Review:

Probability and Statistics

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Random Variables and Densities

- Random variables X represents outcomes or states of world.
  Instantiations of variables usually in lower case: x
  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.)
- Probability mass (density) function $p(x) \geq 0$
  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
- But you have to be careful about the context and about defining random variables and sample spaces carefully. Otherwise you can get in trouble (see, e.g. Simpson's paradox/Prisoner's paradox).

Probability

- We use probabilities $p(x)$ to represent our beliefs $B(x)$ about the states x of the world.
- There is a formal calculus for manipulating uncertainties represented by probabilities.
- Any consistent set of beliefs obeying the *Cox Axioms* can be mapped into probabilities.
  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:
     $B(x \ and \ y) = g[B(x), B(y|x)] = g[B(y), B(x|y)]$

Expectations, Moments

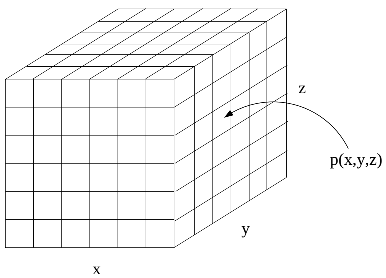
- Expectation of a function $a(x)$ is written $E[a]$ or $\langle a \rangle$

$$E[a] = \langle a \rangle = \sum_x p(x)a(x)$$

  e.g. mean $= \sum_x xp(x)$, variance $= \sum_x (x - E[x])^2 p(x)$
- Moments are expectations of higher order powers.
  (Mean is first moment. Autocorrelation is second moment.)
- Centralized moments have lower moments subtracted away (e.g. variance, skew, curtosis).
- Deep fact: Knowledge of all orders of moments completely defines the entire distribution.

Joint Probability

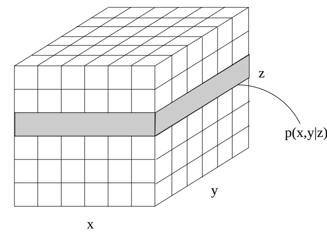
- Key concept: two or more random variables may interact.
  Thus, the probability of one taking on a certain value depends on which value(s) the others are taking.
- We call this a joint ensemble and write
  $p(x, y) = \text{prob}(X = x \text{ and } Y = y)$



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.

$$\boxed{p(x|y) = p(x, y)/p(y)}$$

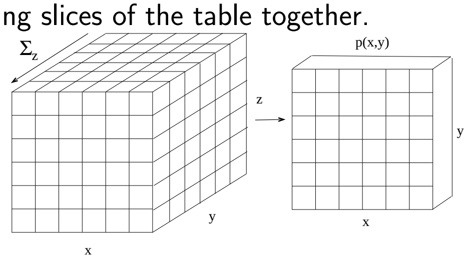


Marginal Probabilities

- 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:

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

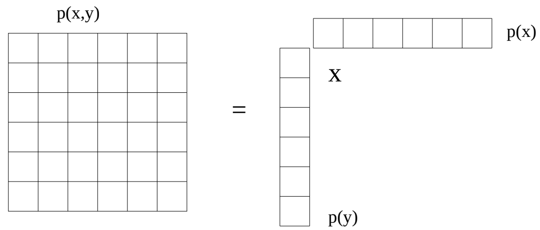
- This gives us a way of "reversing"conditional probabilities.
- Thus, all joint probabilities can be factored by selecting an ordering for the random variables and using the "chain rule":

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

Independence & Conditional Independence

- Two variables are independent iff their joint factors:

$$p(x, y) = p(x)p(y)$$



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

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

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 $q(x)$.

Entropy

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

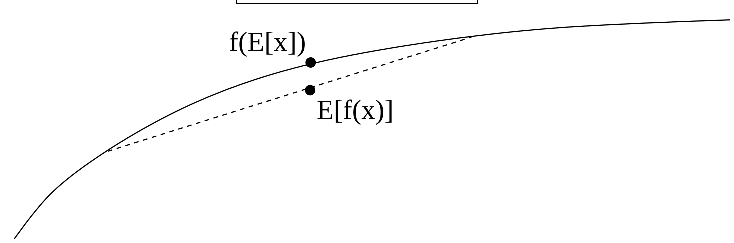
$$\boxed{H(p) = -\sum_x p(x) \log p(x)}$$

- 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 $-\log p$(event)

