02477 – Bayesian Machine Learning: Lecture 3

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Outline

1. Recap: Probabilistic machine learning
2. Recap: Multivariate Gaussian distributions
3. Recap: Linear regression and supervised learning
4. Bayesian linear regression
5. The posterior predictive distribution
6. Dealing with hyperparameters

Recap: Probabilistic machine learning

A probabilistic perspective on making predictions

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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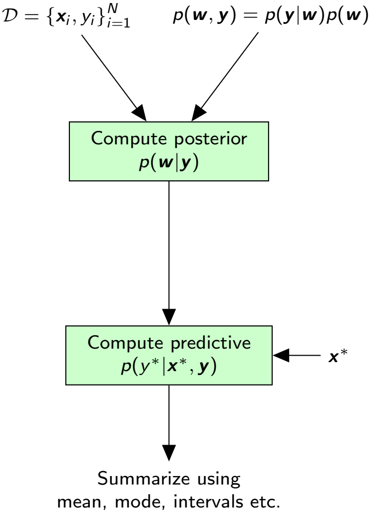
- **Key take-away**: To reason about *y^* given y*, we need to *average the likelihood* for y^* wrt. to the *posterior distribution* $p(\theta|y)$.

Bayesian inference for supervised learning



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

Recap: Multivariate Gaussian distributions

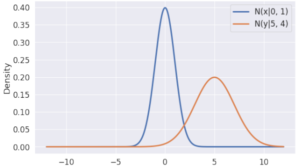
Univariate normal distribution

- The *normal distribution* (also known as the Gaussian)

$$\mathcal{N}(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

- Two parameters: $\mu = \mathbb{E}[x]$ and $\sigma^2 = \mathbb{V}[x]$

- Widely due to Central limit theorems, maximum entropy principle, relation to least squares minimization, nice mathematical properties



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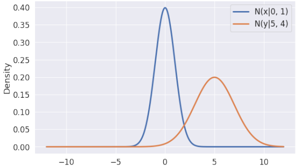

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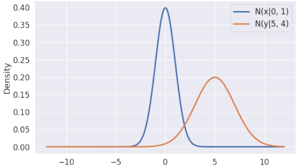
- Let $x \sim \mathcal{N}(m_x, v_x)$ and $y \sim \mathcal{N}(m_y, v_y)$ for $x \perp y$, then

$$x + y \sim \mathcal{N}(m_x + m_y, v_x + v_y)$$



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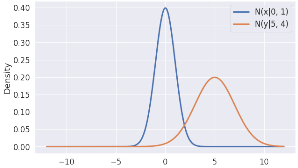

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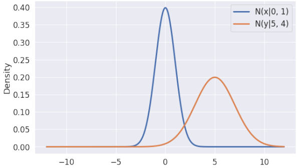

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- Functional form: The *logarithm of a Gaussian density* is a *second order polynomial*

$$\ln \mathcal{N}(x|\mu, \sigma^2) = -\frac{1}{2\sigma^2}x^2 + \frac{\mu}{\sigma^2}x + K$$

The functional form of a Gaussian distribution I

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- Recall we discussed the *functional form* of a Beta distribution
- Let's derive the functional form of the Gaussian

$$\ln \mathcal{N}(x|\mu, \sigma^2) = \ln \left[\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2} \right) \right]$$

The functional form of a Gaussian distribution II: example

- Take-away: the *the functional form* of a univariate Gaussian is

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- Therefore, we conclude $p(x) = \mathcal{N}(x|4, 2)$.

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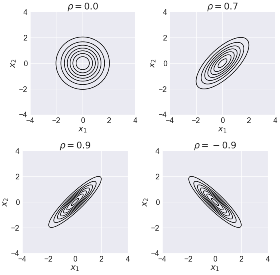
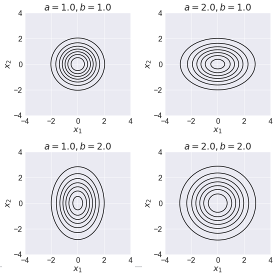
$$p(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{D}{2}} |\boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \mu)^T \boldsymbol{\Sigma}^{-1}(\boldsymbol{x} - \mu)\right)$$

- Two parameters: $\boldsymbol{\mu} = \mathbb{E}[\boldsymbol{x}]$ and $\boldsymbol{\Sigma} = \text{cov}[\boldsymbol{x}]$





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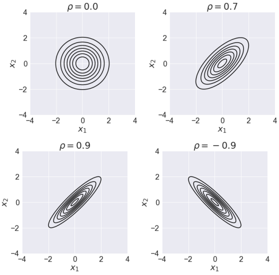
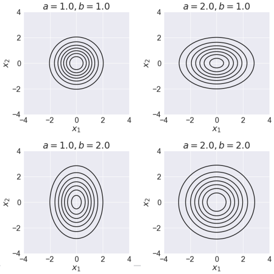
- Covariance matrix for $D = 2$

$$\boldsymbol{\Sigma} = \begin{bmatrix} a & c \\ c & b \end{bmatrix}$$





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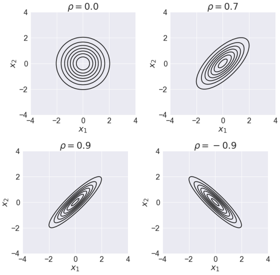
$$p(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{D}{2}} |\boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\mu)^T \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\mu)\right)$$

