## Avoiding Using Least Squares

Justification for fitting data visually:

- Large simplifications in model development mean that eyeballing a fit is reasonable.


## Avoiding Using Least Squares

Justification for fitting data visually:

- Large simplifications in model development mean that eyeballing a fit is reasonable.
- Mathematical methods do not necessarily imply a better fit!


## Avoiding Using Least Squares

Justification for fitting data visually:

- Large simplifications in model development mean that eyeballing a fit is reasonable.
- Mathematical methods do not necessarily imply a better fit!
- You can make objective judgements that computers cannot; you know which data points should be taken more seriously.


## Avoiding Using Least Squares

Justification for fitting data visually:

- Large simplifications in model development mean that eyeballing a fit is reasonable.
- Mathematical methods do not necessarily imply a better fit!
- You can make objective judgements that computers cannot; you know which data points should be taken more seriously.
- Mathematics give precise answers; every answer is fallible.


## Regression

If we have confidence in our data, we may wish to do a regression, a method for fitting a curve through a set of points by following a goodness-of-fit criterion.

## Regression

If we have confidence in our data, we may wish to do a regression, a method for fitting a curve through a set of points by following a goodness-of-fit criterion.

Goal: Formulate mathematically what we do internally: Make the discrepancies between the data and the curve small.

## Regression

If we have confidence in our data, we may wish to do a regression, a method for fitting a curve through a set of points by following a goodness-of-fit criterion.

Goal: Formulate mathematically what we do internally: Make the discrepancies between the data and the curve small.

- Make the sum of the set of absolute deviations small. minimize over all $f$ the sum: $\sum_{\left(x_{i}, y_{i}\right)}\left|y_{i}-f\left(x_{i}\right)\right|$


## Regression

If we have confidence in our data, we may wish to do a regression, a method for fitting a curve through a set of points by following a goodness-of-fit criterion.

Goal: Formulate mathematically what we do internally: Make the discrepancies between the data and the curve small.

- Make the sum of the set of absolute deviations small. minimize over all $f$ the sum: $\sum_{\left(x_{i}, y_{i}\right)}\left|y_{i}-f\left(x_{i}\right)\right|$
- Make the largest of the set of absolute deviations small. minimize over all $f$ the value: $\max _{\left(x_{i}, y_{i}\right)}\left|y_{i}-f\left(x_{i}\right)\right|$


## Regression

If we have confidence in our data, we may wish to do a regression, a method for fitting a curve through a set of points by following a goodness-of-fit criterion.

Goal: Formulate mathematically what we do internally: Make the discrepancies between the data and the curve small.

- Make the sum of the set of absolute deviations small. minimize over all $f$ the sum: $\sum_{\left(x_{i}, y_{i}\right)}\left|y_{i}-f\left(x_{i}\right)\right|$
- Make the largest of the set of absolute deviations small. minimize over all $f$ the value: $\max _{\left(x_{i}, y_{i}\right)}\left|y_{i}-f\left(x_{i}\right)\right|$

One or the other might make more sense depending on the situation.

## Least Squares

A regression method often used is called least squares.

$$
\text { minimize over all } f \text { the sum: } \sum_{\left(x_{i}, y_{i}\right)}\left(y_{i}-f\left(x_{i}\right)\right)^{2}
$$

## Least Squares

A regression method often used is called least squares.

$$
\text { minimize over all } f \text { the sum: } \sum_{\left(x_{i}, y_{i}\right)}\left(y_{i}-f\left(x_{i}\right)\right)^{2}
$$

- A middle ground, giving weight to all discrepancies and more weight to those that are further from the curve.


## Least Squares

A regression method often used is called least squares.

$$
\text { minimize over all } f \text { the sum: } \sum_{\left(x_{i}, y_{i}\right)}\left(y_{i}-f\left(x_{i}\right)\right)^{2}
$$

- A middle ground, giving weight to all discrepancies and more weight to those that are further from the curve.
- Easy to analyze mathematically because this is a smooth function.


