UNIVERSITY OF MANNHEIM
School of Social Sciences

Advanced Quantitative Methods in Political Science: Interpretation and Simulation

Thomas Gschwend | Lisa-Marie Müller | Domantas Undzėnas

Week 7 - 25 March 2026

Leftovers from last week: Fit Measures, Specification and Robustness Checks

Further Model Fit, Specification and Robustness Checks

- *Cross-Validation* (for all types of models)
  - Randomly divide the data set into M approximately equally sized folds (each fold contains about $\frac{N}{M}$ observations)
  - For each $k \in \{1, \ldots, M\}$: estimate the model using all folds except fold k (training data), then evaluate predictive performance on fold k (test data).
  - For inference, we can also average results across the different M estimations.
  - Useful when the data set is too small to set aside a large test sample
  - What does "average results" imply?
    - *Point estimate* is the mean of the estimated point estimates of the M subsets.
    - *Standard error* should account for *within* as well as *across* variance (see King et al. 2001. "Analyzing Incomplete Political Science Data: An Alternative Algorithm for Multiple Imputation". *American Political Science Review* 95: 49 – 69, equation (3))
- *Repeated random sub-sampling validation* (e.g., to test for unobserved heterogeneity)
  - Sample 2/3 of data, run model and collect results. Repeat several (about $M = 20$) times for different samples and combine results per King et al 2001 (aka "Rubin Rule", see above).
- Confront (all) *observable implications* with your observations.

How to get "average results" across M data sets? (aka "Rubin Rule")

- Average point estimates of your quantity of interest q across M sets of estimates

$$\bar{q} = \frac{1}{M} \sum_{k=1}^{M} q_k$$

- Standard errors should account for *within* as well as *across* variance

$$SE(\bar{q})^2 = \frac{1}{M} \sum_{k=1}^{M} SE(q_k)^2 + S_q^2 (1 + \frac{1}{M})$$

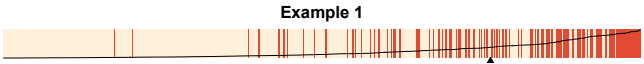
with $S_q^2 = \sum_{k=1}^{M} (q_k - \bar{q})^2 / (M - 1)$

Likelihood-Based Approaches

- Evaluation of model fit through any test statistic that is based on a transformation of the log-likelihood will be a *relative* measure of model fit (e.g., LRT)
- Akaike Information Criterion: $AIC = -2 \cdot lnL + 2p$
  - where p is the number of parameters in the statistical model, and L is maximum of the likelihood function for given model.
  - Pick the model among the possible ones with minimum AIC value. There is no statistical test of difference in AIC.
  - The penalty term ($2p$) does discourage overfitting while rewarding goodness of fit (because of LL).
- Bayesian Information Criterion: $BIC = -2 \cdot lnL + p \cdot ln(N)$
  - where N is the number of observations.
  - Larger penalty term ($p \cdot ln(N)$).
- AIC and BIC work even for non-nested models. Further examples are Vuong test, Bayes factors,....

Assessing Model Fit graphically - Separation Plot

Brian Greenhill, Michael D. Ward, Audrey Sacks. 2011. "The Separation Plot: A New Visual Method for Evaluating the Fit of Binary Models" *American Journal of Political Science*, 55(4): 991-1002.



- Graph fitted values with different colors for each observed outcome.
- Line indicates the predicted probabilities of the observations
- Helpful for identifying clusters of false negatives and false positives (systematic or coding errors)
- Can be also used for models with more than two categorical outcomes!
- In R use e.g, `library(separationplot)`

Intro

What should you take home from this class today?

