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	**Sum rule**	**Conditional**	**Conditional independence**
$p(\boldsymbol{a}, \boldsymbol{b}) = p(\boldsymbol{b}\vert\boldsymbol{a})p(\boldsymbol{a})$	$p(\boldsymbol{b}) = \int p(\boldsymbol{a}, \boldsymbol{b})\mathrm{d}\boldsymbol{a}$	$p(\boldsymbol{a}\vert\boldsymbol{b}) = \frac{p(\boldsymbol{a},\boldsymbol{b})}{p(\boldsymbol{b})}$	$p(\boldsymbol{a}, \boldsymbol{b}\vert\boldsymbol{c}) = p(\boldsymbol{a}\vert\boldsymbol{c})p(\boldsymbol{b}\vert\boldsymbol{c})$

Goal: Given some data y, what can we say about a new observation y^*?

- Step 1: Formulate *joint distribution* for *all variables* of interests

$$p(y^*, y, \theta) = p(y^*, y|\theta)p(\theta) = p(y^*|\theta)p(y|\theta)p(\theta)$$

- Step 2: *Condition* on the *observed data* y

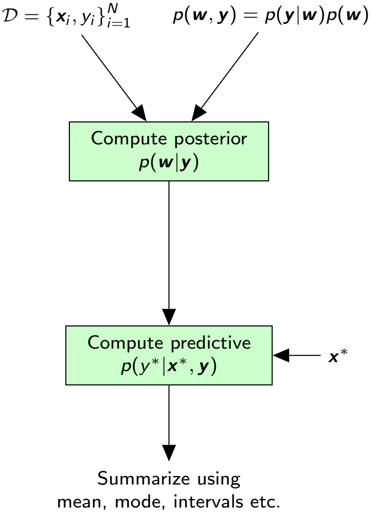
$$p(y^*, \theta|y) = \frac{p(y*, y, \theta)}{p(y)} = \frac{p(y^*|\theta)p(y|\theta)p(\theta)}{p(y)}$$

- Step 3: *Marginalize* out parameter θ using the *sum rule* to get the *posterior predictive distribution*

$$p(y^*|y) = \int p(y^*, \theta|y)\mathrm{d}\theta = \int \frac{p(y^*|\theta)p(y|\theta)p(\theta)}{p(y)}\mathrm{d}\theta = \int p(y^*|\theta)p(\theta|y)\mathrm{d}\theta = \mathbb{E}_{p(\theta|y)}\left[p(y^*|\theta)\right]$$

- **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

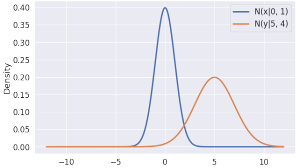
Univariate normal distribution

- 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



$$x \sim N(0,1)$$
$$y = 5 + 2x$$

- Closed under affine transformations

$$x \sim \mathcal{N}(m, v) \quad \Rightarrow \quad a + bx \sim \mathcal{N}(a + bm, b^2 v)$$

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

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

- 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

- 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

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

- Example: suppose we are given the following log density for a random variable x

$$\ln p(x) = -\frac{1}{4}x^2 + 2x + K$$

- We recognize the 2nd order polynomial and conclude that $p(x)$ must be Gaussian

- We determine the *variance* by matching the coefficient for 2nd order term

$$-\frac{1}{2\sigma^2} = -\frac{1}{4} \quad \Rightarrow \quad \frac{1}{\sigma^2} = \frac{1}{2} \quad \Rightarrow \quad \sigma^2 = 2$$

- We determine the *mean* by matching coefficient for 1st order term

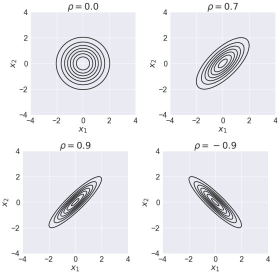
$$\frac{\mu}{\sigma^2} = 2 \quad \Rightarrow \quad \mu = 4$$

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

The multivariate normal distribution

- The *multivariate normal distribution*

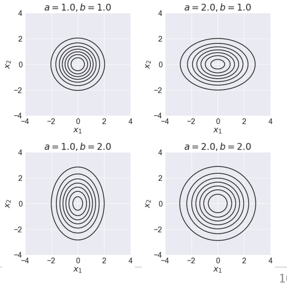
$$p(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{D}{2}} |\boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\mu)^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\mu)\right)$$



