



Model selection in regression

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Selecting the "best" model



There are often:

- many variables to choose
- many models: subtly different configurations
- different costs
- different power
- not an unequivocal "best"

More realistic goal:

Select a "most-satisficing" model – gets you where you want to go, at reasonable cost

Box: "All models are wrong, but some are useful"

Selecting the "best" model



Criteria for model selection

- Sometimes quantifiable
- Sometimes subjective
- Sometimes biased by preconceived ideas
- Sometimes pre-conceived ideas are truly important
- How well do they apply in future samples?

Regression: Opposing criteria

- Good fit, good in-sample prediction
 - Make R² large or MSE small
 - \rightarrow Include many variables
- Parsimony:
 - Keep cost of data collection low, interpretation simple, standard errors small
 - \rightarrow Include few variables

Model selection: the task of selecting a (mathematical) model from a set of **potential** models, given **evidence** and some **goal**.

Statistical goals

- Descriptive/exploratory
 - Describe relations between response & predictors
 - → want precision (+ parsimony ?)
- Scientific explanation
 - Test hypothesis, possibly 'causal' relations
 - $\hfill \rightarrow$ Control/adjust for background variables
 - $\label{eq:product} \rightarrow$ Want precise tests for hypothesized predictors
- Prediction/selection
 - How well will my model predict/select in future samples?
 - \rightarrow Cross-validation methods
- Data mining
 - Sometimes we have a huge # of possible predictors
 - Don't care about explanation
 - Happy with a small % "lift" in prediction

Model selection criteria

• R² = SSR_{model} / SS_{Total}

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- Cannot decrease as more variables added
- \rightarrow look at ΔR^2 as new variables added
- Adjusted R² attempts to adjust for # predictors.

Adj
$$R^2 = 1 - \left(\frac{n-1}{n-p}\right)(1-R^2)$$

• This is on the right track, but antiquated (Wherry, 1931)

Model selection criteria: C_p

- Mallow's C_p: measure of 'total error of prediction' using p parameters
 - est. of

 $\frac{1}{\sigma^2} \sum \left(\underbrace{\operatorname{var}(\hat{y})}_{\text{random error}} + \underbrace{(\hat{y}_{true} - \hat{y}_{\rho})^2}_{\text{bias}} \right)$

- $C_p = (SSE_p / MSE_{all}) (n-2p)$
- Related to AIC and other measures favoring model parsimony

Model selection criteria: C_p

• Relation to incremental F test:

 $C_p = p + (m+1-p) (F_p - 1)$

 F_p = incremental F for omitted predictors, testing H_0 : $\beta_{p+1} = ... = \beta_m = 0$ when there are *m* available predictors.

p = # parameters, including intercept

 H_0 true (no bias) H_0 false (bias) $C_p \approx p$ $C_p > p$ $F_p \approx 1$ $F_p > 1$

```
A "good" model should therefore have Cp \approx p
```

Model selection criteria: Parsimony

- Attempt to balance goodness of fit vs. # predictors
- Akaike Information Criterion (AIC)

$$AIC = n \ln\left(\frac{SSE}{n}\right) + 2p$$

Bayesian Information Criterion (BIC)

$$BIC = n \ln \left(\frac{SSE}{n}\right) + 2(p+2)q - 2q^{2} \text{ where } q = \frac{n\hat{\sigma}^{2}}{SSE}$$

- AIC & BIC
 - Smaller = Better
 - Model comparison statistics, not test statistics no p-values
 - Applicable to all statistical model comparisons
 logistic regression, FA, mixed models, etc.

