	RANDOM VARIABLES AND DENSITIES
REVIEW:	\bullet Random variables X represents outcomes or states of world. Instantiations of variables usually in lower case: x
PROBABILITY AND STATISTICS	We will write $p(x)$ to mean probability $(X = x)$.
	 Sample Space: the space of all possible outcomes/states. (May be discrete or continuous or mixed.)
Sam Roweis	• Probability mass (density) function $p(x) \ge 0$ Assigns a non-negative number to each point in sample space. Sums (integrates) to unity: $\sum_x p(x) = 1$ or $\int_x p(x)dx = 1$. Intuitively: how often does x occur, how much do we believe in x .
	• Ensemble: random variable + sample space+ probability function
October 2, 2002	
Probability	Expectations, Moments
• We use probabilities $p(x)$ to represent our beliefs $B(x)$ about the states x of the world.	• Expectation of a function $a(x)$ is written $E[a]$ or $\langle a \rangle$
 There is a formal calculus for manipulating uncertainties represented by probabilities. 	$E[a] = \langle a \rangle = \sum_{x} p(x)a(x)$
• Any consistent set of beliefs obeying the <i>Cox Axioms</i> can be	e.g. mean = $\sum_{x} x p(x)$, variance = $\sum_{x} (x - E[x])^2 p(x)$
mapped into probabilities.	 Moments are expectations of higher order powers. (Mean is first moment. Autocorrelation is second moment.)
1. Rationally ordered degrees of belief:	

• Centralized moments have lower moments subtracted away

• Deep fact: Knowledge of all orders of moments

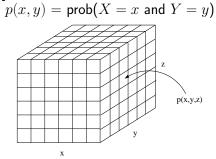
completely defines the entire distribution.

(e.g. variance, skew, curtosis).

- 1. Rationally ordered degrees of belief: if B(x) > B(y) and B(y) > B(z) then B(x) > B(z)
- 2. Belief in x and its negation \bar{x} are related: $B(x) = f[B(\bar{x})]$
- 3. Belief in conjunction depends only on conditionals: B(x and y) = g[B(x), B(y|x)] = g[B(y), B(x|y)]

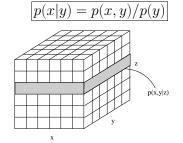
JOINT PROBABILITY

- Key concept: two or more random variables may interact. Thus, the probability of one taking on a certain value depends on which value(s) the others are taking.
- We call this a joint ensemble and write



CONDITIONAL PROBABILITY

- If we know that some event has occurred, it changes our belief about the probability of other events.
- This is like taking a "slice" through the joint table.

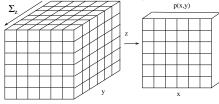


MARGINAL PROBABILITIES

• We can "sum out" part of a joint distribution to get the *marginal distribution* of a subset of variables:

$$p(x) = \sum_{y} p(x, y)$$

• This is like adding slices of the table together.



• Another equivalent definition: $p(x) = \sum_y p(x|y)p(y)$.

BAYES' RULE

• Manipulating the basic definition of conditional probability gives one of the most important formulas in probability theory:

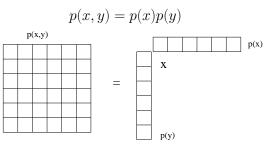
$$p(x|y) = \frac{p(y|x)p(x)}{p(y)} = \frac{p(y|x)p(x)}{\sum_{x'} p(y|x')p(x')}$$

- This gives us a way of "reversing" conditional probabilities.
- Thus, all joint probabilities can be factored by selecting an ordering for the random variables and using the "chain rule":

$$p(x, y, z, \ldots) = p(x)p(y|x)p(z|x, y)p(\ldots | x, y, z)$$

INDEPENDENCE & CONDITIONAL INDEPENDENCE

• Two variables are independent iff their joint factors:



• Two variables are conditionally independent given a third one if for all values of the conditioning variable, the resulting slice factors:

 $p(x,y|z) = p(x|z)p(y|z) \qquad \forall z$

BE CAREFUL!

