Advanced Statistical Inference
Bayesian Logistic Regression

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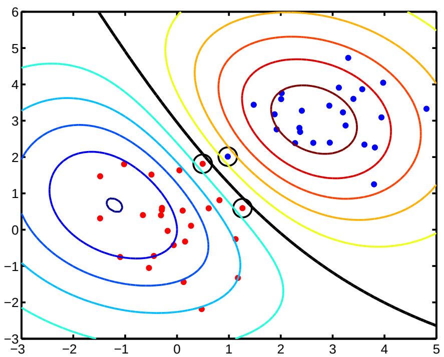
Introduction

- Supervised learning
  - Regression
    - Minimised loss (least squares)
    - Maximised likelihood
    - Bayesian approach
  - **Classification**
- Unsupervised learning
  - Clustering
  - Projection

Classification



- A set of N objects with attributes (usually vector) $\mathbf{x}_n$.
- Each object has an associated response (or label) t_n.
- Binary classification: $t_n = \{0, 1\}$ or $t_n = \{-1, 1\}$,
  - (depends on algorithm).
- Multi-class classification: $t_n = \{1, 2, \ldots, K\}$.

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!

Probabilistic v non-probabilistic classifiers

Classifier is trained on $\mathbf{x}_1, \ldots, \mathbf{x}_N$ and $t_1, \ldots, t_N$ and then used to classify $\mathbf{x}_{\text{new}}$.

- Probabilistic classifiers produce a probability of class membership $P(t_{\text{new}} = k | \mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t})$
  - e.g. binary classification: $P(t_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t})$ and $P(t_{\text{new}} = 0 | \mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t})$.
- Non-probabilistic classifiers produce a hard assignment
  - e.g. $t_{\text{new}} = 1$ or $t_{\text{new}} = 0$.
- Which to choose depends on application....

Probabilistic v non-probabilistic classifiers

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- Probabilities provide us with more information – $P(t_{\text{new}} = 1) = 0.6$ is more useful than $t_{\text{new}} = 1$.
  - Tells us how **sure** the algorithm is.
- Particularly important where cost of misclassification is high and imbalanced.
  - e.g. Diagnosis: telling a diseased person they are healthy is much worse than telling a healthy person they are diseased.
- Extra information (probability) often comes at a cost.
- For large datasets, might have to go with non-probabilistic.

Classification syllabus

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  - 2 are probabilistic.
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    - **Logistic regression.**
  - 2 are non-probabilistic.
    - K-nearest neighbours.
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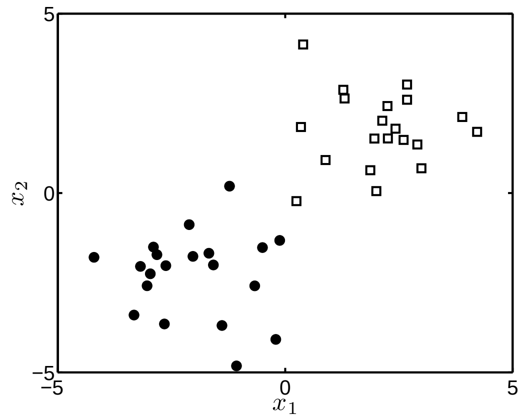
- There are many others!

Some data



Logistic regression

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

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

- Alternative is to directly model $P(T_{\text{new}} = k | \mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t}) = f(\mathbf{x}_{\text{new}}; \mathbf{w})$ with some parameters $\mathbf{w}$.
- We've seen $f(\mathbf{x}_{\text{new}}; \mathbf{w}) = \mathbf{w}^{\mathsf{T}} \mathbf{x}_{\text{new}}$ before – can we use it here?
  - 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.

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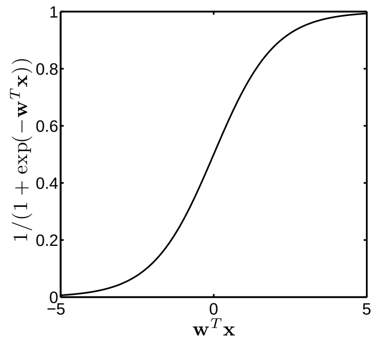
$h(\cdot)$

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

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



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Bayesian logistic regression

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

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

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

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

- Sounds good so far....

