Probabilistic & Unsupervised Learning

Introduction and Foundations

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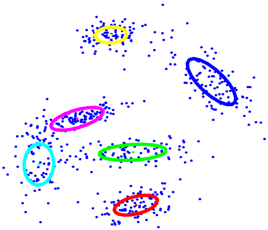
  - **Reinforcement learning.** Rewards or payoffs (and possibly also inputs) depend on actions:

    $$x_1 : a_1 \to r_1, x_2 : a_2 \to r_2, x_3 : a_3 \to r_3 \ldots$$

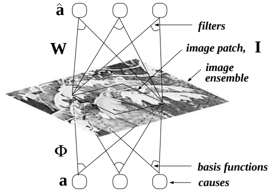
    Find a policy for action choice that maximises payoff.

Unsupervised Learning



Find underlying structure:

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



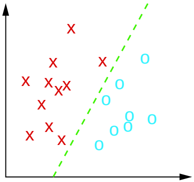
Uses of Unsupervised Learning:

- 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

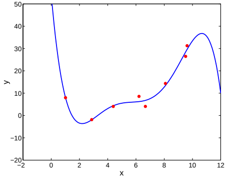
Two main examples:

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 $x \to y$ 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:

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

- 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:

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

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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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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: $\mathcal{D} = \{x_1, \ldots, x_n\}$ 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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- Model selection:

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

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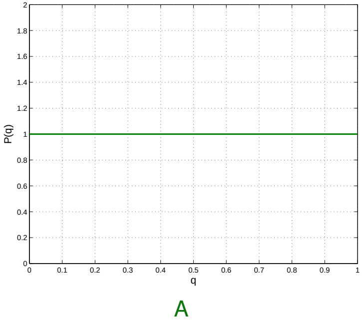

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Learner A believes model $\mathcal{M}_{\text{A}}$: all values of q are equally plausible;

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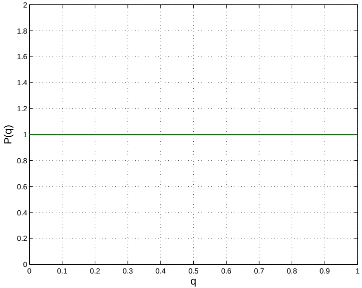

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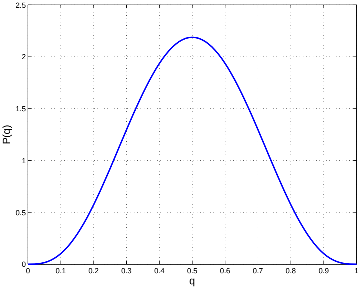

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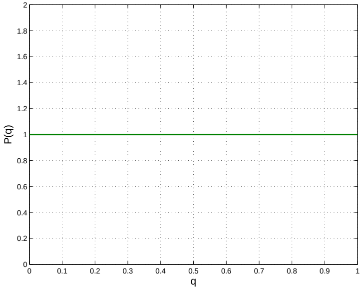

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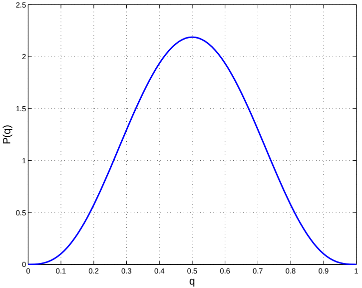

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Both prior beliefs can be described by the Beta distribution:

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

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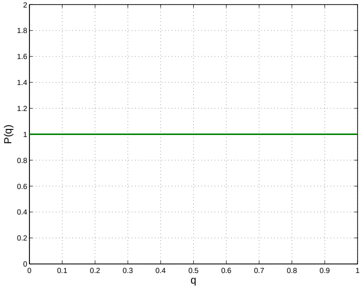
Coin toss: One parameter q — the probability of obtaining *heads*

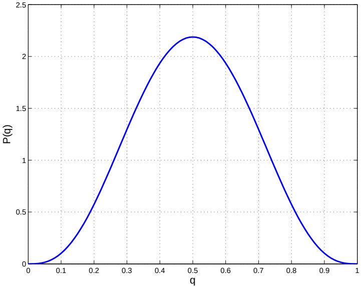
So our space of models is the set of distributions over $q \in [0, 1]$.

