# Bayesian Methods

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(adapted from David Rosenberg's slides)

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# Contents

# Logistics

- Deliverable
  - Homework 4 due today
  - Homework 5 released (due on April 15)
  - Project proposal due tomorrow
    - Make sure each group has a corresponding member
- Codalab
  - Optional but bonus points if you provide a worksheet for reproducibility
  - Tutorial this Thursday during the instructor's office hour

# Introduction

# Recap: typical steps in data science problems

Many problem domains can be formalized as follows:

1. Observe input $x$.
2. Take action $a$.
3. Observe outcome $y$.
4. Evaluate action in relation to the outcome (via a loss function $\ell(a, y)$)

The Three Spaces:

- Input space: $\mathcal{X}$
- Action space: $\mathcal{A}$
- Outcome space: $\mathcal{Y}$

# Some Formalization

## The Spaces

- $\mathcal{X}$: input space
- $\mathcal{Y}$: outcome space
- $\mathcal{A}$: action space

## Prediction Function (or "decision function")

A **prediction function** (or **decision function**) gets input $x \in \mathcal{X}$ and produces an action $a \in \mathcal{A}$ :

$$\begin{aligned} \delta : \quad \mathcal{X} &\rightarrow \mathcal{A} \\ x &\mapsto f(x) \end{aligned}$$

## Loss Function

A **loss function** evaluates an action in the context of the outcome $y$.

$$\begin{aligned} \ell : \quad \mathcal{A} \times \mathcal{Y} &\rightarrow \mathbf{R} \\ (a, y) &\mapsto \ell(a, y) \end{aligned}$$

# Statistical inference

- Observe data $\mathcal{D} = \{y_1, \ldots, y_N\}$
- Assume that data is generated by a family of parametric distributions

$$\{p(y \mid \theta) : \theta \in \Theta\},$$

  - where $p(y \mid \theta)$ is a density on a **sample space** $\mathcal{Y}$, and
  - $\theta$ is a **parameter** in a finite dimensional **parameter space** $\Theta$.
- Assume that data is drawn i.i.d. from $p(y \mid \theta)$.
- The decision-making problem: Infer properties of $p(y \mid \theta)$ given some observed data

# Today's lecture

- How to make decisions given unknown nature/world and limited data?
  - The frequentist approach
  - The Bayesian approach
- Apply the Bayesian approach to conditional models (classification)
  - Learning and prediction

# Frequentist Decision Theory

**Key idea**:

- There exists a true but unknown parameter $\theta^*$.
- We can obtain its estimate $\hat{\theta}$ from a sample $\mathcal{D} \sim p(\mathcal{D} \mid \theta^*)$ using some **point estimator** $\delta$.
    - In general, $\delta : \mathcal{X} \to \mathcal{A}$ is a decision procedure based on data.

**Task**: estimate $\theta$ given i.i.d. samples from $p(y \mid \theta)$ where $\theta \in \Theta$.

How do we choose the best estimator?

$$\textbf{Frequentist risk:}\ R(\theta^*, \delta) = \mathbb{E}_{p(\mathcal{D}|\theta^*)} L(\theta^*, \delta(\mathcal{D})) \tag{1}$$

But we don't know $\theta^*$...

# Desirable Properties of Estimators

Heuristics for selecting a good estimator:

- **Consistent**: As data size $N \to \infty$, we get $\hat{\theta} \to \theta^*$.
  - What assumptions are we making here?
- **Unbiased**: our estimate is correct in expectation.

$$\bar{\theta} \stackrel{\text{def}}{=} \mathbb{E}_{p(\mathcal{D}|\theta^*)}\left[\hat{\theta}\right] = \theta^* \tag{2}$$

$$\text{bias}(\hat{\theta}) = \bar{\theta} - \theta^* \tag{3}$$

- **Minimum variance**:

$$\text{var}(\hat{\theta}) = \mathbb{E}_{p(\mathcal{D}|\theta^*)}\left[\left(\hat{\theta} - \bar{\theta}\right)^2\right] \tag{4}$$

# The bias-variance tradeoff

Do we always want an unbiased estimator?