- We will get to learn tools to improve the interpretation of our results
- Simulations will be our friends
- We will repeat how to simulate *quantities of interest* and apply these tools to a logit example.
- There are two conceptual approaches for defining interesting scenarios: *Average-Case* vs *Observed Value*

Improving Interpretation through Simulating Quantities of Interest

Substantive Interpretation in Non-Linear Models

- Interpreting linear regression coefficients is straightforward because, the effect on Y of a given change in X_j is the same regardless ...
  - ...of the value of that variable
  - ...of the level of all other covariates in the model
- "Holding all other variables constant, ..."
- This is not so in non-linear models!
  - Neither marginal (or discrete) changes with respect to X_j are constant. They are no longer simply equal to a parameter (β_j).
  - The effect on Y of a given change in X_j depends *on values of all other variables* in the model.
  - Thus, each observation i has a different marginal effect.
- Thus, we need another strategy for interpretation and need to invest more time in presenting and interpreting our results.

What Grandma doesn't get - The Ugly Table

Table 1: Logistic Regression Predicting Vote Switching

	Vote switching (= 1)
Small Party	0.998
	(0.228)
Ideology	-7.623
	(3.078)
Candidate	0.806
	(0.214)
Coalition	2.845
	(0.340)
Time	-0.395
	(0.133)
Constant	3.474
	(2.487)
Observations	987

Robust standard errors in parentheses

Criteria for Substantive Interpretation

- Convert raw estimation results in quantities of interest, i.e., express results in substantive terms (e.g., in units of the dependent variable or as probability of an event).
- Convey uncertainty about those quantities.
- Avoid statistical jargon.

General Principles

1. Communicate Substance, Not Statistics
2. When Performing Inference, Convey Uncertainty
3. Graph Data and Results

Communicate Substance, Not Statistics

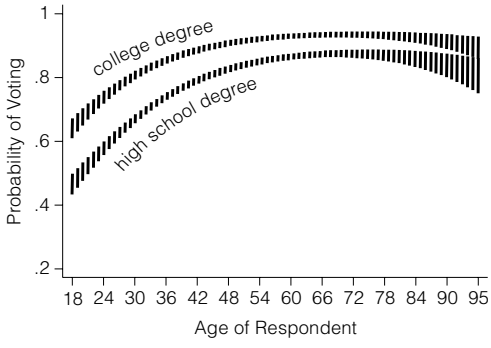
- The coefficient for *Small Party* (.998) is statistically significant
- Other things being equal, for supporters of a small party the likelihood of switching their vote is about 20 percent. That probability decreases to about only 8 percent for large party supporters.

When Performing Inference, Convey Uncertainty

- The coefficient for variable *Small Party* (.998 with a standard error of .23) is statistically significant at the .001 level.
- Other things being equal, for supporters of a small party the likelihood of switching their vote is about 20 (+/- 6) percent. That probability decreases to about only 8 (+/- 2) percent for large party supporters.

Graph Data and Results - Example 1

Figure 1 Probability of Voting by Age



Vertical bars indicate 99-percent confidence intervals

Conceptually three Steps

1. Define a *Quantity of Interest*
   - *Predicted values* $Y|X$ of switching a vote for interesting, "typical" (i.e., mean) or observed values of X. Predicted values are on the same scale as Y.
   - *Expected values* $E(Y|X)$
   - *First differences* $E(Y|X_{j_1}, X) - E(Y|X_{j_2}, X)$, the difference of two expected values (e.g., size of causal effect)
   - *Average marginal (causal) effect*: compute marginal (causal) effect for every observation and then average across them
   - any other quantity
2. Simulate quantity of interest (QoI) and uncertainty around it.
3. Visualize results for interesting scenarios (potentially across all values of a key independent variable)

How to simulate Quantities of Interest?

Strategy for Substantive Interpretation

1. We get QoI as a function of estimated coefficients
2. Where is the uncertainty in a statistical model?
3. Use simulation to account for estimation and fundamental uncertainty
4. Create plots and tables for communicating your results

Where is the Uncertainty?

Recall that we can write any statistical model as

$$
\begin{aligned}
Y_i &\sim f(y_i|\theta_i, \alpha) && \text{stochastic} \\
\theta_i &= g(X_i, \beta) && \text{systematic}
\end{aligned}
$$

1. Estimation Uncertainty: Uncertainty about what the true parameters β and α of the model are. Think of it as caused by small samples. Vanishes if N gets larger.
2. Fundamental Uncertainty: Represented by stochastic component of the model. Exists no matter what (even if model is correct and we would have infinite many observations) because of inherent randomness of the world.

