Predictive Analytics Lecture 4

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Stat 422/722
at The Wharton School of the University of Pennsylvania

February 7 & 8, 2017

Review: Generalizing the Classification Rule

Recall the classification rule $\hat{y} = \mathbb{1}_{\hat{p} \geq 0.5}$. Using 0.5 is a principled default but we can use any rule $p_0 \in (0, 1)$:

$$\hat{y} = \mathbb{1}_{\hat{p} \geq p_0} := \begin{cases} 1 & \text{if} \quad \hat{p} \geq p_0 \\ 0 & \text{if} \quad \hat{p} < p_0 \end{cases}$$

What happens when we change the p_0 threshold? If $p_0 \uparrow \quad \Rightarrow \quad \hat{P} \downarrow$ and $\hat{N} \uparrow$. If $p_0 \downarrow \quad \Rightarrow \quad \hat{P} \uparrow$ and $\hat{N} \downarrow$. Changing p_0 changes the column totals and obviously creates a whole new confusion matrix.

So now it's simple, vary p_0 and pick the best model according to your cost / error / loss function (the *ME* at the moment). Let's just do every p_0!

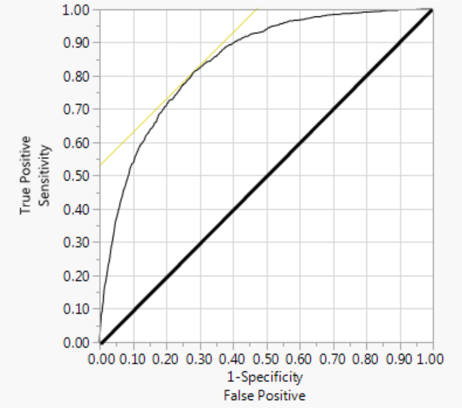
All Possible Confusion Matrices

ROC Table

Prob	1-Specificity	Sensitivity	Sens-(1-Spec)	True Pos	True Neg	False Pos	False Neg
.	0.0000	0.0000	0.0000	0	5163	0	1869
0.8117	0.0000	0.0005	0.0005	1	5163	0	1868
0.8104	0.0000	0.0011	0.0011	2	5163	0	1867
0.8093	0.0000	0.0016	0.0016	3	5163	0	1866
0.8092	0.0000	0.0021	0.0021	4	5163	0	1865
0.8090	0.0000	0.0027	0.0027	5	5163	0	1864
0.8085	0.0000	0.0032	0.0032	6	5163	0	1863
0.8083	0.0000	0.0037	0.0037	7	5163	0	1862
0.8082	0.0000	0.0043	0.0043	8	5163	0	1861
0.8079	0.0000	0.0048	0.0048	9	5163	0	1860
0.8079	0.0000	0.0054	0.0054	10	5163	0	1859
0.8077	0.0000	0.0059	0.0059	11	5163	0	1858
0.8076	0.0002	0.0059	0.0057	11	5162	1	1858
0.8072	0.0002	0.0064	0.0062	12	5162	1	1857
0.8065	0.0002	0.0070	0.0068	13	5162	1	1856
0.8064	0.0002	0.0075	0.0073	14	5162	1	1855
0.8061	0.0002	0.0080	0.0078	15	5162	1	1854

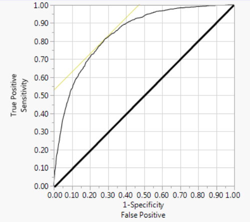
Here, `Prob` is what we denoted p_0.

Receiver-Operator Characteristic Curve



The **ROC Curve**. Each dot represents the sensitivity-specificity tradeoff for each p_0. The starred row of maximum sensitivity + specificity is indicated here by a yellow tangent line.

Area Under the Curve (AUC) Metric



If you built a model by chance the “area under the curve” (or to the right of the curve) on the graph would be ... 0.5 since the graph is a unit square. Under the ROC curve itself (or to its right) is an area ... greater than 0.5. Here, it's 0.844. This metric is called AUC and is widely used as a metric to assess performance of all possible classifiers in this set of models together, it is a composite metric unlike *ME* or anything derived from an individual confusion table.

