3F8: Inference

Bayesian Linear Classification

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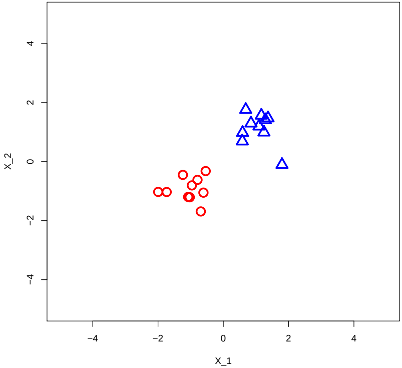
Lent Term

In high dimensions (many basis functions) the data will be **linearly separable**.

Many **w** fit the data equally well. This can lead to **overfitting problems**.



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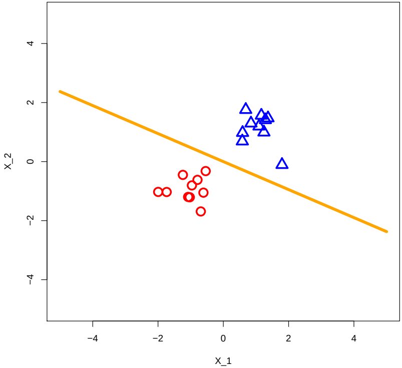

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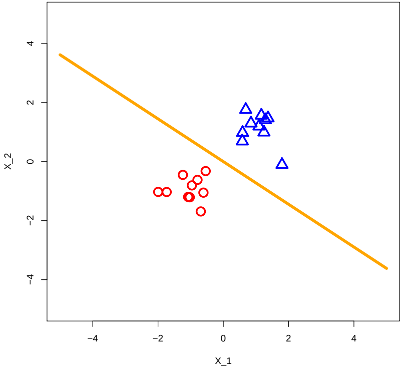

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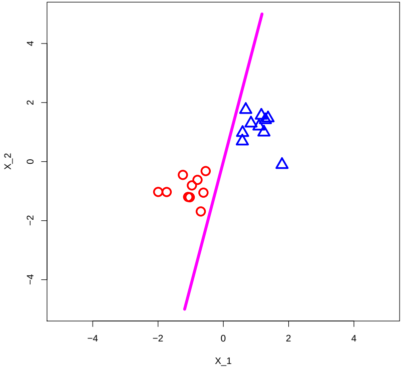

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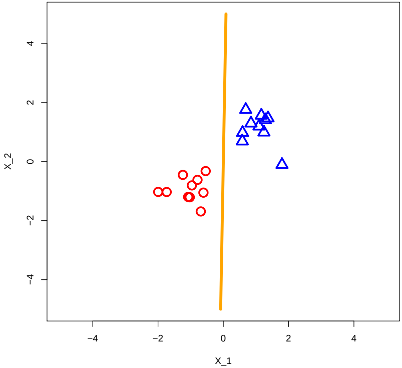

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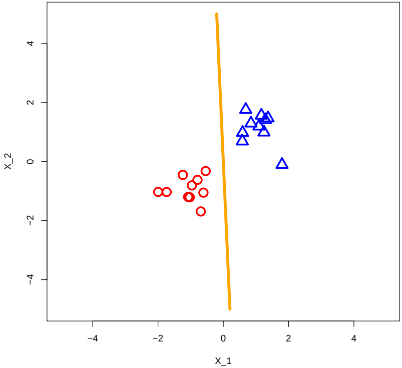

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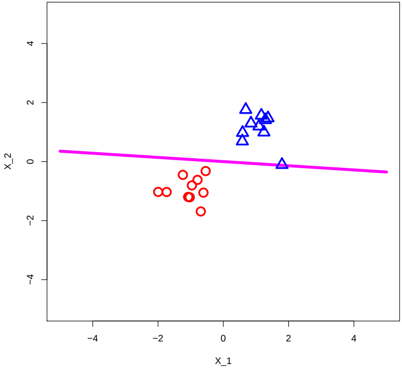