• Watch the context:

e.g. Simpson's paradox

- \bullet Define random variables and sample spaces carefully:
- e.g. Prisoner's paradox

ENTROPY

• Measures the amount of ambiguity or uncertainty in a distribution:

$$H(p) = -\sum_{x} p(x) \log p(x)$$

- Expected value of $-\log p(x)$ (a function which depends on p(x)!).
- H(p) > 0 unless only one possible outcomein which case H(p) = 0.
- Maximal value when p is uniform.
- Tells you the expected "cost" if each event costs $-\log p(\mathsf{event})$

CROSS ENTROPY (KL DIVERGENCE)

• An assymetric measure of the distancebetween two distributions:

$$KL[p||q] = \sum_{x} p(x)[\log p(x) - \log q(x)]$$

- KL > 0 unless p = q then KL = 0
- Tells you the extra cost if events were generated by p(x) but instead of charging under p(x) you charged under q(x).

STATISTICS

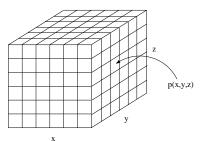
- Probability: inferring probabilistic quantities for data given fixed models (e.g. prob. of events, marginals, conditionals, etc).
- Statistics: inferring a model given fixed data observations (e.g. clustering, classification, regression).
- Many approaches to statistics: frequentist, Bayesian, decision theory, ...

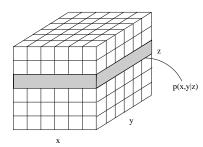
Some (Conditional) Probability Functions

- Probability density functions p(x) (for continuous variables) or probability mass functions p(x = k) (for discrete variables) tell us how likely it is to get a particular value for a random variable (possibly conditioned on the values of some other variables.)
- We can consider various types of variables: binary/discrete (categorical), continuous, interval, and integer counts.
- For each type we'll see some basic *probability models* which are parametrized families of distributions.

(Conditional) Probability Tables

- For discrete (categorical) quantities, the most basic parametrization is the probability table which lists $p(x_i = k^{th} \text{ value})$.
- Since PTs must be nonnegative and sum to 1, for k-ary variables there are k 1 free parameters.
- If a discrete variable is conditioned on the values of some other discrete variables we make one table for each possible setting of the parents: these are called *conditional probability tables* or CPTs.





EXPONENTIAL FAMILY

 \bullet For (continuous or discrete) random variable ${\bf x}$

$$p(\mathbf{x}|\eta) = h(\mathbf{x}) \exp\{\eta^{\top} T(\mathbf{x}) - A(\eta)\}$$
$$= \frac{1}{Z(\eta)} h(\mathbf{x}) \exp\{\eta^{\top} T(\mathbf{x})\}$$

is an exponential family distribution with natural parameter η .

- Function $T(\mathbf{x})$ is a *sufficient statistic*.
- Function $A(\eta) = \log Z(\eta)$ is the log normalizer.
- \bullet Key idea: all you need to know about the data is captured in the summarizing function $T({\bf x}).$

Bernoulli

• For a binary random variable with $p(heads)=\pi$:

$$p(x|\pi) = \pi^x (1-\pi)^{1-x}$$
$$= \exp\left\{\log\left(\frac{\pi}{1-\pi}\right)x + \log(1-\pi)\right\}$$

• Exponential family with:

$$\eta = \log \frac{\pi}{1 - \pi}$$

$$T(x) = x$$

$$A(\eta) = -\log(1 - \pi) = \log(1 + e^{\eta})$$

$$h(x) = 1$$

• The logistic function relates the natural parameter and the chance of heads

$$\pi = \frac{1}{1 + e^{-\eta}}$$

Poisson

• For an integer count variable with rate λ :

$$p(x|\lambda) = \frac{\lambda^{x} e^{-\lambda}}{x!}$$
$$= \frac{1}{x!} \exp\{x \log \lambda - \lambda\}$$

• Exponential family with:

$$\eta = \log \lambda$$
$$T(x) = x$$
$$A(\eta) = \lambda = e^{\eta}$$
$$h(x) = \frac{1}{x!}$$

- \bullet e.g. number of photons ${\bf x}$ that arrive at a pixel during a fixed interval given mean intensity λ
- Other count densities: binomial, exponential.