Let's decompose the square loss. (expectations are over $p(\mathcal{D} \mid \theta^*)$)

$$
\begin{aligned}
\mathbb{E}\left[\left(\hat{\theta}-\theta^*\right)^2\right] &= \mathbb{E}\left[\left(\hat{\theta}-\bar{\theta}+\bar{\theta}-\theta^*\right)^2\right] && (5)\\
&= \mathbb{E}\left[\left(\hat{\theta}-\bar{\theta}\right)^2\right] + 2(\bar{\theta}-\theta^*)\underbrace{\mathbb{E}\left[\left(\hat{\theta}-\bar{\theta}\right)\right]}_{=0 \text{ because } \bar{\theta} \overset{\text{def}}{=} \mathbb{E}\left[\hat{\theta}\right]} + \mathbb{E}\left[(\bar{\theta}-\theta^*)^2\right] && (6)\\
&= \mathbb{E}\left[\left(\hat{\theta}-\bar{\theta}\right)^2\right] + (\bar{\theta}-\theta^*)^2 && (7)\\
&= \operatorname{var}(\hat{\theta}) + \operatorname{bias}^2(\hat{\theta}) && (8)
\end{aligned}
$$

# Example: ridge regression

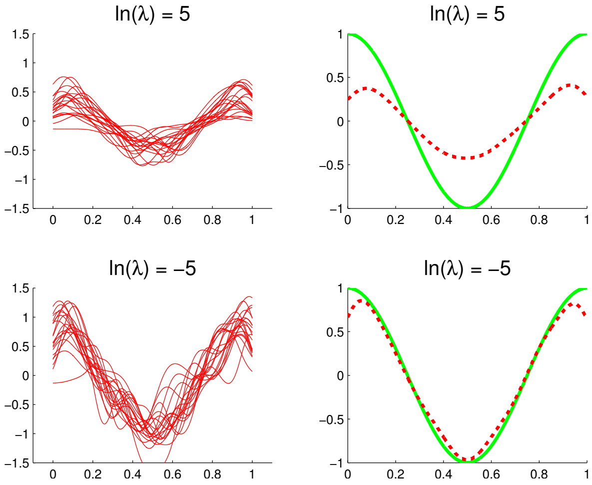



Figure 6.5 from "Machine Learning: a Probabilistic Perspective", K. Murphy.

# Maximum Likelihood Estimation

**Definition**

The **maximum likelihood estimator (MLE)** for $\theta$ in the model $\{p(y \mid \theta) : \theta \in \Theta\}$ is

$$\hat{\theta}_{\text{MLE}} = \underset{\theta \in \Theta}{\arg\max}\, L_{\mathcal{D}}(\theta), \tag{9}$$

$$\text{where } L_{\mathcal{D}}(\theta) \stackrel{\text{def}}{=} p(\mathcal{D} \mid \theta) = \prod_{i=1}^{n} p(y_i \mid \theta) \tag{10}$$

- MLE is consistent but can be biased.
- **Method of moments** is another general approach one learns about in statistics.

# Example: Coin Flipping

**Task**: mode a biased coin.

- Parametric family of mass functions:

$$p(\text{Heads} \mid \theta) = \theta,$$

for $\theta \in \Theta = (0, 1)$.

- Note that every $\theta \in \Theta$ gives us a different probability model for a coin.

# Coin Flipping: Likelihood function

- Data $\mathcal{D} = (H, H, T, T, T, T, T, H, \ldots, T)$
    - $n_h$: number of heads
    - $n_t$: number of tails
- Assume these were i.i.d. flips.
- **Likelihood function** for data $\mathcal{D}$:

$$L_{\mathcal{D}}(\theta) = p(\mathcal{D} \mid \theta) = \theta^{n_h}(1-\theta)^{n_t} \tag{11}$$

# Coin Flipping: MLE

- As usual, easier to maximize the log-likelihood function:

$$\begin{aligned} \hat{\theta}_{\text{MLE}} &= \underset{\theta \in \Theta}{\arg\max} \log L_{\mathcal{D}}(\theta) && (12) \\ &= \underset{\theta \in \Theta}{\arg\max} \left[ n_h \log \theta + n_t \log(1-\theta) \right] && (13) \end{aligned}$$

- First order condition:

$$\begin{aligned} \frac{\partial}{\partial \theta} \ell = \frac{n_h}{\theta} - \frac{n_t}{1-\theta} &= 0 && (14) \\ \iff \theta &= \frac{n_h}{n_h + n_t}. && (15) \end{aligned}$$

- So $\hat{\theta}_{\text{MLE}}$ is the empirical fraction of heads.

# Review

Challenges in statistical inference:

- Unknown data generating process defined by $\theta$
- Cannot observe all data
- Want to infer properties of $\theta$ (and make decisions/predictions)

Frequentist approach:

- Point estimator based on a data sample
- Compare estimators by expected loss over all possible data samples—impossible
- Other metrics: consistency, unbiasedness, variance etc.
- A common estimator: MLE

Next, the Bayesian approach.

