Unsupervised Learning

Week 1: Introduction, Statistical Basics, and a bit of Information Theory

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Three Types of Learning

Imagine an organism or machine which experiences a series of sensory inputs:

$$x_1, x_2, x_3, x_4, \ldots$$

Supervised learning: The machine is also given desired outputs $y_1, y_2, \ldots$, and its goal is to learn to produce the correct output given a new input.

Unsupervised learning: The goal of the machine is to build a model of x that can be used for reasoning, decision making, predicting things, communicating etc.

Reinforcement learning: The machine can also produce actions $a_1, a_2, \ldots$ which affect the state of the world, and receives rewards (or punishments) $r_1, r_2, \ldots$. Its goal is to learn to act in a way that maximises rewards in the long term.

Goals of Supervised Learning

Classification: The desired outputs y_i are discrete class labels.
The goal is to classify new inputs correctly (i.e. to generalize).

Regression: The desired outputs y_i are continuous valued.
The goal is to predict the output accurately for new inputs.

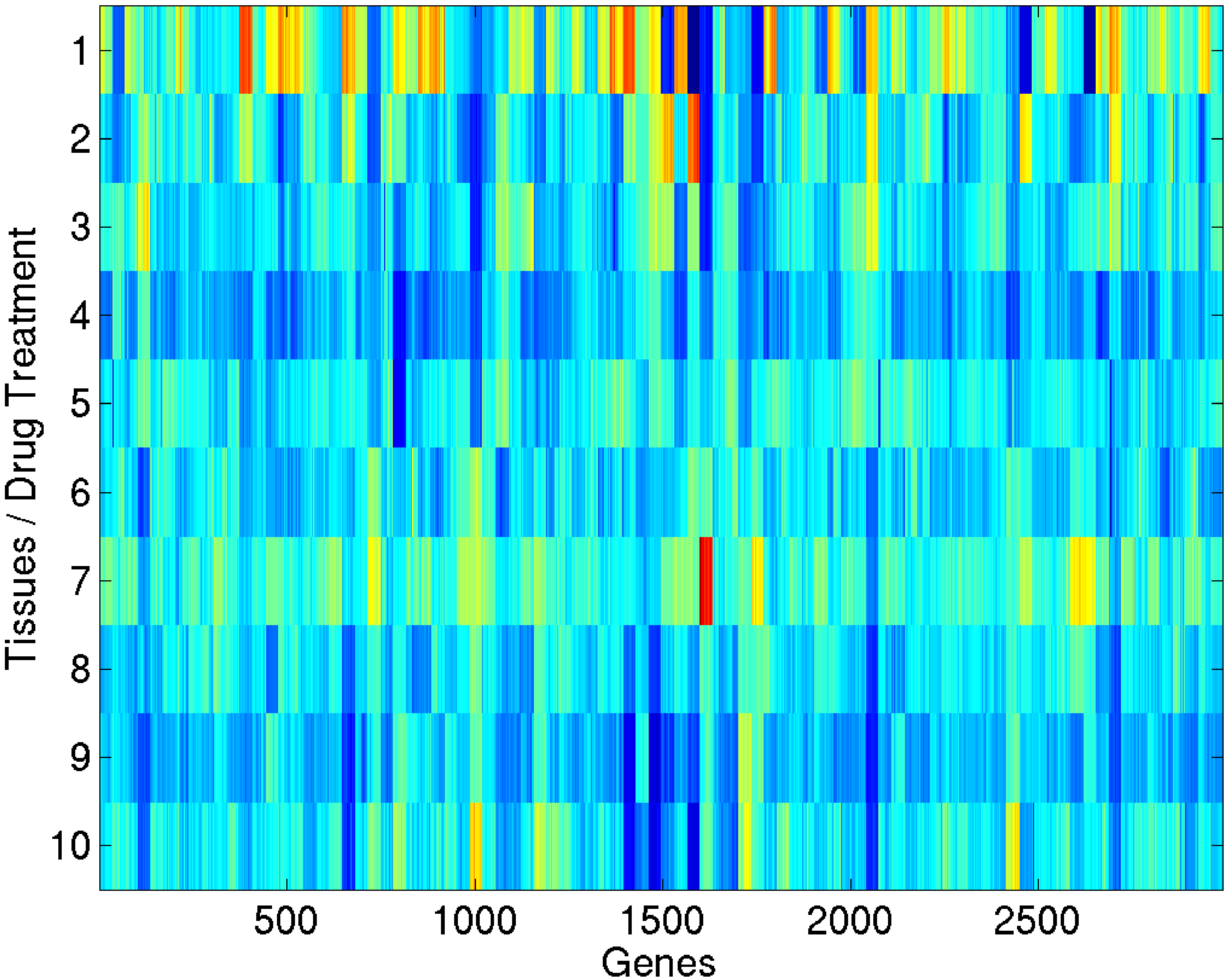
Goals of Unsupervised Learning

To build a model or find useful representations of the data, for example:

- finding clusters
- dimensionality reduction
- finding the hidden causes or sources of the data
- modeling the data density

Uses of Unsupervised Learning

- data compression
- outlier detection
- classification
- make other learning tasks easier
- a theory of human learning and perception



Tissues / Drug Treatment
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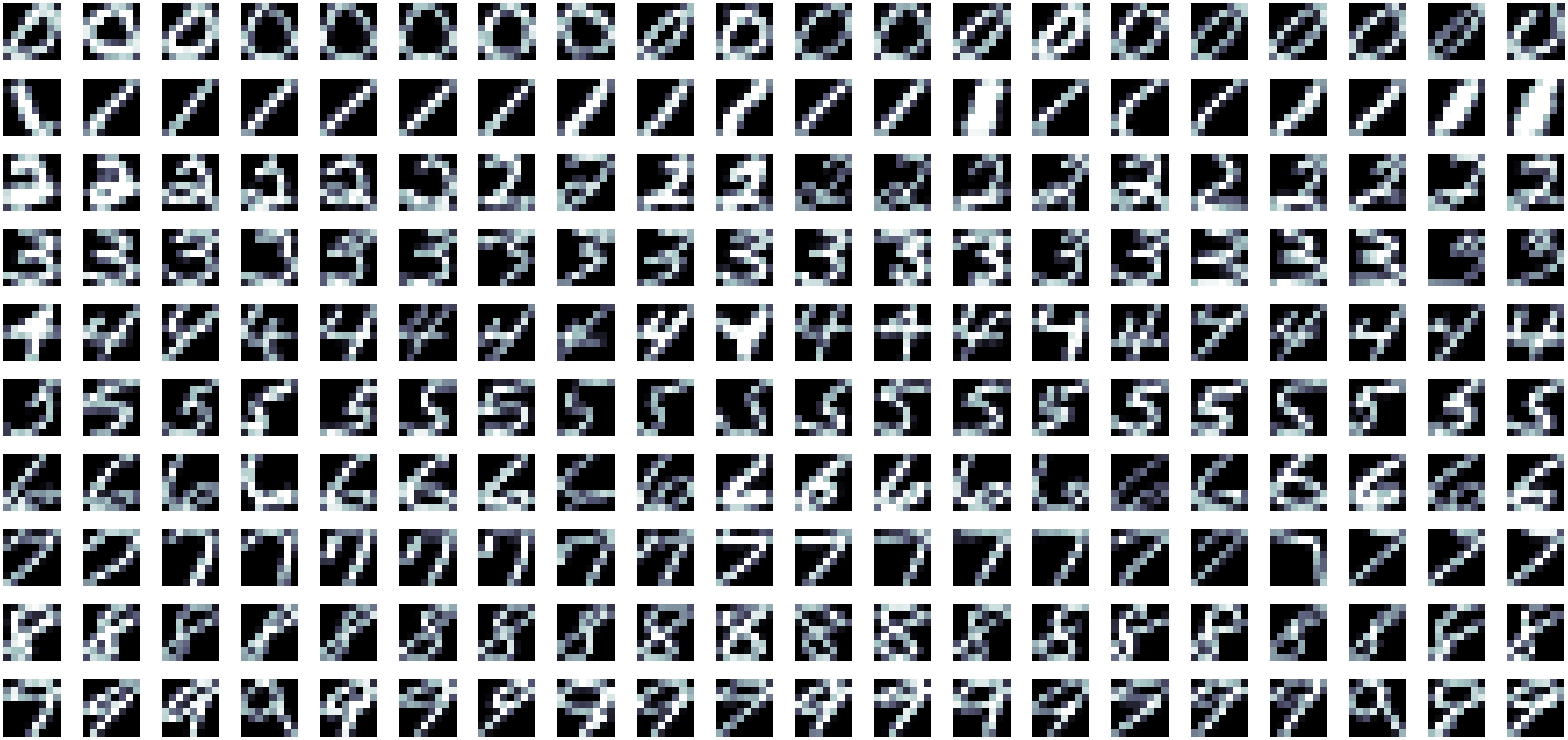
Genes

Handwritten Digits



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Unsupervised Learning - The MIT Press
... From Bradford Books: **Unsupervised Learning** Foundations of Neural Computation Edited by Geoffrey Hinton and Terrence J. Sejnowski Since its founding in 1989 by **...**
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The **Unsupervised Learning** Group (ULG) at UT Austin
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Why a statistical approach?

