Predictive Analytics Lecture 1

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

January 17 & 18, 2017

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I will be using predict and forecast interchangeably.

Examples

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How do we make predictions? We use a *model*.

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Outputs? health, wealth and wisdom

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of a person. A person features health, a person has the characteristic of going to bed early.

What are “observations”?

Generally, inputs and outputs are features of the

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Thus the model relates some *feature(s) of the observation* to other *feature(s) of the observation*. Here, we are relating specific people’s bedtime schedule and waking schedule to their health, wealth and wisdom.

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The Model as a Functional Relationship

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It is traditional to put the outputs on the left hand side. This is assumed that the outputs were measured. This type of observation is called

- old or
- historical or
- known

and predictions here are not needed (obviously). In our aphorism model, for the observation being a known person named Joe:

$$\begin{bmatrix}\text{a measured quantity of Joe's health}\\ \text{a measured quantity of Joe's wealth}\\ \text{a measured quantity of Joe's wisdom}\end{bmatrix} = \text{model}\left(\begin{bmatrix}\text{a measured quantity of Joe's bedtime}\\ \text{a measured quantity of Joe's waketime}\\ \vdots\end{bmatrix}\right)$$

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Now we can hone our definition of prediction. For a

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As an example new person Bob,

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$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \end{bmatrix} = \text{model}\left(\begin{bmatrix} x_1 \\ x_2 \\ \vdots \end{bmatrix}\right)$$

We will use the "hat" symbol (^) to indicate a prediction of the output $\hat{y}$ to distinguish it from the true value of the output y.

More Vocabulary

Even though measured inputs and outputs are features of an observation, they each go by special names that emphasize their roles.

Each output y is called a

- *response* (the model "responds" to inputs)
- *outcome* / *outcome metric* (the result of inputs)
- ~~*endpoint*~~ (only used in clinical trial context)

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Inputs x's then can go by the following terms of art:

- *covariates* (because the vary with the response, co-vary)
- *predictors* (since they will be the inputs used to make predictions)

and they are what we **make use of** to predict. I will try to use "response" and "predictors" in this course.

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Now that we have predictors and responses measured an numeric and an equal sign relating them. We have officially created a *mathematical model*. The word "model" now will be represented as a function, f.

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It is said that the "model **explains** the response". What does this mean?

Science is based on Mathematical Models

We have become quite successful at shrink-wrapping interesting variables in the world around us into simple models with few inputs:

$$
\begin{aligned}
F &= G\frac{m_1 m_2}{d^2} \\
V &= IR \\
K &= \frac{1}{2}mv^2 \\
PV &= nRT
\end{aligned}
$$

It took us thousands of years to figure this out.

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Idea $\to$ English $\to$ Math

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What is the response metric?

Idea → English → Math

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What is the response metric? What does "healthy" mean?

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- Healthy for ages 25-65 (since we can expect health in infanthood and adolescence but not in elderly years)?

ALSO: one also gets a feeling from the wording, there is either "healthy" or "not healthy".

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I there are two levels, it is called *binary* or *dichotomous* and the model would be called a *binary response model* (or a classification) with elements 0 and 1.

Define the response clearly

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We still need a clear definition. Ideas? How about: healthy means no incidence of a “major” disease between the ages of 25–65? This can be assessed with medical records.

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x_1: bedtime schedule

Definition?

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Definition? Average bedtime. How to measure / assess? Survey?

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Definition?

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x_2: waketime schedule

Definition? Average time to rise in the morning assessed via survey

Thus, x_1 and x_2 are a variant of a *timestamp* data type.

Dataframes

The historical *data frame* or *dataset* (or even more colloquially, the "data") can look like:

Healthy? 1 = yes (y)	Average Bedtime (x_1)	Average Waketime (x_2)
1	9:32PM	6:42AM
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We don't know the model yet...

Mathematical Models are Deterministic

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Mathematizing, this becomes $y = f(x_1, x_2)$.

From the wording, it seems the model is unequivocal and deterministic. This meansthat for any input values (the measured values of x_1 and x_2), the output (the response) will have only one unique value.

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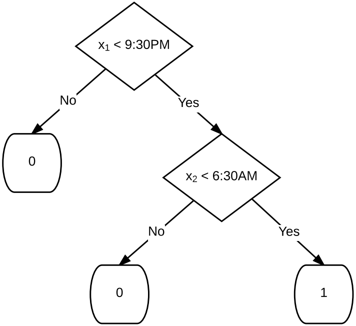
 Thus the functional form likely

looks like a *decision tree model*.



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Thus, this model is **wrong**. Why? We can find at least one person who does not have a matching response when inputs are evaluated in f. Seems obvious but...

Smoking and Lung Cancer

Consider the model with the binary input

- y: contract lung cancer at some point (1) or not (0)
- x_1: smoke 10 pack years or more at some point in a lifetime (1) or not (0) and the response

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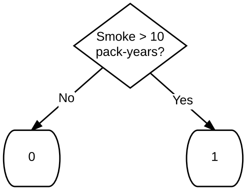

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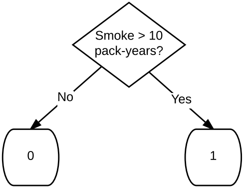


No... in fact "only" 16% of smokers get lung cancer compared to about 0.4% of non-smokers. Thus, the simpel model above is wrong because some responses (that is features of certain individuals) will not "fit" the model. Thus, should we throw out the whole enterprise of modeling?