Simulating Estimation Uncertainty

We account for estimation uncertainty by taking random draws from the approximated "sampling distribution" of all parameters

1. Estimate the model by maximizing the likelihood function (as a canned procedure or using `optim()` in `R`), record the point estimates $\hat{\gamma}$ of all parameters $\gamma = vec(\beta, \alpha)$ and the estimated variance matrix $\hat{V}(\hat{\gamma})$.
2. Draw one vector $\tilde{\gamma} = vec(\tilde{\beta}, \tilde{\alpha})$ from the multivariate normal distribution (representing estimation uncertainty because of CLT), which approximates the sampling distribution we do not have

$$\gamma \sim N\left(\hat{\gamma}, \hat{V}(\hat{\gamma})\right)$$

One draw $\tilde{\gamma}$ is also called *simulated value*.

Logit implementation in R as a running Example

```
ll.logit <- function(theta, y, x) {
# theta consists merely of beta (dim is ncol(X))
  beta   <- theta[1:ncol(X)]
# linear predictor; make sure that X is stored as.matrix
  mu <- X %*% beta
# link function
  p <- 1/(1+exp(-mu))
# individual ll contribution
  ll <- y*log(p) + (1-y)*log(1-p)
# sum
  ll <- sum(ll)
  return(ll)
 }
```

Logit Implementation in R as a running Example

```
# maximize the likelihood function numerically using optim()
res <- optim(c(1,1),                 # starting values
         fn=ll.logit,                # the likelihood function
         control=list(fnscale=-1),   # maximize instead of minimize fct
         y =dat$survived, x = X,     # the data
         method = "BFGS",            # optimization method
         hessian=TRUE)               # return numerical Hessian

cat("MLE Betas\n", res$par, "\n")
cat("Hessian\n")
print(res$hessian)
cat("\nMLE Standard Errors \n", sqrt(diag(solve(-1 * res$hessian))), "\n\n")

# compare with canned logit in R (using standard GLM function)
summary(glm(dat$survived ~ dat$sex, family="binomial"))
```

1. Predicted Values

We can simulate the distribution of predicted values in the following way:

- To simulate *one* predicted value, follow these steps:
  - Step 1: Draw one vector $\tilde{\gamma} = vec(\tilde{\beta}, \tilde{\alpha})$.
  - Step 2: Decide which scenario you wish to compute (i.e., simulate) and, thus, choose one value for *each* explanatory variable in the model (why?). Denote the vector of such values that defines your scenario with X_c.
  - Step 3: Run those values (from step 1 and 2) through link function $g(X_c, \tilde{\beta})$ of systematic component. Denote it by $\tilde{\theta}_c$.
  - Step 4: Finally, to get a predicted value of the chosen scenario $\tilde{Y}_c$, take one random draw from, $f(\tilde{\theta}_c, \tilde{\alpha})$, the stochastic component of the statistical model, to simulate fundamental uncertainty.
- To simulate say $M = 1000$ predicted values, repeat algorithm 1000 times. Use these to plot distribution of simulated predicted values or compute average, standard deviation, percentile values (or anything you want) to summarize this distribution.

2. Expected Values

We can simulate the distribution of expected values similarly:

- To simulate *one* expected value, follow steps 1-4 to generate m predicted values and, then, "average out" fundamental uncertainty (stochastic component) by taking the expectation of these.
  - Step 1: Draw one vector $\tilde{\gamma} = vec(\tilde{\beta}, \tilde{\alpha})$ to account for estimation uncertainty.
  - Step 2: Decide which scenario you wish to simulate and choose X_c, i.e., fix each explanatory variable at particular values.
  - Step 3: Run those values (from step 1 and 2) through link function $g(X_c, \tilde{\beta})$ to get $\tilde{\theta}_c$.
  - Step 4: Draw m values $\tilde{Y}_c^{(k)}$ (with $k = 1, \ldots, m$) from the stochastic component $f(\tilde{\theta}_c, \tilde{\alpha})$ to simulate fundamental uncertainty.
  - Step 5: Average over fundamental uncertainty (stochastic component) by calculating the mean of those m simulations to get one *simulated expected value* $E(Y_c) = \sum_{k=1}^{m} \tilde{Y}_c^{(k)} / m$.
- To simulate, say, $M = 1000$ expected values, repeat algorithm 1000 times. Use these to plot distribution of simulated predicted values or compute an average, std. dev., certain percentile values (or anything you want) to summarize this distribution.

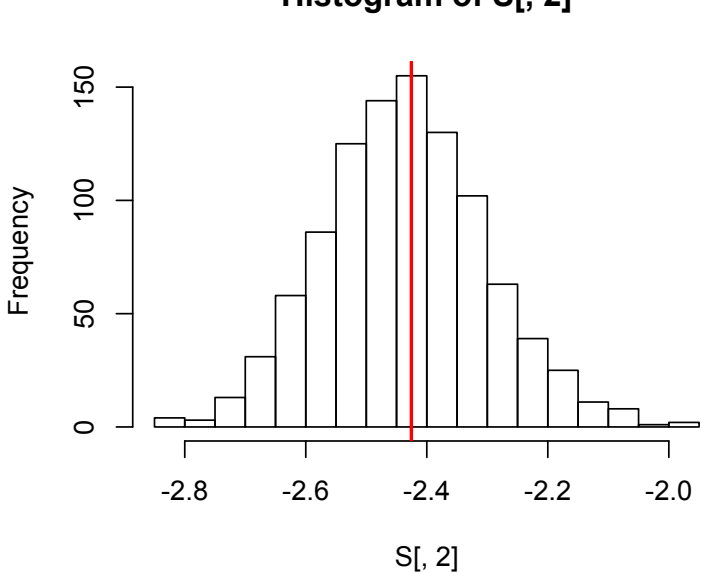
Logit Implementation in R as a running Example

```
# ==========================================
# = Step 1: Simulate Estimation Uncertainty =
# ==========================================

# get gamma and V from optim()
gamma <- res$par
    V <- solve(-res$hessian)

library(MASS)                              # provides mvrnorm
nsim <- 1000                               # N simulations
set.seed(1234)                             # to replicate draws
S <- mvrnorm(nsim, mu = gamma, Sigma = V) # simulations of gamma

dim(S)
# look at simulated distribution in contrast to
# estimated beta coeff (for men)
hist(S[,2], breaks=20)
abline(v=gamma[2], col="red", lwd=2)
```


Histogram of S[, 2]
Frequency
0
50
100
150
-2.8
-2.6
-2.4
-2.2
-2.0
S[, 2]

Logit Implementation in R as a running Example

```
# ================================
# = Step 2: Choose Scenario X_c  =
# ================================

#  set e.g. all covariates to the sample mean
# mean will be applied over columns of X
# Check ?apply for descriptions of all other arguments.
  X_c <-  apply(X, 2, mean)

# ========================================
# = Step 3: Get lp_c (linear predictor)  =
# ========================================

  lp_c<- S %*% X_c
# run it through link-function
  theta_c <- 1/(1+exp(-lp_c))
# summarize simulation results
  mean(theta_c); sd(theta_c)
  quantile(theta_c, c(.025, .975)
  hist(theta_c, breaks=20)
```

Logit Implementation in R as a running Example

```
# ============================================
# = Step 4: Simulate Fundamental Uncertainty  =
# ============================================

# create empty vector to store random draws
  Y_c<-rep(NA,nsim)

  set.seed(1212)    # to be able to replicate draws
  for (i in 1:nsim){
  Y_c[i]<-rbinom(n = 1, size = 1, prob = theta_c[i])
  }

  table(Y_c)

# ================================================
# = Step 5: Average over Fundamental Uncertainty  =
# ================================================

  mean(Y_c)
```