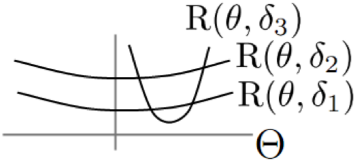
# Bayesian Decision Theory

# Bayesian twist of the frequentist risk

**Task** Design a measure to evaluate some estimator $\delta$.

**Problem** cannot compute the risk without knowing $\theta^*$.

$$R(\theta^*, \delta) = \mathbb{E}_{p(\mathcal{D}|\theta^*)} L(\theta^*, \delta(\mathcal{D})) \tag{16}$$




**Solution** introduce the prior $p(\theta^*)$.

$$\textbf{Bayes risk}: R_B(\delta) = \int R(\theta^*, \delta) p(\theta^*) d\theta^* \tag{17}$$

**Note** Bayes risk is a frequentist concept because it still averages over the data $p(\mathcal{D} \mid \theta^*)$.

# The Bayesian approach

**Key idea**:

- The true $\theta$ is never known but we have **belief** about it (no more $\theta^*$)
- As we observe more data, we can update our beliefs (no expectation over unseen data)

**Key concepts**:

Prior $p(\theta)$, our belief before seeing any data.

Likelihood $p(\mathcal{D} \mid \theta)$.

Marginal likelihood $p(\mathcal{D}) = \int p(\mathcal{D} \mid \theta)p(\theta)d\theta$ (also called evidence)

Posterior probability $p(\theta \mid \mathcal{D})$, our updated belief after seeing $\mathcal{D}$.

Predictive probability $p(y_{\text{new}} \mid \mathcal{D}) = \int p(y_{\text{new}} \mid \theta)p(\theta)d\theta$.

# Expressing the Posterior Distribution

- By Bayes rule, can write the posterior distribution as

$$p(\theta \mid \mathcal{D}) = \frac{p(\mathcal{D} \mid \theta) p(\theta)}{p(\mathcal{D})}.$$

- Let's consider both sides as functions of $\theta$, for fixed $\mathcal{D}$.
- Then both sides are densities on $\Theta$ and we can write

$$\underbrace{p(\theta \mid \mathcal{D})}_{\text{posterior}} \propto \underbrace{p(\mathcal{D} \mid \theta)}_{\text{likelihood}} \underbrace{p(\theta)}_{\text{prior}}.$$

- Where $\propto$ means we've dropped factors independent of $\theta$.

# Posterior risk

Bayesian interpretation of the risk: posterior expected loss.

$$\textbf{posterior risk:}\ r(a \mid \mathcal{D}, p(\theta)) \stackrel{\text{def}}{=} \mathbb{E}_{p(\theta \mid \mathcal{D})}[L(\theta, a)] \qquad \text{where } a = \delta(\mathcal{D}) \tag{18}$$

- Conditioned on observed data and the prior, which are known.
- Average over the posterior distribution of $\theta$.

How to make decisions?

$$\textbf{Bayes action:}\ \delta^*(\mathcal{D}) \stackrel{\text{def}}{=} \arg\min_{a \in \mathcal{A}} \mathbb{E}_{p(\theta \mid \mathcal{D})}[L(\theta, a)] \tag{19}$$

- No need to choose an estimator.
- What might be the practical issue here?

# Coin Flipping: Bayesian Model

- Parametric family of mass functions:

$$p(\text{Heads} \mid \theta) = \theta,$$

  for $\theta \in \Theta = (0, 1)$.

- Need a prior distribution $p(\theta)$ on $\Theta = (0, 1)$.

- Likelihood $p(x \mid \theta)$ is Bernoulli.
- A distribution from the Beta family will do the trick...

# Coin Flipping: Beta Prior

$$\theta \sim \text{Beta}(\alpha, \beta) \tag{20}$$

$$p(\theta) \propto \theta^{\alpha-1}(1-\theta)^{\beta-1} \tag{21}$$

$$\mathbb{E}[\theta] = \frac{\alpha}{\alpha+\beta} \tag{22}$$

Think of $\alpha$ and $\beta$ as our initial counts of head ($h$) and tails ($t$) before seeing any data.

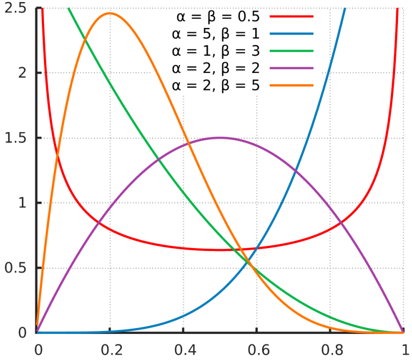



Figure by Horas based on the work of Krishnavedala (Own work) [Public domain], via Wikimedia Commons http://commons.wikimedia.org/wiki/File:Beta_distribution_pdf.svg.

