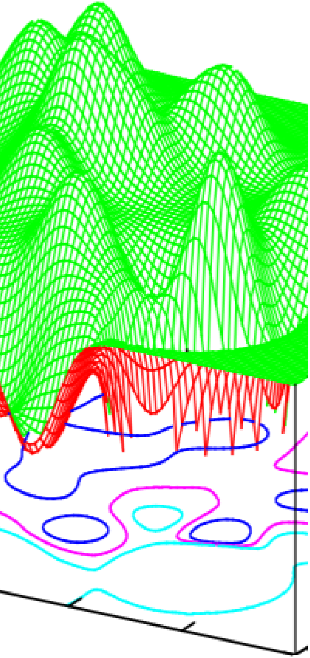

Machine Learning

Bayesian Regression & Classification

learning as inference, Bayesian Kernel Ridge regression & Gaussian Processes, Bayesian Kernel Logistic Regression & GP classification, Bayesian Neural Networks

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Learning as Inference

- The parameteric view

$$P(\beta|\text{Data}) = \frac{P(\text{Data}|\beta)\ P(\beta)}{P(\text{Data})}$$

- The function space view

$$P(f|\text{Data}) = \frac{P(\text{Data}|f)\ P(f)}{P(\text{Data})}$$

- Today:
  - Bayesian (Kernel) Ridge Regression $\leftrightarrow$ Gaussian Process (GP)
  - Bayesian (Kernel) Logistic Regression $\leftrightarrow$ GP classification
  - Bayesian Neural Networks (briefly)

- Beyond learning about specific Bayesian learning methods:

  Understand relations between

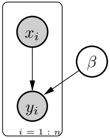
  loss/error ↔ neg-log likelihood

  regularization ↔ neg-log prior

  cost (reg.+loss) ↔ neg-log posterior

Ridge regression as Bayesian inference

- We have random variables $X_{1:n}, Y_{1:n}, \beta$
- We observe data $D = \{(x_i, y_i)\}_{i=1}^n$ and want to compute $P(\beta \mid D)$



- Let's assume:
  $P(X)$ is arbitrary
  $P(\beta)$ is Gaussian: $\beta \sim \mathcal{N}(0, \frac{\sigma^2}{\lambda}) \propto e^{-\frac{\lambda}{2\sigma^2} \|\beta\|^2}$
  $P(Y \mid X, \beta)$ is Gaussian: $y = x^\top \beta + \epsilon \;\; , \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$

Ridge regression as Bayesian inference

- Bayes' Theorem:

$$P(\beta \,|\, D) = \frac{P(D \,|\, \beta)\ P(\beta)}{P(D)}$$

$$P(\beta \,|\, x_{1:n}, y_{1:n}) = \frac{\prod_{i=1}^{n} P(y_i \,|\, \beta, x_i)\ P(\beta)}{Z}$$

$P(D \,|\, \beta)$ is a *product* of independent likelihoods for each observation (x_i, y_i)

Ridge regression as Bayesian inference

- Bayes' Theorem:

$$P(\beta \,|\, D) = \frac{P(D \,|\, \beta)\; P(\beta)}{P(D)}$$

$$P(\beta \,|\, x_{1:n}, y_{1:n}) = \frac{\prod_{i=1}^{n} P(y_i \,|\, \beta, x_i)\; P(\beta)}{Z}$$

$P(D \,|\, \beta)$ is a *product* of independent likelihoods for each observation (x_i, y_i)

Using the Gaussian expressions:

$$P(\beta \,|\, D) = \frac{1}{Z'} \prod_{i=1}^{n} e^{-\frac{1}{2\sigma^2}(y_i - x_i^\top \beta)^2}\; e^{-\frac{\lambda}{2\sigma^2}\|\beta\|^2}$$

Ridge regression as Bayesian inference

- Bayes' Theorem:

$$P(\beta \,|\, D) = \frac{P(D \,|\, \beta)\; P(\beta)}{P(D)}$$

$$P(\beta \,|\, x_{1:n}, y_{1:n}) = \frac{\prod_{i=1}^n P(y_i \,|\, \beta, x_i)\; P(\beta)}{Z}$$

