Probability Densities in Data Mining

Andrew W. Moore
Professor
School of Computer Science
Carnegie Mellon University
www.cs.cmu.edu/~awm
awm@cs.cmu.edu
412-268-7599

Probability Densities in Data Mining

- Why we should care
- Notation and Fundamentals of continuous PDFs
- Multivariate continuous PDFs
- Combining continuous and discrete random variables

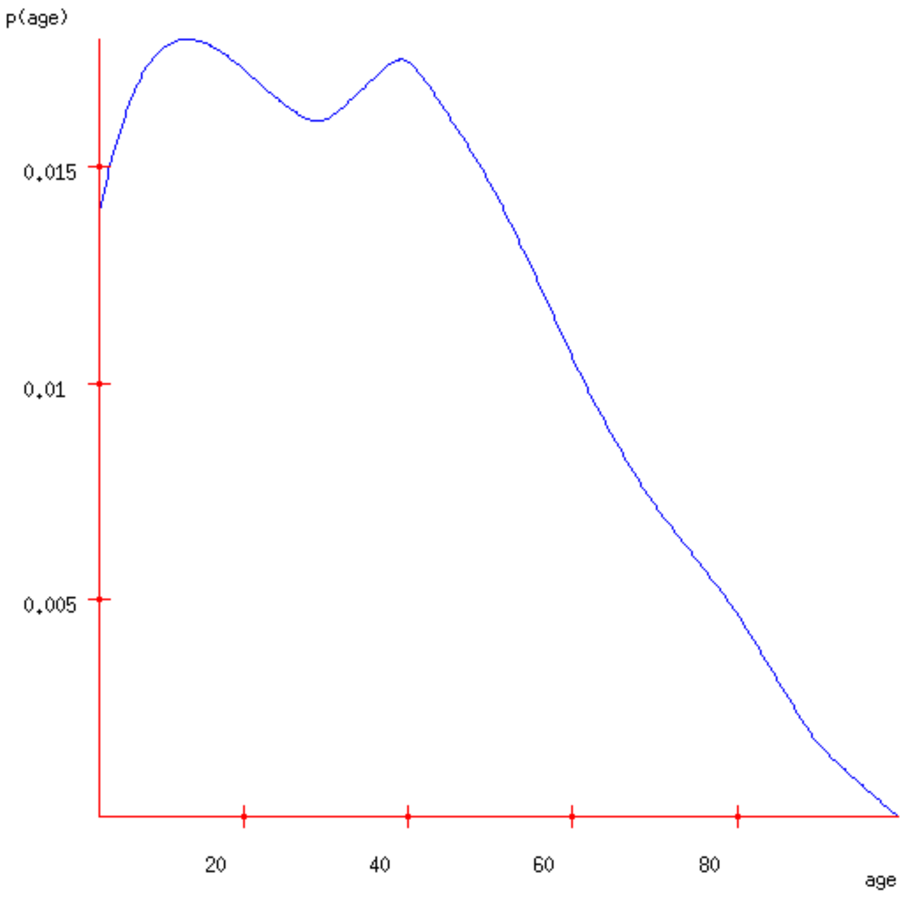
Why we should care

- Real Numbers occur in at least 50% of database records
- Can't always quantize them
- So need to understand how to describe where they come from
- A great way of saying what's a reasonable range of values
- A great way of saying how multiple attributes should reasonably co-occur

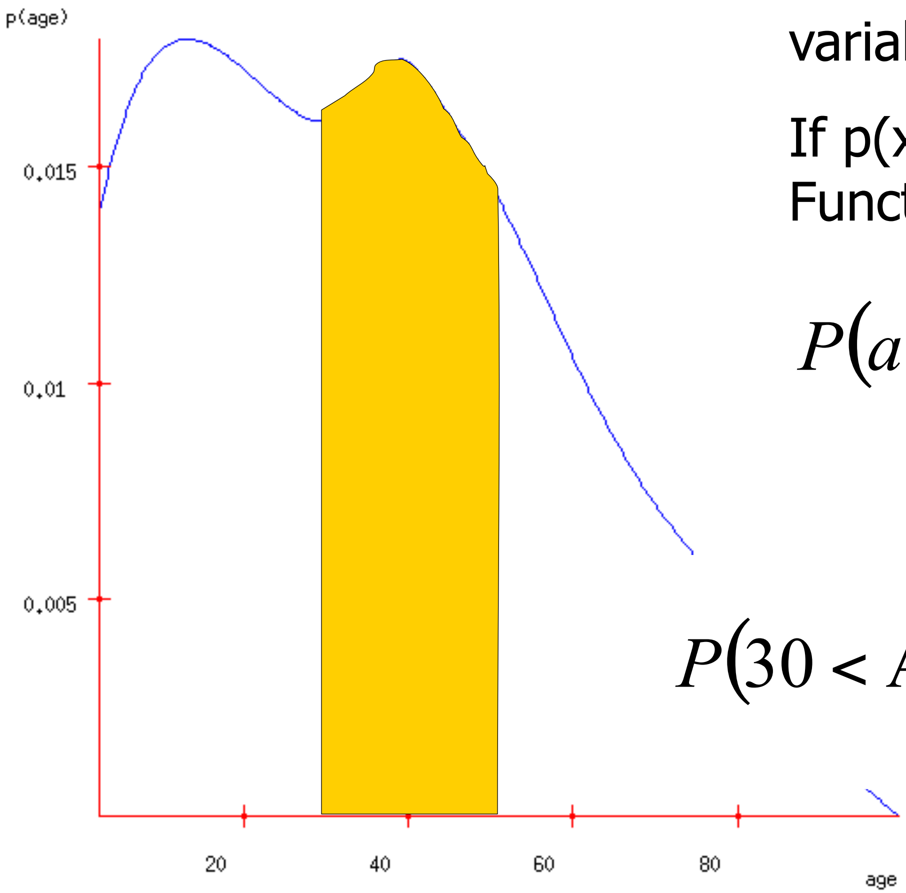
Why we should care

- Can immediately get us Bayes Classifiers that are sensible with real-valued data
- You'll need to intimately understand PDFs in order to do kernel methods, clustering with Mixture Models, analysis of variance, time series and many other things
- Will introduce us to linear and non-linear regression

A PDF of American Ages in 2000



A PDF of American Ages in 2000



Let X be a continuous random variable.

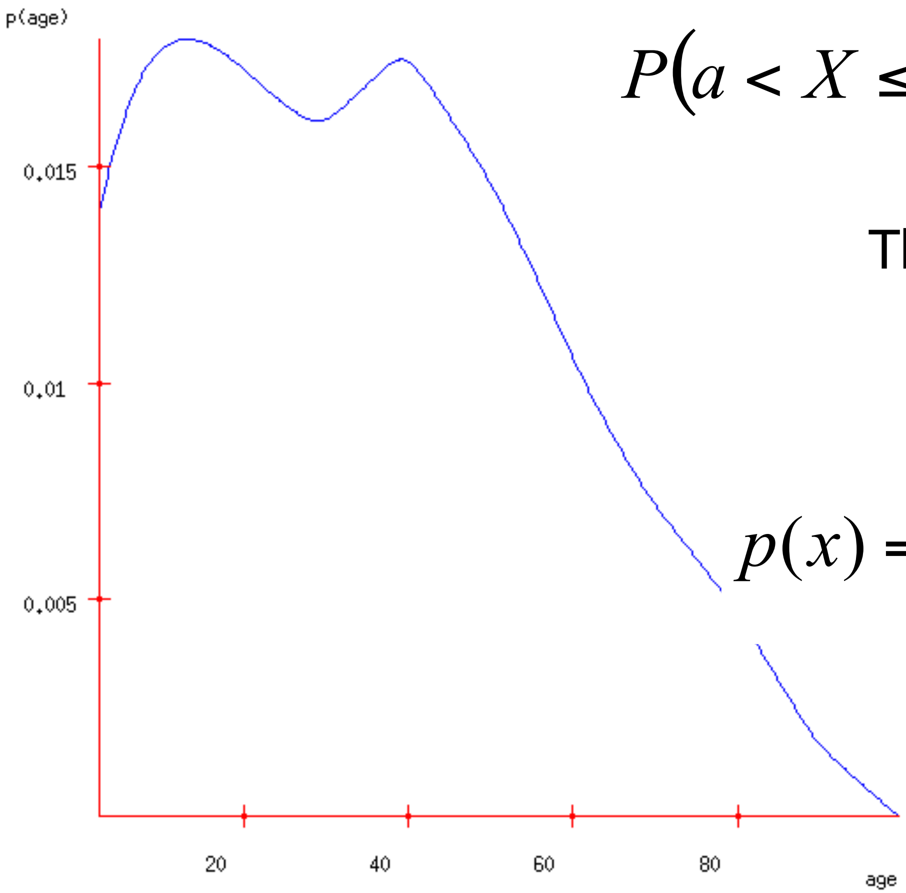
If p(x) is a Probability Density Function for X then…

$$P\left(a < X \le b\right) = \int_{x=a}^{b} p(x)\,dx$$

$$P\left(30 < \text{Age} \le 50\right) = \int_{\text{age}=30}^{50} p(\text{age})\,d\text{age}$$

$= 0.36$

Properties of PDFs



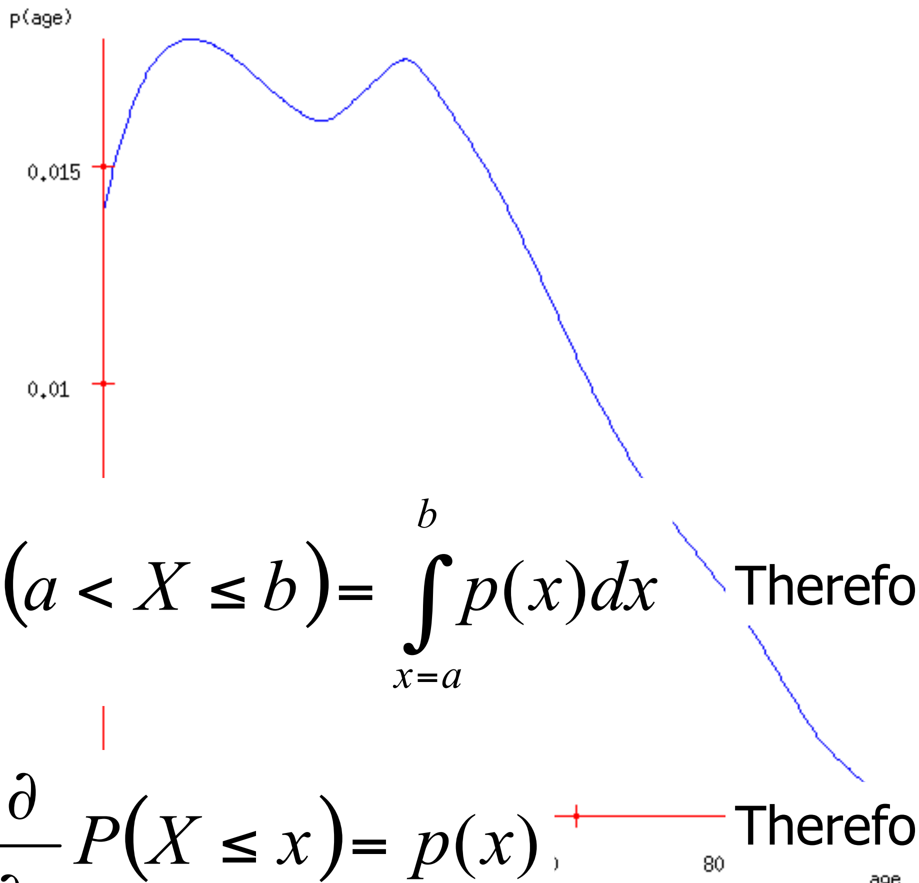
$$P\left(a < X \le b\right) = \int_{x=a}^{b} p(x)\,dx$$

That means…

$$p(x) = \lim_{h \to 0} \frac{P\left(x - \frac{h}{2} < X \le x + \frac{h}{2}\right)}{h}$$

$$\frac{\partial}{\partial x} P\left(X \le x\right) = p(x)$$

Properties of PDFs



$$P(a < X \le b) = \int_{x=a}^{b} p(x)\,dx$$

Therefore…

$$\int_{x=-\infty}^{\infty} p(x)\,dx = 1$$

$$\frac{\partial}{\partial x} P(X \le x) = p(x)$$

Therefore…

$$\forall x : p(x) \ge 0$$

Talking to your stomach

- What's the gut-feel meaning of $p(x)$?