# Coin Flipping: Posterior

- **Prior:**

$$\begin{aligned} \theta &\sim \text{Beta}(h,t) \\ p(\theta) &\propto \theta^{h-1}(1-\theta)^{t-1} \end{aligned}$$

- **Likelihood function**

$$L(\theta) = p(\mathcal{D} \mid \theta) = \theta^{n_h}(1-\theta)^{n_t}$$

- **Posterior density:**

$$\begin{aligned} p(\theta \mid \mathcal{D}) &\propto p(\theta)p(\mathcal{D} \mid \theta) \\ &\propto \theta^{h-1}(1-\theta)^{t-1} \times \theta^{n_h}(1-\theta)^{n_t} \\ &= \theta^{h-1+n_h}(1-\theta)^{t-1+n_t} \end{aligned}$$

What is the posterior distribution?

# Posterior is Beta

- **Prior:**

$$\begin{aligned} \theta &\sim \text{Beta}(h,t) \\ p(\theta) &\propto \theta^{h-1}(1-\theta)^{t-1} \end{aligned}$$

- **Posterior density:**

$$p(\theta \mid \mathcal{D}) \propto \theta^{h-1+n_h}(1-\theta)^{t-1+n_t}$$

- **Posterior is in the beta family**:

$$\theta \mid \mathcal{D} \sim \text{Beta}(h+n_h, t+n_t)$$

- **Interpretation**:
  - Prior initializes our counts with $h$ heads and $t$ tails.
  - Posterior increments counts by observed $n_h$ and $n_t$.

# Conjugate Priors

Interesting that posterior is in the same distribution family as prior.

**Definition**

A family of priors $\pi$ **is conjugate to** a parametric model $P$ (the likelihood) if the posterior is in the same family $\pi$.

Examples:

- The beta family is conjugate to the coin-flipping (i.e. Bernoulli) model.
- The family of all probability distributions is conjugate to any parametric model. [Trvially]

Why use conjugate priors? Mainly for computational convenience.

# Compute the posterior in Coin Flipping

**Likelihood** $p(\text{Heads} \mid \theta) = \theta$ for $\theta \in \Theta = [0,1]$.

**Prior** $\theta \sim \text{Beta}(2,2)$.

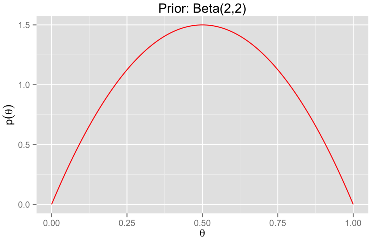
**Data** $\mathcal{D} = \{H, H, T, \ldots, T\}$, 75 heads, 60 tails

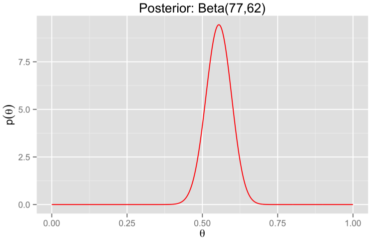
**Posterior** $\theta \mid \mathcal{D} \sim \text{Beta}(77,62)$

**MLE** $\hat{\theta}_{\text{MLE}} = \frac{75}{75+60} \approx 0.556$

- When might the MLE estimate be bad?

Given the posterior, what would be a good estimate of the value $\theta$?



# Bayesian point estimation

**Setup**:

- Data $\mathcal{D}$ generated by $p(y \mid \theta)$, for unknown $\theta \in \Theta$.
- Want to produce a point estimate for $\theta$.

**Approach**:

1. Choose a loss function, e.g., square loss $L(\theta, \hat{\theta}) = \left(\theta - \hat{\theta}\right)^2$.
2. Find an action minimizing the expected risk w.r.t. posterior—Bayes action.

# Bayesian Point Estimation: Square Loss

- Find **action** $\hat{\theta} \in \Theta$ that minimizes **posterior risk**

$$r(\hat{\theta}) = \int \left(\theta - \hat{\theta}\right)^2 p(\theta \mid \mathcal{D})\, d\theta. \tag{23}$$

- Differentiate:

$$\begin{aligned}
\frac{dr(\hat{\theta})}{d\hat{\theta}} &= -\int 2\left(\theta - \hat{\theta}\right) p(\theta \mid \mathcal{D})\, d\theta && (24)\\
&= -2\int \theta p(\theta \mid \mathcal{D})\, d\theta + 2\hat{\theta} \underbrace{\int p(\theta \mid \mathcal{D})\, d\theta}_{=1} && (25)\\
&= -2\int \theta p(\theta \mid \mathcal{D})\, d\theta + 2\hat{\theta} && (26)
\end{aligned}$$

