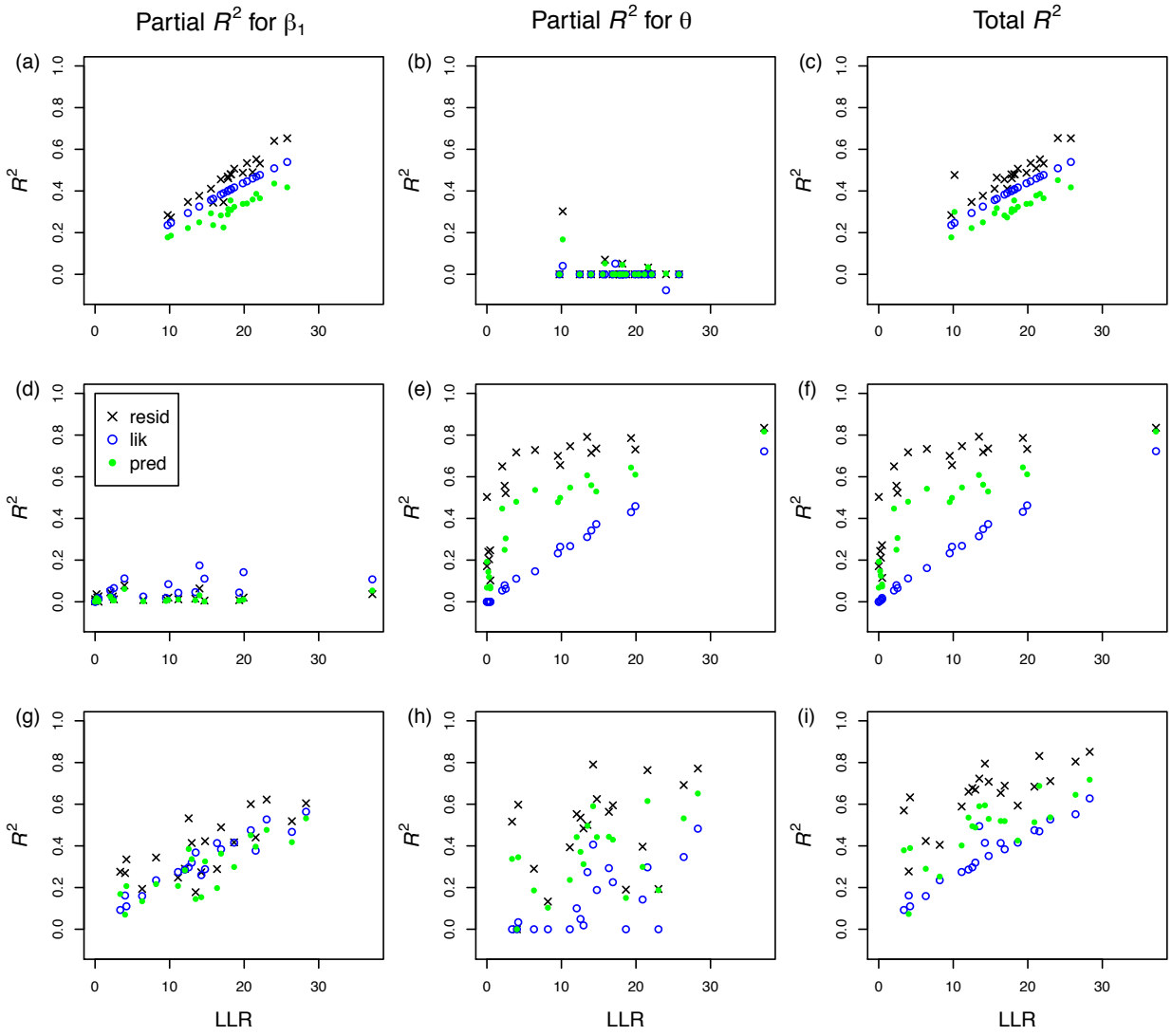

Partial R^2 for β_1
Partial R^2 for θ
Total R^2
(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
(i)
R^2
LLR
resid
lik
pred

