Linear Regression

Fittin' Lines to Data

Dan Wiesenthal

Objectives - Morning

- Linear regression overview
    - Fitting a line
    - Linear relationshiops, Exact vs Inexact
    - Where do we put the line? What is our error metric?
- Expressing our model
    - $y = Mx + b$
    - $Y = \beta_0 + \beta_1 X + \epsilon$
    - Matrix representation
- How good is our model?
    - RSS
    - RSE aka $RMSE$
    - R^2
        - Fraction of variance explained, or, $1 - FUV$
- Compare models (against null)
    - Are all my coefficients not zero?
    - Are some new coefficients not zero?
- Interpreting model output
    - Interpret coefficients from statsmodels
- Assumptions of Linear Regression
    - Linearity
    - Constant Variance (Homoscedasticity)
    - Independence of Errors
    - Normality of Errors
    - Lack of Multicollinearity
- Outliers
    - Types of outliers
    - Detecting outliers
        - Leverage (change in prediction over change in actual)
        - Studentized Residuals
    - Residual plots
- Multicollinearity
    - Perfect
    - Partial
- QQ Plots
    - (Video, ragequit)

Linear Regression Overview

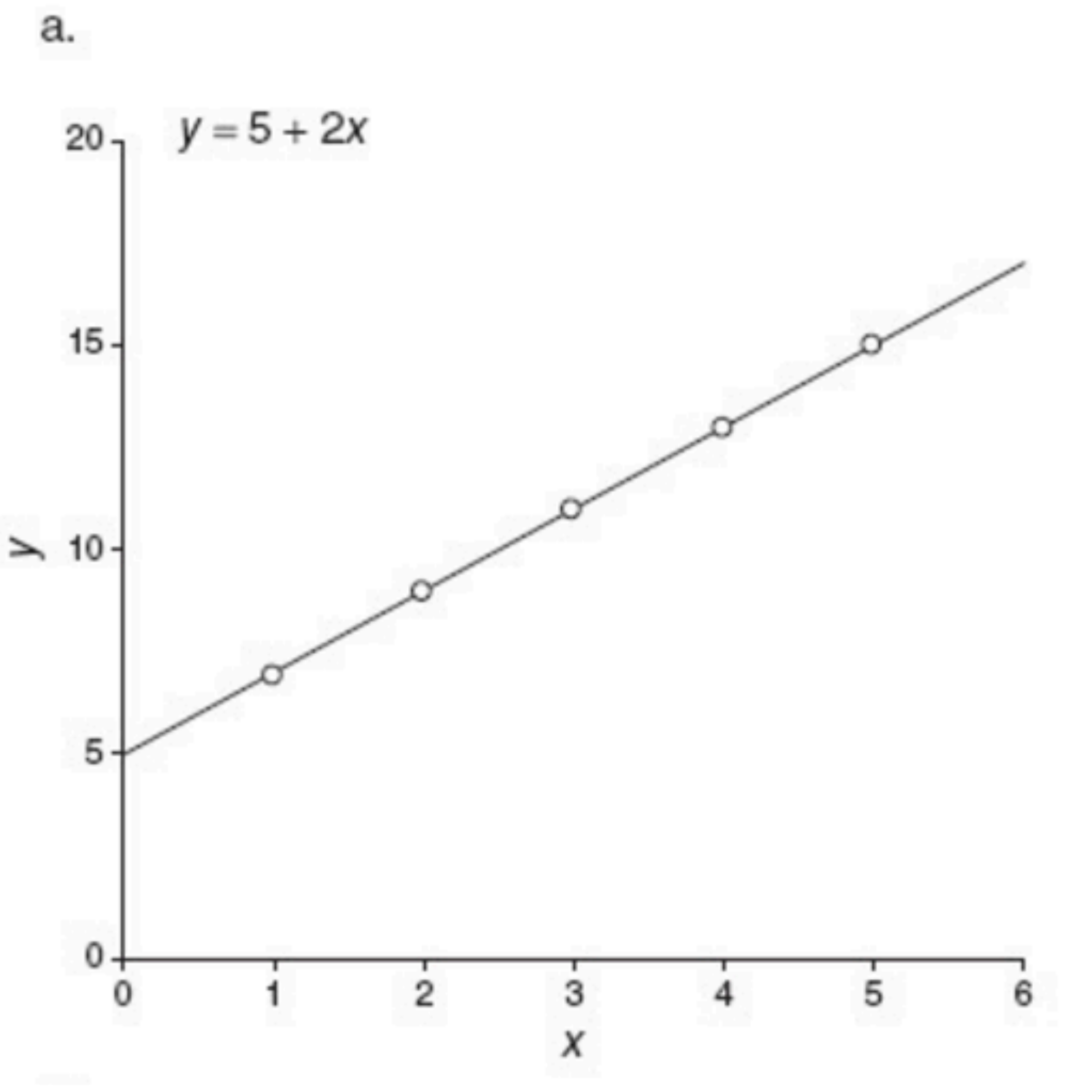
Fitting a line

Linear relationships, Exact vs Inexact

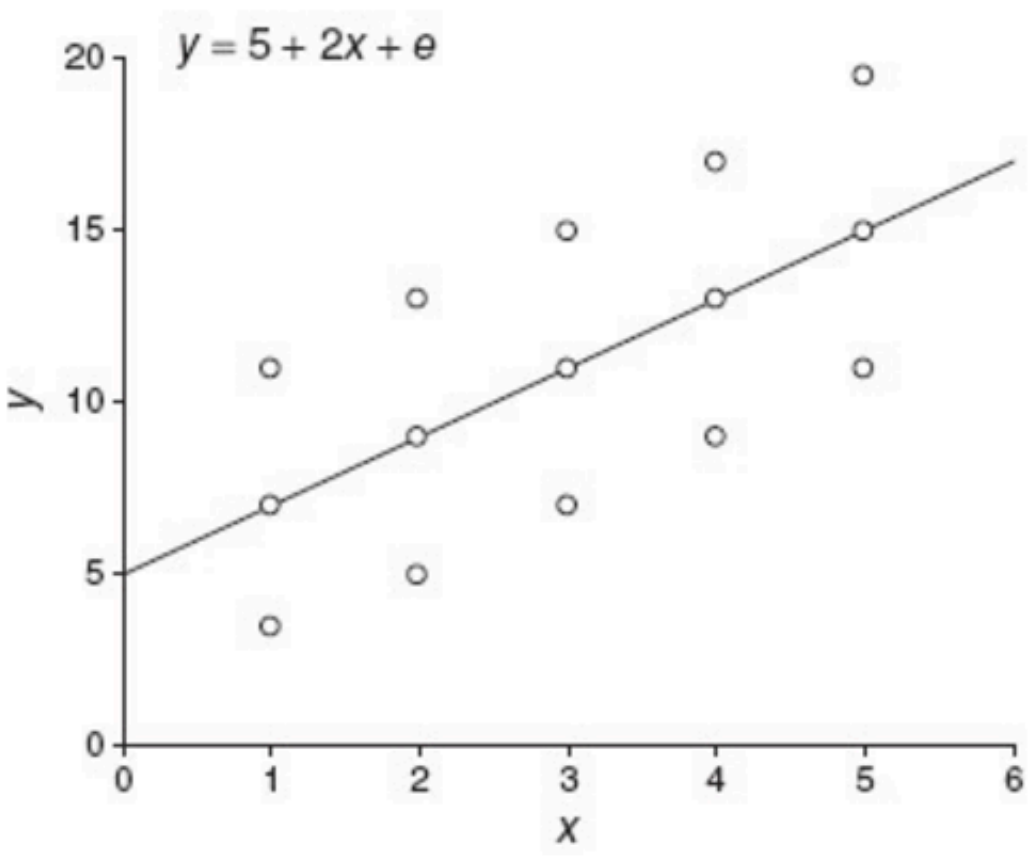
Where do we put the line? What is our error metric?