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Defining a prior

- Choose a Gaussian prior:

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

  - 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:

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

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

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

- and if $t_n = 0$:

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

Posterior

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

- Now things start going wrong.
- We can't compute $p(\mathbf{w}|\mathbf{X},\mathbf{t})$ 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:

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

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What can we compute?

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

- We can compute $p(\mathbf{t}|\mathbf{X},\mathbf{w},\sigma^2)p(\mathbf{w}|\sigma^2)$
  - Define $g(\mathbf{w};\mathbf{X},\mathbf{t},\sigma^2) = p(\mathbf{t}|\mathbf{X},\mathbf{w})p(\mathbf{w}|\sigma^2)$
- Armed with this, we have three options:
  - 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 $p(\mathbf{w}|\mathbf{X},\mathbf{t},\sigma^2)$.
- 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.

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MAP estimate

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

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

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MAP

- When we met maximum likelihood, we could find $\widehat{\mathbf{w}}$ exactly with some algebra.
- Can't do that here (can't solve $\frac{\partial g(\mathbf{w};\mathbf{X},\mathbf{t},\sigma^2)}{\partial \mathbf{w}} = \mathbf{0}$)
- Resort to numerical optimisation:
  1. Guess $\widehat{\mathbf{w}}$
  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.
- Many algorithms exist that differ in how they do step 2.
- e.g. **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

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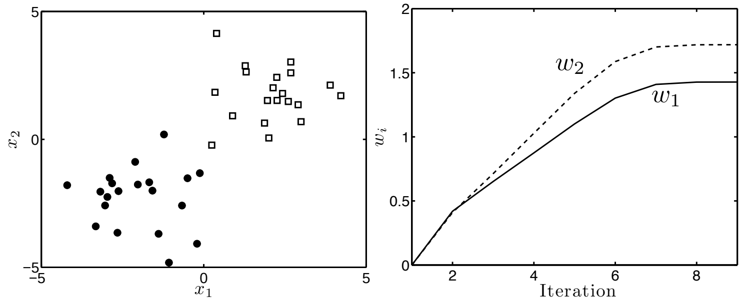

- Left: Data.
- Right: Evolution of $\widehat{\mathbf{w}}$ in numerical optimisation.

Decision boundary

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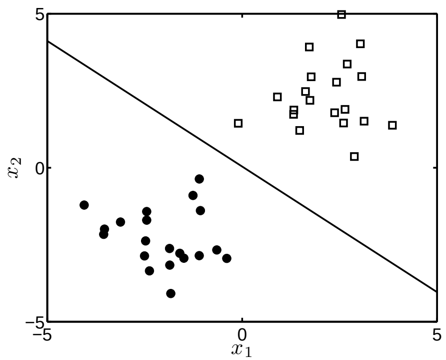
- Once we have $\widehat{\mathbf{w}}$, we can classify new examples.
- Decision boundary is a useful visualisation:



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

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

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

Predictive probabilities

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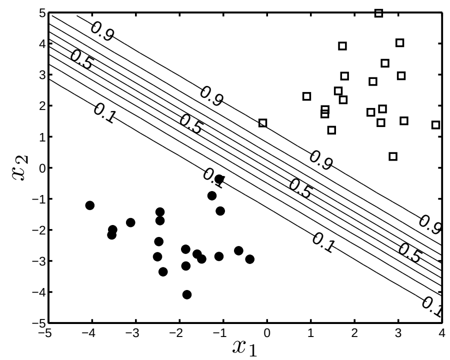


- Contours of $P(T_{\text{new}} = 1|\mathbf{x}_{\text{new}}, \widehat{\mathbf{w}})$.
- Do they look sensible?

