Predictive Analytics Lecture 2

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

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In order to have inference, we need to make explicit random variable model assumptions e.g.

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must be assumed to be something like

$$Y \sim \mathcal{N} \left(\beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p, \sigma^2\right)$$

Is this a reasonable thing to do?

Back to Modeling

We said before that our model for Y was

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assuming we can know the model, there still is \mathcal{E} . Where does it come from?

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assuming we can know the model, there still is \mathcal{E} . Where does it come from? According to determinism a la Laplace, if one knew all the causal information, there would be no error

$$y = t(z_1, z_2, \ldots)$$

i.e t is the deterministic true mathematical model.

Laplace Believes in Demons

Universal determinism and Laplace's demon

Laplace writes:

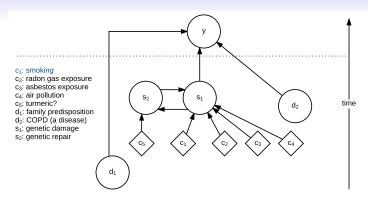
We ought then to regard the present state of the universe as the effect of its anterior state and as the cause of the one which is to follow. Given for one instant an intelligence which could comprehend all the forces by which nature is animated and the respective situation of the beings who compose it – an intelligence sufficiently vast to submit these data to analysis – it would embrace in the same formula the movements of the greatest bodies of the universe and those of the lightest atom; for it, nothing would be uncertain and the future, as the past would be present to its eyes.

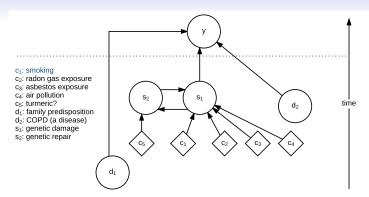
(1814:4)

The vast intelligence here described has come to be known as Laplace's demon. The idea is obviously founded on that of a human scientist (perhaps Laplace himself) using Newtonian mechanics to calculate the future paths of planets and comets. Extrapolating from this success, it was natural to suppose that a sufficiently vast intelligence could calculate the entire future course of the universe. Laplace himself relates his vast intelligence to human successes in astronomy. As he says:

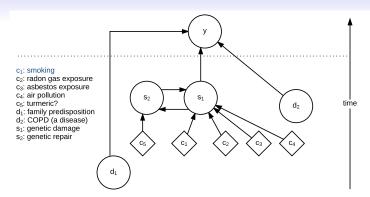
The human mind offers, in the perfection which it has been able to give to astronomy, a feeble idea of this intelligence. Its discoveries in mechanics and geometry, added to that of universal gravity, have enabled it to comprehend in the same analytical expressions the past and future states of the system of the world.

(Laplace 1814: 4)

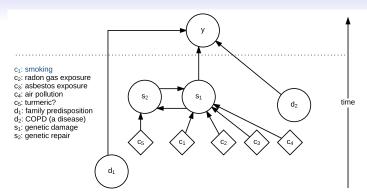




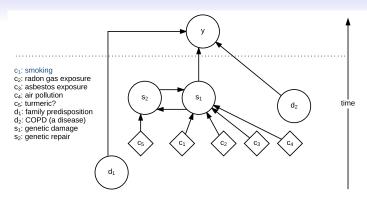
$$y = t($$



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$$Y \sim \operatorname{Bernoulli}(f(c_1))$$

where we saw before that $f(c_1 = 1) = 16\%$ and $f(c_1 = 0) = 0.4\%$ (AKA) "probabilistic causation"). Thus, the response is stochastic only because we lack information. For regression,

$$y = f(x_1,...,x_p) + \underbrace{t(z_1,z_2,...) - f(x_1,...,x_p)}$$

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(i.e. the "noise" is due to ignorance)

Note... some believe that there is still intrinsic randomness in the universe even with all relevant information known. But we are punting on the actual philosophy...

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$$y = s(x_1, \ldots, x_p; \theta_1, \ldots, \theta_\ell) + f(x_1, \ldots, x_p) - s(x_1, \ldots, x_p; \theta_1, \ldots, \theta_\ell)$$

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(LM Inference, Corr.

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noise due to ignorance error

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Further, we then have to estimate the parameters to get a fit:

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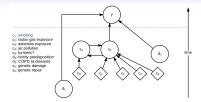
Thus, all predictions have three sources of error.

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Thus, all predictions have three sources of error. What is minimized with non-parametric machine learning?