Statistical Models

Mathematical models such as

$$y = f(x_1, x_2, \ldots)$$

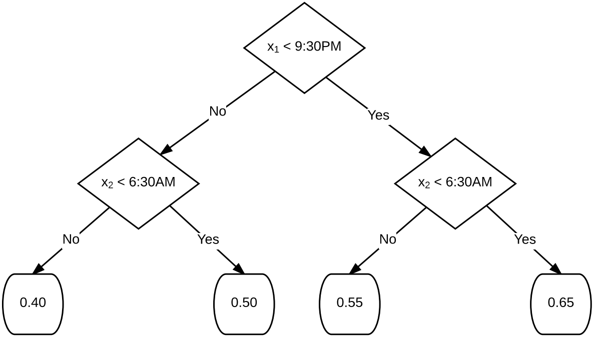
can become forgiving to **errors** in f by allowing for y to be modeled non-deterministically as a random variable (r.v.), uppercase Y. For our case of binary classification, this r.v. is the Bernoulli:

$$Y \sim \text{Bernoulli}\left(f(x_1, x_2, \ldots)\right) := \begin{cases} 1 & \text{with probability } f(x_1, x_2, \ldots) \\ 0 & \text{otherwise} \end{cases}$$

Since the response is now a r.v., we call this a **statistical model**.

A Statistical Model

A more conceivable model f is:



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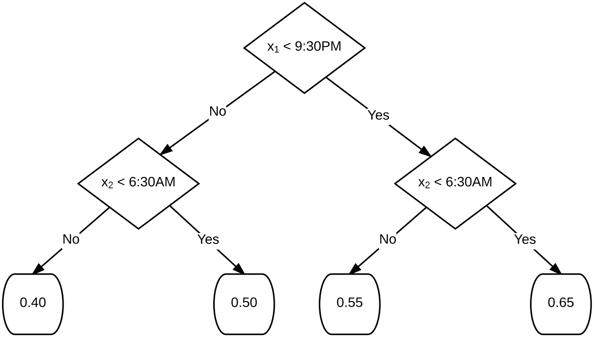

Are there still reasons for x_1 and x_2 to be rigid binary values e.g. 1 if $x_2 <$ 6:30AM? No... but we haven't spoke about model fits nor parameters.... wait...

Is Health Dichotomous?

So, we should really update the text of the aphorism to reflect the introduction of the random variable response. It should read:

Early to bed and early to rise makes a man

Is Health Dichotomous?

So, we should really update the text of the aphorism to reflect the introduction of the random variable response. It should read:

> *Early to bed and early to rise makes a man* ***more likely to be*** *healthy.*

However this seems to still suggest someone is either healthy or not healthy. Didn't the author of the aphorism, to be more accurate, say...

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we need some way to measure a quantity of healthiness on a continuous scale. Open problem. How can you shrink-wrap health into a single number?

QOL: a Response Metric?

One such scale is found in Flanagan (1978) invented the precursor to the modern "Quality of Life Scale" (QOLS) metric based on assessing 7-point Likert scales. It takes 5 minutes and scores range from 16–112. Here are the categories:

Item	English N = 584	Swedish [15] N = 100	Norwegian [17] N = 282	Hebrew [16] N = 100
1. Material and physical well-being	5.6 (1.0)	5.7 (1.4)	5.5 (1.3)	4.3 (1.8)
2. Health	3.9 (1.4)	3.9 (1.6)	4.4 (1.5)	2.3 (1.5)
3. Relationships with parents, siblings and other relatives	5.3 (1.1)	6.0 (1.0)	5.5 (1.5)	5.9 (1.2)
4. Having and raising children	5.6 (1.2)	5.6 (1.6)	5.7 (1.2)	5.9 (1.2)
5. Relationship with spouse or significant other	5.5 (1.4)	5.6 (1.6)	5.5 (1.6)	5.8 (1.2)
6. Relationships with friends	5.4 (1.1)	6.2 (0.9)	5.9 (1.1)	5.4 (1.6)
7. Helping and encouraging others	5.4 (0.9)	5.3 (1.2)	5.2 (1.2)	3.0 (2.0)
8. Participating in organizations and public affairs	4.6 (1.2)	4.9 (1.6)	4.3 (1.6)	2.3 (1.9)
9. Intellectual development	4.7 (1.2)	5.2 (1.4)	4.6 (1.5)	2.1 (1.6)
10. Understanding of self	5.1 (1.1)	5.5 (1.2)	5.3 (1.1)	3.0 (1.8)
11. Occupational role	4.7 (1.4)	5.0 (1.5)	5.3 (1.4)	3.2 (1.8)
12. Creativity/personal expression	4.8 (1.2)	5.0 (1.4)	4.7 (1.6)	2.5 (1.7)
13. Socializing	4.7 (1.2)	5.3 (1.3)	5.1 (1.4)	3.6 (1.9)
14. Passive and observational recreation	5.5 (0.9)	6.0 (1.0)	5.7 (1.1)	3.6 (2.0)
15. Active and participatory recreation	4.0 (1.5)	4.0 (1.7)	4.5 (1.6)	2.2 (1.5)
16. Independence, doing for yourself*	5.0 (1.5)	5.0 (1.7)	5.2 (1.4)	3.8 (1.7)

Making Up Metrics

Yes, metrics are essentially “made up”. Good ones are engineered to carefully capture the information sought. Examples:

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It is most important for these metrics to be monotonic (i.e. higher always means better or worse).
We also would appreciate these metrics being approximately linear. So an increase of 1 "point" on the scale means the same increase/decrease in quality. But that is usually too much to ask.

