Marginal predictions

January 15, 2021

1 Introduction

In this task, we describe various R machineries for displaying predictions in both simple and complex (involving interaction terms) generalized linear models. We first consider existing approaches for *conditioning* predictions and then describe our proposed approach for *marginalized* predictions. These provide a unified and intuitive way of describing relationships from a fitted model, especially complex models involving interaction terms or some kind transformations on the dependent variables whose estimates are usually, but not always, a subject to less clarity of interpretation.

We can derive various quantities from a fitted regression model. The first and most obvious, is the model coefficient estimates. Others include predicted values of the outcome variable—1) predictions at a particular; and 2) mean or median value of the predictors. The first case simply involves evaluation of the fitted model function, say $\hat{f}(X=x)$, at some particular value of x. The second case, chooses the values of the predictor based on its distributional properties.

Most importantly, from these predicted values, we can also generate second class quantities of interest – *conditional* or *marginal* predictions. These quantities describes the change in the predicted value of the dependent variable after changing one independent variable – either a discrete change in the categorical variable(s) or an instantaneous change in continuous variables, while all other variable are held at specified values.

Suppose we are interested in the *conditional* predictions of a particular predictor (hence forth referred as *focal* predictor otherwise *non-focal*), x_f , in the set of predictors. To keep it simple, assume that the model has no interaction terms. Then the idea is to fix the values of *non-focal* predictor(s) at

some typical values – typically determined by averaging in some meaningful way, for example, arithmetic mean and average over the levels of the factors of non-focal continuous and categorical predictors, respectively. This is achieved by averaging the columns of $model\ matrix$, \mathbf{X} , except for the column of focal predictor.

Consider a simple linear model with linear predictor $\eta = \mathbf{X}\beta$ and let $g(\mu) = \eta$ be an identity link function (in the case of simple linear model), where μ is the predicted (expected) value of outcome variable y. Let $\hat{\beta}$ be the estimate of β , together with the estimated covariance matrix $V(\hat{\beta})$ of $\hat{\beta}$. Let the entries of \mathbf{X}^* include all conditioned (non-focal) and focal predictors. The model matrix, \mathbf{X}^* , inherits most of its key properties, for example transformation (e.g., scaling) on the predictors and interactions from the model matrix, \mathbf{X} . Then the predicted values $\hat{\eta}^* = \mathbf{X}^*\hat{\beta}$ represents the conditional predictions of the focal predictor. Alternatively, we can transform these predictions to response scale using $q^{-1}(\hat{\eta}^*)$.

Further, we can compute the standard errors (SEs) of the *conditional* predictions, $\hat{\eta}^*$, for constructing confidence intervals, as the sqrt(diag($\mathbf{X}^*V(\hat{\beta})\mathbf{X}^{*T}$)). When computing *marginal* predictions, the *uncertainty* as a result of *non-focal* predictors are removed. This can be achieved in two ways:

- using variance-covariance matrix, $V(\hat{\beta})$
- using centered model matrix, X^*

1.1 Variance-covariance

The computation of $\hat{\eta}^*$ remains the same as described above. However, to compute SEs $V(\hat{\beta})$ is modified by zeroing-out (the variance-covariance of all non-focal predictors are assigned zero) entries of non-focal terms in $V(\hat{\beta})$. This approach requires centering of the predictors in the model matrix, X. In other words, the fitted model should have centered predictors.

1.2 Centered model matrix

Suppose the non-focal entries in X^* are computed by some kind of averaging. Consider centered X^* , $X_c^* = (X^* - \bar{X}^*)$. It follows that the non-focal entries in X_c^* are all zero. As a result, the SEs are computed as $\operatorname{sqrt}(\operatorname{diag}(\mathbf{X}_c^*V(\hat{\beta})\mathbf{X}_c^{*T}))$, which actually zeros-out. More generally, centering, $\mathbf{X}_c^* = \mathbf{X}^* - k$ (for example $k = E(\mathbf{X}^*)$) impacts on the estimated value

of the intercept and its associated variance. However, the slopes are not affect by this. The implication of this that since *non-focal* terms in \mathbf{X}_c^* are zero, it doesn't matter what their corresponding values are in the variance-covariance matrix. Hence, we can compute *marginal* predictions from non-centered predictors (in other words, fitted models with predictors in their natural scales).