Scientific explanation

- Need to include variable(s) whose effect you are testing
 - Does gasoline price affect consumption?
 - Does physical fitness decrease with age?
- Need to include control variable(s) that could affect the outcome
 - Omitted control variables can bias other estimates
 - E.g., per capita income might affect consumption
 - Weight might affect physical fitness
- Better to risk some reduced precision than bias by including more variables, even if *p*-values NS

Descriptive/Exploratory

- Generally only include variables with strong statistical support (low p values). Choose models with highest adjusted R² or lowest AIC)
 - Parsimony particularly valuable for making in-sample predictions
 - · High precision
 - · Fewer variables to measure
- Models with AIC close to best model are also supported by the data
 - If you need to choose just one, pick the simplest in this group
 - Better to report alternatives, perhaps in a footnote
- Examine whether statistically significant relationships have effects sizes & signs that are meaningful
 - Units of regression coefficients: units of Y/units of X

Example: US Fuel consumption

pop tax nlic inc road driver fuel	Poj Mo Nur Pej Lei Cs Pro	oulation tor fuo mber li r Capion ngth Fo oportion el cons	on (100 el tax icensed ta Pers ederal on lice sumptio	Os) (cents/ driver onal ir Highway nsed dr n (/per	(gal.) rs (1000 ncome (: vs (mi. rivers rson)	Os) \$))	
state	рор	tax	nlic	inc	road	drivers	fuel
AL	3510	7.0	1801	3333	6594	0.513	554
AR	1978	7.5	1081	3357	4121	0.547	628
AZ	1945	7.0	1173	4300	3635	0.603	632
CA	20468	7.0	12130	5002	9794	0.593	524
CO	2357	7.0	1475	4449	4639	0.626	587
СТ	3082	10.0	1760	5342	1333	0.571	457
DE	565	8.0	340	4983	602	0.602	540
FL	7259	8.0	4084	4188	5975	0.563	574

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%include data(fuel); proc reg data=fuel; id state; model fuel = pop tax inc road drivers / selection = rsquare cp aic best=4; run;

Number in				
Model	R-Square	C(p)	AIC	Variables in Model
1	0.4886	27.2658	423.6829	drivers
1	0.2141	65.5021	444.3002	рор
1	0.2037	66.9641	444.9368	tax
1	0.0600	86.9869	452.8996	inc
2	0.6175	11.2968	411.7369	inc drivers
2	0.5567	19.7727	418.8210	tax drivers
2	0.5382	22.3532	420.7854	pop drivers
2	0.4926	28.6951	425.2970	road drivers
3	0.6749	5.3057	405.9397	tax inc drivers
3	0.6522	8.4600	409.1703	pop tax drivers
3	0.6249	12.2636	412.7973	inc road drivers
3	0.6209	12.8280	413.3129	pop road drivers
4	0.6956	4.4172	404.7775	pop tax inc drivers
4	0.6787	6.7723	407.3712	tax inc road drivers
4	0.6687	8.1598	408.8362	pop tax road drivers
4	0.6524	10.4390	411.1495	pop inc road drivers
5	0.6986	6.0000	406.3030	pop tax inc road drivers

NB: C_p always = p for model with all predictors

Variable selection methods

- All possible regressions (or best subsets)
 - proc reg; model ... / selection=rsquare best=;
 - R: leaps package: regsubsets()
 - $2^p 1 : p = 10 \rightarrow 1023 \text{ models!}$
 - Useful overview, but beware of:
 - Effects of collinearity
 - Influential observations (n: small, moderate)
 - Lurking variables: unmeasured, but important
 - → Use R², C_p, AIC to select candidate models, to be explored in more detail, not for final selection

cpplot macro

%*cpplot*(data=fuel,

yvar=fuel, xvar=tax drivers road inc pop, gplot=CP AIC, plotchar=T D R I P, cpmax=20);



Variable selection methods

- Forward selection
 - proc reg; model ... / selection=forward SLentry=.10;
 - At each step, find the variable X_k with the largest partial F_k value

$$F_{k} = \frac{MSR(X_{k} | \text{others})}{MSE(X_{k} + \text{others})}$$

- If Pr(Fk)<SLentry: add to model; else STOP</p>
- Result depends on SLentry (liberal default)