Fig. S11

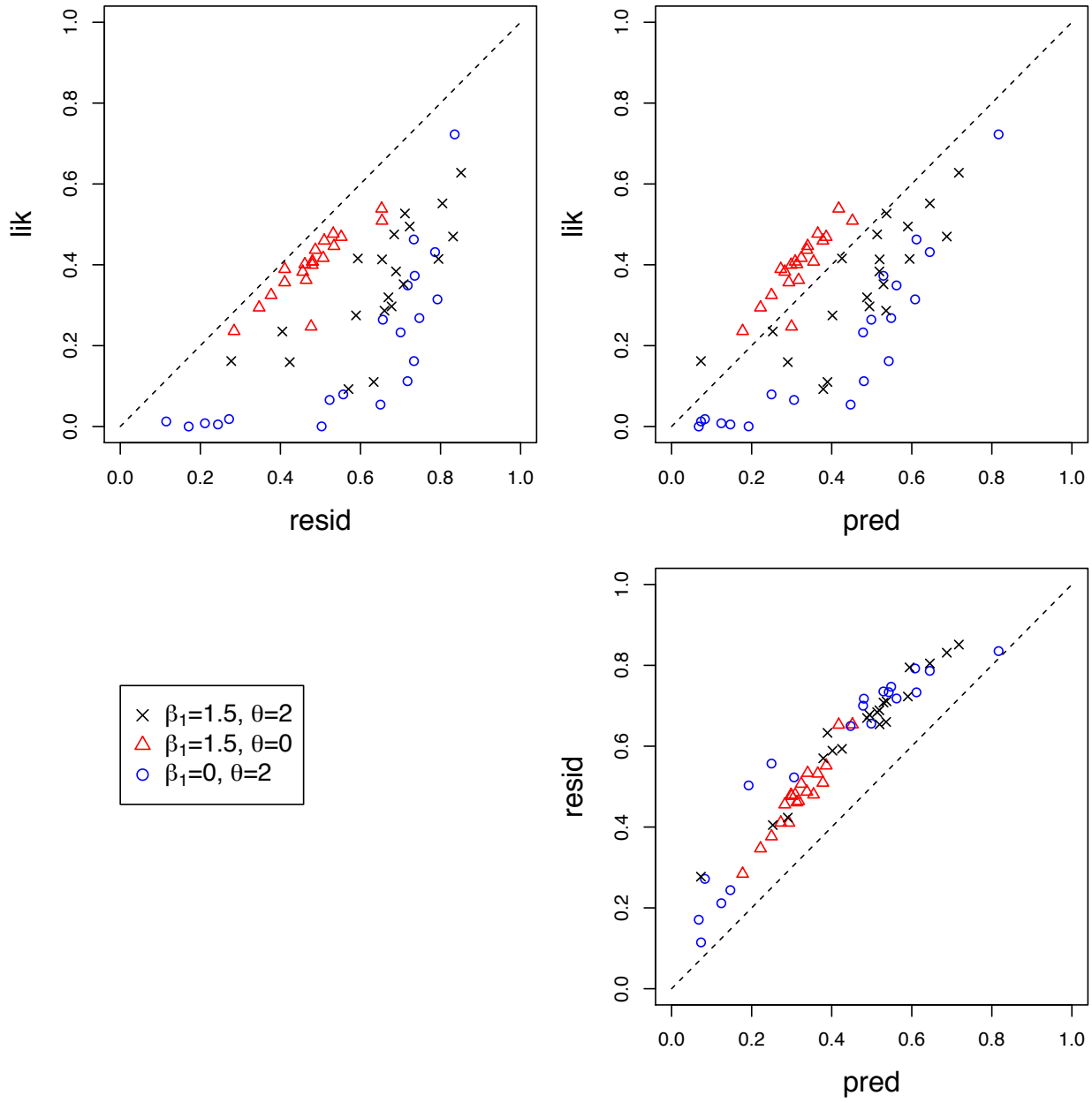
