02477 – Bayesian Machine Learning: Lecture 4

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Outline

Re-cap from last week and a few words about graphical models

Bayesian linear regression model: the key equations

- Linear regression model with Gaussian noise and Gaussian priors

$$y_n = f(\phi(\mathbf{x}_n), \mathbf{w}) + e_n$$

- Given design matrix $\mathbf{\Phi} \in \mathbb{R}^{N\times D}$ and observations $\mathbf{y} \in \mathbb{R}^N$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|0, \alpha^{-1}\mathbf{I}) \qquad (\textit{prior})$$

$$p(\mathbf{y}|\mathbf{w}) = \mathcal{N}(\mathbf{y}|\mathbf{\Phi w}, \beta^{-1}\mathbf{I}) \qquad (\textit{likelihood})$$

$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y}|\mathbf{0}, \beta^{-1}\mathbf{I} + \alpha^{-1}\mathbf{\Phi\Phi}^T) \qquad (\textit{marginal likelihood})$$

$$p(\mathbf{w}|\mathbf{y}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N) \qquad (\textit{posterior})$$

with *posterior parameters*

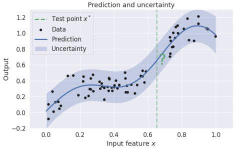
$$\mathbf{m}_N = \beta \mathbf{S}_N \mathbf{\Phi}^T \mathbf{y} \qquad (\textit{posterior mean})$$

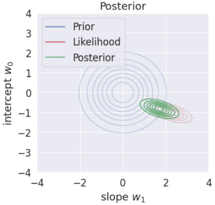
$$\mathbf{S}_N = \left(\alpha \mathbf{I} + \beta \mathbf{\Phi}^T \mathbf{\Phi}\right)^{-1} \qquad (\textit{posterior covariance})$$

- *Two hyperparameters*

  α: prior precision of the regression weights
  β: precision of the measurements

- *Lazy notation*: We should actually write $p(\mathbf{w}|\mathbf{y}, \alpha, \beta)$ etc., but we often suppress dependency of hyperparameter to ease notation





Posterior Predictive distributions

- The *posterior distribution* is $p(\boldsymbol{w}|\boldsymbol{y}) = \mathcal{N}(\boldsymbol{w}|\boldsymbol{m}, \boldsymbol{S})$ with

$$\boldsymbol{m} = \beta \boldsymbol{S} \boldsymbol{\Phi}^T \boldsymbol{y}$$

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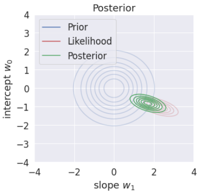
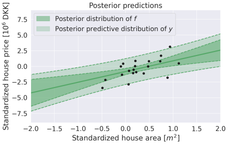


- When making predictions $\boldsymbol{x}^*$ using Bayesian methods, we *average over all possible parameters values weighted by the posterior*

$$f(\boldsymbol{x}^*|\boldsymbol{w}) = \boldsymbol{w}^T \phi(\boldsymbol{x}^*)$$

$$y(\boldsymbol{x}^*) = f(\boldsymbol{x}^*|\boldsymbol{w}) + \epsilon$$



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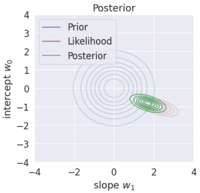

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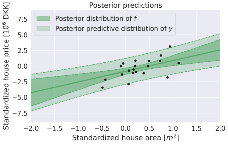

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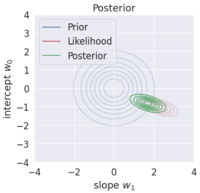

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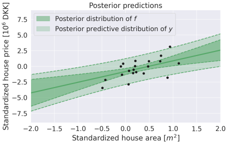

- .. and marginalize with respect to the posterior distribution (sum rule)

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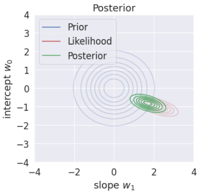

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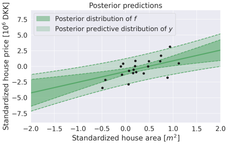

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- This is called *the posterior predictive distribution*

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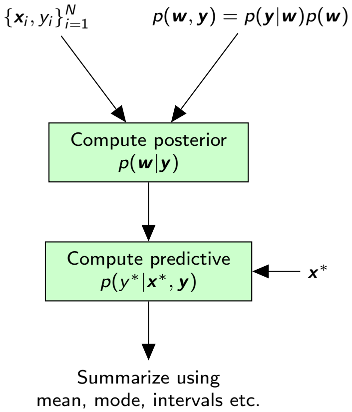
- MAP is sometimes called *poor man's Bayes*, but can still be a useful tool!