Linear Regression Overview

Linear relationships, Exact vs Inexact

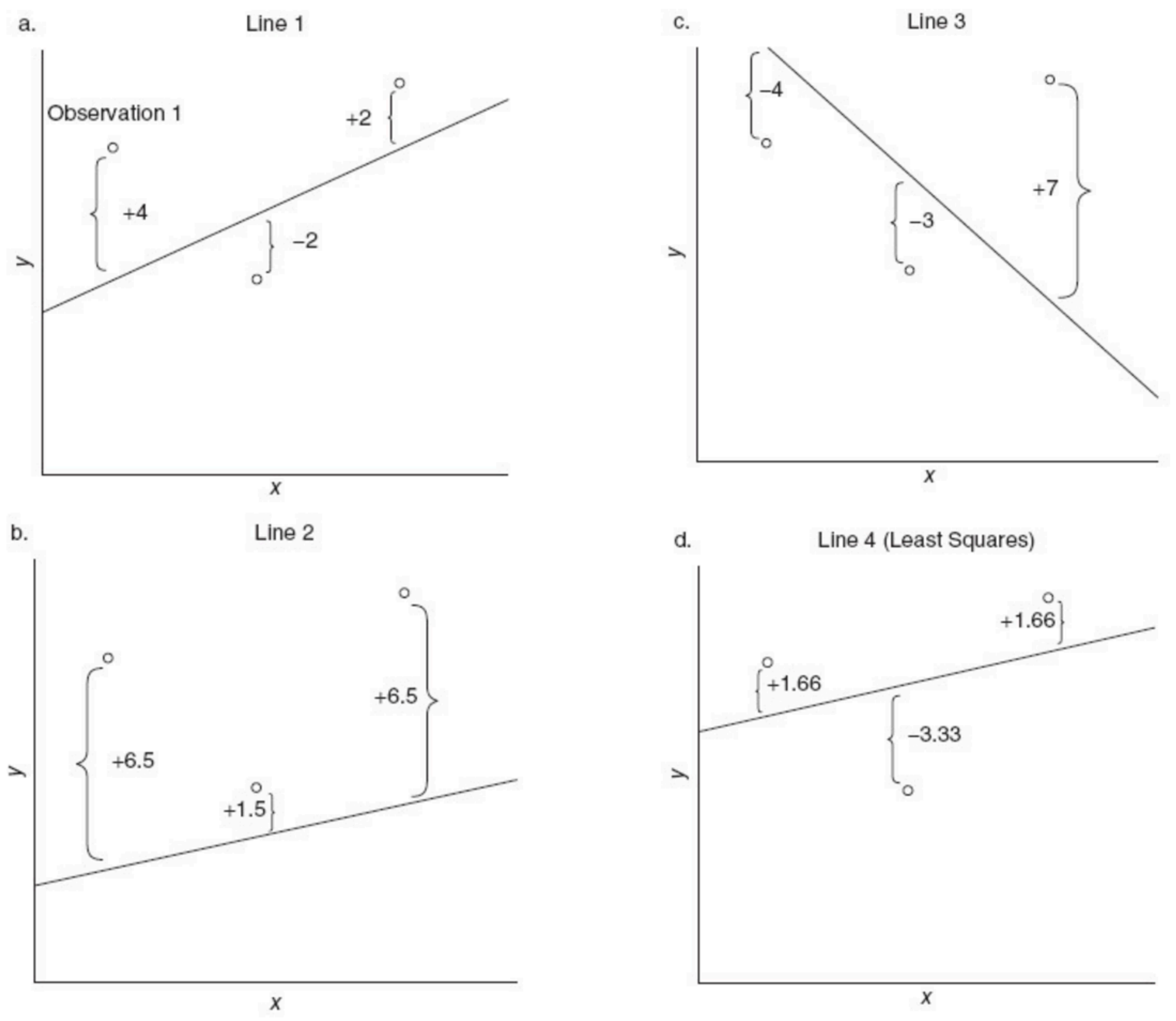


b.



Linear Regression Overview

Where do we put the line? What is our error metric?



- Notes on image:
    - There are many lines possible
    - We don't want to minimize the absolute error, since that could tell us that we have 0 error when we clearly don't have 0 error (upper right)
    - We'll minimize squared error

Expressing our model

Simple (Bivariate) Linear Regression

- The World
  - what you're presuming the world looks like:
$$Y = \beta_0 + \beta_1 X + \epsilon$$
- β_0 and β_1 are unknown constants that represent the intercept and slope
- ϵ, the error term, is i.i.d $N(0, \sigma^2)$

- The Model
  - what you've created from data to estimate the world:
$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$$
- $\hat{\beta}_0$ and $\hat{\beta}_1$ are model coefficient estimates
- $\hat{y}$ indicates the prediction of Y based on $X = x$

Expressing our model

Multiple Linear Regression

- Model in matrix form

$$\begin{aligned}
\mathbf{Y}_{n\times 1} &= \mathbf{X}_{n\times p}\beta_{p\times 1} + \epsilon_{n\times 1} \\
\epsilon &\sim N(\mathbf{0}, \sigma^2\mathbf{I}_{n\times n}) \\
&\boxed{\mathbf{Y} \sim N(\mathbf{X}\beta, \sigma^2\mathbf{I})}
\end{aligned}$$

- Design Matrix X

Target:

$$\mathbf{X} = \begin{bmatrix} 1 & X_{1,1} & X_{1,2} & \cdots & X_{1,p-1} \\ 1 & X_{2,1} & X_{2,2} & \cdots & X_{2,p-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & X_{n,1} & X_{n,2} & \cdots & X_{n,p-1} \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

- Coefficient Matrix β

$$\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{p-1} \end{bmatrix} \qquad \hat{\boldsymbol{\beta}} = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y}$$

How good is our model?

RSS

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

- How far off were we? In, um, raw units (squared).

RSE (aka RMSE)

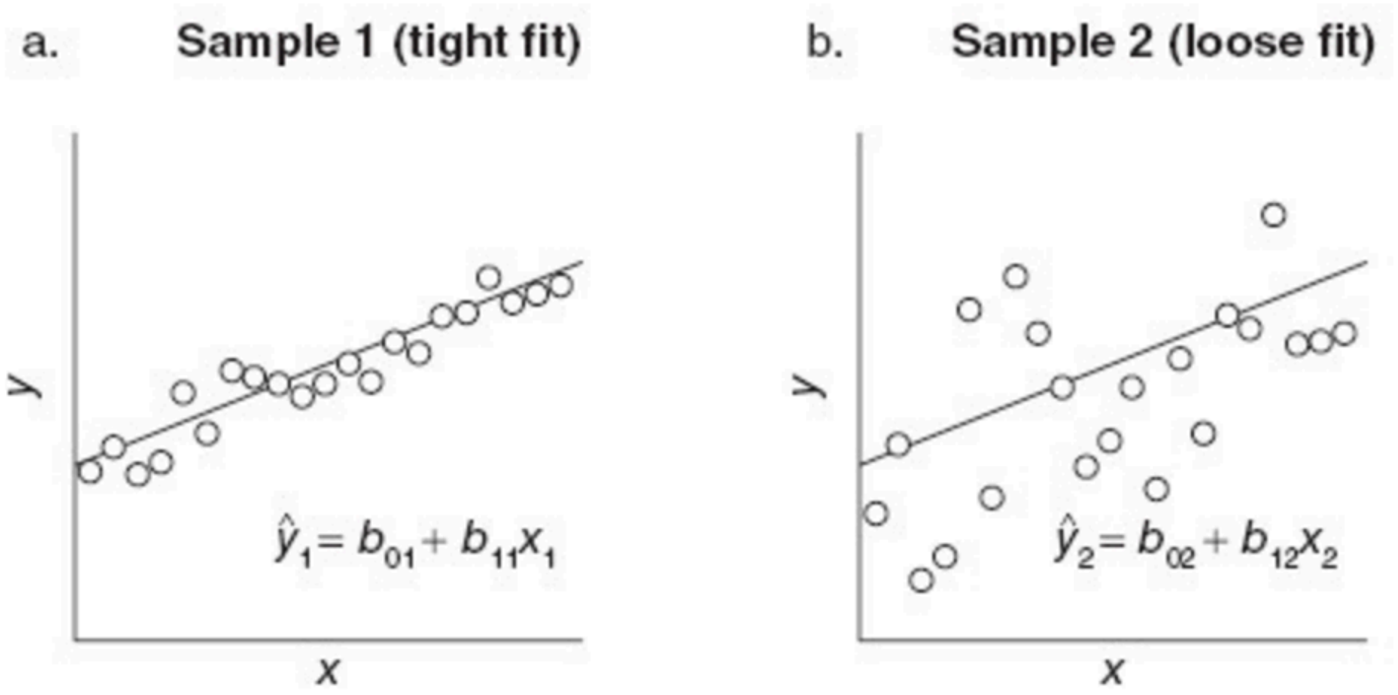
$RSE = RMSE = \sqrt{\frac{RSS}{n-p-1}} = \sqrt{\frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{n-p-1}}$