- A probabilistic model of the data can be used to
  - make inferences about missing inputs
  - generate predictions/fantasies/imagery
  - make decisions which minimise expected loss
  - communicate the data in an efficient way

- Statistical modelling is equivalent to other views of learning:
  - information theoretic: finding compact representations of the data
  - physical analogies: minimising free energy of a corresponding statistical mechanical system

Information, Probability and Entropy

Information is the reduction of uncertainty. How do we measure uncertainty?

Some axioms (informal):

- if something is certain its uncertainty $= 0$

- uncertainty should be maximum if all choices are equally probable

- uncertainty (information) should add for independent sources

This leads to a discrete random variable X having uncertainty equal to the entropy function:

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

measured in *bits* (**bi**nary digi**ts**) if the base 2 logarithm is used or *nats* (**na**tural digi**ts**) if the natural (base e) logarithm is used.

Some Definitions and Intuitions

- Surprise (for event $X = x$): $-\log P(X = x)$
- Entropy = average surpise: $H(X) = -\sum_{X=x} P(X = x)\ \log_2 P(X = x)$
- Conditional entropy

$$H(X|Y) = -\sum_x \sum_y P(x, y) \log_2 P(x|y)$$

- Mutual information

$$I(X;Y) = H(X) - H(X|Y) = H(Y) - H(Y|X) = H(X) + H(Y) - H(X,Y)$$

- Kullback-Leibler divergence (relative entropy)

$$KL(P(X)\|Q(X)) = \sum_x P(x) \log \frac{P(x)}{Q(x)}$$

- Relation between Mutual information and KL: $I(X;Y) = KL(P(X,Y)\|P(X)P(Y))$
- Independent random variables: $P(X,Y) = P(X)P(Y)$
- Conditional independence $X \perp\!\!\!\perp Y|Z$ (X conditionally independent of Y given Z) means $P(X,Y|Z) = P(X|Z)P(Y|Z)$ and $P(X|Y,Z) = P(X|Z)$

Shannon's Source Coding Theorem

A discrete random variable X, distributed according to $P(X)$ has entropy equal to:

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

Shannon's source coding theorem: n independent samples of the random variable X, with entropy $H(X)$, can be compressed into minimum expected code of length $n\mathcal{L}$, where

$$H(X) \leq \mathcal{L} < H(X) + \frac{1}{n}$$

If each symbol is given a code length $l(x) = -\log_2 Q(x)$ then the expected per-symbol length $\mathcal{L}_Q$ of the code is

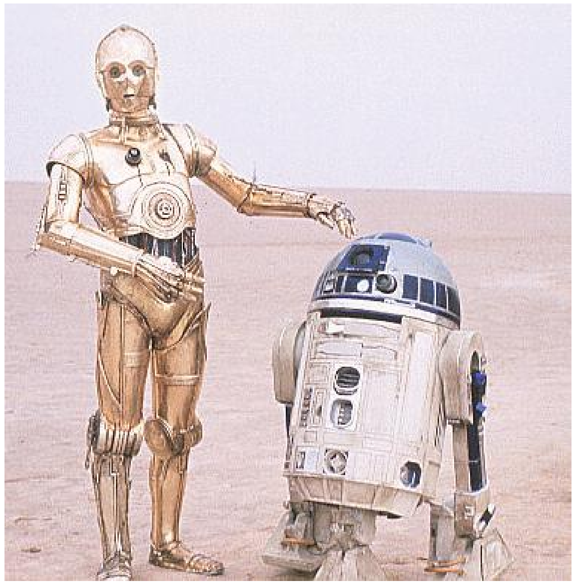
$$H(X) + KL(P\|Q) \leq \mathcal{L}_Q < H(X) + KL(P\|Q) + \frac{1}{n},$$

where the relative-entropy or Kullback-Leibler divergence is

$$KL(P\|Q) = \sum_{x} P(x) \log \frac{P(x)}{Q(x)} \geq 0$$

Learning: A Statistical Approach II

- Goal: to represent the beliefs of learning agents.
- Cox Axioms lead to the following:
  If plausibilities/beliefs are represented by real numbers, then the only reasonable and consistent way to manipulate them is Bayes rule.
- Frequency vs belief interpretation of probabilities
- The Dutch Book Theorem:
  If you are willing to bet on your beliefs, then unless they satisfy Bayes rule there will always be a set of bets ("Dutch book") that you would accept which is guaranteed to lose you money, no matter what outcome!



Basic Rules of Probability

Probabilities are non-negative $P(x) \geq 0 \; \forall x$.