AUC is nice to evaluate overall performance of all possible models... but at the end of the day... you ship **ONE** model! So we still need a means of evaluating our one model from one confusion table.

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$p_0 = 0.5$		$\hat{y}$ 1	0	Totals	Model Errors
y	1	$TP = 1012$	$FN = 857$	$P = 1869$	$FNR = 45.9\%$
	0	$FP = 531$	$TN = 4632$	$N = 5163$	$FPR = 10.2\%$
	Totals	$\hat{P} = 1543$	$\hat{N} = 5489$	$n = 7032$	
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Which numbers did not change? n, P and N. Why?

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Not necessarily... It depends on what your goal is!

Asymmetric Costs in a Classifier

These are always two types of errors but the costs are not always the same.

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Weighted Misclassification Error

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$$ME_w := \frac{1}{n}\sum_{i=1}^{n} c_{FP}\mathbb{1}_{y_i=0\&\hat{y}=1} + c_{FN}\mathbb{1}_{y_i=1\&\hat{y}_i=0}$$

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We now vary p_0 to locate the model that optimizes this error to be minimum.

Minimum Weighted Misclassification Error

Let's assume that $c_{FN} = \$1000$ and $c_{FP} = \$100$ just for the example's sake. Note: this is a **cost ratio** of 10:1 (only the ratio matters for the optimal p_0 solution).

	Prob	TP	TN	FP	FN	COST
1	0.8117	1	5163	0	1868	1868000
2	0.8104	2	5163	0	1867	1867000
3	0.8093	3	5163	0	1866	1866000
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5	0.8090	5	5163	0	1864	1864000
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7	0.8083	7	5163	0	1862	1862000
8	0.8082	8	5163	0	1861	1861000
9	0.8079	9	5163	0	1860	1860000

We now calculate the cost and find the minimum model (i.e. the p_0 to ship). [JMP] Beyond scope: some people select the model with the closest $\#FP/\#FN \approx 10:1$ to match the stakeholder preference of the desired cost ratio. I'm not entirely clear on why this fitness function is used. [JMP ratios sheet]

Expected Value Calculation

You can also imagine assignment of both costs *and* benefits:

$p_0 = 0.1$		$\hat{y}$	
		1	0
y	1	b_{TP}	c_{FN}
	0	c_{FP}	b_{TN}

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and then use the confusion matrix to estimate probabilities:

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The expected value would be?

$$\begin{aligned}\mathbb{E}[T] &= p_{TP} \times b_{TP} + p_{TN} \times b_{TN} + p_{FP} \times c_{FP} + p_{FN} \times c_{FN} \\ &\approx \hat{p}_{TP} \times b_{TP} + \hat{p}_{TN} \times b_{TN} + \hat{p}_{FP} \times c_{FP} + \hat{p}_{FN} \times c_{FN}\end{aligned}$$

Highest expected value model is shipped (ex. from Provost & Fawcett, 2013).

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For example, recall the Telecom churn dataset with one feature (tenure). If the observation has ...

Tenure Time	Churn?	Total Time as a Customer
2	Yes	

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45	No	

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That third observation's response is **censored**. What are we supposed to do??

Dealing with censoring

One option is to disregard all censored observations. Why is this a bad idea?

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This is a very well-studied field with many possible models!

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Assume Y now is time. Time must be positive!

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Interpretation of a unit change in x_1? With all other variables kept constant, a unit change in x_1 will multiply the expected survival by e^{β_1} in a naturally observed new object.

Assumptions of an ELLM

Next up in the recipe... we need to get estimates of the true parameters, we have been denoting these $\left\{\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p\right\}$. How to do so?

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Now the computer crunches away (similar to a logistic regression fit) and we get values of $\left\{\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p\right\}$ back in a split second.