2 Available packages

The following R packages **effects**, **emmeans** and **margins** implement various schemes for constructing *conditional* predictions. However, currently, their ability to compute *marginal* prediction is limited to the use of variance-covariance approach which requires the fitted model to be centered. We propose **varpred** to overcome this limitation.

3 Yet to figure out

- 1. Handling complex interaction
- 2. Zero SEs in the case of variance-covariance approach

4 Illustrations

4.1 Simulation

Consider a simple no-interaction terms simulation:

- $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$ s.t $\epsilon \sim N(0, 1)$ and $\{\beta_0 = -5, \beta_1 = 0.1, \beta_2 = -0.05\}$
 - $-x_1 \sim unif(1,9)$
 - $-x_2$ two level categorical variable
- > set.seed(101)
- > N <- 100
- > x1_min <- 1
- > x1_max <- 9
- > b0 <- 0.3

```
> b1 <- 0.1
> b2 <- -0.6
> x2_levels <- factor(c("A", "B"))
> df <- expand.grid(x1u = runif(n=N, min=x1_min, max=x1_max)</pre>
          , x2u = x2\_levels
+ )
> X <- model.matrix(~x1u + x2u, df)
> betas <- c(b0, b1, b2)
> df$y <- rnorm(nrow(df), mean= X %*% betas, sd=1)</pre>
> df2 <- df
> df <- transform(df
          , x1c = drop(scale(x1u, scale=FALSE))
          , x1s = drop(scale(x1u, center=FALSE))
          , x1sd = drop(scale(x1u))
+ )
> head(df)
      x1u x2u
                                x1c
                                          x1s
                                                    x1sd
            A -0.4524966 -1.222599 0.6940038 -0.5134124
1 3.977587
            A 0.1605887 -3.849588 0.2356505 -1.6165773
2 1.350599
3 6.677472
            A 1.5456482 1.477286 1.1650760 0.6203644
4 6.261523 A -0.4707503 1.061337 1.0925018 0.4456928
5 2.998846
            A 1.3489423 -2.201340 0.5232344 -0.9244202
6 3.400439
            A -0.4111428 -1.799747 0.5933038 -0.7557773
```

4.2 Model fitting

No scaling or centering covariates

```
> df_{temp} \leftarrow drop(df)  # margins doesn't work with transform

> # but we need df to extract attributes :(

> lm_u \leftarrow lm(y \sim x1u + x2u, data = df_{temp})

Centered covariates (x - \bar{x}) model

> lm_c \leftarrow lm(y \sim x1c + x2u, data = df_{temp})

Scaled covariates (x/sdx) model
```

```
> lm_s <- lm(y ~x1s + x2u, data = df_temp)
Both scaled and centered covariates
> lm_sd <- lm(y ~x1sd + x2u, data = df_temp)
Coefficients estimates
> coef_est <- modsummary(fun=coef)</pre>
> print(coef_est)
              lm_c
                     lm_s lm_sd
                                   lm_u
             0.808 0.229
                           0.808 0.229
(Intercept)
             0.111 0.638 0.265
x1c
                                  0.111
x2uB
            -0.535 -0.535 -0.535 -0.535
Log likelihoods
> 11_est <- modsummary(fun=logLik)</pre>
> print(ll_est)
                lm_s
                       lm_sd
        lm_c
                                lm_u
[1,] -272.27 -272.27 -272.27 -272.27
Variance covariance matrix
> vcov_est <- modsummary(fun=function(x)vcov(x), simplify=TRUE
          , combine="rbind", match_colnames = names(coef(lm_u)))
> print(vcov_est)
                  (Intercept)
                                       x2uB model
                                 x1u
lm_c.(Intercept)
                        0.009 0.000 -0.009
                                             lm_c
lm_c.x1c
                        0.000 0.001
                                      0.000
                                             lm_c
lm_c.x2uB
                       -0.009 0.000 0.018
                                             lm_c
lm_s.(Intercept)
                        0.031 -0.024 -0.009
                                             lm_s
lm_s.x1s
                       -0.024 0.026 0.000
                                             lm_s
lm_s.x2uB
                       -0.009 0.000 0.018
                                             lm_s
                        0.009 0.000 -0.009 lm_sd
lm_sd.(Intercept)
lm_sd.x1sd
                        0.000 0.005 0.000 lm_sd
lm_sd.x2uB
                       -0.009 0.000 0.018 lm_sd
lm_u.(Intercept)
                        0.031 -0.004 -0.009
                                             lm_u
lm_u.x1u
                       -0.004 0.001 0.000
                                             lm_u
```