## Least Squares

A regression method often used is called least squares.

$$
\text { minimize over all } f \text { the sum: } \sum_{\left(x_{i}, y_{i}\right)}\left(y_{i}-f\left(x_{i}\right)\right)^{2}
$$

- A middle ground, giving weight to all discrepancies and more weight to those that are further from the curve.
- Easy to analyze mathematically because this is a smooth function.

Calculating minima of smooth functions: (You know how!)


## Least Squares

A regression method often used is called least squares.

$$
\text { minimize over all } f \text { the sum: } \sum_{\left(x_{i} y_{i}\right)}\left(y_{i}-f\left(x_{i}\right)\right)^{2}
$$

- A middle ground, giving weight to all discrepancies and more weight to those that are further from the curve.
- Easy to analyze mathematically because this is a smooth function.

Calculating minima of smooth functions: (You know how!)

- Differentiate with respect to each variable, and set equal to zero.



## Least Squares

A regression method often used is called least squares.

$$
\text { minimize over all } f \text { the sum: } \sum_{\left(x_{i} y_{i}\right)}\left(y_{i}-f\left(x_{i}\right)\right)^{2}
$$

- A middle ground, giving weight to all discrepancies and more weight to those that are further from the curve.
- Easy to analyze mathematically because this is a smooth function.

Calculating minima of smooth functions: (You know how!)

- Differentiate with respect to each variable, and set equal to zero.
- Solve the resulting system of equations.



## Least Squares

A regression method often used is called least squares.

$$
\text { minimize over all } f \text { the sum: } \sum_{\left(x_{i} y_{i}\right)}\left(y_{i}-f\left(x_{i}\right)\right)^{2}
$$

- A middle ground, giving weight to all discrepancies and more weight to those that are further from the curve.
- Easy to analyze mathematically because this is a smooth function.

Calculating minima of smooth functions: (You know how!)

- Differentiate with respect to each variable, and set equal to zero.
- Solve the resulting system of equations.
- Check to see if the solutions are local minima.



## Least Squares Example

Example. Use the least-squares criterion to fit a line $y=m x+b$ to the data: $\{(1.0,3.6),(2.1,2.9),(3.5,2.2),(4.0,1.7)\}$.

## Least Squares Example

Example. Use the least-squares criterion to fit a line $y=m x+b$ to the data: $\{(1.0,3.6),(2.1,2.9),(3.5,2.2),(4.0,1.7)\}$. Intution / Expectations?

## Least Squares Example

Example. Use the least-squares criterion to fit a line $y=m x+b$ to the data: $\{(1.0,3.6),(2.1,2.9),(3.5,2.2),(4.0,1.7)\}$.
Intution / Expectations?
Solution. We need to calculate the sum $S=\sum_{\left(x_{i}, y_{i}\right)}\left[y_{i}-\left(m x_{i}+b\right)\right]^{2}$.

## Least Squares Example

Example. Use the least-squares criterion to fit a line $y=m x+b$ to the data: $\{(1.0,3.6),(2.1,2.9),(3.5,2.2),(4.0,1.7)\}$.
Intution / Expectations?
Solution. We need to calculate the sum $S=\sum_{\left(x_{i}, y_{i}\right)}\left[y_{i}-\left(m x_{i}+b\right)\right]^{2}$. $S=(3.6-1.0 m-b)^{2}+(2.9-2.1 m-b)^{2}+(2.2-3.5 m-b)^{2}+(1.7-4.0 m-b)^{2}$

## Least Squares Example

Example. Use the least-squares criterion to fit a line $y=m x+b$ to the data: $\{(1.0,3.6),(2.1,2.9),(3.5,2.2),(4.0,1.7)\}$. Intution / Expectations?
Solution. We need to calculate the sum $S=\sum_{\left(x_{i}, y_{i}\right)}\left[y_{i}-\left(m x_{i}+b\right)\right]^{2}$. $S=(3.6-1.0 m-b)^{2}+(2.9-2.1 m-b)^{2}+(2.2-3.5 m-b)^{2}+(1.7-4.0 m-b)^{2}$
Expanding, $S=29.1-20.8 b+4 b^{2}-48.38 m+21.2 b m+33.66 m^{2}$