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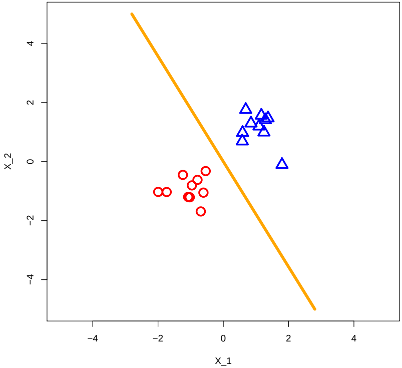

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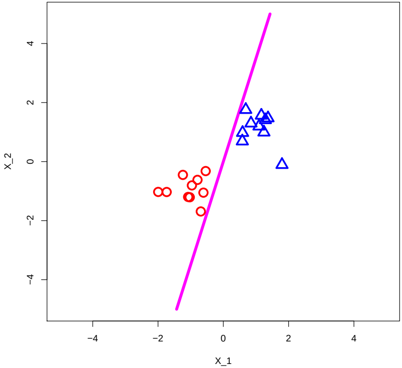

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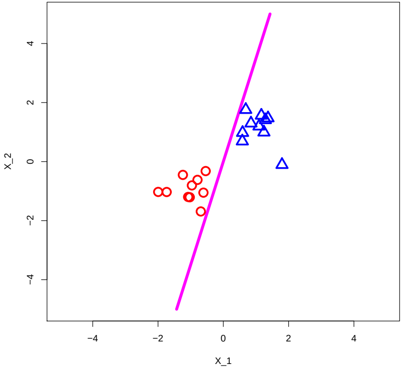

Solution: Bayesian inference.

The prior on $\mathbf{w}$ is

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \lambda^{-1}\mathbf{I})\,.$$

The posterior on $\mathbf{w}$ is

$$p(\mathbf{w}|\mathbf{y}, \widetilde{\mathbf{X}}) \propto \left[\prod_{n_1}^{N} \sigma(y_n \mathbf{w}^{\mathrm{T}} \widetilde{\mathbf{x}}_n)\right] p(\mathbf{w})\,,$$

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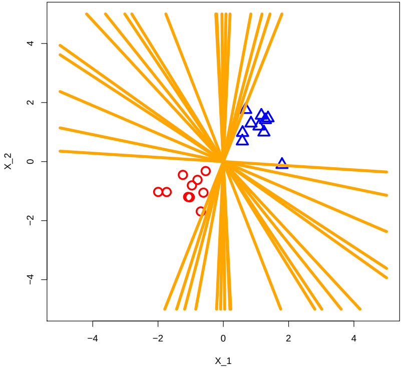

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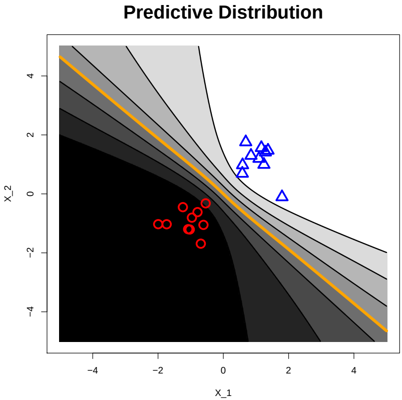

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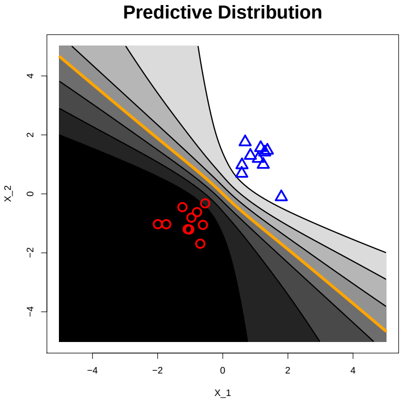

Difference w.r.t. logistic regression: **higher uncertainty** far from data.