Stepwise Selection: Step 1

	Statistic	s for Entry Model		
Variable	Tolerance	R-Square	F Value	Pr > F
tax	1.000000	0.2037	11.76	0.0013
drivers	1.000000	0.4886	43.94	<.0001
road	1.000000	0.0004	0.02	0.8978
inc	1.000000	0.0600	2.93	0.0935
рор	1.000000	0.2141	12.54	0.0009

Variable drivers Entered: R-Square = 0.4886 and C(p) = 27.2658

Stepwise Selection: Step 2 Statistics for Entry								
		Model						
Variable	Tolerance	R-Square	F Value	Pr > F				
+0.4	0.017025	0 5567	6.00	0 0117				
Lax	0.917035	0.5567	0.92	0.0117				
road	0.995887	0.4926	0.36	0.5497				
inc	0.975329	0.6175	(15.17)	0.0003				
рор	0.866451	0.5382	4.83	0.0331				
Variable inc	Entered: R-Squa	are = 0.6175 a	and C(p) = 1	1.2968				

Variable selection methods

Backward elimination

- proc reg; model ... / selection=backward SLstay=.10;
- Start with all variables in the model
- At each step, find the X_k with the **smallest** partial F_k value
- If Pr(Fk)>SLstay: remove from model; else STOP
- Result depends on SLstay (liberal default)

Variable selection methods

Stepwise regression

- proc reg; model ... / selection=stepwise SLentry=.10 SLstay=.10;
- Start with 2 forward selection steps
- Then alternate:
 - Forward step: Add X_k w/ highest F_k if Pr(Fk)<SLentry
 - Backward step: Del X_k w/ lowest F_k if Pr(Fk)>SLstay
 - Until: no variables entered or removed

Summary of Stepwise Selection

Step	Variable Entered	Variable Removed	Label		Number Vars In	Partial R-Square
1 2	drivers inc		Proportion Per Capita	licensed drivers Personal income (\$)	1 2	0.4886 0.1290
3	tax		Motor fuel	tax (cents/gal.)	3	0.0573
4	рор		Population	(1000s)	4	0.0207

Summary of Stepwise Selection

Step	Model R-Square	C(p)	F Value	Pr > F
1	0.4886	27.2658	43.94	<.0001
2	0.6175	11.2968	15.17	0.0003
3	0.6749	5.3057	7.76	0.0078
4	0.6956	4.4172	2.93	0.0942

But:

• Does the model make sense?

• Have all important control variables been included?

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Variable selection in R

leaps package: regsubsets() does a variety of selection methods

library(leaps) fuel.subsets <-	
regsubsets(fuel ~ pop + tax +	inc + road + drivers,
data = fuel,	
nbest = 3,	<pre># best 3 models for each number of predictors</pre>
nvmax = NULL,	# no limit on number of variables
force.in = NULL,	# variables to force in
force.out = NULL,	# exclude from all models
method = "exhaustiv	e") #or, "forward", "backward",
fuel.subsets	

Subset selection object

Call: regsubsets.formula(fuel ~ pop + tax + inc + road + drivers, data = fuel,								
nbest	= 3, nvmax	= NULL, for	ce.in	= NULL,	force.out	= NULL,		
metho	d = "exhaust	ive")						
5 Variabl	es (and int	ercept)						
F	orced in For	ced out						
pop	FALSE	FALSE						
tax	FALSE	FALSE						
inc	FALSE	FALSE						
road	FALSE	FALSE						
drivers	FALSE	FALSE						
3 subsets	of each siz	e up to 5						
Selection	Algorithm:	exhaustive						

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MASS package: **stepAIC()** does forward/backward/stepwise using AIC or BIC

Start: AIC=406.3 fuel ~ pop + tax + inc + road + drivers

	Df	Sum of	Sq	RSS	AIC
- road	1	17	62 1	79106	404.78
<none></none>			1	77344	406.30
- pop	1	117	06 1	89050	407.37
- inc	1	175	65 1	94909	408.84
- tax	1	271	88 2	04533	411.15
- drivers	1	1100	17 2	87361	427.47