$P(D \,|\, \beta)$ is a *product* of independent likelihoods for each observation (x_i, y_i)

Using the Gaussian expressions:

$$P(\beta \,|\, D) = \frac{1}{Z'} \prod_{i=1}^n e^{-\frac{1}{2\sigma^2}(y_i - x_i^\top \beta)^2}\; e^{-\frac{\lambda}{2\sigma^2}\|\beta\|^2}$$

$$-\log P(\beta \,|\, D) = \frac{1}{2\sigma^2}\Big[\sum_{i=1}^n (y_i - x_i^\top \beta)^2 + \lambda \|\beta\|^2\Big] - \log Z'$$

$$-\log P(\beta \,|\, D) \propto L^{\text{ridge}}(\beta)$$

1st insight: The *neg-log posterior* $P(\beta \,|\, D)$ is equal to the cost function $L^{\text{ridge}}(\beta)$!

Ridge regression as Bayesian inference

- Let us compute $P(\beta \mid D)$ explicitly:

$$
\begin{aligned}
P(\beta \mid D) &= \frac{1}{Z'} \prod_{i=1}^{n} e^{-\frac{1}{2\sigma^2}\;(y_i - x_i^\top \beta)^2} \; e^{-\frac{\lambda}{2\sigma^2}\,\|\beta\|^2} \\
&= \frac{1}{Z'}\; e^{-\frac{1}{2\sigma^2}\;\sum_i (y_i - x_i^\top \beta)^2} \; e^{-\frac{\lambda}{2\sigma^2}\,\|\beta\|^2} \\
&= \frac{1}{Z'}\; e^{-\frac{1}{2\sigma^2}\,[(\boldsymbol{y} - \boldsymbol{X}\beta)^\top(\boldsymbol{y} - \boldsymbol{X}\beta) + \lambda \beta^\top \beta]} \\
&= \frac{1}{Z'}\; e^{-\frac{1}{2}\,[\frac{1}{\sigma^2}\,\boldsymbol{y}^\top \boldsymbol{y} + \frac{1}{\sigma^2}\,\beta^\top(\boldsymbol{X}^\top \boldsymbol{X} + \lambda \mathbf{I})\beta - \frac{2}{\sigma^2}\,\beta^\top \boldsymbol{X}^\top \boldsymbol{y}]} \\
&= \mathcal{N}(\beta \mid \hat\beta, \Sigma)
\end{aligned}
$$

This is a Gaussian with covariance and mean

$$
\Sigma = \sigma^2\;(\boldsymbol{X}^\top \boldsymbol{X} + \lambda \mathbf{I})^{-1}\;, \quad \hat\beta = \tfrac{1}{\sigma^2}\;\Sigma \boldsymbol{X}^\top \boldsymbol{y} = (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \mathbf{I})^{-1} \boldsymbol{X}^\top \boldsymbol{y}
$$

- **2nd insight:** The mean $\hat\beta$ is exactly the classical $\operatorname{argmin}_\beta L^{\text{ridge}}(\beta)$.
- **3rd insight:** The Bayesian inference approach not only gives a mean/optimal $\hat\beta$, but also a variance Σ of that estimate!

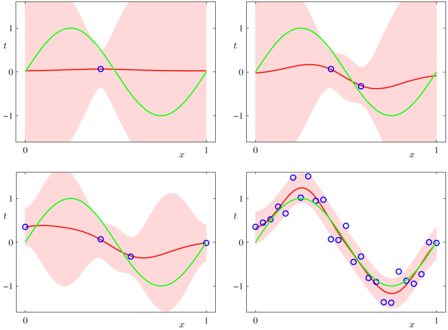
Predicting with an uncertain β

- Suppose we want to make a prediction at x. We can compute the **predictive distribution** over a new observation y^* at x^*:

$$P(y^* \mid x^*, D) = \int_\beta P(y^* \mid x^*, \beta)\ P(\beta \mid D)\ d\beta$$
$$= \int_\beta \mathcal{N}(y^* \mid \phi(x^*)^\top \beta, \sigma^2)\ \mathcal{N}(\beta \mid \hat\beta, \Sigma)\ d\beta$$
$$= \mathcal{N}(y^* \mid \phi(x^*)^\top \hat\beta,\ \sigma^2 + \phi(x^*)^\top \Sigma \phi(x^*))$$

Note $P(f(x) \mid D) = \mathcal{N}(f(x) \mid \phi(x)^\top \hat\beta,\ \phi(x)^\top \Sigma \phi(x))$ without the σ^2

- So, y^* is Gaussian distributed around the mean prediction $\phi(x^*)^\top \hat\beta$:



(from Bishop, p176)

Wrapup of Bayesian Ridge regression

- **1st insight:** The *neg-log posterior* $P(\beta \mid D)$ is equal to the cost function $L^{\text{ridge}}(\beta)$!