Multinomial

 \bullet For a set of integer counts on k trials

$$p(\mathbf{x}|\pi) = \frac{k!}{x_1! x_2! \cdots x_n!} \pi_1^{x_1} \pi_2^{x_2} \cdots \pi_n^{x_n} = h(\mathbf{x}) \exp\left\{\sum_i x_i \log \pi_i\right\}$$

• But the parameters are constrained: $\sum_{i} \pi_{i} = 1$. So we define the last one $\pi_{n} = 1 - \sum_{i=1}^{n-1} \pi_{i}$.

$$p(\mathbf{x}|\pi) = h(\mathbf{x}) \exp\left\{\sum_{i=1}^{n-1} \log\left(\frac{\pi_i}{\pi_n}\right) x_i + k \log \pi_n\right\}$$

٦

• Exponential family with:

$$\eta_i = \log \pi_i - \log \pi_n$$

$$T(x_i) = x_i$$

$$A(\eta) = -k \log \pi_n = k \log \sum_i e^{\eta_i}$$

$$h(\mathbf{x}) = k!/x_1!x_2! \cdots x_n!$$

• The *softmax* function relates the basic and natural parameters:

$$\pi_i = \frac{e^{\eta_i}}{\sum_j e^{\eta_j}}$$

GAUSSIAN (NORMAL)

• For a continuous univariate random variable:

$$p(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$
$$= \frac{1}{\sqrt{2\pi\sigma}} \exp\left\{\frac{\mu x}{\sigma^2} - \frac{x^2}{2\sigma^2} - \frac{\mu^2}{2\sigma^2} - \log\sigma\right\}$$

• Exponential family with:

$$\eta = [\mu/\sigma^2; -1/2\sigma^2]$$
$$T(x) = [x; x^2]$$
$$A(\eta) = \log \sigma + \mu/2\sigma^2$$
$$h(x) = 1/\sqrt{2\pi}$$

• Note: a univariate Gaussian is a two-parameter distribution with a two-component vector of sufficient statistis.

Multivariate Gaussian Distribution

• For a continuous vector random variable:

$$p(x|\mu, \Sigma) = |2\pi\Sigma|^{-1/2} \exp\left\{-\frac{1}{2}(\mathbf{x}-\mu)^{\top}\Sigma^{-1}(\mathbf{x}-\mu)\right\}$$

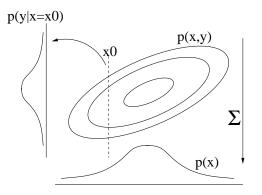
• Exponential family with:

$$\eta = [\Sigma^{-1}\mu; -1/2\Sigma^{-1}]$$
$$T(x) = [\mathbf{x}; \mathbf{x}\mathbf{x}^{\top}]$$
$$A(\eta) = \log |\Sigma|/2 + \mu^{\top}\Sigma^{-1}\mu/2$$
$$h(x) = (2\pi)^{-n/2}$$

- Sufficient statistics: mean vector and correlation matrix.
- Other densities: Student-t, Laplacian.
- For non-negative values use exponential, Gamma, log-normal.

Important Gaussian Facts

• All marginals of a Gaussian are again Gaussian. Any conditional of a Gaussian is again Gaussian.



GAUSSIAN MARGINALS/CONDITIONALS

• To find these parameters is mostly linear algebra: Let $\mathbf{z} = [\mathbf{x}^\top \mathbf{y}^\top]^\top$ be normally distributed according to:

$$\mathbf{z} = \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}; \begin{bmatrix} \mathbf{A} & \mathbf{C} \\ \mathbf{C}^\top & \mathbf{B} \end{bmatrix} \right)$$

where C is the (non-symmetric) cross-covariance matrix between x and y which has as many rows as the size of x and as many columns as the size of y.

The marginal distributions are:

$$\begin{aligned} \mathbf{x} &\sim \mathcal{N}(\mathbf{a}; \mathbf{A}) \\ \mathbf{y} &\sim \mathcal{N}(\mathbf{b}; \mathbf{B}) \end{aligned}$$

and the conditional distributions are:

$$\begin{split} \mathbf{x} | \mathbf{y} &\sim \mathcal{N}(\mathbf{a} + \mathbf{C}\mathbf{B}^{-1}(\mathbf{y} - \mathbf{b}); \mathbf{A} - \mathbf{C}\mathbf{B}^{-1}\mathbf{C}^{\top}) \\ \mathbf{y} | \mathbf{x} &\sim \mathcal{N}(\mathbf{b} + \mathbf{C}^{\top}\mathbf{A}^{-1}(\mathbf{x} - \mathbf{a}); \mathbf{B} - \mathbf{C}^{\top}\mathbf{A}^{-1}\mathbf{C}) \end{split}$$

Moments

- For continuous variables, moment calculations are important.
- We can easily compute moments of any exponential family distribution by taking the derivatives of the log normalizer $A(\eta)$.
- The q^{th} derivative gives the q^{th} centred moment.

$$\frac{dA(\eta)}{d\eta} = \text{mean}$$
$$\frac{d^2A(\eta)}{d\eta^2} = \text{variance}$$

• When the sufficient statistic is a vector, partial derivatives need to be considered.