## Least Squares Example

Example. Use the least-squares criterion to fit a line $y=m x+b$ to the data: $\{(1.0,3.6),(2.1,2.9),(3.5,2.2),(4.0,1.7)\}$.
Intution / Expectations?
Solution. We need to calculate the sum $S=\sum_{\left(x_{i}, y_{i}\right)}\left[y_{i}-\left(m x_{i}+b\right)\right]^{2}$. $S=(3.6-1.0 m-b)^{2}+(2.9-2.1 m-b)^{2}+(2.2-3.5 m-b)^{2}+(1.7-4.0 m-b)^{2}$
Expanding, $S=29.1-20.8 b+4 b^{2}-48.38 m+21.2 b m+33.66 m^{2}$
Calculating the partial derivatives and setting equal to zero:

$$
\left\{\begin{array}{l}
\frac{\partial S}{\partial b}=-20.8+8 b+21.2 m=0 \\
\frac{\partial S}{\partial m}=-48.38+21.2 b+67.32 m=0
\end{array}\right.
$$

## Least Squares Example

Example. Use the least-squares criterion to fit a line $y=m x+b$ to the data: $\{(1.0,3.6),(2.1,2.9),(3.5,2.2),(4.0,1.7)\}$.
Intution / Expectations?
Solution. We need to calculate the sum $S=\sum_{\left(x_{i}, y_{i}\right)}\left[y_{i}-\left(m x_{i}+b\right)\right]^{2}$. $S=(3.6-1.0 m-b)^{2}+(2.9-2.1 m-b)^{2}+(2.2-3.5 m-b)^{2}+(1.7-4.0 m-b)^{2}$
Expanding, $S=29.1-20.8 b+4 b^{2}-48.38 m+21.2 b m+33.66 m^{2}$
Calculating the partial derivatives and setting equal to zero:
$\left\{\begin{array}{l}\frac{\partial S}{\partial b}=-20.8+8 b+21.2 m=0 \\ \frac{\partial S}{\partial m}=-48.38+21.2 b+67.32 m=0\end{array}\right.$
Solving the system of equations gives: $\{b=4.20332, m=-0.605027\}$

## Least Squares Example

Example. Use the least-squares criterion to fit a line $y=m x+b$ to the data: $\{(1.0,3.6),(2.1,2.9),(3.5,2.2),(4.0,1.7)\}$.

## Intution / Expectations?

Solution. We need to calculate the sum $S=\sum_{\left(x_{i}, y_{i}\right)}\left[y_{i}-\left(m x_{i}+b\right)\right]^{2}$. $S=(3.6-1.0 m-b)^{2}+(2.9-2.1 m-b)^{2}+(2.2-3.5 m-b)^{2}+(1.7-4.0 m-b)^{2}$
Expanding, $S=29.1-20.8 b+4 b^{2}-48.38 m+21.2 b m+33.66 m^{2}$
Calculating the partial derivatives and setting equal to zero:

$$
\left\{\begin{array}{l}
\frac{\partial S}{\partial b}=-20.8+8 b+21.2 m=0 \\
\frac{\partial S}{\partial m}=-48.38+21.2 b+67.32 m=0
\end{array}\right.
$$

Solving the system of equations gives: $\{b=4.20332, m=-0.605027\}$
That is, the line that gives the least-squares fit for the data is

$$
y=-0.605027 x+4.20332
$$

## Notes on the Method of Least Squares

- Least squares becomes messy when there are many data points.


## Notes on the Method of Least Squares

- Least squares becomes messy when there are many data points.
- We chose least squares because it was easy. Is it really the "right" method for the job?


## Notes on the Method of Least Squares

- Least squares becomes messy when there are many data points.
- We chose least squares because it was easy. Is it really the "right" method for the job?
- Least squares isn't always easy, for example: $y=C e^{k x}$.


## Notes on the Method of Least Squares

- Least squares becomes messy when there are many data points.
- We chose least squares because it was easy. Is it really the "right" method for the job?
- Least squares isn't always easy, for example: $y=C e^{k x}$.
- You can use least squares on transformed data, but the result is NOT a least-squares curve for the original data.


