

Logistic regression

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May 6, 2019

Reference

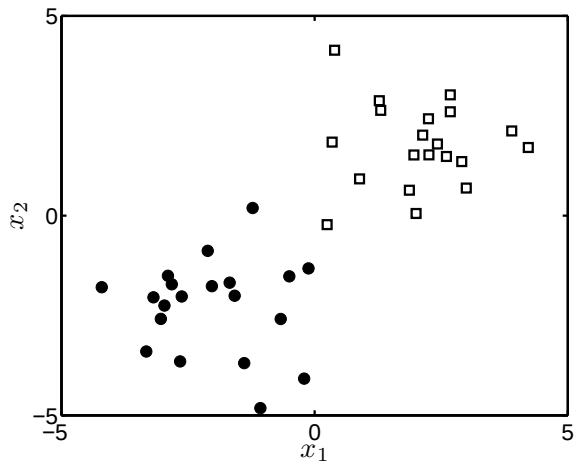
The content and the slides are adapted from

S. Rogers and M. Girolami, A First Course in Machine Learning (FCML), 2nd edition, Chapman & Hall/CRC 2016, ISBN: 9781498738484

Classification syllabus

- ▶ 4 classification algorithms.
- ▶ Of which:
 - ▶ 2 are probabilistic.
 - ▶ Bayes classifier.
 - ▶ **Logistic regression.**
 - ▶ 2 are non-probabilistic.
 - ▶ K-nearest neighbours.
 - ▶ Support Vector Machines.
- ▶ There are many others!

Some data



Logistic regression

- In the Bayes classifier, we built a model of each class and then used Bayes rule:

$$P(t_{\text{new}} = k | \mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t}) = \frac{p(\mathbf{x}_{\text{new}} | t_{\text{new}} = k, \mathbf{X}, \mathbf{t}) P(t_{\text{new}} = k)}{\sum_j p(\mathbf{x}_{\text{new}} | t_{\text{new}} = j, \mathbf{X}, \mathbf{t}) P(t_{\text{new}} = j)}$$

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 - ▶ No – *output is unbounded and so can't be a probability.*

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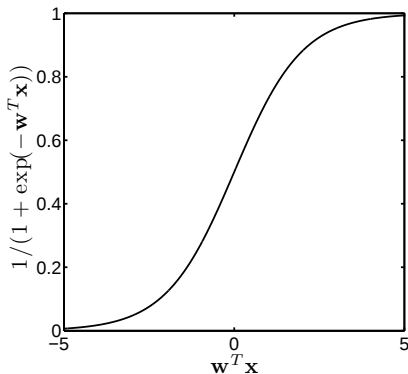
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 - ▶ No – *output is unbounded and so can't be a probability.*
- ▶ But, can use $P(t_{\text{new}} = k | \mathbf{x}_{\text{new}}, \mathbf{w}) = h(f(\mathbf{x}_{\text{new}}; \mathbf{w}))$ where $h(\cdot)$ *squashes* $f(\mathbf{x}_{\text{new}}; \mathbf{w})$ to lie between 0 and 1 – a probability.

$h(\cdot)$

- For logistic regression (binary), we use the sigmoid function:

$$P(t_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \mathbf{w}) = h(\mathbf{w}^T \mathbf{x}_{\text{new}}) = \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x}_{\text{new}})}$$

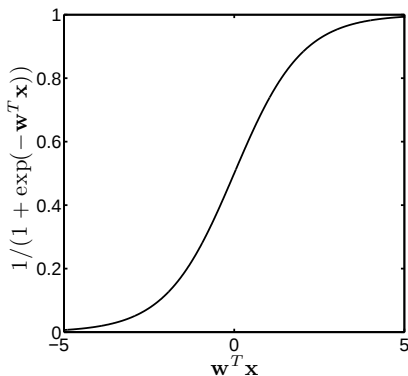


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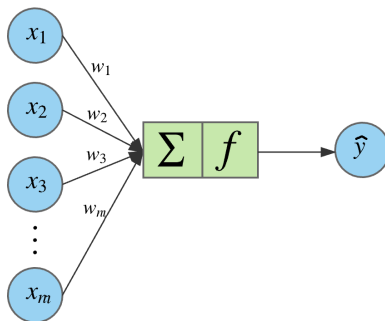
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$$P(T = 1|\mathbf{x}, \mathbf{w}) = h(\mathbf{w}^T \mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x})}$$

$$P(T = 0|\mathbf{x}, \mathbf{w}) = 1 - h(\mathbf{w}^T \mathbf{x}) = \frac{\exp(-\mathbf{w}^T \mathbf{x})}{1 + \exp(-\mathbf{w}^T \mathbf{x})}$$