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.
- 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:
$$\boldsymbol{\mu} = \widehat{\mathbf{w}}, \;\; \boldsymbol{\Sigma}^{-1} = -\left.\frac{\partial \log g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2)}{\partial \mathbf{w} \partial \mathbf{w}^\mathsf{T}}\right|_{\widehat{\mathbf{w}}}$$
- And:
$$\widehat{\mathbf{w}} = \underset{\mathbf{w}}{\operatorname{argmax}} \;\log g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2)$$
- We already know $\widehat{\mathbf{w}}$.

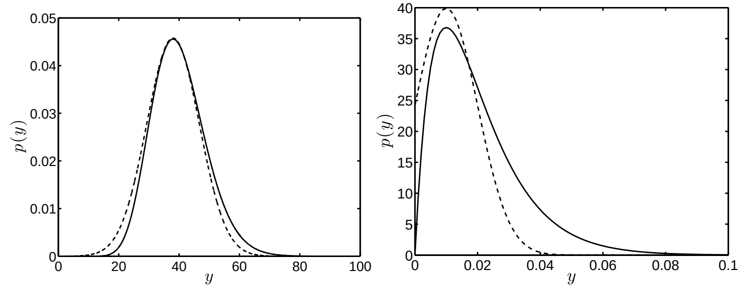
Laplace approximation

- Justification?
- Not covered on this course.
- Based on Taylor expansion of $\log g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2)$ around mode ($\widehat{\mathbf{w}}$).
  - 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

$$\begin{aligned}
p(y|\alpha, \beta) &\propto y^{\alpha-1}\exp(-\beta y)\\
\widehat{y} &= \frac{\alpha-1}{\beta}\\
\frac{\partial \log y}{\partial y^2} &= -\frac{\alpha-1}{y^2}\\
\left.\frac{\partial \log y}{\partial y^2}\right|_{\widehat{y}} &= -\frac{\alpha-1}{\widehat{y}^2}\\
q(y|\alpha, \beta) &= \mathcal{N}\left(\frac{\alpha-1}{\beta}, \frac{\widehat{y}^2}{\alpha-1}\right)
\end{aligned}$$

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

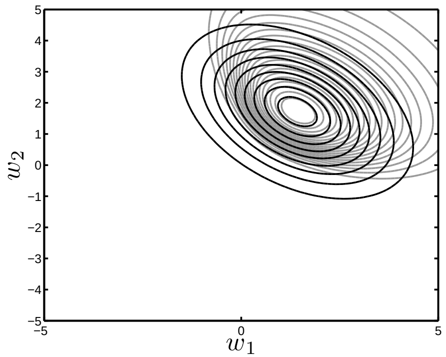


- Solid: true density. Dashed: approximation.
- Left: $\alpha = 20$, $\beta = 0.5$
- Right: $\alpha = 2$, $\beta = 100$
- Approximation is best when density looks like a Gaussian (left).
- Approximation deteriorates as we move away from the mode (both).

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 $\mu = \widehat{\mathbf{w}}$ (that maximises $g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2)$) by Newton-Raphson (already done it – MAP).
- Find:
$$\boldsymbol{\Sigma}^{-1} = -\left.\frac{\partial^2 \log g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2)}{\partial \mathbf{w} \partial \mathbf{w}^\mathsf{T}}\right|_{\widehat{\mathbf{w}}}$$
- (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

- We have $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ as an approximation to $p(\mathbf{w}|\mathbf{X}, \mathbf{t})$.
- Can we use it to make predictions?
- Need to evaluate:

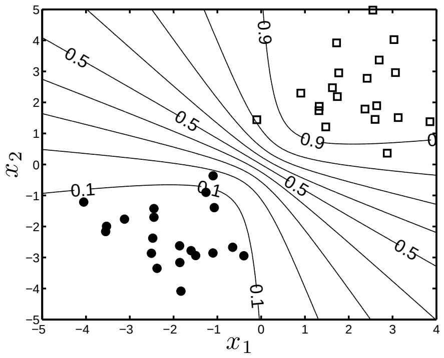
$$\begin{aligned} P(T_{\text{new}} = 1|\mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t}) &= \mathbf{E}_{\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})} \left\{ P(T_{\text{new}} = 1|\mathbf{x}_{\text{new}}, \mathbf{w}) \right\} \\ &= \int \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \frac{1}{1 + \exp(-\mathbf{w}^\mathsf{T} \mathbf{x}_{\text{new}})} \, d\mathbf{w} \end{aligned}$$