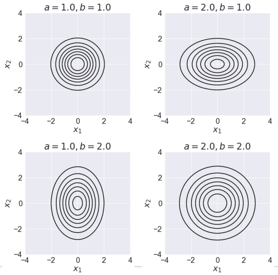
- Two parameters: $\boldsymbol{\mu} = \mathbb{E}[\boldsymbol{x}]$ and $\boldsymbol{\Sigma} = \text{cov}[\boldsymbol{x}]$

- Covariance matrix for $D = 2$

$$\boldsymbol{\Sigma} = \begin{bmatrix} a & c \\ c & b \end{bmatrix}$$

- Correlation coefficient $\rho = \frac{c}{\sqrt{ab}}$





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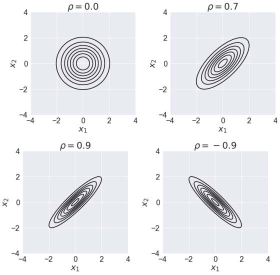

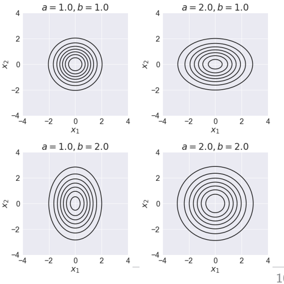

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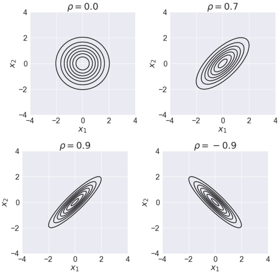

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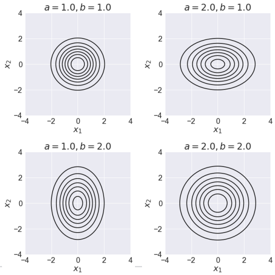

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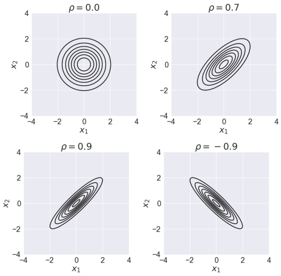

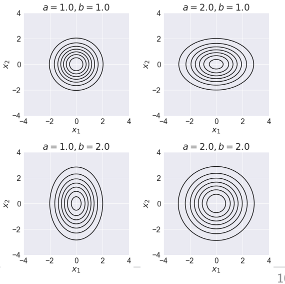

The functional form of multivariate Gaussians

- Consider now the log density, focussing only on terms dependent on $\boldsymbol{x}$.

$$\ln p(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \ln \left[(2\pi)^{-\frac{D}{2}} |\boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp \left(-\frac{1}{2} (\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) \right) \right]$$

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- Key take-aways

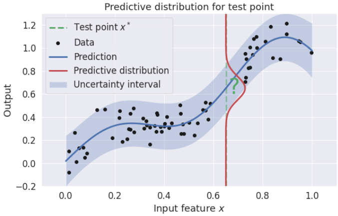
  1. Every time we encounter a distribution with a *quadratic log density*, it must be a Gaussian distribution (if $\boldsymbol{\Sigma}$ is a valid covariance matrix)

  2. We can *match coefficients* of first and second order term to *determine mean and covariance*

Recap: Linear regression and supervised learning

Supervised learning: linear regression

- Dataset $\mathcal{D} = \{(\boldsymbol{x_1}, y_1), (\boldsymbol{x_2}, y_2), \ldots, (\boldsymbol{x_N}, y_N)\}$
  - Input features: $\boldsymbol{x}_i \in \mathbb{R}^D$
  - Targets: $y_i \in \mathbb{R}$



Supervised learning: linear regression

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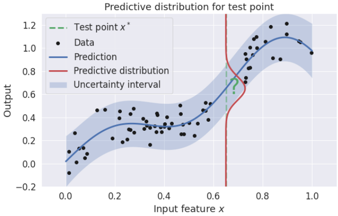
- Additive noise models

$$y_i = f(\boldsymbol{x}_i | \boldsymbol{w}) + \epsilon_i$$



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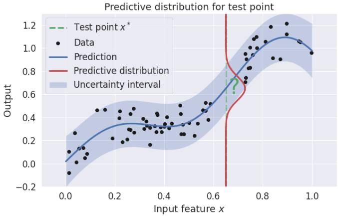
- Linear models are *linear wrt. parameters*, not data!

$$f(\boldsymbol{x}|\boldsymbol{w}) = w_0 + w_1 x_1 + \ldots w_M x_M = \boldsymbol{w}^T \boldsymbol{x}$$



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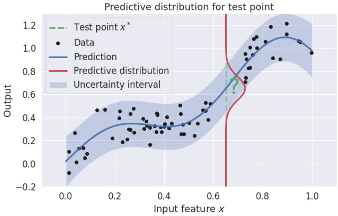
- *Non-linear* feature extractors $\phi(\cdot)$ (basis functions)

$$f(\boldsymbol{x}|\boldsymbol{w}) = \sum_{j=0}^{M} w_j \phi_j(\boldsymbol{x}) = \boldsymbol{w}^T \phi(\boldsymbol{x})$$



Linear regression: the probabilistic model

- The *predictive distribution* of y^* given $\boldsymbol{x}^*$ and the data $\mathcal{D}$ is our goal

$$p\left(y^*|\mathcal{D}, \boldsymbol{x}^*\right)$$

- Model for the "signal"

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

- The gaussian noise ϵ_i is assumed to be *independent and identically distributed (i.i.d)*