Back to Modeling

We now are considering health as a continuous number (the data type is called "continuous") but the model is still deterministic. How to we reengineer the aphorism to allow for stochasticity (randomness)?

Early to bed and early to rise makes a man

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We can then build a statistical model:

$$Y \sim g\left(f(x_1, x_2), \sigma^2, \ldots\right)$$

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where $f(x_1, x_2)$ now represents the mean health for these inputs, σ^2 is now variance around that mean, and the ellipses is a technicality dealing with higher moments such as skew, etc that we will ignore for the purposes of this class. Thus, health scores are realized randomly but the mean health scores are deterministic.

Regression Models

When the response is continuous, the statistical model is called a *regression model*. What does regression mean?

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$$Y = f(x_1, x_2) + \mathcal{E}$$

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Where does $\mathcal{E}$ come from?? Philosophical question... one we will return to soon.

Conditional Expectation

The model can be written even another way to belabor this point:

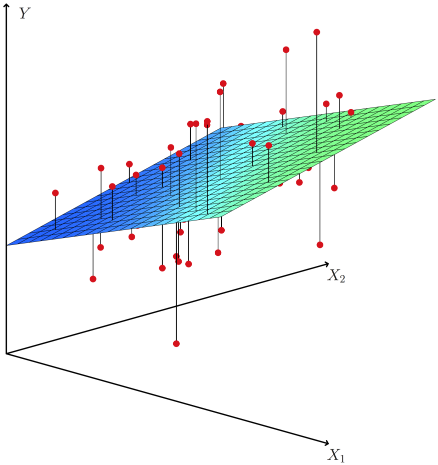
$$Y = \mathbb{E}[Y \mid x_1, x_2] + \mathcal{E}$$

where $\mathbb{E}[Y \mid x_1, x_2]$ is called the "conditional expectation function" or the "conditional mean function" and of course,

$$\mathbb{E}[Y \mid x_1, x_2] = f(x_1, x_2)$$

Specifying the model for f is sometimes called "conditional mean modeling".
How does one think of $\mathbb{E}[Y \mid x_1, x_2]$?

A mock $\mathbb{E}[Y \mid x_1, x_2]$ Illustration



Generalizing the Inputs

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Let's reengineer the aphorism again to allow for grey area:

> ***The earlier*** *to bed and the* ***earlier to*** *rise makes a man healthier on average.*

Bedtime and Waketime Again

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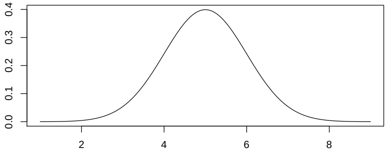
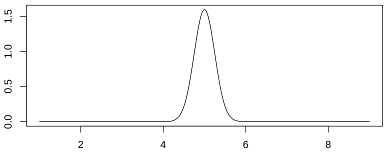
What should we do? Maybe just one number defined as the number of hours after an absurd average bedtime like 5PM? Thus, 9PM $\rightarrow x_1 = 4$ and 2AM $\rightarrow x_1 = 9$, etc. Ditto for waketime to avoid the problem of people on average waking up after 12:59PM.

The Average Is Misleading

We are using average bedtime and waketime. What's wrong with an average?





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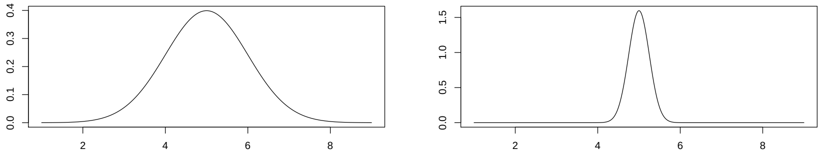

These are two bedtime distributions over many, many years. They both have the same average: 10PM. Who do you think is healthier on average? The person on the right. Why?

Designing Better Inputs

How can we get more "information" out of a person's bedtime and waketime that is relevant to predicting health outcomes?

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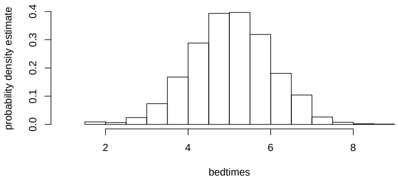
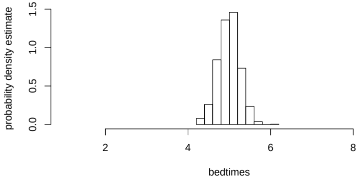
How can we get more "information" out of a person's bedtime and waketime that is relevant to predicting health outcomes?
We likely don't know which piece of the distribution will be helpful, so let's just add all the information. Let's bin by maybe 20min and record the probabilities over many years of being in that bin. For instance, 5 year bins for these two people may look like:





All bin values can be used as inputs. So in this model, $p > 2$. It could be almost 100. This is called **featurization** — designing features and we will talk more about it later.