Probabilities normalise: $\sum_x P(x) = 1$ for discrete distributions and $\int p(x)dx = 1$ for probability densities.

The joint probability of x and y is: $P(x, y)$.

The marginal probability of x is: $P(x) = \sum_y P(x, y)$.

The conditional probability of x given y is: $P(x|y) = P(x, y)/P(y)$
Bayes Rule:

$$P(x, y) = P(x)P(y|x) = P(y)P(x|y) \quad \Rightarrow \quad \boxed{P(y|x) = \frac{P(x|y)P(y)}{P(x)}}$$

Warning: I will not be obsessively careful in my use of p and P for probability density and probability distribution. Should be obvious from context.

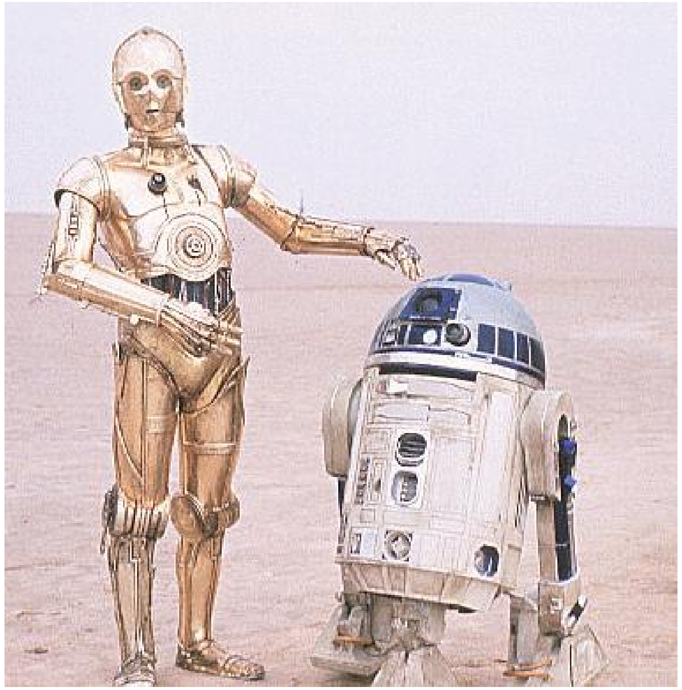
Representing Beliefs (Artificial Intelligence)

Consider a robot. In order to behave intelligently the robot should be able to represent beliefs about propositions in the world:

"my charging station is at location (x,y,z)"

"my rangefinder is malfunctioning"

"that stormtrooper is hostile"



We want to represent the **strength** of these beliefs numerically in the brain of the robot, and we want to know what rules (calculus) we should use to manipulate those beliefs.

Representing Beliefs II

Let's use $b(x)$ to represent the strength of belief in (plausibility of) proposition x.

$0 \leq b(x) \leq 1$		
$b(x) = 0$	x	is definitely **not true**
$b(x) = 1$	x	is definitely **true**
$b(x\|y)$	strength of belief that x is true given that we know y is true	

Cox Axioms (Desiderata):

- Strengths of belief (degrees of plausibility) are represented by real numbers
- Qualitative correspondence with common sense
- Consistency
  - If a conclusion can be reasoned in more than one way, then every way should lead to the same answer.
  - The robot always takes into account all relevant evidence.
  - Equivalent states of knowledge are represented by equivalent plausibility assignments.

Consequence: Belief functions (e.g. $b(x)$, $b(x|y)$, $b(x, y)$) must satisfy the rules of probability theory, including Bayes rule. (see Jaynes, *Probability Theory: The Logic of Science*)

The Dutch Book Theorem

Assume you are willing to accept bets with odds proportional to the strength of your beliefs. That is, $b(x) = 0.9$ implies that you will accept a bet:

$$\begin{cases} x & \text{is true} \quad \text{win} \quad \geq \$1 \\ x & \text{is false} \quad \text{lose} \quad \$9 \end{cases}$$

Then, unless your beliefs satisfy the rules of probability theory, including Bayes rule, there exists a set of simultaneous bets (called a "Dutch Book") which you are willing to accept, and for which **you are guaranteed to lose money, no matter what the outcome**.

The only way to guard against Dutch Books to to ensure that your beliefs are coherent: i.e. satisfy the rules of probability.

Bayesian Learning

Apply the basic rules of probability to learning from data.
Data set: $\mathcal{D} = \{x_1, \ldots, x_n\}$ Models: m, m' etc. Model parameters: θ

Prior probabilities on models: $P(m)$, $P(m')$ etc.