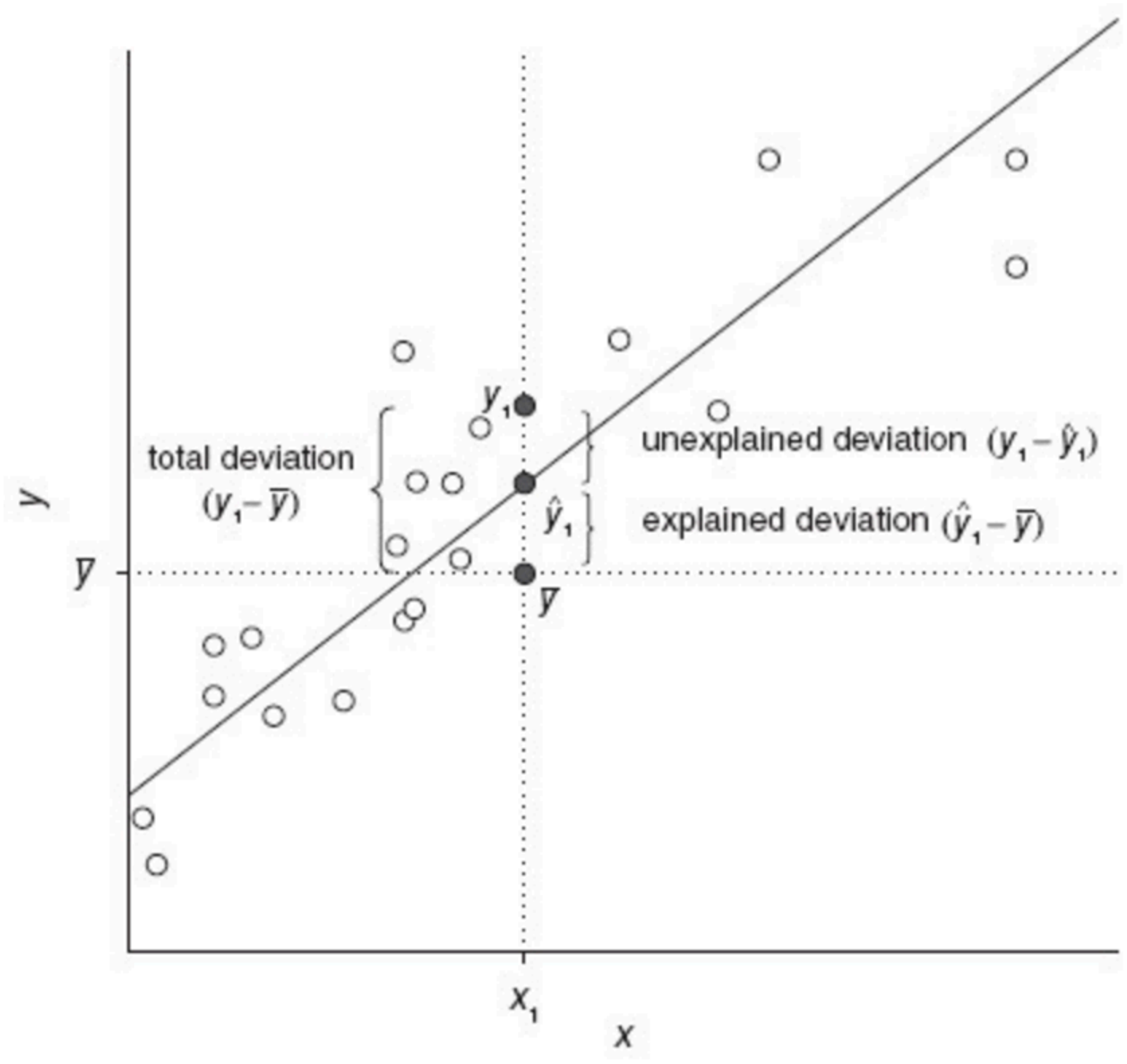
- How far off were we? For, y'know, a typical point. On average. (Controlling for degrees of freedom lost.)
- Similarly, we have the standard error (biased or not depending on dof), $\frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{n-p-1}$

R^2

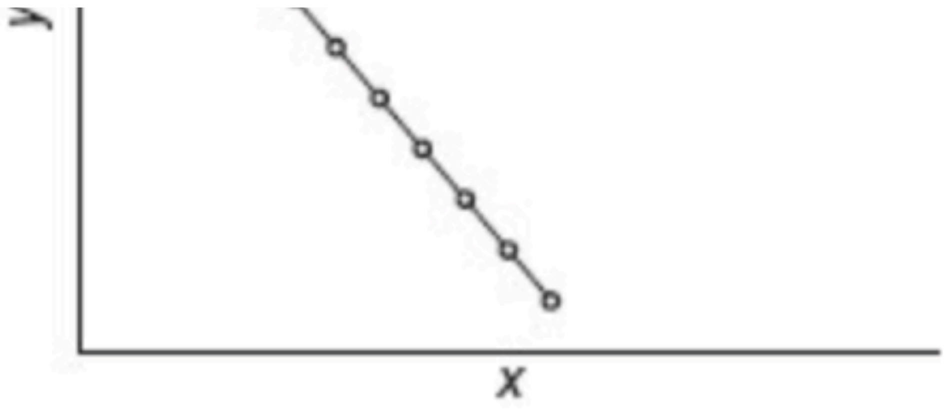
$$1 - FUV = 1 - \frac{Deviation_u}{Deviation_t}$$

- Total deviation, $Deviation_t : (y_1 - \bar{y})$
- Explained deviation, $Deviation_e : (\hat{y_1} - \bar{y})$
- Unexplained deviation, $Deviation_u : (y_1 - \hat{y_1})$

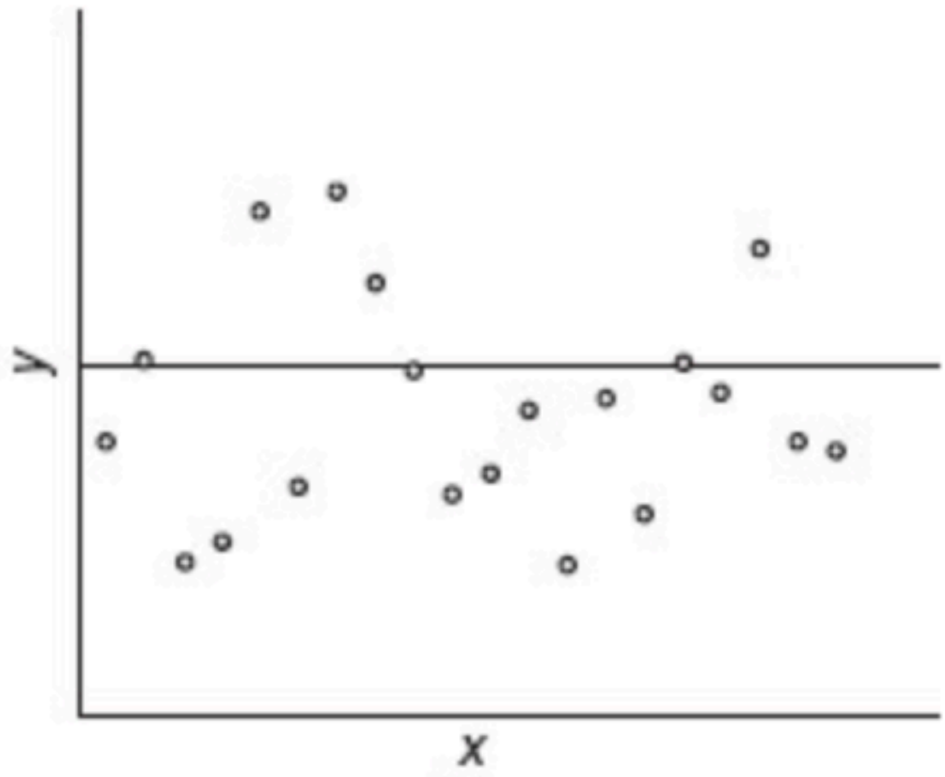



y_1
total deviation $(y_1 - \bar{y})$
unexplained deviation $(y_1 - \hat{y}_1)$
$\hat{y}_1$
explained deviation $(\hat{y}_1 - \bar{y})$
$\bar{y}$
y
x_1
x

