

Probabilistic & Unsupervised Learning

Introduction and Foundations

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What do we mean by learning?



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$$x_1, x_2, x_3, x_4, \dots$$

Describe pattern of data $[p(x)]$, identify and extract underlying structural variables $[x_i \rightarrow y_i]$.

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- ▶ **Reinforcement learning.** Rewards or payoffs (and possibly also inputs) depend on actions:

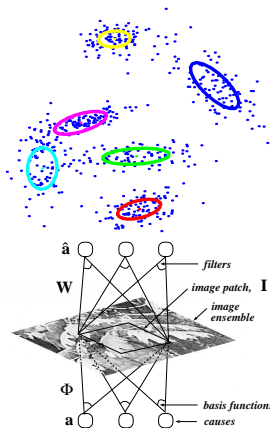
$$x_1 : a_1 \rightarrow r_1, x_2 : a_2 \rightarrow r_2, x_3 : a_3 \rightarrow r_3 \dots$$

Find a policy for action choice that maximises payoff.

Unsupervised Learning

Find underlying structure:

- ▶ separate generating processes (clusters)
- ▶ reduced dimensionality representations
- ▶ good explanations (**causes**) of the data
- ▶ modelling the data density



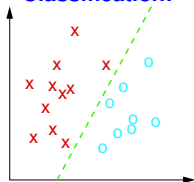
Uses of Unsupervised Learning:

- ▶ structure discovery, science
- ▶ data compression
- ▶ outlier detection
- ▶ input to supervised/reinforcement algorithms (causes may be more simply related to outputs or rewards)
- ▶ a theory of biological learning and perception

Supervised learning

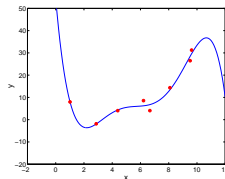
Two main examples:

Classification:



Discrete (class label) outputs.

Regression:



Continuous-values outputs.

But also: ranks, relationships, trees etc.

Variants may relate to unsupervised learning:

- ▶ semi-supervised learning (most x unlabelled; assumes structure of $\{x\}$ and relationship $x \rightarrow y$ are linked).
- ▶ multitask (transfer) learning (predict different y in different contexts; assumes links between structure of relationships).

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The calculus of probabilities naturally handles randomness. It is also the right way to reason about unknown values.

Representing beliefs

Let $b(x)$ represent our strength of belief in (plausibility of) proposition x :

$$0 \leq b(x) \leq 1$$

$$b(x) = 0 \quad x \text{ is definitely **not true**}$$

$$b(x) = 1 \quad x \text{ is definitely **true**}$$

$$b(x|y) \quad \text{strength of belief that } x \text{ is true given that we know } y \text{ is true}$$

Cox Axioms (Desiderata):

- ▶ Let $b(x)$ be real. As $b(x)$ increases, $b(\neg x)$ decreases, and so the function mapping $b(x) \leftrightarrow b(\neg x)$ is monotonically decreasing and self-inverse.
- ▶ $b(x \wedge y)$ depends only on $b(y)$ and $b(x|y)$.
- ▶ Consistency
 - ▶ If a conclusion can be reasoned in more than one way, then every way should lead to the same answer.
 - ▶ Beliefs always take 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 be isomorphic to probabilities, satisfying all the usual laws, including Bayes rule. (See Jaynes, *Probability Theory: The Logic of Science*)

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- ▶ **Bayes Rule:**

$$P(x, y) = P(x)P(y|x) = P(y)P(x|y) \quad \Rightarrow$$

$$P(y|x) = \frac{P(x|y)P(y)}{P(x)}$$

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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:

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

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.**

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But then:

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The only way to guard against Dutch Books is 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.

► Problem specification:

Data: $\mathcal{D} = \{x_1, \dots, x_n\}$ Models: $\mathcal{M}_1, \mathcal{M}_2$, etc. Parameters: θ_i (per model)

Prior probability of models: $P(\mathcal{M}_i)$.

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► Data probability (likelihood)

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(provided the data are independently and identically distributed (iid)).

