Data 401
Machine Learning and Linear Regression

Dennis Sun

September 28, 2016

1. Machine Learning
2. Linear Regression
3. Categorical Predictors

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- **Pros:** Models were super interpretable!
- **Cons:** Performance plateaued quickly. There are too many rules, and we don't know what they are!

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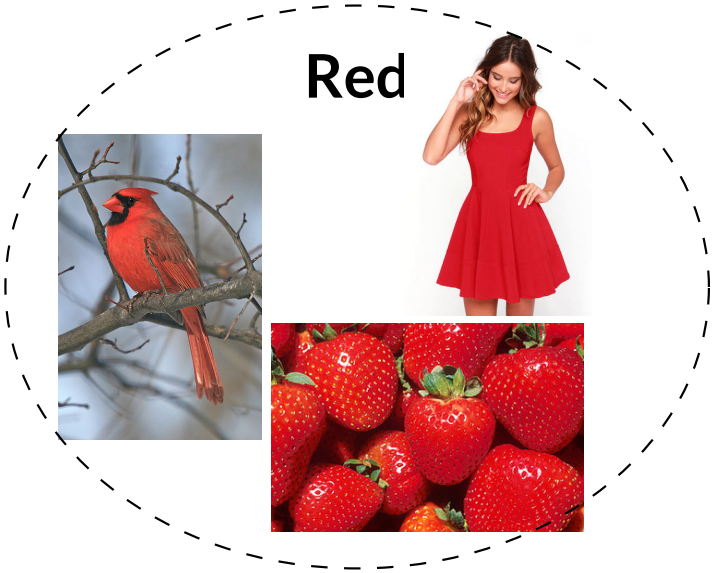

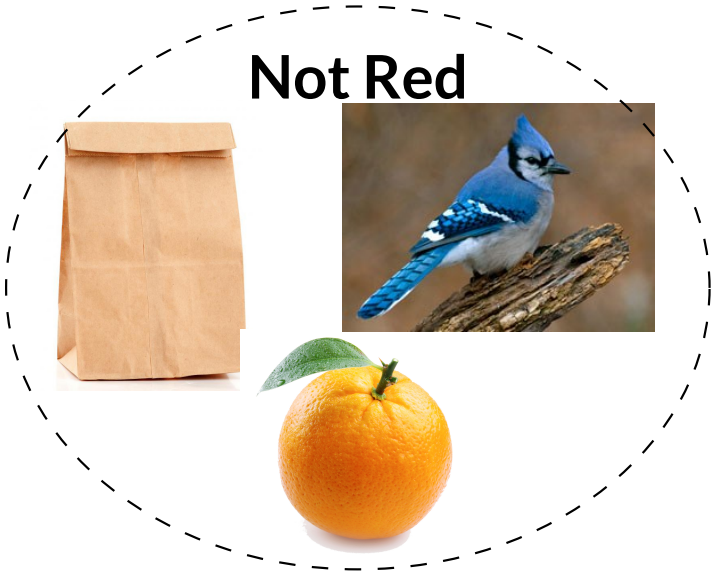

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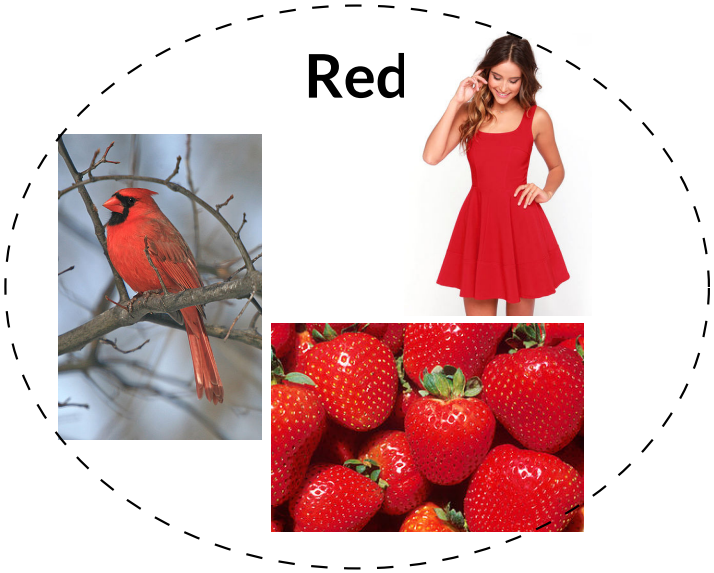