Prior probabilities on model parameters: e.g. $P(\theta|m)$

Model of data given parameters: $P(x|\theta, m)$

If the data are independently and identically distributed then:

$$P(\mathcal{D}|\theta, m) = \prod_{i=1}^{n} P(x_i|\theta, m)$$

Posterior probability of model parameters:

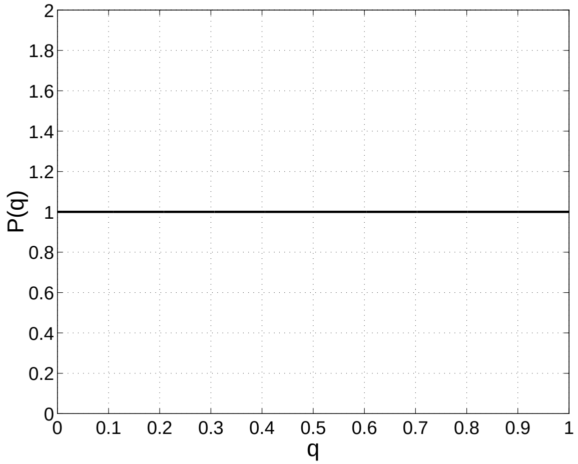
$$P(\theta|\mathcal{D}, m) = \frac{P(\mathcal{D}|\theta, m)P(\theta|m)}{P(\mathcal{D}|m)}$$

Posterior probability of models:

$$P(m|\mathcal{D}) = \frac{P(m)P(\mathcal{D}|m)}{P(\mathcal{D})}$$

Bayesian Learning: A coin toss example

Coin toss: One parameter q — the odds of obtaining *heads*
So our space of models is the set $q \in [0, 1]$.
Learner A believes all values of q are equally plausible;
Learner B believes that it is more plausible that the coin is "fair" $(q \approx 0.5)$ than "biased".



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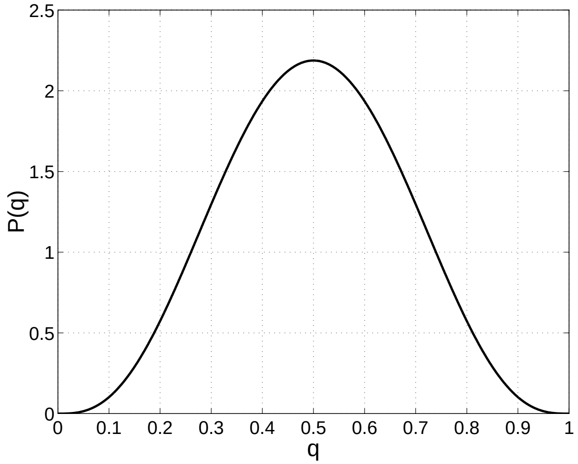


B

These priors beliefs can be described by the Beta distribution:

$$p(q|\alpha_1, \alpha_2) = \frac{q^{(\alpha_1 - 1)}(1-q)^{(\alpha_2 - 1)}}{B(\alpha_1, \alpha_2)} = \mathrm{Beta}(q|\alpha_1, \alpha_2)$$

for A: $\alpha_1 = \alpha_2 = 1.0$ and B: $\alpha_1 = \alpha_2 = 4.0$.

Bayesian Learning: The coin toss (cont)

Two possible outcomes:

$$p(\text{heads}|q) = q \qquad p(\text{tails}|q) = 1 - q \tag{1}$$

Imagine we observe a single coin toss and it comes out *heads*
The probability of the observed data (likelihood) is:

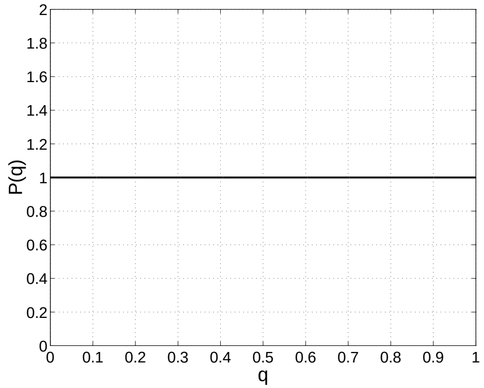
$$p(\text{heads}|q) = q \tag{2}$$

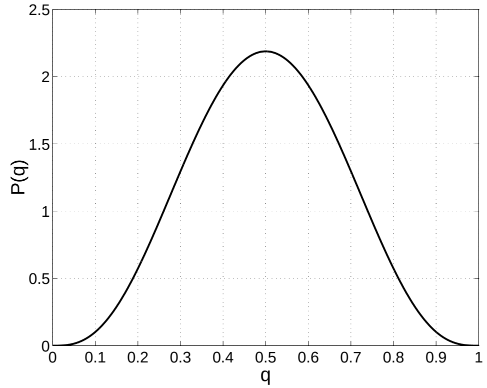
Using Bayes Rule, we multiply the prior, $p(q)$ by the likelihood and renormalise to get the posterior probability:

$$\begin{aligned} p(q|\text{heads}) &= \frac{p(q)p(\text{heads}|q)}{p(\text{heads})} \propto q \, \mathrm{Beta}(q|\alpha_1, \alpha_2) \\ &\propto q \; q^{(\alpha_1 - 1)}(1-q)^{(\alpha_2 - 1)} = \mathrm{Beta}(q|\alpha_1 + 1, \alpha_2) \end{aligned}$$