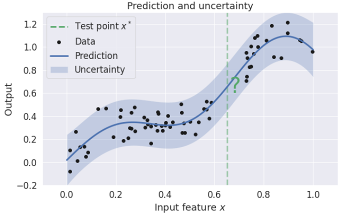
$$y_i = f(\boldsymbol{x}_i|\boldsymbol{w}) + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2)$$

- The *likelihood* for the i'th data point

$$p(y_i|\boldsymbol{x}_i, \boldsymbol{w}, \sigma^2) = \mathcal{N}(y_i|\boldsymbol{w}^T\phi(\boldsymbol{x}_i), \sigma^2)$$

- Using the maximum likelihood solution as a *plug-in* estimator

$$p\left(y^*|\mathcal{D}, \boldsymbol{x}^*\right) = \mathcal{N}(y_i|\hat{\boldsymbol{w}}_{\text{MLE}}^T\phi(\boldsymbol{x}_*), \sigma^2)$$



Estimating the parameters using maximum likelihood

- Given a dataset $\mathcal{D} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \dots, (\boldsymbol{x}_N, y_N)\}$, the *likelihood* for dataset is

$$p(\boldsymbol{y}|\boldsymbol{w}, \sigma^2) = \prod_{n=1}^{N} \mathcal{N}(y_n | f(\boldsymbol{x}_{\boldsymbol{n}}|\boldsymbol{w}), \sigma^2)$$

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- Taking the logarithm and using $f(\boldsymbol{x}_n, \boldsymbol{w}) = \boldsymbol{w}^T \phi(\boldsymbol{x}_n)$

$$\ln p(\boldsymbol{y}|\boldsymbol{w}, \sigma^2) = \sum_{n=1}^{N} \ln \mathcal{N}(y_n|\boldsymbol{w}^T \phi(\boldsymbol{x}_n), \sigma^2)$$

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&= \sum_{n=1}^{N} \left[-\frac{1}{2} \ln(2\pi\sigma^2) - \frac{1}{2\sigma^2} (y_n - \boldsymbol{w}^T \phi(\boldsymbol{x}_n))^2 \right]
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- Maximum likelihood estimator $\hat{\boldsymbol{w}}_{\text{MLE}}$ is equivalent to minimizing sum-of-squares error

$$\hat{\boldsymbol{w}}_{\text{MLE}} = \left(\boldsymbol{\Phi}^T \boldsymbol{\Phi}\right)^{-1} \boldsymbol{\Phi}^T \boldsymbol{y} \qquad \text{(Normal equations)}$$

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$$\hat{\sigma}^2_{\text{MLE}} = \frac{1}{N} \sum_{n=1}^{N} (y_n - \hat{\boldsymbol{w}}_{\text{MLE}}^T \phi(\boldsymbol{x_n}))^2$$

Example: Polynomial regression using maximum likelihood I

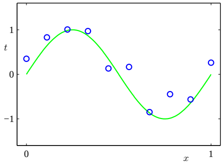
Example from Bishop

- Polynomial basis functions

$$f(x|\boldsymbol{w}) = w_0 + w_1 x + w_2 x^2 + \cdots + w_M x^M = \boldsymbol{w}^T \phi(x)$$

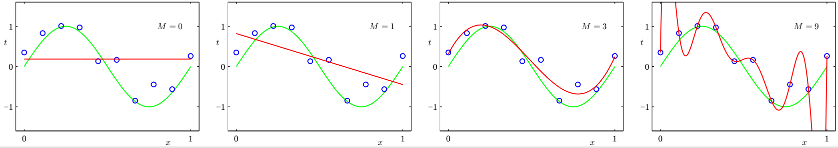
- Feature transformations

$$\phi(x) = \begin{bmatrix} 1 & x & x^2 & \ldots & x^M \end{bmatrix}^T$$



- M controls the *model complexity*: Underfitting vs overfitting

- *Model selection*: How to choose M?

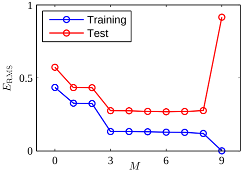


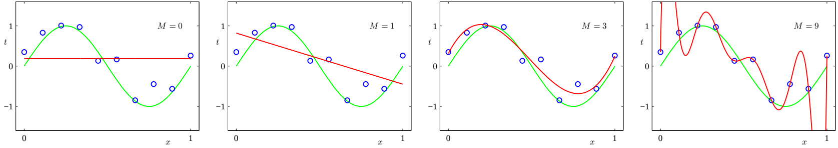
Example: Polynomial regression using maximum likelihood II

- *Cross-validation*
  Split data into training and test sets

- *Overfitting (low training error, high test error)*
  As the function become more flexible we start to fit the noise in the data

- *"Underfitting" (high training error, high test error)*
  When the function is not sufficiently flexible to fit the data





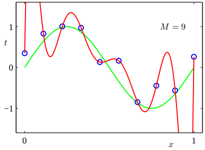
Example: Polynomial regression using maximum likelihood III

- *The optimal model complexity depends on the amount of data*
  The more data the more flexible model we can "afford" to fit

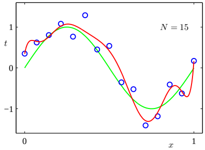
- *Regularization: Controlling the effective model complexity*
  We can use regularization to control the effect model complexity when we have limited data