Bayesian inference for supervised learning



- Same principles for linear regression, logistic regression, neural networks etc. etc.

Hyperparameters and the evidence approximation

- Posterior depends on the hyperparameters α and β (but often suppressed in notation)

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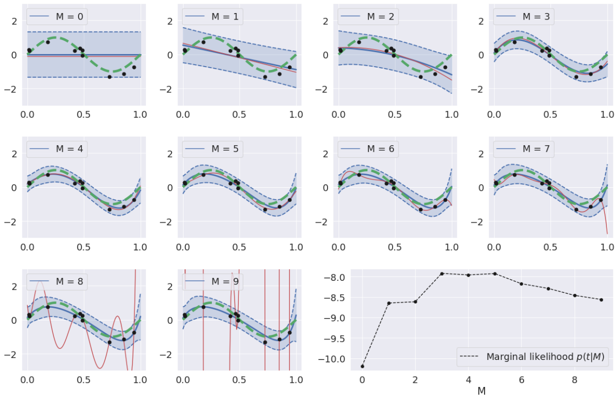
- Equivalent to *poor man's Bayes* on hyperparameter level

Sinusoidal example revisited using the evidence approximation

- Also useful for model selection: $\alpha, \beta, M^* = \arg\max_{\alpha,\beta,M} p(\boldsymbol{y}|\alpha, \beta, M)$



- Implements "Occam's razor": choose the "simplest" model that explain the data
- Often works well for many models, but we should always assess the generalization error

A more general probabilistic perspective on supervised learning

Product rule
$p(\boldsymbol{a}, \boldsymbol{b}) = p(\boldsymbol{b}|\boldsymbol{a})p(\boldsymbol{a})$

Sum rule
$p(\boldsymbol{b}) = \int p(\boldsymbol{a}, \boldsymbol{b})\mathrm{d}\boldsymbol{a}$

Conditional
$p(\boldsymbol{a}|\boldsymbol{b}) = \frac{p(\boldsymbol{a},\boldsymbol{b})}{p(\boldsymbol{b})}$

Conditional independence
$p(\boldsymbol{a}, \boldsymbol{b}|\boldsymbol{c}) = p(\boldsymbol{a}|\boldsymbol{c})p(\boldsymbol{b}|\boldsymbol{c})$

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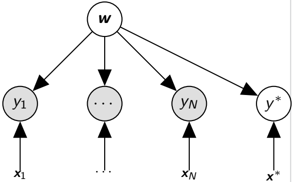

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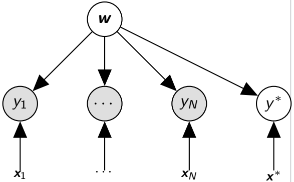

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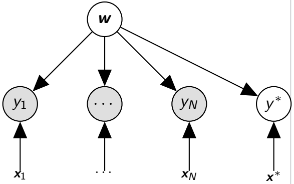

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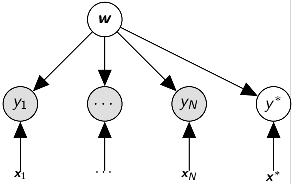

A more general probabilistic perspective on supervised learning

Product rule
$p(\boldsymbol{a}, \boldsymbol{b}) = p(\boldsymbol{b}|\boldsymbol{a})p(\boldsymbol{a})$

Sum rule
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Conditional
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Conditional independence
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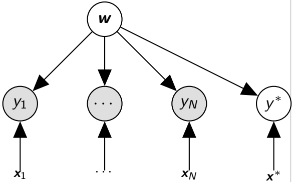

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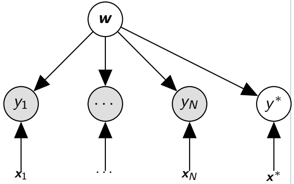