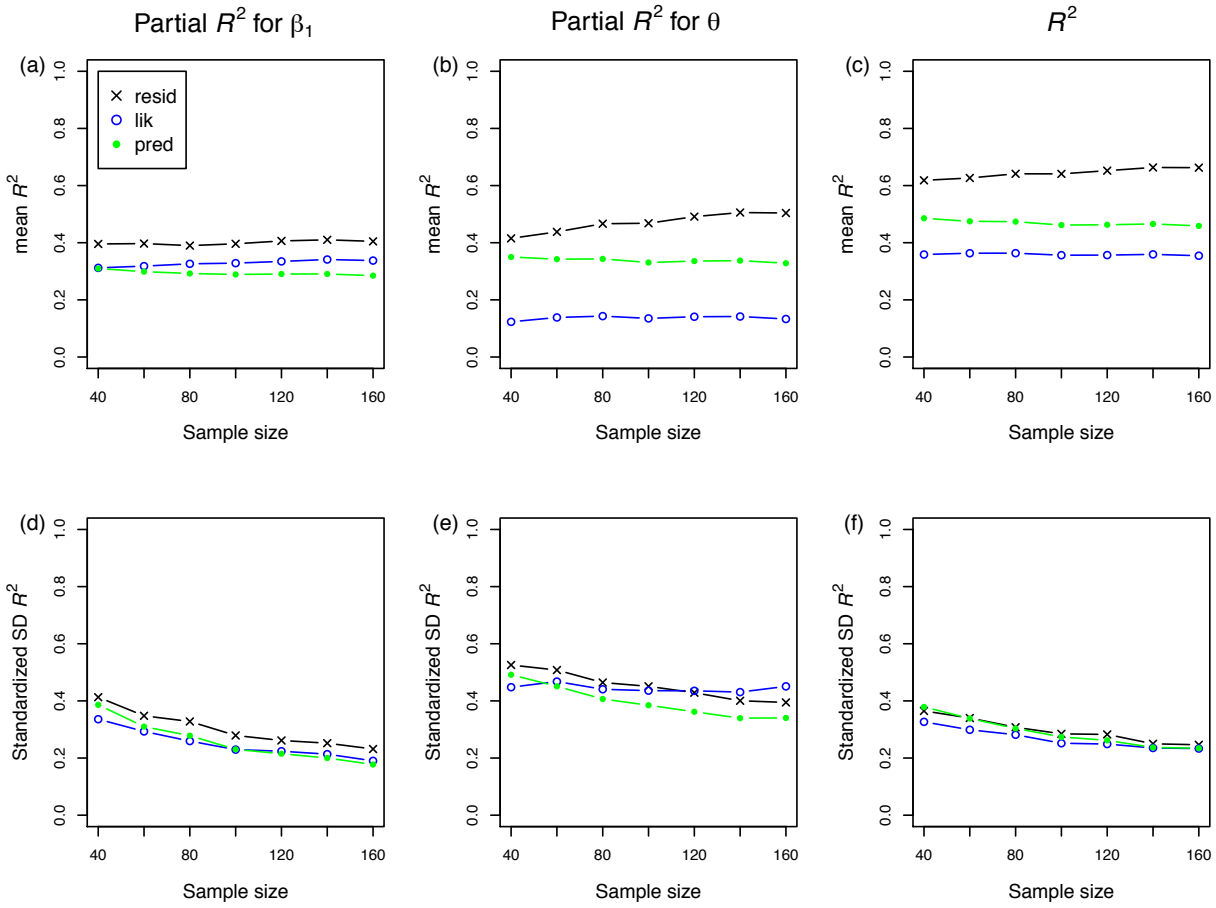