	$M=0$	$M=1$	$M=6$	$M=9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43

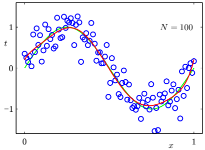
$N = 10$, $M = 9$



$N = 15$, $M = 9$



$N = 100$, $M = 9$



Regularized least squares

- Recall: *Maximum likelihood* is equivalent *minimizng sum-of-squares error*

$$E_D(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N}(y_n - f(x_n|\boldsymbol{w}))^2$$

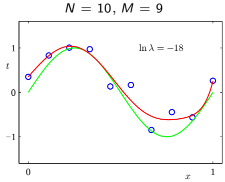
- Adding *penalty term* to prevent weights from becoming too large

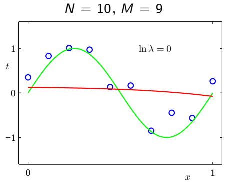
$$\tilde{E}_D(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N}(y_n - f(x_n|\boldsymbol{w}))^2 + \frac{\lambda}{2}||\boldsymbol{w}||^2$$

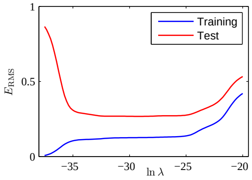
- What happens when $\lambda = 0$? $\lambda \to \infty$?

- Many names: Ridge regression, shrinkage, weight decay

- Regularization parameter λ controls the *effective complexity*



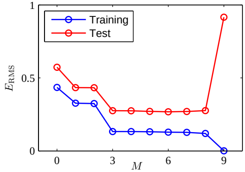


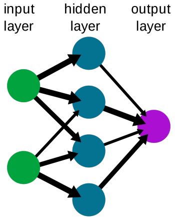


Bayesian linear regression

Bayesian Linear regression: motivation

- *Overfitting*
  Maximum likelihood can be problematic for flexible models
- *Controlling model complexity*
  Limitting number of basis functions and/or regularization?
- *Model selection*
  How to choose the optimal value of λ?
- *Cross-validation*
  Training + validation/development + test
- *Bayesian methods*
  - less prone to overfitting
  - can (often) adapt model complexity automatically
- *Applications in modern machine learning*
  1. Small datasets
  2. Transfer learning
  3. Component in more complex models
  4. Simple uncertainty quantification for neural networks





Bayesian Linear regression: prior and likelihood

- Simplified set-up: assuming σ^2 is fixed and known, then Bayes' rule states

$$p(\boldsymbol{w}|\boldsymbol{y}) = \frac{p(\boldsymbol{y}|\boldsymbol{w})p(\boldsymbol{w})}{p(\boldsymbol{y})}$$

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$$p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{w}, \sigma^2) = \prod_{n=1}^{N} \mathcal{N}(y_n|\boldsymbol{w}^T\phi(\boldsymbol{x}_n), \sigma^2) = \mathcal{N}(\boldsymbol{y}|\boldsymbol{\Phi}\boldsymbol{w}, \sigma^2\boldsymbol{I})$$

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- *The marginal likelihood* is the denominator in Bayes's theorem and is independent of $\boldsymbol{w}$

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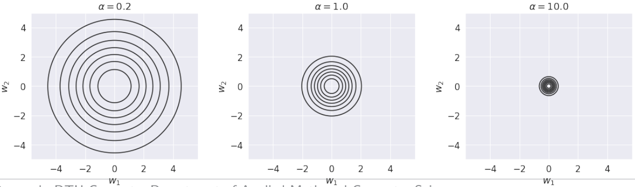

Bayesian Linear regression: The MAP estimator

- The *posterior distribution* of the weights $\boldsymbol{w}$ given the data $\boldsymbol{y}$ is given by

$$p(\boldsymbol{w}|\boldsymbol{y}) = \frac{p(\boldsymbol{y}|\boldsymbol{w})p(\boldsymbol{w})}{p(\boldsymbol{y})} = \frac{\mathcal{N}(\boldsymbol{y}|\boldsymbol{\Phi}\boldsymbol{w}, \sigma^2\boldsymbol{I})\mathcal{N}(\boldsymbol{w}|\boldsymbol{0}, \alpha^{-1}\boldsymbol{I})}{p(\boldsymbol{y})}$$

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- The *mode of the posterior (MAP)* is equivalent to ridge regression with $\lambda = \frac{\alpha}{\beta}$ and to maximum likelihood when $\alpha \to 0$

Deriving the posterior distribution of the weights

Recall the functional form of a generic multivariate Gaussian $\mathcal{N}(\boldsymbol{w}|\boldsymbol{m}, \boldsymbol{S})$

$$\ln \mathcal{N}(\boldsymbol{w}|\boldsymbol{m}, \boldsymbol{S}) = -\frac{1}{2}\boldsymbol{w}^T\boldsymbol{S}^{-1}\boldsymbol{w} + \boldsymbol{m}^T\boldsymbol{S}^{-1}\boldsymbol{w} + \textit{constant}$$

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- Equating coefficients for the second order term

$$\boldsymbol{S}^{-1} = \beta\boldsymbol{\Phi}^T\boldsymbol{\Phi} + \alpha\boldsymbol{I} \quad \iff \quad \boldsymbol{S} = \left(\beta\boldsymbol{\Phi}^T\boldsymbol{\Phi} + \alpha\boldsymbol{I}\right)^{-1}$$