A more complete graphical model

- Lazy, but common notation for Bayesian linear regression

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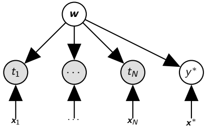
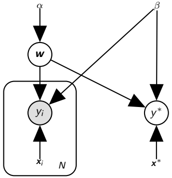


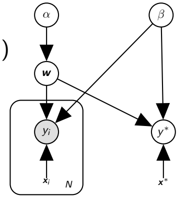
- More complete notation and corresponding graphical model

$$p(y^*, \boldsymbol{y}, \boldsymbol{w}|\alpha, \beta, \boldsymbol{X}, \boldsymbol{x}^*) = p(y^*|\boldsymbol{w}, \beta, \boldsymbol{x}^*)p(\boldsymbol{y}|\boldsymbol{w}, \beta, \boldsymbol{X})p(\boldsymbol{w}|\alpha)$$



- Fully Bayesian inference on hyperparameter level

$$p(y^*, \boldsymbol{y}, \boldsymbol{w}, \alpha, \beta|\boldsymbol{X}, \boldsymbol{x}^*) = p(y^*|\boldsymbol{w}, \beta, \boldsymbol{x}^*)p(\boldsymbol{y}|\boldsymbol{w}, \beta, \boldsymbol{X})p(\boldsymbol{w}|\alpha)p(\alpha)p(\beta)$$



Bayesian vs. classical statistics

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	Frequentist/classical	**Bayesian**
Probability interpretation	Long run frequencies	Degrees of belief

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Bayesian methods for classification

Probabilistic approaches for classification

- Dataset $\mathcal{D} = \{(\boldsymbol{x_1}, y_1), (\boldsymbol{x_2}, y_2), \ldots, (\boldsymbol{x_N}, y_N)\}$
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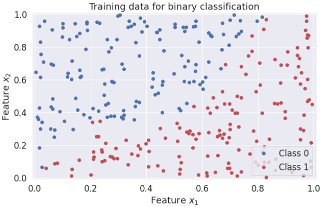

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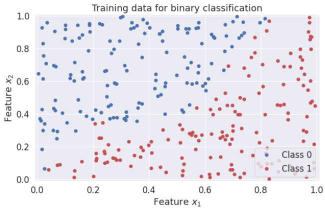

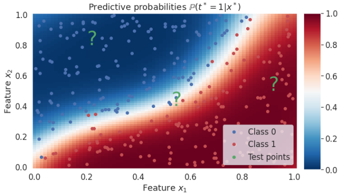

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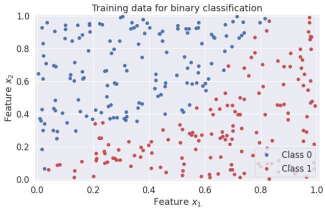

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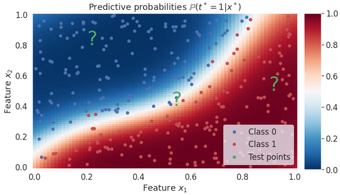

- Two probabilistic approaches
  1. *Discriminative methods*
  2. *Generative methods*

Discriminative vs generative methods

- The *generative approach* models the *joint distribution* $p(\boldsymbol{x}_n, y_n)$, e.g. via Bayes rule

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- Pros and cons for discriminative models
  - \+ Often superior when the assumptions for generative models are wrong
  - \+ Often better calibrated (compared to e.g. generative methods like Naive Bayes etc)
  - \+ Easy to make flexible
  - \- Difficult to handle missing data
  - \- Cannot reason about input data

Bayesian methods for classification: Generative modeling

The generative approach I

- Binary classification $y_n \in \{0, 1\}$

$$p(y_n = 1|\boldsymbol{x}_n) = \frac{p(\boldsymbol{x}_n|y_n = 1)p(y_n = 1)}{p(\boldsymbol{x}_n)}$$

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- Let's plug the result into Bayes' rule

The generative approach II

- The posterior of y_n given the input $\boldsymbol{x}_n$

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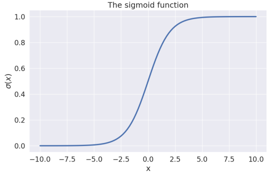