Step: AIC=404.78
fuel ~ pop + tax + inc + drivers

		Df	Sum	of	Sq	RSS	AIC
<1	none>					179106	404.78
-	pop	1		123	L97	191302	405.94
-	inc	1		255	516	204621	409.17
-	tax	1		446	559	223765	413.46
-	drivers	1	-	1210)15	300121	427.56

In stepAIC() :

- k = 2 defines penalty factor for AIC; use k=log(n) for BIC
- scope = list(lower=~1, upper=...) defines the scope of models considered

car package: subsets() plots model selection criteria



Dangers of 'blind' stepwise methods

- Gives R² values that are badly biased high
 - Substantial shrinkage in a future sample
- *F*, *t* (or χ²) statistics for each variable don't have the claimed distribution:
 - *p*-values are wrong, because they don't take selection into account
- Confidence intervals for effects and predicted values are overly narrow
 - Based on one model, not selection from many
- Problems of collinearity: why X4, not X7?
 - Tiny difference in data might select X7

Dangers of 'blind' stepwise methods

- Based on methods (e.g. F tests for nested models) intended to test pre-specified hypotheses.
- Allows us to not think about the problem.
- Generates a lot of output, but most people just look at the final summary.
- "Treat all claims based on stepwise algorithms as if they were made by Saddam Hussein on a bad day with a headache having a friendly chat with George Bush." (From: Stepwise regression = Voodo Regression web page)

Stepwise dangers: demo

title 'Stepwise demo: add 15 random predictors to Fitness data'; %include data(fitnessd);

```
data fitness;
   set fitness;
   array x{15} x1-x15;
   *-- generate the 'artificial' predictors;
   do i=1 to 15;
      x(i) = normal(7654321);
      end;
proc reg data=fitness;
```

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Number in				
Model	R-Square	MSE	Variables in Model	
1	0 7434	7 53394	runtime	Note how often
1	0.1616	04 61497	vic	random prodictore
	0.1616	24.01437		random predictors
	0.1595	24.67582	rstpulse	occur among 'best'
I	0.1584	24.70817	runpuise	modelsl
2	0.7771	6.77903	runtime x10	
2	0.7753	6.83234	runtime x5	
2	0.7650	7.14558	runtime x4	
2	0.7642	7.16842	runtime age	
3	0.8111	5.95669	runtime age runpulse	
3	0.8100	5.99157	runtime runpulse maxpulse	
3	0.8070	6.08587	runtime age x5	
3	0.7986	6.35153	runtime x5 x10	
4	0.8662	4.38138	runtime age runpulse x5	
4	0.8399	5.24242	runtime age maxpulse x5	
4	0.8368	5.34346	runtime age runpulse maxpulse	
4	0.8321	5.49727	runtime runpulse maxpulse x9	
5	0.8795	4.10420	runtime age runpulse x5 x13	
5	0.8780	4.15627	runtime age runpulse x5 x7	
5	0.8767	4.19971	runtime age runpulse maxpulse	x5
5	0.8742	4.28573	runtime age runpulse x5 x11	
	0 8027	3 80744	runtime age runnulse vi v5 vi	2
6	0.0927	3 0/300	runtime age runpulse x5 x7 x1	3
6	0.0000	3.94390	nuntime age nunpulse x5 x7 x1	0 V5 V11
6	0.0000	4.01466	nuntime age nunpulse maxpulse	10
0	0.0001	4.04208	runtime age runpuise x5 XII X	10

Numbers of significant multiple regressions (out of 1,000) based on random data for which the null hypothesis is, by definition, true.



From: Roger Mundry & Charles L. Nunn, "Stepwise Model Fitting and Statistical Inference: Turning Noise 28 into Signal Pollution." *The American Naturalist*, Vol. 173, No. 1 (January 2009), pp. 119-123.