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- Equating coefficients for the first order term

$$\boldsymbol{m}^T\boldsymbol{S}^{-1} = \beta\boldsymbol{y}^T\boldsymbol{\Phi} \quad \iff \quad \boldsymbol{m} = \beta\boldsymbol{S}\boldsymbol{\Phi}^T\boldsymbol{y}$$

Bayesian linear regression model: the key equations

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

$$
\begin{aligned}
p(\boldsymbol{w}) &= \mathcal{N}(\boldsymbol{w}|0, \alpha^{-1}\boldsymbol{I}) && \text{(}\textit{prior}\text{)}\\
p(\boldsymbol{y}|\boldsymbol{w}) &= \mathcal{N}(\boldsymbol{y}|\mathbf{\Phi}\boldsymbol{w}, \sigma^2\boldsymbol{I}) && \text{(}\textit{likelihood}\text{)}\\
p(\boldsymbol{w}|\boldsymbol{y}) &= \mathcal{N}(\boldsymbol{w}|\boldsymbol{m}, \boldsymbol{S}) && \text{(}\textit{posterior}\text{)}\\
p(\boldsymbol{y}) &= \mathcal{N}(\boldsymbol{y}|\mathbf{0}, \sigma^2\boldsymbol{I} + \alpha^{-1}\mathbf{\Phi}\mathbf{\Phi}^T) && \text{(}\textit{marginal likelihood}\text{)}
\end{aligned}
$$

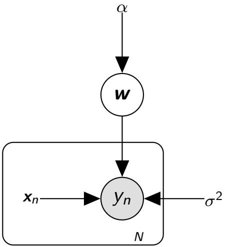
- The *posterior parameters* are given by (using $\beta \equiv \frac{1}{\sigma^2}$)

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

$$
\boldsymbol{S} = \left(\alpha\boldsymbol{I} + \beta\mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}
$$

- *Two hyperparameters*

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



Linear Gaussian-systems in general (see Section 3.3 in Murphy1)

- For *linear* systems: the Gaussian distribution is *conjugate* to itself
- The *posterior* for a *linear* Gaussian model with Gaussian prior is also *Gaussian*

$$p(\boldsymbol{y}|\boldsymbol{z}) = \mathcal{N}(\boldsymbol{y}|\boldsymbol{W}\boldsymbol{z} + \boldsymbol{b}, \boldsymbol{\Sigma}_y) \qquad\qquad p(\boldsymbol{z}) = \mathcal{N}(\boldsymbol{z}|\boldsymbol{\mu}_z, \boldsymbol{\Sigma}_z)$$

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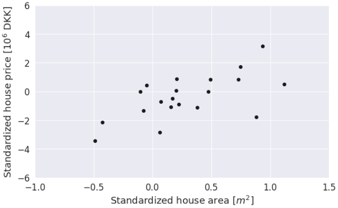
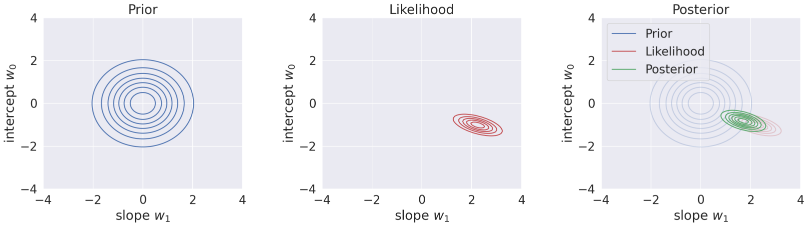
Example

- Simple linear model for fictive house prices

$$f(x|\boldsymbol{w}) = w_0 + w_1 x$$

- The posterior summarizes our beliefs about the parameters after seeing the data





$$p(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}|0, \alpha^{-1}\boldsymbol{I}) \qquad p(\boldsymbol{y}|\boldsymbol{w}) = \mathcal{N}(\boldsymbol{y}|\boldsymbol{\Phi}\boldsymbol{w}, \sigma^2\boldsymbol{I}) \qquad p(\boldsymbol{w}|\boldsymbol{y}) = \mathcal{N}(\boldsymbol{w}|\boldsymbol{m}, \boldsymbol{S})$$

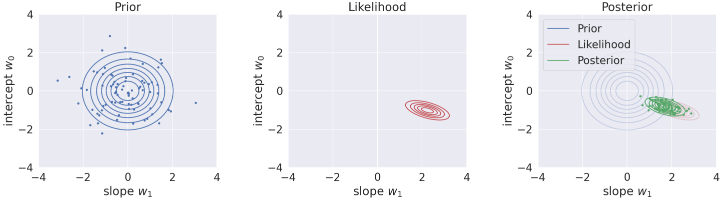
Posterior inference

$$\text{house price} = w_0 + w_1 \cdot \text{area}$$

- Question: Are larger areas associated with bigger house prices?
- We can calculate various probabilities of interest directly from the posterior (analytically or via sampling), e.g.

$$p(w_1 > 0|y) \approx 0.99$$

- No need to remember whether to should use t-tests, F-tests, χ^2-tests etc



The posterior predictive distribution

But how about making predictions?