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: $\alpha_1 = \alpha_2 = 4.0$

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: The coin toss (cont)

Now we observe a toss. Two possible outcomes:

$$p(\mathrm{H}|q) = q \qquad\qquad p(\mathrm{T}|q) = 1 - q$$

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Bayesian learning: The coin toss (cont)

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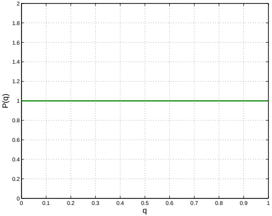
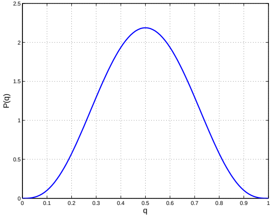
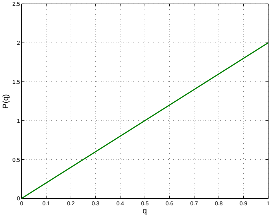
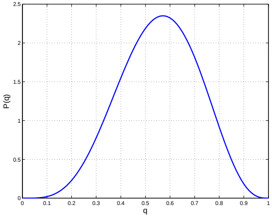
Prior	 Beta$(q \mid 1, 1)$	 Beta$(q \mid 4, 4)$
Posterior	 Beta$(q \mid 2, 1)$	 Beta$(q \mid 5, 4)$

Bayesian learning: The coin toss (cont)

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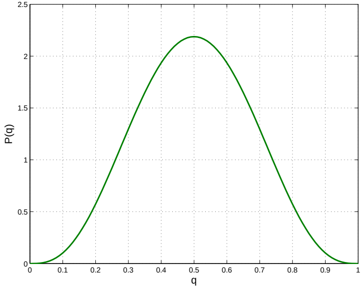

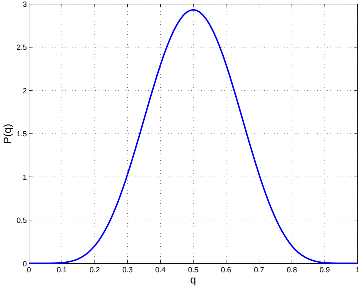

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with $F(\boldsymbol{\tau}, \nu)$ the normaliser, then the posterior is

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

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

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

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

Here,

$\phi(\theta)$	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 τ, with no likelihood equivalent.

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Bayesian coins – comparing models

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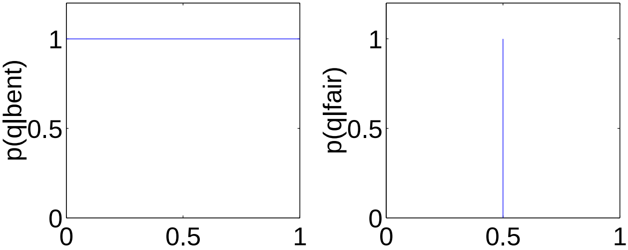

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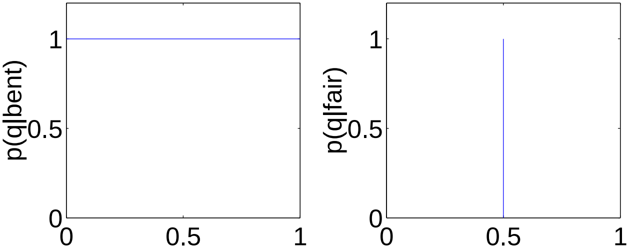

We make 10 tosses, and get: $\mathcal{D} = (\text{T H T H T T T T T T})$.

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How do we make predictions? Could choose the fair model (model selection).

Bayesian coins – comparing models

Which model should we prefer *a posteriori* (i.e. after seeing the data)?

The evidence for the fair model is:

$$P(\mathcal{D}|\text{fair}) = (1/2)^{10} \approx 0.001$$

and for the bent model is:

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

Thus, 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, a two-thirds probability that the coin is fair.