Perceptron



Likelihood

$$\begin{aligned} p(\mathbf{t}|\mathbf{X}, \mathbf{w}) &= \prod_{n=1}^N p(t_n|\mathbf{x}_n, \mathbf{w}) \\ &= \prod_{t_n=1} p(t_n|\mathbf{x}_n, \mathbf{w}) \prod_{t_n=0} p(t_n|\mathbf{x}_n, \mathbf{w}) \\ &= \prod_{t_n=1} h(\mathbf{w}^\top \mathbf{x}_n) \prod_{t_n=0} (1 - h(\mathbf{w}^\top \mathbf{x}_n)) \end{aligned}$$

Cross Entropy

The **negative log-likelihood** is written by

$$\begin{aligned}\mathbf{J}(\mathbf{w}) &= - \sum_{t_n=1} \log h(\mathbf{w}^T \mathbf{x}_n) - \sum_{t_n=0} \log(1 - h(\mathbf{w}^T \mathbf{x}_n)) \\ &= - \sum_{n=1}^N t_n \log h(\mathbf{w}^T \mathbf{x}_n) + (1 - t_n) \log(1 - h(\mathbf{w}^T \mathbf{x}_n))\end{aligned}$$

Minimization of Cross Entropy

We minimize Cross Entropy to infer the model parameters w_j .

$$\frac{\partial \mathbf{J}}{\partial w_j} = - \sum_{n=1}^N [t_n - h(\mathbf{w}^T \mathbf{x}_n)] \mathbf{x}_{n,j}$$

We may use **Gradient Descent** for this purpose:

$$w_j \leftarrow w_j - \eta \frac{\partial \mathbf{J}}{\partial w_j}$$

Multiclass Classification

Data in K classes

$$(\mathbf{x}_1, t_1), \dots (\mathbf{x}_N, t_N),$$

where each $t_n \in \{1 \dots K\}$

One hot representation

Each label $t_n \in \{1 \cdots K\}$ can be represented as a 0/1 K -vector, with

$$t_{n,k} = \begin{cases} 1, & \text{if } t_n = k \\ 0, & \text{otherwise} \end{cases}$$

Softmax Regression

$$P(T = k | \mathbf{x}, \mathbf{w}) = \frac{\exp(-\mathbf{w}^k \mathbf{x})}{\sum_{\ell=1}^K \exp(-\mathbf{w}^\ell \mathbf{x})}$$

That is, we have K parameter vectors $\mathbf{w}^1, \dots, \mathbf{w}^K$ with $\mathbf{w}^k$ used to compute the probability $P(t_{n,k} = 1)$.

Cross Entropy: Multiple Classes

The Cross-Entropy loss is written by

$$\mathbf{J} = - \sum_{n=1}^N \sum_{k=1}^K t_{n,k} \log \frac{\exp(-\mathbf{w}^k \mathbf{x}_n)}{\sum_{\ell=1}^K \exp(-\mathbf{w}^{\ell} \mathbf{x}_n)}$$

Gradient

The **gradient** can be used in Gradient-Descent optimization, or for other purposes.

$$\frac{\partial \mathbf{J}}{\partial w_j^k} = - \sum_{n=1}^N \left[t_{n,k} - \frac{\exp(-\mathbf{w}^k \mathbf{x}_n)}{\sum_{\ell=1}^K \exp(-\mathbf{w}^\ell \mathbf{x}_n)} \right] \mathbf{x}_{n,j}$$

Bayesian logistic regression

- ▶ Recall the Bayesian ideas from few lectures ago....
- ▶ In theory, if we place a *prior* on $\mathbf{w}$ and define a *likelihood* we can obtain a *posterior*:

$$p(\mathbf{w}|\mathbf{X}, \mathbf{t}) = \frac{p(\mathbf{t}|\mathbf{X}, \mathbf{w})p(\mathbf{w})}{p(\mathbf{t}|\mathbf{X})}$$

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- ▶ And we can make predictions by taking expectations (averaging over $\mathbf{w}$):

$$P(t_{\text{new}} = 1|\mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t}) = \mathbf{E}_{p(\mathbf{w}|\mathbf{X}, \mathbf{t})} \{P(t_{\text{new}} = 1|\mathbf{x}_{\text{new}}, \mathbf{w})\}$$

- ▶ Sounds good so far....

Defining a prior

- ▶ Choose a Gaussian prior:

$$p(\mathbf{w}) = \prod_{d=1}^D \mathcal{N}(0, \sigma^2).$$

- ▶ For simplicity, here we assume w_0 is zero.
- ▶ The prior has the parameter σ^2 .
- ▶ Prior choice is *always* important from a data analysis point of view.
- ▶ Previously, it was also important 'for the maths'.
- ▶ This isn't the case today – could choose any prior – no prior makes the maths easier!