- Set to zero:

$$\hat{\theta} = \int \theta p(\theta \mid \mathcal{D})\, d\theta = \mathbb{E}[\theta \mid \mathcal{D}] \qquad \text{posterior mean} \tag{27}$$

# Bayesian Point Estimation: Absolute Loss

- Posterior risk:

$$r(\hat{\theta}) = \int \left|\theta - \hat{\theta}\right| p(\theta \mid \mathcal{D})\, d\theta. \tag{28}$$

$$= \int_{-\infty}^{\hat{\theta}} \left(\hat{\theta} - \theta\right) p(\theta \mid \mathcal{D})\, d\theta + \int_{\hat{\theta}}^{\infty} \left(\theta - \hat{\theta}\right) p(\theta \mid \mathcal{D})\, d\theta \tag{29}$$

- Differentiate:

$$\frac{dr(\hat{\theta})}{d\hat{\theta}} = \int_{-\infty}^{\hat{\theta}} p(\theta \mid \mathcal{D})\, d\theta - \int_{\hat{\theta}}^{\infty} p(\theta \mid \mathcal{D})\, d\theta \tag{30}$$

- Set to zero:

$$\int_{-\infty}^{\hat{\theta}} p(\theta \mid \mathcal{D})\, d\theta = \int_{\hat{\theta}}^{\infty} p(\theta \mid \mathcal{D})\, d\theta \qquad \text{and they sum to one} \tag{31}$$

$$\implies \hat{\theta} \text{ split the area under the curve evenly: posterior median} \tag{32}$$

# Bayesian Point Estimation: Zero-One Loss

- Suppose $\Theta$ is discrete (e.g. $\Theta = \{\text{english}, \text{french}\}$)
- **Zero-one loss:** $\ell(\theta, \hat{\theta}) = 1(\theta \neq \hat{\theta})$
- **Posterior risk**:

$$
\begin{aligned}
r(\hat{\theta}) &= \mathbb{E}\left[1(\theta \neq \hat{\theta}) \mid \mathcal{D}\right] \\
&= \mathbb{P}\left(\theta \neq \hat{\theta} \mid \mathcal{D}\right) \\
&= 1 - \mathbb{P}\left(\theta = \hat{\theta} \mid \mathcal{D}\right) \\
&= 1 - p(\hat{\theta} \mid \mathcal{D})
\end{aligned}
$$

- **Bayes action** is

$$
\hat{\theta} = \operatorname*{arg\,max}_{\theta \in \Theta} p(\theta \mid \mathcal{D})
$$

- This $\hat{\theta}$ is called the **maximum a posteriori (MAP)** estimate.
- The MAP estimate is the **mode** of the posterior distribution.

1. **Define the model**:
   - Choose a parametric family of densities—likelihood:
   $$\{p(\mathcal{D} \mid \theta) \mid \theta \in \Theta\}.$$
   - Choose a distribution $p(\theta)$ on $\Theta$—prior distribution.
2. After observing data $\mathcal{D}$, compute the posterior distribution $p(\theta \mid \mathcal{D})$.
3. Choose action based on $p(\theta \mid \mathcal{D})$ and the loss function.

# Frequentist vs Bayesian

| | Frequentist | Bayesian |
|---|---|---|
| Evaluate a decision | $L(\theta, \delta(\cdot))$ | $L(\theta, \delta(\cdot))$ |
| Handle unknown state of nature ($\theta$) | $\theta^*$ | $\theta$ is a variable—prior, posterior |
| Make decisions | average over (observed and unobserved) data | average over $\theta$ |
| Topics of interests | properties of an estimator (e.g., consistent, unbiased) | compute various quantities, e.g., posterior, marginal etc. |
| History | dominated during the 20th century | dominated before the 20th century |

# Bayesian Conditional Models

# Learning as density estimation

**Setup**

- Observe data $\mathcal{D} = \{y^{(n)}\}_{n=1}^{N}$ assuming $x^{(n)}$'s are fixed.
- Choose a family of parametric distributions:

$$\{p(y \mid x, \theta) : \theta \in \Theta\},$$

**Learning**

- Maximum likelihood estimation:

$$\hat{\theta}_{\text{MLE}} = \underset{\theta \in \Theta}{\arg\max}\, L_{\mathcal{D}}(\theta) = \underset{\theta \in \Theta}{\arg\max}\, p(\mathcal{D} \mid \theta, x) \tag{33}$$

- Assume $y^{(n)}$'s are independent conditioned on $x^{(n)}$.
- Exercise: MLE corresponds to ERM with negative log-likelihood loss.