PARAMETERIZING CONDITIONALS

- When the variable(s) being conditioned on (parents) are discrete, we just have one density for each possible setting of the parents. e.g. a table of natural parameters in exponential models or a table of tables for discrete models.
- When the conditioned variable is continuous, its value sets some of the parameters for the other variables.
- A very common instance of this for regression is the "linear-Gaussian": $p(\mathbf{y}|\mathbf{x}) = \text{gauss}(\theta^{\top}\mathbf{x}; \Sigma)$.
- For discrete children and continuous parents, we often use a Bernoulli/multinomial whose paramters are some function $f(\theta^{\top}\mathbf{x})$.

GENERALIZED LINEAR MODELS (GLMS)

- Generalized Linear Models: $p(\mathbf{y}|\mathbf{x})$ is exponential family with conditional mean $\mu = f(\theta^{\top}\mathbf{x})$.
- The function f is called the *response function*.
- If we chose f to be the inverse of the mapping b/w conditional mean and natural parameters then it is called the *canonical response function*.

$$\eta = \psi(\mu)$$
$$f(\cdot) = \psi^{-1}(\cdot)$$

POTENTIAL FUNCTIONS

• We can be even more general and define distributions by arbitrary *energy* functions proportional to the log probability.

$$p(\mathbf{x}) \propto \exp\{-\sum_k H_k(\mathbf{x})\}$$

• A common choice is to use pairwise terms in the energy:

$$H(\mathbf{x}) = \sum_{i} a_{i}x_{i} + \sum_{\text{pairs } ij} w_{ij}x_{i}x_{j}$$

Special variables

- If certain variables are *always observed* we may not want to model their density. For example inputs in regression or classification. This leads to conditional density estimation.
- If certain variables are *always unobserved*, they are called *hidden* or *latent* variables. They can always be marginalized out, but can make the density modeling of the observed variables easier.
 (We'll see more on this later.)

Multiple Observations, Complete Data, IID Sampling

- \bullet A single observation of the data ${\bf X}$ is rarely useful on its own.
- Generally we have data including many observations, which creates a set of random variables: $\mathcal{D} = \{\mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^M\}$
- Two very common assumptions:
- 1. Observations are independently and identically distributed according to joint distribution of graphical model: IID samples.
- 2. We observe all random variables in the domain on each observation: complete data.

LIKELIHOOD FUNCTION

- So far we have focused on the (log) probability function $p(\mathbf{x}|\theta)$ which assigns a probability (density) to any joint configuration of variables \mathbf{x} given fixed parameters θ .
- But in learning we turn this on its head: we have some fixed data and we want to find parameters.
- Think of $p(\mathbf{x}|\theta)$ as a function of θ for fixed \mathbf{x} :

$$L(\theta; \mathbf{x}) = p(\mathbf{x}|\theta)$$

 $\ell(\theta; \mathbf{x}) = \log p(\mathbf{x}|\theta)$

This function is called the (log) "likelihood".

- Chose θ to maximize some cost function $c(\theta)$ which includes $\ell(\theta)$:
- $c(\theta) = \ell(\theta; D)$ maximum likelihood (ML) $c(\theta) = \ell(\theta; D) + r(\theta)$ maximum a posteriori (MAP)/penalizedML (also cross-validation, Bayesian estimators, BIC, AIC, ...)

Maximum Likelihood

• For IID data:

$$p(\mathcal{D}|\theta) = \prod_{m} p(\mathbf{x}^{m}|\theta)$$
$$\ell(\theta; \mathcal{D}) = \sum_{m} \log p(\mathbf{x}^{m}|\theta)$$

• Idea of maximum likelihod estimation (MLE): pick the setting of parameters most likely to have generated the data we saw:

$$\theta_{\mathrm{ML}}^* = \operatorname{argmax}_{\theta} \ell(\theta; \mathcal{D})$$

• Very commonly used in statistics. Often leads to "intuitive", "appealing", or "natural" estimators.