## Notes on the Method of Least Squares

- Least squares becomes messy when there are many data points.
- We chose least squares because it was easy. Is it really the "right" method for the job?
- Least squares isn't always easy, for example: $y=C e^{k x}$.
- You can use least squares on transformed data, but the result is NOT a least-squares curve for the original data.
- Multivariable least squares can also be done: $w=a x+b y+c z+d$ (Would want to minimize: $\qquad$


## Notes on the Method of Least Squares

- Least squares becomes messy when there are many data points.
- We chose least squares because it was easy. Is it really the "right" method for the job?
- Least squares isn't always easy, for example: $y=C e^{k x}$.
- You can use least squares on transformed data, but the result is NOT a least-squares curve for the original data.
- Multivariable least squares can also be done: $w=a x+b y+c z+d$ (Would want to minimize: $\qquad$
- Least squares measures distance vertically.

A better measure would probably be perpendicular distance.

## Notes on the Method of Least Squares

- Least squares becomes messy when there are many data points.
- We chose least squares because it was easy. Is it really the "right" method for the job?
- Least squares isn't always easy, for example: $y=C e^{k x}$.
- You can use least squares on transformed data, but the result is NOT a least-squares curve for the original data.
- Multivariable least squares can also be done: $w=a x+b y+c z+d$ (Would want to minimize: $\qquad$
- Least squares measures distance vertically. A better measure would probably be perpendicular distance.
- You need to understand the concept of least squares and know how to do least squares by hand for small examples.


## Notes on the Method of Least Squares

- Least squares becomes messy when there are many data points.
- We chose least squares because it was easy. Is it really the "right" method for the job?
- Least squares isn't always easy, for example: $y=C e^{k x}$.
- You can use least squares on transformed data, but the result is NOT a least-squares curve for the original data.
- Multivariable least squares can also be done: $w=a x+b y+c z+d$ (Would want to minimize: $\qquad$
- Least squares measures distance vertically. A better measure would probably be perpendicular distance.
- You need to understand the concept of least squares and know how to do least squares by hand for small examples.
- We'll learn how to use Mathematica to do this for us!


## Price - Demand Curve (p. 111-114)

Example. A company is trying to determine how demand for a new product depends on its price and collect the following data:

| price $p$ | $\$ 9$ | $\$ 10$ | $\$ 11$ |
| :---: | :---: | :---: | :---: |
| demand $d$ | $1200 / \mathrm{mo}$. | $1000 / \mathrm{mo}$. | $975 / \mathrm{mo}$. |

The company has reason to believe that price and demand are inversely proportional, that is, $d=\frac{c}{p}$ for some constant $c$.

## Price - Demand Curve (p. 111-114)

Example. A company is trying to determine how demand for a new product depends on its price and collect the following data:

| price $p$ | $\$ 9$ | $\$ 10$ | $\$ 11$ |
| :---: | :---: | :---: | :---: |
| demand $d$ | $1200 / \mathrm{mo}$. | $1000 / \mathrm{mo}$. | $975 / \mathrm{mo}$. |

The company has reason to believe that price and demand are inversely proportional, that is, $d=\frac{c}{p}$ for some constant $c$.
$\rightarrow$ Use the method of least squares to determine this constant $c$.


## Price - Demand Curve (p. 111-114)

Solution. Since $f(p)=\frac{c}{p}$, then the sum $S=\sum_{\left(p_{i}, d_{i}\right)}\left[d_{i}-\left(\frac{c}{p_{i}}\right)\right]^{2}$.