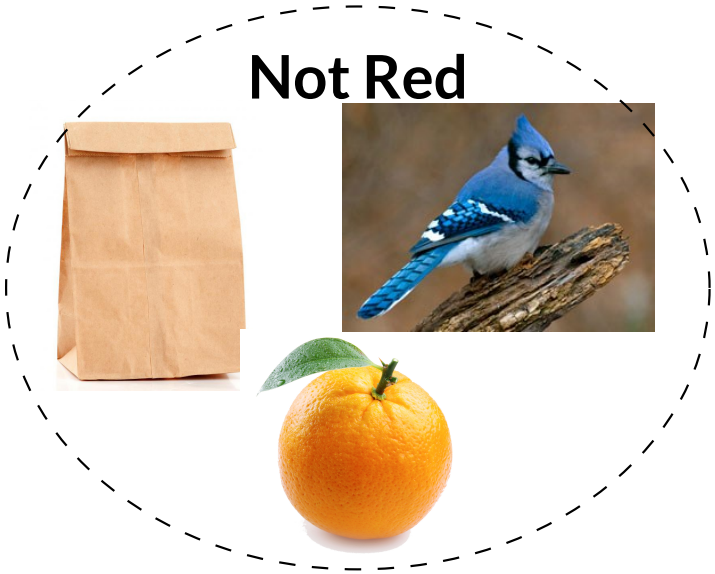

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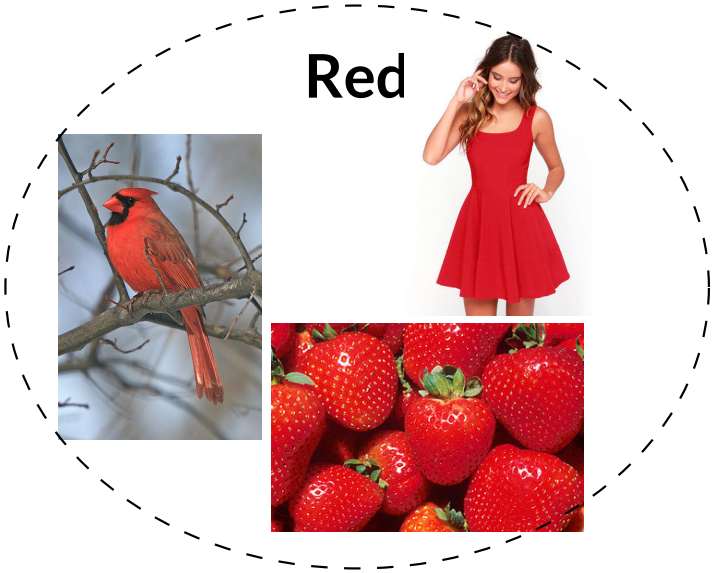

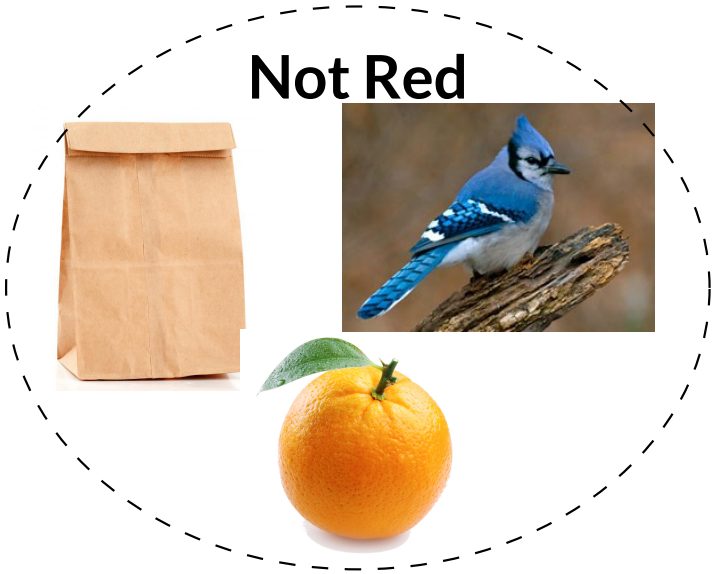

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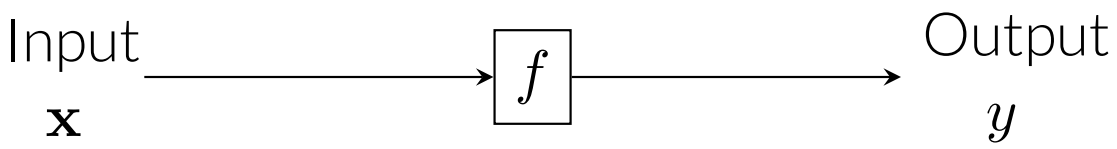