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

- Covariance matrix for $D = 2$

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



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

- Let $\mathbf{x} \sim \mathcal{N}(\mathbf{m}_x, \mathbf{V}_x)$ and $\mathbf{y} \sim \mathcal{N}(\mathbf{m}_y, \mathbf{V}_y)$ for $\mathbf{x} \perp \mathbf{y}$, then

$$\mathbf{a} + \mathbf{B}\mathbf{x} \sim \mathcal{N}(\mathbf{a} + \mathbf{B}\mathbf{m}_x, \mathbf{B}\mathbf{V}_x\mathbf{B}^T)$$
$$\mathbf{x} + \mathbf{y} \sim \mathcal{N}(\mathbf{m}_x + \mathbf{m}_y, \mathbf{V}_x + \mathbf{V}_y)$$

The functional form of multivariate Gaussians

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

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

- 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: $y_i \in \mathbb{R}$

- Additive noise models

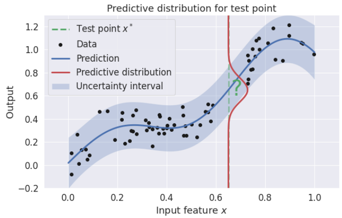
$$y_i = f(\boldsymbol{x}_i | \boldsymbol{w}) + \epsilon_i$$

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

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

- *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)*

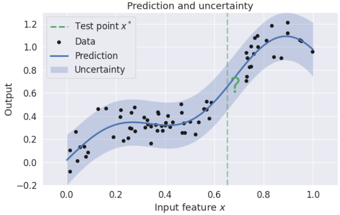
$$y_i = f(\boldsymbol{x}_i | \boldsymbol{w}) + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2)$$

- 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

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



Estimating the parameters using maximum likelihood

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

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

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

$$\begin{aligned}
\ln p(\boldsymbol{y}|\boldsymbol{w}, \sigma^2) &= \sum_{n=1}^{N} \ln \mathcal{N}(y_n | \boldsymbol{w}^T \phi(\boldsymbol{x}_n), \sigma^2) \\
&= \sum_{n=1}^{N} \left[-\frac{1}{2} \ln(2\pi\sigma^2) - \frac{1}{2\sigma^2} (y_n - \boldsymbol{w}^T \phi(\boldsymbol{x}_n))^2 \right] \\
&= -\frac{N}{2} \ln(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{n=1}^{N} (y_n - \boldsymbol{w}^T \phi(\boldsymbol{x}_n))^2
\end{aligned}$$

- Maximum likelihood estimator $\hat{\boldsymbol{w}}_{\text{MLE}}$ is equivalent to minimizing sum-of-squares error

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

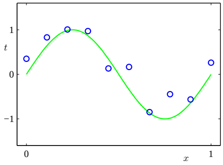
$$\hat{\sigma}^2_{\text{MLE}} = \frac{1}{N} \sum_{n=1}^{N} (y_n - \hat{\boldsymbol{w}}^T_{\text{MLE}} \phi(\boldsymbol{x_n}))^2$$

Example: Polynomial regression using maximum likelihood I

Example from Bishop

- Polynomial basis functions

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

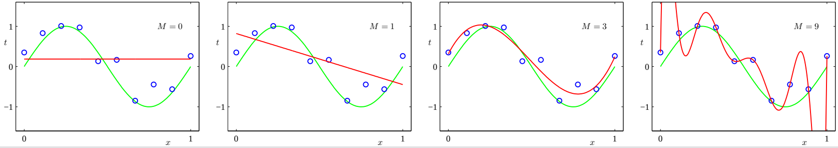


- Feature transformations

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

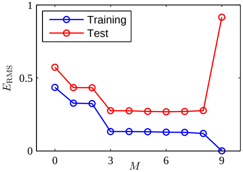
- M controls the *model complexity*: Underfitting vs overfitting

- *Model selection*: How to choose M?