Guided selection

- The haystack: motley collection that remains
 - \rightarrow stepwise (haystack | key + selected promising)
 - Any here worth including?

proc reg; model Y = Age IQ Test2 Test5 X1-X15 / include=4 selection=stepwise SLentry = .15 SLstay=.15;

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- The single most important 'tool' is substantive knowledge of the area and properties of variables
 - Expected sign & magnitude of coefficients?
 - Necessary control variables?
 - What hasn't been measured?
- Never let a computer do your thinking for you.



Are we done yet? Model diagnostics

- Examine model diagnostics for selected models
 - (Just a preview; explained more next week)
 - Influential observations?
 - Partial relations? Outliers?

```
proc reg data=fuel;
    id state;
    model fuel = tax drivers inc pop/ r influence partial;
    plot r. * p. = state
        rstudent. * h. = state ;
    title 'A closer look at the stepwise model';
run;
%inflplot(data=fuel,
    y=fuel, x=tax drivers road inc pop,
    id=state);
%partial(data=fuel,
    yvar=fuel, xvar=tax drivers road inc pop,
    id=state);
```







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-2

log Population Density

-1

Cross-validation & shrinkage

- Fit model in prediction sample [y_{ps} | X_{ps}]
 Cot P² b
 - Get R², **b**_{ps}
- Apply coefficients \boldsymbol{b}_{ps} to validation sample [y_{vs} \mid X_{vs}]
- Cross-validated R^2 : using **b**_{ps} in new sample

 $R_{cv}^2 = r^2(y_{vs}, \hat{y}_{pv})$ where $\hat{y}_{pv} = X_{vs}b_{ps}$

- How much we can expect to lose depends on n/k (k=# predictors)
- Recall goals: most important in prediction; gives realistic assessment for scientific explanation & data mining

TABLE 3.10 Estimated Predictive Power Using the Herzberg Formulas for Small to Fairly Large Subject/Variable Ratios n/k Comment Herzberg Estimate Subject/Variable Ratio The estimated amount Small (5:1) n = 50, = 1 - (n - 1/n - k - 1)(n + k)X 5 shrinkage is great, i.e., k = 10 $+ 1/n)(1 - R^2)$ fixed on the average we expect $R^2 = .50$ ② 1 - 49/39 (61/50) (.50) the predictive power to = .234① be reduced by over 50% Correlation Model X $\hat{o}_{2}^{2} = 1$ random = 1 - 49/39 (48/38) (51/50) (.5)191 10 The shrinkage is s $\hat{p}_{e}^{2} = 1 - 99/89 (111/100) (.50) =$ Moderate (10:1) fairly substantial n = 100, k = 10Correlation Model $R^2 = .50$ $\hat{\rho}_c^2 = 1 - 99/89 (98/88) (101/100) (.5)$ = .374 15 $\hat{p}_c^2 = 1 - 149/139 (161/150) (.50)$ We finally reach a point Fairly Large (15:1) where the expected n = 150, k = 10= .427 amount of shrinkage is $R^2 = .50$ Correlation Model fairly small, i.e., about $\hat{o}_{1}^{2} = 1$ 12% - 149/139 (148/138) (151/150) (.5) = .421



Empirical cross-validation

- Ideal: do CV via replication, but if not...
 - Hold back a portion of the data as the CV sample
 - Fit model to prediction ("training") subset
 - Evaluate R² in hold-back ("validation") subset
 - You "waste" some data, but gain in prediction knowledge
- Can do 'manually' with any software via coding tricks
- Generalized CV methods:
 - Do this several times for different subsets & average
 - K-fold CV: Repeat { omit 1/K; validate on omitted 1/K}
 - There are now a wide variety of methods and algorithms
 - Jackknife, bootstrap, lasso, ...
 - Modern methods use these for model selection!