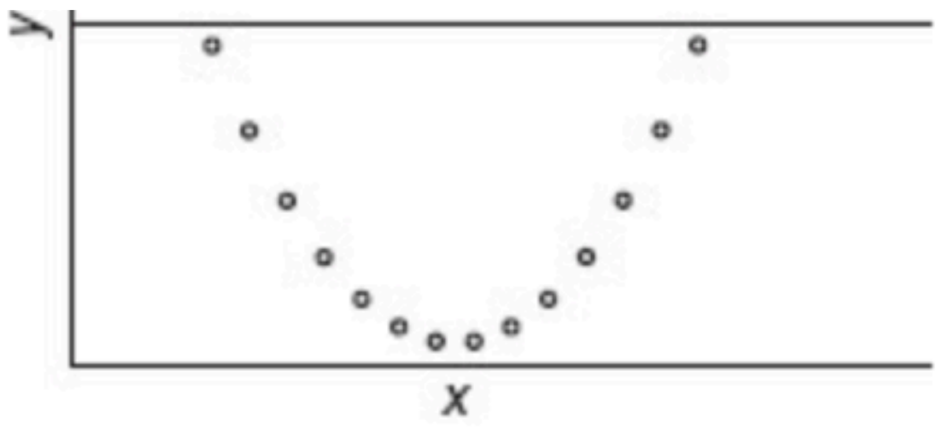
a.
$R^2 = 1$



b. $R^2 = 0$



c. $R^2 = 0$



- Notes on images:
  - We can have two lines with the same slope and intercept, each of which is the best fit line, and they can still be differently "good" fits if the data is spread out
  - If we didn't have a model, we would just predict the mean, so that's what we compare ourselves against to see how good our model is
  - We could have data that clearly has a signal but a low R^2 if we aren't properly modeling it; low R^2 isn't necessarily grounds for concluding there's no signal

Comparing Models

Did I add a useful feature?

1) Set up hypotheses, comparison

$H_0 : \beta_{height} = \beta_{color} = 0$

H_A : at least one of β_{height} or β_{color} is nonzero

Reduced Model:

$$Y = \beta_0 + \beta_{weight} + \beta_{modelyear} + \beta_{cartype}$$

Full Model:

$$Y = \beta_0 + \beta_{weight} + \beta_{modelyear} + \beta_{cartype} + \beta_{height} + \beta_{color}$$

(X's omitted for clarity)

2) Compute F-statistic

$$F = \frac{\frac{(RSS_{reduced} - RSS_{full})}{(p_{full} - p_{reduced})}}{\frac{RSS_{full}}{(n - p_{full} - 1)}}$$

3) Compute p-value

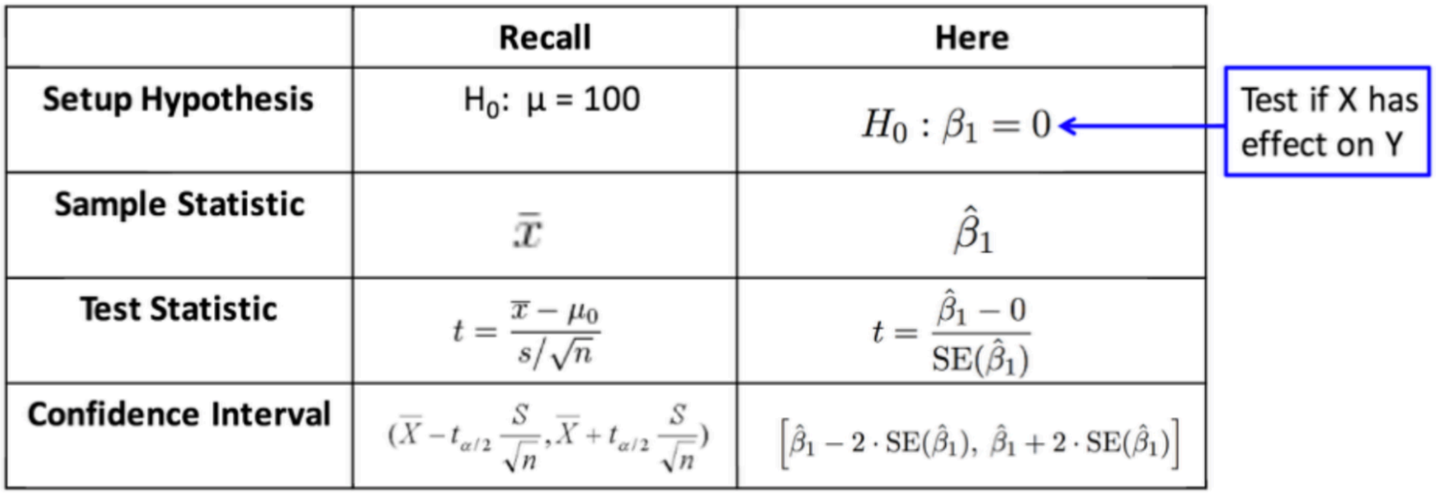
p_val = 1 - scipy.stats.f.cdf(calculated_F, p_full - p_reduced, n - p_full - 1)

Are any of my features useful?

1) Set up hypotheses $H_0 : \beta_1 = \beta_2 = \beta_3 = \ldots = \beta_p = 0$

H_A : at least one β_j is nonzero

2) $F = \frac{\frac{TSS-RSS}{p}}{\frac{RSS}{n-p-1}}$ ~ $F_{p,n-p-1}$



	Recall	Here
Setup Hypothesis	H_0: $\mu = 100$	$H_0 : \beta_1 = 0$
Sample Statistic	$\bar{x}$	$\hat{\beta}_1$
Test Statistic	$t = \frac{\bar{x} - \mu_0}{s/\sqrt{n}}$	$t = \frac{\hat{\beta}_1 - 0}{\mathrm{SE}(\hat{\beta}_1)}$
Confidence Interval	$(\bar{X} - t_{\alpha/2}\frac{S}{\sqrt{n}}, \bar{X} + t_{\alpha/2}\frac{S}{\sqrt{n}})$	$\left[\hat{\beta}_1 - 2 \cdot \mathrm{SE}(\hat{\beta}_1),\ \hat{\beta}_1 + 2 \cdot \mathrm{SE}(\hat{\beta}_1)\right]$

Test if X has effect on Y

Interpreting Model Output

Interpreting coefficients from statsmodels

In [1]:
```
import numpy as np
import random
import pandas as pd
import statsmodels.api as sm
import statsmodels.formula.api as smf
from statsmodels.graphics.regressionplots import influence_plot
import matplotlib.pyplot as plt
%matplotlib inline
```

```
/Users/dan/.virtualenvs/linear_regression_lecture/lib/python2.7/site
-packages/statsmodels/compat/pandas.py:56: FutureWarning: The pandas
.core.datetools module is deprecated and will be removed in a future
version. Please use the pandas.tseries module instead.
  from pandas.core import datetools
```

In [2]:
```
df_gnp = pd.read_csv('http://vincentarelbundock.github.io/Rdatasets/cs
v/datasets/longley.csv', index_col=0)
df_gnp.head()
```

Out[2]:

	GNP.deflator	GNP	Unemployed	Armed.Forces	Population	Year	Employed
1947	83.0	234.289	235.6	159.0	107.608	1947	60.323
1948	88.5	259.426	232.5	145.6	108.632	1948	61.122
1949	88.2	258.054	368.2	161.6	109.773	1949	60.171
1950	89.5	284.599	335.1	165.0	110.929	1950	61.187
1951	96.2	328.975	209.9	309.9	112.075	1951	63.221

In [3]:
```
X = df_gnp.GNP  # Set up our design matrix, X
X = sm.add_constant(X)  # We need to manually add a constant, aka inte
rcept, when working with statsmodels
y = df_gnp.Employed # Set up our target, y
```

In [4]:
```
est = sm.OLS(y, X)
est = est.fit()
est.summary()  # whoa, too much output for the moment

# a utility function to only show the coefficient section of summary
from IPython.core.display import HTML
def short_summary(est):
    return HTML(est.summary().tables[1].as_html())

short_summary(est)
```

```
/Users/dan/.virtualenvs/linear_regression_lecture/lib/python2.7/site
-packages/scipy/stats/stats.py:1334: UserWarning: kurtosistest only
valid for n>=20 ... continuing anyway, n=16
  "anyway, n=%i" % int(n))
```

Out[4]:

	coef	std err	t	P>|t|	[0.025	0.975]
const	51.8436	0.681	76.087	0.000	50.382	53.305
GNP	0.0348	0.002	20.374	0.000	0.031	0.038

Talking points on short summary:

- sanity check
- constant, GNP coefficients
- do they point the right direction
- rough magnitude check (if you have a sense)
- are the p values significant
- oh hey look we have confidence intervals, that's nice