lm_u.x2uB

-0.009 0.000 0.018 lm_u

4.3 Conditional predictions

The function will be used downstream to *tidy* conditional predictions from each of the methods highlighted above.

```
> condsummary <- function(mod_list, fun, resp = "y", simplify = TRUE
           , combine = c("cbind", "rbind"), scale_param = list(), fmethod = NULL)
           focal <- names(mod_list)</pre>
           combine <- match.arg(combine)</pre>
           out <- sapply(focal, function(f){</pre>
                    mod <- mod_list[[f]]</pre>
                    out <- fun(mod, f)</pre>
                    if (inherits(out, c("emmeans", "emmGrid"))) {
                             out <- as.data.frame(out)</pre>
                             oldn <- c(f, "emmean"</pre>
                                      , grep("\\.CL", colnames(out), value=TRUE)
                             newn <- c("xvar", "fit", "lwr", "upr")</pre>
                             colnames(out)[colnames(out) %in% oldn] <- newn</pre>
                    } else if (inherits(out, "eff")) {
                             out <- as.data.frame(out)</pre>
                             oldn <- c(f, "lower", "upper")</pre>
                             newn <- c("xvar", "lwr", "upr")</pre>
                             colnames(out)[colnames(out) %in% oldn] <- newn</pre>
                    } else if (any(colnames(out) %in% c("xvals", "yvals"))) {
                             ## Not proper way to handle margins object.
                             ## Maybe extend cplot to return inheritable object
                             oldn <- c("xvals", "yvals", "lower", "upper")</pre>
                             newn <- c("xvar", "fit", "lwr", "upr")</pre>
                             colnames(out)[colnames(out) %in% oldn] <- newn</pre>
                    } else {
                             out <- data.frame(out)</pre>
                             colnames(out)[colnames(out)%in%f] <- "xvar"</pre>
                    if (combine=="rbind"){
                             out <- cbind.data.frame(out, model = f)</pre>
                             out <- out[, c("xvar", "fit", "lwr", "upr", "model")]</pre>
                    pp <- names(scale_param)</pre>
```

```
if (!is.null(pp)){
                              if(grepl("s$",f)){
                                       vv <- grep("s$",f, value=TRUE)</pre>
                                       xsd <- scale_param[[vv]]</pre>
                                       out[,"xvar"] <- out[,"xvar"]*xsd</pre>
                              if(grepl("c$",f)){
                                       vv <- grep("c$",f, value=TRUE)</pre>
                                       xmu <- scale_param[[vv]]</pre>
                                       out[,"xvar"] <- out[,"xvar"] + xmu</pre>
                              if(grepl("sd$",f)){
                                       vv <- grep("sd$",pp,value=TRUE)</pre>
                                       xmu <- scale_param[[vv]][1]</pre>
                                       xsd <- scale_param[[vv]][2]</pre>
                                       out[,"xvar"] <- out[,"xvar"]*xsd + xmu</pre>
                              }
                    if (!is.null(fmethod)){
                              out[,"method"] <- fmethod</pre>
                    return(out)
           }, simplify = FALSE)
           f <- attr(out, "focal")</pre>
           if (simplify){
                    out <- do.call(combine, out)</pre>
                     if (combine=="cbind") {
                              colnames(out) <- mod</pre>
                     } else {
                              rownames(out) <- NULL
                    }
           attr(out, "response") <- resp</pre>
           return(out)
+ }
```

We start by computing the conditional predictions using each of the methods

(varpred, emmeans, effects, margins). In the first case, the predictions are displayed on the variable level scale-specific values (original (u), mean centered (c), divided by standard deviation (s), and both mean centered and scaled (sd)). In the second case, the predictions are transformed back to the original scale.

```
> simple_models <- list(x1u = lm_u, x1c = lm_c, x1s = lm_s, x1sd = lm_sd)
```