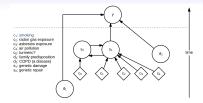
t is Difficult to Model



In order to get t, you'll need to know all these functions explicitly:

$$y = t_y($$

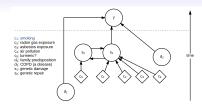
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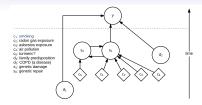
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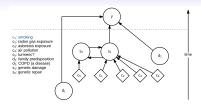
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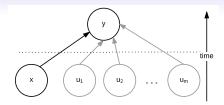
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A "Nice" Type of Ignorance



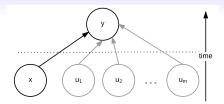
In the situation where the true model is

$$y = g(x) + h_1(u_1) + h_2(u_2) + \ldots + h_m(u_m)$$

and x is observed but u_1, \ldots, u_m are the "unknowns".

$$h_1(u_1) + h_2(u_2) + \ldots + h_m(u_m) \stackrel{\mathcal{D}}{\rightarrow}$$

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(LM Inference, Corr.

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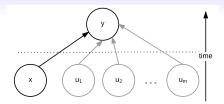
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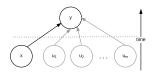
as the number of unseen variables increase (central limit theorem) and if ... they're somewhat independent.

Let
$$\mathcal{E}_0 = \sum_{k=1}^m \mu_k$$
 and $\sigma_{\mathcal{E}}^2 = \sum_{k=1}^m \sigma_k^2$, then

$$y = \underbrace{g(x) + \mathcal{E}_0}_{f(x)} + \mathcal{E}$$
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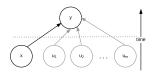
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LM Inference, Corr.

⇒ Causation

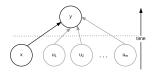
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Also, since x does not affect the other variables in any way, it cannot have an influence on their spread, hence σ^2 is not a function of x. Thus the error spread is the same everywhere across the range of x (homoskedasticity).

Parametric Worldview

We are back to the fundamental statistical problem, $Y = f(x) + \mathcal{E}$ where now we are more "okay" with the noise being normal and homoskedastic for all x.

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We now invoke the parametric worldview. Within that parametric worldview, we will buy into the linear model. Thus,

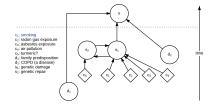
$$Y \sim \mathcal{N} \left(\beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p, \sigma^2\right)$$

But there is one more assumption...

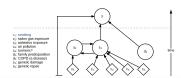
Independence

We now assume that each response is independent of every other response.

Second person:



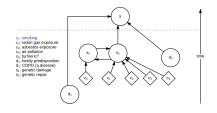
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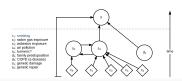
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Second person:



No effect of first person's y_1 (nor any of the unobserved variables which generate the \mathcal{E}_1) on the second person's y (or \mathcal{E}_2).

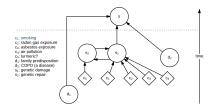
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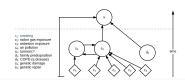
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First person:



No effect of first person's y_1 (nor any of the unobserved variables which generate the \mathcal{E}_1) on the second person's y (or \mathcal{E}_2).

If there are, we need to observe them and rotate them into our estimate of f(x). Examples for this cigarette case?

The Classic OLS Assumptions

Preassuming

• linearity (the parametric assumption)

we then further assume

- independence (most important)
- homoskedasticity (less important)
- normality of \mathcal{E} (least important if n is large)

in order to get ...

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in order to get ... inference. Changing these assumptions gives entirely new modeling techniques and inference. It is called "generalized linear model" theory.

A Different Means of Estimation

Last time, we were working on creating a fit \hat{f} that means we need estimates of all the parameters:

$$\hat{f}(x_1, x_2, \dots, x_p) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \dots + \hat{\beta}_p x_p$$

where the unknown parameters were $\beta_0, \beta_1, \ldots, \beta_p$. Our strategy last time was to minimize SSE via a calculus to obtain $\left\{\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p\right\}$. Why was this arbitrary?

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ight\}$. Why was this arbitrary?

Given the three new assumptions, we now have a completely specified joint probability distribution for our observed data,

$$\mathbb{P}(Y_1 = y_1, Y_2 = y_2, \dots, Y_n = y_n \mid X_1 = x_1, X_2 = x_2, \dots, X_n = x_n)$$

where $\mathbf{x}_i := [x_{i1}, x_{i2}, \dots, x_{ip}]$ i.e. the vector of all known measurements / covariates.