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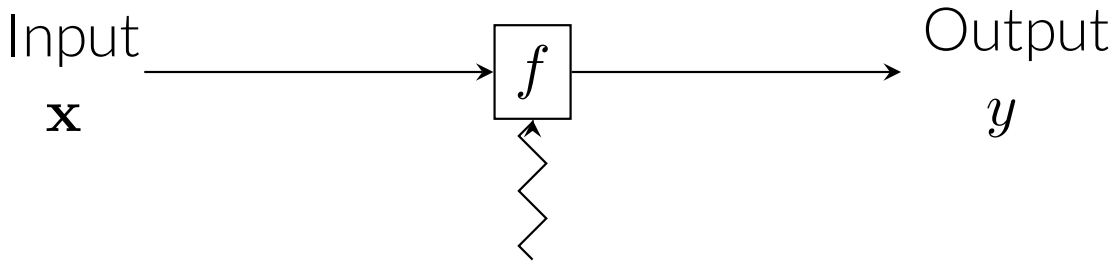

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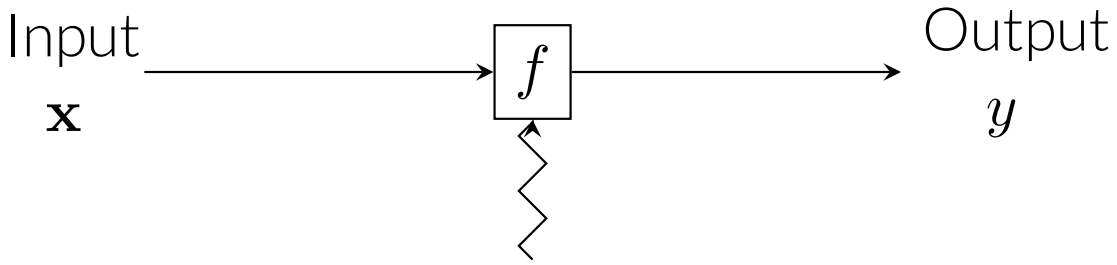

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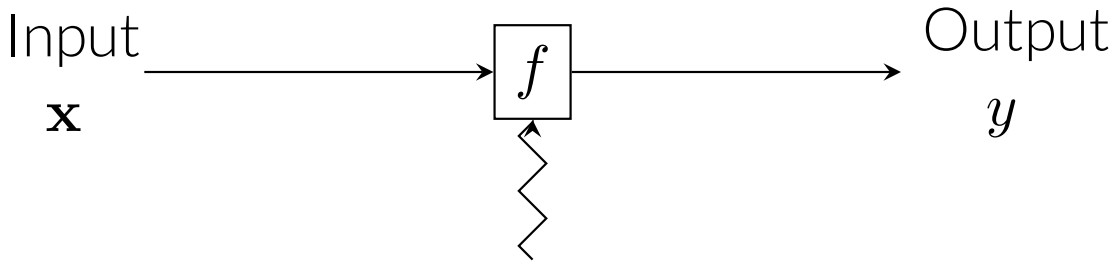

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Linear regression, k-nearest neighbors, random forests, SVMs, and deep learning are all just different ways of estimating f.

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(Multiple) Linear Regression

In linear regression, we assume that f is linear:

$$y = f(\mathbf{x}) + \epsilon = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + ... + \beta_p x_p + \epsilon,$$

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Choose $\beta_0, \beta_1, ..., \beta_p$ to make f fit the training data as best as possible:

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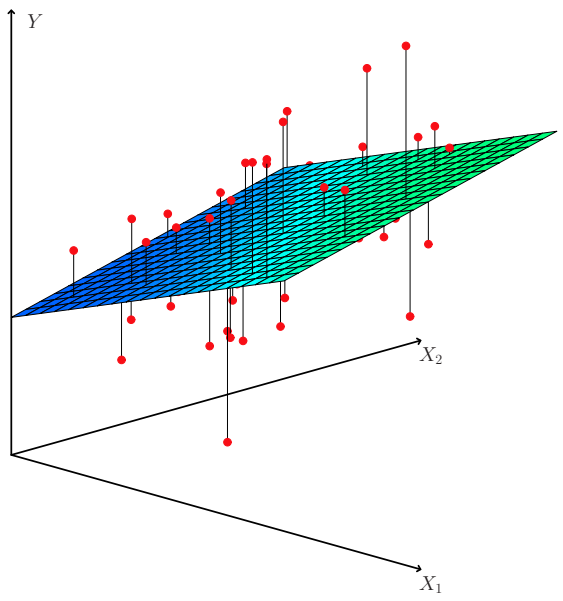