- 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

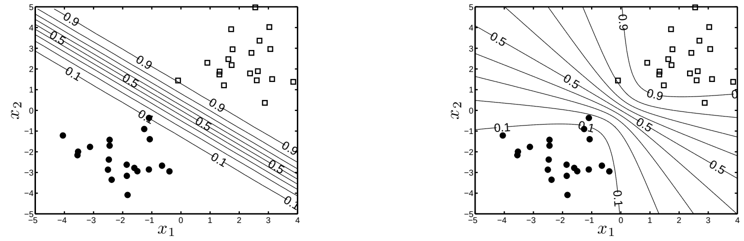
- Draw S samples $\mathbf{w}_1, \ldots, \mathbf{w}_S$ from $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

$$\mathbf{E}_{\mathcal{N}(\boldsymbol{\mu},\boldsymbol{\Sigma})}\left\{P(T_{\text{new}} = 1|\mathbf{x}_{\text{new}}, \mathbf{w})\right\} \approx \frac{1}{S}\sum_{s=1}^{S} \frac{1}{1+\exp(-\mathbf{w}_s^{\mathsf{T}}\mathbf{x}_{\text{new}})}$$

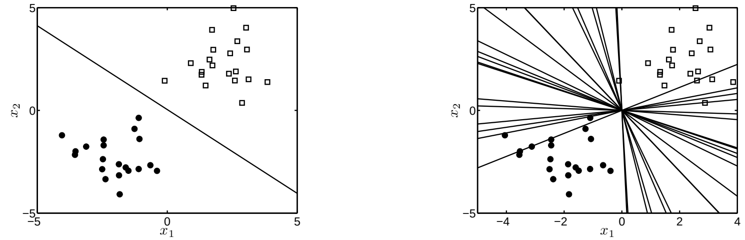


- Contours of $P(T_{\text{new}} = 1|\mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t})$.
- Better than those from the point prediction?

Point prediction v Laplace approximation



Why the difference?



Laplace uses a distribution ($\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$) 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 $P(T_{\text{new}} = 1|\mathbf{x}_{\text{new}}, \mathbf{w}) = h(\mathbf{w}^{\mathsf{T}}\mathbf{w}_{\text{new}})$
- Wanted to make 'Bayesian predictions': average over all posterior values of $\mathbf{w}$.
- Couldn't do it exactly.
- Tried a point estimate (MAP) and an approximate distribution (via Laplace).
- 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.
- 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:

$$p(\mathbf{x}|\text{stuff})$$

- Define function $f(\mathbf{x}) = 1$ if $\mathbf{x}$ in treble 20 and 0 otherwise.
- Probability I hit treble twenty is therefore:

$$\int f(\mathbf{x})p(\mathbf{x}|\text{stuff})\ d\mathbf{x}$$

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

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

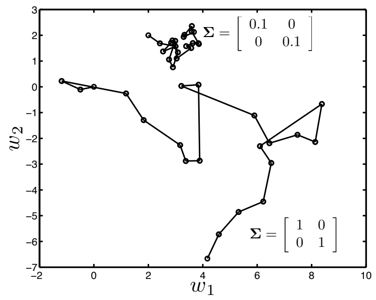
Back to the script: Metropolis-Hastings

- Produces a sequence of samples – $\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_s, \ldots$
- Imagine we've just produced $\mathbf{w}_{s-1}$
- MH firsts proposes a possible $\mathbf{w}_s$ (call it $\widetilde{\mathbf{w}_s}$) based on $\mathbf{w}_{s-1}$.
- MH then decides whether or not to accept $\widetilde{\mathbf{w}_s}$
  - If accepted, $\mathbf{w}_s = \widetilde{\mathbf{w}_s}$
  - If not, $\mathbf{w}_s = \mathbf{w}_{s-1}$
- 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!
- e.g. use a Gaussian centered on $\mathbf{w}_{s-1}$ with some covariance:

$$p(\widetilde{\mathbf{w}_s}|\mathbf{w}_{s-1}, \mathbf{\Sigma}_p) = \mathcal{N}(\mathbf{w}_{s-1}, \mathbf{\Sigma}_p)$$