Jensen's Inequality

- For any concave function $f()$ and any distribution on x,

$$\boxed{E[f(x)] \leq f(E[x])}$$



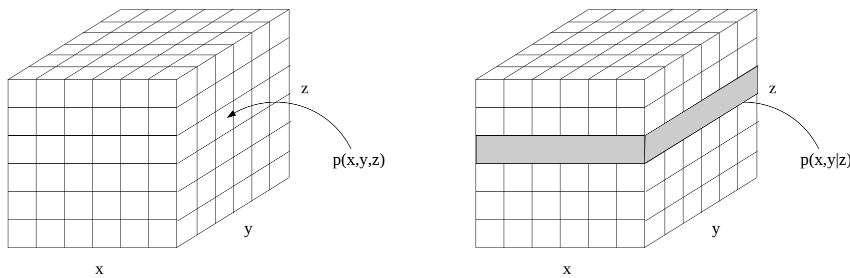
- e.g. $\log()$ and $\sqrt{}$ are concave
- This allows us to bound expressions like $\log p(x) = \log \sum_z p(x, z)$

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*, ...

(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.



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.

Exponential Family

- For (continuous or discrete) random variable $\mathbf{x}$

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

  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.
- Key idea: all you need to know about the data is captured in the summarizing function $T(\mathbf{x})$.

Bernoulli

- For a binary random variable with p(heads)=π:

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

- 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

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

Multinomial

- 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 $\pi_n = 1 - \sum_{i=1}^{n-1}\pi_i$.

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

- 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:

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

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:

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

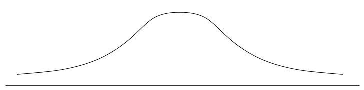
- e.g. number of photons $\mathbf{x}$ that arrive at a pixel during a fixed interval given mean intensity λ
- Other count densities: binomial, exponential.

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:



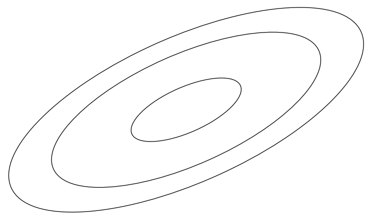
$$\eta = [\mu/\sigma^2\ ;\ -1/2\sigma^2]$$
$$T(x) = [x\ ;\ x^2]$$
$$A(\eta) = \log\sigma + \mu/2\sigma^2$$
$$h(x) = 1/\sqrt{2\pi}$$

- 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.

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 $\mathbf{C}$ is the (non-symmetric) cross-covariance matrix between $\mathbf{x}$ and $\mathbf{y}$ which has as many rows as the size of $\mathbf{x}$ and as many columns as the size of $\mathbf{y}$.
  The marginal distributions are:

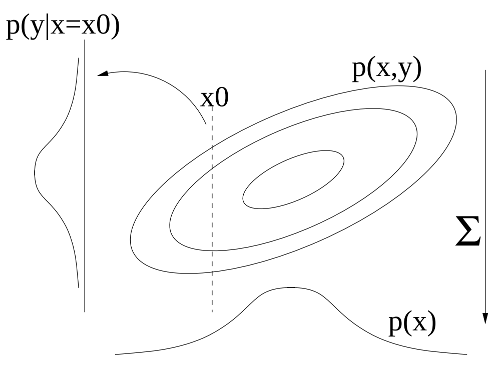
$$\mathbf{x} \sim \mathcal{N}(\mathbf{a};\mathbf{A})$$
$$\mathbf{y} \sim \mathcal{N}(\mathbf{b};\mathbf{B})$$

  and the conditional distributions are:

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

Important Gaussian Facts

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



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.

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

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

Linear-Gaussian 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": $p(\mathbf{y}|\mathbf{x}) = \mathrm{gauss}(\theta^\top \mathbf{x}; \Sigma)$.
- For discrete children and continuous parents, we often use a Bernoulli/multinomial whose paramters are some function $f(\theta^\top \mathbf{x})$.

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 $\ell(\theta)$:

$$c(\theta) = \ell(\theta; \mathcal{D}) \qquad \text{maximum likelihood (ML)}$$
$$c(\theta) = \ell(\theta; \mathcal{D}) + r(\theta) \qquad \text{maximum a posteriori (MAP)/penalizedML}$$

(also cross-validation, Bayesian estimators, BIC, AIC, ...)