Flexible Inputs $p = 2 \rightarrow p \approx 100$

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- Advantage: We can fit more exact rules like if the proportion of times went to bed past 1AM is 10% ... then health drops considerably and then more so for 2AM
- Disadvantage: It makes the model hard to fit and interpret. There are a lot of "degrees of freedom" now (a term you've heard before). A lot more in this later as this is the most important topic in this course.

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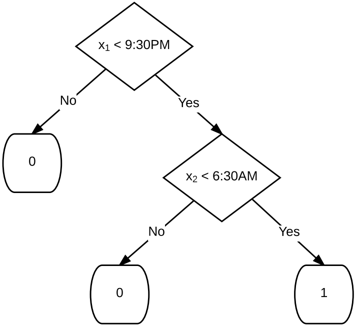
Each predictor and the response have a certain data type. If the data type of the response is categorical (or binary as in two categories), we have a classification model. If the data type of the response is a continuous metric, we have a regression model.

The Aphorism Revisited

Early to bed and early to rise makes a man healthy.

which may imply binary x_1, x_2 and y and thus f likely looks like:



New question: where did this model come from??

History

As the olde englysshe prouerbe sayth in this wyse. Who soo woll ryse erly shall be holy helthy & zely.
- The Book of St. Albans, 1486

Earely to bed and earely to rise, makes a man healthy, wealthy, and wise.
- John Clarke's Paroemiologia Anglo-Latina, 1639 (collection of proverbs)
-Benjamin Franklin, 1735 (popularized it in American English)

We, as a people, built this model and it's been validated over centuries. How did we build it?

Humans as Model Builders

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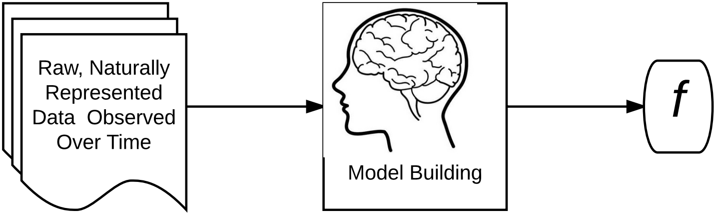

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How many measurements is that? (What's the dimensionality of the input space?) Immeasurable and cannot be defined. But we know it's HUGE! Note: this is technically called **deep learning**.

A Deep Learning Model You've Built

Is this a cat?

Response?

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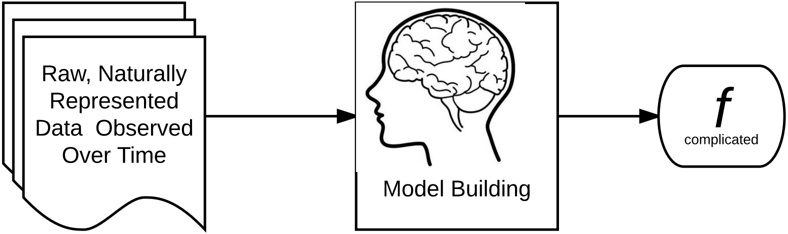
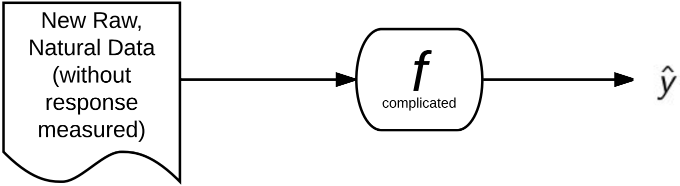
Response? Cat or not (0 or 1 numerically). Predictors in the model? Entire image... raw natural data representation. The brain shrinks the space down to a small number of predictors. You've already built this model (but only in your head... and you don't even know how it works).

Prediction in a Deep-Learned Human Model



Then, in the future...



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- The model cannot be communicated precisely.
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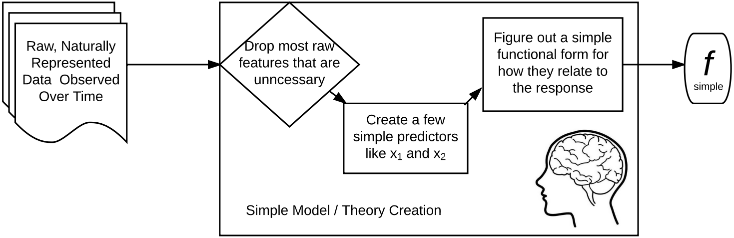
- The functional form cannot be shared.
- And thus no prediction can be made with it (unless it is the same brain that makes the prediction that built the model).

But we Create Simple Models. How?

Early to bed and early to rise makes a man healthy.



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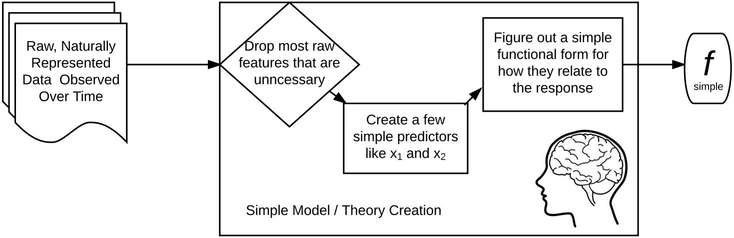

This is the process by which we put forth the model "early to bed and early to rise makes a man healthy".