MH – acceptance

- Choice of acceptance based on the following ratio:

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

- Which simplifies to (all of which we can compute):

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

- 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

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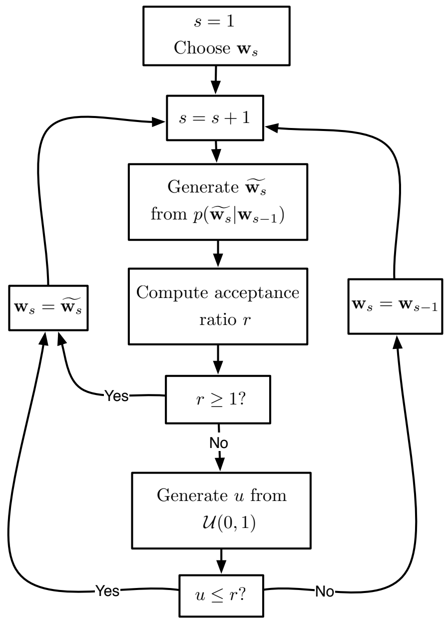

MH – walkthrough 1

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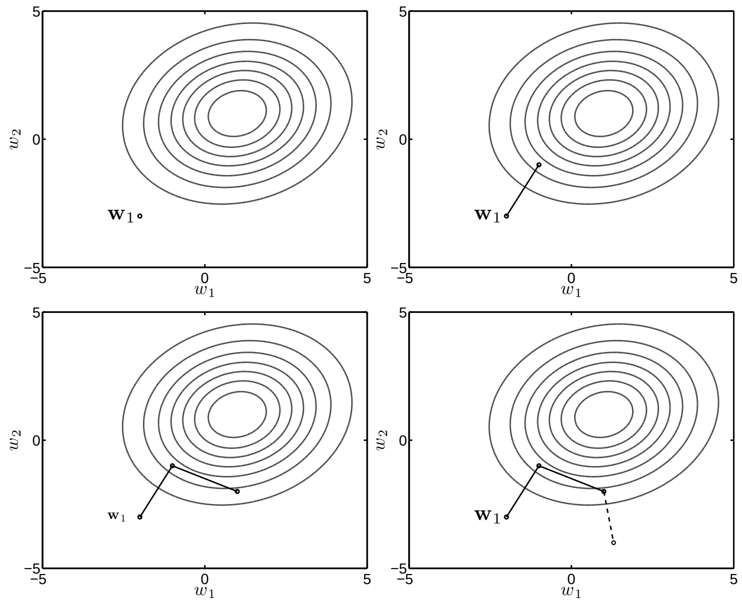

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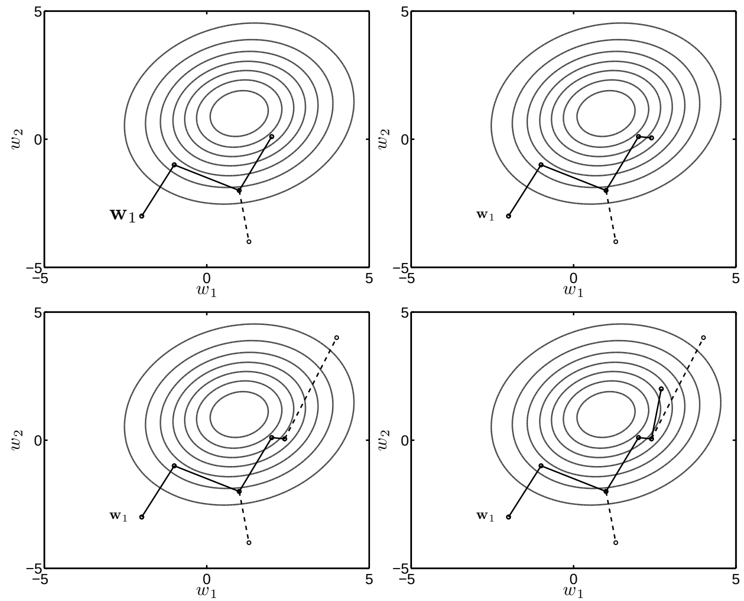
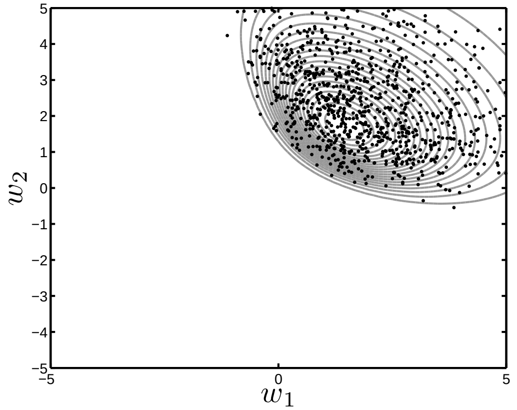