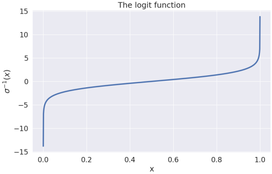

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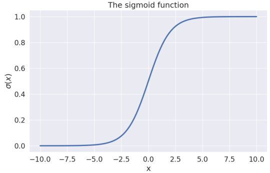

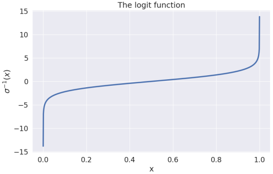

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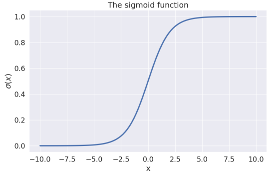

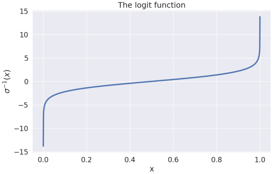

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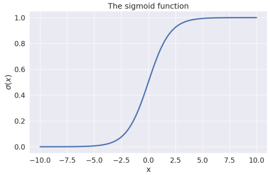
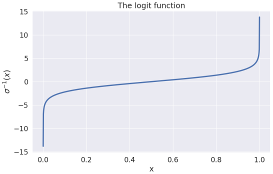
$$p(y_n = 1|\boldsymbol{x}_n) = \frac{1}{1 + \exp(-a)} = \sigma(a)$$





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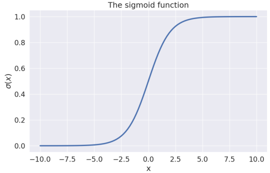
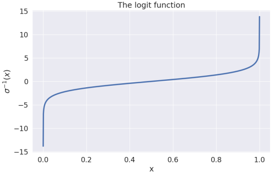
- Recall $\sigma(a)$ is the *logistic sigmoid* function and its inverse is called the *logit* function $a = \ln\left(\frac{\sigma}{1-\sigma}\right)$





The generative approach III: multi-class problems and softmax

- Assume we have K different classes, where $k = 1, \ldots, K$

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- Using similar line of reasoning for K classes

$$p(y_n = k | \boldsymbol{x}_n) = \frac{p(\boldsymbol{x}_n | y_n = k) P(y_n = k)}{\sum_{i=1}^{K} p(\boldsymbol{x}_n | y_n = i) p(y_n = i)} = \frac{\exp(a_k)}{\sum_{j=1}^{K} \exp(a_j)}$$

The generative approach III: multi-class problems and softmax

- Assume we have K different classes, where $k = 1, \ldots, K$

- Define a_k

$$a_k = \ln p(\boldsymbol{x}_n | y_n = k) p(y_n = k)$$

- Using similar line of reasoning for K classes

$$p(y_n = k | \boldsymbol{x}_n) = \frac{p(\boldsymbol{x}_n | y_n = k) P(y_n = k)}{\sum_{i=1}^{K} p(\boldsymbol{x}_n | y_n = i) p(y_n = i)} = \frac{\exp(a_k)}{\sum_{j=1}^{K} \exp(a_j)}$$

- The *normalized exponentials* is the known as the *softmax* function

Example: Gaussian class conditionals

- Binary classification, normal class conditionals with common variance in 1D

$$p(x_n|y_n = 0) = \mathcal{N}(x_n|\mu_0, \sigma^2)$$
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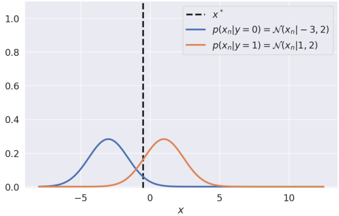

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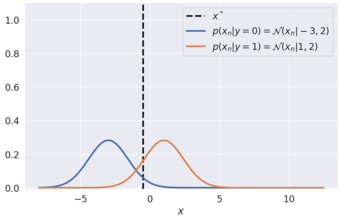

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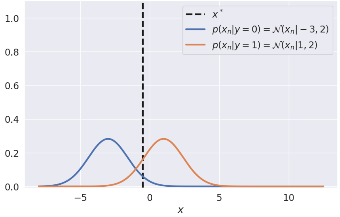