Defining a likelihood

- First assume independence:

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}) = \prod_{n=1}^N p(t_n|\mathbf{x}_n, \mathbf{w})$$

Defining a likelihood

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$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}) = \prod_{n=1}^N p(t_n|\mathbf{x}_n, \mathbf{w})$$

- ▶ We have already defined this – it's our squashing function! If $t_n = 1$:

$$P(t_n = 1|\mathbf{x}_n, \mathbf{w}) = \frac{1}{1 + \exp(-\mathbf{w}^\top \mathbf{x}_n)}$$

- ▶ and if $t_n = 0$:

$$P(t_n = 0|\mathbf{x}_n, \mathbf{w}) = 1 - P(t_n = 1|\mathbf{x}_n, \mathbf{w})$$

Posterior

$$p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2) = \frac{p(\mathbf{t}|\mathbf{X}, \mathbf{w})p(\mathbf{w}|\sigma^2)}{p(\mathbf{t}|\mathbf{X}, \sigma^2)}$$

- ▶ Now things start going wrong.
- ▶ We can't compute $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$ analytically.
 - ▶ Prior is not conjugate to likelihood. No prior is!
 - ▶ This means we don't know the *form* of $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$
 - ▶ And we can't compute the marginal likelihood:

$$p(\mathbf{t}|\mathbf{X}, \sigma^2) = \int p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \sigma^2)p(\mathbf{w}|\sigma^2) d\mathbf{w}$$

What can we compute?

$$p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2) = \frac{p(\mathbf{t}|\mathbf{X}, \mathbf{w})p(\mathbf{w}|\sigma^2)}{p(\mathbf{t}|\mathbf{X}, \sigma^2)}$$

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 - ▶ Sample from $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$.
- ▶ We'll cover *examples* of each of these in turn....
- ▶ These examples aren't the only ways of approximating/sampling.
- ▶ They are also general techniques not unique to logistic regression.

MAP estimate

- ▶ Our first method is to find the value of $\mathbf{w}$ that maximises $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$ (call it $\hat{\mathbf{w}}$).
 - ▶ $g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2) \propto p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$
 - ▶ $\hat{\mathbf{w}}$ therefore also maximises $g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2)$.
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- ▶ Known as MAP (maximum a posteriori) solution.
- ▶ Once we have $\hat{\mathbf{w}}$, make predictions with:

$$P(t_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \hat{\mathbf{w}}) = \frac{1}{1 + \exp(-\hat{\mathbf{w}}^T \mathbf{x}_{\text{new}})}$$

MAP

- ▶ When we met maximum likelihood, we could find $\hat{\mathbf{w}}$ exactly with some algebra.
- ▶ Can't do that here (can't solve $\frac{\partial g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2)}{\partial \mathbf{w}} = \mathbf{0}$)

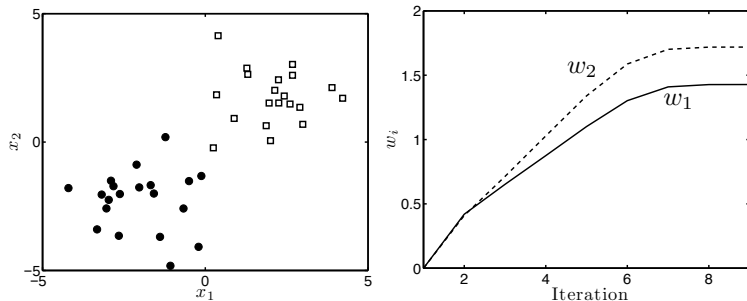
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- ▶ Resort to numerical optimisation:
 1. Guess $\hat{\mathbf{w}}$
 2. Change it a bit in a way that increases $g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2)$
 3. Repeat until no further increase is possible.

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 3. Repeat until no further increase is possible.
- ▶ Many algorithms exist that differ in how they do step 2.
- ▶ e.g. **Gradient Descent** and **Newton-Raphson** (book Chapter 4)
 - ▶ Not covered in this course. You just need to know that sometimes we can't do things analytically and there are methods to help us!

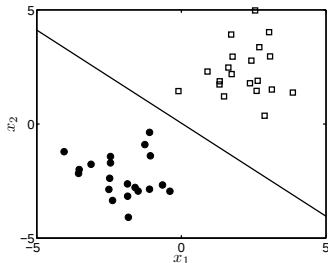
MAP – numerical optimisation for our data



- ▶ Left: Data.
- ▶ Right: Evolution of $\hat{\mathbf{w}}$ in numerical optimisation.
- ▶ We set $\sigma^2 = 10$.