How do we make predictions? Could choose the fair model (model selection).
Or could weight the predictions from each model by their probability (model averaging).
Probability of H at next toss is:

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

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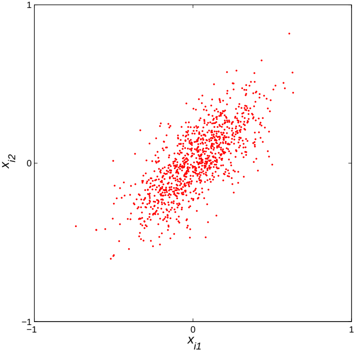
- For the next few weeks we will look at ML and MAP learning in more complex models. We will then return to the fully Bayesian formulation for the few intersting cases where it is tractable. Approximations will be addressed in the second half of the course.

Modelling associations between variables



- Data set $\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$
- with each data point a vector of D features: $\mathbf{x}_i = [x_{i1} \ldots x_{iD}]$
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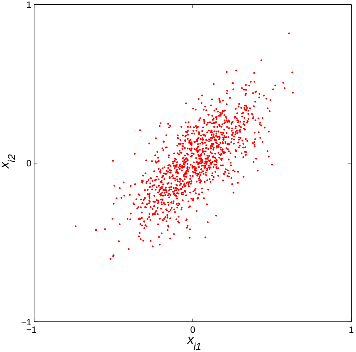

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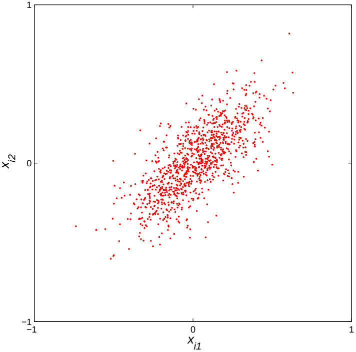

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We can use a multivariate Gaussian model:

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

ML Learning for a Gaussian

Data set $\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, 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:

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

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

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$$\mathrm{Tr}\left[A\right] = \mathrm{Tr}\left[A^\mathsf{T}\right] \qquad \mathrm{Tr}\left[ABC\right] = \mathrm{Tr}\left[CAB\right] = \mathrm{Tr}\left[BCA\right]$$

$$\frac{\partial}{\partial A_{ij}} \mathrm{Tr}\left[A^\mathsf{T} B\right] = \frac{\partial}{\partial A_{ij}} \sum_{mn} A_{mn} B_{mn} = B_{ij}$$

$$\Rightarrow \frac{\partial}{\partial A} \mathrm{Tr}\left[A^\mathsf{T} B\right] = B$$

$$\begin{aligned} \frac{\partial}{\partial A} \mathrm{Tr}\left[A^\mathsf{T} BAC\right] &= \frac{\partial}{\partial A} \mathrm{Tr}\left[F_1(A)^\mathsf{T} B F_2(A) C\right] \text{ with } F_1 \text{ and } F_2 \text{ both identity maps} \\ &= \frac{\partial}{\partial F_1} \mathrm{Tr}\left[F_1^\mathsf{T} B F_2 C\right] \frac{\partial F_1}{\partial A} + \frac{\partial}{\partial F_2} \mathrm{Tr}\left[F_2^\mathsf{T} B^\mathsf{T} F_1 C^\mathsf{T}\right] \frac{\partial F_2}{\partial A} \end{aligned}$$

Refresher – matrix derivatives of scalar forms

We will use the following facts:

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Refresher – matrix derivatives of scalar forms

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&= B F_2 C + B^{\mathsf{T}} F_1 C^{\mathsf{T}} = BAC + B^{\mathsf{T}} A C^{\mathsf{T}}
\end{aligned}$$

$$\frac{\partial}{\partial A_{ij}} \log |A|$$

Refresher – matrix derivatives of scalar forms

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\end{aligned}$$

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

Refresher – matrix derivatives of scalar forms

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&= B F_2 C + B^{\mathsf{T}} F_1 C^{\mathsf{T}} = BAC + B^{\mathsf{T}} A C^{\mathsf{T}}
\end{aligned}$$