If

$p(5.31) = 0.06$ and $p(5.92) = 0.03$

then

when a value X is sampled from the distribution, you are 2 times as likely to find that X is "very close to" 5.31 than that X is "very close to" 5.92.

Talking to your stomach

- What's the gut-feel meaning of p(x)?

If

p(a) = 0.06 and p(b) = 0.03

then

when a value X is sampled from the distribution, you are 2 times as likely to find that X is "very close to" a than that X is "very close to" b .

Talking to your stomach

- What's the gut-feel meaning of p(x)?

If

p(a) = 2z and p(b) = z

then

when a value X is sampled from the distribution, you are 2 times as likely to find that X is "very close to" a than that X is "very close to" b .

Talking to your stomach

- What's the gut-feel meaning of p(x)?

If

$p(a) = \alpha z$ and $p(b) = z$

then

when a value X is sampled from the distribution, you are α times as likely to find that X is "very close to" a than that X is "very close to" b.

Talking to your stomach

- What's the gut-feel meaning of p(x)?

If

$$\frac{p(a)}{p(b)} = \alpha$$

then

when a value X is sampled from the distribution, you are α times as likely to find that X is "very close to" a than that X is "very close to" b .

Talking to your stomach

- What's the gut-feel meaning of p(x)?

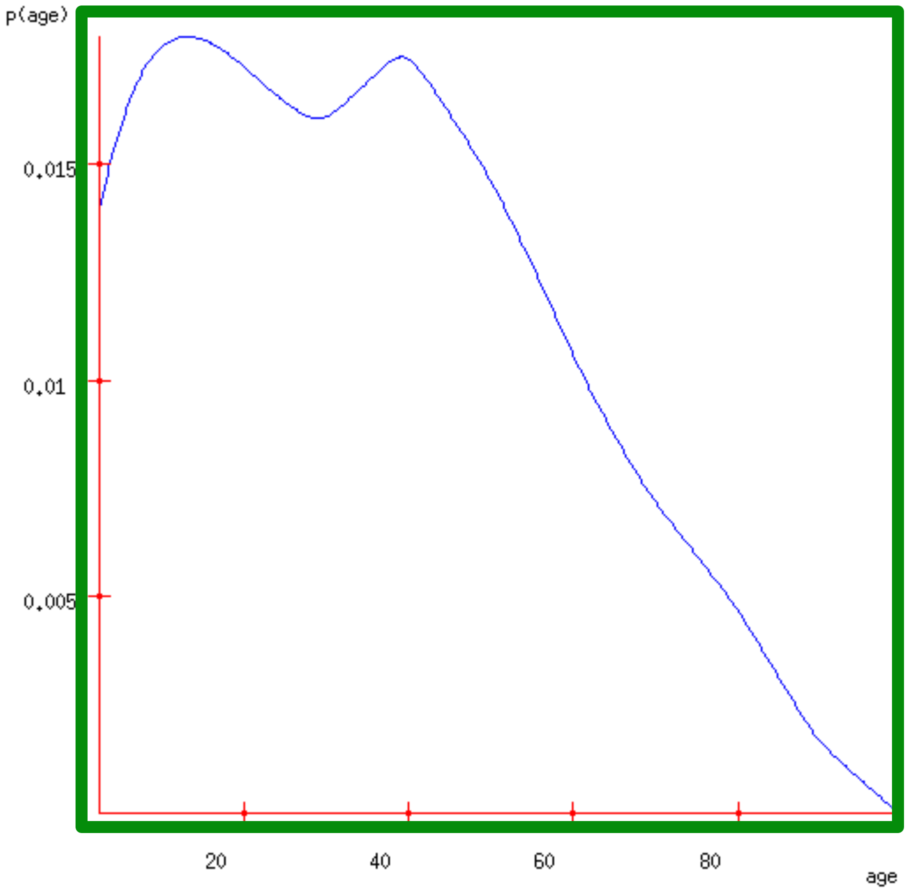
If

$$\frac{p(a)}{p(b)} = \alpha$$

then

$$\lim_{h \to 0} \frac{P(a-h < X < a+h)}{P(b-h < X < b+h)} = \alpha$$

Yet another way to view a PDF



A recipe for sampling a random age.

1. Generate a random dot from the rectangle surrounding the PDF curve. Call the dot (age,d)
2. If d < p(age) stop and return age
3. Else try again: go to Step 1.

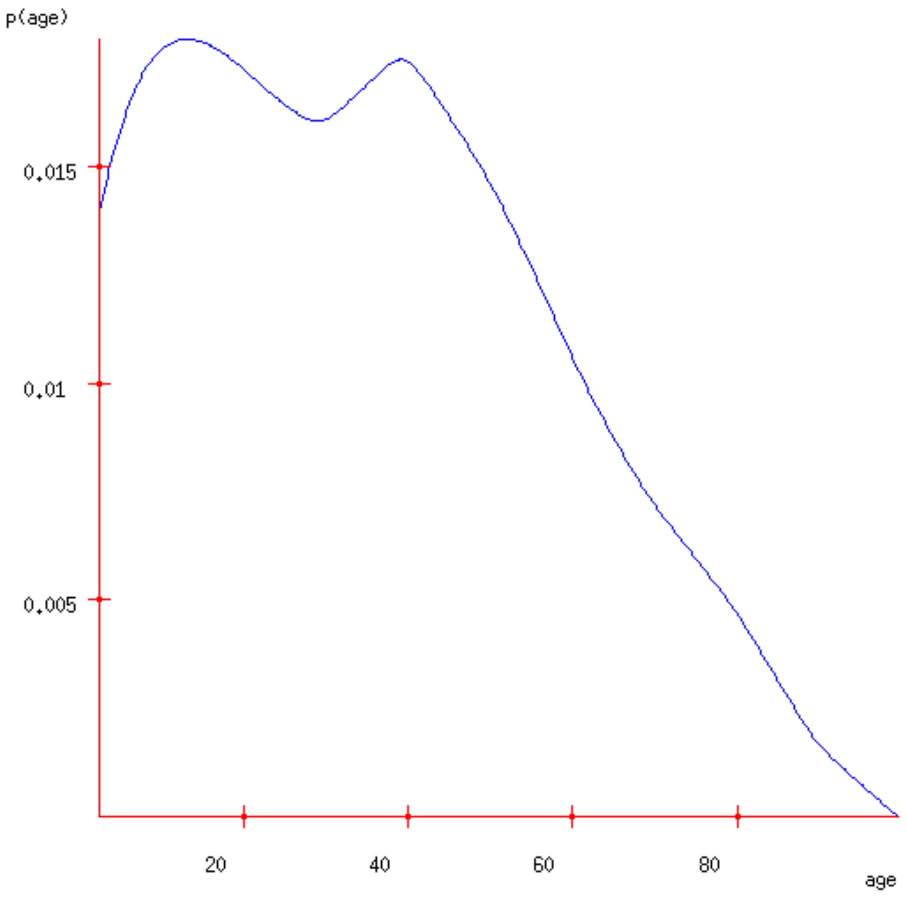
Test your understanding

- True or False:

$$\forall x : p(x) \le 1$$

$$\forall x : P(X = x) = 0$$

Expectations

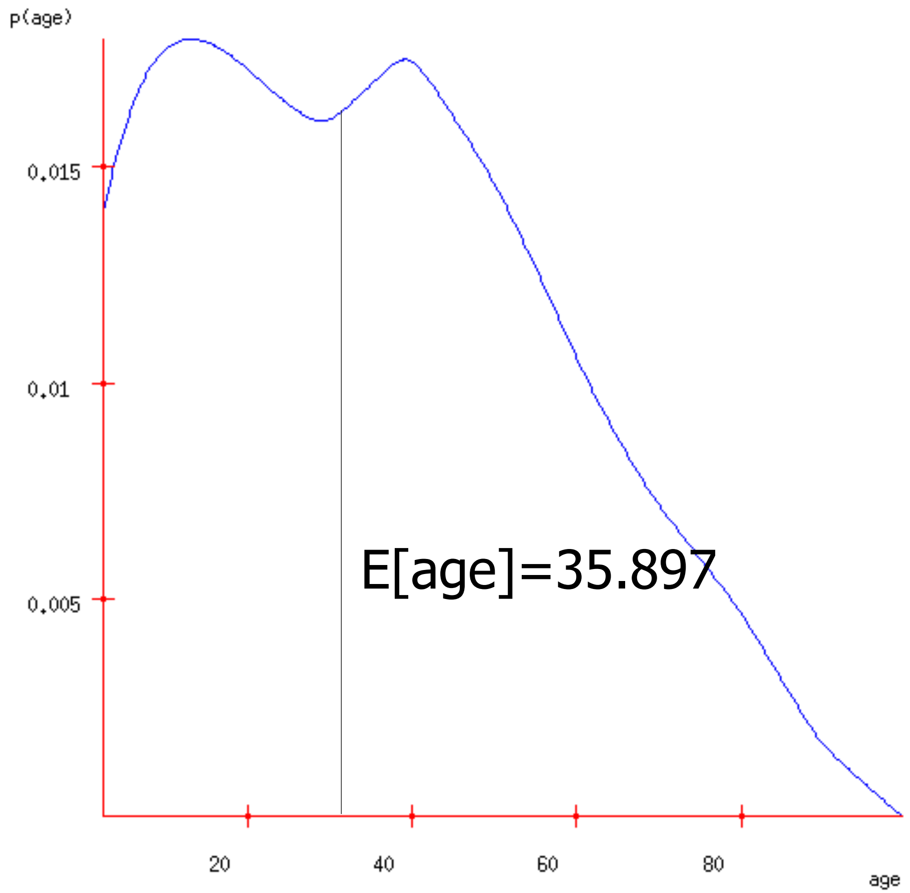


E[X] = the expected value of random variable X

= the average value we'd see if we took a very large number of random samples of X

$$= \int_{x=-\infty}^{\infty} x \, p(x) \, dx$$

Expectations



E[X] = the expected value of random variable X

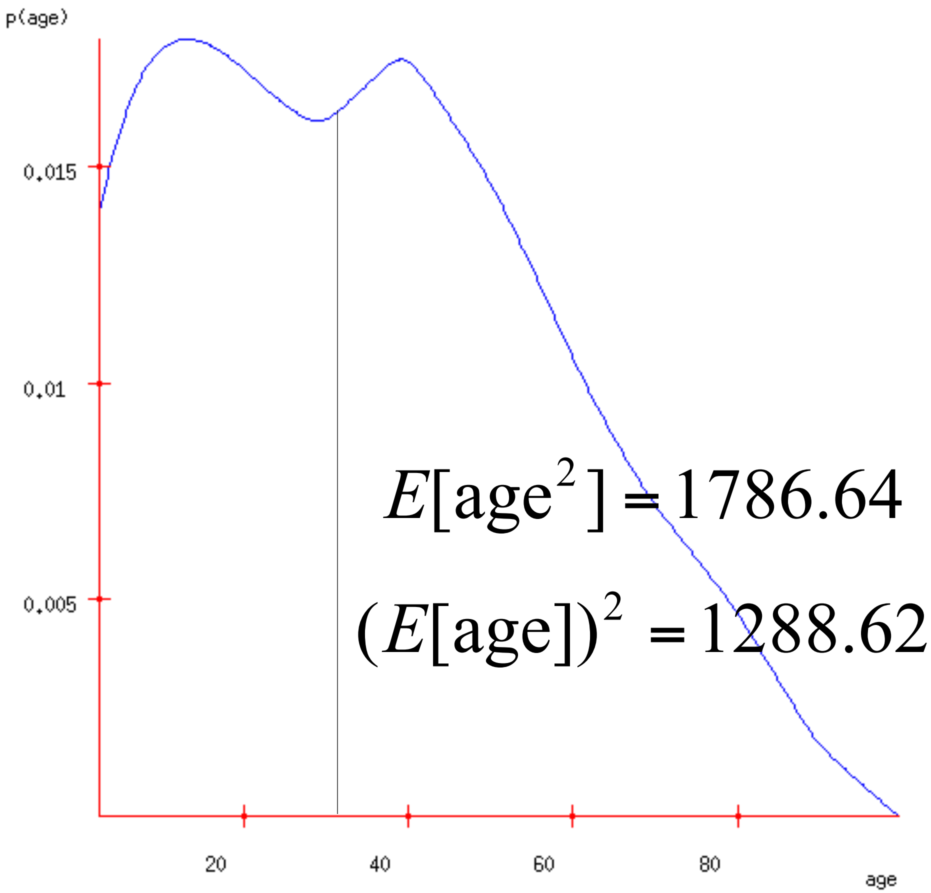
= the average value we'd see if we took a very large number of random samples of X

$$= \int_{x=-\infty}^{\infty} x \, p(x) \, dx$$

= the first moment of the shape formed by the axes and the blue curve

= the best value to choose if you must guess an unknown person's age and you'll be fined the square of your error