**Prediction**

$$p(y \mid x, \hat{\theta}_{\text{MLE}}) \tag{34}$$

# Example: Gaussian linear regression

Model

$$p(y \mid x, \theta) = \mathcal{N}(\theta^T x, \sigma^2) \qquad \text{Assuming known } \sigma^2. \tag{35}$$

Likelihood

$$L_{\mathcal{D}}(\theta) = \prod_{n=1}^{N} p(y^{(n)} \mid x^{(n)}, \theta) \tag{36}$$

$$= \prod_{n=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(y^{(n)} - \theta^T x^{(n)}\right)^2}{2\sigma^2}\right) \tag{37}$$

Solution

$$\hat{\theta}_{\text{MLE}} = \underset{\theta \in \mathbf{R}^d}{\arg\max}\, L_{\mathcal{D}}(\theta) \tag{38}$$

$$= \underset{\theta \in \mathbf{R}^d}{\arg\max} \sum_{n=1}^{N} \left(y^{(n)} - \theta^T x^{(n)}\right)^2 \qquad \text{squared loss} \tag{39}$$

# Regularization via prior

- We want small weights to avoid overfitting. What would be a good prior?

$$\theta \sim \mathcal{N}\left(0, \tau^2 I_d\right) \qquad \text{Why Gaussian?} \tag{40}$$

- Posterior distribution is also a Gaussian distribution:

$$\begin{aligned}
p(\theta \mid \mathcal{D}) &\propto \mathcal{N}(0, \tau^2 I_d)\mathcal{N}(X\theta, \sigma^2 I_N) && (41)\\
&= \mathcal{N}(\mu_P, \Sigma_P) && (42)\\
\mu_P &= \left(X^T X + \frac{\sigma^2}{\tau^2} I_d\right)^{-1} X^T y && (43)\\
\Sigma_P &= \left(\sigma^{-2} X^T X + \tau^{-2} I_d\right)^{-1} && (44)
\end{aligned}$$

- See Rosenberg's notes on multivariate Gaussian.

# MAP (instead of MLE)

- Instead of maximizing the likelihood, let's maximize the posterior distribution to incorporate the prior.

$$p(\theta \mid \mathcal{D}) \propto \underbrace{\exp\left(-\frac{1}{2\tau^2}\|\theta\|^2\right)}_{\text{prior}} \underbrace{\prod_{i=1}^{n} \exp\left(-\frac{(y_i - \theta^T x_i)^2}{2\sigma^2}\right)}_{\text{likelihood}} \tag{45}$$

- To find MAP, sufficient to minimize the negative log posterior (Exercise):

$$\hat{\theta}_{\text{MAP}} = \operatorname*{arg\,min}_{\theta \in \mathbf{R}^d} \left[-\log p(\theta \mid \mathcal{D})\right] \tag{46}$$

$$= \operatorname*{arg\,min}_{\theta \in \mathbf{R}^d} \underbrace{\sum_{i=1}^{n} (y_i - \theta^T x_i)^2}_{\text{log-likelihood}} + \underbrace{\lambda\|\theta\|^2}_{\text{log-prior}} \qquad \lambda \stackrel{\text{def}}{=} \frac{\sigma^2}{\tau^2} \tag{47}$$

- How does the prior control the regularization strength?

# The Bayesian approach

- In Bayesian setting, **there is no selection** from hypothesis space, e.g., $\hat{\theta}_{\text{MLE}}, \hat{\theta}_{\text{MAP}}$.
- We chose a parametric family of conditional densities

$$\{p(y \mid x, \theta) : \theta \in \Theta\},$$

  and a prior distribution $p(\theta)$ on this set.
- Having set our Bayesian model, there are no more decisions to make – just computation...
  - posterior distribution
  - predictive distribution

# Bayesian conditional models

- The **prior distribution** $p(\theta)$ represents our beliefs about $\theta$ before seeing $\mathcal{D}$.
- The **posterior distribution** for $\theta$ is

$$
\begin{aligned}
p(\theta \mid \mathcal{D}, x) &\propto p(\mathcal{D} \mid \theta, x) p(\theta) \\
&= \underbrace{L_{\mathcal{D}}(\theta)}_{\text{likelihood}} \underbrace{p(\theta)}_{\text{prior}}
\end{aligned}
$$

- Posterior represents the updated beliefs after seeing $\mathcal{D}$.

# Bayesian linear regression

Let's derive ridge regression from a Bayesian perspective.