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

Refresher – matrix derivatives of scalar forms

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

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\end{aligned}$$

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

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

Gaussian Derivatives

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

Gaussian Derivatives

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

Gaussian Derivatives

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

Gaussian Derivatives

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

Gaussian Derivatives

$$\begin{aligned}
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&= \frac{1}{2}\sum_n\frac{\partial}{\partial\boldsymbol{\mu}}\left[(\mathbf{x}_n-\boldsymbol{\mu})^{\mathsf{T}}\Sigma^{-1}(\mathbf{x}_n-\boldsymbol{\mu})\right] \\
&= \frac{1}{2}\sum_n\frac{\partial}{\partial\boldsymbol{\mu}}\left[\mathbf{x}_n^{\mathsf{T}}\Sigma^{-1}\mathbf{x}_n + \boldsymbol{\mu}^{\mathsf{T}}\Sigma^{-1}\boldsymbol{\mu} - 2\boldsymbol{\mu}^{\mathsf{T}}\Sigma^{-1}\mathbf{x}_n\right] \\
&= \frac{1}{2}\sum_n\frac{\partial}{\partial\boldsymbol{\mu}}\left[\boldsymbol{\mu}^{\mathsf{T}}\Sigma^{-1}\boldsymbol{\mu}\right] - 2\frac{\partial}{\partial\boldsymbol{\mu}}\left[\boldsymbol{\mu}^{\mathsf{T}}\Sigma^{-1}\mathbf{x}_n\right] \\
&= \frac{1}{2}\sum_n\left[2\Sigma^{-1}\boldsymbol{\mu} - 2\Sigma^{-1}\mathbf{x}_n\right]
\end{aligned}$$

Gaussian Derivatives

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

Gaussian Derivatives

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

$$= \frac{1}{2} \sum_n \frac{\partial}{\partial \boldsymbol{\mu}} \left[(\mathbf{x}_n - \boldsymbol{\mu})^\mathsf{T} \Sigma^{-1} (\mathbf{x}_n - \boldsymbol{\mu}) \right]$$

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$$= \frac{1}{2} \sum_n \frac{\partial}{\partial \boldsymbol{\mu}} \left[\boldsymbol{\mu}^\mathsf{T} \Sigma^{-1} \boldsymbol{\mu} \right] - 2 \frac{\partial}{\partial \boldsymbol{\mu}} \left[\boldsymbol{\mu}^\mathsf{T} \Sigma^{-1} \mathbf{x}_n \right]$$

$$= \frac{1}{2} \sum_n \left[2\Sigma^{-1} \boldsymbol{\mu} - 2\Sigma^{-1} \mathbf{x}_n \right]$$

$$= N\Sigma^{-1} \boldsymbol{\mu} - \Sigma^{-1} \sum_n \mathbf{x}_n$$

$$= 0 \Rightarrow \hat{\boldsymbol{\mu}} = \frac{1}{N} \sum_n \mathbf{x}_n$$

Gaussian Derivatives

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

Gaussian Derivatives

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

Gaussian Derivatives

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$$= \frac{\partial}{\partial \Sigma^{-1}} \left[\frac{N}{2} \log |2\pi I| \right] - \frac{\partial}{\partial \Sigma^{-1}} \left[\frac{N}{2} \log |\Sigma^{-1}| \right]$$

$$+ \frac{1}{2} \sum_n \frac{\partial}{\partial \Sigma^{-1}} \left[(\mathbf{x}_n - \boldsymbol{\mu})^\mathsf{T} \Sigma^{-1} (\mathbf{x}_n - \boldsymbol{\mu}) \right]$$

Gaussian Derivatives

$$
\begin{aligned}
\frac{\partial(-\ell)}{\partial \Sigma^{-1}} &= \frac{\partial}{\partial \Sigma^{-1}} \left[\frac{N}{2} \log |2\pi\Sigma| + \frac{1}{2} \sum_n (\mathbf{x}_n - \boldsymbol{\mu})^\mathsf{T} \Sigma^{-1} (\mathbf{x}_n - \boldsymbol{\mu}) \right] \\
&= \frac{\partial}{\partial \Sigma^{-1}} \left[\frac{N}{2} \log |2\pi I| \right] - \frac{\partial}{\partial \Sigma^{-1}} \left[\frac{N}{2} \log |\Sigma^{-1}| \right] \\
&\quad + \frac{1}{2} \sum_n \frac{\partial}{\partial \Sigma^{-1}} \left[(\mathbf{x}_n - \boldsymbol{\mu})^\mathsf{T} \Sigma^{-1} (\mathbf{x}_n - \boldsymbol{\mu}) \right] \\
&= -\frac{N}{2} \Sigma^\mathsf{T} + \frac{1}{2} \sum_n (\mathbf{x}_n - \boldsymbol{\mu})(\mathbf{x}_n - \boldsymbol{\mu})^\mathsf{T}
\end{aligned}
$$