Expectation of a function



$$E[\text{age}^2] = 1786.64$$

$$(E[\text{age}])^2 = 1288.62$$

μ=E[f(X)] = the expected value of f(x) where x is drawn from X's distribution.

= the average value we'd see if we took a very large number of random samples of f(X)

$$\mu = \int_{x=-\infty}^{\infty} f(x)\, p(x)\, dx$$

Note that in general:

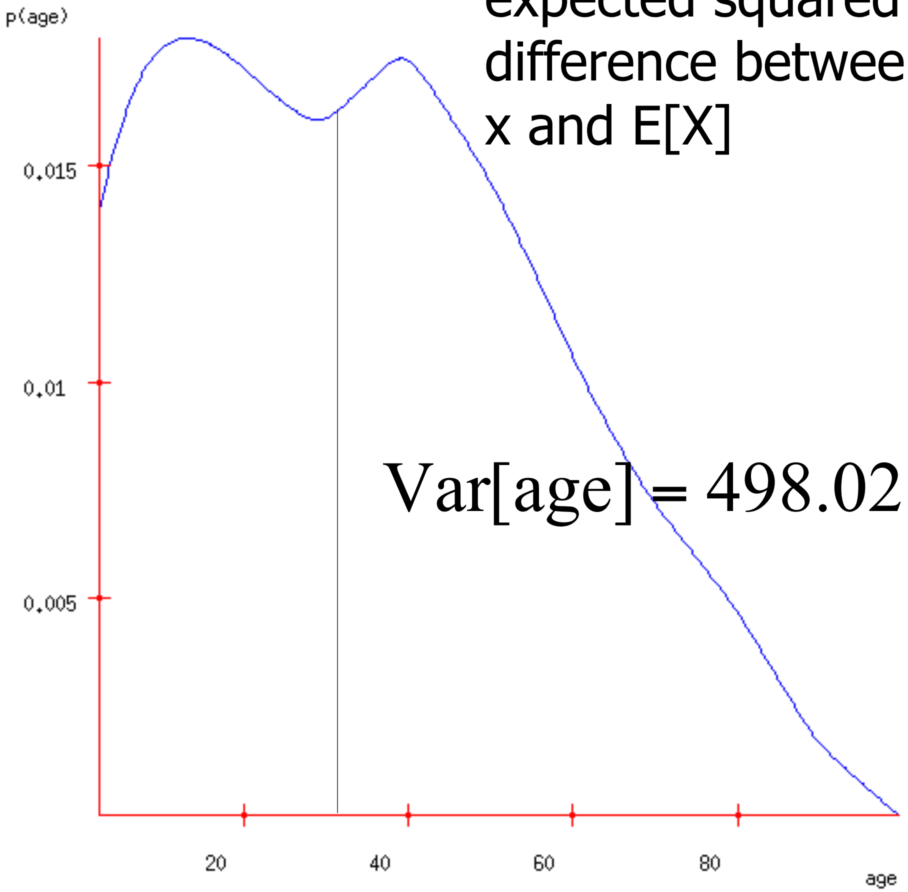
$$E[f(x)] \neq f(E[X])$$

Variance

σ^2 = Var[X] = the expected squared difference between x and E[X]

$$\sigma^2 = \int_{x=-\infty}^{\infty} (x-\mu)^2 \, p(x) \, dx$$

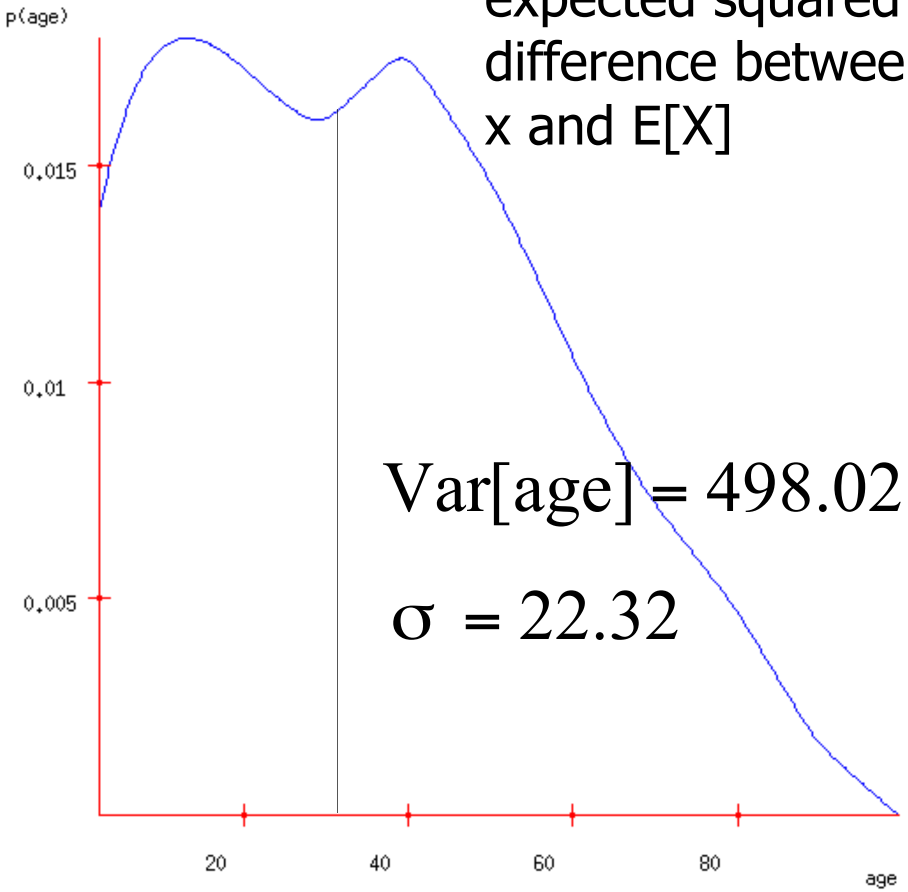
= amount you'd expect to lose if you must guess an unknown person's age and you'll be fined the square of your error, and assuming you play optimally



$\mathrm{Var[age]} = 498.02$

Standard Deviation

σ^2 = Var[X] = the expected squared difference between x and E[X]



$$\mathrm{Var}[age] = 498.02$$

$$\sigma = 22.32$$

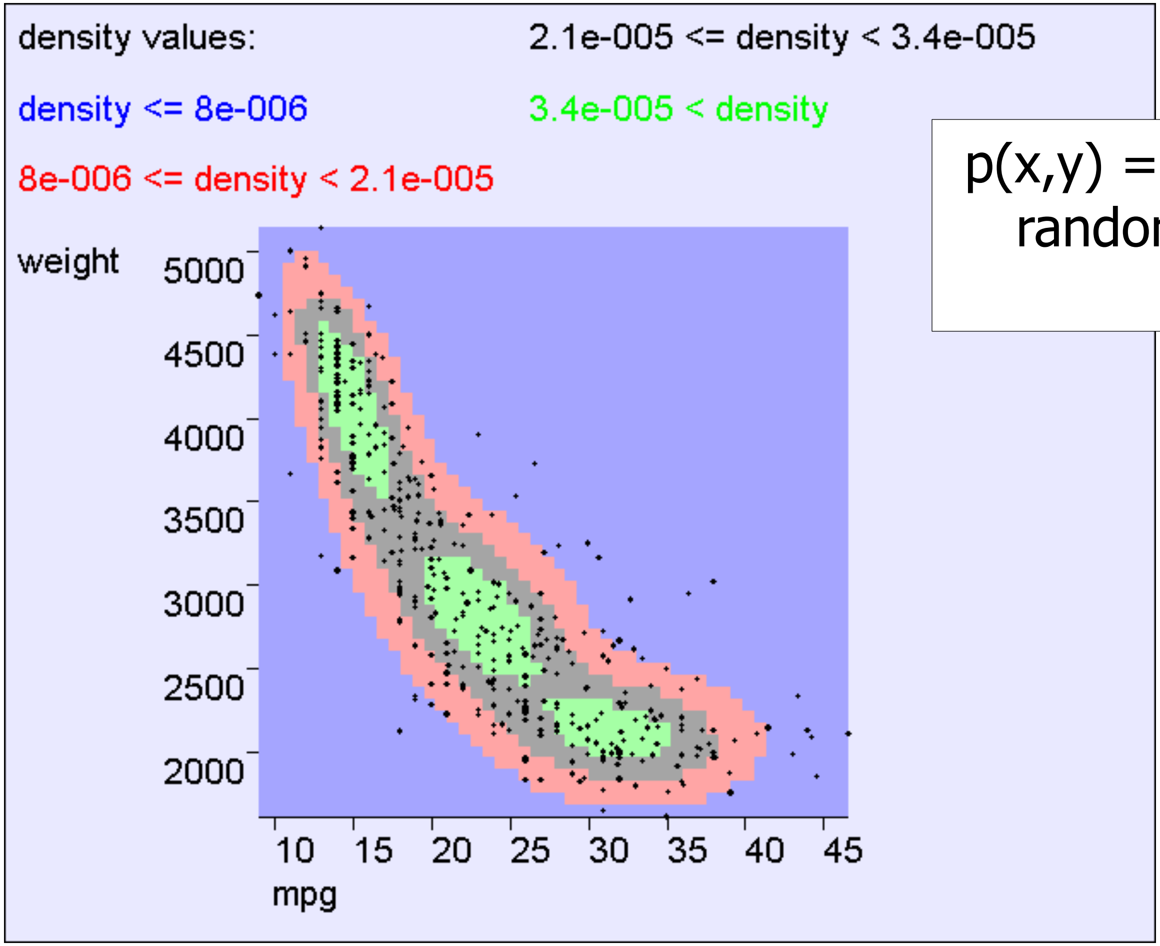
$$\sigma^2 = \int_{x=-\infty}^{\infty} (x-\mu)^2 \, p(x)\, dx$$

= amount you'd expect to lose if you must guess an unknown person's age and you'll be fined the square of your error, and assuming you play optimally