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- Model selection:

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

Bayesian learning: A coin toss example

Coin toss: One parameter q — the probability of obtaining *heads*

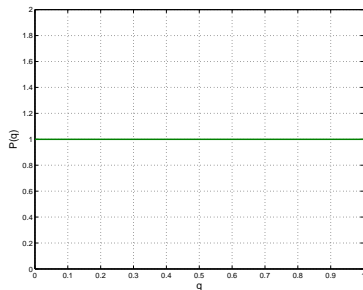
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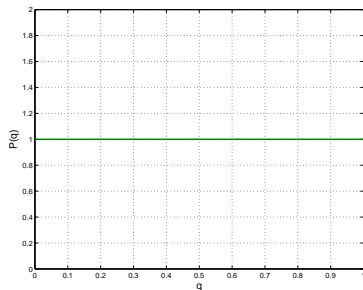
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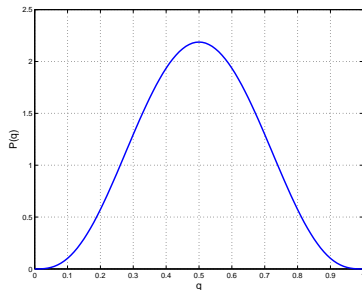
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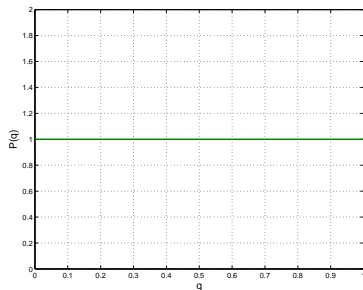
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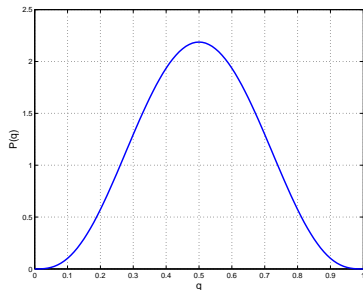
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Both **prior beliefs** can be described by the Beta distribution:

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

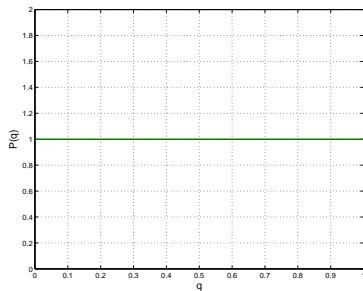
Bayesian learning: A coin toss example

Coin toss: One parameter q — the probability of obtaining *heads*

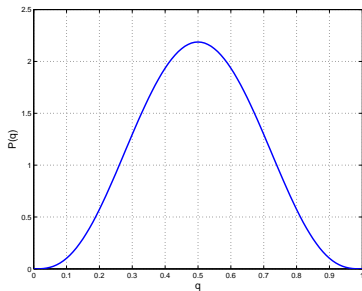
So our space of models is the set of distributions over $q \in [0, 1]$.

Learner A believes model \mathcal{M}_A : all values of q are equally plausible;

Learner B believes model \mathcal{M}_B : more plausible that the coin is “fair” ($q \approx 0.5$) than “biased”.



A: $\alpha_1 = \alpha_2 = 1.0$



B: $\alpha_1 = \alpha_2 = 4.0$

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Bayesian learning: The coin toss (cont)

Now we observe a toss. Two possible outcomes:

$$p(H|q) = q$$

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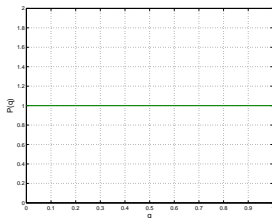
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Bayesian learning: The coin toss (cont)