In [5]:
```
est.summary()  # now let's look at the full summary
```

Out[5]:

OLS Regression Results

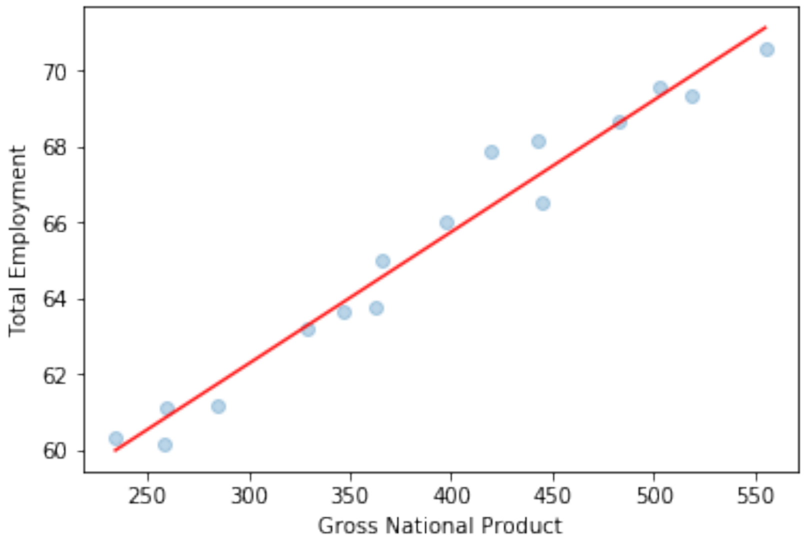
Dep. Variable:	Employed	**R-squared:**	0.967
Model:	OLS	**Adj. R-squared:**	0.965
Method:	Least Squares	**F-statistic:**	415.1
Date:	Mon, 15 May 2017	**Prob (F-statistic):**	8.36e-12
Time:	23:10:49	**Log-Likelihood:**	-14.904
No. Observations:	16	**AIC:**	33.81
Df Residuals:	14	**BIC:**	35.35
Df Model:	1		
Covariance Type:	nonrobust		

	coef	**std err**	**t**	**P>|t|**	**[0.025**	**0.975]**
const	51.8436	0.681	76.087	0.000	50.382	53.305
GNP	0.0348	0.002	20.374	0.000	0.031	0.038

Omnibus:	1.925	**Durbin-Watson:**	1.619
Prob(Omnibus):	0.382	**Jarque-Bera (JB):**	1.215
Skew:	0.664	**Prob(JB):**	0.545
Kurtosis:	2.759	**Cond. No.**	1.66e+03

Let's plot it

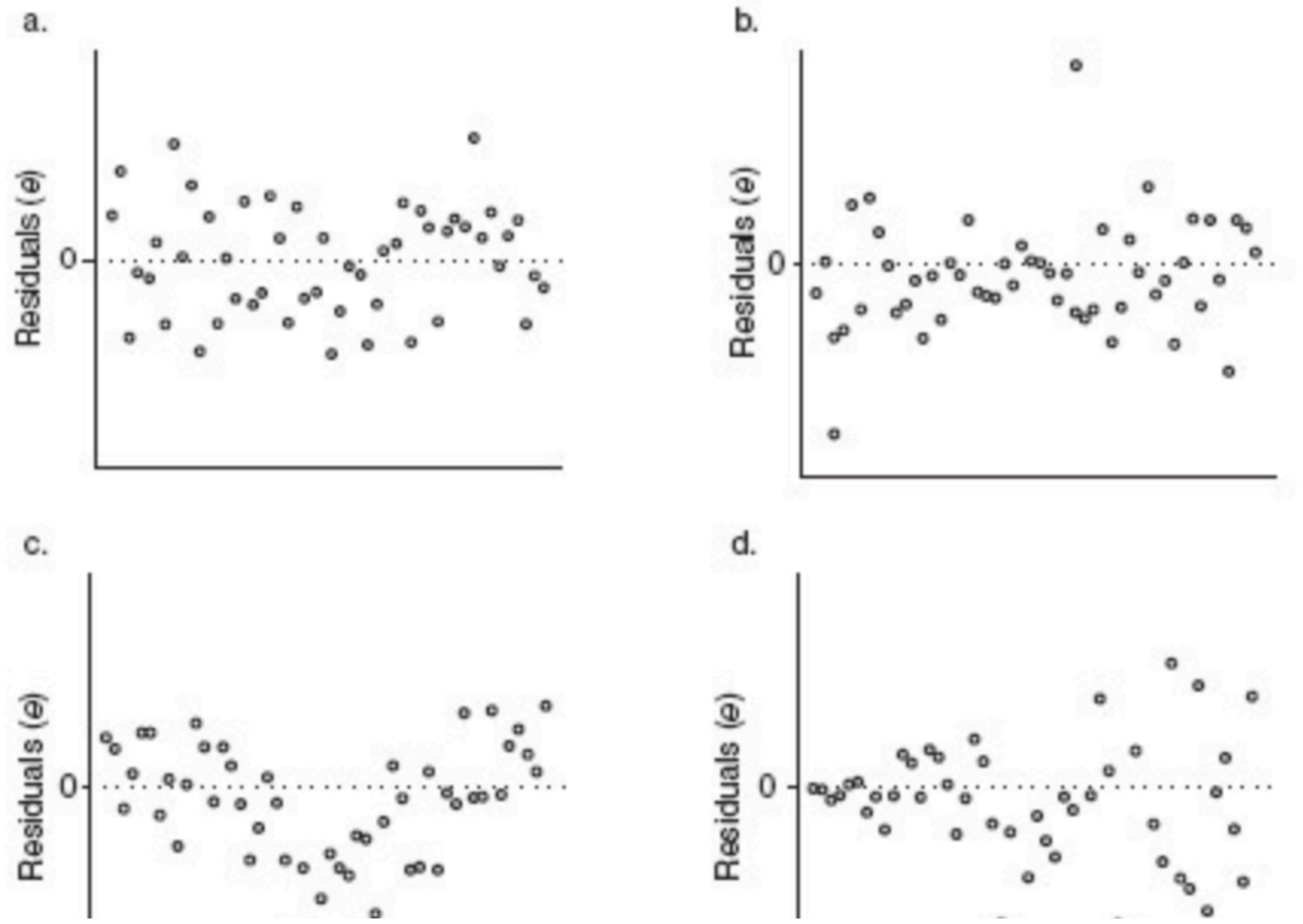
```
In [6]: # We pick 100 hundred points equally spaced from the min to the max
        X_prime = np.linspace(X.GNP.min(), X.GNP.max(), 100)[:, np.newaxis]
        X_prime = sm.add_constant(X_prime)  # add constant as we did before

        # Now we calculate the predicted values
        y_hat = est.predict(X_prime)

        plt.scatter(X.GNP, y, alpha=0.3)  # Plot the raw data
        plt.xlabel("Gross National Product")
        plt.ylabel("Total Employment")
        plt.plot(X_prime[:, 1], y_hat, 'r', alpha=0.9)  # Add the regression l
        ine, colored in red

Out[6]: [<matplotlib.lines.Line2D at 0x1078e6f50>]
```

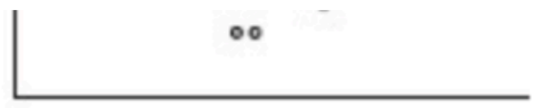


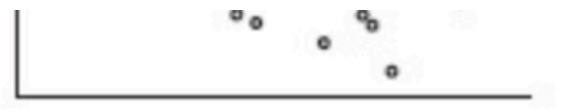
Assumptions of Linear Regression

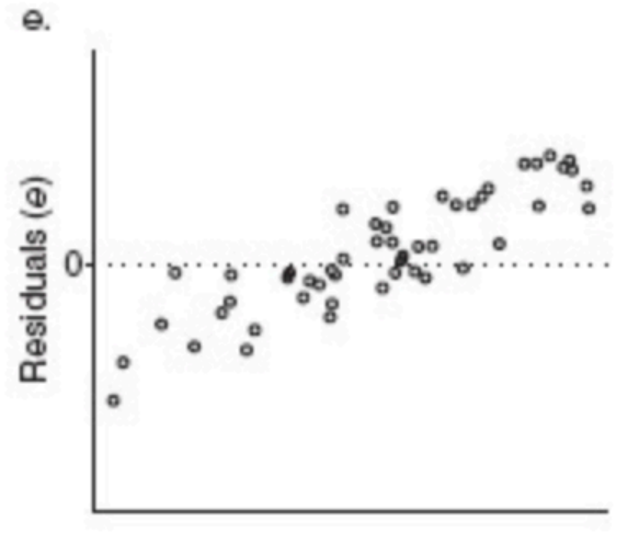
- Assumptions of Linear Regression
  - Linearity
    - We assume it's possible
  - Constant Variance (Homoscedasticity)
    - Our variance shouldn't change as y or X gets bigger
  - Independence of Errors
    - We should gain no information from knowing the error of a different data point
  - Normality of Errors
    - Errors should be normally distributed
  - Lack of Multicollinearity
    - We shouldn't be measuring the same thing in multiple ways

We can't always meet these assumptions, and often have to find ways to combat that reality.