Gaussian Derivatives

$$
\begin{aligned}
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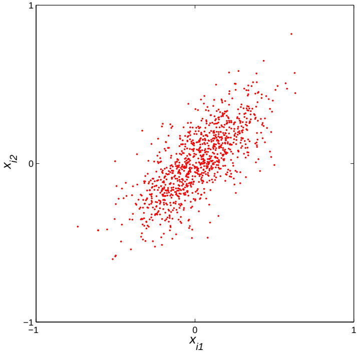
&= \frac{\partial}{\partial \Sigma^{-1}} \left[\frac{N}{2} \log |2\pi I| \right] - \frac{\partial}{\partial \Sigma^{-1}} \left[\frac{N}{2} \log |\Sigma^{-1}| \right] \\
&\qquad + \frac{1}{2} \sum_n \frac{\partial}{\partial \Sigma^{-1}} \left[(\mathbf{x}_n - \boldsymbol{\mu})^\mathsf{T} \Sigma^{-1} (\mathbf{x}_n - \boldsymbol{\mu}) \right] \\
&= -\frac{N}{2} \Sigma^\mathsf{T} + \frac{1}{2} \sum_n (\mathbf{x}_n - \boldsymbol{\mu})(\mathbf{x}_n - \boldsymbol{\mu})^\mathsf{T}
\end{aligned}
$$

$$
= 0 \Rightarrow \hat{\Sigma} = \frac{1}{N} \sum_n (\mathbf{x}_n - \boldsymbol{\mu})(\mathbf{x}_n - \boldsymbol{\mu})^\mathsf{T}
$$

Equivalences



modelling correlations

⇕

maximising likelihood of a Gaussian model

⇕

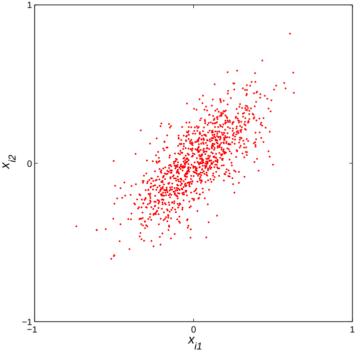
minimising a squared error cost function

⇕

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 $\mathcal{D} = \{(\mathbf{x}_1, \mathbf{y}_1) \ldots, (\mathbf{x}_N, \mathbf{y}_N)\}$
- 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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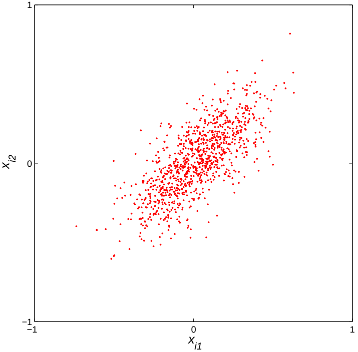

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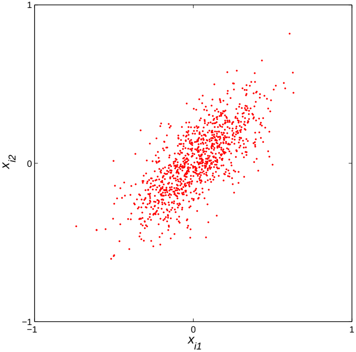
- each $\mathbf{x}_i$ ($\mathbf{y}_i$) is a vector of D_x (D_y) features,
- $\mathbf{y}_i$ is conditionally independent of all else, given $\mathbf{x}_i$.

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

Multivariate Linear Regression

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



- data $\mathcal{D} = \{(\mathbf{x}_1, \mathbf{y}_1) \ldots, (\mathbf{x}_N, \mathbf{y}_N)\}$
- 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 $\mathbf{x}_i$.