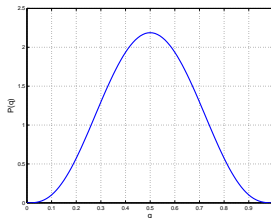
A

Prior



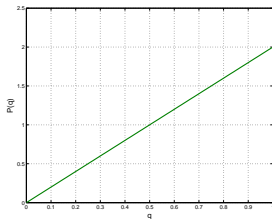
$\text{Beta}(q|1, 1)$

B

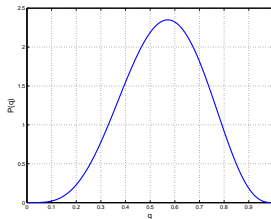


$\text{Beta}(q|4, 4)$

Posterior



$\text{Beta}(q|2, 1)$



$\text{Beta}(q|5, 4)$

Bayesian learning: The coin toss (cont)

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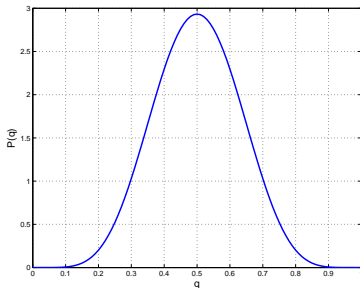
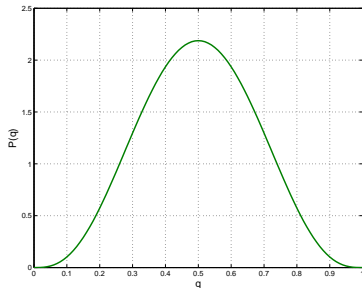
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with $F(\boldsymbol{\tau}, \nu)$ the normaliser, then the posterior is

$$P(\theta|\{x_i\}) \propto P(\{x_i\}|\theta)P(\theta) \propto g(\theta)^{\nu+n} e^{\phi(\theta)^T \left(\boldsymbol{\tau} + \sum_i \mathbf{T}(x_i) \right)}$$

with the normaliser given by $F(\boldsymbol{\tau} + \sum_i \mathbf{T}(x_i), \nu + n)$.

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The posterior given an exponential family likelihood and conjugate prior is:

$$P(\theta|\{x_i\}) = F(\boldsymbol{\tau} + \sum_i \mathbf{T}(x_i), \nu + n) g(\theta)^{\nu+n} \exp \left[\boldsymbol{\phi}(\theta)^\top (\boldsymbol{\tau} + \sum_i \mathbf{T}(x_i)) \right]$$

Here,

$\boldsymbol{\phi}(\theta)$ is the vector of **natural parameters**

$\sum_i \mathbf{T}(x_i)$ is the vector of **sufficient statistics**

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The prior appears to be based on “pseudo-observations”, but:

1. This is different to applying Bayes' rule. **No prior!** Sometimes we can take a uniform prior (say on $[0, 1]$ for q), but for unbounded θ , there may be no equivalent.
2. A valid conjugate prior might have non-integral ν or impossible $\boldsymbol{\tau}$, with no likelihood equivalent.

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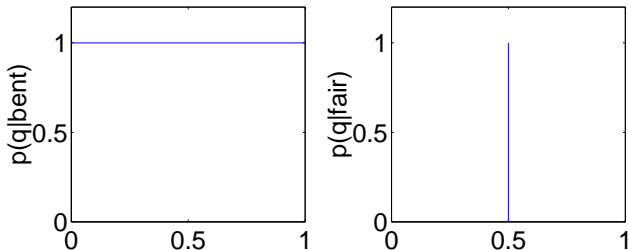
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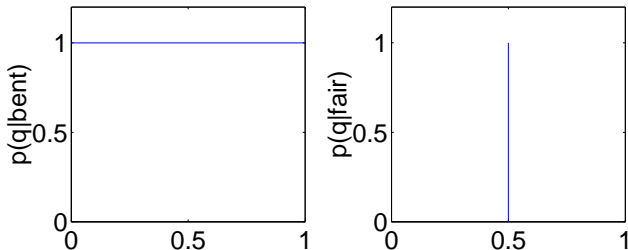


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We make 10 tosses, and get: $\mathcal{D} = (\text{T H T H T T T T T T})$.

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Thus, the posterior for the models, by Bayes rule:

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Or could weight the predictions from each model by their probability (model averaging).