Bayesian Learning: The coin toss (cont)

Prior





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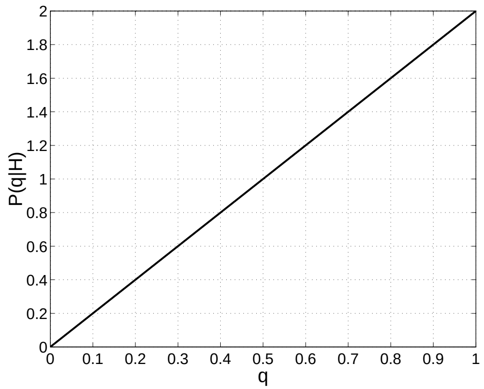
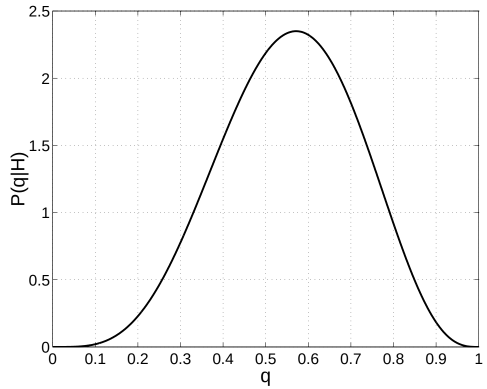




Posterior

Some Terminology

Maximum Likelihood (ML) Learning: Does not assume a prior over the model parameters. Finds a parameter setting that maximises the likelihood of the data: $P(\mathcal{D}|\theta)$.

Maximum a Posteriori (MAP) Learning: Assumes a prior over the model parameters $P(\theta)$. Finds a parameter setting that maximises the posterior: $P(\theta|\mathcal{D}) \propto P(\theta)P(\mathcal{D}|\theta)$.

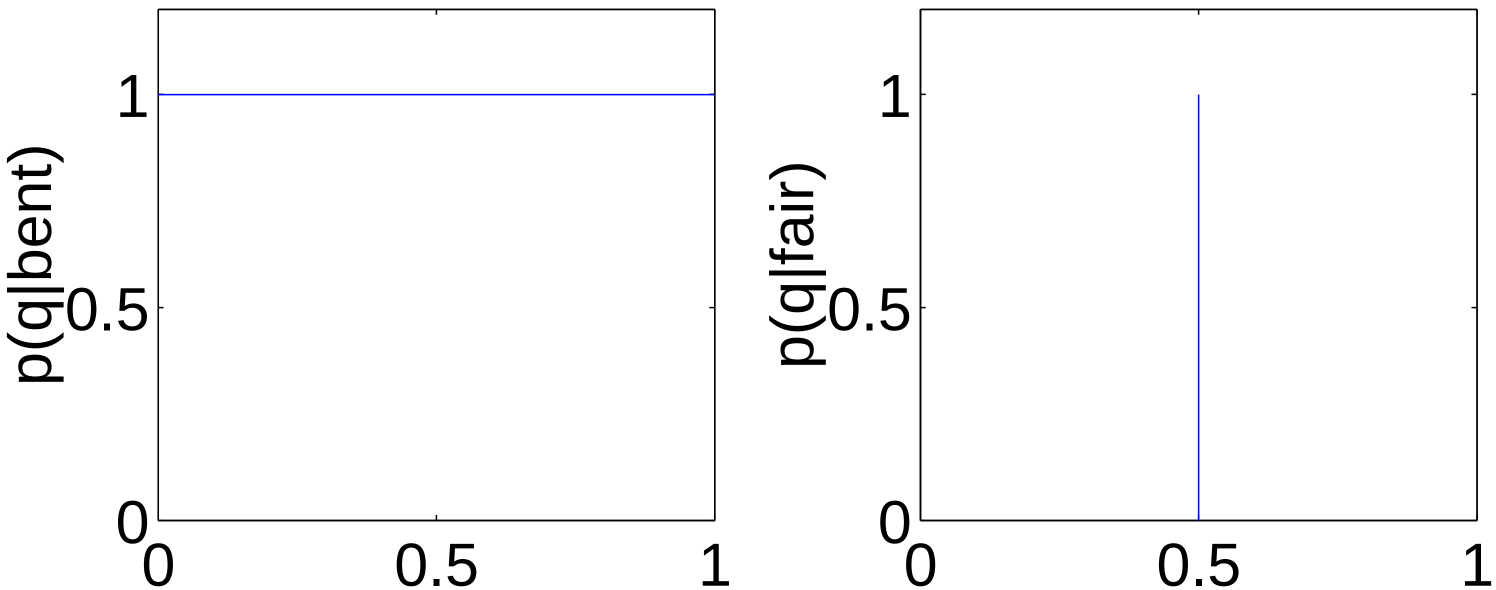
Bayesian Learning: Assumes a prior over the model parameters. Computes the posterior distribution of the parameters: $P(\theta|\mathcal{D})$.