σ = Standard Deviation = "typical" deviation of X from its mean

$$\sigma = \sqrt{\mathrm{Var}[X]}$$

In 2 dimensions

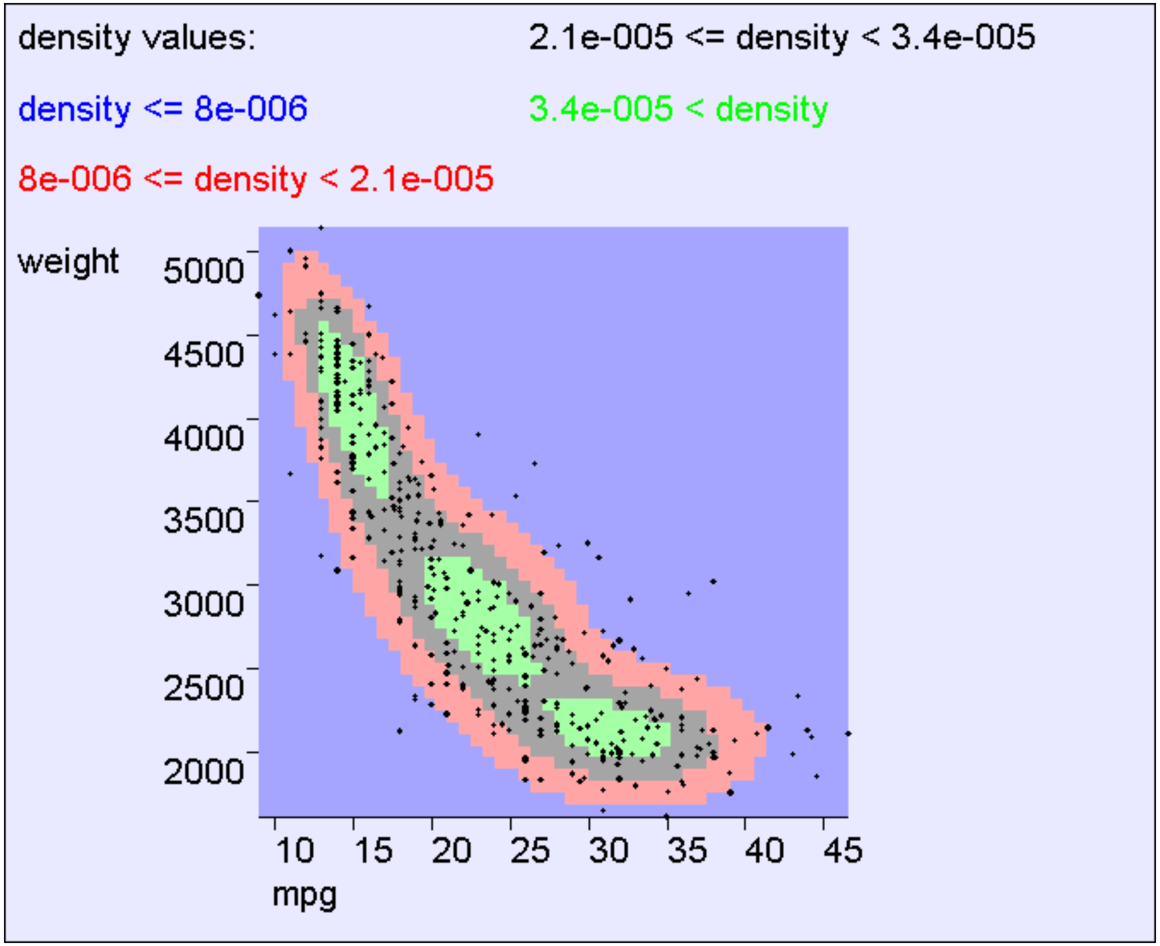


p(x,y) = probability density of random variables (X,Y) at location (x,y)

In 2 dimensions

Let X,Y be a pair of continuous random variables, and let R be some region of (X,Y) space…

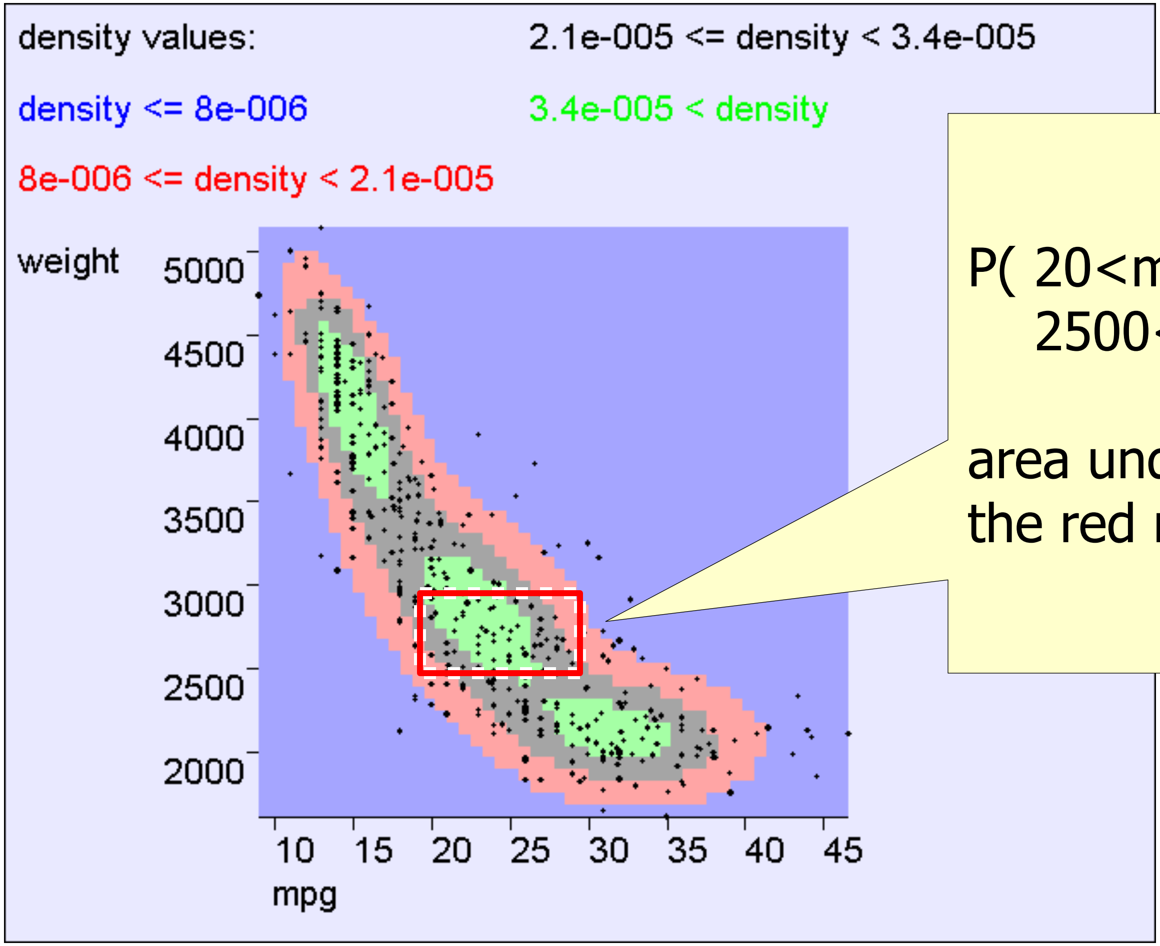
$$P((X,Y)\in R) = \iint_{(x,y)\in R} p(x,y)\,dy\,dx$$



In 2 dimensions

Let X,Y be a pair of continuous random variables, and let R be some region of (X,Y) space…

$$P((X,Y)\in R) = \iint_{(x,y)\in R} p(x,y)\,dy\,dx$$



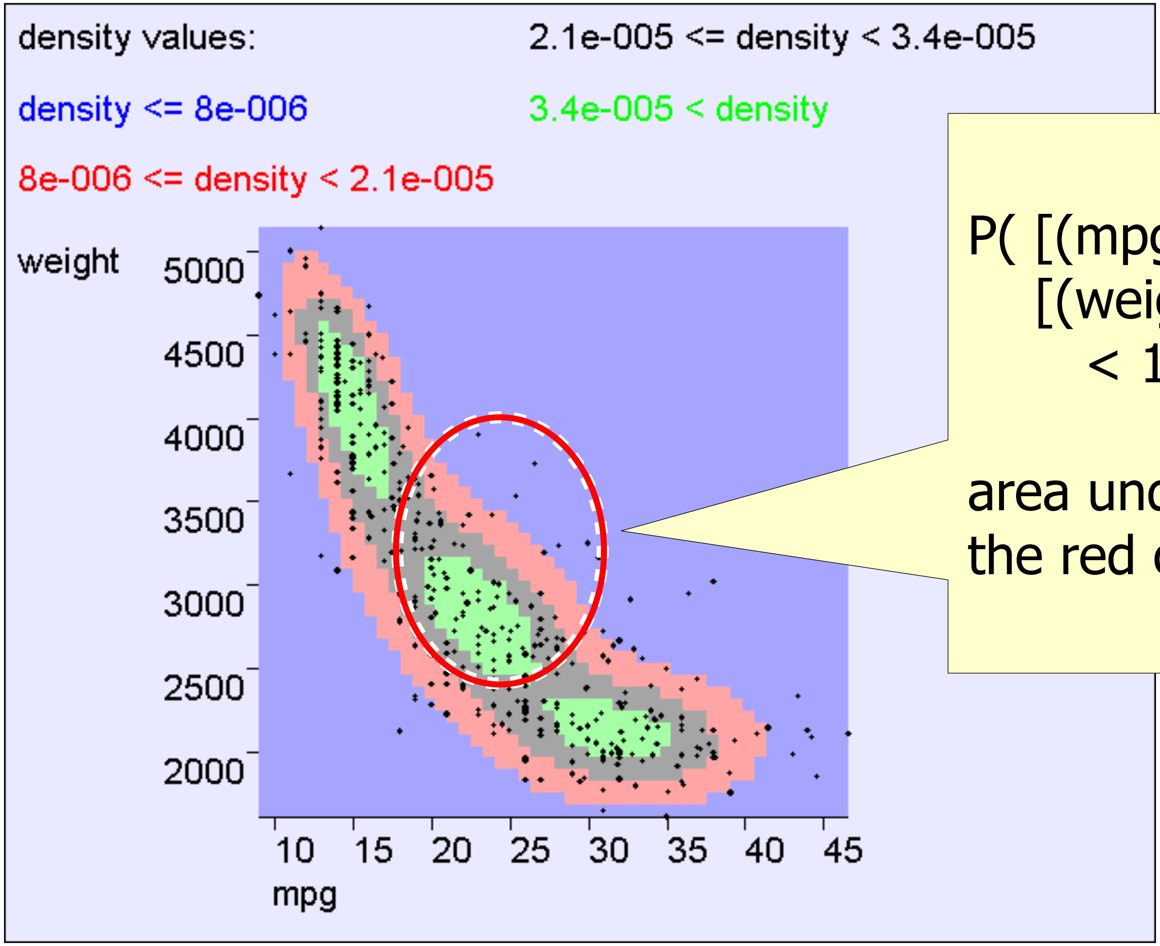
P(20<mpg<30 and
2500<weight<3000) =

area under the 2-d surface within the red rectangle

In 2 dimensions

Let X,Y be a pair of continuous random variables, and let R be some region of (X,Y) space…

$$P((X,Y)\in R) = \iint_{(x,y)\in R} p(x,y)\,dy\,dx$$



P([(mpg-25)/10]^2 + [(weight-3300)/1500]^2 < 1) =

area under the 2-d surface within the red oval

In 2 dimensions

Let X,Y be a pair of continuous random variables, and let R be some region of (X,Y) space…

$$P((X,Y)\in R) = \iint_{(x,y)\in R} p(x,y)\,dy\,dx$$

Take the special case of region R = "everywhere".

Remember that with probability 1, (X,Y) will be drawn from "somewhere".