4.3.1 Continuous predictor

```
> ## varpred
> simple_vpred_all <- condsummary(mod_list=simple_models, fun=function(x, f){</pre>
          dd <- varpred(x, f)</pre>
+ }, simplify = TRUE, combine = "rbind", fmethod = "varpred")
> ## emmeans
> simple_empred_all <- condsummary(mod_list=simple_models, fun=function(x, f){
          spec <- as.formula(paste0("~", f))</pre>
          dd <- emmeans(x, spec=spec, cov.keep=f)</pre>
+ }, simplify = TRUE, combine = "rbind", fmethod = "emmeans")
> ## effects
> simple_efpred_all <- condsummary(mod_list=simple_models, fun=function(x, f){
          dd \leftarrow Effect(f, x, xlevels=100)
+ }, simplify = TRUE, combine = "rbind", fmethod = "effects")
> ## margins
> simple_margpred_all <- condsummary(mod_list=simple_models, fun=function(x, f){
          dd <- cplot(x, f, what="prediction", n=100, draw=FALSE)</pre>
+ }, simplify = TRUE, combine = "rbind", fmethod = "margins")
> ## Combine all the estimates
> simple_pred_all <- do.call("rbind"</pre>
          , list(simple_vpred_all, simple_empred_all, simple_efpred_all, simple_
+ )
> head(simple_pred_all)
                                        upr model method
                  fit
                             lwr
      xvar
1 1.081509 0.08197337 -0.1835256 0.3474723
                                              x1u varpred
2 1.160167 0.09072611 -0.1709771 0.3524294
                                              x1u varpred
3 1.238825 0.09947884 -0.1584477 0.3574054
                                              x1u varpred
4 1.317482 0.10823158 -0.1459380 0.3624011
                                              x1u varpred
```

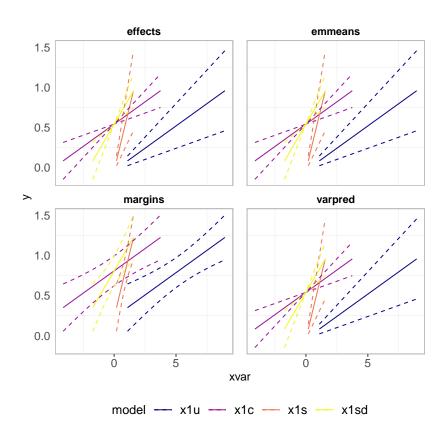


Figure 1: Conditional predictions on the variable-specific values.

Compute predictions and then back transform each predictor to the original scale.

```
> ## Extract scaling parameters
> scale_param <- list(x1s = unlist(attributes(df$x1s))</pre>
          , x1c = unlist(attributes(df$x1c))
          , x1sd = unlist(attributes(df$x1sd))
+ )
> ## varpred
> simple_vpred_spec <- condsummary(mod_list=simple_models, fun=function(x, f){</pre>
                  dd <- varpred(x, f)</pre>
          }, simplify = TRUE, combine = "rbind"
          , scale_param = scale_param, fmethod = "varpred"
+ )
> ## emmeans
> simple_empred_spec <- condsummary(mod_list=simple_models, fun=function(x, f){
                   spec <- as.formula(paste0("~", f))</pre>
                  dd <- emmeans(x, spec=spec, cov.keep=f)</pre>
          }, simplify = TRUE, combine = "rbind"
          , scale_param = scale_param, fmethod = "emmeans"
+ )
> ## effects
> simple_efpred_spec <- condsummary(mod_list=simple_models, fun=function(x, f){
                  dd <- Effect(f, x, xlevels=100)</pre>
          }, simplify = TRUE, combine = "rbind"
          , scale_param = scale_param, fmethod = "effects"
+ )
> ## margins
> simple_margpred_spec <- condsummary(mod_list=simple_models, fun=function(x, f)
                  dd <- cplot(x, f, what="prediction", n=100, draw=FALSE)</pre>
          }, simplify = TRUE, combine = "rbind"
          , scale_param = scale_param, fmethod = "margins"
+ )
> ## Combine all the estimates
> simple_pred_spec <- do.call("rbind"</pre>
          , list(simple_vpred_spec, simple_empred_spec, simple_efpred_spec, simp
+ )
> head(simple_pred_spec)
      xvar
                             lwr
                                        upr model method
1 1.081509 0.08197337 -0.1835256 0.3474723 x1u varpred
```