Decision boundary

- ▶ Once we have $\hat{\mathbf{w}}$, we can classify new examples.
- ▶ Decision boundary is a useful visualisation:

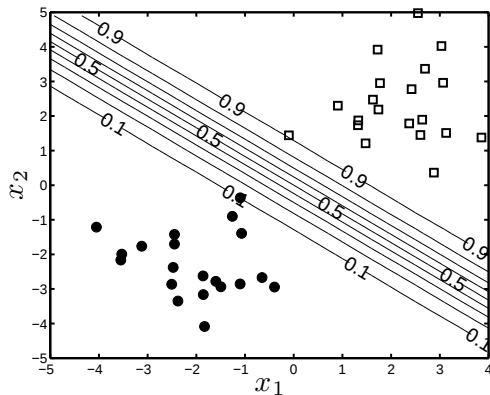


- ▶ Line corresponding to $P(t_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \hat{\mathbf{w}}) = 0.5$.

$$0.5 = \frac{1}{2} = \frac{1}{1 + \exp(-\hat{\mathbf{w}}^T \mathbf{x}_{\text{new}})}.$$

So: $\exp(-\hat{\mathbf{w}}^T \mathbf{x}_{\text{new}}) = 1$. Or: $\hat{\mathbf{w}}^T \mathbf{x}_{\text{new}} = 0$

Predictive probabilities



- ▶ Contours of $P(t_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \hat{\mathbf{w}})$.
- ▶ Do they look sensible?

Roadmap

- ▶ Find the most likely value of $\mathbf{w}$ – a point estimate.
- ▶ **Approximate $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$ with something easier.**
- ▶ Sample from $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$.

Laplace approximation

- ▶ Our second method involves **approximating** $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$ with another distribution.
- ▶ i.e. Find a distribution $q(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$ which is similar.

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- ▶ i.e. Find a distribution $q(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$ which is similar.
- ▶ What is 'similar' ?
 - ▶ Mode (highest point) in same place.
 - ▶ Similar shape?
 - ▶ Might as well choose something that is easy to manipulate!

Laplace approximation

- ▶ Approximate $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$ with a Gaussian:

$$q(\mathbf{w}|\mathbf{X}, \mathbf{t}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- ▶ Where:

$$\boldsymbol{\mu} = \hat{\mathbf{w}}, \quad \boldsymbol{\Sigma}^{-1} = - \left. \frac{\partial^2 \log g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2)}{\partial \mathbf{w} \partial \mathbf{w}^T} \right|_{\hat{\mathbf{w}}}$$

- ▶ And:

$$\hat{\mathbf{w}} = \underset{\mathbf{w}}{\operatorname{argmax}} \log g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2)$$

- ▶ We already know $\hat{\mathbf{w}}$. $\boldsymbol{\Sigma}$ is the negative of the inverse Hessian.

Laplace approximation

- ▶ Justification?
- ▶ Not covered on this course.
- ▶ Based on Taylor expansion of $\log g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2)$ around mode $(\hat{\mathbf{w}})$.
 - ▶ Means approximation will be best at mode.
 - ▶ Expansion up to 2nd order terms 'looks' like a Gaussian.
- ▶ See book Chapter 4 for details.

Laplace approximation – 1D example

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$$\hat{y} = \frac{\alpha - 1}{\beta}$$

- Note, I happen to know what the mode is. You're not expected to be able to work this out!