lik
resid
0.0
0.2
0.4
0.6
0.8
1.0
lik
pred
resid
pred
β1=1.5, θ=2
β1=1.5, θ=0
β1=0, θ=2

Fig. S12


Partial R^2 for β_1
Partial R^2 for θ
R^2
(a)
(b)
(c)
(d)
(e)
(f)
resid
lik
pred
mean R^2
Standardized SD R^2
Sample size
0.0
0.2
0.4
0.6
0.8
1.0
40
80
120
160

SUPPLEMENTARY SECTION 2: R CODE FOR FIGURES A1 AND A2

```
library(lme4)
library(MuMIn)
library(rr2)

inv.logit <- function(x) 1/(1+exp(-x))


# find correction factor for s2d that minimizes the difference between logit
 and Gaussian cumulative distribution functions
optim(par = .85, function(s) {
 x <- .001*(-5000:5000)
 SS <- mean((plogis(x)-pnorm(x, sd=s^.5*pi/3^.5))^2)
 return(SS)
}, method="BFGS")
# [1] 0.8768809


n <- 1000
p <- 10

d <- data.frame(x=0, y=0, u=rep(1:p, each=n/p))
d$u <- as.factor(d$u)

b1 <- 0
sd1 <- 1

nreps <- 100
w <- data.frame(rep=1:nreps)

for(i in 1:nreps){
 d$x <- rnorm(n=n)

 # simulate data from a logit model
 d$prob <- inv.logit(b1 * d$x + rep(rnorm(n=p, sd=sd1), each=n/p))

 # simulate data from a probit model
 #d$prob <- pnorm(b1 * d$x + rep(rnorm(n=p, sd=sd1), each=n/p))

 d$y <- rbinom(n=n, size=1, prob=d$prob)

 # analyze with a logit link function
 z <- glmer(y ~ 1 + (1|u), data=d, family=binomial)
 X <- model.matrix(z)
 mu <- fitted(z)
 Yhat <- X %*% lme4::fixef(z)
 s2.logit <- VarCorr(z)[[1]][1]
 s2w.logit <- exp(mean(log(1/(mu*(1-mu)))))
 s2d <- pi^2/3
 s2d.r <- 0.8768809 * pi^2/3

 w$s2.logit[i] <- s2.logit
 w$s2w.logit[i] <- s2w.logit
 w$s2d[i] <- s2d
 w$s2d.r[i] <- s2d.r

 w$R2.logit.NS[i] <- 1 - s2d/(var(Yhat) + s2.logit + s2d)
```

```
 w$R2.logit.rNS[i] <- 1 - s2d.r/(var(Yhat) + s2.logit + s2d.r)
 w$R2.logit.deltaNS[i] <- r.squaredGLMM(z)[2,2]
 w$R2.logit.w[i] <- 1 - s2w.logit/(var(Yhat) + s2.logit + s2w.logit)

 # analyze with a probit link function
 z.probit <- glmer(y ~ 1 + (1|u), data=d, family=binomial(link="probit"))
 mu.probit <- fitted(z.probit)
 Yhat.probit <- X %*% lme4::fixef(z.probit)
 s2.probit <- VarCorr(z.probit)[[1]][1]
 s2w.probit <- exp(mean(log(mu.probit*(1-
 mu.probit)/dnorm(qnorm(mu.probit))^2)))

 w$s2.probit[i] <- s2.probit
 w$s2w.probit[i] <- s2w.probit

 w$R2.probit.NS[i] <- 1 - 1/(var(Yhat.probit) + s2.probit + 1)
 w$R2.probit.deltaNS[i] <- r.squaredGLMM(z.probit)[2,2]
 w$R2.probit.w[i] <- 1 - s2w.probit/(var(Yhat.probit) + s2.probit +
 s2w.probit)
}

# Fig. S1
par(mfrow=c(1,3))
xlim <- c(0,.8)
ylim <- xlim

plot(w$s2.probit, w$s2.logit/w$s2d, xlim=xlim, ylim=ylim, xlab="s2[probit]",
 ylab="s2[logit]/s2d.NS")
lines(c(0,10),c(0,10), col="red")

plot(w$s2.probit, w$s2.logit/w$s2d.r, xlim=xlim, ylim=ylim,
 xlab="s2[probit]", ylab="s2[logit]/s2d.rNS")
lines(c(0,10),c(0,10), col="red")

xlim <- c(0,.4)
ylim <- xlim
plot(w$s2.probit/w$s2w.probit, w$s2.logit/w$s2w.logit, xlim=xlim, ylim=ylim,
 xlab="s2[probit]/s2w[probit]", ylab="s2[logit]/s2w[logit]")
lines(c(0,10),c(0,10), col="red")


# Fig. S2
par(mfrow=c(2,2))
xlim <- c(0,.45)
ylim <- xlim

plot(w$R2.probit.NS, w$R2.logit.NS, xlim=xlim, ylim=ylim,
 xlab="R2.NS[probit]", ylab="R2.NS[logit]")
lines(c(0,10),c(0,10), col="red")

plot(w$R2.probit.deltaNS, w$R2.logit.deltaNS, xlim=xlim, ylim=ylim,
 xlab="R2.deltaNS[probit]", ylab="R2.deltaNS[logit]")
lines(c(0,10),c(0,10), col="red")

plot(w$R2.probit.NS, w$R2.logit.rNS, xlim=xlim, ylim=ylim,
 xlab="R2.NS[probit]", ylab="R2.rNS[logit]")
lines(c(0,10),c(0,10), col="red")
```

```
plot(w$R2.probit.w, w$R2.logit.w, xlim=xlim, ylim=ylim, xlab="R2.w[probit]",
 ylab="R2.w[logit]")
lines(c(0,10),c(0,10), col="red")
```