Notes on image:

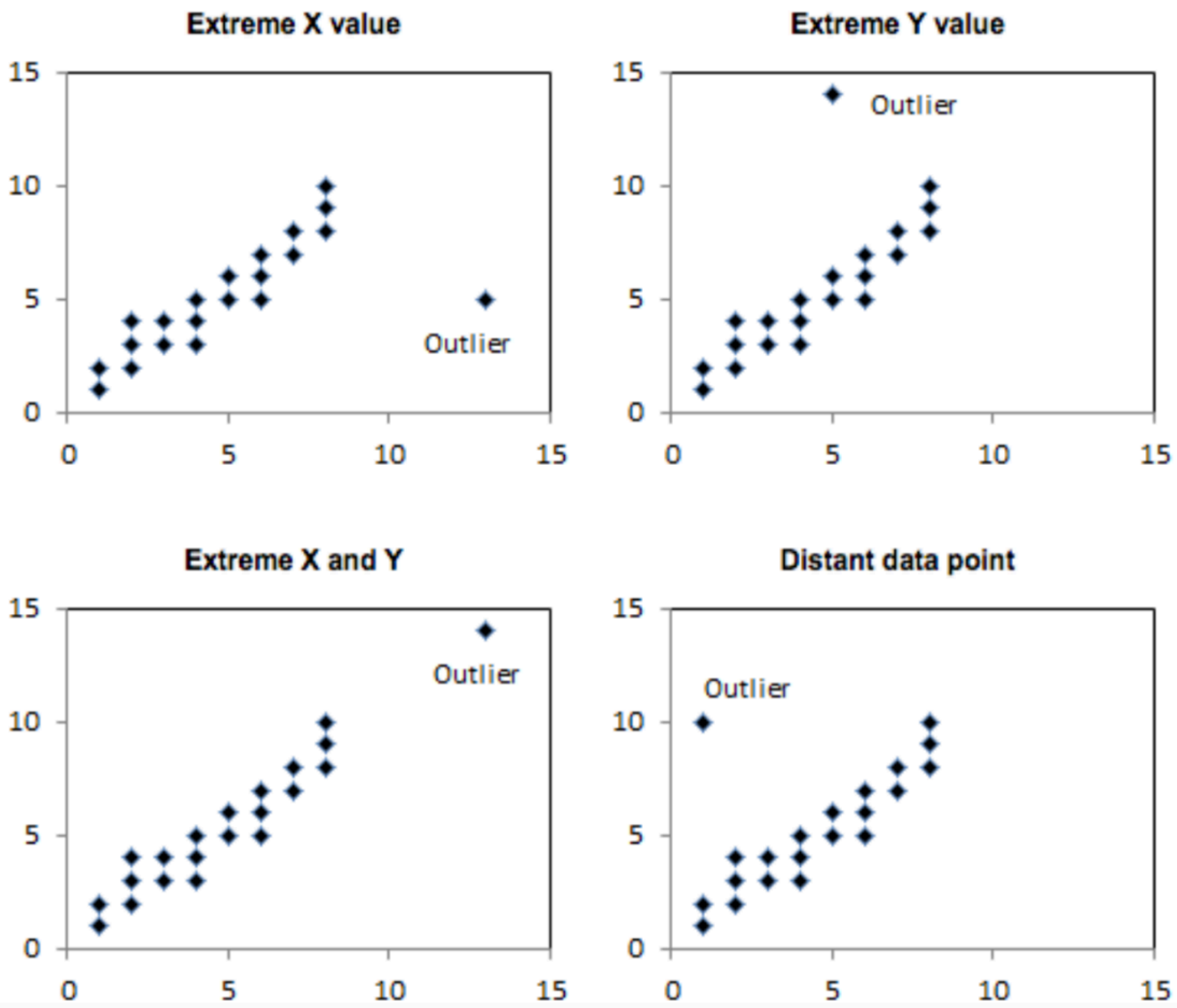
- a looks lovely
- b has some extreme outliers
- c is curvilinear; a change in x does not lead to the same response in y across all values of x
- d violates homoscedasticity; the error variance is not constant but rather depends on x
- e indicates a linear relationship between the residuals and a variable not in the model; we probably want to try to find/measure that variable and add it into our model

Outliers

- Outliers
  - Types of outliers
  - Detecting outliers
    - Leverage (change in prediction over change in actual)
    - Studentized Residuals
  - Residual plots