Difference between Predicted and Expected Values

- Predicted values are draws of Y from the stochastic component that are observed or could be observed (e.g., $\hat{Y} = 1$ or 0)
- Expected values are draws from fixed features of the distribution of Y such as $E(Y)$. Not necessarily observed (e.g., $\pi_i = .6$).
- Predicted values include estimation and fundamental uncertainty
- Expected values average over fundamental uncertainty. The variance of the distribution of expected values (but not of predicted values) go to 0 as N gets large.
- Example use of the distribution of *predicted values*
  - Weather Forecast: Pred. prob. that temperature in Mannheim tomorrow drops below 0^oC.
  - Predicted temperature uncertain because we estimate it and because of natural fluctuations.
- Example use of the distribution of *expected values*
  - Pred. prob. that temperature in Mannheim *on days like tomorrow* drops below 0^oC.
  - Expected temperature is only uncertain because we have to estimate it.
  - We are more certain about expected than actual temperature because we do not care about natural fluctuations.

Further Remarks on Simulating Expected Values

- When $m = 1$ the algorithm to get expected values reduces to the one for predicted values.
- The larger m the better does the algorithm purge away of fundamental uncertainty.
- When $E(Y_c) = \theta_c$, one can skip step 4 and 5. For instance, in the logit model (whenever expected value equals predicted prob. such as for Bernoulli processes), once we have simulated π_i, we do not need to draw Y_c and than average them to get $E(Y_c) = \pi_i$.

```
# results from step 5 (average over fundamental uncertainty)
  mean(Y_c)
  [1] 0.3598

# compare results if we had stopped with step 3
  mean(theta_c)
  [1] 0.3589098
```

3. First Differences

We can simulate the distribution of *first differences* using the same logic as before for simulating expected (as well as predicted) values:

- To draw *one* simulated first difference, follow the following steps.
  - Step 1: Draw one vector $\tilde{\gamma} = vec(\tilde{\beta}, \tilde{\alpha})$.
  - Step 2: Decide which contrast you wish to simulate and choose X_s and X_c, i.e., fix each explanatory variable at particular values.
  - Step 3: Run those values (from step 1 and 2) through link function $g(X_c, \tilde{\beta})$ to get $\tilde{\theta}_c$. Analogously, run $g(X_s, \tilde{\beta})$ to get $\tilde{\theta}_s$.
  - Step 4: Apply the expected value algorithm twice, once for X_s and X_c (we can reuse random draws).
  - Step 5: Take the difference between the two expected values.
- To simulate say $M = 1000$ first differences, repeat algorithm 1000 times. Use these to plot distribution of simulated first difference values, standard deviation, percentile values (or anything you want) to summarize this distribution.

Logit Implementation in R as a running Example

```
# ========================================
# = first differences male vs female     =
# ========================================

# Step 1
# Use simulations of mvrnorm from before

# Step 2
# construct scenario of interest

# set everything to sample mean
  X_1 <- X_2 <- apply(X, 2, mean)

# Now define contrast
  X_1[2] <- 0 # men=0 for female
  X_2[2] <- 1 # men=1 for male
```