Probability of H at next toss is:

$$P(H|\mathcal{D}) = P(H|\mathcal{D}, \text{fair})P(\text{fair}|\mathcal{D}) + P(H|\mathcal{D}, \text{bent})P(\text{bent}|\mathcal{D}) = \frac{2}{3} \times \frac{1}{2} + \frac{1}{3} \times \frac{3}{12} = \frac{5}{12}.$$

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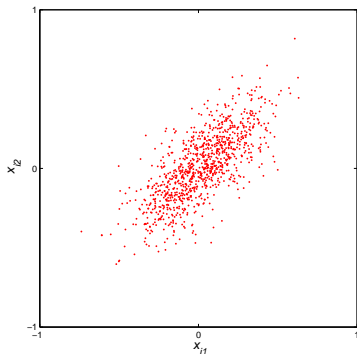
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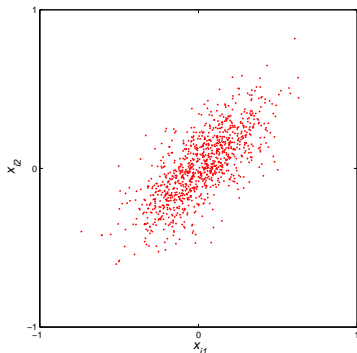
- ▶ **Approximations** may allow us to recover **samples** from posterior, or to find a distribution which is **close** in some sense.
- ▶ Choosing between these and other alternatives may be a matter of definition, of goals (loss function), or of practicality.
- ▶ For the next few weeks we will look at ML and MAP learning in more complex models. We will then return to the fully Bayesian formulation for the few interesting cases where it is tractable. Approximations will be addressed in the second half of the course.

Modelling associations between variables



- ▶ Data set $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$
- ▶ with each data point a vector of D features:
 $\mathbf{x}_i = [x_{i1} \dots x_{iD}]$
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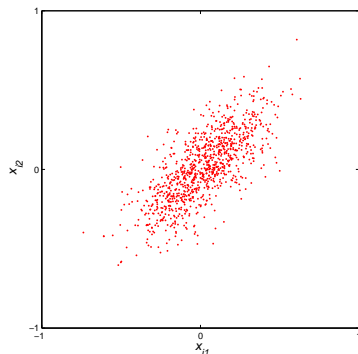
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We can use a multivariate Gaussian model:

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

ML Learning for a Gaussian

Data set $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$, likelihood: $p(\mathcal{D}|\boldsymbol{\mu}, \Sigma) = \prod_{n=1}^N p(\mathbf{x}_n|\boldsymbol{\mu}, \Sigma)$

Goal: find $\boldsymbol{\mu}$ and Σ that maximise likelihood

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Procedure: take derivatives and set to zero:

$$\frac{\partial \ell}{\partial \boldsymbol{\mu}} = 0 \quad \Rightarrow \quad \hat{\boldsymbol{\mu}} = \frac{1}{N} \sum_n \mathbf{x}_n \quad (\text{sample mean})$$

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

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Refresher – matrix derivatives of scalar forms

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$$\mathbf{x}^\top \mathbf{A} \mathbf{y} = \mathbf{y}^\top \mathbf{A}^\top \mathbf{x} = \text{Tr} \left[\mathbf{x}^\top \mathbf{A} \mathbf{y} \right] \quad (\text{scalars equal their own transpose and trace})$$

$$\text{Tr} [A] = \text{Tr} [A^\top] \quad \text{Tr} [ABC] = \text{Tr} [CAB] = \text{Tr} [BCA]$$

$$\frac{\partial}{\partial A_{ij}} \text{Tr} [A^\top B] = \frac{\partial}{\partial A_{ij}} \sum_{mn} A_{mn} B_{mn} = B_{ij}$$

$$\Rightarrow \frac{\partial}{\partial A} \text{Tr} [A^\top B] = B$$

$$\begin{aligned} \frac{\partial}{\partial A} \text{Tr} [A^\top B A C] &= \frac{\partial}{\partial A} \text{Tr} [F_1(A)^\top B F_2(A) C] \quad \text{with } F_1 \text{ and } F_2 \text{ both identity maps} \\ &= \frac{\partial}{\partial F_1} \text{Tr} [F_1^\top B F_2 C] \frac{\partial F_1}{\partial A} + \frac{\partial}{\partial F_2} \text{Tr} [F_2^\top B^\top F_1 C^\top] \frac{\partial F_2}{\partial A} \\ &= B F_2 C + B^\top F_1 C^\top \end{aligned}$$