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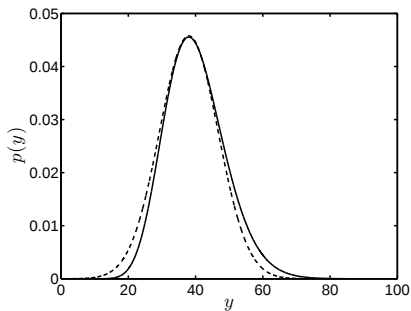
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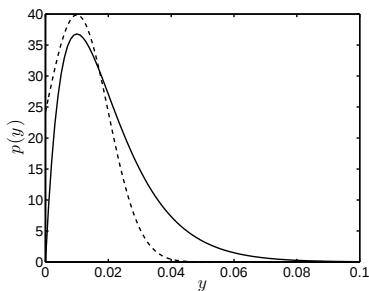
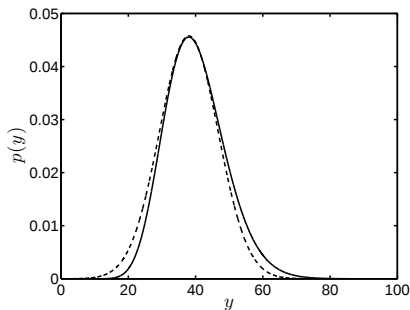
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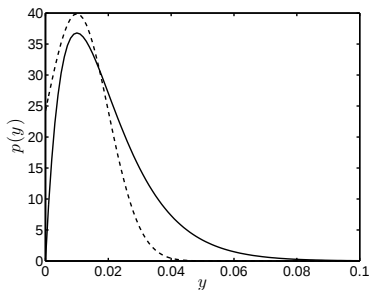
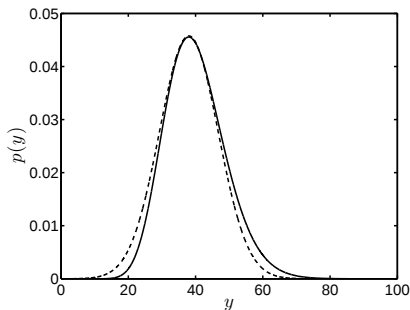
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- ▶ Solid: true density. Dashed: approximation.
- ▶ Left: $\alpha = 20$, $\beta = 0.45$



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- ▶ Right: $\alpha = 2$, $\beta = 100$



- ▶ Solid: true density. Dashed: approximation.
- ▶ Left: $\alpha = 20$, $\beta = 0.45$
- ▶ Right: $\alpha = 2$, $\beta = 100$
- ▶ Approximation is best when density looks like a Gaussian (left).
- ▶ Approximation deteriorates as we move away from the mode (both).

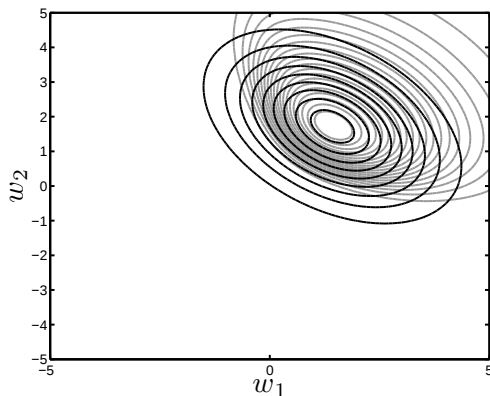
Laplace approximation for logistic regression

- ▶ Not going into the details here.
- ▶ $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2) \approx \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.
- ▶ Find $\boldsymbol{\mu} = \hat{\mathbf{w}}$ (that maximises $g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2)$) by Gradient-Descent or Newton-Raphson (already done it – MAP).
- ▶ Find:

$$\boldsymbol{\Sigma}^{-1} = - \left. \frac{\partial^2 \log g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2)}{\partial \mathbf{w} \partial \mathbf{w}^T} \right|_{\hat{\mathbf{w}}}$$

- ▶ (Details given in book Chapter 4 if you're interested)
- ▶ How good an approximation is it?

Laplace approximation for logistic regression



- ▶ Dark lines – approximation. Light lines – proportional to $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$.
- ▶ Approximation is OK.
- ▶ As expected, it gets worse as we travel away from the mode.

Predictions with the Laplace approximation

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- ▶ Can we use it to make predictions?

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- ▶ Cannot do this! So, what was the point?
- ▶ Sampling from $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ is **easy**
 - ▶ And we can approximate an expectation with samples!

Predictions with the Laplace approximation

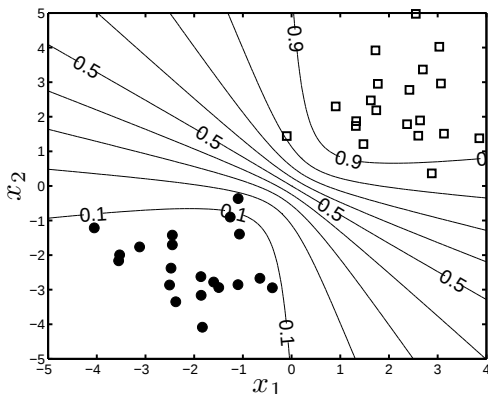
- ▶ Draw S samples $\mathbf{w}_1, \dots, \mathbf{w}_S$ from $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

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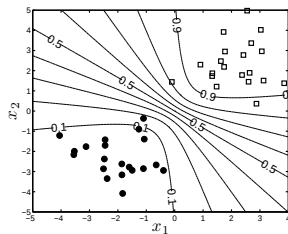
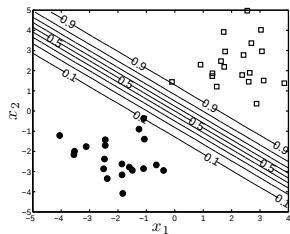
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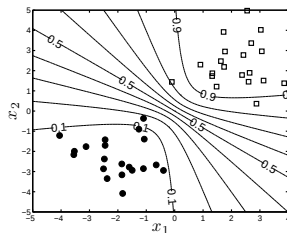
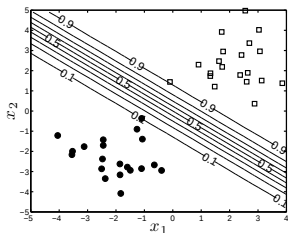
- ▶ Contours of $P(t_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t})$.
- ▶ Better than those from the point prediction?