What's a probability? What's a likelihood?

In general, a parametric density function / mass function of a r.v. looks like the following:

$$\mathbb{P}(x;\theta) = \dots$$

where θ are the ...

What's a probability? What's a likelihood?

In general, a parametric density function / mass function of a r.v. looks like the following:

$$\mathbb{P}(x;\theta) = \dots$$

where θ are the ... tuning knobs on the model. We ask the question "what's the probability of this realization x (the data) assuming the density was parameterized at θ "? Now we ask the inverse question:

$$\mathcal{L}(\theta;x)=\ldots$$

that is "what's the likelihood of these parameters assuming we saw x (the data) come out the way it did"? The \mathcal{L} () denotes the **likelihood** function. Of course, probability and likelihood are

What's a probability? What's a likelihood?

In general, a parametric density function / mass function of a r.v. looks like the following:

$$\mathbb{P}(x;\theta) = \dots$$

where θ are the ... tuning knobs on the model. We ask the question "what's the probability of this realization x (the data) assuming the density was parameterized at θ '? Now we ask the inverse question:

$$\mathcal{L}(\theta;x)=\ldots$$

that is "what's the likelihood of these parameters assuming we saw x (the data) come out the way it did"? The $\mathcal{L}()$ denotes the likelihood function. Of course, probability and likelihood are exactly the same numerically,

$$\mathbb{P}\left(x;\theta\right) = \mathcal{L}\left(\theta;x\right) = \dots$$

but conceptually they couldn't be further apart!

Why not just ask the very common-sense question, what θ (what model within this parametric family) maximizes the probability of seeing what we observe? That would be a good guess as to what θ is.

(LM Inference, Corr.

⇒ Causation)

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Mult. Testing

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$$\mathbb{P}(Y_1 = y_1, Y_2 = y_2, \dots, Y_n = y_n \mid X_1 = x_1, X_2 = x_2, \dots, X_n = x_n) \\
= \prod_{i=1}^n \mathbb{P}(Y_i = y_i \mid X_1 = x_i)$$

How so?

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How so? Each observation is independent of every other. Recall $\mathbb{P}(ABC) = \mathbb{P}(A)\mathbb{P}(B)\mathbb{P}(C)$ if A, B and C are independent.

We can continue,

$$= \prod_{i=1}^{n} \mathbb{P}(Y_i = y_i \mid \boldsymbol{X}_1 = \boldsymbol{x}_i)$$

$$= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2} (y - \mathbb{E}[Y_i \mid \boldsymbol{X}_i])^2\right)$$

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How? Linearity of $\mathbb{E}[Y_i \mid \boldsymbol{X}_i]$. Now we wish to maximize the above over all possible $\beta_0, \beta_1, \dots, \beta_p, \sigma^2$. That's the arg max $\{\mathcal{L}(\theta; x)\}$ step.

Then, by some precalc tricks,

$$= \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} \mathrm{exp}\left(-\frac{1}{2\sigma^2}\mathcal{E}_i^2\right)$$

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Using calculus, the solution to $\left\{\hat{eta}_0,\hat{eta}_1,\ldots,\hat{eta}_{p}
ight\}$ is equivalent to minimizing SSE... What a coincidence!!

Note also: $\hat{\sigma}^2 = \frac{1}{2}SSE = MSE$. Why was there no $\hat{\sigma}^2$ until now?

The Likelihood Ratio (LR)

Imagine two models: (a) the "full" model where $\theta \in \Theta$ and (b) a reduced model where $\theta \in \Theta_R \subset \Theta$. The reduced space has q less degrees of freedom for θ to live within. Consider the ratio of the likelihoods

$$LR := \max_{\theta \in \Theta} \mathcal{L}(\theta; x) / \max_{\theta \in \Theta_R} \mathcal{L}(\theta; x)$$

representing how much

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representing how much more probable the full model is over the restricted model. But is this is this increase in probability **statistically significant?** It turns out as *n* gets large and under pretty forgiving conditions,

$$Q := 2 \underbrace{\ln(LR)}_{\ell(\hat{\theta};x)-} \stackrel{\mathcal{D}}{\underset{\ell(\hat{\theta}_{R};x)}{\longrightarrow}} \chi_{q}^{2}$$