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K-Fold Cross-Validation

Here, we randomly split the data into ${\boldsymbol K}$ distinct blocks of roughly equal size.

- We leave out the first block of data and fit a model.
- 2 This model is used to predict the held-out block
- We continue this process until we've predicted all K held-out blocks

The final performance is based on the hold-out predictions

K is usually taken to be 5 or 10 and leave one out cross–validation has each sample as a block



Example: Simple cross-validation

```
%include data(fitness);
         'Cross-validation of a regression model';
title
/*
o Hold back a portion of the data from the original fit.
o Evaluate how well the model does on the cross-validation sample.
*/
data fit2;
   set fitness;
  if uniform(125741) < .667 /* generate model on 2/3 of data */
     then oxy2 = oxy;
     else oxv2 = ...i
                            /* generate prediction on CV sample */
proc reg data=fit2;
  title2 'Model generation (2/3) sample';
  model oxy2 = age weight runtime runpulse / p;
  output out=stats p=predict r=resid;
proc corr data=stats nosimple;
  /* correlate y, yhat */
   var predict oxy;
   title 'Cross-validation (1/3) sample';
```

Prediction sample:

Dependent Variable: OXY2

		All	arysis or vari	ance	
Source	DF	Sum o Square	f Mean s Square	F Value	Prob>F
Model	4	689.5850	1 172.39625	24.336	0.0001
Error	19	134.5967	7.08404		
C Total	23	824.1817	1		
Root MSE Dep Mean	2 47	2.66159 7.57392	R-square Adj R-sq	0.8367	R ² = 0.84

Analysis of Variance

Validation sample:

Pearson Correlation Coefficients /	Prob > R under Ho PREDICT	: Rho=0 / N = 7 OXY	
PREDICT Predicted Value of OXY2	1.00000 0.0	0.62949 0.1298	R ² = 0.63 ² = 0.40
ОХҮ	0.62949 0.1298	1.00000 0.0	

This simply demonstrates shrinkage of R². In practice, we could average over all folds to get cross-validated estimates of coefficients

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PROC GLMSELECT

- supports all regression & ANOVA models
- partition data: training, validation & testing roles
- selection from large # of effects, variety of criteria
 - Forward, backward, stepwise, least angle regression, lasso
- leave-one-out and k-fold cross validation
- Extensive graphics via ODS Graphics
- In R:
 - DAAG package: cv.lm()
 - bootstrap package: crossval(), ...
 - caret package: extensive facilities for "training", model selection and model averaging

GLMSELECT Example: Baseball data



These use 50% for training, 30% for validation, and 20% for testing

- •Validation ASE chooses smaller model.
- •Regard these as candidate models



DAAG::cv.lm

library(DAAG) fuel.cv <- cv.lm(data=fuel, final.mod, m=3)</pre>

Signif. codes: 0 `***' 0.001 `**' 0.01 `*' 0.05 `.' 0.1 ` ' 1

Analysis of Variance Table

Response: fuel

 Df
 Sum Sq
 Mean
 Sq
 F
 value
 Pr(>F)

 pop
 1
 125996
 125996
 30.25
 1.9e-06

 tax
 1
 162056
 162056
 38.91
 1.6e-07

 inc
 1
 194
 194
 0.05
 0.83

 drivers
 1
 121015
 121015
 29.05
 2.8e-06

 Residuals
 43
 179106
 4165
 --- --- ---

m=3 folds of 16 in each test set

Cross validated tests for model effects



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Summary

- Opposing criteria: goodness of fit vs. parsimony
 - Penalized measures (C_p, AIC, BIC) better
- Different goals
 - Description, explanation, prediction, data mining
 - Require different views of a "good" / "best" model
- Selection methods are tools, not gospel truth
 - Dangers of "blind" stepwise methods
 - Guided selection puts you in the modeling process
- Criticize & validate
 - Regression diagnostics to find/correct problems
 - Cross-validation to check replicability