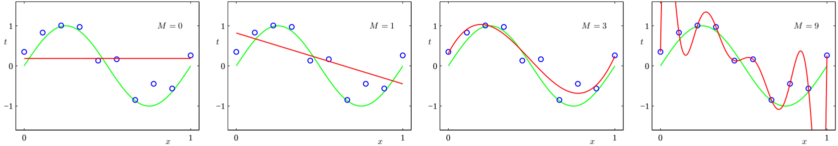
Example: Polynomial regression using maximum likelihood II

- *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

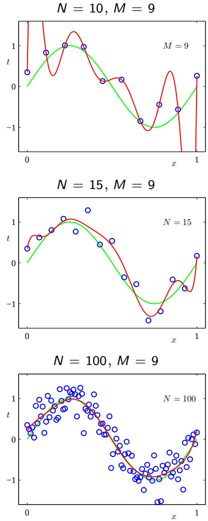


Example: Polynomial regression using maximum likelihood III

- *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

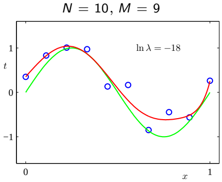
	$M = 0$	$M = 1$	$M = 6$	$M = 9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43



Regularized least squares

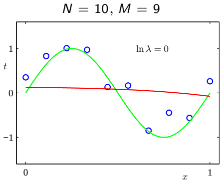
- Recall: *Maximum likelihood* is equivalent *minimizng sum-of-squares error*

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



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

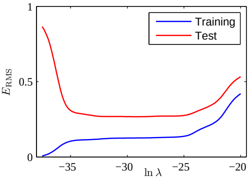
$$\tilde{E}_D(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}(y_n - f(x_n|\mathbf{w}))^2 + \frac{\lambda}{2}||\mathbf{w}||^2$$



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

- Many names: Ridge regression, shrinkage, weight decay

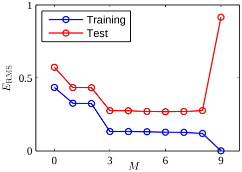
- Regularization parameter λ controls the *effective complexity*

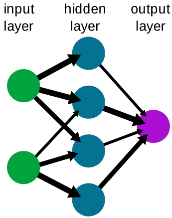


Bayesian linear regression

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

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

- We already know the *likelihood*

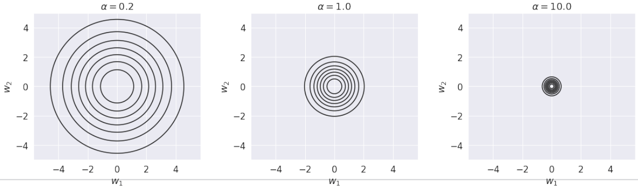
$$p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{w}, \sigma^2) = \prod_{n=1}^{N} \mathcal{N}(y_n|\boldsymbol{w}^T\phi(\boldsymbol{x}_n), \sigma^2) = \mathcal{N}(\boldsymbol{y}|\boldsymbol{\Phi}\boldsymbol{w}, \sigma^2\boldsymbol{I})$$

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

$$p(\boldsymbol{y}) = \int p(\boldsymbol{y}|\boldsymbol{w})p(\boldsymbol{w})\mathrm{d}\boldsymbol{w} = \mathbb{E}_{p(\boldsymbol{w})}\left[p(\boldsymbol{y}|\boldsymbol{w})\right]$$

- The multivariate normal distribution is a *conjugate prior* for the $\boldsymbol{w}$

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



Bayesian Linear regression: The MAP estimator

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

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

- Let's look at the *maximum a posteriori* (MAP) estimate: $\hat{\boldsymbol{w}}_{\mathrm{MAP}} = \arg\max_{\boldsymbol{w}} p(\boldsymbol{w}|\boldsymbol{y})$

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

- Taking the logarithm

$$\begin{aligned}
\ln p(\boldsymbol{w}|\boldsymbol{y}) &\propto \ln \mathcal{N}(\boldsymbol{y}|\boldsymbol{\Phi}\boldsymbol{w}, \sigma^2\boldsymbol{I}) + \ln \mathcal{N}(\boldsymbol{w}|\boldsymbol{0}, \alpha^{-1}\boldsymbol{I}) \\
&= -\frac{N}{2}\ln(2\pi\sigma^2) - \frac{\beta}{2}\sum_{n=1}^{N}(y_n - \boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x}_n))^2 - \frac{D}{2}\ln(2\pi\alpha^{-1}) - \frac{\alpha}{2}\boldsymbol{w}^T\boldsymbol{w} \\
&= -\frac{\beta}{2}\sum_{n=1}^{N}(y_n - \boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x}_n))^2 - \frac{\alpha}{2}\sum_{i=1}^{D} w_i^2 + \text{constant}
\end{aligned}$$