  This is a very very common relation: optimization costs correspond to neg-log probabilities; probabilities correspond to exp-neg costs.

- **2nd insight:** The mean $\hat\beta$ is exactly the classical $\operatorname{argmin}_\beta L^{\text{ridge}}(\beta)$.

  More generally, the most likely parameter $\operatorname{argmax}_\beta P(\beta|D)$ is also the least-cost parameter $\operatorname{argmin}_\beta L(\beta)$. In the Gaussian case, mean and most-likely coincide.

- **3rd insight:** The Bayesian inference approach not only gives a mean/optimal $\hat\beta$, but also a variance Σ of that estimate!

  This is a core benefit of the Bayesian view: It naturally provides a probability distribution over predictions (*"error bars"*), not only a single prediction.

Kernelized Bayesian Ridge Regression

- As in the classical case, we can consider arbitrary features $\phi(x)$
- .. or directly use a kernel $k(x,x')$:

$$\begin{aligned}
P(f(x)\,|\,D) &= \mathcal{N}(f(x)\,|\,\phi(x)^\top\hat\beta,\ \phi(x)^\top\Sigma\phi(x)) \\
\phi(x)^\top\hat\beta &= \phi(x)^\top\boldsymbol{X}^\top(\boldsymbol{X}\boldsymbol{X}^\top+\lambda\mathbf{I})^{\text{-}1}\boldsymbol{y} \\
&= \boldsymbol{\kappa}(x)(\boldsymbol{K}+\lambda\mathbf{I})^{\text{-}1}\boldsymbol{y} \\
\phi(x)^\top\Sigma\phi(x) &= \phi(x)^\top\sigma^2\ (\boldsymbol{X}^\top\boldsymbol{X}+\lambda\mathbf{I})^{\text{-}1}\phi(x) \\
&= \frac{\sigma^2}{\lambda}\phi(x)^\top\phi(x)-\frac{\sigma^2}{\lambda}\phi(x)^\top\boldsymbol{X}(\boldsymbol{X}\boldsymbol{X}^\top+\lambda\mathbf{I}_k)^{\text{-}1}\boldsymbol{X}^\top\phi(x) \\
&= \frac{\sigma^2}{\lambda}k(x,x)-\frac{\sigma^2}{\lambda}\boldsymbol{\kappa}(x)(\boldsymbol{K}+\lambda\mathbf{I}_n)^{\text{-}1}\boldsymbol{\kappa}(x)
\end{aligned}$$

3rd line: As on slide 02:24
last lines: Woodbury identity $(A+UBV)^{\text{-}1}=A^{\text{-}1}-A^{\text{-}1}U(B^{\text{-}1}+VA^{\text{-}1}U)^{\text{-}1}VA^{\text{-}1}$
with $A=\lambda\mathbf{I}$

- In standard conventions $\lambda=\sigma^2$, $P(\beta)=\mathcal{N}(\beta|0,1)$
  – Regularization: scale the covariance function (or features)

Kernelized Bayesian Ridge Regression

is equivalent to Gaussian Processes

(see also Welling: “Kernel Ridge Regression” Lecture Notes; Rasmussen & Williams sections 2.1 & 6.2; Bishop sections 3.3.3 & 6)

- As we have the equations alreay, I skip further math details. (See Rasmussen & Williams)

Gaussian Processes

- The function space view

$$P(f|\text{Data}) = \frac{P(\text{Data}|f)\ P(f)}{P(\text{Data})}$$

- Gaussian Processes define a probability distribution over functions:
  - A function is an infinite dimensional thing – how could we define a Gaussian distribution over functions?
  - For every finite set $\{x_1, .., x_M\}$, the function values $f(x_1), .., f(x_M)$ are Gaussian distributed with mean and cov.