Refresher – matrix derivatives of scalar forms

We will use the following facts:

$$\mathbf{x}^T \mathbf{A} \mathbf{y} = \mathbf{y}^T \mathbf{A}^T \mathbf{x} = \text{Tr} [\mathbf{x}^T \mathbf{A} \mathbf{y}] \quad (\text{scalars equal their own transpose and trace})$$

$$\text{Tr} [\mathbf{A}] = \text{Tr} [\mathbf{A}^T] \quad \text{Tr} [\mathbf{ABC}] = \text{Tr} [\mathbf{CAB}] = \text{Tr} [\mathbf{BCA}]$$

$$\frac{\partial}{\partial \mathbf{A}_{ij}} \text{Tr} [\mathbf{A}^T \mathbf{B}] = \frac{\partial}{\partial \mathbf{A}_{ij}} \sum_{mn} A_{mn} B_{mn} = B_{ij}$$

$$\Rightarrow \frac{\partial}{\partial \mathbf{A}} \text{Tr} [\mathbf{A}^T \mathbf{B}] = \mathbf{B}$$

$$\begin{aligned} \frac{\partial}{\partial \mathbf{A}} \text{Tr} [\mathbf{A}^T \mathbf{BAC}] &= \frac{\partial}{\partial \mathbf{A}} \text{Tr} [\mathbf{F}_1(\mathbf{A})^T \mathbf{B} \mathbf{F}_2(\mathbf{A}) \mathbf{C}] \quad \text{with } \mathbf{F}_1 \text{ and } \mathbf{F}_2 \text{ both identity maps} \\ &= \frac{\partial}{\partial \mathbf{F}_1} \text{Tr} [\mathbf{F}_1^T \mathbf{B} \mathbf{F}_2 \mathbf{C}] \frac{\partial \mathbf{F}_1}{\partial \mathbf{A}} + \frac{\partial}{\partial \mathbf{F}_2} \text{Tr} [\mathbf{F}_2^T \mathbf{B}^T \mathbf{F}_1 \mathbf{C}^T] \frac{\partial \mathbf{F}_2}{\partial \mathbf{A}} \\ &= \mathbf{B} \mathbf{F}_2 \mathbf{C} + \mathbf{B}^T \mathbf{F}_1 \mathbf{C}^T = \mathbf{BAC} + \mathbf{B}^T \mathbf{AC}^T \end{aligned}$$

Refresher – matrix derivatives of scalar forms

We will use the following facts:

$$\mathbf{x}^T \mathbf{A} \mathbf{y} = \mathbf{y}^T \mathbf{A}^T \mathbf{x} = \text{Tr} [\mathbf{x}^T \mathbf{A} \mathbf{y}] \quad (\text{scalars equal their own transpose and trace})$$

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$$\begin{aligned} \frac{\partial}{\partial \mathbf{A}} \text{Tr} [\mathbf{A}^T \mathbf{BAC}] &= \frac{\partial}{\partial \mathbf{A}} \text{Tr} [\mathbf{F}_1(\mathbf{A})^T \mathbf{B} \mathbf{F}_2(\mathbf{A}) \mathbf{C}] \quad \text{with } \mathbf{F}_1 \text{ and } \mathbf{F}_2 \text{ both identity maps} \\ &= \frac{\partial}{\partial \mathbf{F}_1} \text{Tr} [\mathbf{F}_1^T \mathbf{B} \mathbf{F}_2 \mathbf{C}] \frac{\partial \mathbf{F}_1}{\partial \mathbf{A}} + \frac{\partial}{\partial \mathbf{F}_2} \text{Tr} [\mathbf{F}_2^T \mathbf{B}^T \mathbf{F}_1 \mathbf{C}^T] \frac{\partial \mathbf{F}_2}{\partial \mathbf{A}} \\ &= \mathbf{B} \mathbf{F}_2 \mathbf{C} + \mathbf{B}^T \mathbf{F}_1 \mathbf{C}^T = \mathbf{BAC} + \mathbf{B}^T \mathbf{AC}^T \end{aligned}$$