Example: Bernoulli Trials

- We observe M iid coin flips: $\mathcal{D}=H,H,T,H,\ldots$
- Model: $p(H) = \theta$ $p(T) = (1 \theta)$
- Likelihood:

$$\ell(\theta; \mathcal{D}) = \log p(\mathcal{D}|\theta)$$

= $\log \prod_{m} \theta^{\mathbf{x}^{m}} (1-\theta)^{1-\mathbf{x}^{m}}$
= $\log \theta \sum_{m} \mathbf{x}^{m} + \log(1-\theta) \sum_{m} (1-\mathbf{x}^{m})$
= $\log \theta N_{\mathrm{H}} + \log(1-\theta) N_{\mathrm{T}}$

• Take derivatives and set to zero:

$$\frac{\partial \ell}{\partial \theta} = \frac{N_{\rm H}}{\theta} - \frac{N_{\rm T}}{1 - \theta}$$
$$\Rightarrow \theta_{\rm ML}^* = \frac{N_{\rm H}}{N_{\rm H} + N_{\rm T}}$$

Example: Multinomial

- We observe M iid die rolls (K-sided): $\mathcal{D}=3,1,K,2,\ldots$
- Model: $p(k) = \theta_k$ $\sum_k \theta_k = 1$
- Likelihood (for binary indicators $[\mathbf{x}^m = k]$):

$$\ell(\theta; \mathcal{D}) = \log p(\mathcal{D}|\theta)$$

= $\log \prod_{m} \theta_{\mathbf{x}^{m}} = \log \prod_{m} \theta_{1}^{[\mathbf{x}^{m}=1]} \dots \theta_{k}^{[\mathbf{x}^{m}=k]}$
= $\sum_{k} \log \theta_{k} \sum_{m} [\mathbf{x}^{m} = k] = \sum_{k} N_{k} \log \theta_{k}$

 \bullet Take derivatives and set to zero (enforcing $\sum_k \theta_k = 1)$:

$$\frac{\partial \ell}{\partial \theta_k} = \frac{N_k}{\theta_k} - M$$
$$\Rightarrow \theta_k^* = \frac{N_k}{M}$$

Example: Univariate Normal

- We observe M iid real samples: $\mathcal{D}{=}1.18,\text{-}.25,.78,\ldots$
- Model: $p(x) = (2\pi\sigma^2)^{-1/2} \exp\{-(x-\mu)^2/2\sigma^2\}$
- Likelihood (using probability density):

$$\ell(\theta; \mathcal{D}) = \log p(\mathcal{D}|\theta)$$
$$= -\frac{M}{2}\log(2\pi\sigma^2) - \frac{1}{2}\sum_m \frac{(x^m - \mu)^2}{\sigma^2}$$

• Take derivatives and set to zero:

$$\begin{aligned} \frac{\partial \ell}{\partial \mu} &= (1/\sigma^2) \sum_m (x_m - \mu) \\ \frac{\partial \ell}{\partial \sigma^2} &= -\frac{M}{2\sigma^2} + \frac{1}{2\sigma^4} \sum_m (x_m - \mu)^2 \\ \Rightarrow \mu_{\rm ML} &= (1/M) \sum_m x_m \\ \sigma_{\rm ML}^2 &= (1/M) \sum_m x_m^2 - \mu_{\rm ML}^2 \end{aligned}$$

EXAMPLE: UNIVARIATE NORMAL

EXAMPLE: LINEAR REGRESSION

- In linear regression, some inputs (covariates, parents) and all outputs (responses, children) are continuous valued variables.
- For each child and setting of discrete parents we use the model:

$$p(y|\mathbf{x}, \theta) = \text{gauss}(y|\theta^{\top}\mathbf{x}, \sigma^2)$$

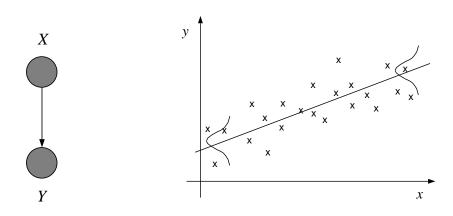
• The likelihood is the familiar "squared error" cost:

$$\ell(\theta; \mathcal{D}) = -\frac{1}{2\sigma^2} \sum_{m} (y^m - \theta^\top \mathbf{x}^m)^2$$