Learning about a coin II

Consider two alternative models of a coin, “fair” and “bent”. A priori, we may think that “fair” is more probable, eg:

$$p(\text{fair}) = 0.8, \qquad p(\text{bent}) = 0.2$$

For the bent coin, (a little unrealistically) all parameter values could be equally likely, where the fair coin has a fixed probability:



We make 10 tosses, and get: T H T H T T T T T T

Learning about a coin. . .

The evidence for the fair model is: $p(\mathcal{D}|\text{fair}) = (1/2)^{10} \simeq 0.001$
and for the bent model:

$$p(\mathcal{D}|\text{bent}) = \int dq\; p(\mathcal{D}|q, \text{bent})p(q|\text{bent}) = \int dq\; q^2(1-q)^8 = \text{B}(3, 9) \simeq 0.002$$

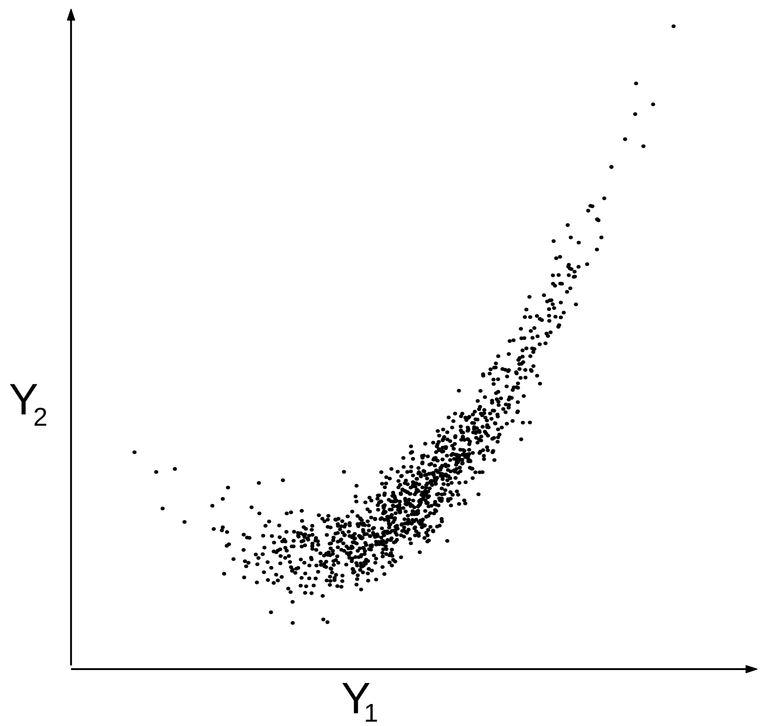
The posterior for the models, by Bayes rule:

$$p(\text{fair}|\mathcal{D}) \propto 0.0008, \qquad p(\text{bent}|\mathcal{D}) \propto 0.0004,$$

ie, two thirds probability that the coin is fair.
How do we make predictions? By weighting the predictions from each model by their probability. Probability of Head at next toss is:

$$\frac{2}{3} \times \frac{1}{2} + \frac{1}{3} \times \frac{3}{12} = \frac{5}{12}.$$

Simple Statistical Modelling: modelling correlations



Assume:

- we have a data set $Y = \{\mathbf{y}_1, \ldots, \mathbf{y}_N\}$
- each data point is a vector of D features: $\mathbf{y}_i = [y_{i1} \ldots y_{iD}]$
- the data points are i.i.d. (independent and identically distributed).