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$$= \frac{\left(\frac{1}{\sqrt{2\pi\hat{\sigma}^{2}}}\right)^{n} \exp\left(-\frac{1}{2\hat{\sigma}^{2}}SSE\right)}{\sqrt{2\pi\hat{\sigma}^{2}}}$$

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$$= \left(\frac{SSE_0}{SSE}\right)^{n/2} \underbrace{\frac{\exp\left(-\frac{n}{2SSE}SSE\right)}{\exp\left(-\frac{n}{2SSE_0}SSE_0\right)}}_{\exp\left(-\frac{n}{2SSE_0}SSE_0\right)}$$

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$$= \frac{\left(\frac{1}{\sqrt{2\pi\hat{\sigma}^{2}}}\right)^{n} \exp\left(-\frac{1}{2\hat{\sigma}^{2}}SSE\right)}{\left(\frac{1}{\sqrt{2\pi\hat{\sigma}^{2}_{0}}}\right)^{n} \exp\left(-\frac{1}{2\hat{\sigma}^{2}}SSE\right)}$$

$$= \left(\frac{SSE_{0}}{SSE}\right)^{n/2} \underbrace{\frac{\exp\left(-\frac{n}{2SSE}SSE\right)}{\exp\left(-\frac{n}{2SSE_{0}}SSE_{0}\right)}}_{1}$$

Now we build the Q statistic:

$$Q = 2 \ln \left(\left(\frac{SSE_0}{SSE} \right)^{n/2} \right) = n \ln \left(\frac{SSE_0}{SSE} \right) \xrightarrow{\mathcal{D}} \chi_p^2$$

This can be used to test

$$H_0: \beta_1 = 0, \beta_2 = 0, \dots, \beta_p = 0$$

 $H_a:$ at least one is non-zero

There is another test for this you've learned about?

Omnibus F-test

$$F = \frac{\frac{SSE_0 - SSE}{p}}{\frac{SSE}{n - p}} = \frac{SSE_0 - SSE}{SSE} \frac{n - p}{p} =$$

Omnibus F-test

Mult. Testing

$$F = \frac{\frac{SSE_0 - SSE}{p}}{\frac{SSE}{n-p}} = \frac{SSE_0 - SSE}{SSE} \frac{n-p}{p} = \left(\frac{SSE_0}{SSE} - 1\right) \frac{n-p}{p} \sim F_{p,n-p}$$

Both tests use the same test statistic, namely SSE_0/SSE (up to constants and a monotonic transformation). It is a harder proof to demonstrate they have the same power for the same n and α (but they do).

Some points

• The likelihood ratio test / F test can also test any subset of the predictors (even one).

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Some points

- The likelihood ratio test / F test can also test any subset of the predictors (even one).
- Thus, we now have inference for every predictor or subset of predictors i.e.
 - Hypothesis testing
 - Confidence intervals

Previously,

$$Y \sim g(\beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p, \sigma^2, \ldots)$$

Do not assume OLS assumptions. We picked L2 loss and minimized to get $\{\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_p\}$. What do these numbers means?

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ight\}$. What do these numbers means? Same thing, except now ... we can "test" each value and provide confidence intervals for each value. You know how "stable" each number is to the the onslaught of the noise.

What you want to say about \hat{eta}_j

[Interpret stolen bases in baseball dataset in JMP].

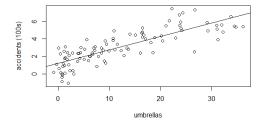
A change in x_j of +1 (a unit increase) causes / induces a β_j difference in its mean response y. Correct?

Umbrella Sales and Car Accidents

Consider a simple example. x: umbrella sales and y: car accidents. What would the relationship look like?

Umbrella Sales and Car Accidents

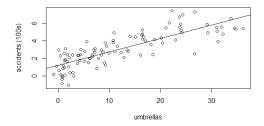
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Umbrella Sales and Car Accidents

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Does 100 more umbrellas sold *cause* 15.3 more car accidents (on average)? No... only an association (assessed by a linear correlation).

Correlation Does Not Imply Causation

What can correlation mean?

- There's a coincidence. How can this be?
- They are consequence from of a common cause (the lurking or counfounding variable). How can this be?
- There is causation

Correlation Does Not Imply Causation

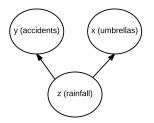
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- There is causation
 - ① x causes y (possibly with intermediates)
 - y causes x (possibly with intermediates)
 - 3 x and y cause each other (cyclic)

(recall time-boundedness property)

Controlling for the Confounder

The confounding variable is likely z = rainfall.



