GP and BO
Probabilistic regression and ML assisted optimization

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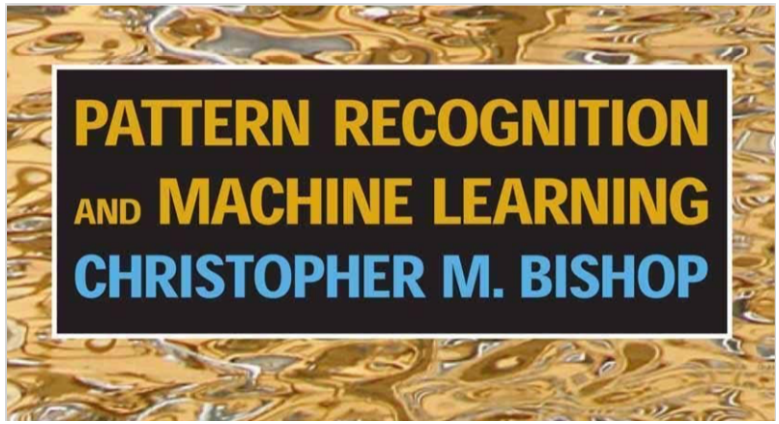
References for today's lecture

Chapter 3 and 6



- Gaussian Processes for ML
- Online material

What about probabilistic regression?

So far we have assumed that for models like,

$$f(\mathbf{x}) = \boldsymbol{\theta}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x})$$

the optimal values of $\boldsymbol{\theta}$ are **deterministic**.

- What if our problem has noise (uncertainty)? $\rightarrow y = \hat{y} + \sigma$

$$y = f(\mathbf{x}) + \epsilon = \boldsymbol{\theta}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}) + \epsilon,$$

where ϵ (noise) can be described probabilistically.

- ϵ is described by a Gaussian distribution with zero mean and variance σ_n^2,

$$\epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

Likelihood, $p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta})$

The probability density of the observations given the parameters,

$$p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta}) = \prod_{i}^{N} p(\mathbf{y}|\mathbf{x}_i, \boldsymbol{\theta}),$$

where,

$$p(\mathbf{y}|\mathbf{x}_i, \boldsymbol{\theta}) = \frac{1}{\sqrt{2\pi}\sigma_n} \exp\left(-\frac{(y_i - \boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}))^2}{2\sigma_n^2}\right)$$

(after some tedious but not complicated algebra we get)

$$p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\Phi}(\mathbf{X})\boldsymbol{\theta}, \sigma_n^2\mathbb{I}) = \frac{1}{(2\pi\sigma_n)^{n/2}} \exp\left(-\frac{(\mathbf{y} - \boldsymbol{\Phi}(\mathbf{X})\boldsymbol{\theta})^2}{2\sigma_n^2}\right)$$

Must probable model

$$p(\mathbf{y}|\mathbf{X},\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\Phi}(\mathbf{X})\boldsymbol{\theta}, \sigma_n^2\mathbb{I}) = \frac{1}{(2\pi\sigma_n)^{n/2}} \exp\left(-\frac{(\mathbf{y}-\boldsymbol{\Phi}(\mathbf{X})\boldsymbol{\theta})^2}{2\sigma_n^2}\right)$$

- What is the most probable $\boldsymbol{\theta}$? (hint: $\ln p(\mathbf{y}|\mathbf{X},\boldsymbol{\theta})$)
- What is the meaning of $\sigma_n^2\mathbb{I}$?
- Is $\boldsymbol{\theta}$ deterministic or probabilistic?

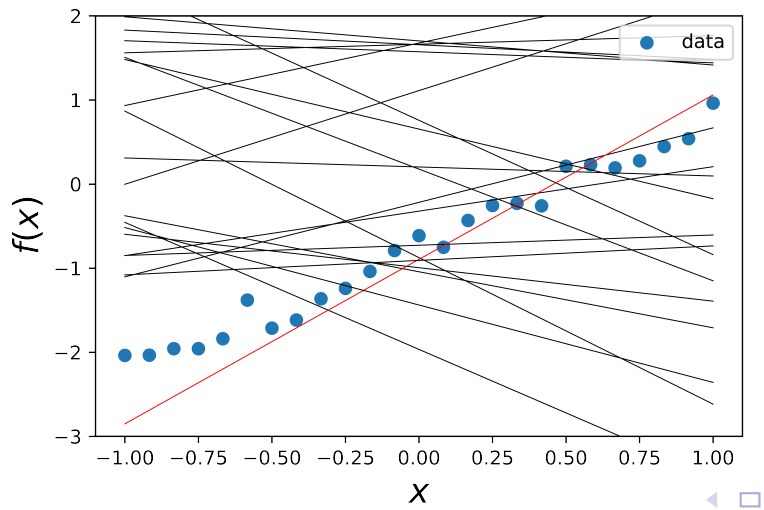
Must probable model

$$p(\mathbf{y}|\mathbf{X},\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\Phi}(\mathbf{X})\boldsymbol{\theta}, \sigma_n^2\mathbb{I}) = \frac{1}{(2\pi\sigma_n)^{n/2}} \exp\left(-\frac{(\mathbf{y}-\boldsymbol{\Phi}(\mathbf{X})\boldsymbol{\theta})^2}{2\sigma_n^2}\right)$$

- What is the most probable $\boldsymbol{\theta}$?

$$\arg\max_{\boldsymbol{\theta}} \ln p(\mathbf{y}|\mathbf{X},\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \left(\underbrace{-\frac{1}{2\sigma_n^2}(\mathbf{y}-\boldsymbol{\Phi}(\mathbf{X})\boldsymbol{\theta})^2}_{\text{linear regression}} + \frac{N}{2}\ln\sigma_n - \frac{N}{2}\ln(2\pi) \right)$$

- Is $\boldsymbol{\theta}$ deterministic or probabilistic?