So..

$$\int_{x=-\infty}^{\infty}\int_{y=-\infty}^{\infty} p(x,y)\,dy\,dx = 1$$

In 2 dimensions

Let X,Y be a pair of continuous random variables, and let R be some region of (X,Y) space…

$$P((X,Y)\in R) = \iint_{(x,y)\in R} p(x,y)\,dy\,dx$$

$$p(x,y) = \lim_{h\to 0} \frac{P\left(x-\frac{h}{2} < X \le x+\frac{h}{2} \quad \wedge \quad y-\frac{h}{2} < Y \le y+\frac{h}{2}\right)}{h^2}$$

In m dimensions

Let $(X_1, X_2, \ldots X_m)$ be an n-tuple of continuous random variables, and let R be some region of $\mathbf{R}^m$ …

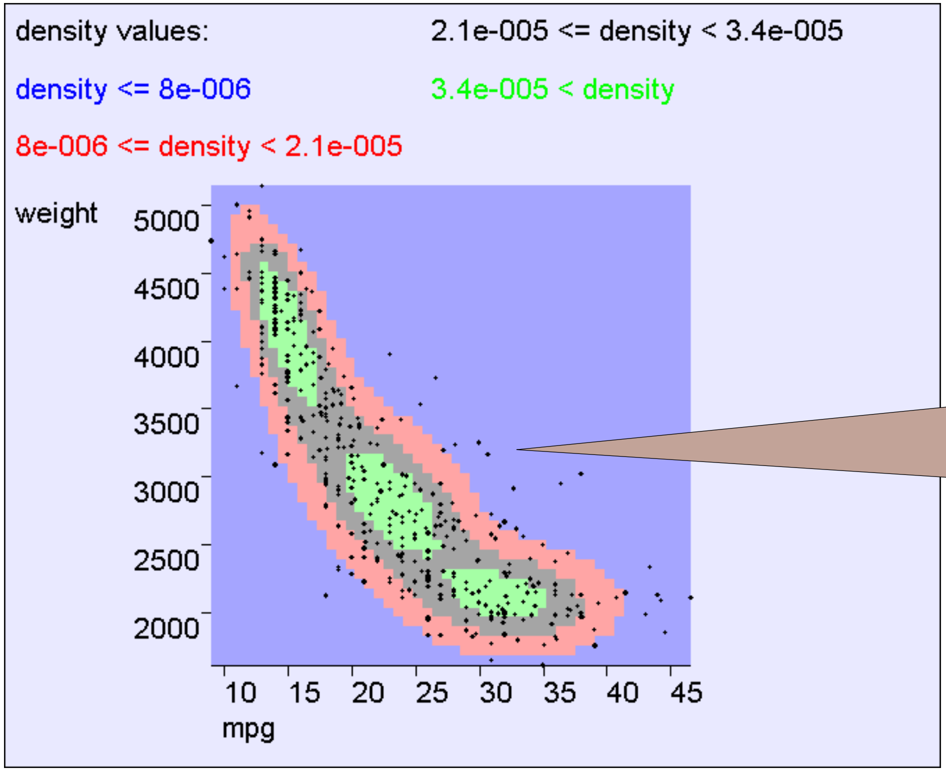
$$P((X_1, X_2, \ldots, X_m) \in R) =$$

$$\underset{(x_1, x_2, \ldots, x_m) \in R}{\iint \cdots \int} p(x_1, x_2, \ldots, x_m)\, dx_m, , \ldots dx_2, dx_1$$

Independence

$$X \perp Y \text{ iff } \forall \mathrm{x}, \mathrm{y} : p(x, y) = p(x)p(y)$$

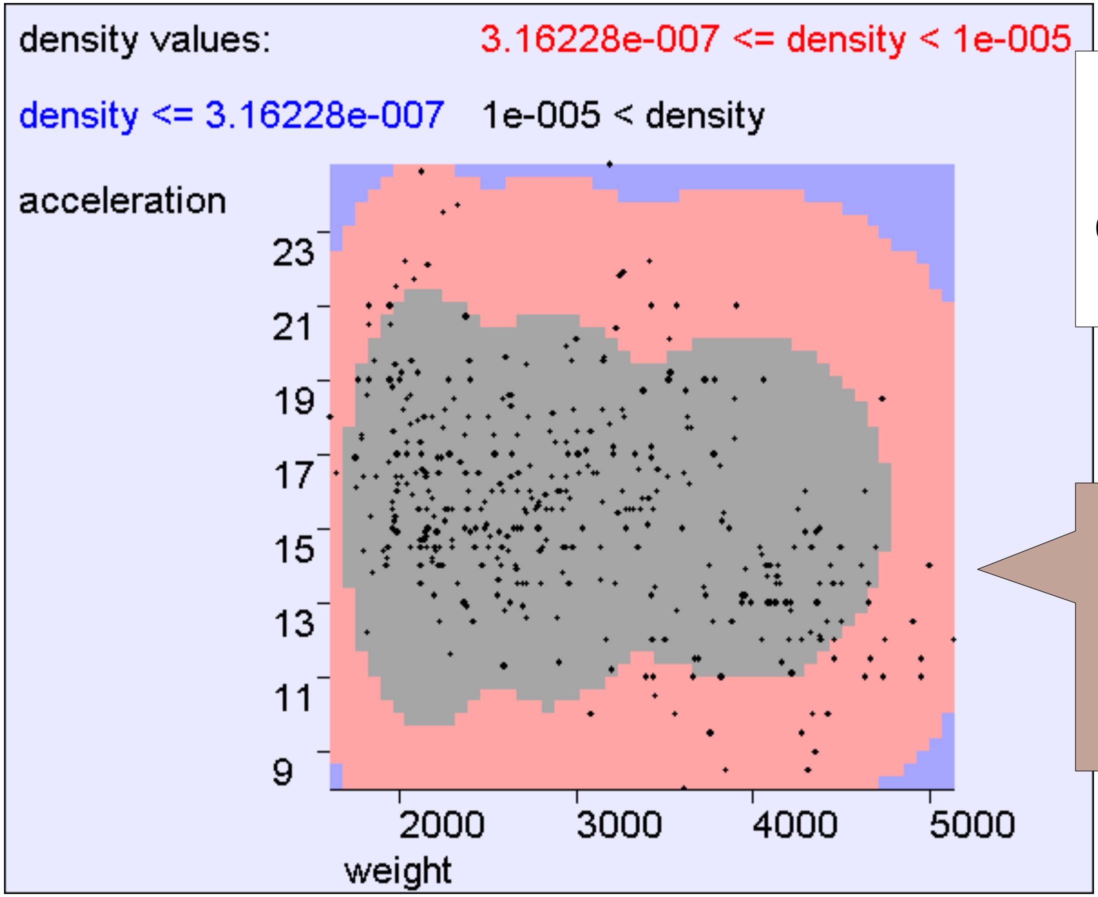
If X and Y are independent then knowing the value of X does not help predict the value of Y



mpg,weight NOT independent

Independence

$$X \perp Y \text{ iff } \forall x, y : p(x,y) = p(x)p(y)$$

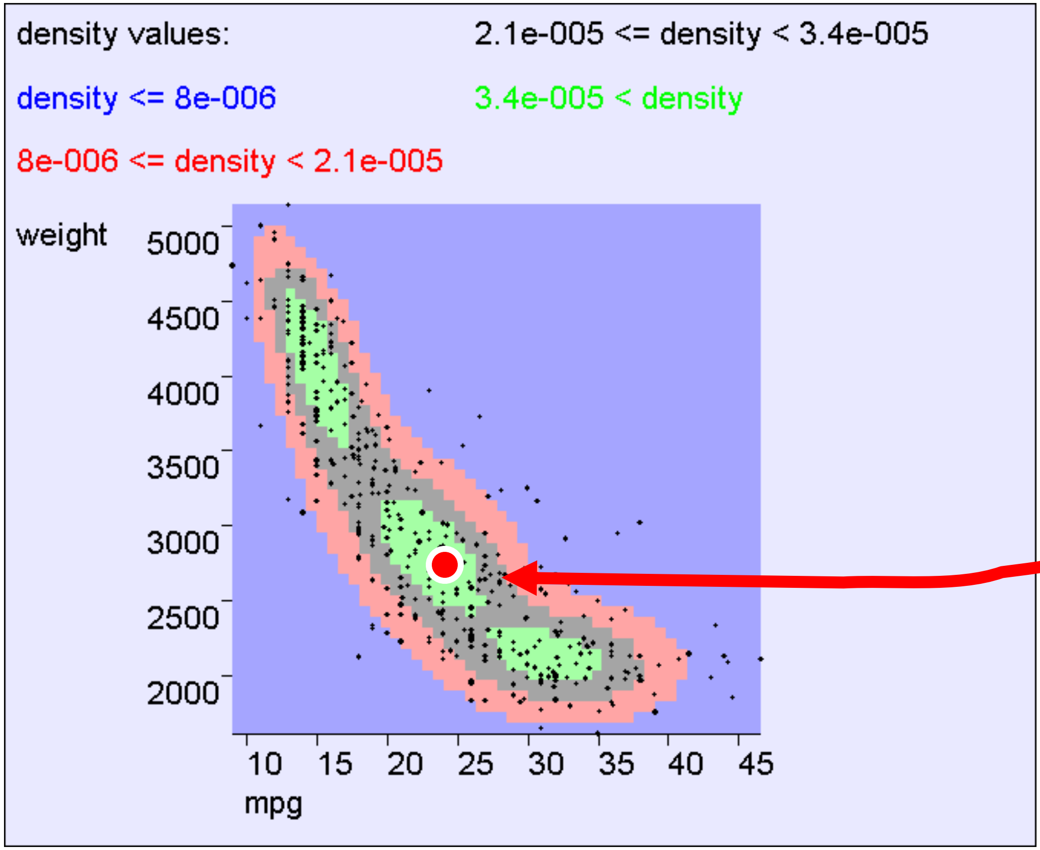


If X and Y are independent then knowing the value of X does not help predict the value of Y

the contours say that acceleration and weight are independent

Multivariate Expectation

$$\boldsymbol{\mu}_{\mathbf{X}} = E[\mathbf{X}] = \int \mathbf{x}\, p(\mathbf{x})\, d\mathbf{x}$$



E[mpg,weight] = (24.5,2600)

The centroid of the cloud

Multivariate Expectation

$$E[f(\mathbf{X})] = \int f(\mathbf{x})\, p(\mathbf{x}) d\mathbf{x}$$

Test your understanding

$$\text{Question : When (if ever) does } E[X+Y] = E[X] + E[Y]\,?$$

- All the time?
- Only when X and Y are independent?
- It can fail even if X and Y are independent?