Multiple Observations, Complete Data, IID Sampling

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

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:

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

- 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,...
- Model: $p(H) = \theta \quad p(T) = (1-\theta)$
- Likelihood:

$$\begin{aligned}\ell(\theta;\mathcal{D}) &= \log p(\mathcal{D}|\theta) \\ &= \log \prod_m \theta^{\mathbf{x}^m} (1-\theta)^{1-\mathbf{x}^m} \\ &= \log\theta \sum_m \mathbf{x}^m + \log(1-\theta)\sum_m (1-\mathbf{x}^m) \\ &= \log\theta N_{\mathrm{H}} + \log(1-\theta) N_{\mathrm{T}}\end{aligned}$$

- Take derivatives and set to zero:

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

Example: Univariate Normal

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

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

- Take derivatives and set to zero:

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

Example: Multinomial

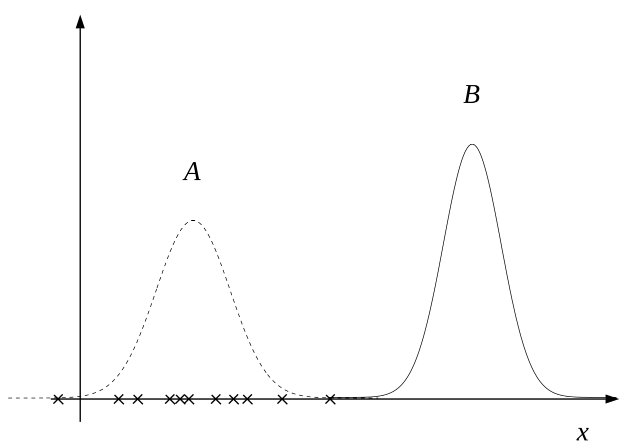
- We observe M iid die rolls (K-sided): $\mathcal{D}$=3,1,K,2,...
- Model: $p(k) = \theta_k \quad \sum_k \theta_k = 1$
- Likelihood (for binary indicators $[\mathbf{x}^m = k]$):

$$\begin{aligned}\ell(\theta;\mathcal{D}) &= \log p(\mathcal{D}|\theta) \\ &= \log \prod_m \theta_{\mathbf{x}^m} = \log \prod_m \theta_1^{[\mathbf{x}^m=1]} \ldots \theta_k^{[\mathbf{x}^m=k]} \\ &= \sum_k \log\theta_k \sum_m [\mathbf{x}^m = k] = \sum_k N_k \log\theta_k\end{aligned}$$

- 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



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:

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

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

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

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

$$\frac{\partial \ell}{\partial \theta} = -\sum_m (y^m - \theta^\top \mathbf{x}^m)\mathbf{x}^m$$

$$\Rightarrow \theta^*_{\mathrm{ML}} = (\mathbf{X}^\top \mathbf{X})^{-1}\mathbf{X}^\top \mathbf{Y}$$

Sufficient Statistics

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

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

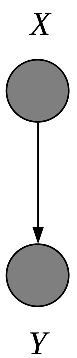
- Equivalently (by the Neyman factorization theorem) we can write:

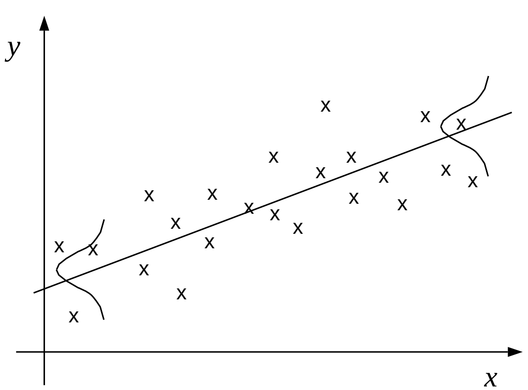
$$p(\mathbf{x}|\theta) = h\left(\mathbf{x}, T(\mathbf{x})\right) g\left(T(\mathbf{x}), \theta\right)$$

- Example: exponential family models:

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

Example: Linear Regression





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. (There are some degenerate exceptions, e.g. the uniform has sufficient statistics of max/min.)

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:

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

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

Learning with Known Model Structure

- 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).
- Many systems we build will be essentially probability models.
- Assume the prior information we have specifies type & structure of the model, as well as the form of the (conditional) distributions or potentials.
- In this case learning $\equiv$ setting parameters.
- Also possible to do "structure learning" to learn model.