Logit Implementation in R as a running Example

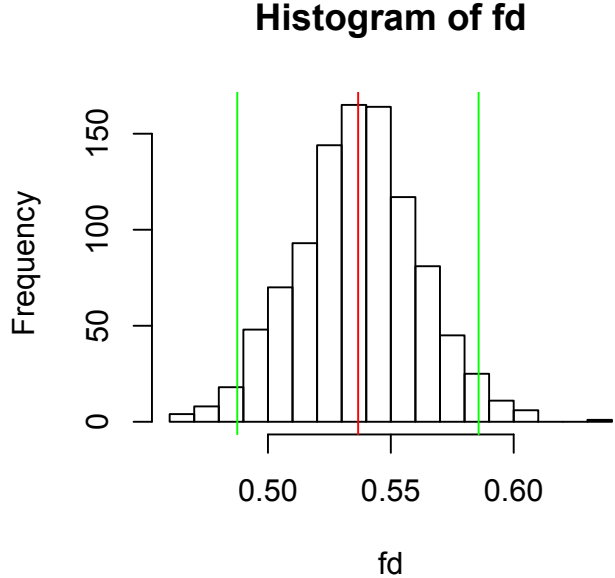
```
# Step 3 (combining step 4 and 5)
# Get theat_c - the linear predictor

   lp_1 <- S %*% X_1
    ev1 <- 1/(1+exp(-lp_1))

   lp_2 <- S %*% X_2
    ev2 <- 1/(1+exp(-lp_2))

# calculate first-difference
# fd = ev(female) - ev(male)
     fd <- ev1 - ev2

mean(fd); sd(fd)
quantile(fd, c(.025, .975))
```


Histogram of fd
Frequency
0
50
100
150
0.50
0.55
0.60
fd

Construction of the Scenario of Interest

There are two conceptual approaches: *Average-Case* vs *Observed Value*

1. So far we have seen examples of the so-called *average-case* approach to define scenario of interest.
   - Set key IV to interesting value, and the other to average (typical) values.
   - Note that those scenarios are hypothetical — they might not actually exist in your data (inference is model dependent!)
   - Nevertheless helpful for theory tests because we often do not hypothesize about an "average case" but about specific conditions under which a relationship holds.

Construction of the Scenario of Interest

There are two conceptual approaches: *Average-Case* vs *Observed Value*

2. The so-called *observed-value* approach is an alternative approach
   - Provides average effect in the data of your key variable of interest holding all other variables at their *observed value*, aka average marginal effect (AME) of that variable.
   - AME of a variable is the average across all individual marginal effects, i.e., the expected change in the probability for a unit change in the key variable of interest holding all other variables at their *observed value*.
   - Used to calculate average treatment effect (ATE), the average of first-difference when unit gets (hyp.) treatment and when it is not, or more generally the treatment effect of a randomly picked observation.

- But mean (average) of the individual marginal effects (AME) holding all other variables at their *observed value* $\neq$ marginal effect at the mean (MEMs).
- It's problematic to calculate counterfactuals that are "far away from the data".

Simulating Parameters - Some Useful Tips

1. Simulate all parameters including ancillary parameters together.
2. Reparameterize to unbounded scale to ...
   - ...make $\tilde{\gamma}$ converge more quickly in n to a multivariate normal. Thus, more reasonable for smaller sample size.
   - ...make maximization algorithm work faster and without explicit constraints.
3. Ideally, all parameters should be unbounded and logically symmetric, e.g.,
   - for non-negative parameters: $\sigma^2 = e^{\eta}$
   - for $0 - 1$ bounded parameters (e.g., probability): $\pi = \frac{1}{1+e^{-\eta}}$.
   - for $-1 \leq \rho \leq 1$, use $\rho = (e^{2\eta} - 1)/(e^{2\eta} + 1)$ (*Fisher's Z transformation*)

   In all three cases, η is unbounded. Reparameterize back to a scale people care about.

Simulating Parameters - More Useful Tips

- Always compute simulations of Y (i.e. predicted values) and use that as a basis for simulating other quantities (of interest).
- If you are interested in simulating functions of Y, say $ln(Y)$ do the following: Simulate $ln(Y)$ and then apply the inverse function $exp(ln(Y))$ to get Y. Y is probably on a meaningful scale we care about. Summarize the distribution of the simulated values with median or mean (for more details, see Rittmann et al. 2023. "How to improve the substantive interpretation of regression results when the dependent variable is logged". *Political Science Research and Methods*, FirstView.)
- Check *approximation error* of your simulation: Run it twice, check no. of digits of precision that do not change. If *not* enough precision for presenting results in a table, increase M (or m) and try again.
- Analytical calculations (e.g., delta method) and other tricks can speed-up simulation and increase precision.