Point prediction v Laplace approximation

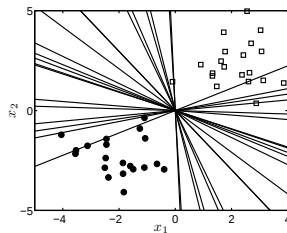
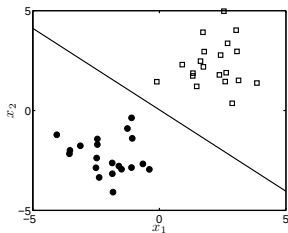


Why the difference?

Point prediction v Laplace approximation



Why the difference?



Laplace uses a distribution ($\mathcal{N}(\mu, \Sigma)$) over $\mathbf{w}$ (and therefore a distribution over decision boundaries) and hence has less certainty.

Summary – roadmap

- ▶ Defined a squashing function that meant we could model $P(t_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \mathbf{w}) = h(\mathbf{w}^T \mathbf{x}_{\text{new}})$
- ▶ Wanted to make ‘Bayesian predictions’: average over all posterior values of $\mathbf{w}$.
- ▶ Couldn’t do it exactly.
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- ▶ Laplace probability contours looked more sensible (to me at least!)
- ▶ Next:
 - ▶ Find the most likely value of $\mathbf{w}$ – a point estimate.
 - ▶ Approximate $p(\mathbf{w} | \mathbf{X}, \mathbf{t}, \sigma^2)$ with something easier.
 - ▶ **Sample from $p(\mathbf{w} | \mathbf{X}, \mathbf{t}, \sigma^2)$.**

MCMC sampling

- ▶ Laplace approximation still didn't let us exactly evaluate the expectation we need for predictions.
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MCMC sampling

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- ▶ But....we could easily sample from it and approximate our approximation.
- ▶ Good news! If we're happy to sample, we can sample directly from $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$ even though we can't compute it!
- ▶ i.e. don't need to use an approximation like Laplace.
- ▶ Various algorithms exist – we'll use *Metropolis-Hastings*

Aside – sampling from things we can't compute

- ▶ At first glance it seems strange – we can roll the die but we can't make it!
- ▶ But – it's pretty common in the world!
- ▶ Darts.....

Darts

- ▶ I want to know the probability that I hit treble 20 when I aim for treble 20.
- ▶ The distribution over where the dart lands when I aim treble 20:

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- ▶ Can't even begin to work out how to write down $p(\mathbf{x}|\text{stuff})$.
- ▶ But can sample – throw S darts, $\mathbf{x}_1, \dots, \mathbf{x}_S$!
- ▶ Compute:

$$\frac{1}{S} \sum_{s=1}^S f(\mathbf{x}_s)$$

Back to the script: Metropolis-Hastings

- ▶ Produces a sequence of samples – $\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_s, \dots$
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- ▶ Two distinct steps – proposal and acceptance.

MH – proposal

- ▶ Treat $\widetilde{\mathbf{w}}_s$ as a random variable conditioned on $\mathbf{w}_{s-1}$
- ▶ i.e. need to define $p(\widetilde{\mathbf{w}}_s | \mathbf{w}_{s-1})$
 - ▶ Note that this does not necessarily have to be similar to posterior we're trying to sample from.
- ▶ Can choose *whatever we like!*

MH – proposal

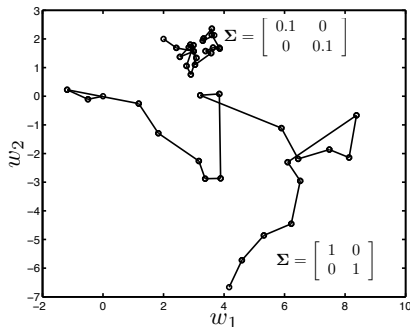
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MH – acceptance