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So Θ would be the space of all $\beta_0, \beta_1, \ldots, \beta_p$ and Θ_R will restrict the space to only β_0 with zeroes for all other "slope" parameters.

$$LR = \frac{\max\limits_{\beta_0, \beta_1, \ldots, \beta_p} \mathcal{L}(\beta_0, \beta_1, \ldots, \beta_p; y_1, \ldots, y_n, c_1, \ldots, c_n, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)}{\max\limits_{\beta_0} \mathcal{L}(\beta_0, \beta_1 = 0, \ldots, \beta_p = 0; y_1, \ldots, y_n, y_n, c_1, \ldots, c_n, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)}$$

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So in the numerator the computer iterates to find $\left\{\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p\right\}$, plugs it in and computes the likelihood and in the denominator the computer independently iterates to find $\left\{\hat{\beta}_0\right\}$, plugs it in and computes the likelihood, then together, the LR.

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We then look at $Q = 2\ln(LR)$ and compare it to the appropriate χ^2 distribution. Here, since we've dropped p parameters / degrees of freedom, we look at the critical $\chi^2_{p,\alpha}$ value.

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Individual Tests in Survival Regression

Let's say we want to test an individual slope coefficient:

$$H_0 : \beta_j = 0, \quad H_a : \beta_j \neq 0$$

(a la the "partial-F test"). We can again use the likelihood ratio test:

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$$LR = \frac{\max\limits_{\beta_0, \beta_1, \ldots, \beta_p} \mathcal{L}\left(\beta_0, \beta_1, \ldots, \beta_p; y_1, \ldots, y_n, c_1, \ldots, c_n, \mathbf{x}_1, \ldots, \mathbf{x}_n\right)}{\max\limits_{\beta_0, \beta_1, \ldots, \beta_{j-1}, \beta_{j+1}, \ldots \beta_p} \mathcal{L}\left(\beta_0, \beta_1, \ldots, \beta_{j-1}, \beta_j = 0, \beta_{j+1}, \ldots \beta_p; y_1, \ldots, y_n, c_1, \ldots, c_n, \mathbf{x}_1, \ldots, \mathbf{x}_n\right)}$$

We then look at $Q = 2\ln(LR)$ and compare it to the appropriate χ^2 distribution. Here, since we've dropped 1 parameter / degrees of freedom; thus we look at the critical $\chi^2_{1,\alpha}$ value.

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Individual Tests in Survival Regression

Let's say we want to test an individual slope coefficient:

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(a la the "partial-F test"). We can again use the likelihood ratio test:

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And again: a χ^2 r.v. with one degree of freedom has the following cool property: $Q \sim \chi^2_1 \Rightarrow \sqrt{Q} \sim \mathcal{N}(0, 1)$ i.e. a "z-score". This is how JMP produces standard errors for survival regression coefficients.

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Multivariable Survival Regression

[JMP]

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- What's wrong with this dataset?? The max survival is 72mo and there's thousands of cases that are censored.
- Evaluating the fitness (i.e. $R^2, RMSE, ME_w$, etc) of survival models is complicated... not covered.

Simple Test of Linearity

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Interpretation of unit change in x : bonus? Depends on the value where you start from (we are moving away from simple interpretations).

Polynomial Regression

Let's try to fit a better curve to bonus — a 4-degree polynomial. Seems to fit better than a quadratic [see LRT in R]. What's the interpretation of a 4-degree polynomial model??

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Let's try to fit a better curve to bonus — a 4-degree polynomial. Seems to fit better than a quadratic [see LRT in R]. What's the interpretation of a 4-degree polynomial model?? Not so intuitive unfortunately. Rarely do we see parametric pre-designed models with more than a quadratic term.

Continuous : Categorical Interactions

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Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	1154.5111	116.733	9.89	<.0001*
BONUS	0.6557937	0.408992	1.60	0.1124
REGION[Midwest]	212.82646	16.25271	13.09	<.0001*
REGION[North]	180.20263	19.96834	9.02	<.0001*
REGION[South]	-250.9858	16.3109	-15.39	<.0001*
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How can we interpret this?