Bivariate Expectation

$$E[f(x,y)] = \int f(x,y)\ p(x,y)dydx$$

$$\text{if } f(x,y) = x \text{ then } E[f(X,Y)] = \int x\ p(x,y)dydx$$

$$\text{if } f(x,y) = y \text{ then } E[f(X,Y)] = \int y\ p(x,y)dydx$$

$$\text{if } f(x,y) = x + y \text{ then } E[f(X,Y)] = \int (x+y)\ p(x,y)dydx$$

$$E[X+Y] = E[X] + E[Y]$$

Bivariate Covariance

$$\sigma_{xy} = \mathrm{Cov}[X,Y] = E[(X-\mu_x)(Y-\mu_y)]$$

$$\sigma_{xx} = \sigma^2{}_x = \mathrm{Cov}[X,X] = Var[X] = E[(X-\mu_x)^2]$$

$$\sigma_{yy} = \sigma^2{}_y = \mathrm{Cov}[Y,Y] = Var[Y] = E[(Y-\mu_y)^2]$$

Bivariate Covariance

$$\sigma_{xy} = \mathrm{Cov}[X,Y] = E[(X-\mu_x)(Y-\mu_y)]$$

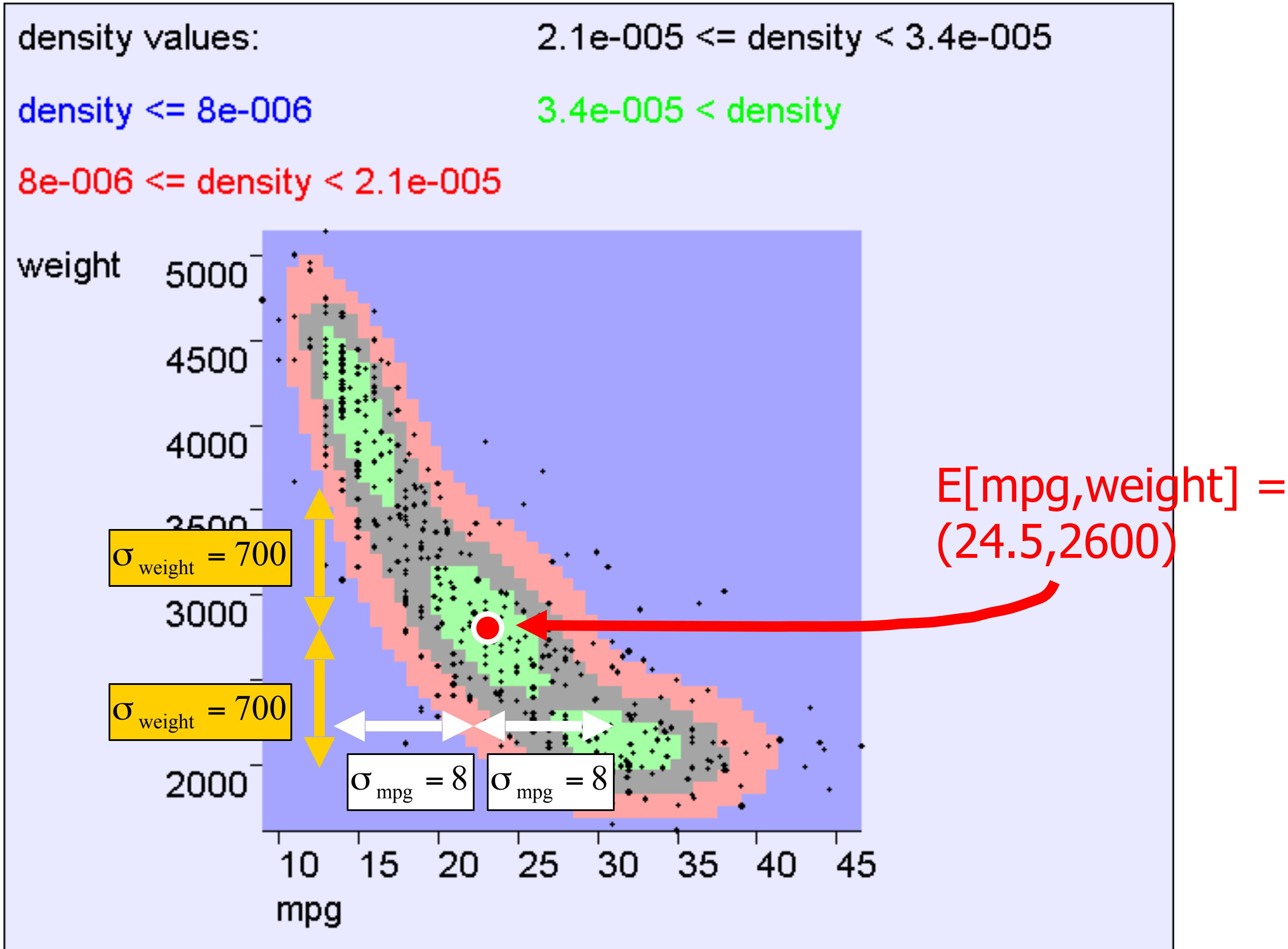
$$\sigma_{xx} = \sigma^2{}_x = \mathrm{Cov}[X,X] = Var[X] = E[(X-\mu_x)^2]$$

$$\sigma_{yy} = \sigma^2{}_y = \mathrm{Cov}[Y,Y] = Var[Y] = E[(Y-\mu_y)^2]$$

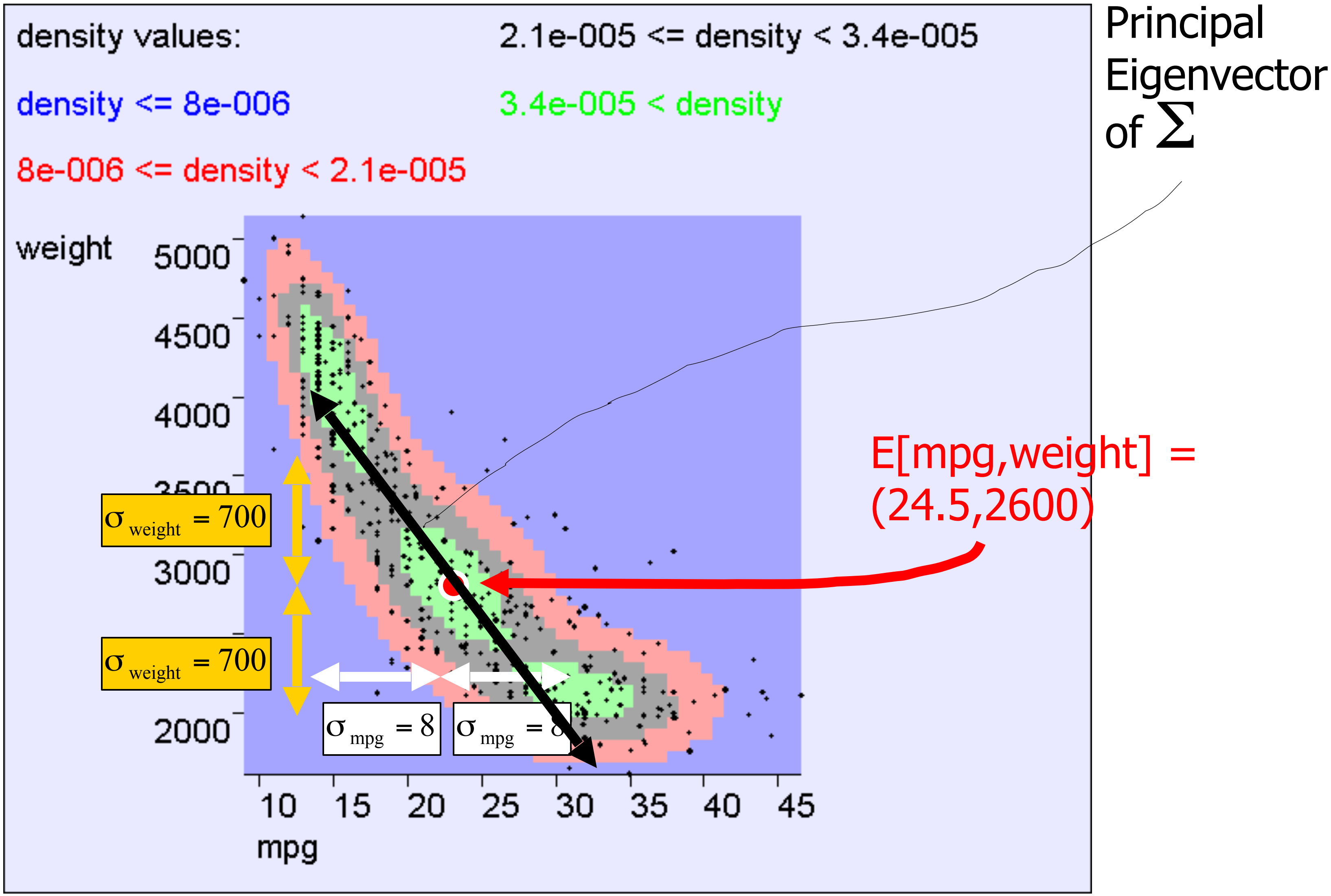
$$\text{Write } \mathbf{X} = \begin{pmatrix} X \\ Y \end{pmatrix}, \text{ then}$$

$$\mathbf{Cov}[\mathbf{X}] = E[(\mathbf{X}-\boldsymbol{\mu}_x)(\mathbf{X}-\boldsymbol{\mu}_x)^T] = \boldsymbol{\Sigma} = \begin{pmatrix} \sigma^2{}_x & \sigma_{xy} \\ \sigma_{xy} & \sigma^2{}_y \end{pmatrix}$$

Covariance Intuition



Covariance Intuition



Covariance Fun Facts

$$\mathbf{Cov}[\mathbf{X}] = E[(\mathbf{X}-\boldsymbol{\mu}_x)(\mathbf{X}-\boldsymbol{\mu}_x)^T] = \boldsymbol{\Sigma} = \begin{pmatrix} \sigma^2_x & \sigma_{xy} \\ \sigma_{xy} & \sigma^2_y \end{pmatrix}$$

- True or False: If $\sigma_{xy} = 0$ then X and Y are independent
- True or False: If X and Y are independent then $\sigma_{xy} = 0$
- True or False: If $\sigma_{xy} = \sigma_x \sigma_y$ then X and Y are deterministically related
- True or False: If X and Y are deterministically related then $\sigma_{xy} = \sigma_x \sigma_y$

How could you prove or disprove these?

General Covariance

Let $\mathbf{X} = (X_1, X_2, \ldots X_k)$ be a vector of k continuous random variables

$$\mathbf{Cov}[\mathbf{X}] = E[(\mathbf{X} - \boldsymbol{\mu}_x)(\mathbf{X} - \boldsymbol{\mu}_x)^T] = \boldsymbol{\Sigma}$$

$$\boldsymbol{\Sigma}_{ij} = Cov[X_i, X_j] = \sigma_{x_i x_j}$$

S is a k x k symmetric non-negative definite matrix

If all distributions are linearly independent it is positive definite

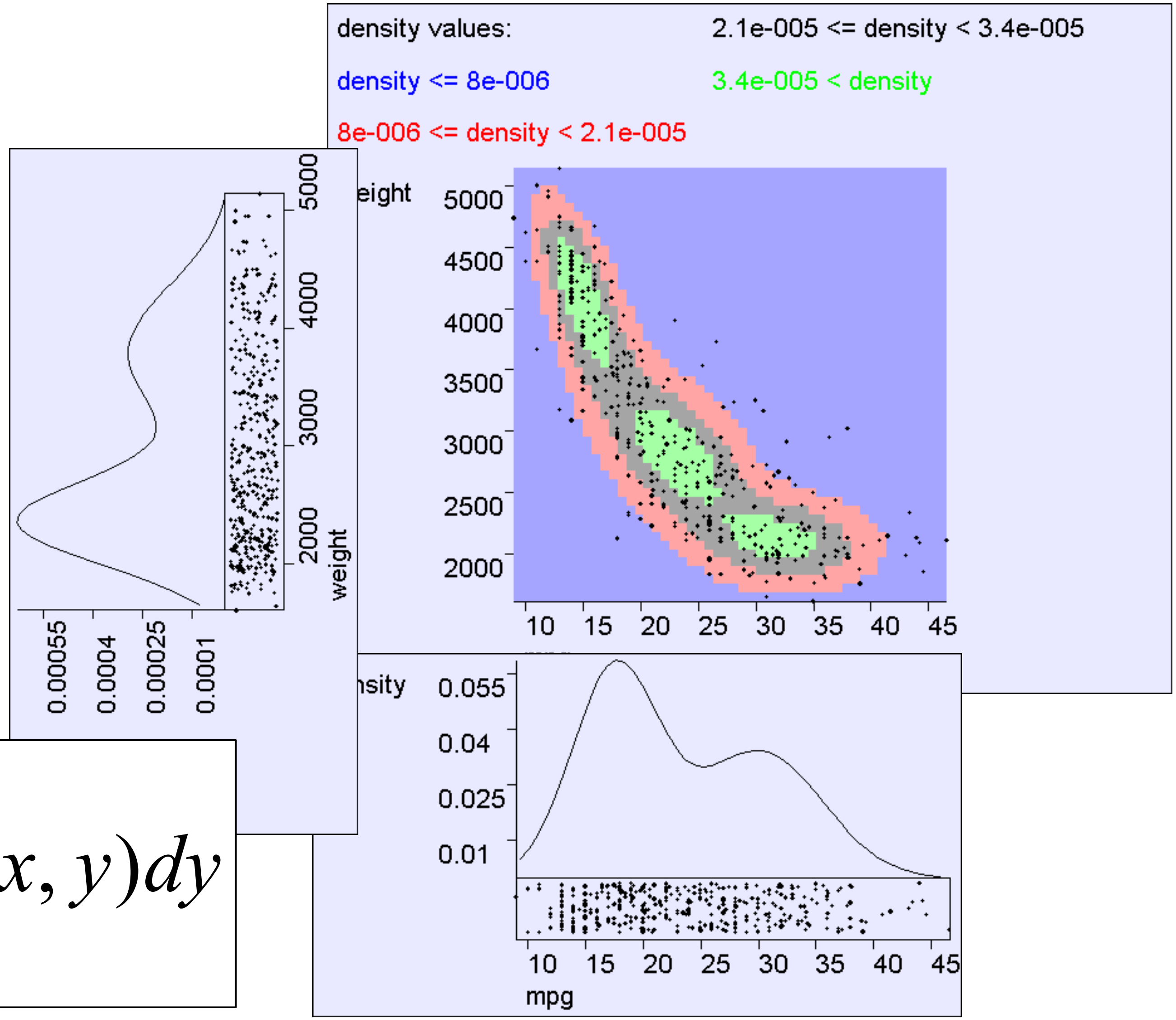
If the distributions are linearly dependent it has determinant zero

Test your understanding

Question : When (if ever) does $Var[X+Y] = Var[X] + Var[Y]$?