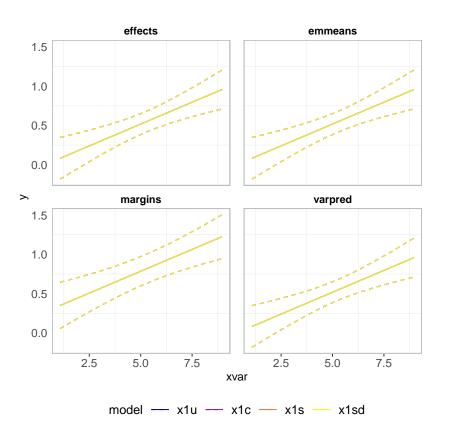


Figure 2: Back-transformed conditional predictions.

4.3.2 Categorical predictors

Here, we are considering case where we are only interested estimating the conditional predictions. In this case, it doesn't matter which of the four models we choose since they will give the same predictions. Later, we'll show how we can estimate marginalized and/or centered (CI) for categorical predictors.

```
> ## varpred
> simple_models_cat <- list(x2u = lm_u)</pre>
> simple_vpred_cat <- condsummary(mod_list=simple_models_cat, fun=function(x, f)
          dd <- varpred(x, f)</pre>
+ }, simplify = TRUE, combine = "rbind", fmethod = "varpred")
> ## emmeans
> simple_empred_cat <- condsummary(mod_list=simple_models_cat, fun=function(x, f
          spec <- as.formula(paste0("~", f))</pre>
          dd <- emmeans(x, spec=spec, cov.keep=f)</pre>
+ }, simplify = TRUE, combine = "rbind", fmethod = "emmeans")
> ## effects
> simple_efpred_cat <- condsummary(mod_list=simple_models_cat, fun=function(x, f
          dd <- Effect(f, x, xlevels=100)</pre>
+ }, simplify = TRUE, combine = "rbind", fmethod = "effects")
> ## margins
> simple_margpred_cat <- condsummary(mod_list=simple_models_cat, fun=function(x,
          dd <- cplot(x, f, what="prediction", n=100, draw=FALSE)</pre>
+ }, simplify = TRUE, combine = "rbind", fmethod = "margins")
> ## Combine all the estimates
> simple_pred_cat <- do.call("rbind"
+
          , list(simple_vpred_cat, simple_empred_cat, simple_efpred_cat, simple_
+ )
> head(simple_pred_cat)
  xvar
             fit
                       lwr
                                 upr model method
     A 0.8077896 0.6202052 0.9953740
                                        x2u varpred
     B 0.2727794 0.0851950 0.4603639
2
                                       x2u varpred
     A 0.8077896 0.6202052 0.9953740
                                       x2u emmeans
4
     B 0.2727794 0.0851950 0.4603639
                                       x2u emmeans
5
     A 0.8077896 0.6202052 0.9953740
                                       x2u effects
     B 0.2727794 0.0851950 0.4603639
                                      x2u effects
```

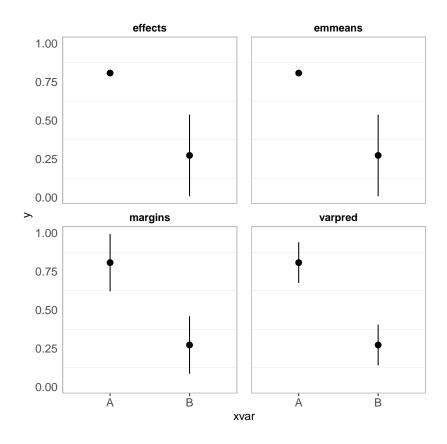


Figure 3: Conditional predictions.

4.4 Marginal predictions

We can implement marginalization by *zeroing-out* the variance of non-focal predictors (possible in all four methods) but this requires that the predictors are centered beforehand. On the other hand, in **varpred** marginal predictions can be obtained by centering the SE estimates.