- We defined a *linear* regression model

$$y_i = \boldsymbol{w}^T \phi(\boldsymbol{x}_i) + \epsilon_i$$

- We derived the *posterior distribution*

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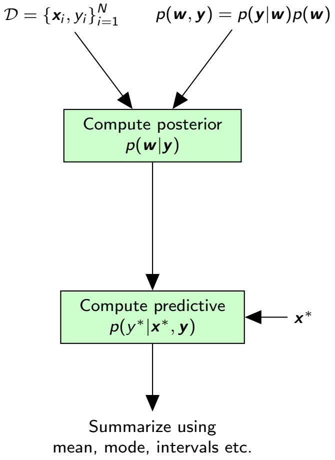

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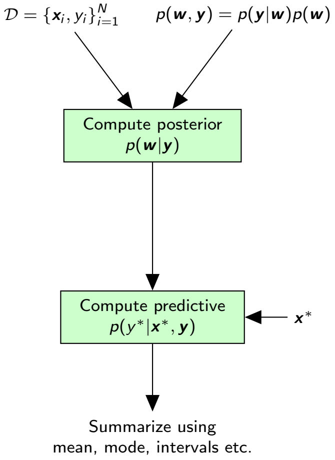

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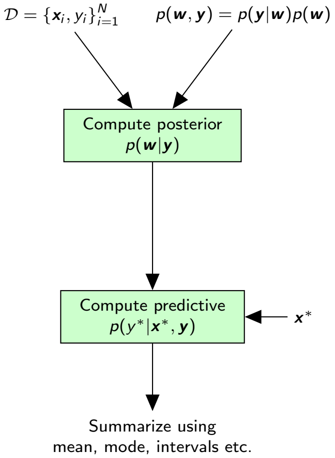

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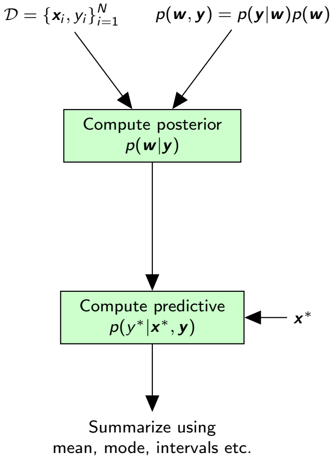

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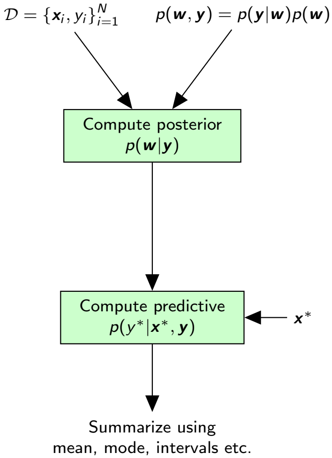

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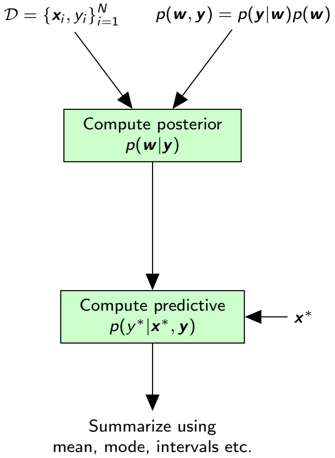
- Can be derived using eq. (3.38) in Murphy1



Quiz time!

$$p(\boldsymbol{w}|\boldsymbol{y}) = \frac{p(\boldsymbol{y}|\boldsymbol{w})p(\boldsymbol{w})}{p(\boldsymbol{y})} \qquad (\textit{Bayes' rule})$$

$$p(\boldsymbol{y}) = \int p(\boldsymbol{y}|\boldsymbol{w})p(\boldsymbol{w})\mathrm{d}\boldsymbol{w} \qquad (\textit{marginal likelihood})$$

$$p(y^*|\boldsymbol{y}, \boldsymbol{x}^*) = \int p(y^*|\boldsymbol{x}^*, \boldsymbol{w})p(\boldsymbol{w}|\boldsymbol{y})\mathrm{d}\boldsymbol{w} \qquad (\textit{Posterior predictive dist.})$$

- Spend 5 minutes DTU Learn quiz: "Lecture 3: Bayesian inference"

Posterior Predictive distributions

Building intuition

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

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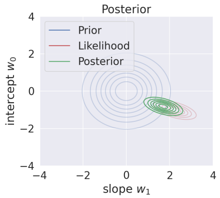

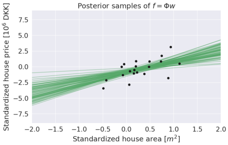

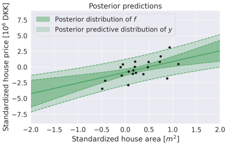

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$$\mathbb{E}\left[f^*\right] =$$

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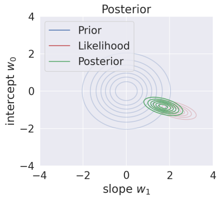

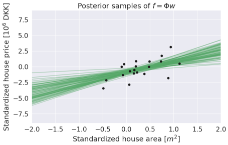

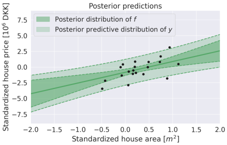

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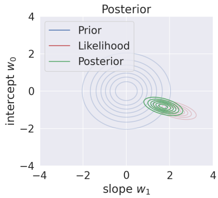

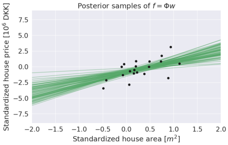

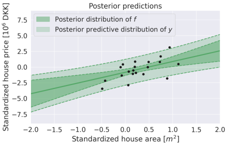

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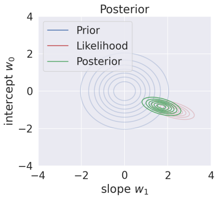