- Gaussian prior:

$$\theta \sim \mathcal{N}(0, \Sigma_0) \tag{48}$$

- Posterior distribution is also Gaussian:

$$\begin{aligned} \theta \mid \mathcal{D} &\sim \mathcal{N}(\mu_P, \Sigma_P) & (49) \\ \mu_P &= \left(X^T X + \sigma^2 \Sigma_0^{-1}\right)^{-1} X^T y & (50) \\ \Sigma_P &= \left(\sigma^{-2} X^T X + \Sigma_0^{-1}\right)^{-1} & (51) \end{aligned}$$

- What are reasonable point estimates of $\theta$? Posterior mode (MAP) and posterior mean:

$$\hat{\theta} = \mu_P = \left(X^T X + \sigma^2 \Sigma_0^{-1}\right)^{-1} X^T y \qquad \text{familiar?} \tag{52}$$

- For the prior covariance $\Sigma_0 = \frac{\sigma^2}{\lambda} I$, we get

$$\hat{w} = \mu_P = \left(X^T X + \lambda I\right)^{-1} X^T y \qquad \text{ridge regression} \tag{53}$$

# Example in 1-Dimension: Setup

- Input space $\mathcal{X} = [-1, 1]$ Output space $\mathcal{Y} = \mathbf{R}$
- Given $x$, the world generates $y$ as

$$y = w_0 + w_1 x + \varepsilon,$$

where $\varepsilon \sim \mathcal{N}(0, 0.2^2)$.

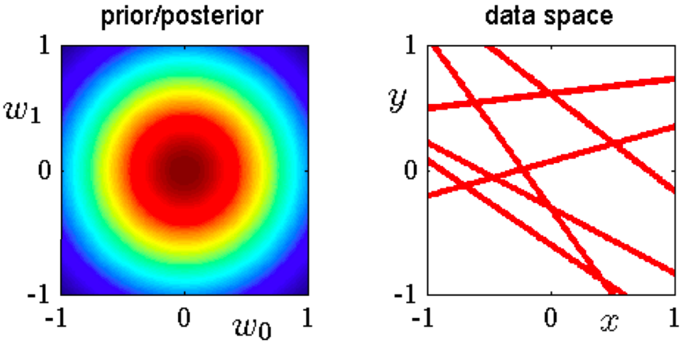
- Written another way, the **conditional probability model** is

$$y \mid x, w_0, w_1 \sim \mathcal{N}\left(w_0 + w_1 x, 0.2^2\right).$$

- What's the parameter space? $\mathbf{R}^2$.
- **Prior distribution:** $w = (w_0, w_1) \sim \mathcal{N}\left(0, \frac{1}{2} I\right)$

# Example in 1-Dimension: Prior Situation

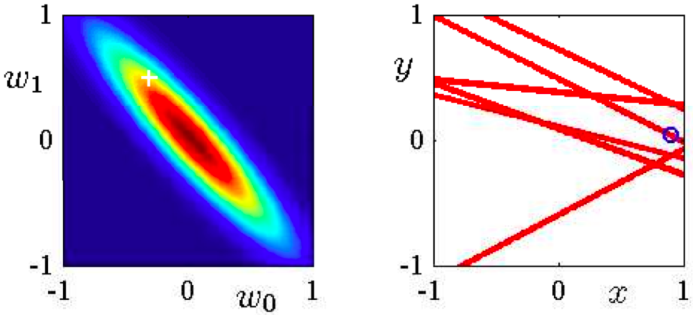
- **Prior distribution:** $w = (w_0, w_1) \sim \mathcal{N}\left(0, \frac{1}{2}I\right)$




- On right, $y = \mathbb{E}[y \mid x, w] = w_0 + w_1 x$, for randomly chosen $w \sim p(w) = \mathcal{N}\left(0, \frac{1}{2}I\right)$.

Bishop's PRML Fig 3.7

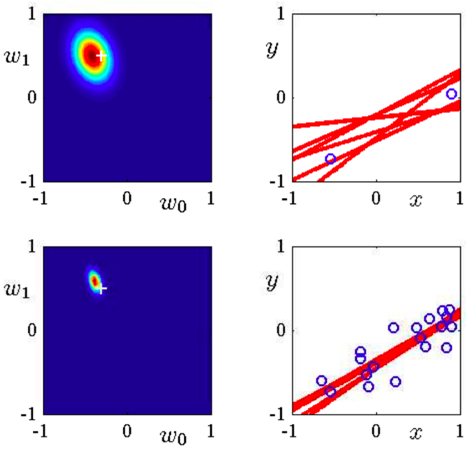
# Example in 1-Dimension: 1 Observation




- On left: posterior distribution; white '+' indicates true parameters
- On right: blue circle indicates the training observation

Bishop's PRML Fig 3.7

# Example in 1-Dimension: 2 and 20 Observations




Bishop's PRML Fig 3.7

# Review

- Task: find a function in a hypothesis space that map $x$ to a distribution of $y$:

$$\{p(y \mid x, \theta) : \theta \in \Theta\}.$$

- In frequentist approach, we choose $\hat{\theta} \in \Theta$, and predict

$$p(y \mid x, \hat{\theta}(\mathcal{D})).$$

- In Bayesian statistics we have two distributions on $\Theta$:
  - the prior distribution $p(\theta)$
  - the posterior distribution $p(\theta \mid \mathcal{D})$.
- Next, prediction by integrating over $\Theta$ w.r.t. $p(\theta \mid \mathcal{D})$.