$$\frac{\partial}{\partial \mathbf{A}_{ij}} \log |\mathbf{A}|$$

Refresher – matrix derivatives of scalar forms

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$$\frac{\partial}{\partial \mathbf{A}_{ij}} \log |\mathbf{A}| = \frac{1}{|\mathbf{A}|} \frac{\partial}{\partial \mathbf{A}_{ij}} |\mathbf{A}|$$

Refresher – matrix derivatives of scalar forms

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$$\frac{\partial}{\partial \mathbf{A}_{ij}} \log |\mathbf{A}| = \frac{1}{|\mathbf{A}|} \frac{\partial}{\partial \mathbf{A}_{ij}} \sum_k (-1)^{i+k} \mathbf{A}_{ik} |\mathbf{A}|_{ik}$$

Refresher – matrix derivatives of scalar forms

We will use the following facts:

$$\mathbf{x}^T \mathbf{A} \mathbf{y} = \mathbf{y}^T \mathbf{A}^T \mathbf{x} = \text{Tr} [\mathbf{x}^T \mathbf{A} \mathbf{y}] \quad (\text{scalars equal their own transpose and trace})$$

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$$\frac{\partial}{\partial \mathbf{A}_{ij}} \log |\mathbf{A}| = \frac{1}{|\mathbf{A}|} \frac{\partial}{\partial \mathbf{A}_{ij}} \sum_k (-1)^{i+k} \mathbf{A}_{ik} |\mathbf{A}|_{ik} = \frac{1}{|\mathbf{A}|} (-1)^{i+j} |\mathbf{A}|_{ij}$$

Refresher – matrix derivatives of scalar forms

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$$\frac{\partial}{\partial \mathbf{A}_{ij}} \log |\mathbf{A}| = \frac{1}{|\mathbf{A}|} \frac{\partial}{\partial \mathbf{A}_{ij}} \sum_k (-1)^{i+k} A_{ik} |[A]_{ik}| = \frac{1}{|\mathbf{A}|} (-1)^{i+j} |[A]_{ij}|$$

$$\Rightarrow \frac{\partial}{\partial \mathbf{A}} \log |\mathbf{A}| = (\mathbf{A}^{-1})^T$$

Gaussian Derivatives

$$\frac{\partial(-\ell)}{\partial\boldsymbol{\mu}} = \frac{\partial}{\partial\boldsymbol{\mu}} \left[\frac{N}{2} \log |2\pi\Sigma| + \frac{1}{2} \sum_n (\mathbf{x}_n - \boldsymbol{\mu})^\top \Sigma^{-1} (\mathbf{x}_n - \boldsymbol{\mu}) \right]$$

Gaussian Derivatives

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Gaussian Derivatives

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Gaussian Derivatives

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Gaussian Derivatives

$$\frac{\partial(-\ell)}{\partial \Sigma^{-1}}$$

Gaussian Derivatives

$$\frac{\partial(-\ell)}{\partial \Sigma^{-1}} = \frac{\partial}{\partial \Sigma^{-1}} \left[\frac{N}{2} \log |2\pi \Sigma| + \frac{1}{2} \sum_n (\mathbf{x}_n - \boldsymbol{\mu})^\top \Sigma^{-1} (\mathbf{x}_n - \boldsymbol{\mu}) \right]$$