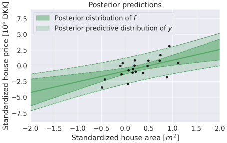

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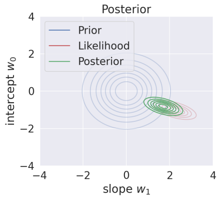

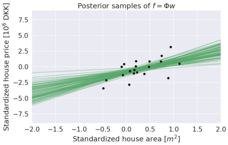

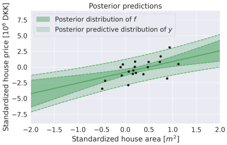

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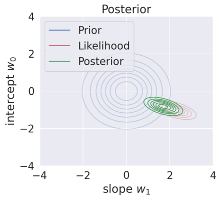

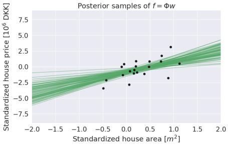

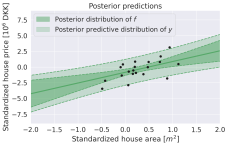

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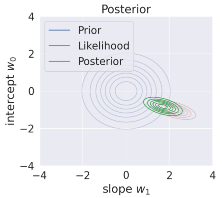

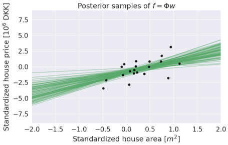

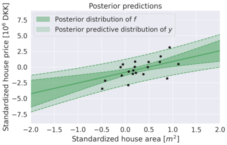

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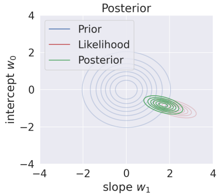

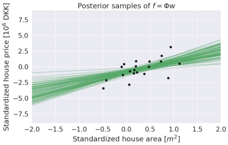

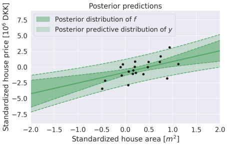

Posterior Predictive distributions

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

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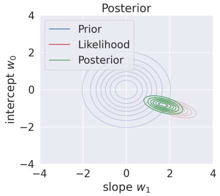

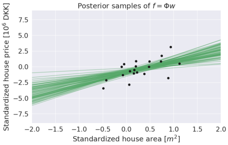

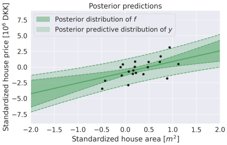

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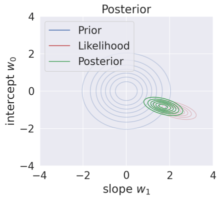
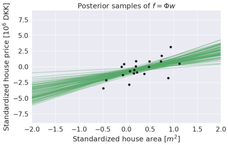
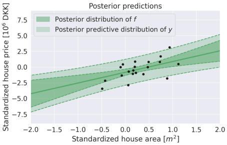
since $\mathbb{V}[\epsilon] = \sigma^2$







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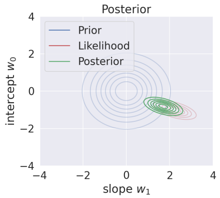
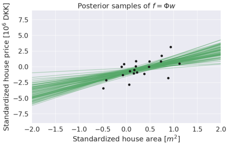
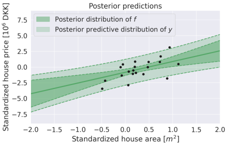
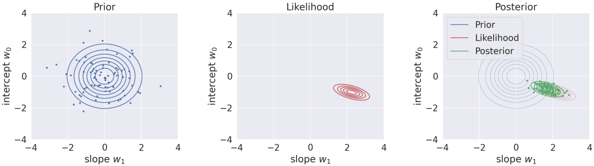
- We can also compute the *prior* predictive distribution.







Prior and posterior predictive distributions



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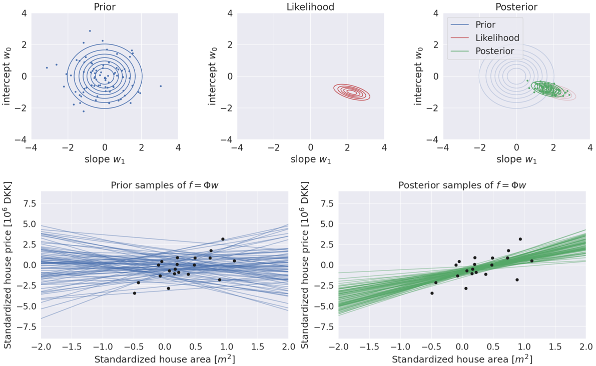

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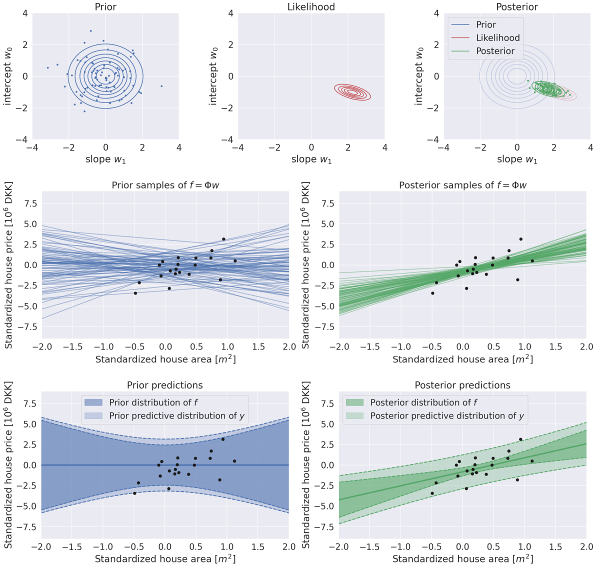
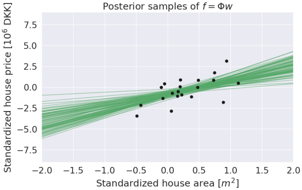
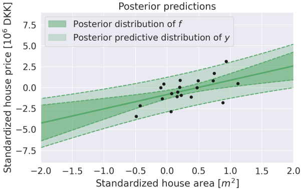


