

Predictive Analytics Lecture 4

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Stat 422/722

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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 $p_0 \in (0, 1)$:

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

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

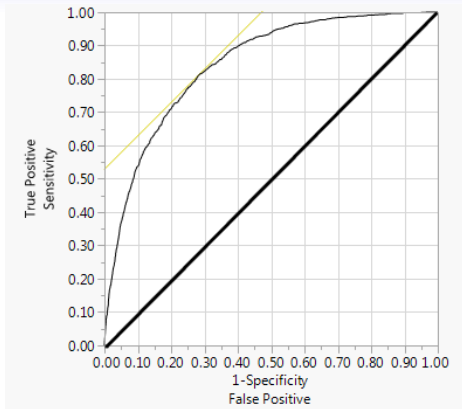
So now it's simple, vary p_0 and pick the best model according to your cost / error / loss function (the *ME* at the moment). Let's just do every p_0 !

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

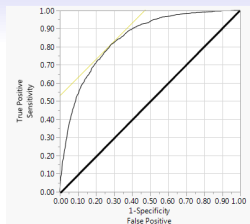
Here, Prob is what we denoted p_0 .

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.

Churn Example Where $p_0 = 0.10$

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		1	0		
y	1	$TP = 1012$	$FN = 857$	$P = 1869$	$FNR = 45.9\%$
	0	$FP = 531$	$TN = 4632$	$N = 5163$	$FPR = 10.2\%$
Totals		$\tilde{P} = 1543$	$\tilde{N} = 5489$	$n = 7032$	
Use errors		$FDR = 34.3\%$	$FOR = 15.6\%$		$ME = 19.7\%$

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

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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.

	Prob	TP	TN	FP	FN	COST
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We now calculate the cost and find the minimum model (i.e. the p_0 to ship). [JMP]

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We now calculate the cost and find the minimum model (i.e. the p_0 to ship). [JMP] Or alternatively, we can select the model with the closest $FN/FP \approx 10 : 1$ to match the stakeholder preference of the desired cost ratio. Why would this be good?

Expected Value Calculation

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

$p_0 = 0.1$		\hat{y}	
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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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8		Yes	9
45		No	

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Tenure	Time	Churn?	Total Time as a Customer
2		Yes	3
8		Yes	9
45		No	unknown

That third observation's response is **censored**.

New Type of Response Metric: TTL

What if your response was time? For example:

- Time for a patient to live (typical in clinical trials)?
- How long will a customer be a customer?
- How long will a car engine last?

What kind of data type is the response? Continuous. But what does response look like at the time of sampling?

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	3
8	Yes	9
45	No	unknown

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

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

The Exponential Model

Assume Y now is time. Time must be positive!

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$$p(y) = \frac{1}{\mu} e^{-\frac{1}{\mu}y} \quad \text{and} \quad F(y) = 1 - e^{-\frac{1}{\mu}y}$$

with mean $\mathbb{E}[Y] = \mu$ where $\mu > 0$.

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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.

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

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

$$LR = \frac{\max_{\beta_0, \beta_1, \dots, \beta_p} \mathcal{L}(\beta_0, \beta_1, \dots, \beta_p; \mathbf{y}_1, \dots, \mathbf{y}_n, \mathbf{c}_1, \dots, \mathbf{c}_n, \mathbf{x}_1, \dots, \mathbf{x}_n)}{\max_{\beta_0} \mathcal{L}(\beta_0, \beta_1 = 0, \dots, \beta_p = 0; \mathbf{y}_1, \dots, \mathbf{y}_n, \mathbf{y}_n, \mathbf{c}_1, \dots, \mathbf{c}_n, \mathbf{x}_1, \dots, \mathbf{x}_n)}$$

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

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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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$$LR = \frac{\max_{\beta_0, \beta_1, \dots, \beta_p} \mathcal{L}(\beta_0, \beta_1, \dots, \beta_p; y_1, \dots, y_n, c_1, \dots, c_n, x_1, \dots, x_n)}{\max_{\beta_0, \beta_1, \dots, \beta_{j-1}, \beta_{j+1}, \dots, \beta_p} \mathcal{L}(\beta_0, \beta_1, \dots, \beta_{j-1}, \beta_j = 0, \beta_{j+1}, \dots, \beta_p; y_1, \dots, y_n, c_1, \dots, c_n, x_1, \dots, x_n)}$$

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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Is the reduction expected? Yes. Why are these numbers so large? (1) Likely the exponential model is not a great fit here since the tail is too long and the memorylessness property is not realistic. Also, (2) Dataset is not a good sample... was not **designed** for survival.

Multivariable Survival Regression

[JMP]

- Do these coefficients make sense?

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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??

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?? Not so intuitive unfortunately. Rarely do we see parametric pre-designed models with more than a quadratic term.

Continuous : Categorical Interactions

It's possible that bonuses may have differential effects in the different American "regions". The way to test this is to allow for a differential slope for each region. [JMP]

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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*
(BONUS-279.521)*REGION[Midwest]	-3.171339	0.639193	-4.96	<.0001*
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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?