4.5 zeroed-out covariance matrix

We **zero_vcov** function in **varpred** to transform the variances of non-focal predictors to zero. For example:

```
> lm_u_vcov <- vcov(lm_u)
> print(lm_u_vcov)
             (Intercept)
                                   x1u
                                                 x2uB
             0.030729586 -4.169417e-03 -9.047842e-03
(Intercept)
            -0.004169417 8.017823e-04 -3.588329e-19
x1u
x2uB
            -0.009047842 -3.588329e-19 1.809568e-02
> ## x1u is the focal variable
> lm_u_vcov_zero <- zero_vcov(lm_u, focal_vars = "x1u")</pre>
> print(lm_u_vcov_zero)
            (Intercept)
                                 x1u x2uB
(Intercept)
                      0 0.000000000
                      0 0.0008017823
                                         0
x1u
x2uB
                      0 0.000000000
                                         0
```

We'll repeat the same procedure in conditional predictions section but modify the functions to incorporate *zeroed-out* covariance matrix.

4.5.1 Continuous predictor

Notice that the modification in each of the method function call to pass either covariance matrix or function. In particular, in **varpred**, it is passed as **vcov**, **emmeans** and **effects** as **vcov**, and **margins** as **vcov**. However, this seems not to work currently in **cplot** which computes the predictions in **margins**.

```
+ spec <- as.formula(paste0("~", f))
+ dd <- emmeans(x, spec=spec, cov.keep=f, vcov. = zero_vcov(x, f))
+ }, simplify = TRUE, combine = "rbind", fmethod = "emmeans")
> ## effects
> simple_efpred_all <- condsummary(mod_list=simple_models, fun=function(x, f){
+ dd <- Effect(f, x, xlevels=100, vcov. = function(x, complete=FALSE)zer
+ }, simplify = TRUE, combine = "rbind", fmethod = "effects")
> ## margins
> simple_margpred_all <- condsummary(mod_list=simple_models, fun=function(x, f){
+ dd <- cplot(x, f, what="prediction", n=100, draw=FALSE, vcov=function(x, f), simplify = TRUE, combine = "rbind", fmethod = "margins")
> ## Combine all the estimates
> simple_pred_all <- do.call("rbind"
+ , list(simple_vpred_all, simple_empred_all, simple_efpred_all, simple_
+ )</pre>
```

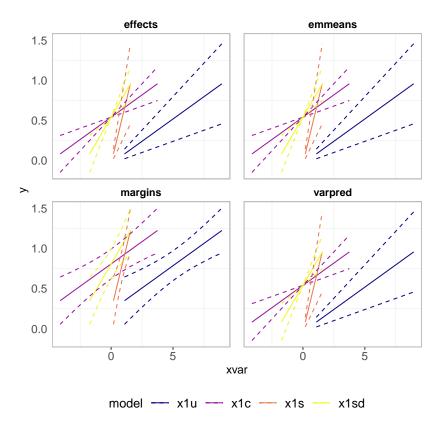


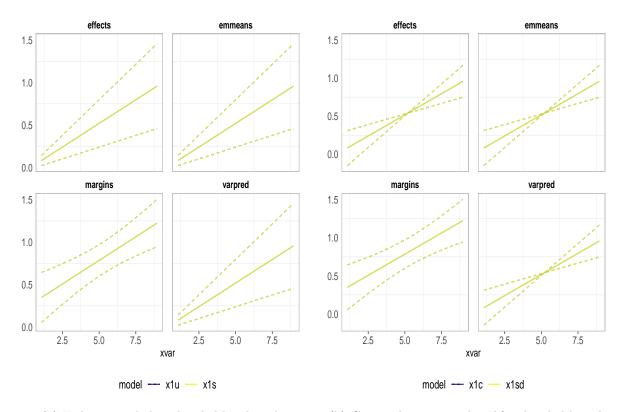
Figure 4: Marginal predictions with the zeroed-out covariances on the variable-specific scale.

Also, we repeat above implementation but back-transform the predictions to original scale (unscale – uncenter and/or unscale) by modifying the previous code to include scaling parameters. To clearly distinguish between what happens when apply various scaling schemes, we separately do the plots (see Figure 5).

4.6 Centered model matrix

Marginal predictions in **effects** and **emmeans** require models fitted with transformed predictors. However, in **varpred** we can use model fitted using predictors on their original scale and estimate marginal predictions. In our

example, we use the unscaled model lm_u and simply set isolate=TRUE. The predictions (see Figure 6) are similar to Figure 5 b (except for the margins).



- (a) Either unscaled or devided by the sd.
- (b) Centered or centered and/or devided by sd.