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How can we interpret this? Could we also interact two continuous features? Two categorical features? Could we interact features with others' polynomials? Yes, yes, yes...

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- 99.9% on splines (polynomials on steroids) which may not be fake??

How do we know?

Recall the Modeling Basics

In lecture 1 we spoke about how

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By including all sorts of polynomials and interactions, we become more nonparametric thereby losing the benefits of the parametric worldview of s... (i.e. parsimony, interpretability and inference) but gaining a closer fit of the true f. But what could go wrong if we take this liberty?

Non-germane footnote: recall that we fit $\hat{s}$ which generally speaking fails to estimate s correctly (model error) and s generally speaking fails to represent f correctly since its a parametric model which lacks flexibility.

Recall the Modeling Basics

In lecture 1 we spoke about how

$$Y = f(x_1, \ldots, x_p) + \mathcal{E}$$

where $x_1, \ldots, x_p$ denotes predictors available (including all polynomials and interactions and whatnot!) and $\mathcal{E}$ denotes **irreducible error** due to information not available (and thus independent of $x_1, \ldots, x_p$), the inaccessible information.

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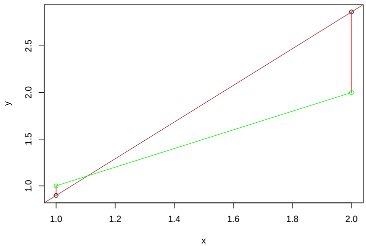
Any value different from f is not **generalizable** as the conditional mean minimizes squared error.

But the BIG problem is: we don't know what the form of f is and we don't know the individual values of $\mathcal{E}$. Thus, we have NO WAY to know if we've overfit (as of now)!

When Does This Happen?

Essentially, when p gets closer to n. Here's the linear model case with $n = 2$ and there's one slope so $p = 1$ (+1 for the intercept) so really, the number of predictors is 2 since there is two degrees of freedom. [R demo]



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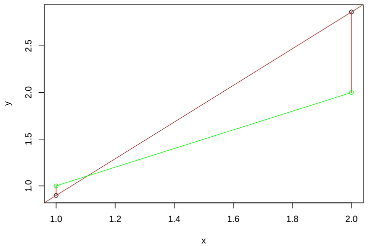

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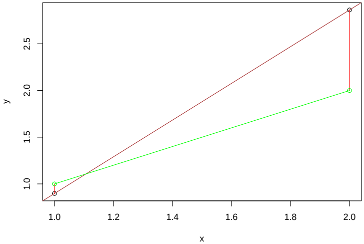

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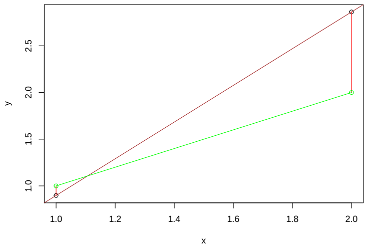

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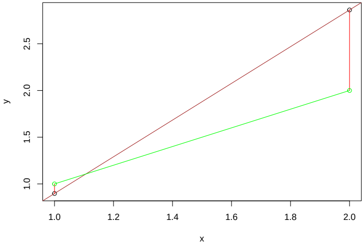

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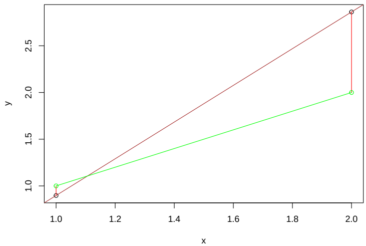

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Let's return to the [R demo] to witness the cost of overfitting. How did we demonstrate overfittedness? We used "new data" not in the dataframe generated from the same realization process as the historical dataframe (our sample). Hence this new data is called **out of sample (oos)** data. And then we calculated familiar metrics such as SSE, RMSE, R^2 but since these are done oos, we call them oosSSE, oosRMSE, oosR^2 and they are our **out of sample statistics**. Everything we spoke about previously we will now call **in-sample statistics**.