Models we are Good and Bad At

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Bad at Building Statistical Models when...

inputs are already derivative features of the raw data representation, are numeric and there a lot of them (p large), and noise is large ($\mathbb{V}\text{ar}\left[\mathcal{E}\right] >> 0$).

We are Frequently Bad...

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The clinicians make a diagnosis on the basis of a quick meeting and a whole bunch of numeric variables: age, serum glucose, blood pressure, symptom measurements... difficult models for us to build.

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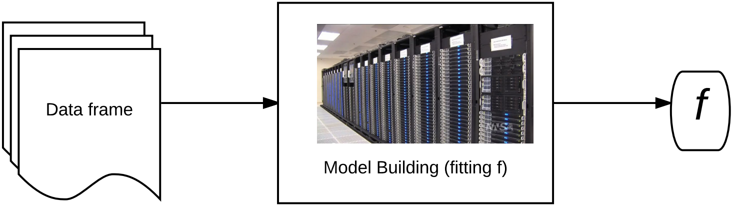
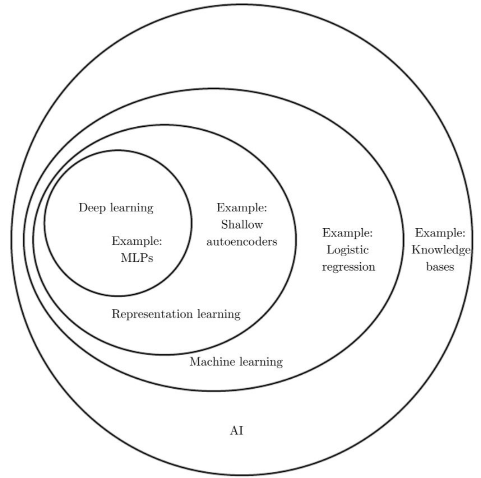


Luckily, yes. And this is a main advantage of artificial intelligence.

Types of AI?



(Fig 1.4 in Goodfellow et al., 2017)

What Does Input to AI Look Like?

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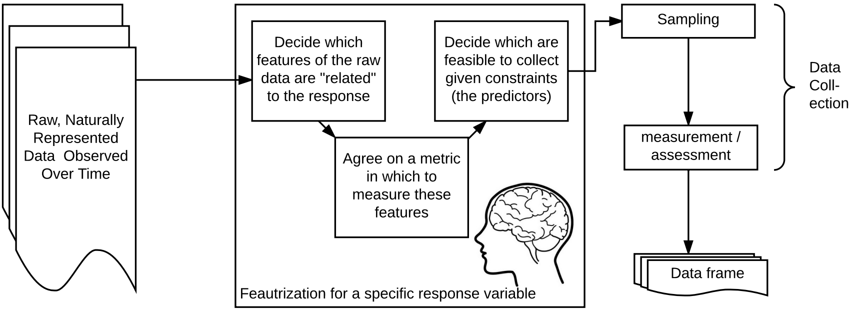
Can we enter all this into a computer? No, not now, possibly not ever. Also, willl be using statistical modeling so it needs well-defined measurements. So we need to “featurize” and then “collect data”.

What is Featurization & Data Collection?



What is featurization?

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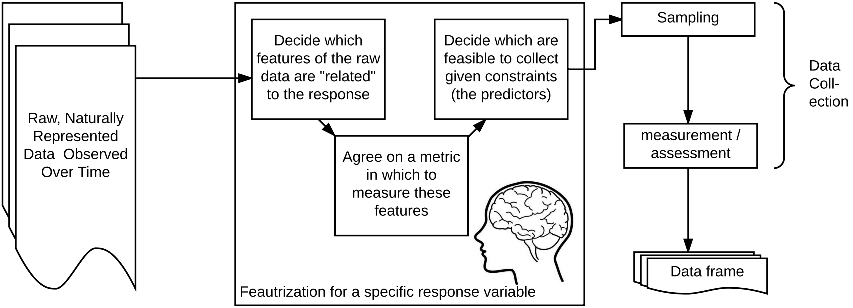

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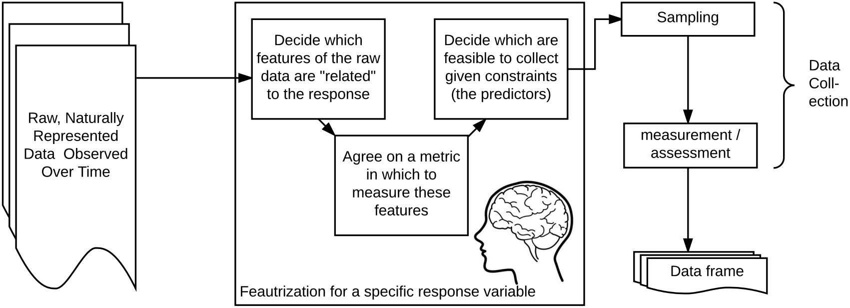