 \bullet The ML parameters can be solved for using linear least-squares:

$$\begin{aligned} \frac{\partial \ell}{\partial \theta} &= -\sum_{m} (y^m - \theta^\top \mathbf{x}^m) \mathbf{x}^m \\ \Rightarrow \theta^*_{\mathrm{ML}} &= (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{Y} \end{aligned}$$

EXAMPLE: LINEAR REGRESSION



SUFFICIENT STATISTICS

- A statistic is a function of a random variable.
- $\bullet \ T(\mathbf{X})$ is a "sufficient statistic" for \mathbf{X} if

$$T(\mathbf{x}^1) = T(\mathbf{x}^2) \quad \Rightarrow \quad L(\theta; \mathbf{x}^1) = L(\theta; \mathbf{x}^2) \quad \forall \theta$$

 \bullet Equivalently (by the Neyman factorization theorem) we can write:

 $p(\mathbf{x}|\theta) = h\left(\mathbf{x}, T(\mathbf{x})\right) g\left(T(\mathbf{x}), \theta\right)$

• Example: exponential family models:

$$p(\mathbf{x}|\theta) = h(\mathbf{x}) \exp\{\eta^{\top} T(\mathbf{x}) - A(\eta)\}$$

SUFFICIENT STATISTICS ARE SUMS

- In the examples above, the sufficient statistics were merely sums (counts) of the data: Bernoulli: # of heads, tails Multinomial: # of each type Gaussian: mean, mean-square Regression: correlations
- As we will see, this is true for all exponential family models: sufficient statistics are average natural parameters.
- Only exponential family models have simple sufficient statistics.

MLE FOR EXPONENTIAL FAMILY MODELS

• Recall the probability function for exponential models:

$$p(\mathbf{x}|\theta) = h(\mathbf{x}) \exp\{\eta^{\top} T(\mathbf{x}) - A(\eta)\}$$

• For iid data, sufficient statistic is $\sum_m T(\mathbf{x}^m)$:

$$\ell(\eta; \mathcal{D}) = \log p(\mathcal{D}|\eta) = \left(\sum_{m} \log h(\mathbf{x}^m)\right) - MA(\eta) + \left(\eta^\top \sum_{m} T(\mathbf{x}^m)\right)$$

• Take derivatives and set to zero:

$$\begin{split} \frac{\partial \ell}{\partial \eta} &= \sum_m T(\mathbf{x}^m) - M \frac{\partial A(\eta)}{\partial \eta} \\ \Rightarrow \frac{\partial A(\eta)}{\partial \eta} &= \frac{1}{M} \sum_m T(\mathbf{x}^m) \\ \eta_{\text{ML}} &= \frac{1}{M} \sum_m T(\mathbf{x}^m) \end{split}$$

recalling that the natural moments of an exponential distribution are the derivatives of the log normalizer.

FUNDAMENTAL OPERATIONS WITH DISTRIBUTIONS

- Generate data: draw samples from the distribution. This often involves generating a uniformly distributed variable in the range [0,1] and transforming it. For more complex distributions it may involve an iterative procedure that takes a long time to produce a single sample (e.g. Gibbs sampling, MCMC).
- Compute log probabilities.

When all variables are either observed or marginalized the result is a single number which is the log prob of the configuration.

- *Inference*: Compute expectations of some variables given others which are observed or marginalized.
- Learning.

Set the parameters of the density functions given some (partially) observed data to maximize likelihood or penalized likelihood.

BASIC STATISTICAL PROBLEMS

- Let's remind ourselves of the basic problems we discussed on the first day: *density estimation, clustering classification* and *regression*.
- Density estimation is hardest. If we can do joint density estimation then we can always condition to get what we want:

 $\begin{array}{l} \text{Regression: } p(\mathbf{y}|\mathbf{x}) = p(\mathbf{y},\mathbf{x})/p(\mathbf{x}) \\ \text{Classification: } p(c|\mathbf{x}) = p(c,\mathbf{x})/p(\mathbf{x}) \\ \text{Clustering: } p(c|\mathbf{x}) = p(c,\mathbf{x})/p(\mathbf{x}) \ c \ \text{unobserved} \end{array}$

Learning

- In AI the bottleneck is often knowledge acquisition.
- Human experts are rare, expensive, unreliable, slow.
- But we have lots of data.
- Want to build systems automatically based on data and a small amount of prior information (from experts).