## Price - Demand Curve (p. 111-114)

Solution. Since $f(p)=\frac{c}{p}$, then the sum $S=\sum_{\left(p_{i}, d_{i}\right)}\left[d_{i}-\left(\frac{c}{p_{i}}\right)\right]^{2}$.
Specifying datapoints gives

$$
S=\left[1200-\frac{c}{9}\right]^{2}+\left[1000-\frac{c}{10}\right]^{2}+\left[975-\frac{c}{11}\right]^{2}
$$

## Price - Demand Curve (p. 111-114)

Solution. Since $f(p)=\frac{c}{p}$, then the sum $S=\sum_{\left(p_{i}, d_{i}\right)}\left[d_{i}-\left(\frac{c}{p_{i}}\right)\right]^{2}$.
Specifying datapoints gives

$$
S=\left[1200-\frac{c}{9}\right]^{2}+\left[1000-\frac{c}{10}\right]^{2}+\left[975-\frac{c}{11}\right]^{2}
$$

Setting the derivative equal to zero gives

$$
\frac{d S}{d c}=\frac{-2}{9}\left[1200-\frac{c}{9}\right]+\frac{-2}{10}\left[1000-\frac{c}{10}\right]+\frac{-2}{11}\left[975-\frac{c}{11}\right]=0
$$

## Price - Demand Curve (p. 111-114)

Solution. Since $f(p)=\frac{c}{p}$, then the sum $S=\sum_{\left(p_{i}, d_{i}\right)}\left[d_{i}-\left(\frac{c}{p_{i}}\right)\right]^{2}$.
Specifying datapoints gives

$$
S=\left[1200-\frac{c}{9}\right]^{2}+\left[1000-\frac{c}{10}\right]^{2}+\left[975-\frac{c}{11}\right]^{2}
$$

Setting the derivative equal to zero gives

$$
\frac{d S}{d c}=\frac{-2}{9}\left[1200-\frac{c}{9}\right]+\frac{-2}{10}\left[1000-\frac{c}{10}\right]+\frac{-2}{11}\left[975-\frac{c}{11}\right]=0
$$

Solving for $c$ gives $c \approx 10517$.


## New York City Temperature (similar to p. 158)

The graph of average weekly temperature in New York City from Jan. 2010 to Dec. 2012 gives the distinct impression of a $\qquad$ .


## New York City Temperature (similar to p. 158)

The graph of average weekly temperature in New York City from Jan. 2010 to Dec. 2012 gives the distinct impression of a $\qquad$ .

We need to determine the constants in:

$$
\operatorname{Temp}(t)=A+B \sin (C(t-D))
$$



## New York City Temperature (similar to p. 158)

The graph of average weekly temperature in New York City from Jan. 2010 to Dec. 2012 gives the distinct impression of a $\qquad$ .

We need to determine the constants in:

$$
\operatorname{Temp}(t)=A+B \sin (C(t-D))
$$



Mathematica has a hard time finding all four constants at once. Using knowledge of the seasons, we can make assumptions about $C$ and $D$. We can assume that $C=$ $\qquad$ .

## New York City Temperature (similar to p. 158)

The graph of average weekly temperature in New York City from Jan. 2010 to Dec. 2012 gives the distinct impression of a $\qquad$ .

We need to determine the constants in:

$$
\operatorname{Temp}(t)=A+B \sin (C(t-D))
$$



Mathematica has a hard time finding all four constants at once. Using knowledge of the seasons, we can make assumptions about $C$ and $D$. We can assume that $C=$ $\qquad$ .

For $D$, find when the sine passes through zero.
Since January is coldest and July is hottest, the zero should occur in April; guess $D \approx 0.3$.

## New York City Temperature (similar to p. 158)

The graph of average weekly temperature in New York City from Jan. 2010 to Dec. 2012 gives the distinct impression of a $\qquad$ .

We need to determine the constants in:

$$
\operatorname{Temp}(t)=A+B \sin (C(t-D))
$$



Mathematica has a hard time finding all four constants at once. Using knowledge of the seasons, we can make assumptions about $C$ and $D$. We can assume that $C=$ $\qquad$ .

For $D$, find when the sine passes through zero. Since January is coldest and July is hottest, the zero should occur in April; guess $D \approx 0.3$.

Fitting to $\operatorname{Temp}(t)=A+B \sin [2 \pi(t-0.3)]$ gives: $\operatorname{Temp}(t)=56.5+20.6 \sin [2 \pi(t-0.3)]$