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Integration with respect to $p(\mathbf{w}, \mathbf{y}|\widetilde{\mathbf{X}}) = \left[\prod_{n_1}^{N} \sigma(y_n \mathbf{w}^\mathsf{T} \widetilde{\mathbf{x}}_n)\right] p(\mathbf{w})$ over $\mathbf{w}$ is intractable (**how do you know?**), but this is required to compute

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Use **approximate Bayesian inference**. Different approaches are possible:

1. Draw a sequence of asymptotically unbiased samples from $p(\mathbf{w}|\mathbf{y}, \widetilde{\mathbf{X}})$ (Monte Carlo methods).
2. Approximate $p(\mathbf{w}|\mathbf{y}, \widetilde{\mathbf{X}})$ with a simpler distribution (e.g. a Gaussian) (Deterministic approximate inference).

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The Laplace approximation

Fits a **Gaussian** (why Gaussian?) approximation to the posterior.

The univariate case:

Consider a scalar continuous variable w with

$$p(w|\mathcal{D}) = \frac{1}{Z} f(w) \,,$$

where $f(w) = p(w, \mathcal{D})$ for some data $\mathcal{D}$ and $Z = \int f(w) dw$.

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A choice for m can be the **MAP solution**. We find a **mode** w_{MAP} of $p(w|\mathcal{D})$:

$$\left.\frac{df(w)}{dw}\right|_{w=w_{\text{MAP}}} = 0$$

Any **optimization algorithm** can be used for this purpose.

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We consider a **truncated Taylor expansion** of $\log f(w)$ center at w_{MAP}:

$$\log f(w) \approx \log f(w_{\text{MAP}}) - \frac{1}{2} a (w - w_{\text{MAP}})^2 , \quad a = -\frac{d^2}{dw^2} \log f(w) \Big|_{w = w_{\text{MAP}}}$$

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Taking the exponential we obtain:

$$f(w) \approx f(w_{\text{MAP}}) \exp\left\{ -\frac{a}{2} (w - w_{\text{MAP}})^2 \right\} = \tilde{q}(w) \quad q(w) = \mathcal{N}(w | w_{\text{MAP}}, a^{-1}) \,,$$

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Only defined if $a > 0$: f must have **negative second derivative** at w_{MAP}.
Beware of saddle points when finding w_{MAP}!

Example

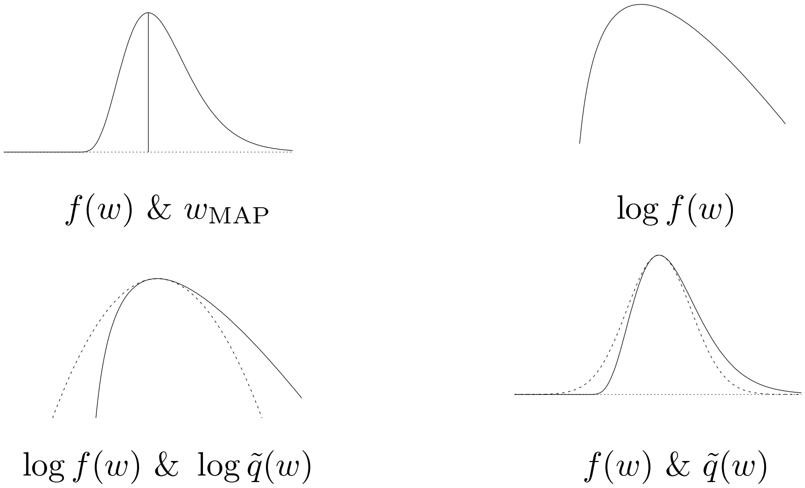

Figure: David J.C. MacKay. Information Theory, Inference, and Learning Algorithms. 2003.

The multi-variate case:

Now $\mathbf{w}$ is a d-dimensional vector and $p(\mathbf{w}|\mathcal{D}) = \frac{1}{Z} f(\mathbf{w})$.