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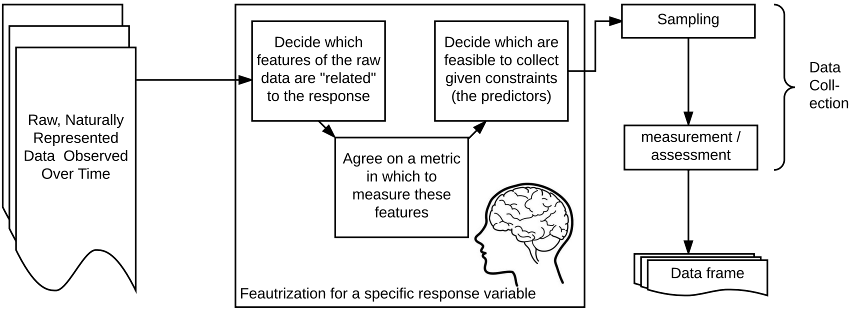

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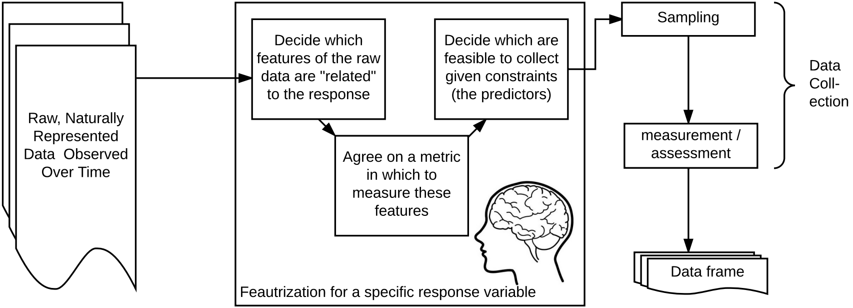
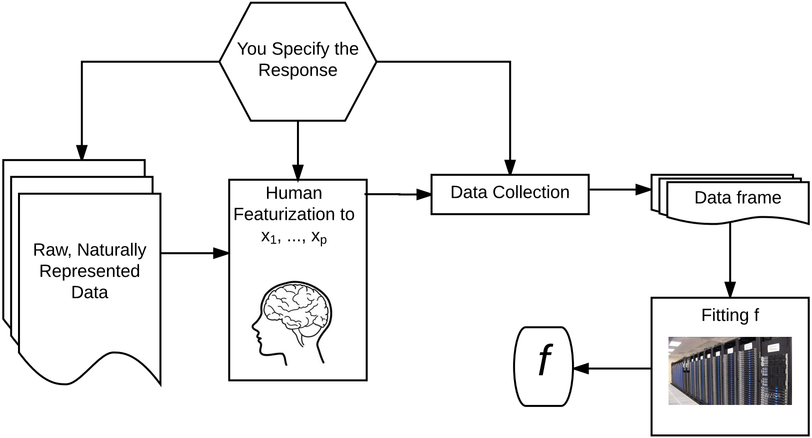
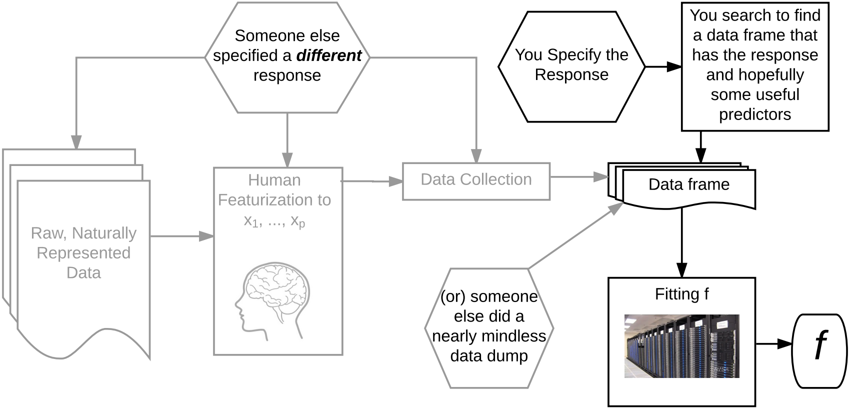


What is featurization? Deciding predictors. What is data collection? (a) sampling units then (b) measuring the numeric values of the predictors (note: some measurements may be missing).

What is Good Machine Learning?



What is Day-Day Machine Learning?

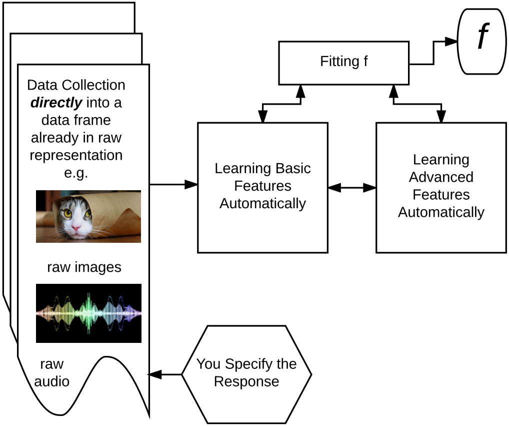


This is bad... but it's what we generally do all day...