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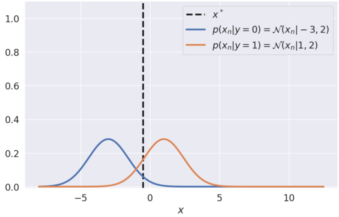

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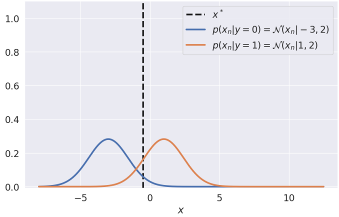

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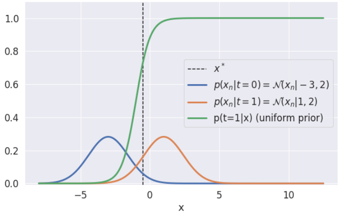
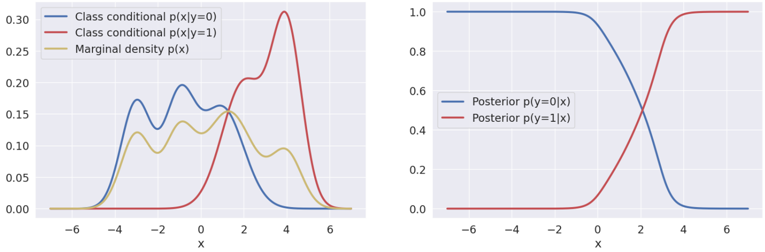


Example 2: More complex distributions



Bayesian methods for classification: Discriminative modelling

Discriminative modelling for binary classification

- In the generative model, we defined *priors* $p(y_n = 1) = \pi_1$ and a set of *class-conditionals* $p(\mathbf{x}_n|y_n = 1)$, applied Bayes rule and ended up with

$$a(\mathbf{x}_n) = \ln \frac{\pi_1 p(\mathbf{x}_n|y_n = 1)}{\pi_0 p(\mathbf{x}_n|y_n = 0)} = \ln \frac{p(y_n = 1|\mathbf{x}_n)}{p(y_n = 0|\mathbf{x}_n)}$$

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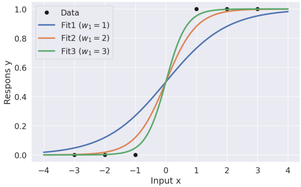
- We *estimate* $\boldsymbol{w}$ using maximum likelihood, MAP or Bayesian inference with the likelihood function

$$p(\boldsymbol{y}|\boldsymbol{w}, \boldsymbol{X}) = \prod_{n=1}^{N} \sigma(\phi(\boldsymbol{x}_n)^T \boldsymbol{w})^{y_n} \left(1 - \sigma(\phi(\boldsymbol{x}_n)^T \boldsymbol{w})\right)^{1-y_n}$$

Maximum likelihood estimator for logistic regression: Quiz

Set-up

- Consider a simple dataset with $N = 6$, $\phi(x) = x$



- Logistic regression likelihood

$$p(\boldsymbol{y}|w_1) = \prod_{n=1}^{N} \sigma(w_1 x_n)^{y_n} \left(1 - \sigma(w_1 x_n)\right)^{1-y_n}$$

- One parameter: w_1

Questions (5mins)

- Spend 5 minutes DTU Learn quiz: "Lecture 4: Logistic regression"

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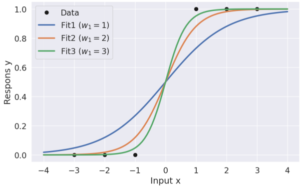

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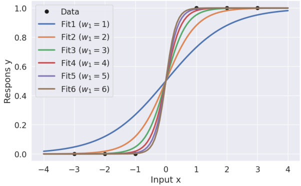

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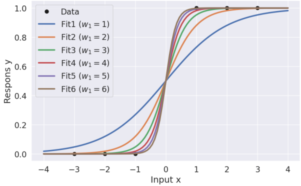

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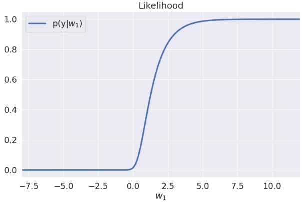

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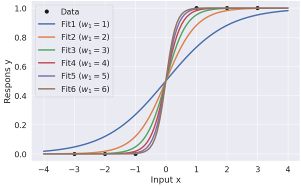