- 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 $\mathcal{N}(\boldsymbol{w}|\boldsymbol{m}, \boldsymbol{S})$

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

- We focus on term that depends on $\boldsymbol{w}$. From the previous slide, we have

$$\begin{aligned}
\ln p(\boldsymbol{w}|\boldsymbol{y}) &= -\frac{\beta}{2}\sum_{n=1}^{N}(y_n - \boldsymbol{w}^T\phi(\boldsymbol{x}_n))^2 - \frac{\alpha}{2}\boldsymbol{w}^T\boldsymbol{w} + \text{constant} \\
&= -\frac{\beta}{2}(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{w})^T(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{w}) - \frac{\alpha}{2}\boldsymbol{w}^T\boldsymbol{w} + \text{constant} \\
&= -\frac{\beta}{2}\left(\boldsymbol{y}^T\boldsymbol{y} - 2\boldsymbol{y}^T\boldsymbol{\Phi}\boldsymbol{w} + \boldsymbol{w}\boldsymbol{\Phi}^T\boldsymbol{\Phi}\boldsymbol{w}\right) - \frac{\alpha}{2}\boldsymbol{w}^T\boldsymbol{w} + \text{constant} \\
&= -\frac{\beta}{2}\left(-2\boldsymbol{y}^T\boldsymbol{\Phi}\boldsymbol{w} + \boldsymbol{w}\boldsymbol{\Phi}^T\boldsymbol{\Phi}\boldsymbol{w}\right) - \frac{\alpha}{2}\boldsymbol{w}^T\boldsymbol{w} + \text{constant} \\
&= -\frac{1}{2}\boldsymbol{w}^T\left(\beta\boldsymbol{\Phi}^T\boldsymbol{\Phi} + \alpha\boldsymbol{I}\right)\boldsymbol{w} + \beta\boldsymbol{y}^T\boldsymbol{\Phi}\boldsymbol{w} + \text{constant}
\end{aligned}$$

- Equating coefficients for the second order term

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

- Equating coefficients for the first order term

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

Bayesian linear regression model: the key equations

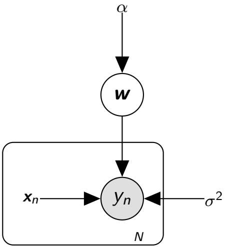
- Given design matrix $\boldsymbol{\Phi} \in \mathbb{R}^{N \times D}$ and observations $\boldsymbol{y} \in \mathbb{R}^N$:

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

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

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

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



- *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*

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

- The *joint* distribution $p(\boldsymbol{z}, \boldsymbol{y}) = \mathcal{N}\left(\begin{bmatrix}\boldsymbol{z}\\ \boldsymbol{y}\end{bmatrix} |\boldsymbol{\mu}, \boldsymbol{\Sigma}\right)$

$$\boldsymbol{\mu} = \begin{bmatrix}\boldsymbol{\mu}_z \\ \boldsymbol{W}\boldsymbol{\mu}_z + \boldsymbol{b}\end{bmatrix} \qquad \boldsymbol{\Sigma} = \begin{bmatrix}\boldsymbol{\Sigma}_z & \boldsymbol{\Sigma}_z\boldsymbol{W}^T \\ \boldsymbol{W}\boldsymbol{\Sigma}_Z & \boldsymbol{\Sigma}_y + \boldsymbol{W}\boldsymbol{\Sigma}_z\boldsymbol{W}^T\end{bmatrix}$$