Figure 5: Back-transformed marginal predictions.

```
> ## Centered predictions from unscaled model
```

> plot(vpred_c)

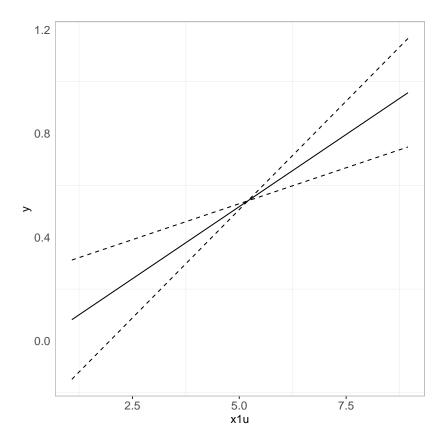


Figure 6: Using **varpred** to obtain marginal predictions from unscaled model.

4.6.1 Categorical predictors

Back to categorical predictor, x2u. The reference (base) category has not variance and has such we can not use the zeroed-out covariance approach to estimate CI for the marginalized predictions. However, if we can figure out how to center model matrix in the computation of CIs, we can actually use model with unscaled categorical predictors and estimate marginal predictions for centered categorical predictors. Currently, only **varpred** provide this

> vpred_c <- varpred(lm_u, focal = "x1u", isolate = TRUE)

functionality.

```
> ## varpred
> simple_models_cat <- list(x2u = lm_u)</pre>
> simple_vpred_cat <- condsummary(mod_list=simple_models_cat, fun=function(x, f)
          dd <- varpred(x, f, isolate=TRUE)</pre>
+ }, simplify = TRUE, combine = "rbind", fmethod = "varpred")
> ## emmeans
> simple_empred_cat <- condsummary(mod_list=simple_models_cat, fun=function(x, f
          spec <- as.formula(paste0("~", f))</pre>
          dd <- emmeans(x, spec=spec, cov.keep=f, vcov. = zero_vcov(x, f))</pre>
+ }, simplify = TRUE, combine = "rbind", fmethod = "emmeans")
> ## effects
> simple_efpred_cat <- condsummary(mod_list=simple_models_cat, fun=function(x, f
          dd <- Effect(f, x, xlevels=100, vcov. = function(x, complete=FALSE)zer
+ }, simplify = TRUE, combine = "rbind", fmethod = "effects")
> ## margins
> simple_margpred_cat <- condsummary(mod_list=simple_models_cat, fun=function(x,
          dd <- cplot(x, f, what="prediction", n=100, draw=FALSE, vcov=function(</pre>
+ }, simplify = TRUE, combine = "rbind", fmethod = "margins")
> ## Combine all the estimates
> simple_pred_cat <- do.call("rbind"</pre>
          , list(simple_vpred_cat, simple_empred_cat, simple_efpred_cat, simple_
+ )
> head(simple_pred_cat)
             fit
                                   upr model method
                         lwr
1
     A 0.8077896 0.675147365 0.9404318
                                         x2u varpred
     B 0.2727794 0.140137215 0.4054217
                                         x2u varpred
     A 0.8077896 0.807789595 0.8077896 x2u emmeans
     B 0.2727794 0.007494985 0.5380639
                                         x2u emmeans
     A 0.8077896 0.807789595 0.8077896 x2u effects
     B 0.2727794 0.007494985 0.5380639
                                         x2u effects
> class(simple_pred_cat) <- c("jdeffects", "data.frame")</pre>
> simple_pred_cat_plot <- (plot(simple_pred_cat)</pre>
          + facet_wrap(~method)
          + theme(legend.position="bottom")
+ )
```

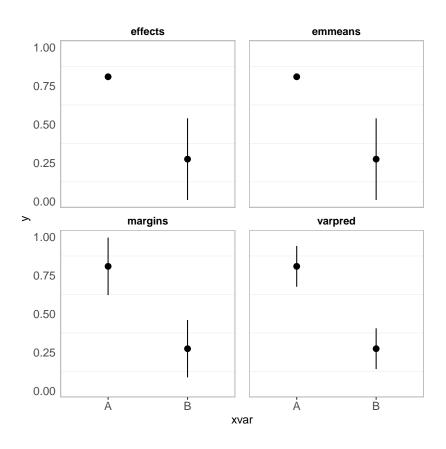


Figure 7: Conditional predictions.