Bayesian linear model

• "In the Bayesian formalism we need to specify a prior over the parameters, expressing our beliefs about the parameters before we look at the observations" [1]

$$\boldsymbol{\theta} \sim \mathcal{N}(\mathbf{0}, \Sigma_\theta)$$

Goal: Infer the posterior distribution over the weights.

Bayes rule

$$\underbrace{p(\boldsymbol{\theta}|\mathbf{X}, \mathbf{y})}_{\textit{posterior}} \approx \underbrace{p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta})}_{\textit{likelihood}} \underbrace{p(\boldsymbol{\theta})}_{\textit{prior}}$$

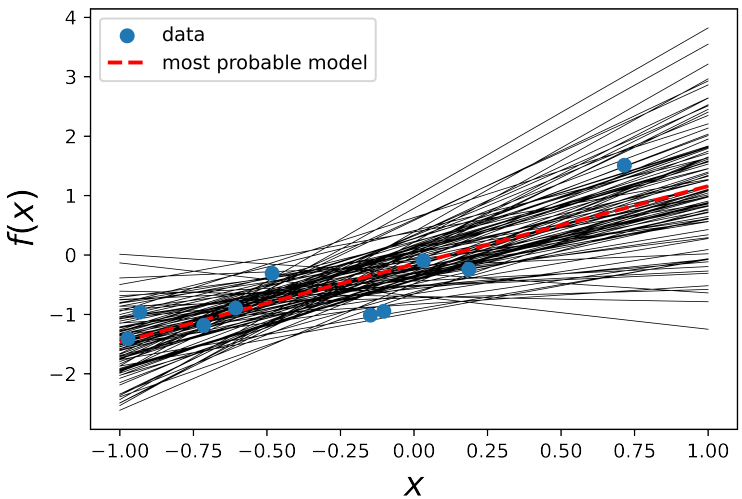
• What is the solution of $\arg\max_\theta \ln p(\boldsymbol{\theta}|\mathbf{X}, \mathbf{y})$?

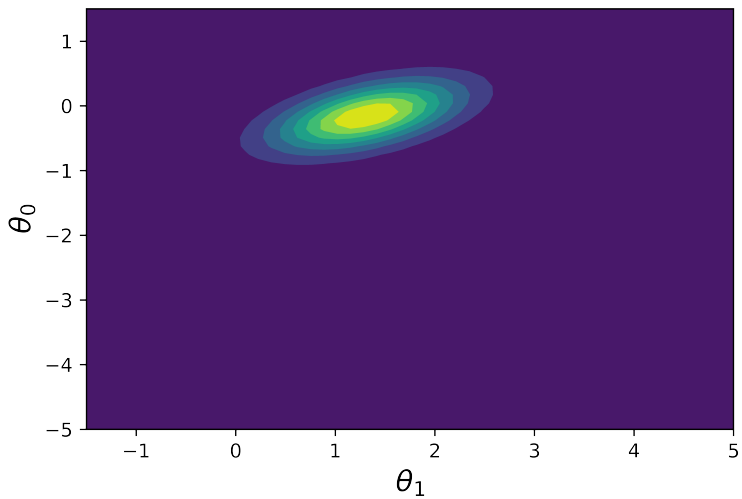
$$\begin{aligned} p(\boldsymbol{\theta}|\mathbf{X}, \mathbf{y}) &\approx \mathcal{N}(\boldsymbol{\Phi}(\mathbf{X})\boldsymbol{\theta}, \sigma_n^2 \mathbb{I})\ \mathcal{N}(\mathbf{0}, \lambda^{-1}\mathbb{I}) \\ \mathcal{N}(\mathbf{0}, \lambda^{-1}\mathbb{I}) &\propto \exp\left(-\frac{1}{\lambda}\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{\theta}\right) \end{aligned}$$

[1] GP book

Bayesian linear model

$$[\theta_1, \theta_0] \sim p(\boldsymbol{\theta}|\mathbf{X}, \mathbf{y})$$





Gaussian Process

$$p(\theta|\mathbf{\Phi}(\mathbf{X}), \mathbf{y}) \approx p(\mathbf{y}|\mathbf{\Phi}(\mathbf{X}), \theta)\ p(\theta)$$

- Same as kernel ridge regression!!
- Let's use the matrix identity trick and write the equations in terms of kernel function
- What about prediction?

$$p(y(\mathbf{x})|\mathbf{x}, \mathbf{\Phi}(\mathbf{X}), \mathbf{y}) = \int \theta^{\mathrm{T}} \phi(\mathbf{x}) p(\theta|\mathbf{X}, \mathbf{y}) d\theta$$

- Ensamble average!
- $p(y(\mathbf{x})|\mathbf{x}, \mathbf{\Phi}(\mathbf{X}), \mathbf{y})$ is also a Gaussian distribution!!

$$\begin{aligned}
\mu(\mathbf{x}) &= \mathbf{k}(\mathbf{x}, \mathbf{X})^{\top} \left(K(\mathbf{X}, \mathbf{X} + \sigma_n^2 \mathbb{I})\right)^{-1} \mathbf{y} = \sum_i^N \alpha_i k(\mathbf{x}, \mathbf{x}_i) \\
\sigma(\mathbf{x}) &= k(\mathbf{x}, \mathbf{x}) - \mathbf{k}(\mathbf{x}, \mathbf{X})^{\top} \left(K(\mathbf{X}, \mathbf{X} + \sigma_n^2 \mathbb{I})\right)^{-1} \mathbf{k}(\mathbf{x}, \mathbf{X})
\end{aligned}$$