One of the simplest forms of unsupervised learning: model the **mean** of the data and the **correlations** between the D features in the data

We can use a multi-variate Gaussian model:

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

ML Estimation of a Gaussian

Data set $Y = \{\mathbf{y}_1, \ldots, \mathbf{y}_N\}$, likelihood: $p(Y|\mu, \Sigma) = \prod_{n=1}^{N} p(\mathbf{y}_n|\mu, \Sigma)$

Maximize likelihood ⇔ maximize log likelihood
Goal: find μ and Σ that maximise log likelihood:

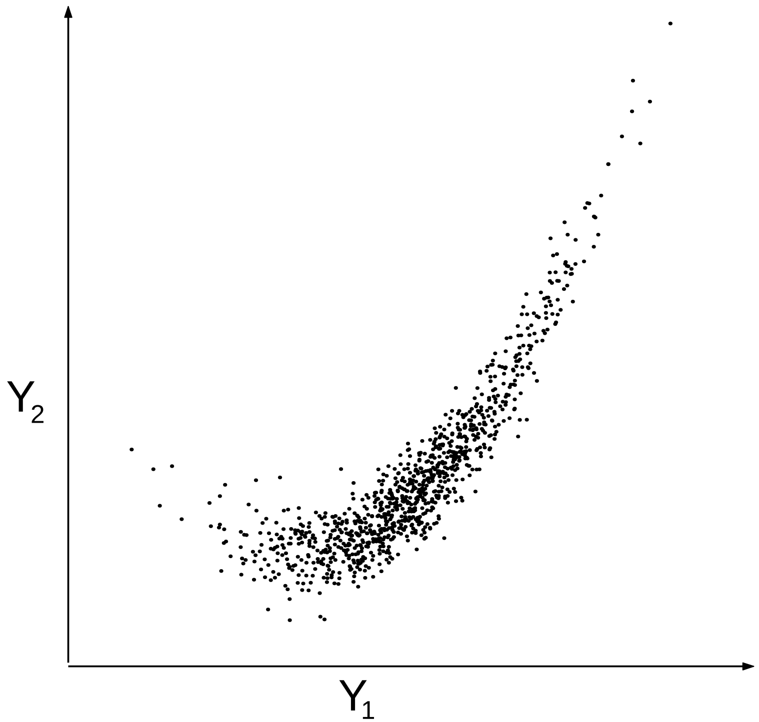
$$\begin{aligned} \mathcal{L} &= \log \prod_{n=1}^{N} p(\mathbf{y}_n|\mu, \Sigma) = \sum_n \log p(\mathbf{y}_n|\mu, \Sigma) \\ &= -\frac{N}{2} \log |2\pi\Sigma| - \frac{1}{2} \sum_n (\mathbf{y}_n - \mu)^\top \Sigma^{-1} (\mathbf{y}_n - \mu) \end{aligned} \tag{3}$$

Note: equivalently, minimise $-\mathcal{L}$, which is *quadratic* in μ
Procedure: take derivatives and set to zero:

$$\frac{\partial \mathcal{L}}{\partial \mu} = 0 \quad \Rightarrow \quad \hat{\mu} = \frac{1}{N} \sum_n \mathbf{y}_n \quad \text{(sample mean)}$$

$$\frac{\partial \mathcal{L}}{\partial \Sigma} = 0 \quad \Rightarrow \quad \hat{\Sigma} = \frac{1}{N} \sum_n (\mathbf{y}_n - \hat{\mu})(\mathbf{y}_n - \hat{\mu})^\top \quad \text{(sample covariance)}$$

Note



modelling correlations

$\Updownarrow$

maximising likelihood of a Gaussian model

$\Updownarrow$

minimising a squared error cost function

$\Updownarrow$

minimizing data coding cost in bits (assuming Gaussian distributed)

Error functions, noise models, and likelihoods

- **Squared error:** $(y-\mu)^2$
  Gaussian noise assumption, y is real-valued

- **Absolute error:** $|y-\mu|$
  Exponential noise assumption, y real or positive

- **Binary cross entropy error:**
  $-y\log p-(1-y)\log(1-p)$
  Binomial noise assumption, y binary

- **Cross entropy error:** $\sum_i y_i \log p_i$
  Multinomial noise assumption, y is discrete (binary unit vector)

Three Limitations

- What about higher order statistical structure in the data? $\Rightarrow$ nonlinear and hierarchical models

- What happens if there are outliers? $\Rightarrow$ other noise models

- There are $D(D+1)/2$ parameters in the multi-variate Gaussian model. What if D is very large?

  $\Rightarrow$ dimensionality reduction

End Notes

For some matrix identities and matrix derivatives see:
`www.cs.toronto.edu/∼roweis/notes/matrixid.pdf`

Also, see Tom Minka's notes on matrix algebra at CMU.
`http://www.stat.cmu.edu/∼minka/papers/matrix.html`