# The Predictive Distribution

- Without any data, the **prior predictive distribution** is given by

$$p(y \mid x) = \int p(y \mid x; \theta) p(\theta)\, d\theta.$$

  - This is an average of all conditional densities in our family, weighted by the prior.
- Once we see data $\mathcal{D}$, the **posterior predictive distribution** is given by

$$p(y \mid x, \mathcal{D}) = \int p(y \mid x; \theta) p(\theta \mid \mathcal{D})\, d\theta.$$

  - This is an average of all conditional densities in our family, weighted by the posterior.

# What if we don't want a full distribution on $y$?

- Once we have a predictive distribution $p(y \mid x, \mathcal{D})$,
    - we can easily generate single point predictions.
- $x \mapsto \mathbb{E}\left[y \mid x, \mathcal{D}\right]$, to minimize expected square error.
- $x \mapsto \text{median}[y \mid x, \mathcal{D}]$, to minimize expected absolute error
- $x \mapsto \arg\max_{y \in \mathcal{Y}} p(y \mid x, \mathcal{D})$, to minimize expected 0/1 loss
- Each of these can be derived from $p(y \mid x, \mathcal{D})$.

# Bayesian linear regression: Predictive Distribution

Let's go back to Gaussian linear regression:

$$\theta \sim \mathcal{N}(0, \Sigma_0) \qquad \text{prior} \qquad (54)$$

$$y^{(n)} \mid x^{(n)}, \theta \sim \mathcal{N}(\theta^T x^{(n)}, \sigma^2) \qquad \text{likelihood} \qquad (55)$$

**Predictive Distribution**

$$p(y_{\text{new}} \mid x_{\text{new}}, \mathcal{D}) = \int p(y_{\text{new}} \mid x_{\text{new}}, \theta) p(\theta \mid \mathcal{D})\, d\theta \qquad (56)$$

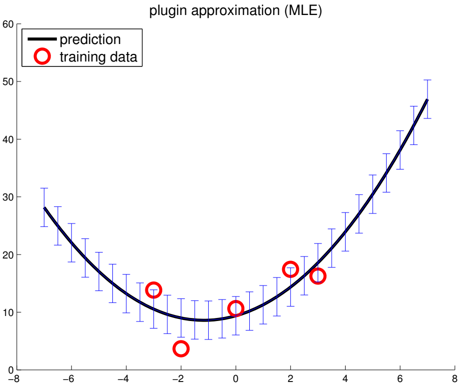
$$= \mathcal{N}(\eta_{\text{new}}, \sigma^2_{\text{new}}) \qquad \text{also a Gaussian} \qquad (57)$$

$$\eta_{\text{new}} = \mu_P^T x_{\text{new}} \qquad \text{MAP prediction} \qquad (58)$$

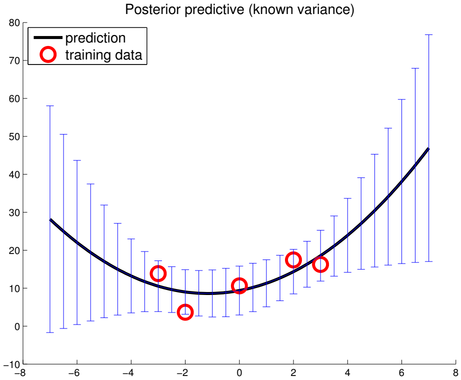
$$\sigma^2_{\text{new}} = \underbrace{x_{\text{new}}^T \Sigma_P x_{\text{new}}}_{\text{from variance in } \theta} + \underbrace{\sigma^2}_{\text{inherent variance in } y} \qquad \text{principled way to handle uncertainty} \qquad (59)$$

# Prediction uncertainty

Predictive distributions allow mean prediction with error bands.




(a) MLE: constant error bars




(b) Posterior: larger error bars where training points are few

Murphy. *Machine Learning: a Probabilistic Perspective*, Fig.7.12(a)(b)

# Conclusion

Frequentist
- Average over data (both observed and unobserved)
- No principled way to choose estimators
- Less computation

Bayesian
- Average over parameters (subjective prior)
- Uncertainty estimation "for free"
- Computationally intensive

Bayesian methods
1. Specify likelihood / model
2. Choose (conjugate) prior
3. Bayesian inference...