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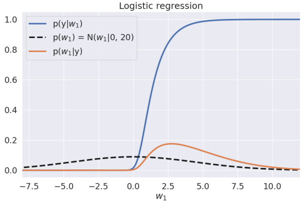


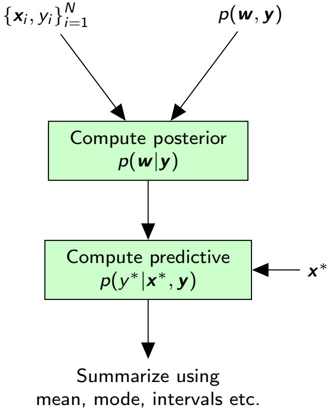
This is a general problem for linearly separable datasets. A prior can fix this

$$p(w_1|\mathbf{y}) \propto p(w_1|\mathbf{y})p(w_1)$$

Bayesian logistic regression

Bayesian supervised learning

- For conjugate models, both the posterior and predictive distributions can be computed analytically



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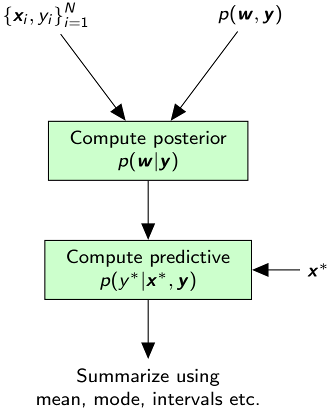
- The real strength of the Bayesian framework lies in the modelling flexibility



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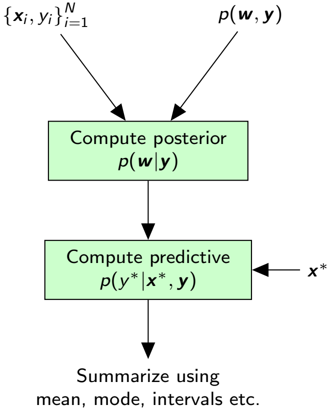

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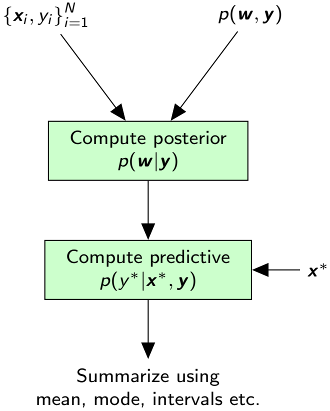

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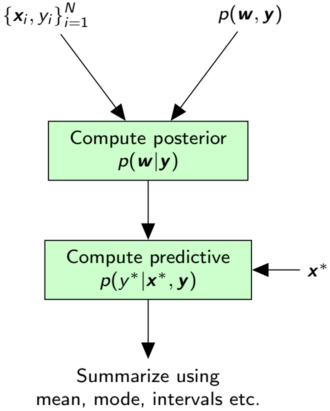
- ... and we will discuss different strategies to evaluate the predictive distribution



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- Likelihood for logistic regression

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- Clearly, we need $p(\boldsymbol{y})$ as well

$$p(\boldsymbol{y}) = \int p(\boldsymbol{y}|\boldsymbol{w}) p(\boldsymbol{w}) \mathrm{d}\boldsymbol{w}$$

Bayesian logistic regression II

- General problem: we *cannot* compute the posterior mean analytically

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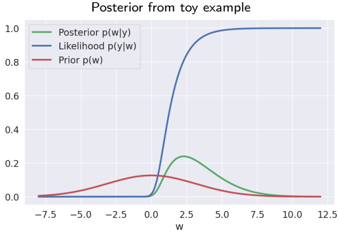

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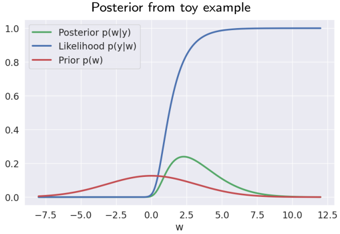

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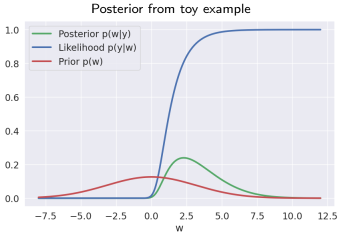