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

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

Multivariate Linear Regression – ML estimate

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

$$
\begin{aligned}
\ell &= \sum_i \log p(\mathbf{y}_i | \mathbf{x}_i, \mathsf{W}, \Sigma_y) \\
&= -\frac{N}{2} \log |2\pi \Sigma_y| - \frac{1}{2} \sum_i (\mathbf{y}_i - \mathsf{W}\mathbf{x}_i)^{\mathsf{T}} \Sigma_y^{-1} (\mathbf{y}_i - \mathsf{W}\mathbf{x}_i)
\end{aligned}
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$$\frac{\partial(-\ell)}{\partial \mathrm{W}}$$

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$$\frac{\partial(-\ell)}{\partial \mathrm{W}} = \frac{\partial}{\partial \mathrm{W}} \left[\frac{N}{2} \log |2\pi\Sigma_y| + \frac{1}{2} \sum_i (\mathbf{y}_i - \mathrm{W}\mathbf{x}_i)^{\mathsf{T}} \Sigma_y^{-1} (\mathbf{y}_i - \mathrm{W}\mathbf{x}_i) \right]$$

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$$= \frac{1}{2} \sum_i \frac{\partial}{\partial \mathrm{W}} \left[(\mathbf{y}_i - \mathrm{W}\mathbf{x}_i)^{\mathsf{T}} \Sigma_y^{-1} (\mathbf{y}_i - \mathrm{W}\mathbf{x}_i) \right]$$

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\frac{\partial(-\ell)}{\partial \mathrm{W}} &= \frac{\partial}{\partial \mathrm{W}}\left[\frac{N}{2}\log|2\pi\Sigma_y| + \frac{1}{2}\sum_i (\mathbf{y}_i - \mathrm{W}\mathbf{x}_i)^\mathsf{T}\Sigma_y^{-1}(\mathbf{y}_i - \mathrm{W}\mathbf{x}_i)\right] \\
&= \frac{1}{2}\sum_i \frac{\partial}{\partial \mathrm{W}}\left[(\mathbf{y}_i - \mathrm{W}\mathbf{x}_i)^\mathsf{T}\Sigma_y^{-1}(\mathbf{y}_i - \mathrm{W}\mathbf{x}_i)\right] \\
&= \frac{1}{2}\sum_i \frac{\partial}{\partial \mathrm{W}}\left[\mathbf{y}_i^\mathsf{T}\Sigma_y^{-1}\mathbf{y}_i + \mathbf{x}_i^\mathsf{T}\mathrm{W}^\mathsf{T}\Sigma_y^{-1}\mathrm{W}\mathbf{x}_i - 2\mathbf{x}_i^\mathsf{T}\mathrm{W}^\mathsf{T}\Sigma_y^{-1}\mathbf{y}_i\right]
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\frac{\partial(-\ell)}{\partial \mathrm{W}} &= \frac{\partial}{\partial \mathrm{W}}\left[\frac{N}{2}\log|2\pi\Sigma_y| + \frac{1}{2}\sum_i (\mathbf{y}_i - \mathrm{W}\mathbf{x}_i)^{\mathsf{T}}\Sigma_y^{-1}(\mathbf{y}_i - \mathrm{W}\mathbf{x}_i)\right] \\