Posterior Predictive distributions

Epistemic and aleatoric uncertainty





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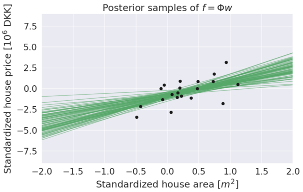

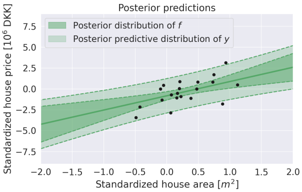

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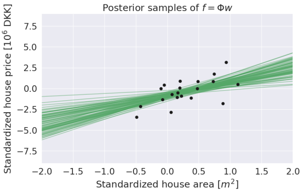

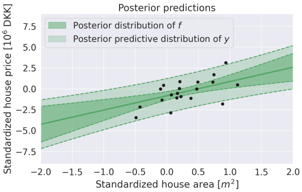

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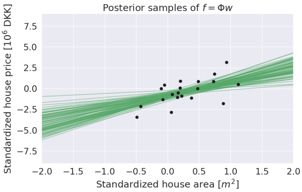

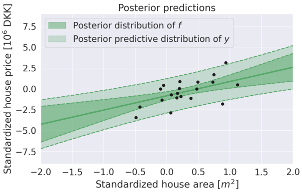

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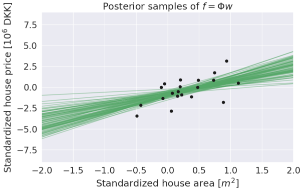
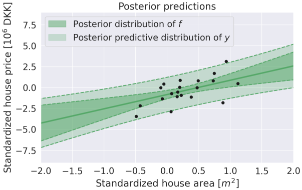
- A couple of questions for you:
  1. What happens to the predictive variance when $N \to \infty$?
  2. Why is the uncertainty "U-shaped"?
  3. Why does the aleatoric uncertainty appear to dominate the total uncertainty near the data?



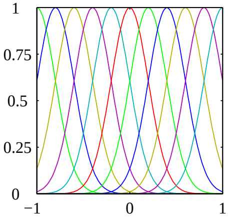


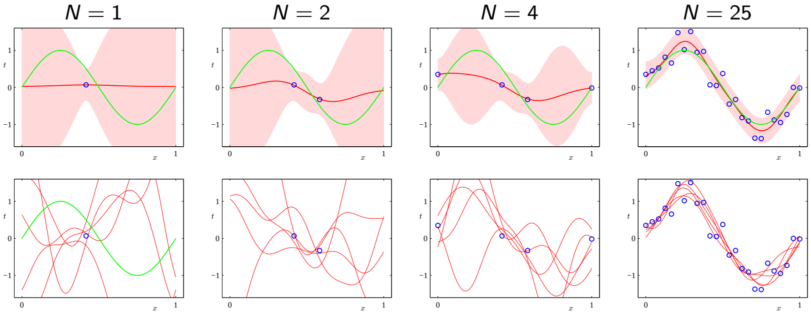
Example: posterior predictive distributions

- *Predictive distributions* for simple sinoidal toy dataset using Gaussian Basis functions

- Samples from the posterior

Feature extractors $\phi_i(x)$





Dealing with hyperparameters

But what about the hyperparameters?

- The Bayesian linear regression model

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

$$p(\boldsymbol{y}|\boldsymbol{w}) = \mathcal{N}(\boldsymbol{y}|\boldsymbol{\Phi}\boldsymbol{w}, \sigma^2\boldsymbol{I}) \qquad \textit{(likelihood)}$$

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

$$p(\boldsymbol{y}) = \mathcal{N}(\boldsymbol{y}|\boldsymbol{0}, \sigma^2\boldsymbol{I} + \alpha^{-1}\boldsymbol{\Phi}\boldsymbol{\Phi}^T) \qquad \textit{(marginal likelihood)}$$

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- ... and integrate them out

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- ... but this is not analytically tractable. Later in the course we will learn tools to deal with this in general

The evidence approximation

- How to deal with this bastard?

$$p(y^*|\boldsymbol{y}) = \int\int\int p(y^*|\boldsymbol{w},\beta)p(\boldsymbol{w}|\boldsymbol{y},\alpha,\beta)p(\alpha,\beta|\boldsymbol{y})\mathrm{d}\boldsymbol{w}\mathrm{d}\alpha\mathrm{d}\beta$$

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- We can estimate $\hat{\alpha},\hat{\beta}$ by *optimizing the marginal likelihood* $p(\boldsymbol{y}|\alpha,\beta)$

$$\hat{\alpha},\hat{\beta} = \arg\max_{\alpha,\beta} \log p(\boldsymbol{y}|\alpha,\beta)$$

Sinoidal example revisited using the evidence approximation