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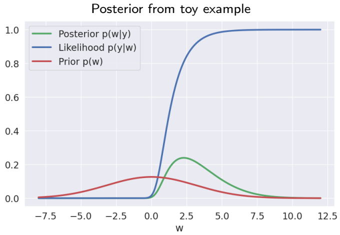

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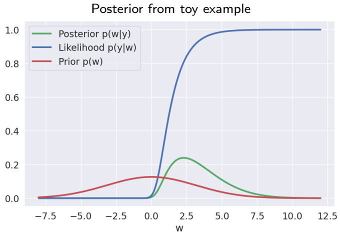

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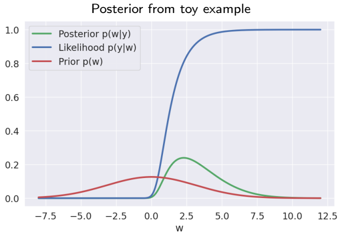

Laplace approximations

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- The *Laplace approximation* is a method for approximating intractable probability densities

- Assume we have a posterior distribution of interest $p(\boldsymbol{w}|\boldsymbol{y})$

$$p(\boldsymbol{w}|\boldsymbol{y}) = \frac{p(\boldsymbol{y}|\boldsymbol{w})p(\boldsymbol{w})}{p(\boldsymbol{y})} = \frac{1}{Z}f(\boldsymbol{w}) \approx \mathcal{N}(\boldsymbol{w}|\boldsymbol{m}, \boldsymbol{S})$$

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- That is, we approximate the posterior mean using the MAP and the posterior covariance using the curvature at the MAP solution.

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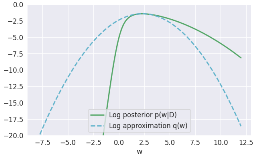

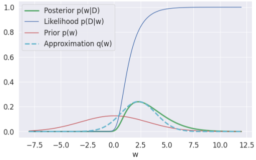

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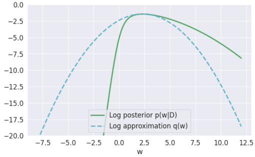

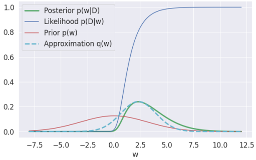

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  1. Simple and well-understood
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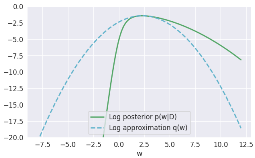
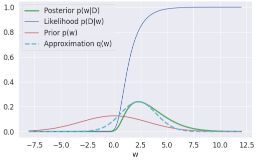
  3. Gives good results for many problems





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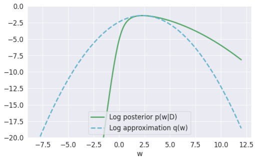
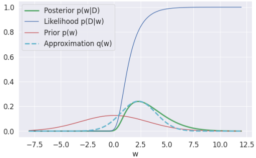
- Limitations

  1. Only applies to continuous parameters
  2. Gaussian (symmetric distribution, thin tails)
  3. Only capture local properties of $p(\boldsymbol{w}|\boldsymbol{y})$ near $\boldsymbol{w}_{\text{MAP}}$
  4. Does not work for hierarchical models in general





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- Very useful for model selection, parameter tuning etc

The posterior predictive distribution

How to make predictions?

- For classification, we need the predictive distribution for a new input $\boldsymbol{x}^*$. The likelihood for a input data point $\boldsymbol{x}*$ is

$$p(y^* = 1|\boldsymbol{w}, \boldsymbol{x}^*) = \sigma(\phi(\boldsymbol{x}^*)^T \boldsymbol{w})$$

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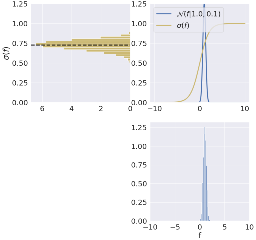
Evaluating predictive distributions for logistic regression

How does uncertainty in f affect the distribution of $\sigma(f)$?

$$p(y^* = 1|\boldsymbol{y}, \boldsymbol{x}^*) = \int \sigma(f)\mathcal{N}(f|\mu, \sigma^2)\mathrm{d}f$$