The illustration shows that if you change x obviously y doesn't change whatsoever (causes always precede their dependent effects an assumption known as temporal boundedness)

[Show regression in R]

A Proper Interpretation of \hat{eta}_j

Consider $\hat{\beta}_j$ estimates β_j . Imagine n is large and the confidence interval is really small. So basically, $\hat{\beta}_i = \beta_i \neq 0$. Interpretation?

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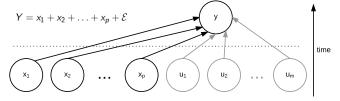
Another object naturally observed with exactly the same features except that x_j is increased by 1 unit will have a $\hat{\beta}_j \pm \mathbb{SE}\left[\hat{\beta}_j\right]$ difference in its mean response y. (Not much difference except accounting for model estimation error).

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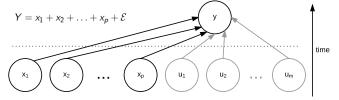
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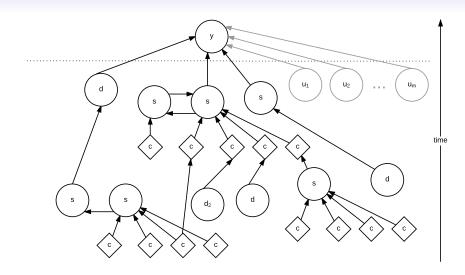
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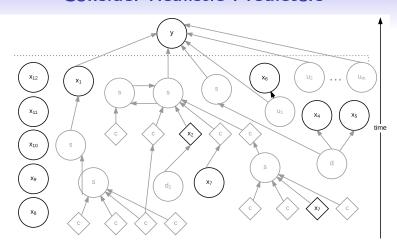


(causal for all p features ... how can the illustration be updated for one variable?)

2 -OR- If we've run a randomized experiment manipulating x_j among the objects AND assuming an linear additive effect of x_j on y.

Consider a Realistic Model





Grey variables and known to be dependent but the values are unknown and the u_k 's are the "unknown unknowns".

Some observations from the previous illustration:

• Maybe some of the predictors x_1, \ldots, x_p are causal, but most are likely not.

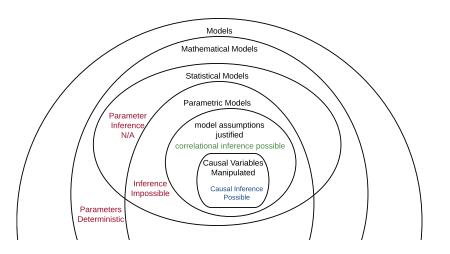
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- Of the ones that are not causal due to a confounder, you may have an idea of the lurking variables but it is unlikely you can measure them. Think college GPA vs SAT with confounder true IQ / ability.
- If some variables are causal, it is unlikely they have an additive causal effect; their effect is likely moderated by many other interacting variables possibly in non-linear ways.

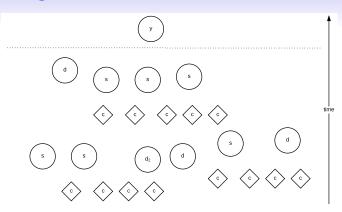
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- Some predictors are completed independent of the response.
- A linear model for y on x_1, \ldots, x_p is likely far from the truth (not related to our discussion on causality).

Inference and Causality

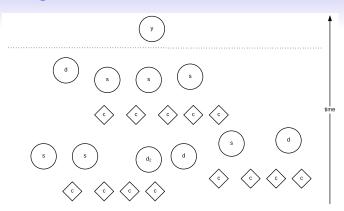


Sidebar: Theories are Hard...



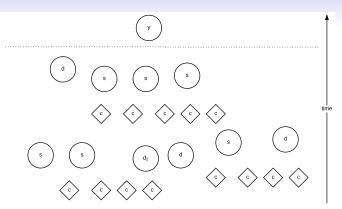
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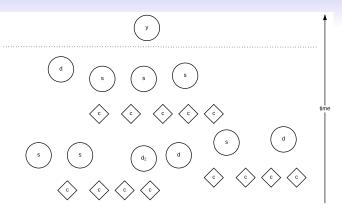
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More on OLS Coefficient Interpretation

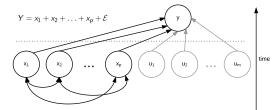
The linear regression coefficient interpretation again: another object naturally observed with exactly the same features except that x_j is increased by 1 unit will have a $\hat{\beta}_j \pm \mathbb{SE}\left[\hat{\beta}_j\right]$ difference in its mean response y.