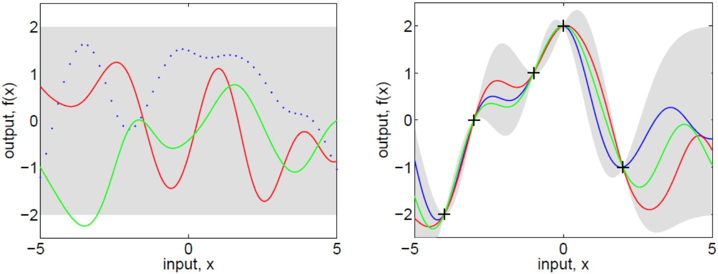
$$\begin{aligned} \langle f(x_i) \rangle &= \mu(x_i) \qquad \text{(often zero)} \\ \langle [f(x_i) - \mu(x_i)][f(x_j) - \mu(x_j)] \rangle &= k(x_i, x_j) \end{aligned}$$

  Here, $k(\cdot, \cdot)$ is called **covariance function**

- Second, Gaussian Processes define an observation probability

$$P(y|x, f) = \mathcal{N}(y|f(x), \sigma^2)$$

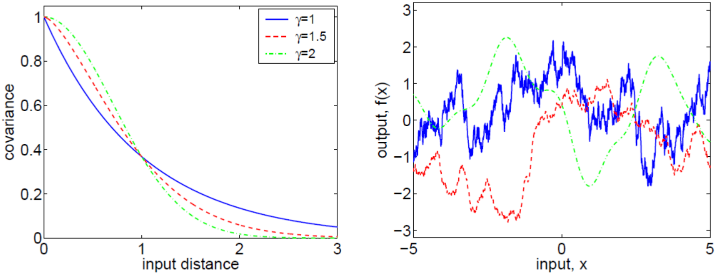
Gaussian Processes



(a), prior (b), posterior

(from Rasmussen & Williams)

GP: different covariance functions

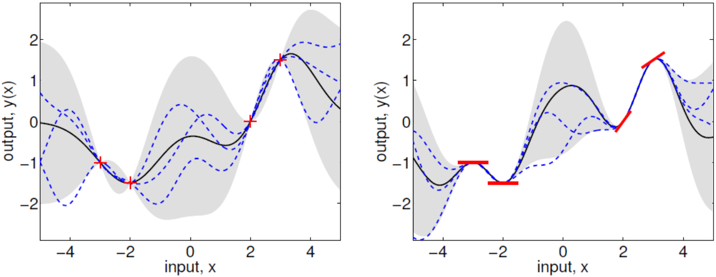


(from Rasmussen & Williams)

- These are examples from the γ-exponential covariance function

$$k(x, x') = \exp\{-|(x - x')/l|^{\gamma}\}$$

GP: derivative observations



(from Rasmussen & Williams)

- Bayesian Kernel Ridge Regression = Gaussian Process

- GPs have become a standard regression method
- If exact GP is not efficient enough, many approximations exist, e.g. sparse and pseudo-input GPs

Bayesian (Ridge) Logistic Regression

Bayesian Logistic Regression

- f now defines a logistic probability over $y \in \{0, 1\}$:

$$\begin{aligned} P(X) &= \text{arbitrary} \\ P(\beta) &= \mathcal{N}(\beta|0, \frac{2}{\lambda}) \propto \exp\{-\lambda\|\beta\|^2\} \\ P(Y\!=\!1 \,|\, X, \beta) &= \sigma(\beta^\top \phi(x)) \end{aligned}$$

- Recall

$$L^{\text{logistic}}(\beta) = -\sum_{i=1}^{n} \log p(y_i \,|\, x_i) + {\color{red}\lambda\|\beta\|^2}$$

- Again, the parameter posterior is

$$P(\beta|D) \propto P(D \,|\, \beta)\ P(\beta) \propto \exp\{-L^{\text{logistic}}(\beta)\}$$