Outliers

Types of outliers



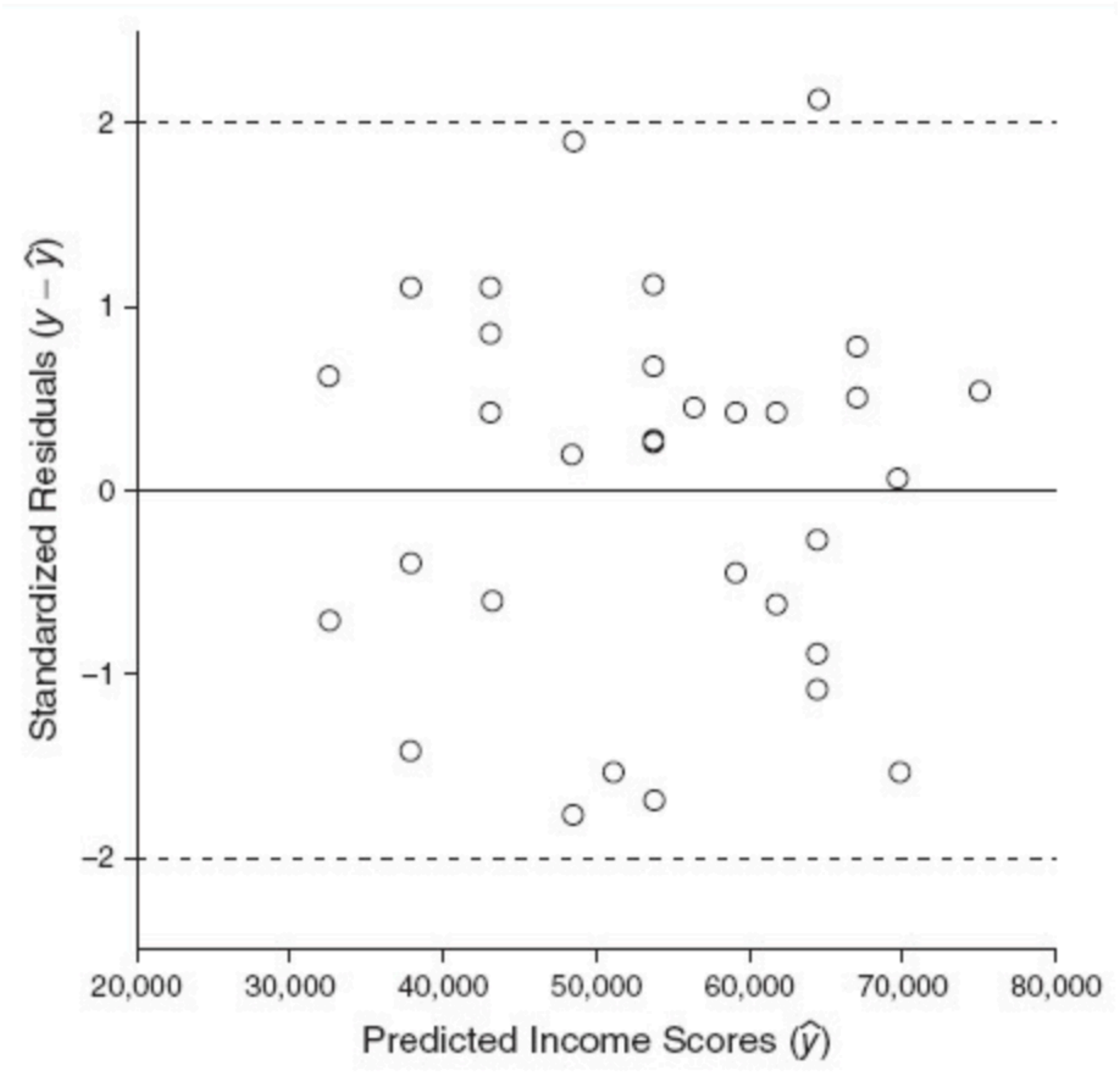
Outliers

Detecting outliers

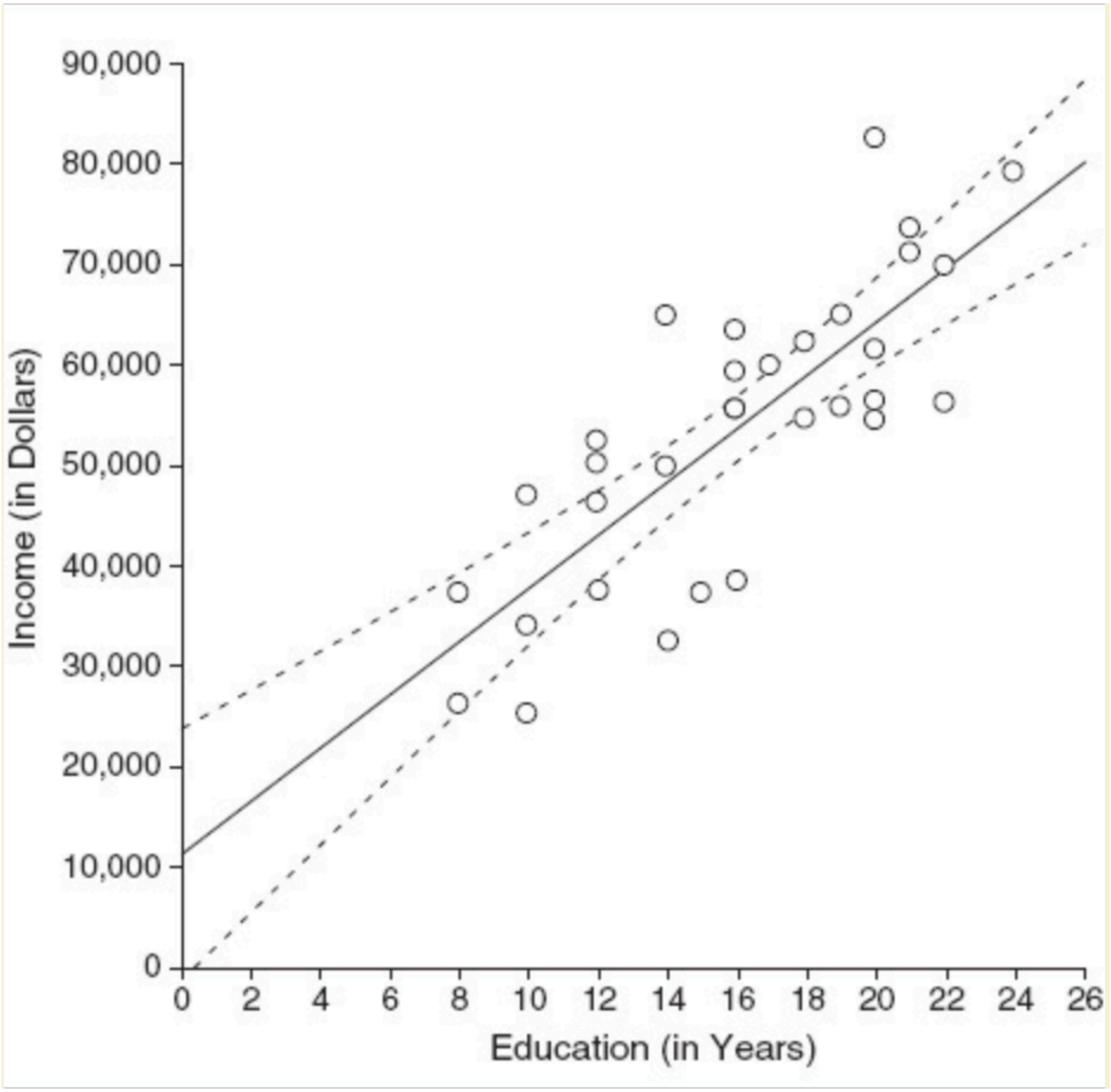
Visually

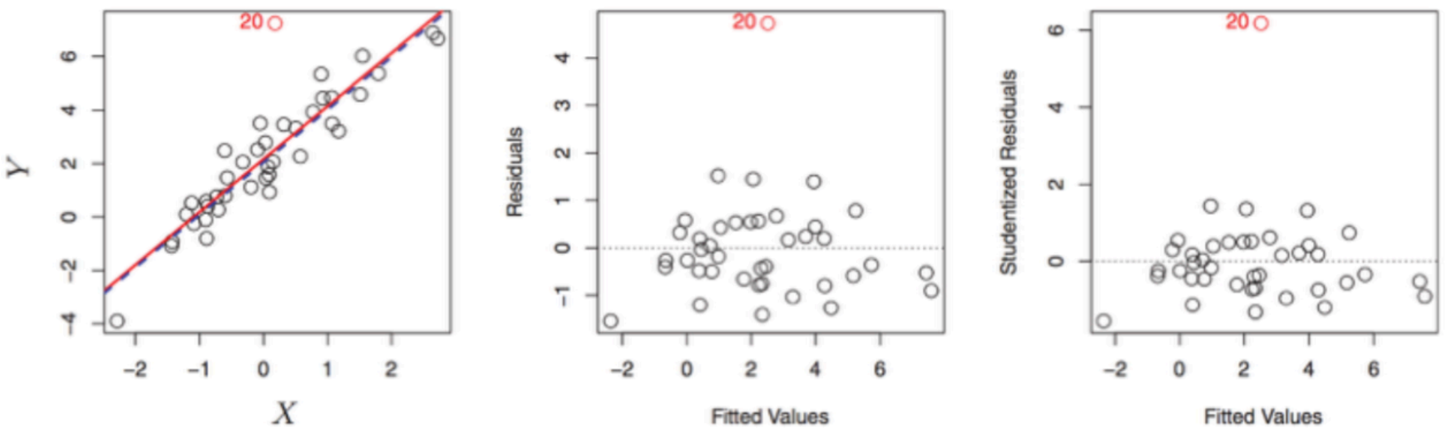
We can make a **residual plot** to help identify outliers visually. In this case, we plot the residuals by the fitted/predicted value, y.

Even better, we can **standardize** by dividing by the standard error. This allows us to see which points are outliers in a common way, perhaps by checking whether they're above or below 2 (roughly 95% of our data is covered by that region).



Even better still, we can **"Studentize"** the errors by dividing, not by the "global" standard error for our model, but by the standard error of our model at the particular value of y where the residual occurred. Our confidence intervals change depending on how much data we have seen in a particular region. If we've seen a lot of data, our intervals are tight; otherwise, they are wide. So, it takes "more" for a data point to be considered an outlier if it is in a region in which we have little data.




20
Y
X
Residuals
Fitted Values
Studentized Residuals
Fitted Values

Outliers

Detecting outliers

Programmatically

Leverage

- A high-leverage point is an observation with an unusual X value.
- It does not necessarily have a large effect on the regression model (it could lie right along the best fit line of a model fit without it).
- Most common measure is the "hat value": $h_{ii} = (H)_{ii}$
- The ith diagonal of the hat matrix
$$H = X(X^T X)^{-1} X^T$$
is the leverage of the particular data point
- Heuristic explanation: dragging a single point upwards and seeing how much the prediction line follows. If, for a fixed x, we perturb y and $\hat{y_i}$ moves a little, then it is low leverage; if it moves a lot, then it is high leverage. So you can think of it as $h_{ii} = \frac{d\hat{y_i}}{dy_i}$

We can use Leverage to Studentize our errors

- The variance of the ith residual is
$$var(\hat{\epsilon_i}) = \sigma^2 (1 - \frac{1}{n} - \frac{(x_i - \bar{x})^2}{\sum_{j=1}^{n} (x_j - \bar{x})^2})$$
- The corresponding Studentized residual is then
$$t_i = \frac{\hat{\epsilon_i}}{\hat{\sigma}\sqrt{1 - h_{ii}}}$$
where $\sigma\hat{}$ is an appropriate estimate of σ (basically square root of RSE)

Now that we have either standardized (divided by "global" standard error) or studentized (divided by "local" standard error) residuals, we can use them to programmatically identify outlier points. Roughly 95% of our data will fall within ± 2 standardized/studentized errors. We likely don't want to throw out 1 in 20 data points, though, so perhaps we'll cut anything off if it's outside the ± 3 bounds. Note, if we do find outliers we usually train two models, one with them and one without. Also we might chase down the story behind the outlier data points, if we can (was data entered incorrectly? was there a tsunami that day? did the servers go down?).