Baseball Data Questions

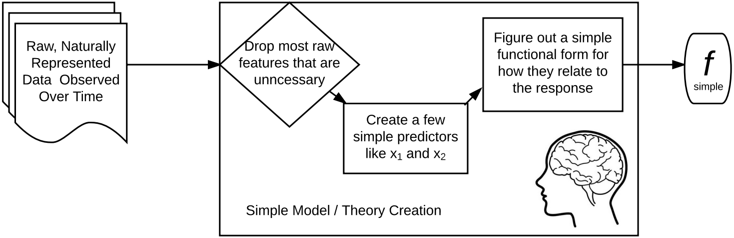
- Response?
- Predictors?
- $n = ?$ $p = ?$
- How was this data frame likely collected?
- Do you think by studying this dataset you can predict salaries?

Aside: what is Deep Learning?



Learning complex features automatically (the cutting edge).
Software running self-driving cars use this.

What are we really bad at?



Figuring out those functional forms... and the computer excels at it.

The Fundamental Statistical Problem

We know our response variable, we've picked features, made measurements and now have an $n \times (p+1)$ data frame. We know the response looks like

$$Y = f(x_1, x_2, \ldots, x_p) + \mathcal{E}$$

where f represents the conditional mean $\mathbb{E}[Y \mid x_1, x_2, \ldots, x_p]$ and the $\mathcal{E}$ r.v. is random noise added atop the conditional mean but we don't know f!

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So we have to learn / infer f the best we could from the historical dataset. We denote this fit $\hat{f}$. What does this mean in the baseball data?

Two Worldviews: (I) Parametric

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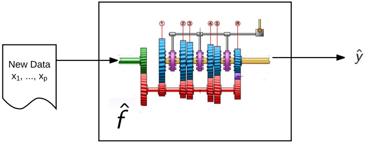
- We would like to know how f works, but it's likely very complex, so it's not our top priority.
- Absolute prediction accuracy is indeed our #1 focus. It's the bottom line. We want $f \approx \hat{f}$ as close as possible.

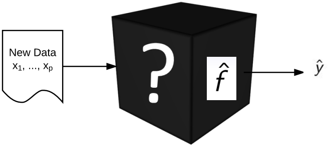
Two Worldviews

The process to find $\hat{f}$ is known by many names:

- parametric modeling
- model fitting
- statistical modeling
- white box modeling



- non-parametric modeling
- function fitting
- function approximation
- response surface methodology
- machine learning
- black box modeling



What is a Parametric Model?

If we see f is a parametric model, we mean that

$$f(x_1, x_2, \ldots, x_p) \approx s(x_1, x_2, \ldots, x_p; \theta_1, \theta_2, \ldots, \theta_\ell)$$

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$$s(x_1, x_2, \ldots, x_p) = \beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p$$

with p predictors, there are $p + 1$ degrees of freedom (the intercept is also a knob that can be twisted). It is traditional to call the θ's in the linear model β's due to historical reasons.

What is $\hat{f}$ in a linear model?

Then we need to create a fit $\hat{f}$ that means we need estimates of all the parameters:

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

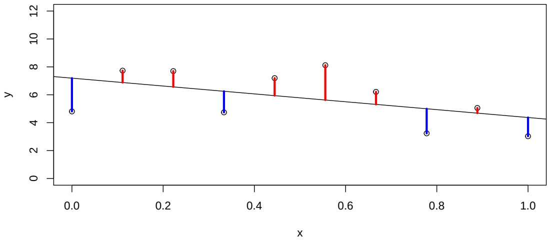
then we can use $\hat{f}$ on new data (where the response is not observed), say $x_1^*, x_2^*, \ldots, x_p^*$ to get a prediction:

$$\hat{y} = \hat{f}(x_1^*, x_2^*, \ldots, x_p^*)$$

Where do we get $\left\{\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p\right\}$ from?

What defines a good fit?

Consider the simple linear regression (one predictor) i.e. $s(x) = \beta_0 + \beta_1 x$ thus we need to figure out $\hat{\beta}_0$ and $\hat{\beta}_1$, constituting the model fitting. Let's say given data, we guess that $\hat{\beta}_0 = 7.2$ and $\hat{\beta}_1 = -2.8$. Would this be a good fit?



The line is our $\hat{y}(x)$ i.e. all possible predictions. Seems sometimes we undershot the response (the red) i.e. $y - \hat{y} > 0$ and sometimes overshot the response (the blue) i.e. $y - \hat{y} < 0$.

The Role of the Residuals

We call $e_i := y_i - \hat{y}_i$ the ith residual. Since we fit all of our historical data there are n residuals $e_1, \ldots, e_n$. Wouldn't it be nice to keep these small?

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- Minimize $e_1, \ldots, e_n$ while
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What does "minimize $e_1, \ldots, e_n$" mean? We need to define an overall error metric. This is called the **loss function**.

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Luckily the computer does all of this for you and it just pops out its answer $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p$.

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We won't have time to get into custom and asymmetric cost functions. But you need to keep this in mind when you consider the predictions you make with all of the $\hat{f}$'s we discuss in this class.