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&= \frac{1}{2}\sum_i \frac{\partial}{\partial \mathrm{W}}\left[\mathbf{y}_i^{\mathsf{T}}\Sigma_y^{-1}\mathbf{y}_i + \mathbf{x}_i^{\mathsf{T}}\mathrm{W}^{\mathsf{T}}\Sigma_y^{-1}\mathrm{W}\mathbf{x}_i - 2\mathbf{x}_i^{\mathsf{T}}\mathrm{W}^{\mathsf{T}}\Sigma_y^{-1}\mathbf{y}_i\right] \\
&= \frac{1}{2}\sum_i \left[\frac{\partial}{\partial \mathrm{W}}\mathrm{Tr}\left[\mathrm{W}^{\mathsf{T}}\Sigma_y^{-1}\mathrm{W}\mathbf{x}_i\mathbf{x}_i^{\mathsf{T}}\right] - 2\frac{\partial}{\partial \mathrm{W}}\mathrm{Tr}\left[\mathrm{W}^{\mathsf{T}}\Sigma_y^{-1}\mathbf{y}_i\mathbf{x}_i^{\mathsf{T}}\right]\right]
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&= \frac{1}{2} \sum_i \frac{\partial}{\partial \mathrm{W}} \left[(\mathbf{y}_i - \mathrm{W}\mathbf{x}_i)^\mathsf{T} \Sigma_y^{-1} (\mathbf{y}_i - \mathrm{W}\mathbf{x}_i) \right] \\
&= \frac{1}{2} \sum_i \frac{\partial}{\partial \mathrm{W}} \left[\mathbf{y}_i^\mathsf{T} \Sigma_y^{-1} \mathbf{y}_i + \mathbf{x}_i^\mathsf{T} \mathrm{W}^\mathsf{T} \Sigma_y^{-1} \mathrm{W} \mathbf{x}_i - 2\mathbf{x}_i^\mathsf{T} \mathrm{W}^\mathsf{T} \Sigma_y^{-1} \mathbf{y}_i \right] \\
&= \frac{1}{2} \sum_i \left[\frac{\partial}{\partial \mathrm{W}} \mathrm{Tr} \left[\mathrm{W}^\mathsf{T} \Sigma_y^{-1} \mathrm{W} \mathbf{x}_i \mathbf{x}_i^\mathsf{T} \right] - 2 \frac{\partial}{\partial \mathrm{W}} \mathrm{Tr} \left[\mathrm{W}^\mathsf{T} \Sigma_y^{-1} \mathbf{y}_i \mathbf{x}_i^\mathsf{T} \right] \right] \\
&= \frac{1}{2} \sum_i \left[2\Sigma_y^{-1} \mathrm{W} \mathbf{x}_i \mathbf{x}_i^\mathsf{T} - 2\Sigma_y^{-1} \mathbf{y}_i \mathbf{x}_i^\mathsf{T} \right]
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&= \frac{1}{2}\sum_i \left[\frac{\partial}{\partial \mathrm{W}}\mathrm{Tr}\left[\mathrm{W}^\mathsf{T}\Sigma_y^{-1}\mathrm{W}\mathbf{x}_i\mathbf{x}_i^\mathsf{T}\right] - 2\frac{\partial}{\partial \mathrm{W}}\mathrm{Tr}\left[\mathrm{W}^\mathsf{T}\Sigma_y^{-1}\mathbf{y}_i\mathbf{x}_i^\mathsf{T}\right]\right] \\
&= \frac{1}{2}\sum_i \left[2\Sigma_y^{-1}\mathrm{W}\mathbf{x}_i\mathbf{x}_i^\mathsf{T} - 2\Sigma_y^{-1}\mathbf{y}_i\mathbf{x}_i^\mathsf{T}\right] \\
= 0 \Rightarrow \widehat{\mathrm{W}} &= \sum_i \mathbf{y}_i\mathbf{x}_i^\mathsf{T}\left(\sum_i \mathbf{x}_i\mathbf{x}_i^\mathsf{T}\right)^{-1}
\end{aligned}
$$