- The *posterior* distribution of $\boldsymbol{z}$ given $\boldsymbol{y}$

$$p(\boldsymbol{y}|\boldsymbol{z}) = \mathcal{N}\left(\boldsymbol{z}|\boldsymbol{\mu}_{z|y}, \boldsymbol{\Sigma}_{z|y}\right)$$
$$\boldsymbol{\Sigma}_{z|y}^{-1} = \boldsymbol{\Sigma}_z^{-1} + \boldsymbol{W}^T\boldsymbol{\Sigma}_y\boldsymbol{W}$$
$$\boldsymbol{\mu}_{z|y} = \boldsymbol{\Sigma}_{z|y}\left[\boldsymbol{W}^T\boldsymbol{\Sigma}_y^{-1}(\boldsymbol{y} - \boldsymbol{b}) + \boldsymbol{\Sigma}_z^{-1}\boldsymbol{\mu}_z\right]$$

- The *marginal* distribution $\boldsymbol{y}$

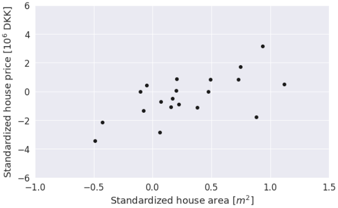
$$p(\boldsymbol{y}) = \mathcal{N}(\boldsymbol{y}|\boldsymbol{W}\boldsymbol{\mu}_z + \boldsymbol{b}, \boldsymbol{\Sigma}_y + \boldsymbol{W}\boldsymbol{\Sigma}_z\boldsymbol{W}^T)$$

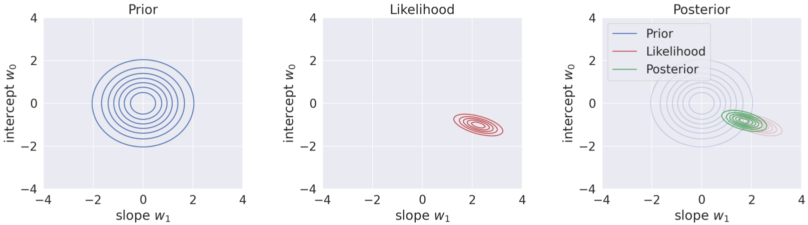
Example

- 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





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

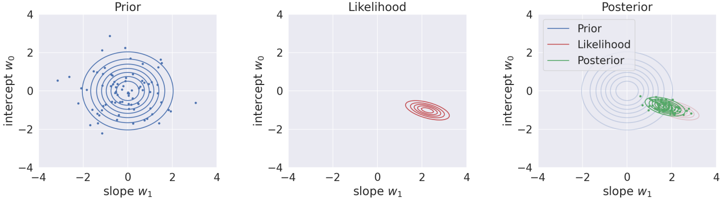
Posterior inference

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

- 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*

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

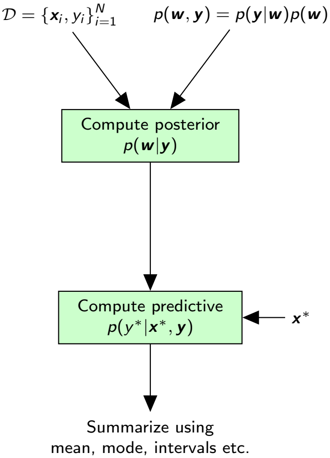
- Next goal: *making predictions* for new $\boldsymbol{x}^*$

$$p(y^*|\boldsymbol{x}^*, \boldsymbol{w}) = \mathcal{N}(y^*|\boldsymbol{w}^T \underbrace{\phi(\boldsymbol{x}^*)}_{\phi_*}, \sigma^2)$$

- The *posterior predictive distribution* is given by

$$\begin{aligned} p(y^*|\boldsymbol{y}, \boldsymbol{x}^*) &= \int \underbrace{p(y^*|\boldsymbol{x}^*, \boldsymbol{w})}_{\text{Pred. likelihood}} \underbrace{p(\boldsymbol{w}|\boldsymbol{y})}_{\text{Posterior}} \mathrm{d}\boldsymbol{w} \\ &= \int \mathcal{N}(y^*|\boldsymbol{w}^T \phi_*, \sigma^2) \mathcal{N}(\boldsymbol{w}|\boldsymbol{m}, \boldsymbol{S}) \mathrm{d}\boldsymbol{w} \\ &= \mathcal{N}(y^*|\mathbf{m}^T \phi_*, \phi_*^T \boldsymbol{S} \phi_* + \sigma^2) \end{aligned}$$

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



Quiz time!