What do we mean by naturally observed?

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The linear regression coefficient interpretation again: another object naturally observed with exactly the same features except that x_j is increased by 1 unit will have a $\hat{\beta}_j \pm \mathbb{SE}\left[\hat{\beta}_j\right]$ difference in its mean response y.

What do we mean by naturally observed? This other object is realized from the same joint distribution as all other observations. This means that whatever multicollinearity / covariance structure exists between the predictors, $\{\mathbb{C}\text{ov}[X_j, X_k]\}$, will give rise to the predictor values in the other object.



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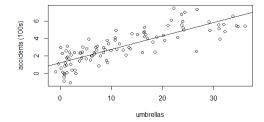
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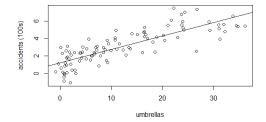
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But isn't getting the adjustments the whole reason we do linear regression??

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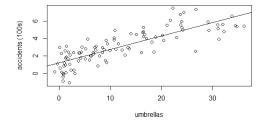


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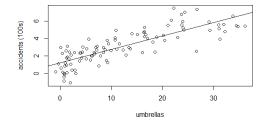
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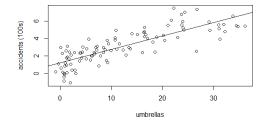
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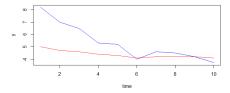
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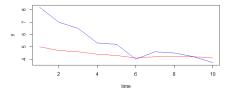
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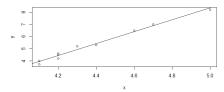


Are they linearly predictive of one another?

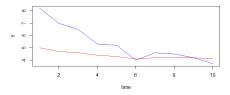
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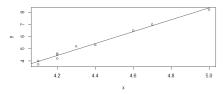
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 $R^2 \approx 99\%$, F test $p_{\rm val} \approx 1 \times 10^{-8}$. [R demo]

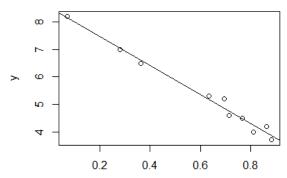
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Be careful about featurization... try to at least have some inkling of an idea for a causal dependency for the response on the predictors... I "found" this using by running that demo code for a few hours...

pval = 1.76e-08 r = 10108802



[JMP Baseball data]

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When is an individual t-test / F-test / LR test valid? When you are looking to test one single theory. Imagine you wished to test $H_a: \beta_{\text{num}} \mid_{\text{RBIs}} \neq 0$. Here's all you "see" then:

4	Parameter Estimates				
	Term	Estimate	Std Error	t Ratio	Prob> t
	Intercept	223.11467			
	batting_average	3043.1916			
	on_base_pct	-3528.013			
	num_runs	7.1003087			
	num_hits	-2.69827			
	num_doubles	1.3683081			
	num_triples	-17.92163			
	num_home_runs	19.483221			
	num_rbi	17.415071	5.068232	3.44	0.0007*
	num_walks	5.8147456			
	num_str_outs	-9.585548			
	num_stolen_bases	13.043869			
	num_errors	-9.553269			
	indic_free_agency	1372.8859			
	indic_free_agent_1991	-280.7903			
	indic_arb_elig	783.59223			
	indic arb 1991	352.11393			

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Imagine K tests. The strictest correction will be when considering that they fail to reject H_0 implying that their p values are $\sim \mathrm{U}\left(0,\,1\right)$. A rejection occurs at $p<\alpha$ which has probability α . This is called the false positive rate / Type I error.