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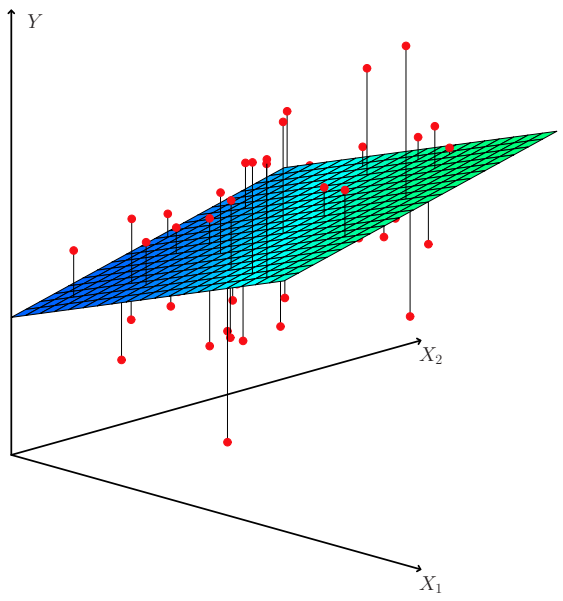

When $p > 2$, we can't visualize it, but we can still do the math.

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We can stack our training data into matrices and vectors:

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} \qquad X = \begin{pmatrix} 1 & x_{11} & \dots & x_{1p} \\ 1 & x_{21} & \dots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \dots & x_{np} \end{pmatrix} \qquad \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}.$$

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Notice that $X\boldsymbol{\beta}$ is the vector of **predictions** or **fitted values** for the observations in our training set:

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and $\mathbf{y} - X\boldsymbol{\beta}$ is the vector of **residuals**:

$$\mathbf{y} - X\boldsymbol{\beta} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} - \begin{pmatrix} \beta_0 + \beta_1 x_{11} + \ldots + \beta_p x_{1p} \\ \vdots \\ \beta_0 + \beta_1 x_{n1} + \ldots + \beta_p x_{np} \end{pmatrix}$$

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No! Remember, one of the challenges of data science is **big data**. It'll be hard to *load* a 10 GB file into R, much less run `lm` on it.

As a data scientist, you will need to understand the nuts and bolts because you may need to implement these methods from scratch.

Solving for $\boldsymbol{\beta}$

How do we find $\boldsymbol{\beta}$ that minimizes

$$L(\boldsymbol{\beta}) = \sum_{i=1}^{n} (y_i - (\beta_0 x_{i0} + \beta_1 x_{i1} + ... + \beta_p x_{ip}))^2,$$

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This is a linear system of $p + 1$ equations with $p + 1$ unknowns.

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Now if we solve for $\boldsymbol{\beta}$, we obtain

$$\hat{\boldsymbol{\beta}} = (X^T X)^{-1} X^T \mathbf{y}$$

Multiple Regression in Code

In-Class Exercise

Open the notebook `Implementing Linear Regression.ipynb` *and implement the* `lm` *function, assuming that all predictors are quantitative. Check that your function returns the same coefficients as scikit-learn.*

Hints:

- `np.dot` *can be used to multiply matrices.*
- `X.T` *returns the transpose of the matrix* `X`.
- `np.linalg.inv` *can be used to invert matrices.*

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What do you think the estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ will be?

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So the predicted price of a car with three cylinders would be $\beta_0 + \beta_1$, while for one with four cylinders it would be $\beta_0 + \beta_1 + \beta_2$.

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An ordinal variable is like a categorical variable, except that the levels have an ordering.

For example, the number of cylinders is (arguably) an ordinal variable, with levels two, three, four, five, six, eight, twelve.

For ordinal variables, we also expand the variable into $k-1$ binary variables. But we often code it slightly differently:

$$\begin{pmatrix} \text{two} \\ \text{three} \\ \text{four} \\ \text{five} \\ \vdots \end{pmatrix} \longrightarrow X = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 1 & 0 & \cdots & 0 \\ 1 & 1 & 1 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \end{pmatrix}.$$

So the predicted price of a car with three cylinders would be $\beta_0 + \beta_1$, while for one with four cylinders it would be $\beta_0 + \beta_1 + \beta_2$.

Each coefficient β_j represents the change in price from level $j-1$ to level j (rather than from a common baseline to level j).

Multiple Regression with Categorical Predictors

In-Class Exercise

Now, modify your `lm` *function so that it automatically handles categorical variables.*

Hints:

- *Read the documentation on Pandas' "categorical" data type. It is analogous to* `R`*'s factors.*