The same principle can be applied. The truncated Taylor series is

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Only defined if $\mathbf{A}$ **positive definite**. **Beware of saddle points!**

Example: probit regression

The posterior distribution is:

$$p(\mathbf{w}|\mathcal{D}) \propto p(\mathbf{y}|\mathbf{w}, \widetilde{\mathbf{X}})p(\mathbf{w}) = f(\mathbf{w}), \quad \log f(\mathbf{w}) = \log p(\mathbf{y}|\mathbf{w}, \widetilde{\mathbf{X}}) + \log p(\mathbf{w}).$$

Let $\Phi(\cdot)$ be the standard Gaussian cdf. Then, we have that:

$$\log f(\mathbf{w}) = \sum_{n=1}^{N} \log \Phi(y_n \mathbf{w}^{\mathrm{T}} \widetilde{\mathbf{x}}_n) - \frac{1}{2}\lambda \mathbf{w}^{\mathrm{T}}\mathbf{w} + \text{const}.$$

Let $\mathbf{w}_{\text{MAP}}$ be the maximizer of f. Computing the negative Hessian at $\mathbf{w}_{\text{MAP}}$:

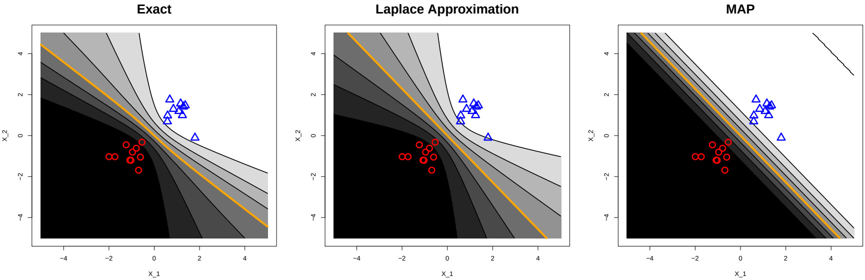
$$\mathbf{A} = \sum_{n=1}^{N} \left[v_n(s_n + v_n)\widetilde{\mathbf{x}}_n \widetilde{\mathbf{x}}_n^{\mathrm{T}} \right] + \lambda \mathbf{I}, \quad v_n = \frac{\mathcal{N}(s_n|0,1)}{\Phi(s_n)}, \quad s_n = y_n \mathbf{w}_{\text{MAP}}^{\mathrm{T}} \widetilde{\mathbf{x}}_n.$$

We then have $q(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{w}_{\text{MAP}}, \mathbf{A}^{-1})$ and $Z \approx f(\mathbf{w}_{\text{MAP}})\sqrt{\frac{(2\pi)^d}{|\mathbf{A}|}}$.

An approx. **predictive distribution** is obtained by replacing $p(\mathbf{w}|\mathcal{D})$ with $q(\mathbf{w})$:

$$p(y_\star|\widetilde{\mathbf{x}}_\star, \mathbf{y}) \approx \int p(y_\star|\widetilde{\mathbf{x}}_\star, \mathbf{w}) q(\mathbf{w}) d\mathbf{w} = \int \Phi(y_\star \mathbf{w}^{\mathrm{T}} \widetilde{\mathbf{x}}_\star) \mathcal{N}(\mathbf{w}|\mathbf{w}_{\mathrm{MAP}}, \mathbf{A}^{-1}) d\mathbf{w}\,,$$

$$= \Phi\left(\frac{y_\star \mathbf{w}_{\mathrm{MAP}}^{\mathrm{T}} \widetilde{\mathbf{x}}_\star}{\sqrt{\widetilde{\mathbf{x}}_\star^{\mathrm{T}} \mathbf{A}^{-1} \widetilde{\mathbf{x}}_\star + 1}}\right)\,.$$



Uncertainty increases in regions where there is **no data**.

The MAP predictive uncertainty is **constant** along the decision border.

Considerations for the Laplace approximation

- The Hessian can be approximated by numerical differences.
- Multiple possible solutions on multi-modal distributions, one per mode.
- Often, the posterior is more and more Gaussian as $N \to \infty$.
- Does not work with discrete random variables or discrete likelihoods.
- Fails to capture global properties, only considers curvature at the mode.
- A change of variables changes the solution (a defect or an opportunity).