- Choice of acceptance based on the following ratio:

$$r = \frac{p(\widetilde{\mathbf{w}}_s | \mathbf{X}, \mathbf{t}, \sigma^2)}{p(\mathbf{w}_{s-1} | \mathbf{X}, \mathbf{t}, \sigma^2)} \frac{p(\mathbf{w}_{s-1} | \widetilde{\mathbf{w}}_s, \boldsymbol{\Sigma}_p)}{p(\widetilde{\mathbf{w}}_s | \mathbf{w}_{s-1}, \boldsymbol{\Sigma}_p)}.$$

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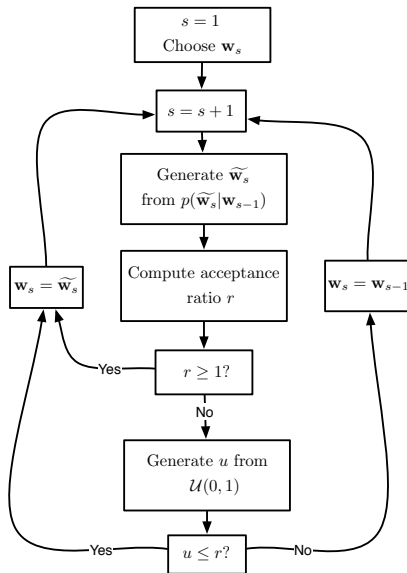
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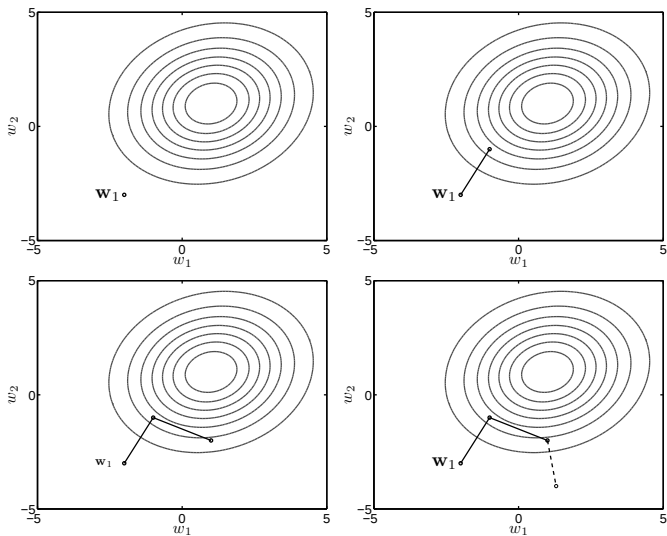
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- ▶ We now use the following rules:
 - ▶ If $r \geq 1$, accept: $\mathbf{w}_s = \widetilde{\mathbf{w}}_s$.
 - ▶ If $r < 1$, accept with probability r .
- ▶ If we do this enough, we'll eventually be sampling from $p(\mathbf{w} | \mathbf{X}, \mathbf{t})$, no matter where we started!
 - ▶ i.e. for any $\mathbf{w}_1$

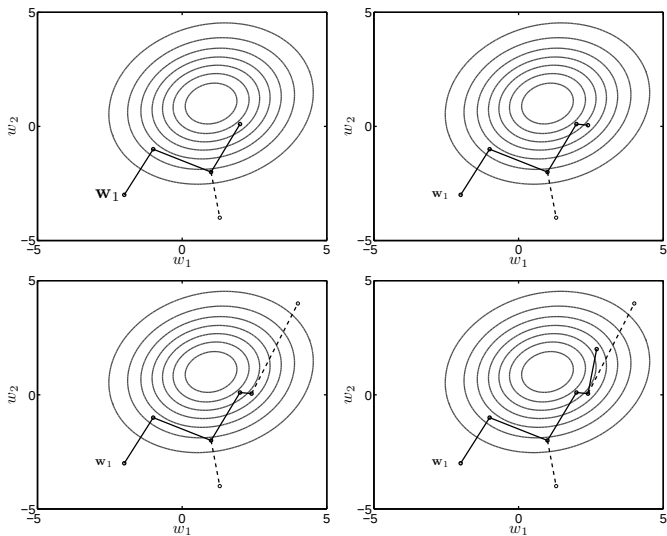
MH – flowchart



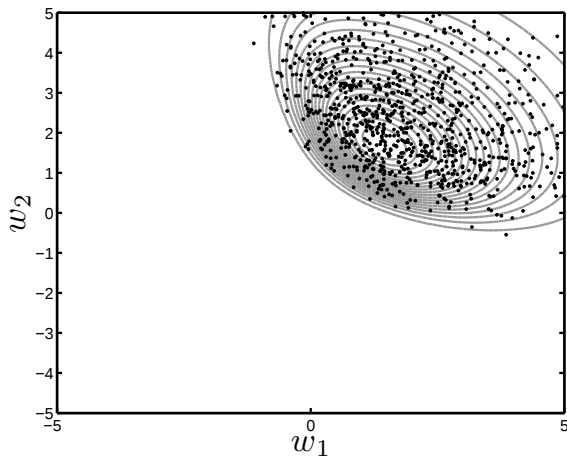
MH – walkthrough 1



MH – walkthrough 2



What do the samples look like?