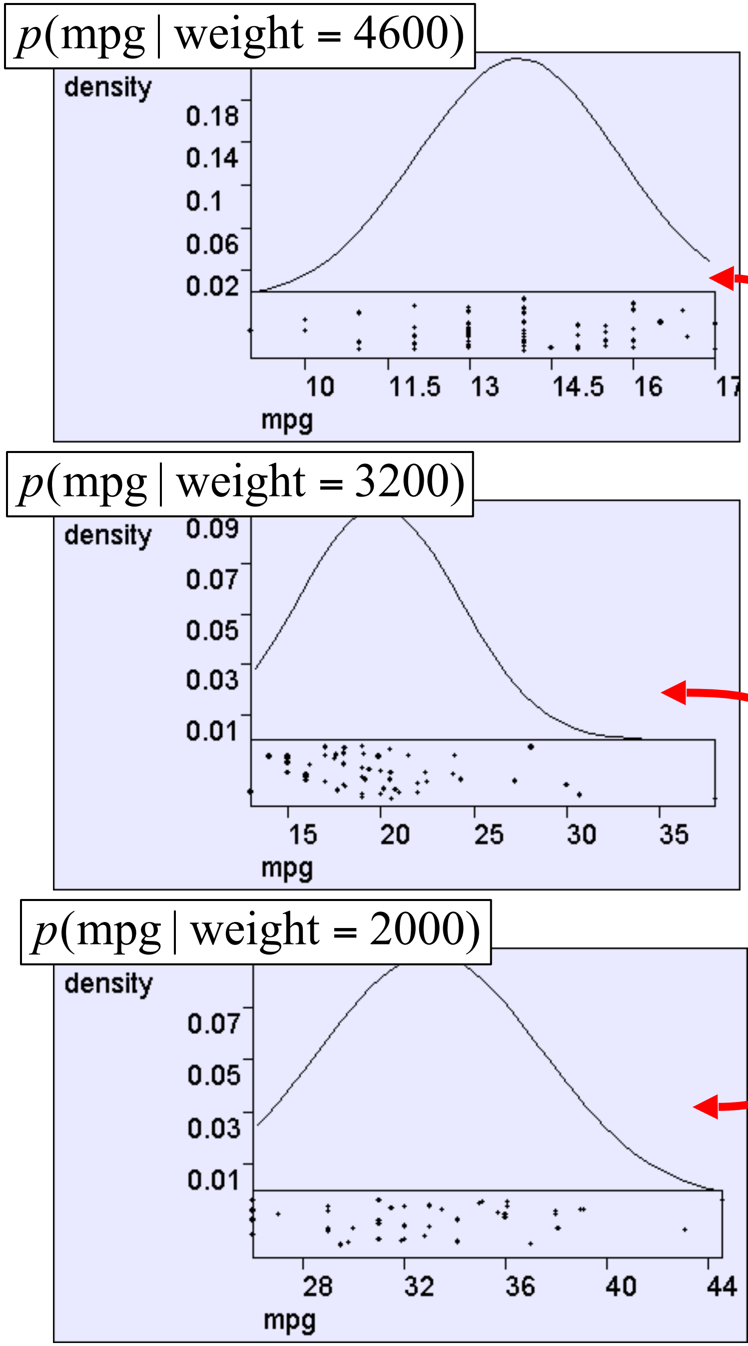
- All the time?
- Only when X and Y are independent?
- It can fail even if X and Y are independent?

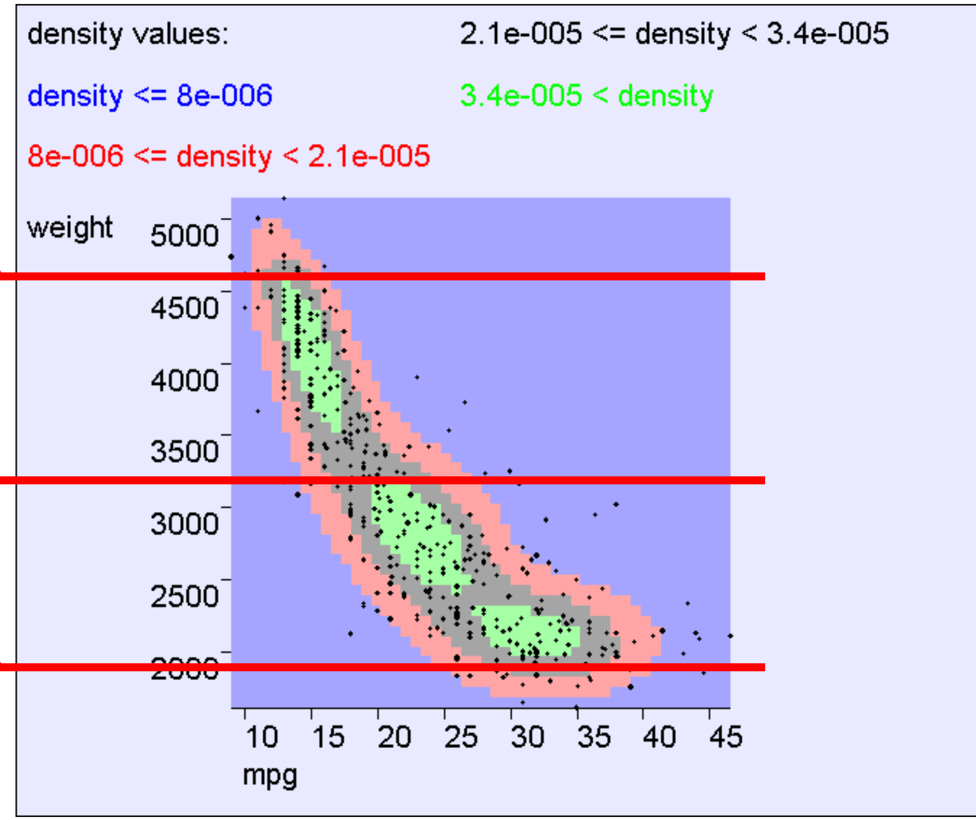
Marginal Distributions



$$p(x) = \int_{y=-\infty}^{\infty} p(x,y)\,dy$$

Conditional Distributions



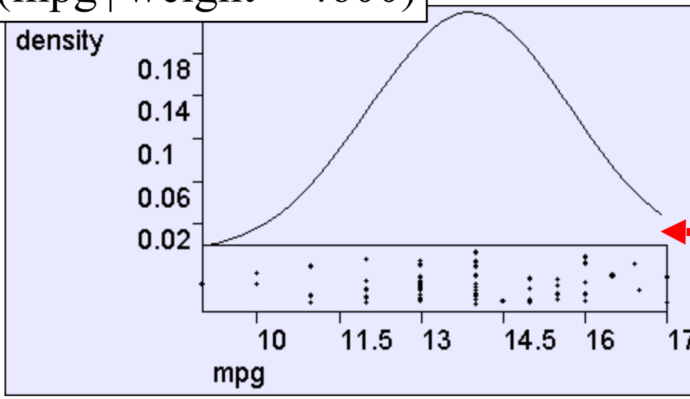


$$p(x \mid y) =$$

$$\text{p.d.f. of } X \text{ when } Y = y$$

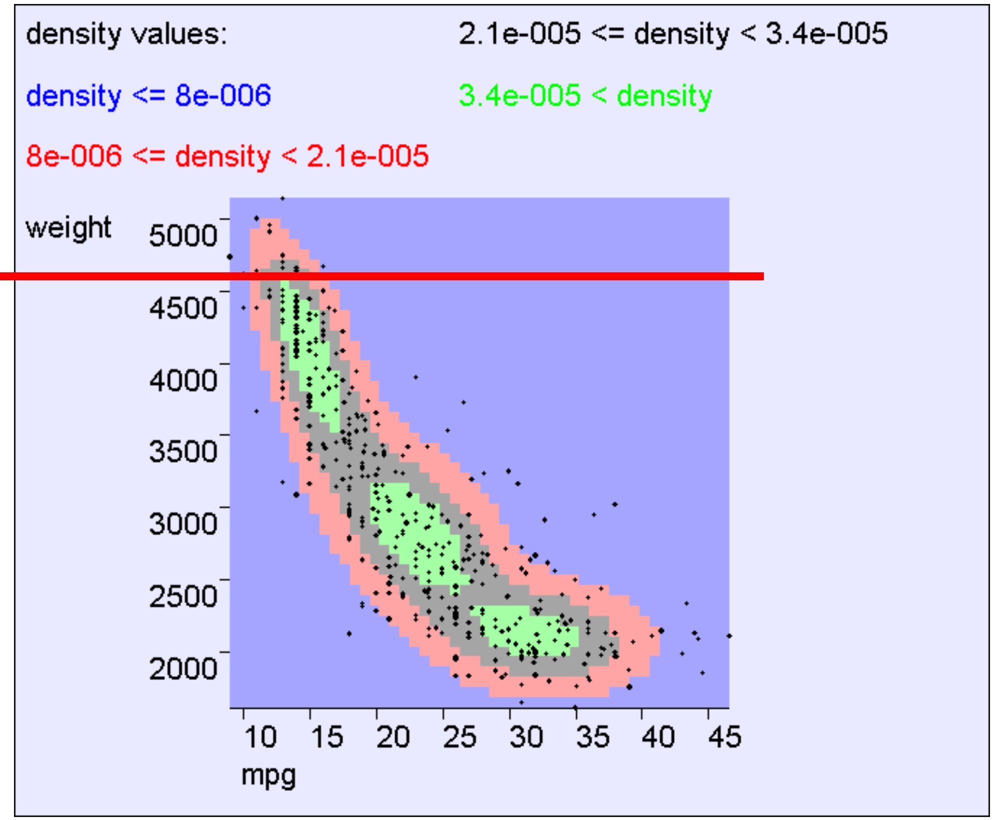
Conditional Distributions

$p(\text{mpg} \mid \text{weight} = 4600)$



$$p(x \mid y) = \frac{p(x, y)}{p(y)}$$

Why?