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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)

Recall the Modeling Basics

In lecture 1 we spoke about how

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

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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?

Going Too Far

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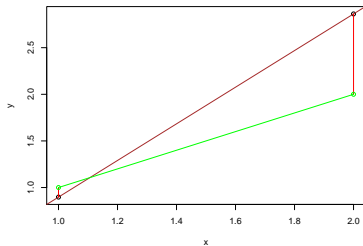
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Any value different from f is not **generalizable** as the conditional mean minimizes squared error.

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?

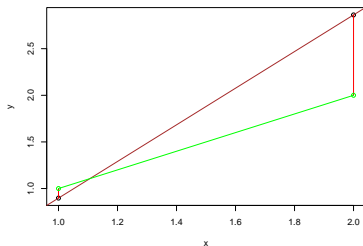
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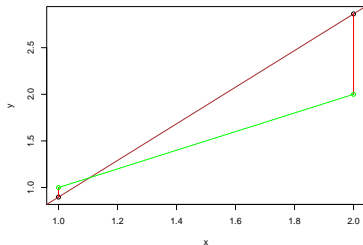
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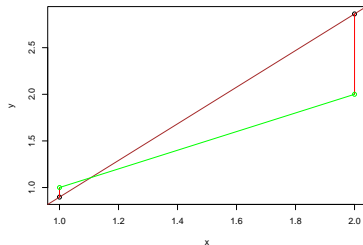
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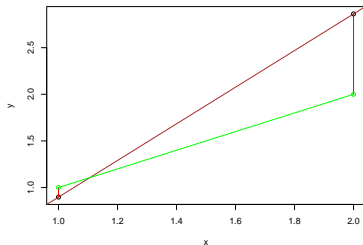
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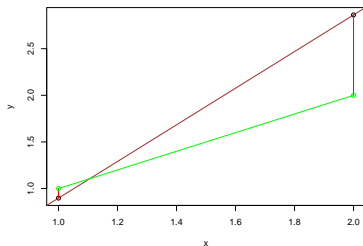
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Assessing Overfitting and its Cost to You

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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, oos R^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.

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It is easy to assess if you have access to the data-generating process — you can just generate more data and see how you do. But in the real world, you only have a limited set of historical data from the data-generating process. What to do?

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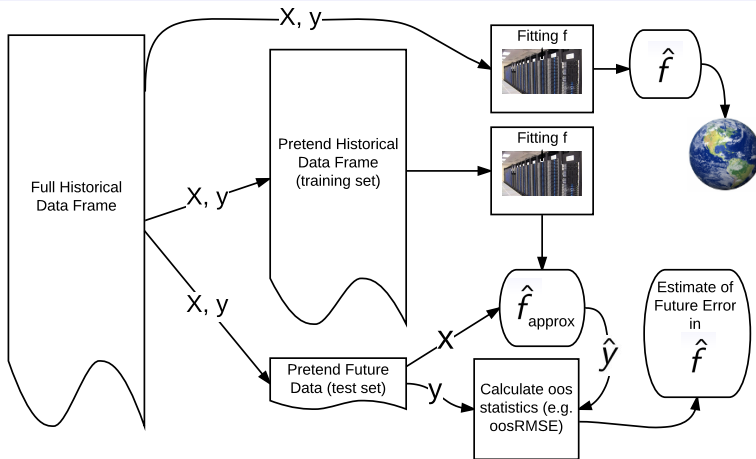
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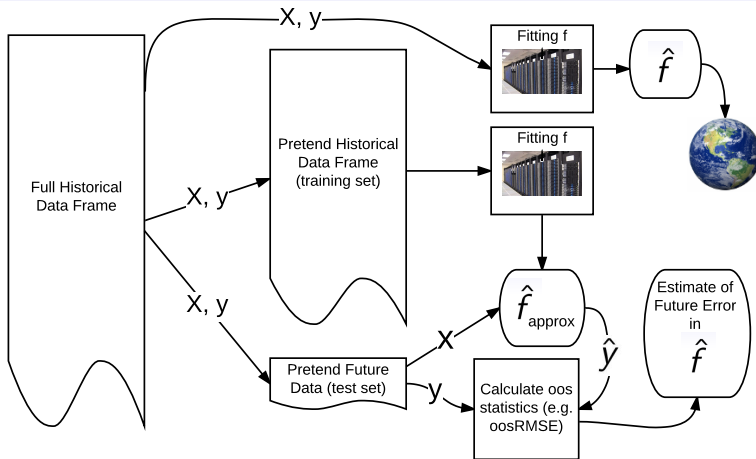
Building the model on the training set and predicting on the test set and comparing these predictions to the real, known values of the response in the test set constitutes *out of sample validation*. Why is it called that?

Model Fitting with OOS Validation



Can oos metrics be better than in-sample metrics (on average)?

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A Possible Spin on Validation

Procedure outlined above:

- 1 Split dataframe into training and test.

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Does the following procedure also seem reasonable?

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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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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...