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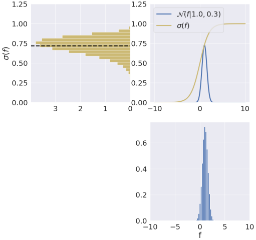

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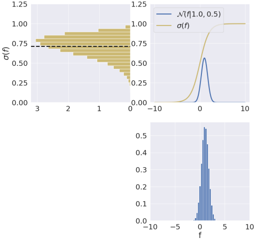

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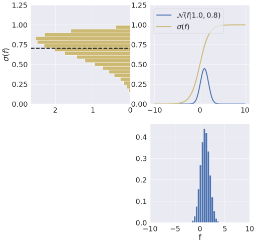

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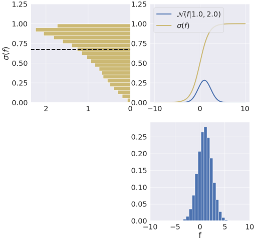

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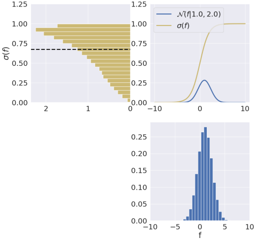

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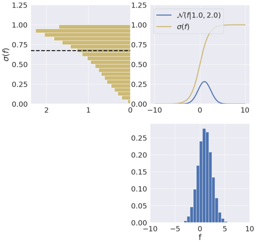

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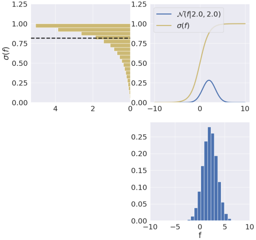

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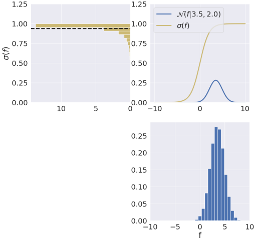

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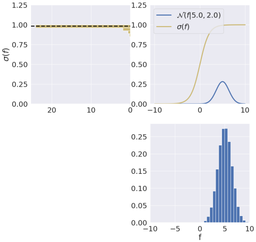

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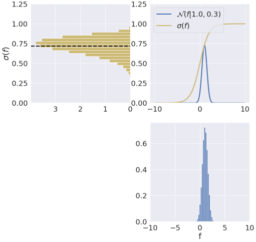

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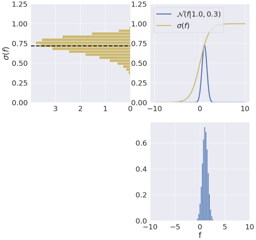

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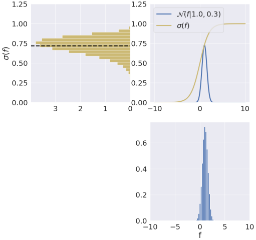

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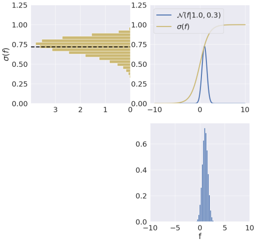

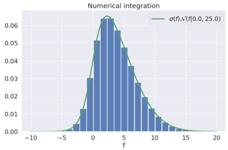

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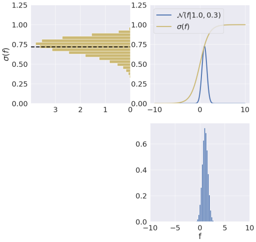

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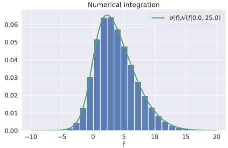
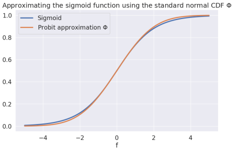


  3. Probit approximation

$$\sigma(y) \approx \Phi\left(y\sqrt{\frac{\pi}{8}}\right)$$

where Φ is the CDF of the standard normal



Let's zoom out and summarize

- We introduced *logistic regression* as a *discriminative* approach for binary classification
- We saw to use the *Laplace approximation* to approximate the *posterior* of the weights
- We briefly discussed three strategies to compute *the predictive distribution*
  1. Sampling
  2. Numerical integration
  3. Probit approximation