- 1000 samples from the posterior using MH.

Predictions with MH

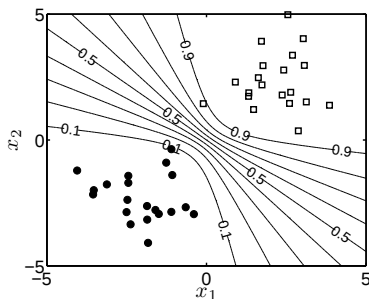
- ▶ MH provides us with a set of samples – $\mathbf{w}_1, \dots, \mathbf{w}_S$.
- ▶ These can be used like the samples from the Laplace approximation:

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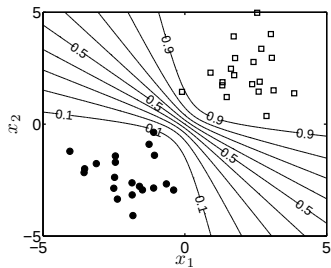
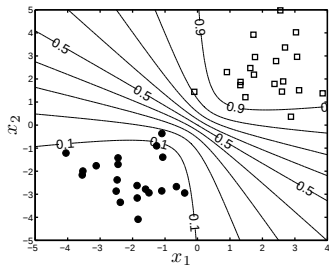
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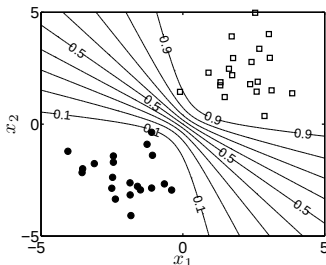
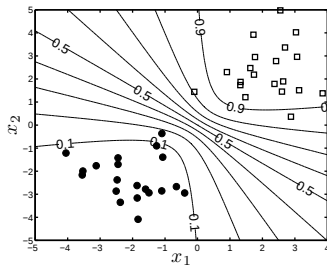
- ▶ Contours of $P(t_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t}, \sigma^2)$

Laplace vs. MH

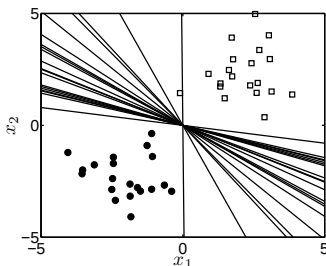
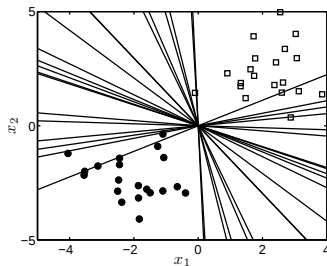


Why?

Laplace vs. MH

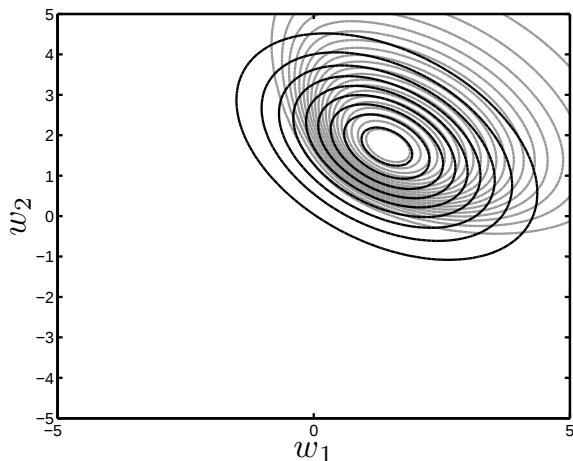


Why?



Laplace approximation (left) allows some *bad* boundaries

Laplace vs. MH



Approximate posterior allows some values of w_1 and w_2 that are very unlikely in true posterior.

Summary

- ▶ Introduced logistic regression – a probabilistic binary classifier.
- ▶ Saw that we couldn't compute the posterior.
- ▶ Introduced *examples of* three alternatives:
 - ▶ Point estimate – MAP solution.
 - ▶ Approximate the density – Laplace.
 - ▶ Sample – Metropolis-Hastings.
- ▶ Each is better than the last (in terms of predictions)....
- ▶ ...but each has greater complexity!
- ▶ To think about:
 - ▶ What if posterior is multi-modal?