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

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

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

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

Posterior Predictive distributions

Building intuition

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

- Two *model quantities* of interest

$$f^* = f(\boldsymbol{x}_*) = \boldsymbol{w}^T \boldsymbol{\phi}_*$$
$$y^* = y(\boldsymbol{x}_*) = \boldsymbol{w}^T \boldsymbol{\phi}_* + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

- Computing the *posterior* mean and variance

$$\mathbb{E}\left[f^*\right] = \mathbb{E}\left[\boldsymbol{w}^T \boldsymbol{\phi}_*\right] = \mathbb{E}\left[\boldsymbol{w}^T\right] \boldsymbol{\phi}_* = \boldsymbol{m}^T \boldsymbol{\phi}_*$$
$$\mathbb{V}\left[f^*\right] = \mathbb{V}\left[\boldsymbol{w}^T \boldsymbol{\phi}_*\right] = \boldsymbol{\phi}_*^T \mathbb{V}\left[\boldsymbol{w}^T\right] \boldsymbol{\phi}_* = \boldsymbol{\phi}_*^T \boldsymbol{S} \boldsymbol{\phi}_*$$

- Hence, the *posterior distribution* of f^* given the data $\boldsymbol{y}$ is

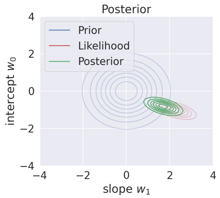
$$p(f^*|\boldsymbol{y}, \boldsymbol{x}_*) = \mathcal{N}(f^*|\mathbf{m}^T \boldsymbol{\phi}_*, \boldsymbol{\phi}_*^T \boldsymbol{S} \boldsymbol{\phi}_*)$$

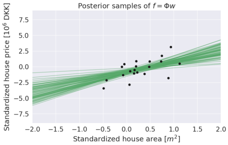
- and the *posterior predictive distribution* for y^* becomes

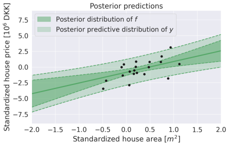
$$p(y^*|\boldsymbol{y}, \boldsymbol{x}_*) = \mathcal{N}(y^*|\mathbf{m}^T \boldsymbol{\phi}_*, \boldsymbol{\phi}_*^T \boldsymbol{S} \boldsymbol{\phi}_* + \sigma^2)$$

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

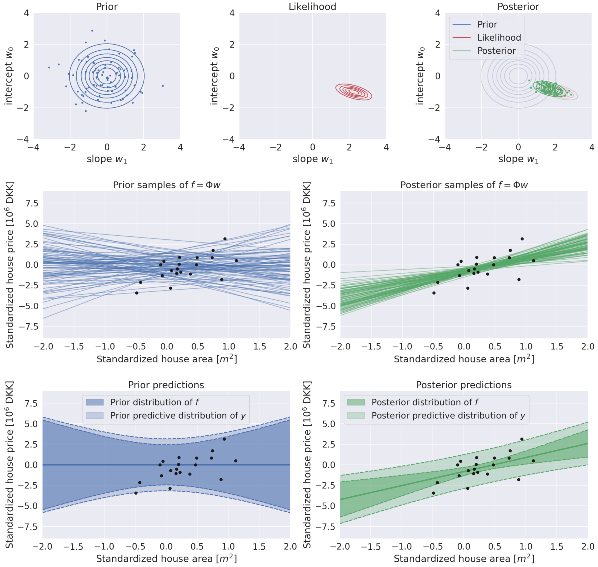
- We can also compute the *prior* predictive distribution.







Prior and posterior predictive distributions



Posterior Predictive distributions

Epistemic and aleatoric uncertainty

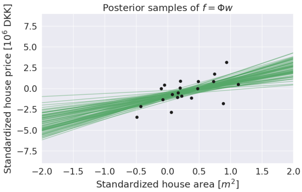
- The *posterior predictive distribution* of $y^* = \boldsymbol{w}^T \phi(\boldsymbol{x}^*) + \epsilon$ is

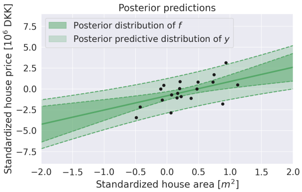
$$p(y^*|\boldsymbol{y}, \boldsymbol{x}_*) = \mathcal{N}(y^*|\mathbf{m}^T \phi_*, \phi_*^T \boldsymbol{S} \phi_* + \sigma^2)$$

- Variance: The first term is due to parameter uncertainty (*epistemic/reducible*) and the second term is due to measurement noise (*aleatoric/irreducible*)

- The term $\phi(\boldsymbol{x}_*)^T \boldsymbol{S} \phi(\boldsymbol{x}_*)$ is the *posterior uncertainty projected to data space*

- 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?