	In Sample	Out of Sample
RMSE	2.0	84.7
R^2	99.9%	9.5%

Overfitting can get arbitrarily bad and this is an extreme example.

Assessments in the Real World

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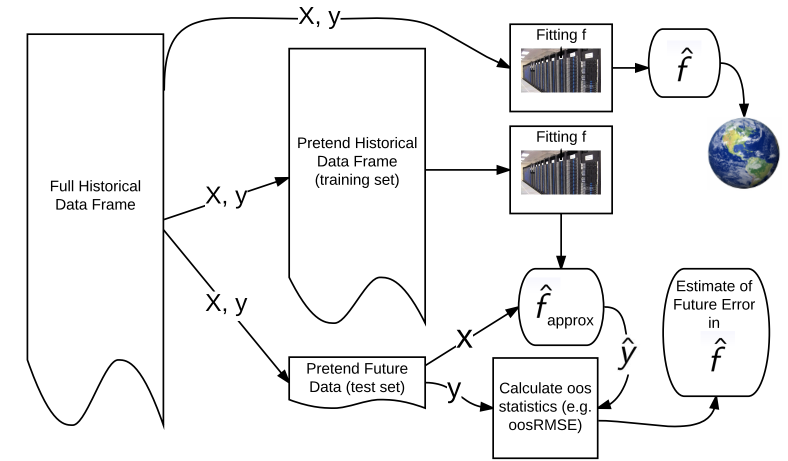
Building the model on the training set and predicting on the test set and comparing these predictions to the real, known values of the response in the test set constitutes *out of sample validation*. Why is it called that?

Model Fitting with OOS Validation



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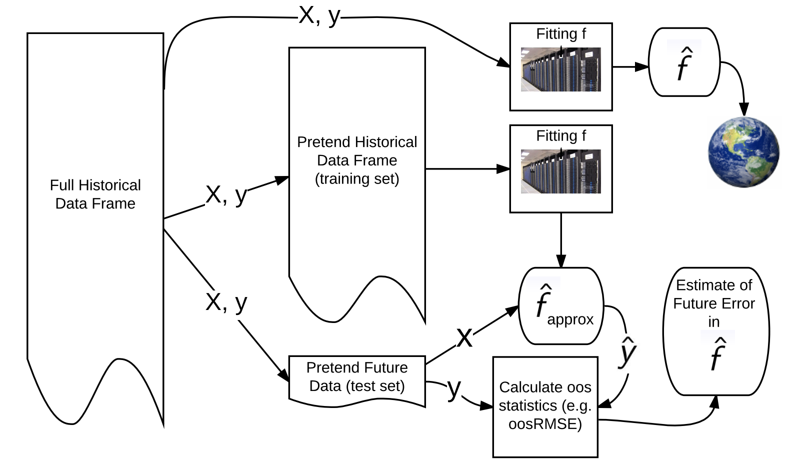

Can oos metrics be better than in-sample metrics (on average)? No...

A Possible Spin on Validation

Procedure outlined above:

1. Split dataframe into training and test.

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7. Calculate estimate of future generalization error of model B.
8. Pick whichever model has better generalization error.

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The oos validation is only valid if...

you treat the test set as a lockbox. Once you open it up, that's it!

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Note: the in-sample and oos statistics are statistics! Thus, they are random!

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[JMP Cols...Modeling Utilities...Make Validation Col...fit model... validation option is the validation col...crossvalidation tab] Note: "RASE" = root average squared error = root mean squared error = oosRMSE. "Validation" = "test". "Freq" is the sample sizes in training and test. Looks like we were overoptimistic by 6x the standard error on predictions! Substantial overfitting.

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Let's look at three models for the White Wine data. Here the response is wine quality as measured by professional raters and features are 11 features (e.g. acidity, sugar, pH and alcohol content).

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[JMP col validation... fit all models with validation ... save prediction formula cols... analyze model... model comparison]
Conclusions? Model C looks the best. Where to go from here?

What did I do that wasn't legal? Remember a few slides ago? I looked at the test set four times! We need to solve this problem...