$$p(x \mid y) = \text{p.d.f. of } X \text{ when } Y = y$$

Independence Revisited

$$X \perp Y \text{ iff } \forall \mathrm{x}, \mathrm{y} : p(x, y) = p(x)p(y)$$

It's easy to prove that these statements are equivalent…

$$\forall \mathrm{x}, \mathrm{y} : p(x, y) = p(x)p(y)$$

$$\Leftrightarrow$$

$$\forall \mathrm{x}, \mathrm{y} : p(x \mid y) = p(x)$$

$$\Leftrightarrow$$

$$\forall \mathrm{x}, \mathrm{y} : p(y \mid x) = p(y)$$

More useful stuff

$$\int_{x=-\infty}^{\infty} p(x \mid y)\,dx = 1$$

(These can all be proved from definitions on previous slides)

$$p(x \mid y, z) = \frac{p(x, y \mid z)}{p(y \mid z)}$$

$$p(x \mid y) = \frac{p(y \mid x)\,p(x)}{p(y)}$$

Bayes Rule

Mixing discrete and continuous variables

$$p(x, A = v) = \lim_{h \to 0} \frac{P\left(x - \frac{h}{2} < X \leq x + \frac{h}{2} \wedge A = v \right)}{h}$$

$$\sum_{v=1}^{n_A} \int_{x=-\infty}^{\infty} p(x, A = v)dx = 1$$

$$p(x \mid A) = \frac{P(A \mid x)p(x)}{P(A)}$$

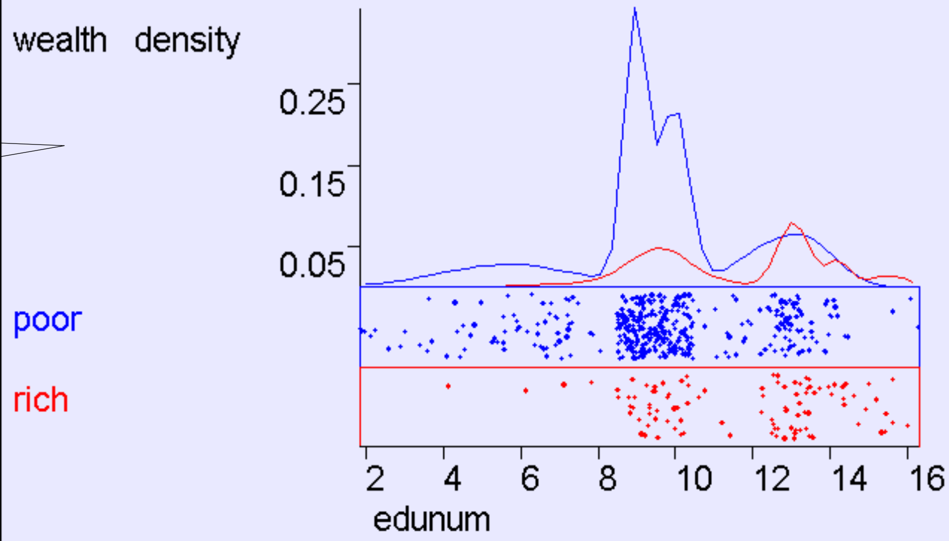
Bayes Rule

$$P(A \mid x) = \frac{p(x \mid A)P(A)}{p(x)}$$

Bayes Rule

Mixing discrete and continuous variables

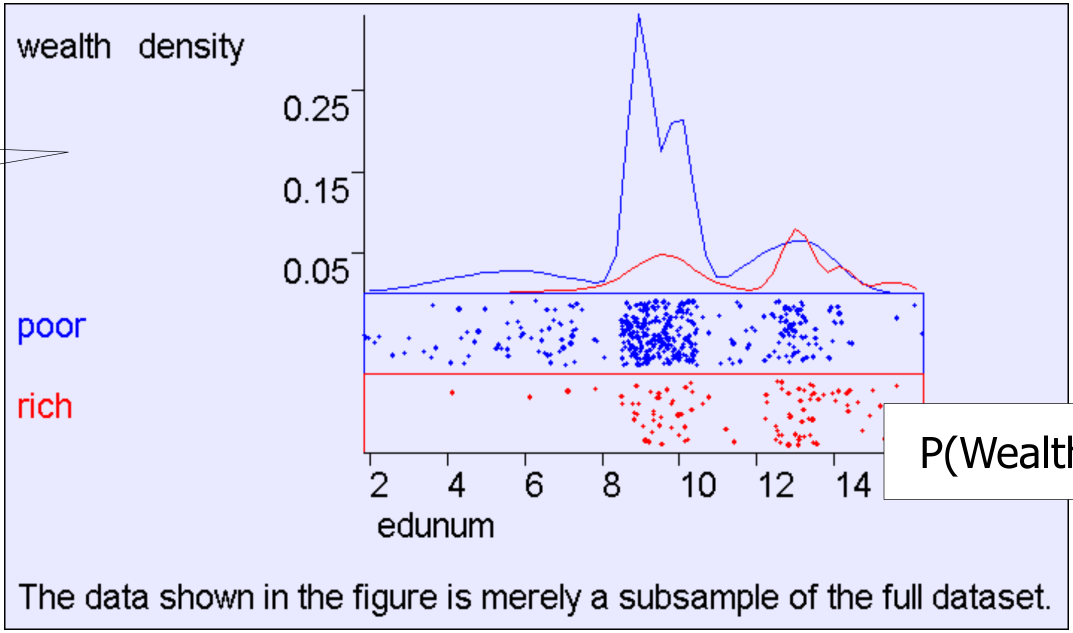
P(EduYears,Wealthy)



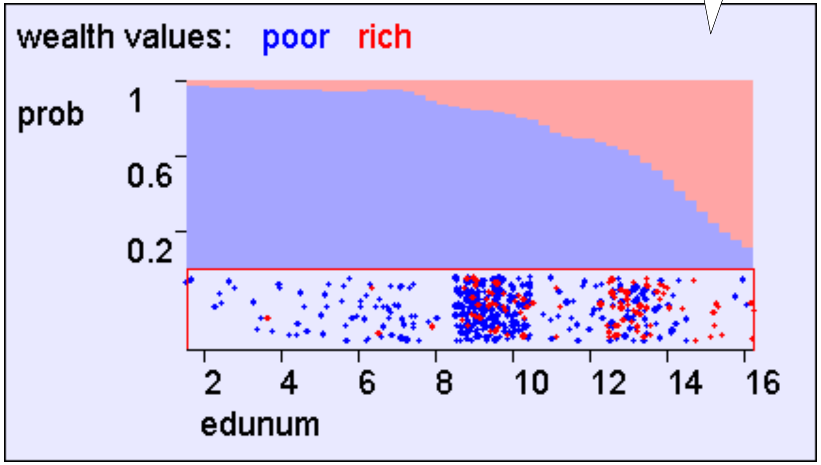
The data shown in the figure is merely a subsample of the full dataset.

Mixing discrete and continuous variables

P(EduYears,Wealthy)

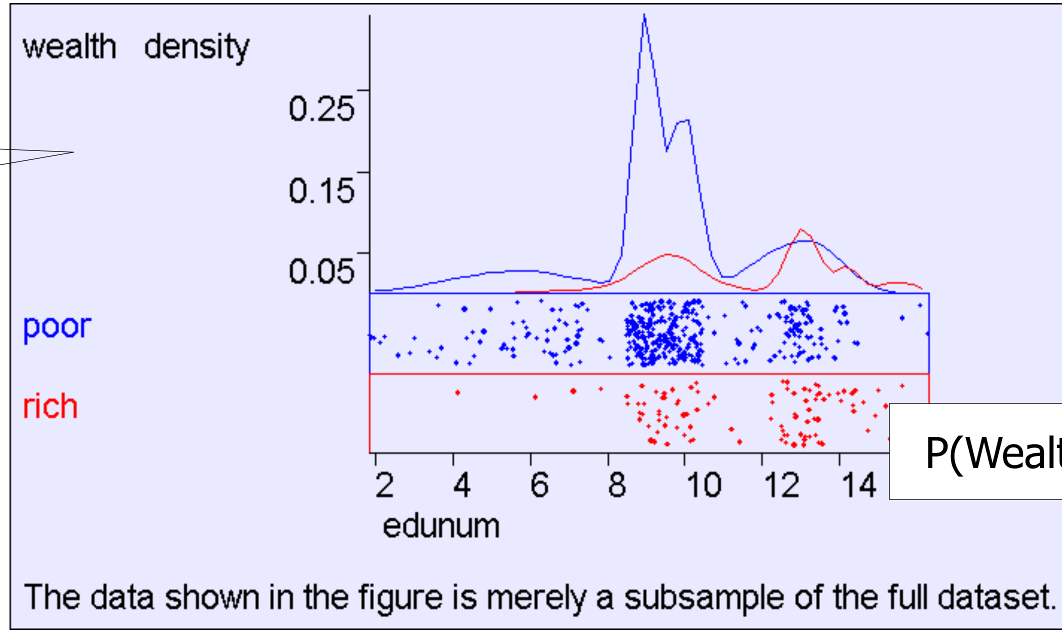


P(Wealthy| EduYears)



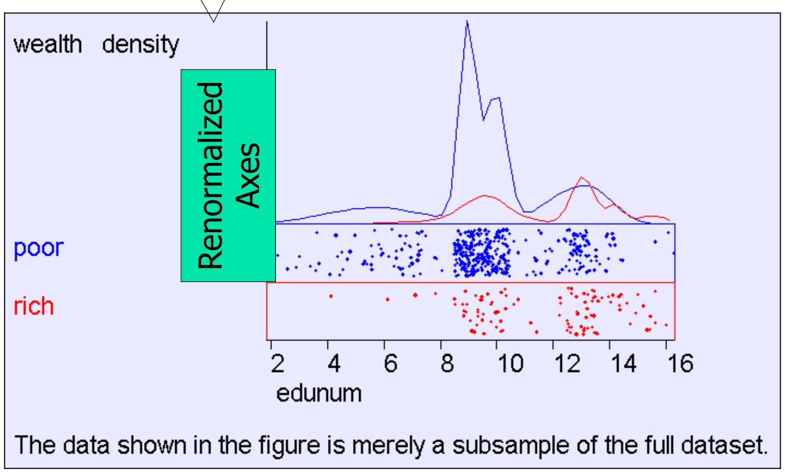
Mixing discrete and continuous variables

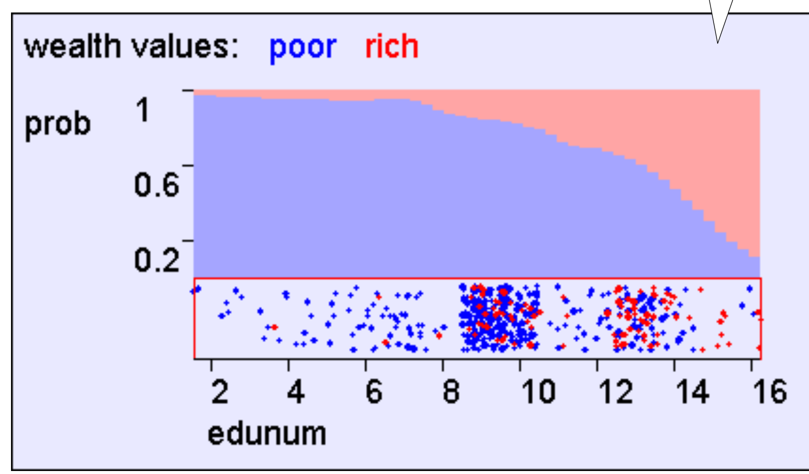
P(EduYears,Wealthy)



P(Wealthy| EduYears)

P(EduYears|Wealthy)





What you should know

- You should be able to play with discrete, continuous and mixed joint distributions
- You should be happy with the difference between p(x) and P(A)
- You should be intimate with expectations of continuous and discrete random variables
- You should smile when you meet a covariance matrix
- Independence and its consequences should be second nature

Discussion

- Are PDFs the only sensible way to handle analysis of real-valued variables?
- Why is covariance an important concept?
- Suppose X and Y are independent real-valued random variables distributed between 0 and 1:
  - What is p[min(X,Y)]?
  - What is E[min(X,Y)]?
- Prove that E[X] is the value u that minimizes E[(X-u)^2]
- What is the value u that minimizes E[|X-u|]?