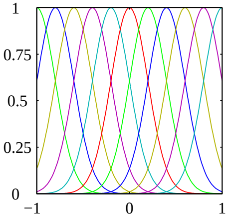


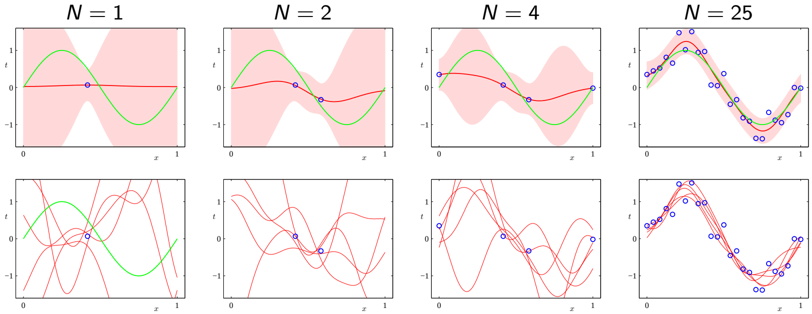


Example: posterior predictive distributions

- *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

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

- A fully Bayesian solution would require us to impose priors on α, β (recall $\beta = \frac{1}{\sigma^2}$)

$$p(\alpha, \beta|\boldsymbol{y}) \propto p(\boldsymbol{y}|\alpha, \beta)p(\alpha, \beta)$$

- ... and integrate them out

$$
\begin{aligned}
p(y^*|\boldsymbol{y}) &= \iiint p(y^*|\boldsymbol{w}, \beta)p(\boldsymbol{w}|\boldsymbol{y}, \alpha, \beta)p(\alpha, \beta|\boldsymbol{y})\, \mathrm{d}\boldsymbol{w}\mathrm{d}\alpha\mathrm{d}\beta \\
&= \mathbb{E}_{p(\alpha,\beta|\boldsymbol{y})}\left[\quad \mathbb{E}_{p(\boldsymbol{w}|\boldsymbol{y},\alpha,\beta)}\left[p(y^*|\boldsymbol{w}, \beta)\right] \quad\right]
\end{aligned}
$$

- ... 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?

$$p(y^*|\boldsymbol{y}) = \iiint p(y^*|\boldsymbol{w},\beta)p(\boldsymbol{w}|\boldsymbol{y},\alpha,\beta)p(\alpha,\beta|\boldsymbol{y})\mathrm{d}\boldsymbol{w}\mathrm{d}\alpha\mathrm{d}\beta$$
$$= \mathbb{E}_{p(\alpha,\beta|\boldsymbol{y})}\left[\quad \mathbb{E}_{p(\boldsymbol{w}|\boldsymbol{y},\alpha,\beta)}\left[p(y^*|\boldsymbol{w},\beta)\right] \quad\right]$$

- *The evidence approximation*, *maximum likelihood type II*, *Empirical Bayes*

- If the posterior is sharply peaked around $\hat{\alpha}$ and $\hat{\beta}$, then $p(\alpha,\beta|\boldsymbol{y})$ can be approximated by a Dirac's delta distribution

$$p(y^*|\boldsymbol{y}) \approx \mathbb{E}_{p(\boldsymbol{w}|\boldsymbol{y},\hat{\alpha},\hat{\beta})}\left[p(y^*|\boldsymbol{w},\beta)\right]$$

- Assume we impose a *flat prior* on α and β, then

$$p(\alpha,\beta|\boldsymbol{y}) \propto p(\boldsymbol{y}|\alpha,\beta)p(\alpha,\beta) \propto p(\boldsymbol{y}|\alpha,\beta)$$

- 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