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$$lpha_{\mathit{FWER}} := \mathbb{P}\left(\geq 1 \; \mathsf{rejection}\right) = 1 - \mathbb{P}\left(0 \; \mathsf{rejections}\right) = 1 - \binom{\mathcal{K}}{0} lpha^0 \left(1 - lpha\right)^{\mathcal{K}}$$

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Bonferroni Correction

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Bonferroni Correction

What does the Sidak Correction assume among the K tests? Independence. Can we assume that here? No. There is multicollinearity which means \mathbb{C} ov $\left[\hat{\beta}_i,\hat{\beta}_j\right] \neq 0$. What can we do now? Call event R a rejection. Recall inclusion exclusion:

$$\mathbb{P}(R_1 \cup R_2) = \mathbb{P}(R_1) + \mathbb{P}(R_2) - \mathbb{P}(R_1 \cap R_2)$$

$$\alpha_{FWER} = \alpha + \alpha - \boxed{?}$$

which can be used to demonstrate Boole's Inequality:

$$\mathbb{P}\left(\bigcup_{k=1}^{K} R_{k}\right) \leq \sum_{k=1}^{K} \mathbb{P}\left(R_{k}\right)$$

$$\alpha_{FWER} \leq \sum_{k=1}^{K} \alpha = K\alpha$$

Meaning if I want the typical $\alpha_{FWER} = 5\%$, I'd better set the individual rejection at 5%/K. This is known as the Bonferroni Correction.

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$$\mathbb{P}\left(\frac{\left(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}\right)^{\top} \left(\boldsymbol{X}^{T} \boldsymbol{X}\right)^{-1} \left(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}\right)}{\rho MSE} \leq F_{\alpha, p, n-p}\right) = 1 - \alpha$$

This also account for every possible contrast you'd ever want to test e.g. H_a : $\beta_3 + \beta_7 \neq \beta_5 - \beta_2$.

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I can't figure out how to do this in JMP, so if it is on the homework, we will do it in R.

Omnibus F test as a "Correction"

Recall:

$$R^2 = \frac{SSE_0 - SSE}{SSE_0} =$$

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$$= \frac{R^{2}}{1 - R^{2}} \times \underbrace{\frac{n-p}{p}}_{\text{penalty for too many features}}_{\text{unexolained to unexolained}}$$

[R Demo]

Hypothesis Testing: a Review

Conceptually, let's act out the introduction of data assuming H_0 , H_a and some predetermined level α .

 H_0 : UFOs do not exist

 H_a : UFOs do exist

and the inverse:

 H_0 : UFOs do exist

 H_a : UFOs do not exist

"Flipping" the null and the research hypothesis represents a completely different framing. The Type II error is now controlled for.

Hypothesis Testing: a Review

For regression, we can consider the same:

$$H_0: \beta_i = 0$$

$$H_a: \beta_j \neq 0$$

and the inverse:

$$H_0: \beta_j \neq 0$$

$$H_a: \beta_j = 0$$

[R Demo]

An Equivalence Test

We are trying to prove $\beta_j = 0$ so we first assume $\beta_j \neq 0$ and wait until we have enough evidence (an "equivalence test"). Can you think of a situation you would need this type of control?

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We first define δ , a margin of practical equivalence, so if $\beta \in [-\delta, \delta]$ than practically speaking we believe it to be zero. You need to set δ yourself. Then we run two tests at level α :

$$H_0: \beta_j \ge \delta$$
 $H_0: \beta_j \le -\delta$
 $H_a: \beta_i < \delta$ $H_a: \beta_i > -\delta$

This is known as TOST (two one sided tests) which is equivalent to taking the intersection of two α -sized one sided confidence intervals, i.e. a two sided confidence interval at level 2α . Thus, we reject H_0 if:

$$Cl_{eta_j,\mathbf{1}-lpha}:=\left[\hat{eta}_j\pm t_{lpha,n-p-1}\mathbb{S}\mathsf{E}\left[\hat{eta}_j
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[R demo]

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- Optimal Design

Question: assume OLS and that we only care about inference for β_1 . We can sample any x values live in their set \mathbb{X} e.g. $\in [x_m, x_M]$. What should the n values be?

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- ② Uniform spacing: $\{0, 0.111, 0.222, \dots, 0.999\}$

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- Something else?

[R demo]

Recall the formula from Stat 102 / 613:

$$\mathbb{SE}\left[\hat{eta}_1
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- ② Minimize the numerator, MSE i.e. minimize the SSE. Can we do this? Yes by picking the closest $\hat{\beta}_1$ to β_1 (which we already do).