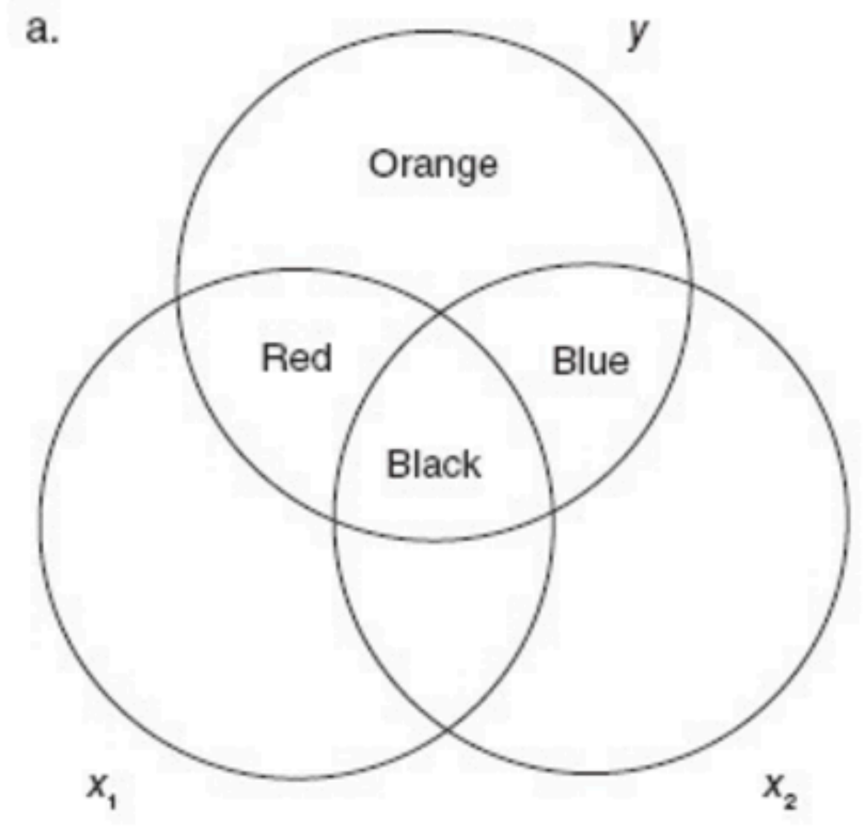
Multicollinearity

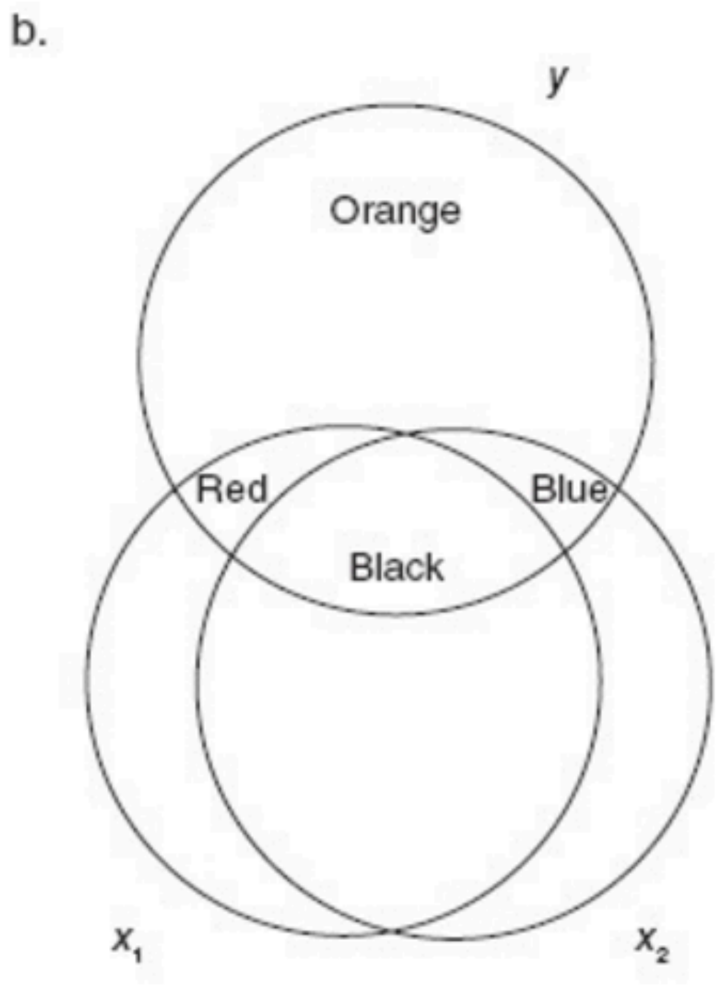
Measuring the same thing two different ways.

If we had the grade of every class for a student, as well as their GPA, we have multicollinearity because GPA is a linear function of their grades.

Could also just be married_is_True and married_is_False as features.

- Perfect vs Partial
  - Perfect
    - Your model will often fail to run/converge (some libraries will still be ok, but don't count on it)
    - Unlikely to occur in practice, unless you goof
      - Consider a case where β_1 and β_2 measure "years since graduating Galvanize" and "years as a data scientist", and of course these are the same ;)
      - If the true "value" for the coefficient is 10, our model could assign weights to β_1 and β_2 of (10, 0), (0, 10), (5, 5)... or any combination between these, and get the same values.
  - Partial
    - Uncertainty in the model coefficients becomes large
    - Does not necessarily affect model accuracy or bias the coefficients





Notes on image:

- Here x_1 and x_2 are both correlated with the dependent variable, and are correlated with each other.
- If they are relatively less correlated with each other (top), then the "black" region of their overlap is smaller. If they're relatively more correlated with each other (bottom), then the "black" region of their overlap is larger. The variation that each variable captures of the target is its circle; when the circles overlap heavily, we don't know which variable to give credit to, as their overlapping region could go to either. One of them could get full credit for it, no credit for it, or somewhere in between, which means the coefficient values are going to vary widely.

Multicollinearity

- Correlation Matrix / Scatterplot Matrix / Bivariate Correlations
    - Can only pick up pairwise effects
- Variance Inflation Factors, VIF
    - I heard you liked regression, so I put some regression in your regression so you can regress while you regress
    - Regress each of the independent variables on all the other independent variables
        - If any of these auxiliary R^2 values are near 1, there is high multicollinearity
        - Makes sense: if we can predict one variable with the others... it's collinear with them
    - For each of the predictor variables j:

$$VIF = \frac{1}{1 - R_j^2}$$

    - This measures how much the variance of the regression coefficients is inflated relative to the noninflated baseline of linearly independent predictors
    - In the best case:
        - We can't predict our jth feature with the others, so R_j^2 is 0
        - This means VIF is 1, and x_j is linearly independent of the other independent variables
    - If $VIF > 10$, then multicollinearity is probably a problem
        - 10 is a rule of thumb; you may be more or less conservative

Why do we subtract and invert rather than just talking about auxiliary R^2 values, where lower is better? Good. Question. (Perhaps fancy terms are correlated with salary for statisticians... a Salary Inflation Factor ;)

- What should I do if I have high multicollinearity?
    - Try to gather more data
    - Consider combining multiple intercorrelated variables into one
    - Don't interpret coefficients, just use your model to predict
    - Discard the offending variable(s)
    - What if I created multicollinearity by adding polynomial terms?
        - Say I added x_{40} and x_{40}^2 because there was a quadratic trend in x_{40}
        - Now I have two variables that exhibit high multicollinearity
        - I can subtract the mean and use the deviations (and squared deviations) as variables in the model; this reduces multicollinearity, but also changes the interpretation of the coefficients

QQ Plots

Watch this: https://www.youtube.com/watch?v=X9_ISJ0YpGw (https://www.youtube.com/watch?v=X9_ISJ0YpGw)

(ragequit QQ)

jupyter nbconvert Linear_Regression.ipynb --to slides --post serve

```
In [ ]:
```