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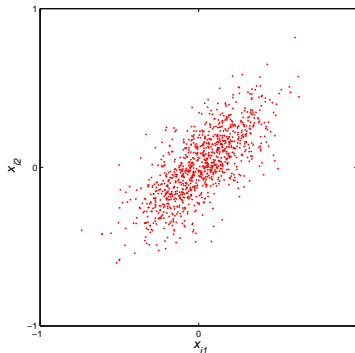
Gaussian Derivatives

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Gaussian Derivatives

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Equivalences



modelling correlations



maximising likelihood of a Gaussian model



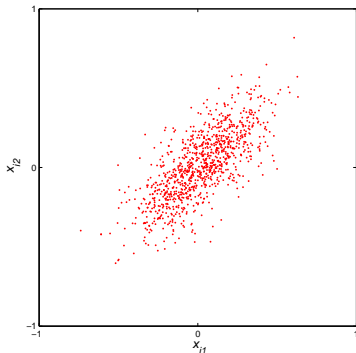
minimising a squared error cost function



minimizing data coding cost in bits (assuming Gaussian distributed)

Multivariate Linear Regression

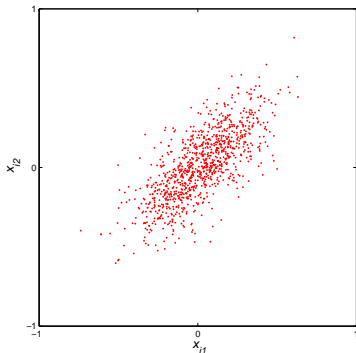
The relationship between variables can also be modelled as a **conditional** distribution.



- ▶ data $\mathcal{D} = \{(\mathbf{x}_1, \mathbf{y}_1) \dots, (\mathbf{x}_N, \mathbf{y}_N)\}$
- ▶ each \mathbf{x}_i (\mathbf{y}_i) is a vector of D_x (D_y) features,
- ▶ \mathbf{y}_i is conditionally independent of all else, given \mathbf{x}_i .

Multivariate Linear Regression

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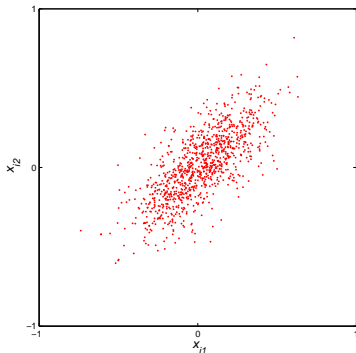


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A simple form of supervised (predictive) learning: model \mathbf{y} as a **linear** function of \mathbf{x} , with **Gaussian** noise.

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A simple form of supervised (predictive) learning: model \mathbf{y} as a **linear** function of \mathbf{x} , with **Gaussian** noise.

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

Multivariate Linear Regression – ML estimate

ML estimates are obtained by maximising the (conditional) likelihood, as before:

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Let y_i be scalar (so that W is a row vector) and write \mathbf{w} for the column vector of weights.

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- ▶ Gaussian models are also used for regression in **Gaussian Process Models**. We'll see these later too.

Three limitations of the multivariate Gaussian model

- ▶ What about higher order statistical structure in the data?
- ▶ What happens if there are outliers?
- ▶ There are $D(D + 1)/2$ parameters in the multivariate Gaussian model. What if D is very large?

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⇒ dimensionality reduction

End Notes

- ▶ It is very important that you *understand* all the material in the following cribsheet:
<http://www.gatsby.ucl.ac.uk/teaching/courses/ml1-2014/cribsheet.pdf>
- ▶ The following notes by (the late) Sam Roweis are quite useful:
 - ▶ Matrix identities and matrix derivatives:
<http://www.cs.nyu.edu/~roweis/notes/matrixid.pdf>
 - ▶ Gaussian identities:
<http://www.cs.nyu.edu/~roweis/notes/gaussid.pdf>
- ▶ Here is a useful statistics / pattern recognition glossary:
<http://alumni.media.mit.edu/~tpminka/statlearn/glossary/>
- ▶ Tom Minka's in-depth notes on matrix algebra:
<http://research.microsoft.com/en-us/um/people/minka/papers/matrix/>