Multivariate Linear Regression – Posterior

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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Then the log posterior on **w** is

$$\log P(\mathbf{w}|\mathcal{D}, \mathsf{A}, \sigma_y) = \log P(\mathcal{D}|\mathbf{w}, \mathsf{A}, \sigma_y) + \log P(\mathbf{w}|\mathsf{A}, \sigma_y) - \log P(\mathcal{D}|\mathsf{A}, \sigma_y)$$

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&= -\frac{1}{2}\mathbf{w}^{\mathsf{T}}\left(\mathrm{A} + \sigma_y^{-2}\sum_i \mathbf{x}_i\mathbf{x}_i^{\mathsf{T}}\right)\mathbf{w} + \mathbf{w}^{\mathsf{T}}\sum_i (y_i\mathbf{x}_i)\sigma_y^{-2} + \text{const}
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&= -\frac{1}{2}\mathbf{w}^{\mathsf{T}} \underbrace{(\mathrm{A} + \sigma_y^{-2}\sum_i \mathbf{x}_i\mathbf{x}_i^{\mathsf{T}})}_{\Sigma_w^{-1}}\mathbf{w} + \mathbf{w}^{\mathsf{T}}\sum_i (y_i\mathbf{x}_i)\sigma_y^{-2} + \mathrm{const}
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&= -\frac{1}{2}\mathbf{w}^{\mathsf{T}}\Sigma_w^{-1}\mathbf{w} + \mathbf{w}^{\mathsf{T}}\Sigma_w^{-1}\,\Sigma_w\sum_i (y_i\mathbf{x}_i)\sigma_y^{-2} + \text{const}
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&= -\frac{1}{2}\mathbf{w}^{\mathsf{T}}\underbrace{(\mathrm{A} + \sigma_y^{-2}\sum_i \mathbf{x}_i\mathbf{x}_i^{\mathsf{T}})}_{\Sigma_w^{-1}}\mathbf{w} + \mathbf{w}^{\mathsf{T}}\sum_i (y_i\mathbf{x}_i)\sigma_y^{-2} + \text{const} \\
&= -\frac{1}{2}\mathbf{w}^{\mathsf{T}}\Sigma_w^{-1}\mathbf{w} + \mathbf{w}^{\mathsf{T}}\Sigma_w^{-1}\underbrace{\Sigma_w\sum_i (y_i\mathbf{x}_i)\sigma_y^{-2}}_{\boldsymbol{\mu}_w} + \text{const}
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&= -\frac{1}{2}\mathbf{w}^{\mathsf{T}}\Sigma_w^{-1}\mathbf{w} + \mathbf{w}^{\mathsf{T}}\Sigma_w^{-1}\underbrace{\Sigma_w \sum_i (y_i\mathbf{x}_i)\sigma_y^{-2}}_{\boldsymbol{\mu}_w} + \text{const} \\
&= \log \mathcal{N}\left(\Sigma_w {\textstyle\sum_i} (y_i\mathbf{x}_i)\sigma_y^{-2}, \Sigma_w\right)
\end{aligned}$$

MAP and ML for linear regression

As the posterior is Gaussian, the MAP and posterior mean weights are the same:

$$\mathbf{w}^{\text{MAP}} = \underbrace{\left(A + \frac{\sum_i \mathbf{x}_i \mathbf{x}_i^{\mathsf{T}}}{\sigma_y^2}\right)^{-1}}_{\Sigma_w} \frac{\sum_i y_i \mathbf{x}_i}{\sigma_y^2}$$

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Compare this to the (transposed) ML weight vector for scalar outputs:

$$\mathbf{w}^{\text{ML}} = \widehat{\text{W}}^{\top} = \left(\sum_i \mathbf{x}_i \mathbf{x}_i^{\top}\right)^{-1} \sum_i y_i \mathbf{x}_i$$

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Compare this to the (transposed) ML weight vector for scalar outputs:

$$\mathbf{w}^{\text{ML}} = \widehat{\text{W}}^{\text{T}} = \left(\sum_i \mathbf{x}_i \mathbf{x}_i^{\text{T}}\right)^{-1} \sum_i y_i \mathbf{x}_i$$

- The prior acts to "inflate" the apparent covariance of inputs.

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- As A is positive (semi)definite, shrinks the weights towards the prior mean (here $\mathbf{0}$).

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Compare this to the (transposed) ML weight vector for scalar outputs:

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- The prior acts to “inflate” the apparent covariance of inputs.
- As A is positive (semi)definite, shrinks the weights towards the prior mean (here $\mathbf{0}$).
- If $A = \alpha I$ this is known as the ridge regression estimator.

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- If $A = \alpha I$ this is known as the ridge regression estimator.
- The MAP/shrinkage/ridge weight estimate often has lower squared error (despite bias) and makes more accurate predictions on test inputs than the ML estimate.

MAP and ML for linear regression

As the posterior is Gaussian, the MAP and posterior mean weights are the same:

$$\mathbf{w}^{\text{MAP}} = \underbrace{\left(A + \frac{\sum_i \mathbf{x}_i \mathbf{x}_i^\top}{\sigma_y^2}\right)^{-1}}_{\Sigma_w} \frac{\sum_i y_i \mathbf{x}_i}{\sigma_y^2} = \left(A\sigma_y^2 + \sum_i \mathbf{x}_i \mathbf{x}_i^\top\right)^{-1} \sum_i y_i \mathbf{x}_i$$

Compare this to the (transposed) ML weight vector for scalar outputs:

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- An example of prior-based regularisation of estimates.

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  Posterior, or even ML, estimation is not possible in closed form $\Rightarrow$ iterative methods such as gradient ascent or iteratively re-weighted least squares (IRLS).
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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

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  $\Rightarrow$ 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/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/`