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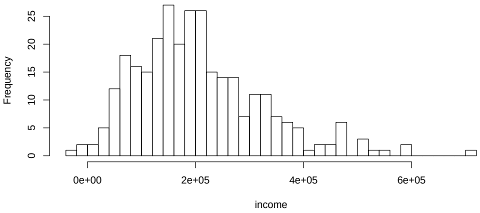
Consider a dataset for income among HS grads that didn't go to college. You have $n = 1,000$ historical responses (the incomes). Here they are:



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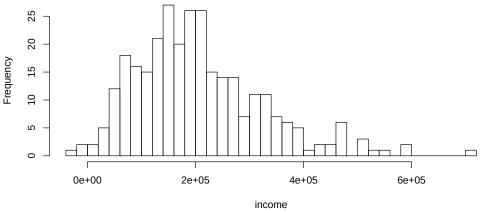

Imagine there was no predictors but you still would like to produce predictions. What would you do?

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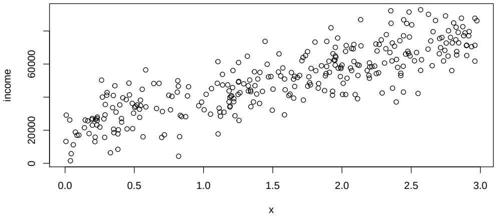
Shoot Blind

The best guess (i.e. the one with minimal SSE) is the average $\hat{y} = \bar{y}$ for any new observation. Using this prediction model, albeit very basic, the SSE is 115512239042 (usually called SST).

Now imagine you had a predictor... let's say some measure of work ethic or intelligence, call it x. Here's a plot:



(see in R)

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$$\begin{aligned} R^2 &:= \frac{SSE_0 - SSE}{SSE_0} \times \frac{n-1}{n-1} = \frac{\frac{1}{n-1} SSE_0 - \frac{1}{n-1} SSE}{\frac{1}{n-1} SSE_0} \\ &= \frac{\frac{1}{n-1} \sum_{i=1}^{n} (y_i - \bar{y})^2 - \frac{1}{n-1} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\frac{1}{n-1} \sum_{i=1}^{n} (y_i - \bar{y})^2} \\ &= \frac{s_y^2 - s_e^2}{s_y^2} \approx \frac{\mathbb{V}\mathrm{ar}[Y] - \mathbb{V}\mathrm{ar}[E]}{\mathbb{V}\mathrm{ar}[Y]} \end{aligned}$$

where $\mathbb{V}\mathrm{ar}[Y]$ is what was inexplicable before and $\mathbb{V}\mathrm{ar}[E]$ is what is inexplicable after. R^2 is really an *estimate* of the pctg var. explained.

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How about the following metric?

$$s_e = \sqrt{s_e^2} = \sqrt{\frac{1}{n-1} SSE} = \sqrt{\frac{1}{n-1} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2}$$

This is our best guess of the standard error of our estimate e, our residual (AKA "RMSE"). What is a standard error?

Recall the Empirical Rule

If $X \sim \mathcal{N}\left(\mu, \sigma^2\right)$, then

- $\mu \pm 1\sigma$ contains 68% of the realization values
- $\mu \pm 2\sigma$ contains 95% of the realization values
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Thus for a realization x,

- $x \pm 1\sigma$ contains μ 68% of the time
- $x \pm 2\sigma$ contains μ 95% of the time
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Stretch the Empirical Rule

If σ is unknown then,

- $x \pm 1s$ contains μ about 68% of the time
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and if the distribution of X is non-normal but not too funky,

- $x \pm 1s$ contains μ about about 68% of the time
- $x \pm 2s$ contains μ about about 95% of the time
- $x \pm 3s$ contains μ about about 99.7% of the time

Why is RMSE useful?

In our case, the r.v. is $Y \mid X_1, \ldots, X_p$ which is centered at $\mu = \mathbb{E}[Y \mid x_1, \ldots, x_p]$ and generally speaking, non-normal. $\hat{y} \approx \mu$ and $s_e \approx \mathbb{S}\mathrm{E}[Y \mid X]$. Thus,

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- $\hat{y} \pm 1s_e$ contains 68% of the response values for a specific $x_1, \ldots, x_p$
- $\hat{y} \pm 2s_e$ contains 95% of the response values for a specific $x_1, \ldots, x_p$
- $\hat{y} \pm 3s_e$ contains 99.7% of the response values for a specific $x_1, \ldots, x_p$

Thus RMSE gives you an approximate means of assessing how variable the real response y could be give your predicted response $\hat{y}$.

All Three are Equivalent

Minimizing SSE, maximizing R^2 and minimizing s_e all give equivalent fits.

$$
\begin{aligned}
& SSE \\
R^2 \quad &:= \quad \frac{SSE_0 - SSE}{SSE_0} \\
s_e \quad &= \quad \sqrt{s_e^2} = \sqrt{\frac{1}{n-1} SSE} = \sqrt{\frac{1}{n-1} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2}
\end{aligned}
$$

R^2 vs. F test

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

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

must be assumed to be something like

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

(we will explore next time)

In this case R^2 will be related to F, the omnibus test statistic for whether the model has any signal whatsoever.

$$F = \frac{\frac{SSE_0 - SSE}{p-1}}{\frac{SSE}{n-p}} = \frac{SSE_0 - SSE}{SSE} \frac{n-p}{p-1}$$