What do the samples look like?

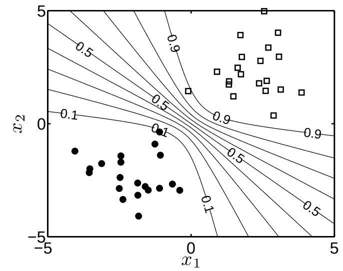


- 1000 samples from the posterior using MH.

Predictions with MH

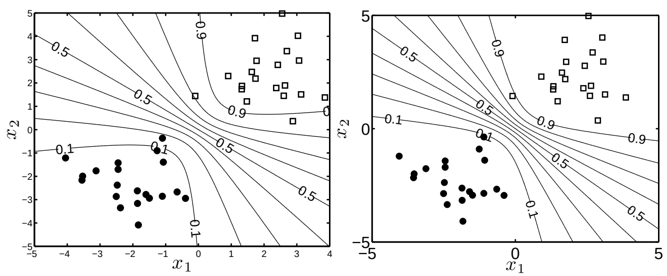
- MH provides us with a set of samples – $\mathbf{w}_1, \ldots, \mathbf{w}_S$.
- These can be used like the samples from the Laplace approximation:

$$P(t_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t}, \sigma^2) = \mathbf{E}_{p(\mathbf{w}|\mathbf{X},\mathbf{t},\sigma^2)} \{P(t_{\text{new}} | \mathbf{x}_{\text{new}}, \mathbf{w})\}$$
$$\approx \frac{1}{S} \sum_{s=1}^{S} \frac{1}{1 + \exp(-\mathbf{w}_s^\mathsf{T} \mathbf{x}_{\text{new}})}$$

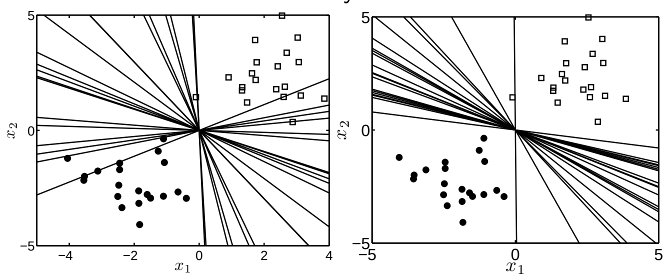


- Contours of $P(t_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t}, \sigma^2)$

Laplace v MH

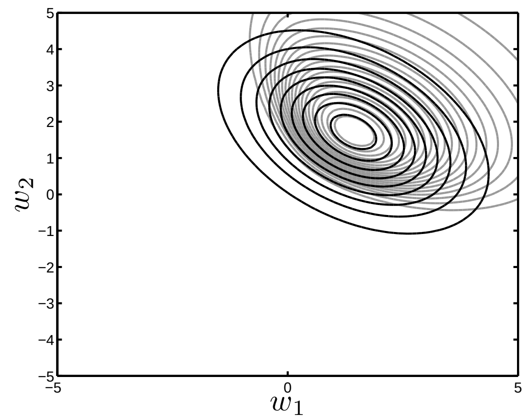


Why?



Laplace approximation (left) allows some <u>bad</u> boundaries

Laplace v 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?