Bayesian Logistic Regression

- Use **Laplace approximation** (2nd order Taylor for L) at $\beta^* = \text{argmin}_\beta L(\beta)$:

$$
\begin{aligned}
L(\beta) &\approx L(\beta^*) + \bar\beta^\top \nabla + \frac{1}{2}\bar\beta^\top H \bar\beta\ , \quad \bar\beta = \beta - \beta^* \\
P(\beta|D) &\propto \exp\{-\bar\beta^\top \nabla - \frac{1}{2}\bar\beta^\top H \bar\beta\} \\
&= \mathcal{N}[\bar\beta \,|\, -\nabla, H] = \mathcal{N}(\bar\beta \,|\, -H^{\text{-}1}\nabla, H^{\text{-}1}) \\
&= \mathcal{N}(\beta|\beta^*, H^{\text{-}1}) \qquad \text{(because } \nabla = 0 \text{ at } \beta^*\text{)}
\end{aligned}
$$

- Then the predictive distribution of the *discriminative function* is also Gaussian!

$$
\begin{aligned}
P(f(x)\,|\,D) &= \textstyle\int_\beta P(f(x)\,|\,\beta)\ P(\beta\,|\,D)\ d\beta \\
&= \textstyle\int_\beta \mathcal{N}(f(x)\,|\,\phi(x)^\top\beta, 0)\ \mathcal{N}(\beta\,|\,\beta^*, H^{\text{-}1})\ d\beta \\
&= \mathcal{N}(f(x)\,|\,\phi(x)^\top\beta^*, \phi(x)^\top H^{\text{-}1}\phi(x)) \ =:\ \mathcal{N}(f(x)\,|\,f^*, s^2)
\end{aligned}
$$

- The predictive distribution over the label $y \in \{0, 1\}$:

$$
\begin{aligned}
P(y(x){=}1\,|\,D) &= \textstyle\int_{f(x)} \sigma(f(x))\ P(f(x)|D)\ df \\
&\approx \varphi(\sqrt{1 + s^2\pi/8} f^*)
\end{aligned}
$$

the approximation replaced σ by the probit function $\varphi(x) = \int_{-\infty}^x \mathcal{N}(0, 1)dx$.

Kernelized Bayesian Logistic Regression

- As with Kernel Logistic Regression, the MAP discriminative function f^* can be found iterating the Newton method $\leftrightarrow$ iterating GP estimation on a *re-weighted* data set.
- The rest is as above.

Kernel Bayesian Logistic Regression

is equivalent to Gaussian Process Classification

- GP classification became a standard classification method, if the prediction needs to be a meaningful probability that takes the *model uncertainty* into account.

Bayesian Neural Networks

General non-linear models

- Above we always assumed $f(x) = \phi(x)^\top \beta$ (or kernelized)
- Bayesian Learning also works for non-linear function models $f(x, \beta)$
- Regression case:
  $P(X)$ is arbitrary.
  $P(\beta)$ is Gaussian: $\beta \sim \mathcal{N}(0, \frac{\sigma^2}{\lambda}) \propto e^{-\frac{\lambda}{2\sigma^2} \|\beta\|^2}$
  $P(Y \mid X, \beta)$ is Gaussian: $y = f(x, \beta) + \epsilon \ , \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$

General non-linear models

- To compute $P(\beta|D)$ we first compute the most likely

$$\beta^* = \underset{\beta}{\operatorname{argmin}} L(\beta) = \underset{\beta}{\operatorname{argmax}} P(\beta|D)$$

- Use Laplace approximation around β^*: 2nd-order Taylor of $f(x, \beta)$ and then of $L(\beta)$ to estimate a Gaussian $P(\beta|D)$

- Neural Networks:
  – The Gaussian prior $P(\beta) = \mathcal{N}(\beta|0, \frac{\sigma^2}{\lambda})$ is called **weight decay**
  – This pushes “sigmoids to be in the linear region”.

Conclusions

- Probabilistic inference is a very powerful concept!
  - Inferring about the world given data
  - Learning, decision making, reasoning can view viewed as forms of (probabilistic) inference
- We introduced Bayes' Theorem as the fundamental form of probabilistic inference
- Marrying Bayes with (Kernel) Ridge (Logisic) regression yields
  - Gaussian Processes
  - Gaussian Process classification