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We seek the best linear approximation of f(x) which is $\beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p$. We pick the x's to give us the best linear approximation. What criteria? JMP gives two ways:

$$\bullet \ \, \mathsf{Note:} \, \, \mathbb{V}\mathsf{ar}\left[\hat{\beta}_{0},\hat{\beta}_{1},\ldots,\hat{\beta}_{p}\right] = \sigma^{2}\left(\boldsymbol{X}^{T}\boldsymbol{X}\right)^{-1}$$

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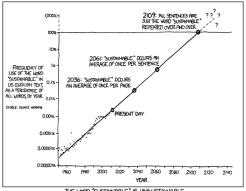
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[R Demo] What did we learn? For linear models with no polynomials or interactions, keep the observations as close to the minimimums and maximums as possible. For linear models with polynomials and interactions (more non-parametric than parametric), keep most towards the minimums and maximums and some in the center of the input space.

Extrapolation

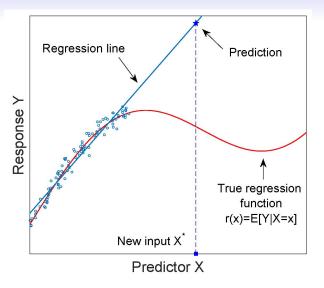
Data driven approaches are all focused on accuracy during interpolation.



THE WORD "SUSTAINARI E" IS UNSUSTAINARI E.

Extrapolation brings trouble. It is important to ask the question for a new observation x^* if it is within the space of x's in the historical data. (Hardly anyone does this... but you should)! Be aware that extrapolation methods of different algorithms differ considerably! [R Demo]

Reconciliation of those Silly Cartoons



Modeling Categorical Responses

Previously the response y was continuous and via the OLS assumptions we obtained the statistical model,

$$Y \stackrel{ind}{\sim} \mathcal{N}\left(\beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p, \sigma^2\right)$$

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We need a "link function" to connect the linear function to the restricted support of the response:

$$\lambda(f_{\mathbb{R}}(x_1,\ldots,x_p))=f(x_1,\ldots,x_p)$$

And the parametric assumption would be

$$\lambda(s_{\mathbb{R}}(x_1,\ldots,x_p;\theta_1,\ldots,\theta_\ell))=s(x_1,\ldots,x_p;\theta_1,\ldots,\theta_\ell)$$

And assuming a linear form:

$$\lambda(\beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p) = ?$$

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Let's investigate what the first one means. Define $p := \mathbb{P}(Y = 1)$. We can think about probability in another way:

$$odds(Y = 1) := \frac{p}{1 - p}$$

So if odds = 4:1, what is p? This means that the probability of the event happening is four times more likely than the complement happening. Or... of 4+1 runs, 4 will be a yes. What is the range of odds?

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What is the range of the logit function? All of $\mathbb R$. Hence, we can now set this equal to our $s_{\mathbb{R}}$ function. In the linear modeling context,

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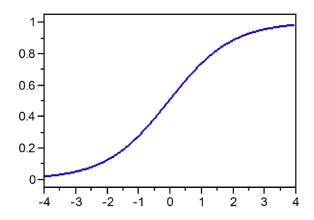
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Thus, a change in the linear model becomes a linear change in log-odds. This is (I would say) the most interpretable link function situation we've got.

The Logistic Function



How to Obtain a Model Fit

A model fit would mean we estimate $\{\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_p\}$. We initially did this estimation for regression (continuous y) by defining a loss function, SSE, and finding the optimal solution via calculus. What do we do now??

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1 Linear-Logistic conditional expectation

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- Linear-Logistic conditional expectation
- Independence

$$\mathbb{P}(Y_1 = y_1, Y_2 = y_2, \dots, Y_n = y_n \mid X_1 = x_1, X_2 = x_2, \dots, X_n = x_n) \\
= \prod_{i=1}^n \mathbb{P}(Y_i = y_i \mid X_1 = x_i)$$

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$$= \prod_{i=1}^{n} \left(\frac{e^{\beta_0 + \beta_1 x_1 + \dots + \beta_\rho x_\rho}}{1 + e^{\beta_0 + \beta_1 x_1 + \dots + \beta_\rho x_\rho}} \right)^{y_i} \left(1 - \frac{e^{\beta_0 + \beta_1 x_1 + \dots + \beta_\rho x_\rho}}{1 + e^{\beta_0 + \beta_1 x_1 + \dots + \beta_\rho x_\rho}} \right)^{1 - y_i}$$

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How? This does not have a simple, closed form solution. The computer iterates numerically and converges on the values of the parameters that maximize the above and these are shipped to you as $\left\{\hat{\beta}_0,\hat{\beta}_1,\ldots,\hat{\beta}_p\right\}$. This is called "running a logistic regression".

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